The research highlighted in this book is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

Visit https://bluewaters.ncsa.illinois.edu/science-teams for the latest on Blue Waters-enabled science and to watch the 2019 Blue Waters Symposium presentations.
The National Center for Supercomputing Applications (NCSA) was funded in 1986 to enable discoveries not possible anywhere else. We have a long history of doing things that have not been done before. The Blue Waters Project admirably continued that tradition and spawned new avenues of research and discovery for NCSA and our partners.

We are leading the way in multimeessenger astrophysics (MMA). In fact, we were recently awarded over $20 million in grants in MMA areas that would not have been possible without the discoveries Blue Waters helped achieve. MMA combines data from cosmic messengers such as gravitational waves, neutrinos, and electromagnetic waves. We are bringing together large-scale computing, data science, artificial intelligence (AI), machine learning (ML), and software development not only to advance these domains but to develop techniques, technologies and software that may transfer to other domains as well.

We’re helping to marry medicine and technology as a partner with the Carle Illinois College of Medicine, the world’s first engineering-based medical school. And for many years we’ve partnered with Mayo Clinic to advance precision medicine—drugs or treatments designed for small groups rather than large populations—by applying ML and AI.

We are incorporating ML and AI into agriculture as a partner in the University of Illinois’ new Center for Digital Agriculture. With the Institute for Genomic Biology, the College of Agricultural, Consumer and Environmental Sciences, and the Grainger College of Engineering we’ll be facilitating student education in the use of technology in agriculture as well as assisting farmers and agricultural industries to advance digital agriculture to keep pace with the ways technology is transforming how we feed and support a growing global population.

In addition, we recently launched the Center for Artificial Intelligence Innovation at NCSA that will focus on leveraging past and existing research projects to develop software to amplify current AI and ML research areas and explore new ones.

Earlier in 2020 I was privileged to be part of a delegation of University of Illinois leaders that participated in discussions on the next frontier of AI, data science, and design thinking with Illinois alumnus Tom Siebel and his staff at C3.ai. In his remarks, Illinois’ Vice Chancellor for Academic Affairs and Provost Andreas Cangellaris commented that “no matter how powerful the computers are, the real power comes from the people behind them.”

Blue Waters is not just a peak petascale system; it is a true sustained-petascale system, specifically designed to be well balanced and deliver petascale computing power and productivity across a variety of applications. Because of this balance, for almost seven years the Blue Waters Project has enabled remarkable work in biology, chemistry, physics, geosciences, cosmology and astrophysics, atmospheric science, and many other fields such as agriculture, economics, political science, and the social sciences.

You’ll find these remarkable discoveries in the pages that follow. Discoveries that were made by the people behind the computer—the extraordinary NCSA staff and the scientists they support in their quest for frontier science. They are leading by example. And as the leader of NCSA, I would not have it any other way.

Dr. William “Bill” Gropp
Director
National Center for Supercomputing Applications
I take great pride in the Blue Waters Project and in the outstanding science and project teams that make Blue Waters an exceptional open resource for research.

Every year I write how Blue Waters enabled computational, data analysis, and now machine learning/artificial intelligence investigations that could not be done otherwise. Once again, as you go through this report you will see the many accomplishments that carry the badge indicating “Only on Blue Waters” to signify that the research would not have been possible on other open-science resources deployed at the time.

Throughout the years, increasing numbers of projects have been identified as involving “data intensive” processing or as incorporating machine learning/artificial intelligence. This shift is another indication of the leadership of Blue Waters and the impact it is making. Many projects do not just involve data-intensive processing or machine learning but instead are combining these methods with multiscale and multiphysics simulation to achieve cutting-edge results. As I have said before, Blue Waters is an easy catalyst for excellence because of its exceptional balance of computing and I/O capabilities, along with thoroughly supporting teams using different methods while also helping science teams integrate different methods within their work to achieve remarkable new results.

As a leadership-class compute system, Blue Waters is intended to help pioneer amazing science and engineering discoveries. We designed it to be a balanced system in which its computational, interconnect, external network, and storage system work together to deliver unprecedented petascale and highly usable computing capabilities to the national research community. Blue Waters was conceived to accelerate the science frontier and to rapidly expand the adoption of new methods into other best-of-breed and “frontier” uses. This supercomputer boot-strapping process is how the world moved from the first 2D atmospheric circulation model to being able to accurately predict weather 10 to 15 days in advance, from studying basic fluid dynamics to using computing for complete aircraft and ship design, and for moving from studying small molecules to understanding the basic principles of life.

One of the most unexpected and remarkable successes of Blue Waters in 2019 was the role it played in a gerrymandering decision reached by Ohio’s Sixth District Court, where Blue Waters used Ms. Buffett’s “Champaign” tool an analysis conducted on Blue Waters and based on more than three million simulations of possible electoral maps. Ms. Buffett used a novel evolutionary Markov chain Monte Carlo algorithm designed to take advantage of Blue Waters’ massively parallel architecture to produce an array of map scenarios that could be compared to the current map. Further, she served as an expert witness and presented results from her simulations on Blue Waters to objectively compare biased and unbiased redistricting.

Making high-performance computing (HPC) available to more of our scientific community is important to the Blue Waters Project team. To expand participation in the use of Blue Waters resources and services, a new category of Broadening Participation allocations was announced in 2017, a component of the Innovation and Exploration allocations managed by NCSA. Through this, over 3.7 million node-hours of the original contractual requirements for our broadening participation programs were awarded to us, we were able to operate the Blue Waters supercomputer an additional 18 months beyond original plans, providing nearly seven years of access to Blue Waters instead of the five years originally planned by NSF. We were also able to add additional programs not in our original project scope, such as the aforementioned Broadening Participation allocations, as well as the Blue Waters Graduate Fellowships, our Petascale Application Improvement Discovery (PAID) program, and our Virtual School.

Continued service and operations only make sense if a system is reliable and resilient. Blue Waters is the most monitored and studied system in the world, with dozens of publications about its reliability and resiliency. The original contractual requirements for our system were set to 150 node failures per month, and no more than six systemic outages per month. In reality, for the past five years we averaged only one or two node outages per day, and the mean time between system interruptions ranges from three to six months.

Another way to explain this is that Blue Waters has 49,508 AMD CPU module sockets. We recently went back and reevaluated all the AMD CPU modules that had been taken out of the system, many as a preemptive measure. The analysis found there were 154 modules, or only 0.3 percent, that were defective. When equipped with Mean Time Between Failure (MTBF) over the six-and-a-half years, this indicates an MTBF of over 2,000 years for a CPU module.

Talented, dedicated individuals at NCSA and our partner institutions have maintained the system, supported our science and engineering partners in achieving breakthrough research, improved tools and processes, and trained the next generation of computational researchers. This publication celebrates the accomplishments of our partners and the researchers, educators, and students they support but also celebrates the dedication and innovation of the Blue Waters staff.

The end of the NSF funding for Blue Waters "broad access" phase is not the end of the story. Blue Waters will continue providing groundbreaking insight as it transitions to being a high-performance computational and data resource for the National Geospatial-Intelligence Agency (NGA). Blue Waters will focus ninety percent of the system resources on NGA-related projects, with ten percent of Blue Waters reserved for use by researchers at the University of Illinois at Urbana-Champaign. As Illinois’ Vice Chancellor for Academic Affairs and Provost Andreas C. C. Caragliulis commented, “no matter how powerful the computers are, the real power comes from the people behind them.” NGA will be building upon the amazingly impactful ArcticDEM research of Paul Morris of the University of Minnesota, which mapped the Arctic Circle, and the REMA research of Ian Howett of The Ohio State University, which mapped Antarctica. NGA will be funding the operations of Blue Waters to make high-resolution topographic maps of the entire Earth and other related projects associated with its mission to "map and model the world." We dreamed that was possible when Blue Waters entered production in 2013?

I am so thankful to have been able to work with everyone on the Blue Waters Project these past years. Together, we changed the world. And we’ll keep changing it. I cannot wait to see what discoveries we will uncover!”

Dr. William T.C. Kramer

Director and Principal Investigator
Blue Waters Project
The Blue Waters supercomputer began full service operations at the National Center for Supercomputing Applications in April 2013. Funded by the National Science Foundation, the University of Illinois and the State of Illinois, the primary goal of Blue Waters is to enable productive frontier research with a well-balanced leadership class computational and data analysis system that can process vast amounts of data in a precise, time-efficient manner. Funds for operation and management included a $134 million dollar grant awarded by the NSF to cover 7 years of Blue Waters’ service.

Blue Waters ended its role as an NSF Track-1 leadership supercomputer in 2019 but continues to serve as the world’s largest, non-classified geospatial system. The impressive computing capacity of Blue Waters has afforded research, development, and educational opportunities for communities locally and globally.

Throughout its life, teams have used Blue Waters for an impressive number of science discoveries. These discoveries are then shared with the world when teams publish their results. To date, over 1,300 papers have been presented at conferences and published in 244 journals. This number continues to grow as teams further analyze the vast amounts of data generated on Blue Waters.

THE SYSTEM

Blue Waters is currently the largest system ever built and delivered by supercomputer manufacturer Cray. It comprises 49,500 processor modules in 288 liquid-cooled cabinets, containing both AMD Interlagos CPUs and NVIDIA Kepler (K20x) GPUs.

With all its parts Blue Waters weighs about 576,000 pounds, or more than 288 tons. The size was necessary for the ambitious computing goals of the system.

Blue Waters was the first sustained petascale system, with more than 1.3 quadrillion (1.3 x 10^15) sustained calculations per second for a very wide range of large scale applications. Operating at peak performance, the supercomputer is capable of reaching 10 times its sustained computing power, reaching up to 13.34 petaflops (13.34 x 10^15).

Solving scientific problems requires prolonged computation, making the primary focus of Blue Waters sustained petascale performance. Thanks to the work of contributors to the Blue Waters project, researchers can get many science applications to run at a sustained petaflop. Running this many calculations per second opens the door for scientists and engineers to gain new insights into everything from the smallest biological processes to the largest cosmic events.

Storing this data requires a global addressable memory as impressive as its computing ability. Blue Waters has 1.66 petabytes (1,660,000 GB) of memory and has 26 usable petabytes of data storage provided by the Cray Sonexion storage appliances.
For long periods of storage, a nearline tape environment was built. At its peak, the Blue Waters nearline system stored over 35 petabytes of user data on its 11,600 miles of tape, which would stretch about half-way around the earth’s equator.

From July 2012 through March 2020 Blue Waters transferred 157.2 petabytes of data to and from its file systems from external sources.

THE BUILDING

Safely housing and supporting this massive computing system required the construction of the National Petascale Computing Facility. This state of the art facility spans 88,000 square feet, with the machine room housing Blue Waters taking up about 30,000 square feet of six foot raised floor. NPCF provides 24MW of electricity for computing and data equipment. In order to keep the supercomputer from overheating, NPCF has a water-cooling system capable of cycling at a peak flow rate of 9,600 gallons per minute.

In cool months, about 40-50 percent of the year, the facility uses its own evaporative cooling towers so almost no energy is used for water cooling. This system helped enable the NPCF to become one of the first computing facilities to achieve a Leadership in Energy and Environmental Design (LEED) Gold certification.

OUTREACH

Having exposure to a supercomputer like Blue Waters is not just a boon for research, but also for education. The project has given students first-hand experience with Blue Waters through the creation of 139 undergraduate internship opportunities as well as 50 graduate fellowships. But student involvement does not end there. Almost half of the Blue Waters users are graduate students, and they have been a fundamental part of the science teams. In fact, the average allocation time used per graduate student was 388,663 node hours. In addition to students being an active part of the research on Blue Waters, over its years of service 12.6 million node hours have been made available for educational projects.

Beyond this direct access to the machine, graduate students and postdocs had access to numerous experiences and training that contributed to their research projects through their Blue Waters experience. These projects serve to help develop a broader community of petascale computing experts. Reaching a community further than just those with accounts on Blue Waters has been important as well. The webinars/seminars created have had over 50,000 viewers and the training sessions and workshops created have had over 10,000 viewers. These are preserved online and will continue to serve the community into the future.

Some of these educational efforts included Virtual School of Computational Science and Engineering summer school events, virtual courses available at 27 institutions—including minority-serving institutions (MSI) and those in the Established Program to Stimulate Competitive Research (EPSCoR) program—and the International High Performance Computing Summer School. These programs gave well over six thousand students the opportunity to learn about petascale computing.

Exposure to the supercomputer is not just limited to those wishing to conduct research or work in the field of supercomputing. Over the years of operation over 14,000 people have toured the NPCF to see the Blue Waters supercomputer in person. These tours let people see for themselves how far computing technology has come and learn about the great research advances being made in our community.

WHAT’S NEXT

Although Blue Waters has ended its role as an NSF Track-1 supercomputer it is still serving to help make tremendous gains in our knowledge of the world. The Blue Waters Project, National Geospatial-Intelligence Agency, University of Minnesota and The Ohio State University are collaborating on the production of a digital elevation model (DEM) of the entire Earth.

EarthDEM follows the successful ArcticDEM and REMA projects which helped researchers in tracking geological changes, such as ice cap collapse, in the Arctic and Antarctic. Having publicly accessible, high-resolution topography of the entire world gives researchers the ability to assess landscape changes, no matter how remote the area.
BLUE WATERS METRIC INFORMATION

DEMOGRAPHICS OF BLUE WATERS USER BASE
- Graduate Students 44%
- Undergraduate Students 10%
- Faculty 10%
- University Research Staff (excluding postdoctorates) 7%
- Center Researcher Staff 2%
- Industrial Users 2%
- Center Non-Researcher Staff 2%
- Other 7%
- Postdoctorate 17%
- NSF 84.03%
- GLCPC 2.46%
- Innovation 1.81%
- Training and Education 0.43%
- NCSA Industry 0.11%

PROJECTS BY ALLOCATION TYPES
- NSF 18%
- Innovation 10%
- GLCPC 8%
- NCSA Industry 2%
- Illinois 44%

USERS IN ALLOCATION TYPES
- NSF 36%
- Innovation 9%
- Training and Education 9%
- GLCPC 7%
- NCSA Industry 2%
- Illinois 37%

USERS IN ALLOCATION TYPES
- NSF 922,183
- GLCPC 154,754
- Innovation and Exploration 91,766
- NCSA Industry 28,220
- Training and Education 21,822
- Illinois 100,014

NODE HOURS USED BY ALLOCATION TYPES
- NSF 84.03%
- GLCPC 2.46%
- Innovation 1.81%
- Training and Education 0.43%
- NCSA Industry 0.11%
- Illinois 11.16%

AVERAGE USER NODE USE BY ALLOCATION TYPES
- NSF 922,183
- GLCPC 154,754
- Innovation and Exploration 91,766
- NCSA Industry 28,220
- Training and Education 21,822
- Illinois 100,014
<table>
<thead>
<tr>
<th>Page</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>Simulating Two-Fluid MHD Turbulence and Dynamos in Star-Forming Molecular Clouds and a New Paradigm for Computational Astrophysics for Spherical Systems</td>
</tr>
<tr>
<td>16</td>
<td>The Computational Keys to the Supernova Puzzle: How Multiple 3D Radiation/Hydrodynamic Models Can Unlock the Supernova Mystery</td>
</tr>
<tr>
<td>18</td>
<td>Shedding Light on Supermassive Binary Black Hole Mergers</td>
</tr>
<tr>
<td>20</td>
<td>Accretion Dynamics of Supermassive Black Hole Binaries</td>
</tr>
<tr>
<td>24</td>
<td>The Epoch of the First Luminous Black Holes: Evolving the BlueTides Simulation into the First Billion Years of Cosmic History</td>
</tr>
<tr>
<td>26</td>
<td>Advancing First-Principle Symmetry-Guided Nuclear Modeling for Studies of Nucleosynthesis and Fundamental Symmetries in Nature</td>
</tr>
<tr>
<td>28</td>
<td>Magnetized Models of Giant Impacts</td>
</tr>
<tr>
<td>30</td>
<td>Cosmic Reionization on Computers</td>
</tr>
<tr>
<td>32</td>
<td>Elucidating the Alignment Mechanism for Black Hole Accretion Disks Subjected to Lens–Thirring Torques</td>
</tr>
<tr>
<td>34</td>
<td>Understanding the Origins of the Stars and Galaxies in our Universe</td>
</tr>
<tr>
<td>36</td>
<td>Deep Learning at Scale for the Construction of Galaxy Catalogs with the Dark Energy Survey</td>
</tr>
<tr>
<td>38</td>
<td>Characterization of Numerical Relativity Waveforms of Eccentric Binary Black Hole Mergers</td>
</tr>
<tr>
<td>40</td>
<td>Fusing Numerical Relativity and Deep Learning to Detect Eccentric Binary Black Hole Mergers Using Higher-Order Waveform Multiples</td>
</tr>
<tr>
<td>42</td>
<td>Data- and Compute-Intensive Challenges for Observational Astronomy in the Great Survey Era</td>
</tr>
<tr>
<td>44</td>
<td>Modal Decompositions of Shock Interactions</td>
</tr>
<tr>
<td>46</td>
<td>Plasma Plasma Spacecraft Interactions</td>
</tr>
<tr>
<td>48</td>
<td>The Spreading of Three-Dimensional Magnetic Reconnection in Asymmetric Geometry</td>
</tr>
<tr>
<td>50</td>
<td>Assembling a Map of the Universe: Shapes and Mass Distribution for the Dark Energy Survey</td>
</tr>
<tr>
<td>52</td>
<td>Petascale Simulations of Binary Neutron Star Mergers</td>
</tr>
<tr>
<td>54</td>
<td>Development of a Scalable Gravity Solver for Enzo-I</td>
</tr>
<tr>
<td>56</td>
<td>Simulating Galaxy Formation Across Cosmic Time</td>
</tr>
<tr>
<td>58</td>
<td>Processing Dark Energy Camera Data to Make the World’s Best Map of the Night Sky</td>
</tr>
<tr>
<td>60</td>
<td>Coupling the Solar Wind and Local Interstellar Medium in the Era of the New Horizons, Interstellar Boundary Explorer, Parker Solar Probe, Ulysses, and Voyager Spacecraft</td>
</tr>
<tr>
<td>62</td>
<td>Interior Dynamics of Young Stars Revealed by 3D Hydrodynamic Simulations</td>
</tr>
<tr>
<td>64</td>
<td>Modeling of Galaxy Populations</td>
</tr>
<tr>
<td>66</td>
<td>Effects of Active Galaxy Feedback on the Intracluster Medium</td>
</tr>
<tr>
<td>70</td>
<td>Feeding Black Holes: Tilt with a Twist</td>
</tr>
<tr>
<td>72</td>
<td>Scaling the RAYSE-R-15 MHD Model to Over 100,000 Cores with Efficient Hybrid OpenMP and MPI Parallelization</td>
</tr>
<tr>
<td>74</td>
<td>Numerical Study on the Fragmentation Condition in a Primordial Accretion Disk</td>
</tr>
<tr>
<td>75</td>
<td>Merging Black Holes and Neutron Stars</td>
</tr>
</tbody>
</table>
SIMULATING TWO-FLUID MHD TURBULENCE AND DYNAMOS IN STAR-FORMING MOLECULAR CLOUDS AND A NEW PARADIGM FOR COMPUTATIONAL ASTROPHYSICS FOR SPHERICAL SYSTEMS

EXECUTIVE SUMMARY

We are at the threshold of a new data-rich and simulation-rich era in star-formation studies. The question of how stars form is fascinating in and of itself and has a great impact on several other areas of astrophysics. The consensus is that a predominant amount of star formation in our galaxy takes place in molecular clouds, and more specifically in giant molecular clouds (GMC).

The project aims to study magnetic field evolution in partially ionized plasmas as well as developing and applying a new paradigm for simulating magnetohydrodynamics (MHD) on geodesic meshes that cover the sphere with no coordinate singularities and no loss of accuracy at the poles.

RESEARCH CHALLENGE

Our understanding of the star-formation process has reached the point where advanced observational capabilities are required. Consequently, NASA has made multimillion-dollar investments in the High-resolution Airborne Wideband Camera Plus (HAWC+) instrument aboard the Stratospheric Observatory for Infrared Astronomy airborne observatory with the specific goal of understanding the turbulent nature of star-forming clouds. At the same time, high-resolution simulations that include the appropriate physics of GMCs are also of critical importance. The PhDs are theorists who are participating in a multiyear, funded NASA proposal to obtain observational data associated with turbulence in the Perseus GMC.

The PhDs have also done the leading simulations of two-fluid MHD simulations on a range of XSEDE and PRAC resources [4,7–10]. At the original resolutions of 512 × 3 and smaller, the team would have been unable to match the observations from HAWC+. With the new generation of simulations, with a 1,0242 zone and upwards resolution, the researchers were able to obtain a well-defined inertial range in two-fluid and dynamo simulations. This ensured that NASA’s investment in HAWC+ is being matched by well-resolved observations.

The most compelling motivation for understanding two-fluid, ambipolar diffusion-mediated turbulence, in fact, comes from recent observations. Differences in the linewidths between neutral and ionized tracers have led to the suggestion that the dissipation of turbulence from ambipolar diffusion sets in on scales smaller than 0.0018 parsecs in the Messier 17 nebula [2].

A breakthrough realization by Xu and Lazarian [7] claimed that magnetic fields would grow in a partially ionized plasma (known as the dynamo problem) at rates that are very different from the growth in a fully ionized plasma. Their prediction was that while magnetic fields grow exponentially in a fully ionized plasma, they grow only quadratically in a partially-ionized plasma. However, confirmation of the theory requires a highly resolved turbulent flow. Fig. 1 (from [10]) shows the evolution of magnetic energy with time in a two-fluid dynamo. The right panel shows magnetic field growth in a partially ionized plasma. The inset on the left shows the initial growth of magnetic energy, with the red curve representing the research team’s highly resolved simulations and the blue curves showing the best fit to a quadratic. The agreement with theory is very good and has been documented. The study of the magnetic energy spectra is also significant and is shown in Fig. 2. The peak in the magnetic energy spectrum is predicted to evolve with time at a set rate, and the results of this project conform to theory. These results have also been published [10].

METHODS & CODES

The core MHD algorithms in the research group’s Riemann code are based on higher-order Godunov schemes. The team has been on the forefront of the effort to develop high-accuracy schemes for computational astrophysics in general and computational MHD in particular. Two-fluid methods have been described in [3,5,6]. The team has also published its breakthrough work on divergence-free MHD on geodesic meshes [11]. The method made several advances on higher-order-accurate reconstruction, including the reconstruction of divergence-free magnetic fields on isoparametrically mapped meshes.

RESULTS & IMPACT

Several large-scale simulations have been completed or are ongoing on Blue Waters. The key points from these simulations have been documented above and are being readied for publication in 2019. The new work represents a substantial improvement in resolution as well as in the details of input physics and accuracy of the simulation code. In addition, the first results on geodesic mesh MHD have been published [11], showing the petascale scalability on Blue Waters for the new code.

WHY BLUE WATERS

The simulations reported here are extremely CPU-intensive. The goal of this project is to use the petascale computing power of Blue Waters to push the resolution, accuracy, and fidelity of the simulations much higher in order to match theory with the observations coming from NASA-funded instruments.

PUBLICATIONS & DATA SETS


THE COMPUTATIONAL KEYS TO THE SUPERNova PUZZLE: HOW MULTIPLE 3D RADIATION/HYDRODYNAMIC MODELS CAN UNLOCK THE SUPERNova MYSTERY

EXECUTIVE SUMMARY

The mechanism of supernova explosions is a long-standing problem in theoretical astrophysics. Its obstinacy is intertwined with the long sense that it is necessary to address the phenomena and the challenging numerical context, involving the coupling of multidimensional hydrodynamics with neutrino radiation transfer in violently turbulent flow. This project explores solutions to this decades-old conundrum with the state-of-the-art 3D code Fornax. The overarching goal is to determine the solutions to this decades-old conundrum with the state-of-the-art 3D code Fornax. The mechanism of explosion, explosion energies, residual neutron star masses, nucleosynthesis, and explosion morphologies. Various other observational diagnostics such as radioactive nickel yields, neutrino and gravitational-wave signatures, and newly born pulsar kicks are also of interest. This initiative is enabled by the novel algorithms in Fornax that yield speedups of factors of five to ten over previous codes. This enables multiple 3D simulations, rather than just one, to be performed each year and, hence, permits a previously unprecedented exploration of parameter space.

RESEARCH CHALLENGE

Core-collapse supernovae dramatically announce the death of massive stars and the birth of neutron stars and black holes. During this violent process, a combination of high-density nuclear physics, multidimensional hydrodynamics, radiation transport, and neutrino physics determines whether and how the star explodes. However, the precise mechanism of explosion has not been pinned down, and this 50-year-old puzzle is one of the central remaining unsolved problems in theoretical astrophysics. Nevertheless, we are now at a crossroads. An early phase of modern supernova theory involved routine spherical simulations. This allowed explorations in parameter and progenitor space to fully characterize the phenomenon as a function of all-important quantities. Mistakes could be made quickly and an overarching understanding in 1-D could be achieved. However, researchers knew that the cores were unstable to hydrodynamic overturn and turbulence that could not be captured in one dimension. The next phase of discovery occurred when techniques and hardware advanced sufficiently so that 2D calculations became as routine as 1-D had been. This phase gave scientists a glimpse of the effects of turbulence and convection with state-of-the-art neutrino transport. At the end of this phase, a few 3D simulations appeared, but each of these simulations required approximately one year of simulation time on high-performance computers. In summary, the main advantages of the Fornax code are its efficiency owing to its explicit nature, its excellent strong scaling to hundreds of thousands of cores, its ability to perform the most advanced spherical simulations of any available high-performance computing resource.

METHODS & CODES

The research team developed a new multidimensional, multiphysics simulation program, Fornax, for the study of core-collapse supernovae. Fornax is a directionally unsplit Godunov-type code that employs spherical coordinates, solves the moving-frame, multiphysics, two-moment, velocity-dependent transport equations that Ov1(3), solves the M1 tensor closure for the second and third moments of the radiation fields, and employs a dendritic spherical grid. Fluxes at cell faces are computed with an HLLC Riemann solver based on left and right states reconstructed from the underlying volume-averaged states. Three species of neutrino are followed using an explicit Godunov characteristic method applied to the radiation transport operators and an implicit solver for the radiation source terms. In this way, the radiative transport and transfer are handled locally, without the need for a global solution on the entire mesh.

RESULTS & IMPACT

Using Blue Waters, the research team has performed a suite of 3D runs of the collapse, bounce, and explosion (most often) of 9-, 10-, 11-, 12-, 13-, 14-, 15-, 16-, 17-, 18-, 19-, 25-, and 60-solar-mass progenitor massive stars. This is the most extensive set of 3D supernova simulations with the necessary realism ever performed. Moreover, the team has been able to conduct the high-resolution full-physics simulations ever performed, calculate the gravitational wave and neutrino signatures, explore pulsar kick speeds, and establish debris morphologies and compositions.

WHY BLUE WATERS

For the team’s code, Fornax, the Blue Waters architecture in the MPI/CPU context, with its large per-node memory and rapid interconnect, provides the quickest turnaround for these 3D supernova simulations of any available high-performance computing resource.

PUBLICATIONS & DATA SETS

10.1007/s11214-017-0450-9.
10.1093/mnras/stx809.
10.1093/mnras/stz270.
10.1093/mnras/stx809.
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10.1093/mnras/stx809.
10.1093/mp/cty040.
10.1093/mnras/stx809.
10.1093/mp/cty040.
EXECUTIVE SUMMARY

Observing electromagnetic and gravitational waves from supermassive binary black holes and their environments promises to provide important new information about both strong-field gravity and galaxy evolution. Since little theoretical understanding about the details of these accreting binary black hole systems exists, the aim of this project is to continually advance the realism and rigor of simulations of these systems. The problem is complicated because dynamical general relativity, plasma physics, and radiation physics all must be calculated together over vast spatial and temporal scales.

This past year, the research team finished performing the first magnetohydrodynamics (MHD) simulations of black holes with their own mini-disks surrounded by a circumbinary disk. The team also created the first detailed electromagnetic predictions consistent with simulations using postproduction radiation transport. These predictions will be critical to the success of electromagnetic searches and source characterization leading up to the launch of the Laser Interferometer Space Antenna (LISA), which will provide important new information about both strong-field gravity and galaxy evolution. Since little theoretical understanding about the details of these accreting binary black hole systems exists, the aim of this project is to continually advance the realism and rigor of simulations of these systems. The problem is complicated because dynamical general relativity, plasma physics, and radiation physics all must be calculated together over vast spatial and temporal scales.

RESEARCH CHALLENGE

Realistic accretion disk simulations are particularly challenging because they involve a multitude of physical processes interacting over large dynamic ranges in space and time. In actual systems, gas is collected at scales a million times larger than the black holes themselves, yet many cells per black hole width must be used to capture the relativistic plasma dynamics in their vicinity. Reliable angular momentum transport of gas through the disk requires solving the MHD equations of motion at sufficiently high resolution to adequately resolve the responsible internal magnetic stresses. Consistency between the gas’s thermodynamics and radiation model is desirable to produce self-consistent predictions of the light produced by the modeled systems, which is the ultimate goal of this program. Then, transporting the produced light to a distant observer requires researchers to calculate how light moves in the curved time-dependent spacetime of the black hole binary, and how it scatters and is absorbed by intervening gas; i.e., investigators must solve the general relativistic geodesic and radiative transfer equations. All this sophistication is built so scientists can confidently predict what electromagnetic counterparts may exist to the extremely bright gravitational wave sources LISA will see over cosmological distances. Since LISA is planned to launch in more than a decade, researchers can begin to search for these systems with predictions in hand. The research group’s simulations may discover features that are unique to binaries and inform the search for them.

METHODS & CODES

The research team used the flux conservative GRMHD code called HARM3D. It is written in a covariant way such that arbitrary spacetime metrics and coordinate systems may be used without the need to modify core routines. The team also tested and used the new code Patchwork/MHD coupled with HARM3D to enable the most sophisticated and longest simulations yet. This allowed the placement of meshes with different refinement/coordinate and topologies in a way ideal for the system, increasing the efficiency of the simulations and extending them by an order of magnitude in time. It enabled the team to capture the behavior of a region between the black holes that was excluded in prior 3D simulations and to achieve a resolution unprecedented in magnetized 3D simulations of accreting binaries.

RESULTS & IMPACT

The research team’s continued research program focused on 3D MHD simulations of the black hole mini-disks and circumbinary disk interactions has advanced the field in a number of ways. During a previous allocation period, the team discovered a new phenomenon in which the irregular circumbinary flow can modulate the rate of accretion onto the mini-disks in a quasiperiodic fashion, causing them to be depleted and then refilled as they passed by the over-density feature in the circumbinary disk [1]. During the most recent allocation period, the team continued the simulation of three binary black hole orbits to 12 orbits [3]. This allowed the team to probe the mini-disks quasiperiodic behavior deeper into the late stages of the relativistic binary black hole inspiral. The research group showed that the quasiperiodicity in the mini-disks evolution is driven by the interaction of the individual black holes with a localized over-density feature in the circumbinary, which orbits the binary at a well-defined beat frequency with respect to the orbiting black holes. Since the mass inflow times onto each black hole during the late stages of inspiral are comparable to the variability of the mass supply owing to the over-density, the mini-disks masses and accretion rate onto each black hole are strongly modulated at this beat frequency. This constitutes a distinctive electromagnetic signature, the sort that could distinguish supermassive black hole binary systems from typical accreting single supermassive black holes. The research team subsequently explored how all these changes when the disk is tilted with respect to the binary’s orbit, since the gas fed to the system need not always be aligned. The team has completed a first survey and are analyzing the results as of August 2019 (Fig. 1).

The team performed first-of-its-kind radiative transfer calculations in time-dependent general relativity using the simulation’s data as an emitting source in order to predict the electromagnetic emission from the mini-disks. A range of viewing angles and observation frequencies were surveyed for all time steps of data to explore the energy, time, and angle dependence of the emission [2]. This calculation resulted in the first electromagnet-
ACCRETION DYNAMICS OF SUPERMASSIVE BLACK HOLE BINARIES

Allocation: NSF PRC/16,600 Knh
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Collaborators: Scott Noble1, J. Kroulik2, Mark Avara3, Dennis Bowen4, Vassilios Mewes1
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EXECUTIVE SUMMARY
The plasma dynamics and electromagnetic emission of a supermassive black hole binary embedded in a gaseous astrophysical environment is integral to the story of galaxy evolution and the growth of supermassive black holes. The future launch of the Laser Interferometer Space Antenna (LISA) and an enhanced view of the sky enabled by upcoming X-ray and time-domain telescopes will provide a multimessenger view of these binary systems. To meaningfully identify the specific electromagnetic signals coming from a supermassive black hole binary approaching merger requires numerical explorations on Blue Waters of their full nonlinear behavior. With this allocation, the research team has performed the first 3D GRMHD simulation of an electromagnetically active supermassive black hole binary to over 30 orbits. This became possible with the development of a new multimesh code, PatchworkMHD, which removed significant limitations on meshes, coordinates, and geometry from prior simulations, provided better efficiency, and will ultimately enable the first parameter space survey in 3D–MHD simulations of these binary systems.

RESEARCH CHALLENGE
Understanding the behavior of supermassive black hole binaries in an empty region of space requires proper evolution of a dynamical general relativistic spacetime. When such a system is embedded in a gaseous environment in which plasma falls toward the black holes forming accretion disks, the system can become incredibly bright, and only then will electromagnetic telescopes detect them. Simulations of these accreting systems are particularly challenging as they involve a multitude of physical processes interacting over large dynamic ranges in space and time. The gas is collected at scales over a million times larger than the black holes themselves, yet a realistic grid-based numerical study requires many grid cells spanning the width of the black hole in order to capture the relativistic plasma dynamics in their vicinity. The demands grow further because realistic angular momentum transport in the gas of the disk requires solving the magnetohydrodynamic (MHD) equations of motion at sufficiently high resolution to adequately resolve the responsible internal magnetic stresses. Furthermore, consistency between the gas’s thermodynamics and a radiation model is desirable to produce reliable predictions of the light produced by the systems, which is the ultimate goal of this program. Transporting the produced light to the equivalent of an Earth-based telescope requires researchers to calculate how light moves in the curved time-dependent spacetime of the black hole binary and how it is scattered and absorbed by intervening gas. This requires numerically solving the general relativistic geodesic and radiative transfer equations.

METHODS & CODES
The research team used the flux conservative GRMHD code called HARM3D. It is written in a covariant way such that arbitrary spacetime metrics and coordinate systems may be used without the need to modify core routines. The team has also used the new code PatchworkMHD coupled with HARM3D to enable the most sophisticated and longest simulations of supermassive black hole binaries yet (Fig. 1). PatchworkMHD allows the placement of meshes with different refinement/coordinates and topologies in a way that is ideal for the system (Fig. 2). This ability has increased the efficiency of the simulations, extending them by an order of magnitude in time. It also allowed the team to capture the behavior of a region between the black holes that was excluded in prior 3D simulations and to achieve a resolution unprecedented for magnetized 3D simulations of accreting binaries.

RESULTS & IMPACT
This continued research program focused on 3D MHD simulations of minidisk and circumbinary disk interactions has advanced the field in a number of ways. During a previous allocation, the research team discovered a new phenomenon in which the irregular circumbinary flow can modulate the rate of accretion onto the minidisks, leading them to be depleted and then refilled as they pass by the over-density feature in the circumbinary disk, producing quasi-periodic electromagnetic emission [1–3]. An extension of this early simulation to 12 orbits provides enough temporal overlap for quantitative comparison to the team’s newest 30-orbit simulation using the new PatchworkMHD infrastructure. With better resolution, the first 3D GRMHD evolution of the region where material sloshes from orbit around one black hole in the binary to the other, and with enough orbits to start constraining and identifying light-curve properties unique to these systems, the team’s most recent simulation has provided a number of new insights soon to be published [4]. The research group has discovered that at this separation there is significant interaction among the materials orbiting each black hole. The team has also discovered symmetry breaking important to observations that only 3D simulations capture, and have constrained how the magnetic field threading each black hole evolves through these final stages prior to merger (Fig. 1). Insights in this last domain help the team to understand potential electromagnetic signatures from relativistic jets in supermassive black hole binaries, producing complementary observables to those coming from the disks. The large number of orbits performed in this simulation is enough to evolve the binary through a gravitational-wave decay to half its starting separation. The team has therefore finally been able to capture the coupled evolution of the circumbinary disk and the accreting black holes through their final stages. This work of starts to fill the gap between nonrelativistic studies of widely separate binaries and fully relativistic studies that capture the black hole merger. There is much yet to be discovered in how these regimes connect; the tools that the research team has developed and tested on Blue Waters are well suited for taking the next steps. Analysis and interpretation of the combined postprocessing data products for both the simulation published in [3] as well as the 30-orbit [4] simulations are underway and will provide much more detail, especially with regard to a time-dependent electromagnetic view of supermassive black hole systems.

WHY BLUE WATERS
Using PatchworkMHD, the research team was able to run binary simulations with 30 times the prior efficiency, which—coupled with the scale of resources available only on Blue Waters—has enabled the team to perform the first physical parameter-space study of these systems in 3D GRMHD.

PUBLICATIONS & DATA SETS
ACHIEVING PROBABILISTIC CLASSIFICATION OF COSMIC WEB PARTICLES USING RAPIDLY GENERATED TRAINING DATA: A METHOD FOR CLASSIFYING GALAXIES INTO THEIR COSMIC WEB STRUCTURAL GROUPS USING SUPERVISED MACHINE LEARNING

EXECUTIVE SUMMARY

The cosmic web consists of a network of galaxies and dark matter: long, strandlike filaments connect between spheroidal galaxy clusters, leaving underdense void regions in between. Knowing whether a galaxy is a member of a halo (the dark matter clump around which clusters form), filament, or void provides substantial information about its surrounding environment, which helps in understanding how it formed and will evolve. However, current methods are limited: direct classification algorithms are generally inefficient, while deep learning-based methods are inconsistent with one another. Therefore, the research group created a novel classification method using supervised machine learning. They train the algorithm using quickly generated data that visually approximates the cosmic web using predetermined generation algorithms. Then, with the help of the high memory capacity of Blue Waters, the researchers use the trained algorithm to classify galaxies in simulated data. While the training data lack much of the detail seen in observed/simulated data, it takes substantially less computational power to create. A simulation of cosmic web formation with 16 million particles requires tens of thousands of node-hours on a supercomputer, whereas the team’s method can generate training data with the same number of particles in less than an hour on a laptop computer. The researchers have demonstrated that this method provides enough information for the machine learning algorithm to “learn” to correctly classify particles in more realistic data sets. Although it is trained using simpler data, the robustness of machine learning helps the algorithm bridge the information gap, providing classification at a substantially cheaper cost.

RESEARCH CHALLENGE

Current methods used to classify galaxies into cosmic web structural groups typically utilize neural networks, as direct algorithms are too computationally intense. However, arbitrary hyperparameters and inconsistent cosmic web class definitions lead to substantial disagreement among methods. In addition, owing to these hyperparameters, it is difficult to establish self-consistency for a given method.

METHODS & CODES

Training data is generated by sampling particles from pre-determined toy model structures. Halos are produced by sampling particles from a spherical Gaussian distribution and then distributed randomly throughout the region. Filaments consist of particles populated in a uniform cylinder around randomly generated Bezier curves (https://github.com/dhermes/bezier), while voids are a uniform background distribution. Measurements of the k-nearest neighbors provide information about the local density magnitude, while the explained variance ratio calculated from a principal component analysis decomposition measures the density field directionality. A random forest algorithm was trained using the results of these measurements on each particle, and the trained algorithm was used to classify particles in an N-body simulation. Though these classifications cannot be directly verified owing to a lack of true class values, the researchers demonstrated the robustness of the method by comparing these predictions to those made on another toy model data set.

RESULTS & IMPACT

Currently, the team is working on a final write-up of the results. Work to date has demonstrated that the methodology does provide a robust method for classifying particles at a much lower computational cost. In addition, the team’s verification methods have shown that the method achieves probabilistic classification, providing additional information to use when studying the formation and evolution of galaxies. Although the optimal configuration of measurements and toy model parameters remains to be found, the research group has demonstrated the effectiveness of using a supervised method trained with fast generated data, and they expect that future optimization will lead to improvements in particle classification that is naturally accompanied by information on the classification confidence. This will change the field of cosmology by simplifying and improving the efficiency of particle classification, enabling greater understanding of the cosmic web and its effects on other structures.

WHY BLUE WATERS

Blue Waters provided substantial benefit through its high-memory nodes. Although toy model generation is extremely fast and efficient, performing measurements on the N-body simulation requires considerably more memory than is available on a laptop or a single Blue Waters node. Segmenting the particle field does not avoid this issue because of the size of the required files, and analysis would take an unreasonable amount of time. Blue Waters’ nodes had enough memory to load the segmented files and analyze them, and by parallelizing the analysis across several nodes, it allowed computations that would normally require several weeks on a high-capacity remote machine to be completed in less than a day.
THE EPOCH OF THE FIRST LUMINOUS BLACK HOLES: EVOLVING THE BLUE TIDES SIMULATION INTO THE FIRST BILLION YEARS OF COSMIC HISTORY

Allocation: NSF PRC/4,400 Kosh
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Collaborators:

The application runs required essentially the full system: The researchers used 20,250 nodes (648,000 core equivalents—the new version of the code can scale higher, but the team left a safety margin) using 57 GB/node (89%). This application thus uses 1.15 PB of memory—something Blue Waters can provide, as it is 90% of the available memory. Running such large jobs on a regular basis in a very timely fashion obviously requires advanced resource management, and the way the Blue Waters project has been set up made this possible.

PUBLICATIONS & DATA SETS


Figure 1: Left—The current (as of 2019) quasar sample in the early Universe. Thirty new quasars at \( z \approx 6 \) (the first billion years) were discovered recently. Right: The large-scale environment surrounding the first massive black hole in Blue Tides. Bottom: Blue Tides galaxies as they would be seen by the Webb telescope.

The previous phase of the Blue Tides (BT) simulation made direct contact with the observations of the giant record holding black hole, making predictions for its host galaxy. Remarkably, the sample of early Universe quasars has grown tremendously over the last year, with 30 more quasars having been found from the first billion years of the universe. The researchers would like to study those types of objects directly with Blue Tides, if they are able to. In order to do so, the researchers found a method that enables the rapid black hole growth necessary to reach these giant masses and make predictions for upcoming telescopes. In order to make contact with this much larger sample, it was necessary to evolve Blue Tides forward in time, reaching into a new regime where hundreds of thousands of galaxies in the simulation volume are forming stars, and the Universe is at a new level of complexity.

METHODS & CODES

Blue Tides is run on the entire set of compute nodes on Blue Waters using the latest version of the research team’s MP-Gadget code. The general characteristics of the GADGET family of codes are those of a flexible Tree-PM-SPH solver for cosmological fluids of dark matter, gas, and stars. In addition to the basic physics of gravity and hydrodynamics, the code also contains numerous further physics modules covering aspects of star formation and black hole growth. The MP-Gadget code variant was developed to be lean, efficient, and scalable. As the simulation progresses, the computation starts to become dominated by the hydrodynamics solver as more galaxies form. This part of the code has traditionally been the hardest to scale, with timesteps getting very small in highly clustered regions of very high density. These regions, however, are the most interesting ones, where the observable massive galaxies and quasars form. The MP-Gadget hydro-solver is MPI/thread hybridized, and the team has recently further improved the threading efficiency. More threads mean fewer MPI ranks, and thus easier over-decomposition.

RESULTS & IMPACT

As the cosmic web of gas and dark matter was evolving in Blue Tides at an ever-increasing pace, a large sample of massive black holes had formed in the simulation volume over the course of the current run. With such a set of objects, the researchers can now carry out statistical tests on the whole population, and test cosmological models quantitatively. The host galaxies of these black holes have detailed stellar properties available: They all tend to be highly star-forming but have a wide range of kinematic characteristics (disks, bulges), and lie in a variety of large-scale environments. The assembly of each galaxy happens at the same time that the central black holes grow, and for approximately 30 objects the black hole outshines the galaxy significantly and the object would be observed as a quasar.

With the large-scale simulation volume, the researchers have made many predictions on what the James Webb Space Telescope (JWST) will see when pointed at such early quasars after its launch in 2021. By comparison, the Blue Tides simulation box is ten thousand times larger in angular area than the field of view of JWST’s Near Infrared Camera, allowing the rare regions where quasars form to be translated into mock JWST observations. JWST should reveal an assortment of black hole galaxies, including compact spheroids, and isolated galaxies.

WHY BLUE WATERS

A complete simulation of the Universe at the epochs the researchers are studying requires a small enough particle mass to model the dwarf galaxies, which significantly contribute to the summed ionizing photon output of all sources. It also requires an enormous volume (on the order of 1 cubic gigaparsec or Gpc, where 1 Gpc is \( 3 \times 10^{10} \) cubic light years) in order to capture the rarest and brightest objects: the first quasars. The first requirement is therefore equivalent to a high particle density, and the second to a large volume.

Previous calculations on smaller high-performance computing systems have either fulfilled the first requirement in a small volume, or the second with large particle masses, thus only resolved for large galaxies. With Blue Waters, however, the research team has reached the point where the required number of particles (about one trillion) could be contained in memory, and the petaflop computing power was available to evolve them forward in time. Blue Waters, therefore, has made possible this qualitative advance, allowing arguably the first complete simulation (at least in terms of the hydrodynamics and gravitational physics) of the creation of the first galaxies and large-scale structures in the Universe.

The application runs required essentially the full system: The researchers used 20,250 nodes (648,000 core equivalents—the
ADVANCING FIRST-PRINCIPLE SYMMETRY-GUIDED NUCLEAR MODELING FOR STUDIES OF NUCLEOSYNTHESIS AND FUNDAMENTAL SYMMETRIES IN NATURE

EXECUTIVE SUMMARY

The Blue Waters (BW) system has enabled modeling of nuclear wave functions with unprecedented accuracy for light- and medium-mass nuclei, capitalizing on advances feasible with the SA–NCSM and Blue Waters computational power. This targets nuclei far from stability with collective and cluster substructures, while pinpointing key features in magnesium isotopes—important for providing accurate predictions for deformed and, on nucleosynthesis simulations. This method capitalizes on a new symmetry of the nucleus. The SA–NCSM utilizes physically relevant model spaces using ultralarge model spaces with concomitant computer code LSU3shell [3−5], that embraces the first-principles concept and capitalizes on a new symmetry of the nucleus. The SA–NCSM solves the time-independent Schroedinger equation as a Hamiltonian matrix eigenvalue problem. The main computational task is to evaluate a large symmetric Hamiltonian matrix and to obtain the lowest-lying eigenvectors that correspond to the experimental regime. Accuracy is based on the degree of con- vergence, which is linked to the size of the model space that can be achieved. The SA–NCSM utilizes physically relevant model space of significantly reduced dimensionality compared to ul- tralarge model spaces encountered by standard ab initio approaches. These theoretical advances [2,6,7], coupled with the computational power of the Blue Waters system, have allowed the team to reach medium-mass nuclei that are inaccessible experimentally and to other ab initio methods.

RESULTS & IMPACT

The nucleus of interest represent a considerable challenge requiring computational power of nearly the entire BW machine and its system memory. Two graduate students have carried forward these studies and have had the unique opportunity to work with supercomputers and massively parallel programming environments. The following list describes the results and their impact:

- While enhanced deformation and cluster substructures are difficult to describe from first principles, the SA–NCSM and the BW system have allowed the first ab initio descriptions of deformed nuclei using chiral interactions [2,6,7]. The team has continued to study emergent deformation and clustering in nuclei, from first principles, for Mg isotopes and their mirror nuclei. In addition to calculations for Mg and F, Mg and Ne, new results are now available for Mg and Na, and the challenging Mg (Fig. 1). For Mg, new observations have revealed an anomaly in a specific type of collective transition, which has been explained by the SA–NCSM model as shape mixing.

- For neutron experiments, it is important to reduce uncertainties related to the response of the detector nucleus to the neutron. Response functions are now feasible for intermediate-mass nuclei, such as Mg, the next-generation detector ingredient. As an illustration, BW has allowed the team to carry forward large-scale ab initio calculations for the response for Ne (Fig. 2). Such calculations are important for studies of nuclear com- pressibility, which in turn inform the equation of state for neu- tron stars. In addition, various peaks in the response function can provide further insight into clustering substructures and collective degrees of freedom.

- Ab initio modeling of open-shell intermediate-mass nuclei is now feasible, and these, in turn, are used to study nuclei on the proton drip line, such as Ar, by nuclear systematics, key to further under- standing the origin and production of heavy elements. For example, ab initio calculations for Ne, and especially the neg- ative parity states (Fig. 2), as well as for O, are used to calcu- late alpha decay probabilities, which enter as a critical input into reaction rates for (n,α) and proton capture reactions. In- deed, the alpha-induced reaction for O is currently not well understood but has been suggested to have the largest effect on nucleosynthesis simulations. This ab initio modeling is im- portant for providing accurate predictions for deformed and, in the future, heavy nuclei of interest to understand the β process nucleosynthesis, one of the most challenging problems in astrophysics today.

WHY BLUE WATERS

Currently, only the BW system provides resources required for these ab initio studies of medium-mass isotopes with cut- ting-edge accuracy. To illustrate the level of complexity, appli- cations to medium-mass nuclei require more than hundreds of exabytes of memory to store the Hamiltonian matrix. In order to capitalize on advances feasible with the SA–NCSM and Blue Waters’ capabilities, and with the help of the BW staff, the re- search team managed to improve scalability and performance of its code. As a result, the team’s largest production runs efficient- ly utilized 715,712 concurrent threads running on 22,368 Cray

Figure 1: First ever ab initio description of collective features in magnesium (Mg) isotopes. SA–NCSM calculations are performed on ultralarge model spaces using concomitant computer code LSU3shell [3–5], that embraces the first-principles concept and capitalizes on a new symmetry of the nucleus. The ab initio SA– NCSM solves the time-independent Schroedinger equation as a Hamiltonian matrix eigenvalue problem. The main computation- al task is to evaluate a large symmetric Hamiltonian matrix and to obtain the lowest-lying eigenvectors that correspond to the experimental regime. Accuracy is based on the degree of con- vergence, which is linked to the size of the model space that can be achieved. The SA–NCSM utilizes physically relevant model space of significantly reduced dimensionality compared to ultralarge model spaces encountered by standard ab initio approach- es. These theoretical advances [2,6,7], coupled with the computa- tional power of the Blue Waters system, have allowed the team to reach medium-mass nuclei that are inaccessible experimentally and to other ab initio methods.

Figure 2: The first ab initio response of the deformed Ne to an external probe vs. the energy transfer, resolving a clear evidence (the highest peak) for a giant monopole resonance and intriguing nuclear communality. Other emerging features detected within the SA–NCSM model are also shown, enhanced collectivity (P1) and clustering (P2). XEB compute nodes to solve the nuclear eigenvalue problem with a memory footprint of up to 750 terabytes of data. Clearly, the BW system represents a unique computational platform that al- ready plays a crucial role in advancing ab initio nuclear theory toward new domains.

PUBLICATIONS & DATA SETS


ACKNOWLEDGMENTS

The Blue Waters (BW) system has enabled modeling of nuclear wave functions with unprecedented accuracy for light- and medium-mass nuclei, capitalizing on advances feasible with the SA–NCSM and Blue Waters computational power. This targets nuclei far from stability with collective and cluster substructures, while pinpointing key features in magnesium isotopes—important for providing accurate predictions for deformed and, on nucleosynthesis simulations. This method capitalizes on a new symmetry of the nucleus. The SA–NCSM utilizes physically relevant model spaces using ultralarge model spaces with concomitant computer code LSU3shell [3−5], that embraces the first-principles concept and capitalizes on a new symmetry of the nucleus. The ab initio SA–NCSM solves the time-independent Schroedinger equation as a Hamiltonian matrix eigenvalue problem. The main computational task is to evaluate a large symmetric Hamiltonian matrix and to obtain the lowest-lying eigenvectors that correspond to the experimental regime. Accuracy is based on the degree of convergence, which is linked to the size of the model space that can be achieved. The SA–NCSM utilizes physically relevant model space of significantly reduced dimensionality compared to ultralarge model spaces encountered by standard ab initio approaches. These theoretical advances [2,6,7], coupled with the computational power of the Blue Waters system, have allowed the team to reach medium-mass nuclei that are inaccessible experimentally and to other ab initio methods.
MAGNETIZED MODELS OF GIANT IMPACTS

Allocation: Exploratory/30 Knh, 300 Knh
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Co-PI: Patrick Mullen

EXECUTIVE SUMMARY

The giant impact hypothesis suggests that about 4.5 billion years ago, a highly energetic, off-centered collision between a Mars-sized body and the proto-Earth formed a massive debris disk about the early Earth. It is from this orbiting disk of debris that the Moon is thought to have coalesced. Numerical simulations of the giant impact require massively parallel, high-resolution, multiphysics simulations. The research team's models, applied to the Blue Waters supercomputer, are unique in that they are the first to address the dynamical importance of any magnetic field the impactor and/or proto-Earth may have possessed. These simulations have found that the natural consequence of a magnetized Moon-forming giant impact is a disk of debris hosting a toroidal magnetic field. A series of high-resolution numerical experiments also demonstrated that magnetic field strengths are amplified by as many as three to four orders of magnitude following the impact and early disk evolution.

RESEARCH CHALLENGE

Shortly after the formation of the solar system, the giant impact hypothesis suggests that a Mars-sized impactor, Theia, struck the proto-Earth in an off-centered collision. This giant impact sent liquid and vaporized silicates into orbit around the proto-Earth, forming a protolunar disk from which the moon is thought to have coalesced. Three-dimensional simulations of this impact have been studied extensively; however, all of them have neglected the potential role of magnetic fields [1,2]. Therefore, the research group employed the Blue Waters supercomputer to study the dynamical importance of magnetic fields in the giant impact and the early evolution of the protolunar disk.

METHODS & CODES

The team applied the astrophysical magnetohydrodynamics code Athena++ [6]. Athena++, written in C++, operates in a purely Eulerian framework and uses a hybrid parallelization model based on OpenMP/MPI. The code employs a task-based execution model: each thread works on whichever tasks are presently available during a given timestep. Athena++ is modular; the included physics (such as magnetic fields, self-gravity, equation of state, diffusion, and the like) in addition to the choice of integrator/reconstruction method and coordinate system, are set as configure options at build time.

RESULTS & IMPACT

The research team's simulations initialize the impactor and proto-Earth with dipole magnetic fields. The Moon-forming giant impact wraps and winds these magnetic field lines into a toroidal configuration in the debris disk. Shear and turbulence in the disk amplify these field strengths by nearly four orders of magnitude in approximately one month after initial contact [4]. Thus, with even a modest initial field strength for the impactor and proto-Earth, these simulations demonstrate that magnetic fields could become dynamically important in a short timescale compared to the lifetime of the protolunar disk. In particular, magnetic fields may drive a fluid instability in the disk that causes turbulence to mix vaporized rock between the protolunar disk and the Earth. Such magnetic turbulence may help explain the isotopic similarities between the Earth and the Moon [4].

WHY BLUE WATERS

A large computational domain is required to contain the giant impact. In addition, a high-resolution model is necessary to accurately model dynamically important shocks and capture the onset of turbulence in the disk. Further, long integrations are required to evolve the simulation from initial impact to approximately one month after the formation of the protolunar disk. The Blue Waters supercomputer enables these large-scale, multiphysics simulations in which the team has applied as many as 128 Blue Waters XE nodes to a 1,024^3 (~200-km linear resolution) simulation.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Cosmic reionization—the process of ionization of the bulk of cosmic gas by ultraviolet radiation from the first galaxies and quasars—is the last frontier of modern cosmology. The Cosmic Reionization on Computers (CROC) project produced several numerical simulations of reionization that self-consistently modeled all relevant physics from radiative transfer to gas dynamics and star formation in simulation volumes of over 100 comoving Mpc. This was necessary to model a representative sample of high-mass galaxies, and a spatial resolution approaching 100 parsecs in physical units, which is necessary to reliably model star formation in galaxies. These simulations, therefore, cover the full range of spatial, temporal, and mass scales important for studying reionization.

The primary motivation for focusing on reionization now is the expected major advance in observational capabilities: the James Webb Space Telescope (the next flagship NASA mission) is scheduled to launch in 2021, and studying galaxies responsible for cosmic reionization is one of its primary goals. Studies of intergalactic gas will be propelled forward by the deployment of 30-meter telescopes, several of which will become operational in the first half of the next decade. Other novel observational tools will follow in the second half of the next decade.

METHODS & CODES

In order to reach the required dynamic range, the research team relied on the adaptive mesh refinement technique. The simulations are run with the adaptive refinement tree code, a publicly available cosmological simulation code developed and supported by the research group. The code includes all necessary physical modules for simulating cosmic reionization (dynamics of dark matter and gas, atomic processes, interstellar chemistry, star formation and stellar feedback, radiative transfer of ionizing and UV radiation). ART is MPI-OpenMP parallel and scales perfectly on this type of simulation to about 50,000 cores, with parallel scaling remaining acceptable to about 100,000 cores.

RESULTS & IMPACT

CROC simulations are defining the state of the art in this field. By virtue of including all the relevant physics and extending to volumes that are required to properly capture the process of reionization, they are creating a physically plausible model of cosmic reionization that can be matched against any existing observational data. Such comparisons have been made by the research group in the last several years in a series of papers. However, the most constraining observational data set that exists today is the distribution of optical depth in the spectra of distant quasars. Over 100 quasars during the reionization epoch have been discovered so far, and for almost 70 of them, high-resolution and high-quality spectra exist. These data probe the largest spatial scales relevant for reionization of about 70 comoving Mpc.

During the second year of this project, the team focused on two separate scientific questions: (1) how galaxies influence and shape the distribution of ionized gas on large scales; and (2) how the brightest known quasars affect galaxies and gas in their vicinity. Both of these questions are at the frontier of modern research and promise to develop into new, independent areas of study in the next several years. An example of cosmic gas distribution from one of the team’s simulations is shown in Fig. 1.

Figure 1: Slice through the simulation box. Subregions show the cosmic gas overdensity 1 + δ, neutral hydrogen fraction xHI, and gas temperature T.
ELUCIDATING THE ALIGNMENT MECHANISM FOR BLACK HOLE 
ACCRETION DISKS SUBJECTED TO LENSE–THIRRING TORQUES

Allocation: GLCP/C/288 Koh
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EXECUTIVE SUMMARY

The research team uses Blue Waters to study astrophysical accretion onto a spinning black hole in which there is a misalignment (tilt) between the orbital axis of the incoming gas and the black hole rotation axis. Astrophysicists have long expected that an initially misaligned orbiting accretion disk would align with the black hole’s spin axis at some location near the hole. A detailed understanding of this alignment process has, however, been limited owing to the assumption of a phenomenological viscosity to describe the internal dissipation necessary for alignment. The team’s simulations capture the physical internal stresses due to magnetohydrodynamic turbulence without reliance on phenomenological viscosity; such simulations are only possible with the high grid resolution made feasible by Blue Waters. The investigation probes how a time-steady transition might be achieved between an inner disk region aligned with the equatorial plane of the central mass’s spin and an outer region orbiting in a different plane.

RESEARCH CHALLENGE

Accretion disks occur in a wide variety of astrophysical systems. Whenever the disk’s angular momentum is oblique to the angular momentum of the central object(s), a torque causes rings within the disk to precess, twisting and warping it. Because the torque weakens rapidly with increasing radius, it has been thought that some unspecified “friction” brings the inner portions of such disks into alignment with the equator of the central object. Despite considerable theoretical effort, researchers are still unable to predict the alignment radius for a disk. Nearly all previous work on this topic has assumed that such a disk’s internal stresses can be described by a parameterized isotropic viscosity. However, there is a well-established physical mechanism for internal stresses in accretion disks—correlated magnetohydrodynamic (MHD) turbulence, driven by the magnetorotational instability [1,2].

Simulating MHD turbulence in a tilted disk is demanding. To evolve MHD turbulence, a simulation must have a timestep that is very short compared to an orbital time, whereas the precession timescale of orientation transition is many orbital periods long. This project’s numerical simulations investigate how twisted disks align when their mechanics are described only in terms of real forces, including MHD turbulence. The aim is to develop a predictive model for the location of alignment fronts in disks subjected to alignment torques.

METHODS & CODES

The research team used a simplified disk model first studied in [3], consisting of an isothermal disk orbiting a point-mass in Newtonian gravity with a Keplerian angular velocity distribution and including only a lowest-order post-Newtonian term to represent the relativistic Lense–Thirring torque. This idealized model allowed the team to focus on the important physical processes governing alignment; these can be studied in isolation and in detail. They examined the influence of black hole tilt on the alignment process, evolving three models where the tilt angle is changed without altering anything else. This approach stands in contrast to those efforts that simulate model disks in the full general-relativistic context.

The simulations were done with a Fortran-95 version of Zeus, an operator-split code that solves the equations of compressible MHD by time-explicit finite-differencing [4] using the constrained transport algorithm [5] to preserve the divergence-free property of the magnetic field. Zeus uses domain decomposition and MPI for parallelization.

RESULTS & IMPACT

The project team investigated the effects of black hole tilt angle on accretion disk alignment, modeling three initial black hole tilts of 6°, 12°, and 24° using both magnetohydrodynamic (and inviscid) hydrodynamic evolutions. By considering a single sound speed and a simple underlying disk model, the researchers isolated the effect of tilt amplitude, which is found to have a limited influence on alignment. The imposed tilt angle simply sets the “unit,” and the resulting dynamics are determined by ratios in terms of that unit. The radial shape of the transition region between the aligned inner disk and unaligned outer disk, as well as the location of the head of the alignment front, are very nearly identical once the black hole tilt (see Fig. 11) is scaled out. Tilt does have some secondary effects. The steady state warp within the alignment front increases at a slightly faster rate with tilt than with simple proportionality. Another effect is a small decrease in the initial alignment front velocity with increasing tilt.

Purely hydrodynamic disks behave similarly, but because the amplitude of the disk warp is a function of the tilt angle for a given disk thickness, higher tilt angles have larger relative warp values. From this it follows that bending waves produced in the disk are increasingly nonlinear, and hence more dissipative. Bending waves propagating through the disk without hindrance proceed solid-body precession which, in turn, can end alignment at an earlier time compared to an MHD disk where the turbulence inhibits wave propagation [6]. In this work, the hydrodynamic models saw a rapid diminution of precession phase gradient in the outer disk, which brought alignment to a halt and reversed the motion of the alignment front.

Some simulations of tilted disks have either seen evidence for a possible separation of the inner and outer disk [7], or clear disk breaking, whether the central object is a binary or a spinning black hole (e.g. [8]). In this project’s simulations, even when the initial misalignment is 24°, which, for the sound speed studied, is four vertical scale heights at the disk fiducial radius, the surface density remains a smooth function of radius; i.e., the team found no examples in which the disk inner-aligned and outer-misaligned regions separated, or “broke.”

WHY BLUE WATERS

The research team has used Blue Waters to compute new thin disk simulations subject to Lense–Thirring torque with unprecedented resolution to explore the mechanisms behind, and scaling properties of, disk alignment. The unique high-performance capabilities of Blue Waters enabled key maximum-resolution simulations.

PUBLICATIONS & DATA SETS


Figure 1: Logarithmic density contours for disk tilt angles of 6° (top), 12° (middle), and 24° (bottom) after 20 orbits of applied torque. The inner disk regions have aligned with the black hole equatorial plane (overlaid line), and the transition from alignment to outer obliquity occurs at approximately the same radius.
UNDERSTANDING THE ORIGINS OF THE STARS AND GALAXIES IN OUR UNIVERSE

EXECUTIVE SUMMARY

This research uses Blue Waters to explore the origins of galaxies and the nature of dark matter. At a fundamental level, the study of galaxies and stars seeks to answer the question, “How did we get from the Big Bang to the Milky Way?” This is an immensely challenging question, involving the interplay among gravity, fluid dynamics, radiation, matter, and stars exploding as supernovae, giving rise to explosive outflows of material from galaxies that can reach the observable Universe. The physics is chaotic and wildly nonlinear, and the range of timescales is tremendous (from one to ten billion years). As such, massive numerical simulations that can follow all of these processes are required. By using numerical simulations, the researchers have gained fundamental insights into why galaxies today look as they do and, in the process, have strongly constrained the allowed nature of the dark matter.

RESEARCH CHALLENGE

The program seeks to understand the origin and nature of galaxies, using massively parallel simulations that follow the birth and evolution of galaxies and stars from the very early Universe to the present. The simulations model the origins, evolution, internal structure, and observable properties of galaxies ranging in size from the smallest observed “dwarf” galaxies (with just a few thousand stars) to the Milky Way and Andromeda (“the Local Group”). Deep and fundamental questions remain unresolved in this area, including, simply, “How did we get from the Big Bang to the Milky Way?” as well as, “Why did the Universe form so few stars (compared to what it could have done)?” Further questions include, “Why did stars form when and where they did?” and “How can we use galaxies to probe the fundamental nature of dark matter?” At the heart of these issues lies the fact that stars, once they form, are not passive actors within a galaxy: they shine and emit tremendous amounts of energy in the form of light (radiation), stellar winds, and supernova explosions. This energy can blow material out of the galaxy entirely and completely alter the evolutionary history of galaxies.

But these stellar and galactic processes remain poorly understood, in large part because they: (1) couple very small and very large scales in the Universe and require simulations with enormous dynamic range to model them, and (2) involve a diverse range of physics including (but not limited to) gravity, fluid dynamics, magnetic fields, conduction and viscosity, radiation–matter interactions, interstellar chemistry, and stellar evolution. The simulations run on Blue Waters incorporated all of these processes into the highest-resolution simulations yet completed, allowing the research team to address these questions for the first time at the level of detail needed to make observable predictions. Billions of dollars are being invested in new telescopes and instruments to explore these questions experimentally; these simulations are critical tools to make detailed predictions and leverage these transformative observations.

METHODS & CODES

The researchers have run a large suite of cosmological, high-resolution simulations including detailed treatments of the physics of the interstellar medium, star formation, feedback in radiation and supernovae, magnetic fields, and cosmic rays. The simulations use the feedback in realistic environments (FIRE) physics and supernovae, magnetic fields, and cosmic rays. The simulations use the feedback in realistic environments (FIRE) physics methods in the GIZMO code, a new massively parallel multiphysics, hybrid Lagrangian–Eulerian finite-element, high-order, radiation-hydrodynamics code (unique in numerical methods employed).

RESULTS & IMPACT

These cosmological simulations target galaxies from the faintest dwarfs through to the Milky Way and run at the ultrahigh resolution and realism required to interpret the next generation of observations. The petascale resources of Blue Waters allow the researchers to resolve each galaxy with approximately one billion particles and follow them self-consistently over their entire history in realistic cosmological settings. When the interstellar medium is resolved into dense molecular clouds, massive stars naturally form and then inject large quantities of energy and momentum into the surrounding medium via “stellar feedback”: this feedback is critical to produce realistic galaxies and generate the powerful galactic winds observed, radically altering the baryon cycle between galaxies and the circumgalactic medium. The simulations model the physics of galaxy formation with unprecedented realism, uniquely incorporating not only all of the important stellar feedback mechanisms (radiation pressure, photo-heating, stellar winds, supernovae, cosmic rays) but also magnetic fields, physical (anisotropic) Bragginski conduction and viscosity, passive scalar (metal) diffusion, and explicit, multivavelength radiative hydrodynamics.

This work represents the culmination of several years of research supported by the National Science Foundation, and it has been critical in enabling the science of the FIRE project: a collaboration of theorists across 13 different major institutions. The program has revealed fundamental new insights into how stars alter their galactic environments and has changed observational inferences about the nature of dark matter in those galaxies. The simulations are also being used to support an outreach component involving high school students and teachers, and undergraduate students, as well as a large science team using these simulations. The simulations have already been utilized to make predictions specifically for next-generation telescopes including (but not limited to) JWST, LSST, Gaia, and HST, in order to constrain the origin of the heavy elements in the Universe, and test theories of galaxy and star formation, the reionization history of the early Universe, the effects of fundamental plasma physics in the circum- and intergalactic medium, and the nature of cold dark matter.

WHY BLUE WATERS

Blue Waters was critical for this research because the enormous computational challenges detailed in this report required more than 100 million CPU-hours on tens of thousands of processors with tens of terabytes of active memory to store and evolve the immensely complex physical systems, which produced petabytes of data products. No other facility could have enabled this research.

PUBLICATIONS & DATA SETS


Figure 1: Simulations of a Milky Way-like galaxy. Observed starlight (mock images) is shown with overlaid intensity maps showing mock carbon monoxide (molecular gas). X-rays, and dust emission. The “Galaxy Merger” portion shows a mock Hubble image during a galaxy collision, where rival “bursts” of star formation are triggered.

Figure 2: Mock Hubble map of a simulated galaxy pair in a Semi-ana-rich star. Hylenomolecular molecular cloud complexes and young star clusters are visible within the “Milky Way” (galactic disk). The research team’s combination of physics and resolution allows them to model galactic structure with unprecedented realism.
DEEP LEARNING AT SCALE FOR THE CONSTRUCTION OF GALAXY CATALOGS WITH THE DARK ENERGY SURVEY

EXECUTIVE SUMMARY

The scale of ongoing and future electromagnetic surveys poses formidable challenges to classifying astronomical objects. Pioneering efforts on this front include citizen science campaigns adopted by the Sloan Digital Sky Survey (SDSS). SDSS data sets have recently been used to train neural network models to classify galaxies in the Dark Energy Survey (DES) that overlap the footprint of both surveys. The research team has demonstrated that knowledge from deep learning algorithms, pretrained with real-object images, can be transferred to classify galaxies that overlap both SDSS and DES surveys, achieving a state-of-the-art accuracy of 99.6%. In addition, the team has demonstrated that this process can be completed within just eight minutes using distributed training. The researchers also used their neural network classifier to label 10,000 DES galaxies that do not overlap previous surveys. Further, the team has shown that these new data sets can be combined with recursive training to create DES galaxy catalogs in preparation for the Large Synoptic Survey Telescope era.

RESEARCH CHALLENGE

The classification of astrophysical objects has been pursued in the past using a diverse set of tools. For instance, galaxies have been classified using their photometric properties, achieving classification accuracies of around 85% [1]. Other methods of classifying galaxies according to their morphology have taken into account their physical properties across multiple wavelengths. For instance, the method introduced in [2] considered a sample of galaxies from the Sloan Digital Sky Survey (SDSS) [3] using the five SDSS filters (u, g, r, i, z) and then used a combination of shapelet decomposition and principal components analysis (PCA). Other methods for galaxy classification include Concentration—Asymmetry—Smoothness [4] and machine learning, including artificial neural networks and PCAs [5].

In recent years, citizen science campaigns have played a key role in classifying thousands of celestial objects in astronomical surveys. SDSS is an archetypical example of a successful approach to classifying hundreds of thousands of galaxies. As electromagnetic surveys continue to increase their depth and coverage, campaigns of this nature may lack scalability. For example, within six years of operation, the Dark Energy Survey (DES) [6] observed over three hundred million galaxies, a number that will be surpassed by the observing capabilities of the Large Synoptic Survey Telescope (LSST) [7]. In brief, there is a pressing need to explore new approaches to maximize the science throughput of next-generation electromagnetic surveys. A promising paradigm is the convergence of deep learning and large-scale computing to address the imminent increase in data volume, complexity, and latency of observations of LSST-type surveys.

METHODS & CODES

The research team used a subset of SDSS Data Release (DR) 7 images for which it had high confidence classifications through the Galaxy Zoo project, i.e., the team only chose galaxies with a debiased probability greater than 0.985 for combined spirals and 0.926 for ellipticals, respectively. Samples of these images are shown in Fig. 1. The team chose these cutoff thresholds to ensure that: (1) the galaxies used for training the neural network had robust and accurate classifications; and (2) the representation of both classes in the training and test data sets were balanced. The team then divided these images into three separate data sets for training, validation, and testing. The validation set was used to monitor the accuracy and loss when training and fine-tuning the deep neural network, and hence served to optimize hyperparameters such as learning rate and number of epochs for training.

Two test sets were carefully constructed so that the images in each set lay both in the SDSS and DES footprints. The first test set consisted of images with a Galaxy Zoo classification confidence similar to that of the training set, i.e., a high probability cut-off was introduced. This test set was hence labeled High Probability (HP) Test Set, and there were two versions, one for each survey: HP SDSS and HP DES. Just as in the training set, the images for SDSS were obtained from SDSS DR7 and the corresponding images for DES were obtained from the DES DR1 data release. Furthermore, a second test set was created without introducing any probability thresholds on the Galaxy Zoo classification confidence. This set consisted of almost all galaxies lying in both the SDSS and DES footprints, and hence was labeled Full Overlap (FO) Test Set. Again, there were two versions: FO SDSS and FO DES. The motivation behind creating this second test set was that the galaxy profiles in the unlabeled DES data set would more closely match these in the FO test sets. Hence, the FO test set served as a good evaluation metric of the performance of the neural net on the ultimate task of classifying all unlabeled galaxies in the DES catalogue.

The team used open-source software stacks for its studies. The deep learning APIs used were Keras [8] and TensorFlow [9]. For the classification problem, the team did transfer learning starting with the Xception model [10], which had been pretrained with the ImageNet data set [11]. The researchers chose this neural network model because it outperforms many other state-of-the-art neural network models, including Inception-v3, ResNet-152, and VGG16, on the ImageNet validation data set, and it has been suggested that better ImageNet architectures are capable of learning better transferable representations [12]. More importantly, the research team carried out several experiments and found that Xception performed as well as or nominally better on the validation and testing galaxy data sets compared to many other state-of-the-art architectures.

RESULTS & IMPACT

This is the first application of deep transfer learning combined with distributed training for the classification of DES galaxies that overlap the footprint of the SDSS survey, achieving state-of-the-art accuracies of 99.6%. The research team has also used its neural network classifier to label over 10,000 DES galaxies that had not been observed in previous surveys. Using t-SNE visualizations (see [13] and Fig. 2), the research group found that deep transfer learning was effective to abstract morphological information from the galaxy images to clearly identify two distinct classes of galaxies in the unlabeled DES data set.

WHY BLUE WATERS

Blue Waters was essential to extract and curate the data sets used to train, validate, and test the team’s neural network models at scale. Staff provided support to deploy the software stacks, to use them at scale, and to carry out all the analyses reported in this study.

PUBLICATIONS & DATA SETS

CHARACTERIZATION OF NUMERICAL RELATIVITY WAVEFORMS OF ECCENTRIC BLACK HOLE MERGERS

Allocation: Illinois/325 Knh
PI: Eli Huerta
Co-PIs: Roland Haue, Gabrielle Allen, Ed Seidel
Collaborator: Sarah Habib

EXECUTIVE SUMMARY

An accurate description of the physics of eccentric binary black holes (BBHs) throughout the late-inspiral, merger, and ringdown requires numerical relativity (NR). Once NR simulations are post-processed and extracted [1], it is necessary to quantify the eccentricity and other orbital parameters that uniquely identify them. Existing methods to measure eccentricity based on the BH trajectories in NR simulations do not provide a sound approach, given that these trajectories are gauge-dependent. The research team circumvents this limitation by introducing a gauge-invariant method that characterizes an NR waveform by comparing it to a large array of semianalytical waveforms, dubbed ENIGMA waveforms, that are written in the gauge used to detect gravitational waves with the Laser Interferometer Gravitational-Wave Observatory detectors. The researchers quantify the circularization of eccentric BBHs near merger and quantify the impact of higher-order waveform modes in the morphology of eccentric BBH waveforms. This study is timely and relevant to characterizing future observations of eccentric BBHs.

RESEARCH CHALLENGE

The research team explored a variety of gauge-invariant objects to directly compare NR and ENIGMA (eccentric, nonspinning, inspiral, Gaussian-process merger approximation) waveforms. The researchers found that the dimensionless object Ma, where a is the mean orbital frequency and M stands for the total mass of the BBH, provides a robust approach to capture the signatures of eccentricity. To compute Ma for NR waveforms, the team uses the relation \( M_a = -\frac{f}{2\pi M} \), where a and b represent the plus and cross polarizations of an NR waveform h+a h. The ENIGMA waveform model produces this gauge-invariant quantity by providing, as input parameters, the mass-ratio of the BBH system and the initial eccentricity, \( e_0 \), and mean anomalous, \( l_0 \), of the system at a fiducial GW frequency \( f_0 \) from which the waveform is produced. The team removes junk radiation from the NR waveform by applying a Savitsky–Golay filter. Since input parameters are required to produce ENIGMA waveforms, seed values are initialized for \( f_0 \) and \( l_0 \). The researchers provide an informed guess of the GW frequency using the relation \( f_0 \sim \omega_0/(2\pi M) \), where \( \omega_0=\gamma \omega_0 \) and \( \gamma \) is the time at which the NR waveform is free from junk radiation. \( \omega_0 \) is analytically initialized to \( a \), a value manually determined to be optimal through verification of a few NR waveforms. Orbital eccentricity does not require a seed value since the range of possible values is consistent for all catalogued waveforms. The algorithm starts with a grid search in the 2D parameter space of \( (f_0, e_0) \) and iteratively refines it. The researchers densely sample the frequency range \( 0.5\text{Hz} \leq f_0 \leq 5\text{Hz} \), and the eccentricity range \( 0 \leq e_0 \leq 0.5 \). For each coordinate pair, an ENIGMA Ma is produced using the specified \( (f_0, e_0) \) values and the seeded \( l_0 \). The resulting Ma time evolution is then compared to that of the original NR waveform. Parameters are chosen that minimize the difference between two properties of the ENIGMA and NR evolutions: time duration of the first orbital cycle and the maximum change in \( M_a \) during the first cycle. Throughout the entire search, \( l_0 \) is held constant. After completing the grid search, the chosen \( (f_0, e_0) \) parameters are further refined iteratively. In this stage, initial GW frequency and orbital eccentricity are independently varied stepwise to increase precision. The team used this method to characterize the 89 NR waveforms presented in [3].

RESULTS & IMPACT

This research addresses two topics: (1) the rate of circularization of eccentric BBH mergers, and (2) the importance of including higher-order waveform modes for an accurate modeling of these astrophysical systems. For the second topic, the researchers have constructed NR waveforms that include either the modes \( (l, |m|) = (2, 2), (2, 1), (3, 2), (3, 1), (4, 2), (4, 1) \), or just the \( l=|m|=2 \) mode. For the second-order modes that include higher-order modes, the team has quantified the parameters of space that maximize the contribution of these modes for GW detection. Upon constructing these NR waveforms, the researchers compute the overlap between these NR waveforms so that those only include the leading-order quadrupole term. Figure 2 presents results for these calculations for a variety of astrophysically motivated scenarios. These indicate that the inclusion of higher-order modes does not quantitatively modify the morphology of higher-order NR waveforms that describe equal-mass eccentric BBH mergers. However, NR waveforms that describe asymmetric mass-ratio and eccentric BBH mergers have a much richer topology that requires the inclusion of higher-order waveform modes.

WHY BLUE WATERS

Blue Waters was critical in producing a catalog of NR waveforms and enabling the research team to postprocess and characterize these waveforms in situ and at scale. While this analysis was to be prohibitive in a campus cluster-sized resource, the analysis can be completed within a few minutes on Blue Waters for a catalog of over 100 NR waveforms.

PUBLICATIONS & DATA SETS

FUSING NUMERICAL RELATIVITY AND DEEP LEARNING TO DETECT ECCENTRIC BINARY BLACK HOLE MERGERS USING HIGHER-ORDER WAVEFORM MULTIPOLES

Allocation: Illinois/845 Krah
PI: Eli Huerta
Collaborators: Adam Rebei, Sibo Wang, Daniel Johnson, Sarah M. Habib, Roland Haas, Daniel George

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EXECUTIVE SUMMARY

An ever-increasing number of gravitational wave detections with the LIGO (Laser Interferometer Gravitational-Wave Observatory) and Virgo observatories has firmly established the existence of binary black hole mergers. Using a catalog of numerical relativity simulations that describes eccentric black holes mergers with mass-ratios \(1 \leq q \leq 10\), and eccentricities \(e \approx 0.18\) ten gravitational wave cycles before the merger event, the research team determined the mass-ratio, eccentricity, and binary inclination angle combinations that maximize the contribution of the higher-order waveform multipoles \((l, |m|)\) for gravitational wave detection. The researchers then explored the implications of these results in the context of stellar-mass black holes that are detectable by LIGO detectors and showed that compared to models that only include the \((2, 2)\) mode, the inclusion of higher-order waveform multipoles can increase the signal-to-noise ratio of eccentric binary black hole mergers by up to approximately 45% for mass-ratio binaries \(q \leq 10\).

RESEARCH CHALLENGE

Motivated by recent electromagnetic observations that suggest the existence of compact binary populations in galactic cluster M22 [1] and in the galactic center [2], and considering that eccentricity provides one of the cleanest signatures to identify these compact binary populations, the research team studied the detectability of these signals in LIGO. LIGO relies on waveform models to detect gravitational waves in its data stream. While numerical relativity simulations are free from approximation errors and represent the actual gravitational waves produced by colliding black holes, these simulations are too expensive to use directly. Approximate models, on the other hand, will often ignore all subdominant modes in the gravitational waves, potentially resulting in a reduced detection accuracy in LIGO. Assessing the impact of these approximations is only possible using high-fidelity numerical simulations covering a sizable region of the black hole parameter space accessible to LIGO. Computing this many numerical relativity waveforms with sufficient accuracy is a formidable challenge since Einstein’s equations of general relativity are among the most complex partial differential equations encountered in modern physics.

METHODS & CODES

The researchers used the Einstein Toolkit, a community-driven, open source astrophysics framework. The toolkit is OpenMP+MPI hybrid parallelized and uses automatic code generation to create compute kernels for general relativity. It employs eighth-order finite-differencing stencils in space and fourth-order accurate time integration. Adaptive mesh refinement including subcycling in time is used to resolve both the centers of the black holes as well as the gravitational waves far away from the black holes where they are detectable by LIGO.

RESULTS & IMPACT

The research team showed that the inclusion of higher-order waveform multipoles can increase the signal-to-noise ratio of eccentric binary black hole mergers by up to approximately 45% for mass-ratio binaries \(q \leq 10\). Fig. 1 shows a representative waveform prediction with or without including higher-order modes. Generally speaking, higher-order modes add extra structure to the waveform, with more complex structure being present in eccentric black hole collisions than in purely circular inspirals and collisions. Fig. 2 shows the relative increase in signal-to-noise ratio depending on the sky-location of the source. The improvement obtained by including higher-order modes is most prominent in regions of the sky where the \((2, 2)\) mode is strongly suppressed. Including these modes will thus be critical to search for and find astrophysically motivated eccentric black hole collisions. Furthermore, the team showed that machine learning can accurately reconstruct higher-order waveform multipole signals embedded in real LIGO data.

WHY BLUE WATERS

Only Blue Waters provides the compute capabilities to simulate the hundreds of binary black hole collisions required to construct a waveform catalog suitable to explore the effect of higher-order multipoles on detectability by LIGO.

PUBLICATIONS & DATA SETS

DATA- AND COMPUTE-INTENSIVE CHALLENGES FOR OBSERVATIONAL ASTRONOMY IN THE GREAT SURVEY ERA

EXECUTIVE SUMMARY

This Blue Waters project is motivated by the data- and compute-intensive challenges posed by the large-survey telescopes of the coming decade, including the Large Synoptic Survey Telescope (LSST) and the Square Kilometer Array (SKA), among others. These science goals of these telescopes require high data acquisition rates and concomitant innovations in data analysis methods, some very compute-intensive and requiring resources on the scale of Blue Waters. The specific subprojects included in this parent project report include: (1) exoplanet detectability in largescale surveys and optimal new approaches to exoplanet detection and parameter estimation in general; and (2) development of new statistical estimators for dark matter distribution and clustering in large-scale cosmological simulations and surveys in anticipation of LSST and related surveys.

RESEARCH CHALLENGE

This project is focused on data- and compute-intensive problems posed by the next generation of telescopes in observational astronomy, specifically those forming part of the imminent Great Survey Era, such as the LSST [1] and the Square Kilometer Array (SKA) [2]. Their science goals require high data acquisition rates with concomitant requirements for novel compute-intensive analysis approaches given their considerably more complex instrumental data models. Specific areas of focus include: (1) development and characterization of new algorithmic approaches for transiting exoplanet detection and parameter estimation, particularly for future large surveys; (2) development of new statistical estimators for the distribution and properties of dark matter for use as discriminants of cosmological models and in preparation for future large-scale surveys such as LSST; and (3) algorithmic challenges that are foundational to radio-interferometric imaging for highly data-intensive future telescopes such as the SKA.

The relevance of this research with Blue Waters centers on the temporary state-of-practice in spectral estimation and detection. This specific research project focuses on the use of the estimator for the counts-in-cells probability distribution function (PDF), $f(N)$, which defines the probability of finding $N$ galaxies in a cosmological volume $V$. Although computational-intensive to estimate, this PDF contains significant embedded information on the properties of dark matter. The team's specific research interest is on the use of this distribution function as a discriminator of cosmological models and also as an assessment of its application to future survey data from LSST.

In the past year, the research team has applied the counts-in-cells PDF estimator for dark matter halos to the Dark Energy Universe Simulations (DEUS) [4] on Blue Waters. They have obtained measurements between redshifts $z = 0$ to $z = 4$ at both linear and nonlinear scales and have compared the best fits of four analytical models to the measured counts-in-cells distributions. The resulting counts-in-cells distributions, $f(N)$, as a function of redshift $z$, cell-size, and cosmological model are shown in Fig. 1. The team has also used Blue Waters to compute particularly expensive fits to PDF models where variable precision arithmetic is required owing to very large numerical coefficients. The percentage difference between $f(N)$ for different cosmological dark energy models is a few percent at small $z$ but can be significantly higher at high $z$, and therefore provide a useful manner to separate different dark energy models; here, the researchers consider quintessence and phantom dark energy against standard cold dark matter cosmology.

The research team's work in radio-interferometric calibration and imaging complications concerns the most computational-challenging problems for future data-intensive telescopes in this field.

WHY BLUE WATERS

The specific research conducted under this allocation explores new computationally intensive approaches to data analysis in this discipline. Several key projects are not practical without petascale resources. In addition, the codes bases used in a number of these research subprojects are based on serial community codes in a parallel framework and therefore benefit particularly from the balanced architecture of Blue Waters.

RESULTS & IMPACT

The research subproject into exoplanet detection and estimation (with Jamila Serena Taaki) is strongly informed by the contemporary state-of-practice in spectral estimation and detection. A code framework has been developed and deployed on Blue Waters to evaluate the statistical performance of new transiting exoplanet estimators against data from the Kepler satellite [3], including algorithms based on marginalization, Monte Carlo methods, and new Bayesian approaches. In a research subproject (with Di Wen), the team has explored the cosmological analysis of large-survey data with application for future telescopes such as LSST, specifically the development and characterization of estimators for the statistical properties of the distribution of dark matter in large-scale N-body cosmological simulations. This specific research project focuses on the use of the estimator for the counts-in-cells probability distribution function (PDF), $f(N)$, which defines the probability of finding $N$ dark matter halos in a cosmological volume $V$. Although computational-intensive to estimate, this PDF contains significant embedded information on the properties of dark matter. The team's specific research interest is on the use of this distribution function as a discriminator of cosmological models and also as an assessment of its application to future survey data from LSST. In the past year, the research team has applied the counts-in-cells PDF estimator for dark matter halos to the Dark Energy Universe Simulations (DEUS) [4] on Blue Waters. They have obtained measurements between redshifts $z = 0$ to $z = 4$ at both linear and nonlinear scales and have compared the best fits of four analytical models to the measured counts-in-cells distributions. The resulting counts-in-cells distributions, $f(N)$, as a function of redshift $z$, size, and cosmological model are shown in Fig. 1. The team has also used Blue Waters to compute particularly expensive fits to PDF models where variable precision arithmetic is required owing to very large numerical coefficients. The percentage difference between $f(N)$ for different cosmological dark energy models is a few percent at small $z$ but can be significantly higher at high $z$, and therefore provide a useful manner to separate different dark energy models; here, the researchers consider quintessence and phantom dark energy against standard cold dark matter cosmology. The research team's work in radio-interferometric calibration and imaging complications concerns the most computationally-challenging problems for future data-intensive telescopes in this field.

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PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY

Hypersonic flows involving Edney type IV/V shock wave-boundary layer interaction (SWBLI) systems are characterized by complex multilength-scale features that include the triple point, separation bubble, shear layer, and shocklets. These features lead to a complex flow dynamics that is characterized by thermal nonequilibrium downstream of the bow shock as a result of the small residence time of the flow, a low-frequency unsteadiness associated with the laminar separation bubble (caused by a strong pressure rise along the surface), the potential growth of the Kelvin–Helmholtz instability in the shear layer at the contact surface of the triple point, periodic oscillations of the shocklet, and the potential growth of the Kelvin–Helmholtz instability in the shear layer at the contact surface of the triple point. Governing the triple point, separation bubble (caused by a strong pressure rise along the surface), and shocklet phenomena are the triple point, separation bubble, shear layer, and shocklet phenomena. The triple point, separation bubble, shear layer, and shocklet are key elements in the complex flow dynamics that results in unsteady state streamwise velocity fields. These simulations show for the first time that self-excited perturbations are present even at two orders of magnitude lower order Reynolds number in hypersonic flow. They also show that the estimate of the spanwise wavelength of flow structures is 9 mm, which is twice the size of the separation length defined as the distance between the separation and reattachment points. The case started from a precomputed 2D base flow field extruded in the spanwise direction and was expanded in the spanwise direction and was expanded in the spanwise direction. Such runs require about 86,000 Blue Waters node-hours to simulate an unsteady flow for 0.1 ms.

RESEARCH CHALLENGE

Given the complexity of the 3D finite span simulation, it is pertinent first to understand the behavior of the 2D base flow under self-excited, spanwise homogeneous perturbations by simulating flow over the double wedge of a chosen span length with periodic flow domain boundaries in the spanwise direction. Such perturbations could be generated inside the laminar separation bubble and grow, or the shock system might amplify the disturbances naturally present in the free stream. Growing perturbations may have a range of different wavelengths; however, this work involves the wavelength for which the growth is maximum since the spanwise periodic flow structures will exhibit this particular wavelength. The spanwise periodic cases can shed light on the stability of the base flow under self-excited oscillations, the wavelength of spanwise periodic structures, their origin, and their role in the complex flow dynamics. The perturbations present in the separation bubble may have a range of dominant frequencies. One of the broader objectives of this research is to find out if there is a link between the frequency of shock oscillation and the characteristic frequency associated with the growth and shrinkage of the separation bubble. The second challenge of this work is the development and verification of a linear stability analysis framework that takes into account thermal nonequilibrium, thereby extending its application to hypersonic SWBLI systems.
EXECUTIVE SUMMARY

High-fidelity numerical plasma modeling has been a key aspect for predicting physics in plasma. Using Blue Waters, the researcher conducted a series of numerical studies on a variety of plasma-based flows such as space plasma–surface interactions including modeling spacecraft contamination from electric propulsion thrusters and anomalous spacecraft charging in low Earth orbit. These simulations are unique in that both electrons and ions are treated as computational particles. In order to do this, a GPU-based code, called CHAOS, was developed during the researcher’s previous Blue Waters projects, and has demonstrated an 85% strong scaling. Given the immense range of length and timescales in plasma-based flows, a parallel computing architecture such as Blue Waters is necessary for their self-consistent numerical modeling.

RESEARCH CHALLENGE

Solar cell arrays provide onboard power for most spacecraft in orbits around Earth. These arrays have about a 1,000 V potential drop along their span, using wires to interconnect multiple dielectric photocells (Fig. 1). The positive potential of the interconnects attracts ambient electrons, creating an additional current loop that drains power generated by the solar panels. When the voltage across the interconnect is increased beyond a certain limit, the current dramatically shoots up, causing a large parasitic current. This phenomenon is known as “snap over.” The major contribution of the collection current to the interconnect comes from the secondary electrons emitted by nearby dielectric surfaces. The objective of this work is to model plasma physics near solar panel interconnects using a kinetic particle-in-cell approach and to establish how plasma surface interactions affect parasitic current.

METHODS & CODES

The modeling was performed with the direct simulation Monte Carlo (DSMC) particle-in-cell (PIC) code, CHAOS (CUDA-based hybrid approach for octree simulations) that was developed to study neutral flows through porous media under a previous Blue Waters effort and was reported earlier. The approach utilizes the Morton Z-curve octree structure and a volume-of-fluids approach to compute volume of cut-leaf nodes using ray-tracing, which is very efficient on GPUs [1]. The code has been used previously to model ion thruster plume contamination of spacecraft in the backflow region in a fully kinetic manner [2]. To model the snap-over phenomenon, the secondary electron emission process has been added to the code to model electron emission yields from magnesium fluoride, a typical dielectric, as a function of the incident ambient electron energy at the surface. It is assumed that every secondary electron that is emitted by the dielectric surface also leaves a positive charge on the surface. Emitted electrons are assumed to have an energy of 1 eV with velocities taken from a cosine distribution.

Fig. 2 shows a key result from the research that was recently presented [3]. The left-hand side (LHS) chart shows the time variation of surface potential at three numerical probes that are approximately 0.075, 0.15, and 0.31 mm from the interconnect (IC), and the right-hand side (RHS) chart shows the accumulating surface charge on the dielectric photosensitive material as a function of time. When the secondary electron emission (SEE) is included, the dielectric discharges more slowly and to a higher potential, attracting more primary electrons from the ambient plasma. The surface charge on probes two and three for an emissive dielectric surface reaches a steady value at a higher charge than the charge for a nonemissive dielectric surface, as expected. However, at probe one, which lies very close to the IC, the charge collected on the surface keeps falling (RHS), even when the electric potential has reached a steady value (LHS). This shows that the region near probe 1 behaves as a conductor and collects an electron current similar to that of the IC.

These results have been obtained with a potential drop of 250 V across the IC. The effect of SEE is to cause electrons to gain kinetic energy of up to 250 eV initially when the surface is charged to a potential of 250 V at t = 0. This incident electron energy gives a yield of about 3.0 secondary electrons that charges the surface locally positively and emits two additional electrons near the dielectric. The more positive dielectric surface allows electrons in front of the dielectric with SEE to gain a higher z-velocity than without SEE, thereby increasing the total electron flux on the solar panel surface.

To understand the sensitivity of the results to the energy at which electrons are emitted from the dielectric material, additional simulations were performed wherein the emitted energy was reduced from 1 to 0.1 eV. The PI found that electrons have a higher density near the dielectric surface for the higher emitted energy case because the electrons emitted from the dielectric surface are attracted toward the same positively charged dielectric surface, and the ones that are emitted with the lower kinetic energy are more likely to be coincident on the dielectric surface, effectively negating the positive charge on the surface caused by the secondary electron emissions. This was also evident in the time discharging of the surface electric potential where the time variation of surface potential on probes two and three for the lower emitted energy case was closer to the case without SEE than the higher energy emitted case. Since a major fraction of emitted secondary electrons is coincident on the dielectric surface for the lower energy emitted case, they do not reach the interconnect, causing a 25% decrease in the IC current for the lower energy emitted case.

With BLUE WATERS

As efficient as the algorithms are in the CHAOS code, the kinetic modeling of electrons in the presence of heavy ion masses such as positive atomic oxygen or xenon is rare because such simulations are computationally challenging. The ability to perform heterogeneous computing on a large number of combined CPU/GPU nodes is unique to the Blue Waters architecture. This hardware has enabled the PI to demonstrate the first ever such simulations of plasma-based flows.

Figure 1: Computational domain of ambient plasma in front of solar cell array. Two dielectric elements are shown with the interconnect (IC) lying at 0.75 mm on the surface and their relationship to a typical solar cell array on a spacecraft.

Figure 2: Electric potential and dielectric charging as a function of distance from the interconnect for simulations with and without secondary electron emission (SEE). Solid lines and closed circles indicate no SEE and with SEE, respectively.
THE SPREADING OF THREE-DIMENSIONAL MAGNETIC RECONNECTION IN ASYMMETRIC GEOMETRY

EXECUTIVE SUMMARY

Earth’s magnetosphere—a region formed from its magnetic fields—shields the planet from constant bombardment by super-sonic solar winds. However, this magnetic shield, called the magnetopause, can be eroded by various plasma mechanisms. Among them, magnetic reconnection is arguably the most active process. Reconnection not only allows the transport of solar wind plasmas into Earth’s magnetosphere but also releases the magnetic energy and changes the magnetic topology. At Earth’s magnetopause, magnetic reconnection proceeds between the shocked solar wind plasmas and the magnetosphere plasmas. Magnetic properties of magnetic reconnection in such asymmetric geometry remain unclear. The research team used first-principle simulations to explore the 3D kinetic physics that control this critical energy conversion process.

RESEARCH CHALLENGE

Massive solar eruptions drive magnetic storms that impact Earth’s magnetosphere and space weather. The consequential electromagnetic waves, electric currents, and energetic particles can harm satellites, astronauts, GPS systems, radio communication, and power grids on the ground. Magnetic reconnection is the critical player in solar wind–magnetosphere coupling, and space weather in general. Fundamental questions in reconnection research include: Is there a simple principle that determines the orientation of the reconnection x-line (the null line where magnetic reconnection occurs) in such an asymmetric current sheet? How fast does reconnection spread out from a point source? The answers to these questions remain unclear given our current understanding of magnetic reconnection, and the research team aims to study its 3D nature. This work is a crucial step in the quest for predicting the location and rate of flux transfer at Earth’s magnetopause, and will thus improve the forecast of space weather.

RESULTS & IMPACT

The spreading of magnetic reconnection in asymmetric current sheets was studied in the third year of this project. The result has an application to the reconnection that occurs at Earth’s magnetopause. The research team initiated reconnection at the center of a large simulation domain to minimize the boundary effect. The resulting x-line had sufficient freedom to develop along an optimal orientation, and the signal of fast reconnection spread out from two ends of the x-line. The team measured the spreading speed and found that it exhibited a strong dependence on the thickness of the initial current sheet. They mapped out a criterion for the Alfvénic spreading of fast reconnection and explored its physics origin. While the criterion appears to be stringent, this study suggests that under typical conditions at Earth’s magnetopause, the reconnection x-line is unlikely to demonstrate Alfvénic spreading at the local Alfvén speed regardless of the guide field strength. An Alfvénic spreading is expected only if the typically thick magnetopause current sheet is substantially compressed (perhaps by the solar wind) to a state strongly unstable to the collisionless tearing instability.

These results compared favorably with recent magnetopause observations using SuperDARN radars and THEMIS satellites. In addition, this new result is important to NASA’s ongoing Magnetospheric Multiscale Mission, which was designed to study the kinetic physics of the reconnection x-line. The results could also be relevant to the ongoing European Space Agency (ESA)–Japan Aerospace Exploration Agency (JAXA)–Chinese Academy of Sciences joint mission, Solar Wind Magnetosphere–Ionosphere Link Explorer, which will study the development of reconnection lines at Earth’s magnetopause using X-ray and UV imagers.

WHY BLUE WATERS

Because the x-line has a dimension down to the electron scale, a fully kinetic description is necessary. Given the available computational capability, it has become possible to use a first-principle kinetic simulation to investigate the dynamics of the x-line in a reasonably large 3D system that spans from the electron kinetic scale to the magnetohydrodynamics scale. A representative 3D run in this project traces the motion of two trillion charged particles under the interaction of self-generated electromagnetic fields, which are evaluated on six billion grids. The output data easily have a size of hundreds of terabytes for each run. Blue Waters provides not only the computational resource for the calculation but also the online storage for the output and restart files.

PUBLICATIONS & DATA SETS

ASSEMBLING A MAP OF THE UNIVERSE: SHAPES AND MASS DISTRIBUTION FOR THE DARK ENERGY SURVEY

Allocation: Illinois/460 Kohl
PI: Felipe Menanteau
Collaborators: Robert Gruendl, Donald Peterson, Erin Sheldon

EXECUTIVE SUMMARY

The Dark Energy Survey (DES) has performed a 5,000 square-degree wide field survey in five optical bands of the southern sky and a 30 square-degree deep supernova survey with the aim of understanding the nature of dark energy and the accelerating Universe. DES used the 3 square-degree CCD (Charge-Coupled Device) camera (DECam) installed at the prime focus on the Blanco 4-m telescope at the Cerro Tololo Interamerican Observatory (CTIO) in Northern Chile. DECam consists of a 570 megapixel camera installed at the prime focus on the Blanco 4-m telescope at the Cerro Tololo Interamerican Observatory (CTIO) in Northern Chile. DECam consists of 62 fully depleted, 250-micron-thick 2,048 × 4,096 CCDs combined with four 2,048 × 2,048 guider and eight 2,048 × 2,048 autofocus CCDs. For 575 nights from 2013–2019, DES scanned the sky to perform a 5,000 square-degree wide field survey. Over five observing seasons, DES measured shapes, positions, fluxes, and colors for approximately 300 million galaxies and discovered and measured light curves for 3,500 supernovae, using these measurements to deliver powerful new constraints on cosmic acceleration and dark energy. Each image arrives from CTIO in Chile at the National Center for Supercomputing Applications (NCSA), Urbana, Illinois within minutes of being observed and is usually processed by the nightly processing pipeline within the next 24 hours. These nightly pipelines are critical for the near-real-time supernovae analyses, and also provide rapid feedback about overall data quality as the survey progresses. The other cosmological probes (weak lensing and galaxy clustering) rely on the combination of all survey observations to form a data release with unprecedented depth but at the cost of averaging over instrumental changes and varying atmospheric conditions.

The DESDM software and workflows (using HTCondor) have already been implemented and exercised as part of previous allocations on Blue Waters. In addition, the atomic pieces of the DES Y6A1 release comprised 131,602 reduced, calibrated exposures and 10,169 COADD tiles and catalogs that cover the 5,000 square degree survey volume. These form the inputs for the joint analyses.

METHODS & CODES

DES uses the state-of-the-art 3 square-degree DECam, a 570 megapixel camera installed at the prime focus on the Blanco 4-m telescope at the Cerro Tololo Interamerican Observatory (CTIO) in Northern Chile. DECam consists of 62 fully depleted, 250-micron-thick 2,048 × 4,096 CCDs combined with four 2,048 × 2,048 guider and eight 2,048 × 2,048 autofocus CCDs. For 575 nights from 2013–2019, DES scanned the sky to perform a 5,000 square-degree wide field survey. Over five observing seasons, DES measured shapes, positions, fluxes, and colors for approximately 300 million galaxies and discovered and measured light curves for 3,500 supernovae, using these measurements to deliver powerful new constraints on cosmic acceleration and dark energy. Each image arrives from CTIO in Chile at the National Center for Supercomputing Applications (NCSA), Urbana, Illinois within minutes of being observed and is usually processed by the nightly processing pipeline within the next 24 hours. These nightly pipelines are critical for the near-real-time supernovae analyses, and also provide rapid feedback about overall data quality as the survey progresses. The other cosmological probes (weak lensing and galaxy clustering) rely on the combination of all survey observations to form a data release with unprecedented depth but at the cost of averaging over instrumental changes and varying atmospheric conditions.

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RESULTS & IMPACT

During the early years of the DES survey, new algorithms for measuring the galaxy properties were developed, but these require a joint analysis of combined images (COADDs) with the individual nightly observations that make up the survey on a per-object (galaxy) basis. The Blue Waters allocation was used to perform these analyses.

New measurement algorithms have been developed to cope with the increased astronomical survey depth, as the density of sources (stars and galaxies) projected along any line of sight in the survey volume is high enough that the projected object images overlap. Further, modern survey methodologies to obtain those depths rely on the combination of many images taken over many years in varied conditions (e.g., atmospheric turbulence). Three advanced measurement algorithms have been developed by the DES Collaboration to make precise measurements based on the initial data release products. These include:

- **MOF (Multi-Object Multiband Fitting)**, which simultaneously fits basic galaxy shapes and fluxes to each object and its neighbors;
- **SOF (Single-Object Multi-Band Fitting)**, which performs a similar fit but masks neighboring object as a cross-check to the MOF analysis and
- **Shear**, which makes a detailed shape analysis of an object and its neighbors.

These new catalogs are more precise and minimize the systematic uncertainties imprinted on the survey data. As an example of how these new catalogs will be used by the DES Collaboration, Fig. 1 shows the mass map from the first year of DES observations inferred from weak lensing measurements [1].
PETHASCLE SIMULATIONS OF BINARY NEUTRON STAR MERGERS

Allocation: NSF PRAC/200 Kobe
PI: Philipp Misn
Co-PI: David Radice
Collaborators: Roland Haas, Erik Schnetter, Sebastiano Bernuzzi

1University of California, Berkeley
2University of Jena
3National Center for Supercomputing Applications
4Perimeter Institute
5University of Iowa

EXECUTIVE SUMMARY

The gravitational wave and electromagnetic data from the collision between two neutron stars, GW170817 [1], is revolutionizing our understanding of the origin of the heavy elements, of the nature of short gamma-ray bursts, and of the properties of matter at extreme densities. To fully exploit the potential of multimessenger observations, the research team performed ab initio simulations of binary neutron star mergers and computed their gravitational wave and electromagnetic signatures. These simulations were enabled by both Blue Waters’ capacity for massively parallel high-resolution simulations and high throughput for large sets of simulations at smaller scales. The simulations revealed a new mechanism that could power mildly relativistic outflows during mergers and could be revealed by radio observations months to years after merger. The team also found that the electromagnetic (EM) signal is very sensitive to the merger outcome, i.e., whether a black hole was formed promptly or with some delay. They used this observation to develop a novel way to constrain neutron star radii using joint electromagnetic and gravitational wave observations of neutron star mergers. The simulations showed that the outflows powered by mergers could inject positrons in the interstellar medium, and the researchers suggested that neutron star mergers could provide a solution to the decades-old puzzle concerning the origin of cold positrons in the galactic center and some of the dwarf galaxies. Gravitational waveforms, ejecta data, and nucleosynthesis yields from the simulations are publicly available at www.computational-relativity.org and zenodo.org.

The team has performed the first general-relativistic magnetohydrodynamics (MHD) turbulence simulations of neutron star merger remnants including nuclear and neutrino physics. These simulations allowed them to quantify the role magnetic fields play in angular momentum transport in the remnant, and they showed that the lifetime of the remnant can change significantly when including magnetic field effects. The results from these simulations will also be used to inform initial conditions for long-term follow-up simulations of merger remnants.

WHY BLUE WATERS

The MHD turbulence simulations of neutron-star merger remnants that resolve the magnetorotational instability would have been impossible without Blue Waters’ capability. Blue Waters’ capacity is also crucial for a quick turnaround in the team’s numerical relativity neutron-star merger simulations. No other machine allows for the throughput of many of these simulations concurrently to generate the theoretical predictions needed for Laser Interferometer Gravitational-Wave Observatory and EM follow-up.

PUBLICATIONS & DATA SETS

DEVELOPMENT OF A SCALABLE GRAVITY SOLVER FOR ENZO–E

EXECUTIVE SUMMARY

Blue Waters was used to develop and profile a highly scalable version of the Enzo cosmological adaptive mesh refinement (AMR) code called Enzo–E (E for extreme scale) [6]. In this project, the research team illustrated the weak scaling results of the domain-decomposed AMR Poisson solver using a suite of dark matter clustering simulations.

RESEARCH CHALLENGE

Improved computational models of the intergalactic medium (IGM) are needed to extract information encoded in the high-resolution optical spectra of distant quasars. That information includes the physical state of the mostly primordial gas pervading the Universe but also the dark matter that shapes the gas into discrete intergalactic absorption line systems (the Lyman-α forest). Discrete intergalactic absorption line systems (the Lyman-α forest) are needed to extract information encoded in the high-resolution optical spectra of distant quasars. That information includes the physical state of the mostly primordial gas pervading the Universe but also the dark matter that shapes the gas into discrete intergalactic absorption line systems (the Lyman-α forest).

METHODS & CODES

Including galaxies in simulations of the IGM poses severe resolution requirements that can be addressed using adaptive mesh refinement (AMR) around galaxies. However, Enzo’s AMR capability is not sufficiently scalable to permit a full frontal assault on this problem. For this reason, the research team has been developing a successor to the Enzo code called Enzo–E built on an entirely new highly scalable AMR framework called Cello [3]. The combined code—Enzo–E/Cello—uses the Charm++ parallel object-jected framework for parallelization. The team has implemented the proven scalable Forest-of-Octrees AMR algorithm [4] on top of Charm++ and has obtained excellent parallel scaling results on Blue Waters as a prelude to the target application.

Solving the elliptic Poisson equation on the Forest-of-Octrees adaptive mesh is a prerequisite for cosmological applications. In the past year, the team has developed such a solver and profiled it on Blue Waters. Fig. 1 shows its application to a pure dark matter N-body simulation. The left side shows the projection of the dark matter density onto the adaptive mesh at redshift 7.5 in a cubic volume 6 comoving megaparsecs on a side. The right side shows the projection of the adaptive mesh, with levels of refinement encoded in color: root grid = dark blue; levels 1, 2, 3, 4 = light blue, green, yellow, and red, respectively. Each square is the projection of a block of 16 × 16 × 16 computational cells. The right side shows the projection of the adaptive mesh, with levels of refinement encoded in color: root grid = dark blue; levels 1, 2, 3, 4 = light blue, green, yellow, and red, respectively. Each square is the projection of a block of 16 × 16 × 16 computational cells, on which the gravitational potential was solved using the following method. First, the dark matter particle masses were assigned to the grid block that contains them using Cloud-In-Cell interpolation. Second, the matter densities were projected to the root grid (level 0). Third, the global gravitational potential was computed on the root grid using a V-cycle multigrid solver. Fourth, the gravitational potential was interpolated from the root grid to the facets of each octree. Fifth, the gravitational potential was computed for each octree using a multilevel iterative solver (BICGStab).

RESULTS & IMPACT

The DD (domain-decomposed) Poisson solver described above was implemented and tested on Blue Waters in the context of dark matter-only cosmological structure formation simulations. Weak scaling results are shown in Fig. 2. The research team plotted wall time per timestep versus timestep for four simulations in box sizes 3, 6, 12, and 24 comoving megaparsecs on a side, with root grid resolutions of 643, 1283, 2563, and 5123 cells. These correspond to 4, 8, 16, and 323 arrays of blocks of 163 cells each. Each root grid block is the base of a separate octree, which refines as structure forms. With 8 root grid blocks per core, the simulations were run on 8, 64, 512, and 4,096 cores of Blue Waters. At early times, before cycle 100, mesh refinement had not begun, and the execution time was dominated by the global multigrid solver. At later times, up to a factor of 100 more refined blocks at all levels were created to resolve structure formation. Execution time was dominated by the BICGStab tree solver. The fact that the curves from different runs bunch together at late times indicated favorable weak scaling of the DD solver.

WHY BLUE WATERS

It is essential to have a petascale resource like Blue Waters to develop an application for exascale machines. The sheer size, the favorable queue structure, and the excellent throughput at large core counts were instrumental during the code development and test phase of this research. In the process of developing the DD solver, certain synchronization issues only showed up at large scale (P > 1,000). It was essential to be able to turn around large test runs quickly as the research team diagnosed the problem.

PUBLICATIONS & DATA SETS


Methods & Codes

Including galaxies in simulations of the IGM poses severe resolution requirements that can be addressed using adaptive mesh refinement (AMR) around galaxies. However, Enzo’s AMR capability is not sufficiently scalable to permit a full frontal assault on this problem. For this reason, the research team has been developing a successor to the Enzo code called Enzo–E built on an entirely new highly scalable AMR framework called Cello [3]. The combined code—Enzo–E/Cello—uses the Charm++ parallel object-ject framework for parallelization. The team has implemented the proven scalable Forest-of-Octrees AMR algorithm [4] on top of Charm++ and has obtained excellent parallel scaling results on Blue Waters as a prelude to the target application. Solving the elliptic Poisson equation on the Forest-of-Octrees adaptive mesh is a prerequisite for cosmological applications. In the past year, the team has developed such a solver and profiled it on Blue Waters. Fig. 1 shows its application to a pure dark matter N-body simulation. The left side shows the projection of the dark matter density onto the adaptive mesh at redshift 7.5 in a cubic volume 6 comoving megaparsecs on a side. The right side shows the projection of the adaptive mesh, with levels of refinement encoded in color: root grid = dark blue; levels 1, 2, 3, 4 = light blue, green, yellow, and red, respectively. Each square is the projection of a block of 16 × 16 × 16 computational cells. The right side shows the projection of the adaptive mesh, with levels of refinement encoded in color: root grid = dark blue; levels 1, 2, 3, 4 = light blue, green, yellow, and red, respectively. Each square is the projection of a block of 16 × 16 × 16 computational cells, on which the gravitational potential was solved using the following method. First, the dark matter particle masses were assigned to the grid block that contains them using Cloud-In-Cell interpolation. Second, the matter densities were projected to the root grid (level 0). Third, the global gravitational potential was computed on the root grid using a V-cycle multigrid solver. Fourth, the gravitational potential was interpolated from the root grid to the facets of each octree. Fifth, the gravitational potential was computed for each octree using a multilevel iterative solver (BICGStab). Finally, the potential was smoothed across all the leaf nodes of all octrees using Jacobi smoothing.

RESULTS & IMPACT

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PUBLICATIONS & DATA SETS


SIMULATING GALAXY FORMATION ACROSS COSMIC TIME

Allocation: NSF PRAC/1,500 Knh
PI: Brian O'Shea
Co-PI: David C. Collins, John H. Wise
Collaborators: Cameron J. Hummels, Britton D. Smith, Molly S. Peeples, John D. Regan, Jason Tumlinson, Lauren Corlies

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2Florida State University
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4California Institute of Technology
5University of Edinburgh
6Space Telescope Science Institute
7Dublin City University
8SST Corporation
9University of Arizona

EXECUTIVE SUMMARY

This project addresses two fundamental questions in galaxy formation: How do the first stars and galaxies influence the rest of cosmological structure formation over the following 13 billion years? And how does the cycling of gas into and out of galaxies through cosmic inflows and supernova-driven winds regulate the behavior of these galaxies?

The research team addresses these questions via a suite of physics-rich, high-dynamic-range adaptive mesh refinement simulations done with the Enzo code (enzo-project.org), which has been modified to scale to large core counts on Blue Waters. Through these simulations, the researchers have gained key insights into the formation of the first supermassive black holes and into the ways in which the circumgalactic gas around galaxies acts as a "thermostat" that regulates star formation.

RESEARCH CHALLENGE

The primary goals of this research are to understand two fundamental issues in galaxy formation: the birth and growth of the first generations of galaxies and their connections to present-day galaxies like the Milky Way; and the "baryon cycle" in galaxies like the Milky Way; in other words, the movement of gas into and out of galaxies, and how this regulates the behavior of star formation in galaxies.

Both of these questions are critical to interpreting observations of galaxies over the age of the Universe through both current observatories (such as the Hubble Space Telescope and the 10-meter Keck telescope on Mauna Kea) and future observatories (such as the James Webb Space Telescope and the Large Synoptic Survey Telescope). All of the calculations needed to study these problems require simulations with extremely high dynamic range in space and time, complex physics (often including radiation transport and nonequilibrium gas chemistry), and large simulation volumes.

METHODS & CODES

The researchers' simulation tool of choice is the Enzo code [1,2; http://enzo-project.org], an open source and community-developed software platform for studying cosmological structure formation. Enzo allows the inclusion of all the critical physical components needed to study galaxy formation—gravity, dark matter dynamics, fluid dynamics, the microphysics of plasmas, and prescriptions for star formation and feedback—and can scale to large numbers of CPUs. All analysis was done with the yt code [3; http://yt-project.org].

RESULTS & IMPACT

The main results involve the growth of supermassive black holes in the early Universe and the cycling of gas into and out of galaxies. The former result [4,5] demonstrates a novel "direct collapse" mechanism for gas clouds to turn into intermediate-mass black holes (with masses of thousands or tens of thousands of solar masses) rather than first turning into stars. This is important because it provides the first plausible formation mechanism for the extremely massive (hundreds of millions to billions of solar masses) black holes seen in the early Universe. The project has also demonstrated that the frequency with which these black holes form is consistent with the frequency that early-Universe supermassive black holes are observed.

The second set of important results involves the exploration of gas cycling into and out of galaxies [6–8]. Simulations demonstrate that massively increased physical resolution in the "circumgalactic medium"—the gas outside the stellar disk of a galaxy but is bound to the galaxy by gravity, and composes almost half of the mass of the baryons in the galaxy—is incredibly important. The work suggests that increasing the resolution by more than an order of magnitude beyond previous state-of-the-art calculations results in the appearance of both spatial and chemical features that are seen in observations but not in previous simulations. This research is revolutionizing the understanding of the interface between the stellar component of galaxies and the diffuse corona of gas that surrounds them and provides predictions of observational quantities relating to quasar absorption line spectra and to the direct emission of radiation from the circumgalactic medium, as observed by Keck's KCWI instrument.

WHY BLUE WATERS

The simulations used to properly model galaxies in both the early Universe and the present day require extremely high spatial and temporal dynamic ranges and also require complex physics—most importantly, radiation transport and nonequilibrium gas chemistry. Furthermore, large simulation volumes (and thus many resolution elements) are needed to model the many early galaxies that will merge together to create a Milky Way-like galaxy at the present day, and in the research team's present-day galaxy simulations, huge numbers of cells are required to accurately resolve the circumgalactic gas. Taken together, this project requires the use of a supercomputer with large memory and disk space to accommodate the tremendous data set sizes; large computational resources; and an extremely high bandwidth, low-latency communication network to enable significant scaling of the radiation transport code. Blue Waters is the only machine available to the academic community that fits all of these requirements.

PUBLICATIONS & DATA SETS

PROCESSING DARK ENERGY CAMERA DATA TO MAKE THE WORLD’S BEST MAP OF THE NIGHT SKY

EXECUTIVE SUMMARY

The Dark Energy Camera (DECam) on the Blanco 4-meter telescope has been a premier instrument for making astronomical surveys during its seven years of operation. The largest of these surveys is the Dark Energy Survey (DES), whose data was processed by the National Center for Supercomputing Applications (NCSA). In addition to DES, DECam has produced 200,000 exposures from various smaller surveys. These smaller surveys were processed with multiple pipelines, many of which have known deficiencies. In addition, their processed data are not publicly available for search. The research team is processing these 200,000 exposures along with the original DES data. This meta-survey will immediately be much deeper than any survey of similar size. It will be used to study Milky Way structure, galaxy clusters, and solar system objects. It will also provide the “before” image for astronomical transients in multimessenger astronomy.

RESEARCH CHALLENGE

The DECam has a three square degree field of view, and each image it produces contains 50 million pixels [1]. This has made it a major instrument for making astronomical surveys that cover large areas of the sky. The largest of these surveys, the Dark Energy Survey (DES) [2], was made with nearly half of the DECam observing time, and its data were processed at NCSA with a highly developed image processing pipeline. Smaller DECam surveys like the Dark Energy Camera Legacy Surveys [3] and the Dark Energy Camera Plane Survey [4] comprise months of DECam data and cover thousands of square degrees. However, they were processed with multiple pipelines that are known to be quantitatively inferior to the DES pipeline. In addition, while the raw data for these surveys are publicly available, searchable catalogs are not. The research team is processing all DECam data with the DES pipeline and releasing it publicly. For many applications, this will increase the effective DES area from 5,500 square degrees to 25,000 square degrees, or roughly 60% of the sky.

METHOD & CODES

The research team uses the DES image processing pipeline [5]. In addition to correcting or masking camera artifacts with the most recent proven algorithms, the pipeline uses human-inspected calibration images and a superior background subtraction method based on principle component analysis of the background [6]. The net result of these improvements is that DES reduced data have a photometric (brightness) precision of 0.5%. DECam data reduced with other pipelines have a photometric precision of between 2% and 6%, depending on the pipeline.

RESULTS & IMPACT

Using Blue Waters, the researchers have processed 66,740 DECam exposures. This comprises 33 TB of raw data turned into 100 TB of processed data. These data cover roughly 15,000 square degrees of the sky, with an average coverage of 12 exposures in any given area. These images are the deepest available over most of this new area. The research team has given early access to these data to DES scientists. Preliminary results (with publications forthcoming) include the discovery of new outer Milky Way structures, improved observations of galaxy clusters, and the discovery of solar system objects (asteroids). The Milky Way structures will be used to trace the ancient collisions the Milky Way has had with its neighbors that have led to its current form. Images of galaxy clusters will be used to determine their masses, and through these measurements, to understand the growth of cosmological structure in the Universe. The discovery of new solar system objects helps complete a census of nearby objects, including those that may someday impact Earth. All of these discoveries required the new depth and wide area that these data provide and could not have been made had the data not been processed with Blue Waters and made available through this project.

In addition to this ongoing research, the team’s survey will provide the template, or “before” image, needed to detect astronomical transients, including those initially detected with the Laser Interferometer Gravitational-Wave Observatory and other multimessenger detectors. Having archival templates will allow these objects to be studied as they are dynamic instead of hours or days later when the data have been fully analyzed.

WHY BLUE WATERS

The challenges of processing 33 TB of raw data into 100 TB of usable images and catalogs extend beyond the hundreds of thousands of core hours needed to perform the processing. This work involved the importation of a large, specialized software stack; constant transfer of large files across limited network space; and millions of calls to a central database to organize the processing and data. The Blue Waters staff showed the system’s versatility by working with the research team to solve each of these problems so that data could be processed quickly with minimal human interaction and transferred back to the home system reliably. This allowed the team not only to perform the necessary computations but to present the astronomical community with a usable and exciting new data set before other groups even thought to begin to reduce the data.

Figure 1: The spatial distribution of g-band DECam data processed by the DECADE (DECam All Data Everywhere) team. These data cover half the night sky to unprecedented depth.

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EXECUTIVE SUMMARY

The research team has investigated physical phenomena occurring near the solar wind's interaction with the local interstellar medium (LISM). These include: (1) the effect of non-Maxwellian plasma distribution on the SW–LISM interaction; (2) the propagation of coronal mass ejections, constrained by multi-viewpoint images, through the solar wind flow governed by photospheric magnetograms; (3) transient phenomena affecting space weather at Earth and other planets; (4) magneto-hydrodynamic (MHD) instabilities and magnetic reconnection in the presence of turbulence; (5) the effect of nonthermal pickup ions (PUIs) on spacecraft measurements; (6) energetic neutral atom observations from the Interstellar Boundary Explorer (IBEX) through direct 3D, MHD–kinetic simulations; (6) the heliospheric effect on the observed anisotropy of galactic cosmic rays with energies on the order of TeV and the origin of this anisotropy; and (7) the global structure of the solar wind flow along the Parker Solar Probe (PSP) trajectory. Our simulations help interpret IBEX, New Horizons, PSP, Ulysses, and Voyager measurements, as well as air shower observations.

RESEARCH CHALLENGE

The Grand Challenge of this research is to investigate fundamental physical phenomena that start on the solar surface and result in solar wind acceleration and propagation through interplanetary space toward the boundary of the heliosphere, where the solar wind interacts with the local interstellar medium. The research team studied plasma instabilities, magnetic reconnection, cosmic ray transport, and kinetic effects of partial ionization in plasma. These included the birth/death of secondary neutral atoms and nonthermal PUIs, and phenomena driven by MHD turbulence. Most of the research team’s simulations were data-driven and also validated by observations from such space missions as IBEX [1]; New Horizons (NH) [2], PSP [3], Ulysses [4], Voyager [5], and the fleet of near-Earth spacecraft.

To drive the coronal model, the researchers used the wealth of magnetogram data accompanied by the satellite missions STE-REO and SOHO observations. This allowed the team to develop a new approach, preserving the shape and speed of a coronal mass ejection as well as the plasma mass and poloidal magnetic field fluxes carried by it. Simulations were especially focused on the interstellar mission of Voyager 1 and 2 (V1 and V2) spacecraft, which crossed the entire heliosphere and are now traversing the LISM. For the first time in the history of mankind, we are acquiring in situ information on the properties of LISM plasma, energetic particles, and magnetic fields at the heliospheric boundary. Voyager data are complemented by the IBEX observations of energetic neutral atoms (ENAs) in different energy bands. Since ENAs are born owing to charge exchange of nonthermal PUIs with other neutrals, the team was able to investigate the effect of non-Maxwellian proton distribution function on the heliospheric structure and support the interstellar origin of the IBEX ribbon.

METHODS & CODES

The researchers solved the equations of ideal MHD coupled with the kinetic Boltzmann equation describing the transport of neutral atoms. In a less strict approach, the flow of atoms was modeled with a few systems of the Euler gas dynamic equations describing the atom populations that differ by the domain of their origin. The team has developed both fluid dynamics and kinetic models for PUIs and turbulence generated by kinetic instabilities of their distribution function. All these are components of a Multi Scale Fluid-Kinetic Simulation Suite—an adaptive mesh refinement code built on the Chombo framework.

RESULTS & IMPACT

• The team has developed a powerful data-driven solar model that allowed for the simulation of the solar wind flow and interplanetary magnetic field as a function of time along the Earth; New Horizons spacecraft; and Pluto, Neptune, and Uranus trajectories.
• This work represents a substantial breakthrough in modeling flows of partially ionized plasma in the presence of PUIs by designing special boundary conditions for the latter at the heliospheric termination shock. This is of utmost importance because such boundary conditions are intrinsically kinetic.
• The team has developed a unique solar wind model that is based on synchronous vector magnetograms from the Solar Dynamic-Observatory. This made it possible, for the first time in the history of solar wind simulations, to create a mathematically consistent model of solar corona.
• This study has analyzed quantitatively the distribution of quantities in the heliospheric boundary layer—a region of interstellar plasma in front of the heliopause that is characterized by depressed plasma density and enhanced interstellar magnetic field. The MHD instabilities and magnetic reconnection have been analyzed with high resolution in space and time, owing to the high computing power of Blue Waters.

• The research group's numerical simulations have shown features of magnetic reconnection near the heliopause in the southern hemisphere and, in particular, near the point where Voyager 2 crossed the heliopause.
• The researchers have reproduced the 5 TeV cosmic ray anisotropy observed in the Tibet air shower experiment. It has been demonstrated that the heliosphere provides most of the higher-than-dipole contributions to this anisotropy. The cosmic ray anisotropy in the pristine LISM has been derived and the likely source of this anisotropy has been identified.
• The team's new, data-driven coronal mass ejection simulations have been extended to involve the poloidal magnetic flux observations in the photosphere, which improves the quality of simulations tremendously.
• This project's numerical simulation results have found their way to the broader space science community and received publicity. A few internal and national press releases were focused on this research, powered by Blue Waters.

WHY BLUE WATERS

Blue Waters is not just a supercomputer with higher-than-usual allocation opportunities. It comes with an efficient and highly professional support staff, who responded to all our concerns and were very helpful in the development of job scheduling and visualization strategies. The PAID and Student Fellowship opportunities were also extremely valuable.

PUBLICATIONS & DATA SETS

INTERIOR DYNAMICS OF YOUNG STARS REVEALED BY 3D HYDRODYNAMIC SIMULATIONS

Collaborators: Isabelle Baraffe, Tom Goffrey, MUltidimensional Stellar Implicit Code developers’ team

EXECUTIVE SUMMARY

Our current understanding of the evolution of stars is drawn from one-dimensional calculations based on simple phenomenological approaches and fitted observational data. To interpret the data produced from the recent space missions CoRoT, Kepler, and GAIA, as well as to understand new high-quality data from the upcoming missions TESS and PLATO, it is necessary to study realistic stellar conditions using three-dimensional hydrodynamic simulations.

RESULTS & IMPACT

Early results from a simulation performed on Blue Waters are shown in Figs. 1 and 2. In Fig. 1, radial velocities are shown in a spherical wedge that fills 80% of the star’s radius. Smaller-scale convective flows are visible near the surface, while the extent of these radial flows is larger, deep in the stellar interior. Although these flows are of a length scale similar to the stellar radius, they also clearly have small-scale features that are important for diffusion and chemical mixing. The research team is currently producing a long time-sequence of data in order to perform a complete statistical analysis of these convective flows and the consequences for mixing when they overshoot the convection zone.

One of the consequences of convective plumes overshooting into the radiative zone is the mixing of colder fluid into a hotter layer, potentially changing the temperature gradients within the stellar interior. Fig. 2 shows that heat becomes trapped in waves that are excited in the overshooting layer. A full study of this phenomenon is underway and will be completed using the simulations currently running on Blue Waters.

This work is expected to result in improved models for stellar evolution, which the researchers expect to be included in open-source code such as MESA. As a result of this project, stellar physicists will be better able to understand how a young star such as that in this project’s simulations can evolve into a sun.

WHY BLUE WATERS

The research team has carried out its simulations on Blue Waters because of the large grid size and large number of timesteps necessary for simulations of a star. Simulations of this size would be expected to run continuously for several years on a university-size system and can be completed on Blue Waters in less than a year. Blue Waters’ staff played an essential role in the success of this project by installing the Trilinos library, used by MUSIC.

METHODS & CODES

This project used the MUltidimensional Stellar Implicit Code (MUSIC), a code that has been designed and developed under a European Research Council Advanced Grant over the last six years. MUSIC solves fully compressible fluid equations in a spherical geometry using a second-order finite volume method and MPI–FORTRAN. MUSIC also uses fully implicit time integration in order to cover long windows of stellar dynamics. The time integration algorithm is second-order and centers on a Jacobian–Free Newton–Krylov method using physics-based preconditioning. Each aspect of the design of MUSIC has been chosen to seamlessly extend one-dimensional stellar evolution calculations into three dimensions.
Clusters of galaxies are both a useful probe of cosmology and a laboratory for understanding galactic feedback processes. However, modeling galactic-scale feedback processes in the context of a cluster presents a computational challenge because of the large dynamic range involved. Through the use of a highly scalable N-body/hydrodynamics code running on Blue Waters, the research team is tackling this challenging problem. The results show that models that have successfully reproduced the morphology and number densities of field galaxies can also produce realistic models of cluster galaxies. Large computational resources with high-performance networks are necessary for these calculations, however.

RESEARCH CHALLENGE

Groups and clusters of galaxies are the largest bound objects in the Universe, containing more than half of its warm-hot diffuse gas and a significant fraction of all galaxies. Consequently, understanding the physical processes that occur in group and cluster environments, including the interactions among the dark matter, hot diffuse gas, stars, and active galactic nuclei (AGN), is key to gaining insights into the evolution of baryons and galaxies across the age of the Universe. Furthermore, galaxy clusters are one of the few places where the majority of the baryons are visible via X-ray and microwave. In contrast to field galaxies, where feedback from supernovae and AGN puts gas into a mostly invisible circumgalactic medium, feedback from cluster galaxies will impact the state of the intracluster medium (ICM). Hence, clusters will provide very tight constraints on our understanding of the physical processes that occur in group and cluster environments, including the interactions among the dark matter, hot diffuse gas, stars, and active galactic nuclei (AGN).

METHODS & CODES

The research team used the highly scalable N-body/hydrodynamics code ChaNGa to model the formation and evolution of a population of galaxies in a Coma-sized galaxy cluster, including their contribution to and interaction with the ICM. This code is built on the Charm++ [1] parallel programming infrastructure. It leverages the object-based virtualization and data-driven style of computation inherent in Charm++ to adaptively overlap communication and computation and achieve high levels of resource utilization on large systems. The code has been shown to scale well to 500,000 cores on Blue Waters [2].

The code includes a well-constrained model for star formation and feedback, with improved implementation of supermassive black hole formation, growth, mergers, and feedback [3,4]. In a previous Blue Waters allocation, the team demonstrated that these models can reproduce populations of field galaxies at intermediate-to-high redshift [5] and can reproduce the observed stellar mass–halo mass relationship of galaxies from dwarfs up to galaxy groups [4].

These simulations are being compared to observations of clusters to understand the physical and temporal origin of their morphologies. The model ICW will be compared to X-ray and microwave data via the Sunyaev–Zeldovich effect to understand the relationship among these observables and the underlying gas properties. Finally, the overall mass distribution will be used to better understand how these clusters gravitationally amplify the light from background galaxies.

RESULTS & IMPACT

The team’s simulations are advancing the state of the art in simulations of galaxy clusters, particularly in the relationship among galactic processes and the cluster environment. The research has shown that the supermassive black holes (SMBHs) at the center of galaxies can effectively regulate the star formation rate in cluster galaxies just as they do in field galaxies. Furthermore, the processes that establish the observed relationship between the SMBH mass and the stellar mass of the galaxy is independent of the galactic environment and is determined by the correlation between SMBH accretion rate and the star formation rate. On the other hand, the state of the gas in the core of the cluster is not determined by the SMBH feedback but, rather, is set by the mergers of larger substructures. The team’s high-resolution simulations allow them to make predictions about the multiphase structure of the cluster gas and how it can be observed with the Hubble Space Telescope and future UV-capable space telescopes (Fig. 1).

WHY BLUE WATERS

Our scientific goals require modeling over a large dynamic range in mass and space. We have demonstrated that mass resolutions on the order of 10^7 solar masses are needed to accurately follow star formation and galaxy morphology. Likewise, we need to model a galaxy cluster on the order of 10^15 solar masses that is comparable to those observed over a range of redshifts. Hence, simulations require approximately 10 billion particles. Such simulations can only be run on the largest computers available. Furthermore, the long-range nature of gravity requires a high-performance, low-latency network to perform the calculations.

PUBLICATIONS & DATA SETS


EFFECTS OF ACTIVE GALAXY FEEDBACK ON THE INTRACLUSTER MEDIUM

EXECUTIVE SUMMARY

The research team has used Blue Waters to apply a novel approach to a key question regarding the intracluster medium (ICM), the hot plasma trapped in the gravitational potential wells of galaxy clusters. This approach involves a subgrid model for black hole accretion to study the ability of jets to efficiently and uniformly deposit heat into the ICM. The model improves on existing techniques by directly measuring the accretion rate onto the black hole, linking it to a model of the accretion disk, and using the result to determine the feedback efficiency. In 2019, the researchers have used parts of this framework to study the role of jet precession and ICM turbulence in making feedback more isotropic.

RESEARCH CHALLENGE

Loss by the ICM should cause the gas to lose pressure support against gravity, condensing to form stars at prodigious rates. Generally, this star formation is not observed; instead, cluster central galaxies are overwhelmingly “red and dead” with little or no star formation and very old stellar populations. Some heating process must offset the radiative cooling. The most likely candidate is energy input by the supermassive (approximately 10^9 solar mass) black holes (SMBHs) found at the centers of clusters. When actively accreting matter and producing relativistic jets, these are the central engines of what are called active galactic nuclei (AGN). High-resolution X-ray and radio observations clearly show AGN disturbing and heating the ICM gas.

However, tuning the amount of feedback to match the cooling rate and distributing it so that the gas is evenly heated are serious theoretical problems. This requires connecting processes occurring in accretion disks around black holes smaller than the solar system with plasma physics as much as 30,000 light years away. The modeling of AGN feedback usually involves a subgrid model and considerable simplification of the complex physics involved in the region surrounding the AGN’s central black hole. Those approaches still have major shortcomings. Often, the multiphase structure of the gas is not incorporated, and accretion rates are estimated using spherically symmetric models applied to data on scales much larger than the accretion region. The efficiency of feedback is taken to be a constant, tuned to roughly reproduce the central entropies of clusters.

The research team’s approach, which borrows from techniques used in star formation and stellar evolution, applies a sink particle model to directly measure the accretion rate onto the black hole plus accretion disk system. The core of the cluster is resolved at scales of a few light years, allowing the complex gas structure in the vicinity of the AGN to be directly simulated. The efficiency and mode of feedback, as well as the growth rate of the black hole, are determined by matching the sink particle formalism to a model of the accretion disk that is informed by accretion disk simulations in the literature.

METHODS & CODES

This work uses the adaptive mesh refinement (AMR) hydrodynamics plus N-body code FLASH 4. FLASH 4's AMR is an Eulerian flow simulation method that allows high-resolution meshes to be placed only in regions of interest. It also uses a hydrodynamics solver based on the piecewise-parabolic method. In local idealized simulations, turbulent stirring is imposed in a manner that follows a Kolmogorov-like spectrum by adding a divergence-free, time-correlated velocity evolved by an Ornstein–Uhlenbeck random process. Radiative cooling using a metallicity-dependent cooling function assures that the gas reaches the densities needed to trigger feedback events.

RESULTS & IMPACT

The researchers have used parts of the subgrid framework outlined above to study the ability of jet precession and turbulence to isotropize heating of the ICM. Accretion rates are measured using fluxes on a control surface surrounding the AGN, and feedback efficiency is held constant. They allow the AGN jet to precess, constraining the precession angle and period with observations of jet morphology in radio and X-ray maps. In some simulations, they introduce turbulent stirring to model the effects of galaxy wakes and cluster mergers. The team used recent Hitomi observations of the Perseus cluster to set the stirring energy. They have conducted isolated cluster-core simulations with stationary and precessing jets as well as without turbulence and with weak or strong turbulence corresponding to different turbulent velocity dispersion values. Fig. 1 shows an example of the evolution of accretion rate in the team’s simulations. The researchers have found that precession helps jets deposit energy in a more distributed manner but suppresses accretion onto the SMBH by sweeping away a larger volume of gas. Larger precession angles seem to contribute to a time lag between accretion and feedback.

Fig. 2 shows an example of one of the runs with both precessing jets and turbulent driving. The researchers have discovered that while turbulent driving itself enhances the kinetic energy of the ICM and triggers accretion, with precessing jets and weaker turbulent driving, the gas primarily passes through strong shocks produced by the jet, and cavity-like structures are formed. However, the situation changes with stronger turbulence, where the jet material gets blown away and the accretion process is enhanced by inflows of hot gas, allowing more energy to be deposited in the ICM. This coupling between jet precession and turbulent driving thus helps to regulate AGN feedback.

WHY BLUE WATERS

Numerous complex physical processes are involved in the ICM. The required dynamic ranges in space and time are very large. These features make the ICM a natural setting for simulation studies that exploit the unique characteristics of Blue Waters. The researchers’ improved approach to measuring accretion rates and introducing feedback increases the complexity of the simulations in the innermost region close to the SMBH, which inevitably increases the cost. The computing ability of Blue Waters provides resources for such calculations to be done.

PUBLICATIONS & DATA SETS

GRavitational and Electromagnetic Signatures from Binary Black Hole–neutron Star Mergers: A jet Engine for Short Gamma-ray Bursts

EXECUTIVE SUMMARY

Recently, the LIGO/Virgo scientific collaboration reported the detection of gravitational waves likely produced by a black hole–neutron star (BHNS) system (source S190426c). No electromagnetic counterparts were linked to this event. Using general relativistic magnetohydrodynamic simulations of a BHNS undergoing merger, the research team surveyed different configurations that differ in the spin of the BH (a/MBH = −0.5, 0, 0.5, 0.75); in the mass ratio (q = 3:1, q = 5:1); and in the orientation of the magnetic field (aligned and tilted by 90° with respect to the orbital angular momentum). Only for configurations with a MNS > 0.5 and aligned magnetic fields did the team find collimated, magnetically confined jets whose luminosity was consistent with typical short gamma-ray bursts and significant mass outflows that can induce detectable kilonova. By contrast, in case q = 5:1 the remnant disk and magnetic field were too small to drive a jet and generate significant mass outflows or counterpart electromagnet luminosity. High mass ratio BHNS may therefore be the progenitors of S190426c.

RESEARCH CHALLENGE

Inspiraling and merging black hole–neutron star binaries are not only important sources of gravitational waves (GWs) but are also promising candidates for coincident electromagnetic (EM) counterparts. In particular, these systems are thought to be progenitors of short gamma-ray bursts (GRBs) [1–4].

Coincident detection of GWs with EM signals from compact binary mergers containing neutron stars (NSs) could give new insight into their sources: GWs are sensitive to the density profile of NSs and their measurement enforces tight constraints on the equation of state of NSs [5]. Postmerger EM signatures, on the other hand, can help to explain, for example, the phenomenon of GRBs and the role of BHNS mergers in triggering the nucleosynthesis processes in their ejecta. BHNS mergers have attracted a great deal of attention recently because of the first-ever candidate detection of GWs from a BHNS system (90% confidence) reported by the LIGO/VIRGO scientific collaboration [6]. As a crucial step to solidifying the role of BHNS as multimessenger systems, the research team reported results from general relativistic simulations of BHNS configurations underlying merger that differ in the spin of the BH (a/MBH = −0.5, 0, 0.5, 0.75); in the mass ratio (q = 3:1, q = 5:1); and in the orientation of the magnetic field (aligned and tilted by 90° with respect to the orbital angular momentum), to determine their impact in the EM luminosity, ejecta, and other EM counterparts [7,8].

METHODS & CODES

Magnetohydrodynamic (MHD) numerical simulations in full general relativity require the solution of the Einstein field equations to determine the gravitational field as well as the relativistic MHD equations to determine the flow of matter and the electromagnetic fields. Together, the equations constitute a large system of highly nonlinear, multidimensional, partial differential equations in space and time. The researchers solved the above equations through their completely independent Illinois GRASHM code, which has been built over many years on the Cactus infrastructure and uses the Carpet code for adaptive mesh refinement but employs the team’s own algorithms and coding [9]. This code utilizes state-of-the-art high-resolution shock-capturing methods to evolve scenarios involving either vacuum or matter spacetimes, with or without magnetic fields. It utilizes the Baumgart–Shapiro–Shibata–Nakamura formulation of the Einstein field equations with puncture gauge conditions. It solves the magnetic induction equation by introducing a vector potential and employs a generalised Lorentz gauge condition to reduce the spurious appearance of strong magnetic fields on refinement level boundaries [9].

RESULTS & IMPACT

In agreement with the researchers’ earlier calculations, where the star is seeded with a dipole magnetic field that extends from the interior to the stellar surface [4,10], they found that the BHNS mergers listed above led to a disk + BH remnant with a rest-mass ranging from ~10−6Msun to ~10−3Msun, and dimensionless spin ranging from a/MNS = −0.33 to 0.85. The early evolution, tidal disruption, and the merger phases are unaltered by the dynamically weak initial magnetic field. In the postmerger phase, the researchers found that by around ∆t = −300Msun = (80MNS) (1Msun)/ms after the GW peak emission a magnetically driven jet is launched in the case where the spin of the BH companion is equal or larger than a/MNS = 0.5. The lifetimes of the jet [∆t = 0.7(MNS/1-4Msun)s] and outgoing Poynting luminosity [Lpoynting(1-104erg/s)] are consistent with observations of typical sGRBs [11], as well as with the Blandford–Znajek [12] mechanism for launching jets and their associated Poynting luminosities. In contrast, by the time the team terminated its simulations, they did not find any indication of an outflow in the other cases; in the nonspinning case (a/MBH = 0) and mass-ratio q = 3:1, a persistent fallback debris toward the BH was observed until the end of the simulation, the magnetic field above the BH poles was wound into a helical configuration, but the magnetic pressure gradients were still too weak to overcome the fallback ram pressure, and thus it is expected that a longer simulation will be required if a jet were to emerge. However, if the fallback debris timescale is longer than the disk accretion timescale (∆t = 0.36 (MNS/1.4Msun)), the launching of a jet in this case may be suppressed. In the counter-rotating q = 3:1 BHNS configurations (a/MBH = −0.5) the star plunges quickly into the BH, leaving an “envelope” BH with a negligibly small accretion disk containing less than 1% of the rest-mass of the NS. Similar behavior was observed in the BHNS configuration with mass ratio q = 5:1. Finally, in the tilted magnetic field case, the team did not find a coherent poloidal magnetic field component remaining after the BHNS merger; hence, the jet ingredient for jet launching was absent. The dynamical ejecta produced in the nonspinning q = 5:1 and the counter-rotating BHNS configurations were too small to be resolved (~10−0Msun) and it may indicate that high mass-ratio BHNS or counter-rotating BHNS configurations may not be accompanied by either kilonovae or short gamma-ray bursts because they underproduce a negligible amount of mass and form negligibly small accretion disks onto the remnant BH. The researchers have concluded that these two configurations may be the progenitors of the BHNS candidate S190426c.

WHY BLUE WATERS

Blue Waters provides the required computational power to simulate those cosmic sources in a timely manner. By adding OpenMP support to our message-passing interface (MPI)-based code, scalability on multicore machines has improved greatly. With the Blue Waters high-performance interconnect and processors, the team’s hybrid OpenMP/MPI code exhibits greater scalability and performance than on any other supercomputer they have used. Recently, the researchers were able to build their code with the Blue Waters Intel compilers. This resulted in a significant boost of the code’s performance by about 30%, making Blue Waters unique for tackling the astrophysical problems the team wants to address.

PUBLICATIONS & DATA SETS


METHODS & CODES

Using the research team’s new code, H-AMR [2] (pronounced “hammer”), which includes adaptive mesh refinement, local adaptive timestepping, and runs efficiently on GPUs, the research team was able to overcome the above challenges. H-AMR performs 10 times faster on a GPU than on a similar vintage 16-core CPU. H-AMR is parallelized via MPI with domain decomposition and scales well to thousands of GPUs, achieving weak scaling efficiency of 85% on 4,096 GPUs on the Blue Waters supercomputer. The performance of the code allowed the team to study tilted discs at higher resolutions and over longer durations than was previously possible.

RESULTS & IMPACT

The simulations carried out on Blue Waters’ GPU partition revealed that the frame dragging of a spinning black hole can tear up tilted accretion disks into several individually precessing subdisks [1]. This can lead to complex, variable disk emission as the orientation of subdisks changes in time, and high-energy emission, as a result of jets running into subdisks.

WHY BLUE WATERS

Access to Blue Waters has been instrumental in obtaining these groundbreaking results, which require not only enormous amounts of computing power but also fast interconnect speeds to make use of hundreds of XK nodes. As in the past, Mark Van Moer helped enormously with 3D visualization.

PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY

Accretion disks are typically tilted relative to the black hole rotational equator. Lack of symmetries makes numerical studies of such disks particularly challenging, especially on the curved spacetime of a rapidly spinning black hole. The GPU partition of Blue Waters enabled the research team for the first time to simulate such disks in full general relativity. The team found that, contrary to standard expectations, tilted disks tear up into individually precessing subdisks. If torn disks are prevalent around black holes, this calls for a reconsideration of the black hole accretion theory.

RESEARCH CHALLENGE

Tilted accretion is common in astrophysical systems. In fact, researchers expect that nearly all black hole accretion disks are tilted at some level relative to the black hole rotational equator. This is because the gas that approaches the black hole from large distances has no idea which way the black hole is spinning. However, studies of such tilted accretion are extremely challenging, especially in the crucial regime of luminous, radiatively efficient accretion that powers bright quasars. Such accretion disks are razor-thin and difficult to resolve numerically, requiring high resolutions and adaptive grids to follow the body of the disk as it moves through the computational grid.

Figure 1: The inner part of a disk of half-thickness $h/r = 0.03$ tilted by 60° tears off from the outer misaligned part of the disk and precesses independently. This is the first demonstration of the disk tearing in a GRMHD (general relativistic magnetohydrodynamic) numerical simulation.
SCALING THE BATS–R–US MHD MODEL TO OVER 100,000 CORES WITH EFFICIENT HYBRID OPENMP AND MPI PARALLELIZATION

Allocation: GLCP/PC360 Keh
Collaborator: Hongyang Zhou1

EXECUTIVE SUMMARY

This project aims to optimize and improve multilevel parallelization of the computationally most expensive components of the space weather modeling framework. One of the most important and computationally expensive models in the framework is the BATS–R–US magnetohydrodynamic (MHD) code. With pure MPI parallelization it is limited to about 32,000 cores owing to memory constraints. The research team has designed and implemented an efficient hybrid MPI + OpenMP parallelization. The main idea is to assign grid blocks consisting of hundreds of grid cells to each OpenMP thread. This is much easier to implement than a cell-by-cell multithreading approach, and it is also more efficient. The new version of the code can scale to over 100,000 cores on Blue Waters while maintaining high efficiency.

RESEARCH CHALLENGE

While pure MPI parallelization can be near optimal in terms of speed, the total number of cores used can be limited by the memory usage. In our BATS–R–US MHD code [1], for example, most but not all of the data are distributed over the processes. In particular, the description of the adaptive tree of the grid blocks is stored on all the MPI processes so that finding neighbor blocks or finding the grid block covering some spatial location can be done efficiently. The size of this array grows with the problem size and eventually can become a bottleneck. This issue can be mitigated by using OpenMP parallelization because the amount of memory occupied by the repeated arrays on a given node will be reduced proportionally with the number of MPI processes per node. Correspondingly, one can scale the model to a larger number of cores. With dozens of cores per node on current architectures this difference is significant, by a factor of 15 to 30 or even more.

Adding OpenMP into a complex MPI parallel code is not simple. BATS–R–US consists of about 250,000 lines of Fortran 90 code without counting comments and empty lines. The workload is distributed over a large fraction of the source code. The goal is to add OpenMP parallelization that obtains good performance with a reasonable development time investment.

The team's primary goal is to allow scaling BATS–R–US to hundreds of thousands of cores on new computers to solve large problems efficiently. Further, the researchers’ work and experiences should help in making similar projects run smoothly and efficiently.

METHODS & CODES

The team’s multiphysics code BATS–R–US can solve various partial differential equations with a large variety of numerical schemes on a block adaptive grid. The grid blocks consist of a fixed number of grid cells, typically 4 x 4 x 4 to 8 x 8 x 8 cells, although their physical size may vary. The code loops over grid blocks and performs various computations such as calculating fluxes and sources for each grid cell and then updates the grid cell value, etc. There are two possible implementation strategies for OpenMP: (1) parallelize the loops over grid cells (fine-grained) or (2) parallelize loops over grid blocks (coarse-grained).

The team chose the coarse-grained option for several reasons. In the overall algorithm, the loops over the cells contain less work than the loops over the blocks. There are many more loops over cells than loops over blocks, so a fine-grained approach would require adding more OpenMP parallel sections. For many loops over the grid cells the work per cell may be insufficient to make the OpenMP parallelization efficient given the overhead of starting and closing the multithreaded section. A significant difficulty with the coarse-grained approach is finding and resolving race conditions. It took significant effort for the team to find the appropriate tool. Intel's Inspector turned out to be invaluable.

RESULTS & IMPACT

The team’s strategy required relatively modest code changes: only 609 OpenMP directive lines were added to the 250,000-line source code. Most of the changes were declaring variables as thread private or moving module variables into subroutines when convenient. The team also learned to look out for variable initializations, which make local subroutine variables behave as shared by default.

Fig. 1 shows that by using the OpenMP + MPI parallelization, BATS–R–US can run on more than 500,000 cores. Running 32 threads per node requires communication between the two sockets; still, the performance is about 50% of the ideal scaling, which is quite reasonable. With 16 threads per node BATS–R–US can scale up to approximately 250,000 cores and obtain around 80% of the ideal performance. In comparison, the pure MPI parallelization can run only up to about 16,000 cores before running out of memory. The researchers obtained similar results when running the code with an implicit solver. The team also learned that for some compilers, switching on the OpenMP library can severely impact code performance (a slowdown of up to a factor of three) even if only one thread is used per MPI process. It is important to make sure that the code is portable and performs well for a compiler that runs efficiently with the OpenMP library. The researchers also found that the pinning of the OpenMP threads (assigning them to the proper CPU cores with respect to the MPI processes) can be quite complicated and the proper settings vary from platform to platform and even from compiler to compiler. A simple C code reporting of which core is used by a certain thread and MPI process is invaluable to verify that the pinning works as expected.

WHY BLUE WATERS

Blue Waters provided a platform with the appropriate hardware, software, and computing environment to make good progress with this project. On most systems it is practically impossible to run on more than about 10,000 cores with reasonable turnaround times. On Blue Waters, the team could scale up to about 500,000 cores. The variety of compilers allowed for testing the efficiency of the hybrid parallelization comprehensively and identifying some of the not-so-well-known problems.

PUBLICATIONS & DATA SETS

NUMERICAL STUDY ON THE FRAGMENTATION CONDITION IN A PRIMORDIAL ACCRETION DISK

Allocation: Illinois/1,000 Knh
PI: Matthew Turk1
Co-PIs: Wei-Ting Liao1, His–Yu Schive1
1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

This project uses Blue Waters to study the accretion flow that surrounds the first luminous objects known as Population III stars. These early-stage protostars are believed to be surrounded by massive accretion disks where competition between gravity and turbulence leads to the formation of multiple stellar objects. The goals of the project are to understand the multiplicity of the first stellar systems as well as to find the limits on the final mass of individual Population III stars. The research team also aims to uncover the unique roles of both turbulence and gravity on the resulting variability of the accreted mass that governs the final mass of Population III stars.

RESEARCH CHALLENGE

The simulation will provide a numerical model that furthers our understanding of the formation of Population III stars and their possible observable quantities.

METHODS & CODES

This work uses GAMER-2 [1] in conjunction with GRACKLE [2]. The numerical scheme allows the team to explore the accretion flow instability while self-consistently evolving the primordial chemistry.

RESULTS & IMPACT

The simulation suggests that the primordial accretion disks are highly turbulent and, thus, the formation of companion stars could be delayed. Using Blue Waters, the team aims to deepen the understanding of the conditions under which companion protostars may form and how it may impact the initial mass function of primordial stars.

WHY BLUE WATERS

Blue Waters provides the environment that ensures high performance and scalability. GAMER-2 has been optimized and tested to run efficiently on Blue Waters.

MERGING BLACK HOLES AND NEUTRON STARS

Allocation: NSF PRAC/200 Knh
PI: Saul A. Teukolsky1
1Cornell University

EXECUTIVE SUMMARY

The primary purpose of the project is the numerical solution of Einstein’s equations of general relativity. The goal is to track the coalescence and merger of binary black hole systems and to calculate the emitted gravitational waves (GWs). Another goal is to carry out a similar project for binary systems containing a black hole and one or two neutron stars. The work is aimed at providing theoretical predictions that can be compared with the signals measured by the National Science Foundation’s LIGO (Laser Interferometer Gravitational-Wave Observatory) GW detector.

RESEARCH CHALLENGE

The primary scientific objective of this project is to theoretically underpin and improve the ability of LIGO to extract the rich information that the observed GWs carry. Gravitational waves provide a new window on the universe that will enable scientists to test their understanding of fundamental physics as well as learn about the most extreme events in the cosmos.

METHODS & CODES

Most of the computations are done with the SpEC code (spectral Einstein code) developed by the collaboration. The numerical methods that are used make it the fastest and most accurate code for treating black holes. The research team is also developing a new code, SpECTRE, that will include innovative methods to treat neutron star systems.

RESULTS & IMPACT

The researchers have released a new version of their public catalog of gravitational waveforms for use by all scientists, largely through simulations on Blue Waters. The new version increased the size of the catalog from 174 waveforms to 2,018. These waveforms have already been employed to produce a very accurate waveform model that LIGO can use in its data analysis, and will meet most of LIGO’s needs for the next two to three years.

WHY BLUE WATERS

The research team’s numerical code runs most efficiently on 50 to 70 processors for each waveform. Blue Waters’ nodes are perfectly sized for using one or two nodes per waveform and exploring hundreds of different parameter values to develop the team’s catalog.

PUBLICATIONS & DATA SETS

Image Processing to Build a Multitemporal Vegetation Elevation Ecosystem Model of the Great Lakes Basin
Petascale Processing of Satellite Earth Observations
Large-Scale Remote Monitoring of Invasive Species Dynamics Through a Petascale High-Performance Computing System
Deforestation of the Amazon Forest: Understanding Hydroclimate Impacts by Tracing the Water that Evaporates from the Forest
Forecasting Volcanic Unrest and Eruption Potential Using Statistical Data Assimilation
Monitoring Field-Scale Crop Water Use Using a Satellite Data-Driven Mechanistic Modeling Approach
Building an Objective Seasonal Forecasting System for U.S. Corn and Soybean Yields
Inflow and Outflow from Thunderstorms: Tracking Their Influence on Precipitation and Further Growth
Petascale Polar Topography Production
High-Resolution Numerical Simulations of Convection Initiation over the Sierras de Córdoba Mountains in Argentina
Simulations of Violently Tornadic Supercells and Damaging Thunderstorms
Prediction of Geomagnetic Secular Variation with Large-Ensemble Geomagnetic Data Assimilation
Machine Learning for Error Quantification in Simulating the Climate Impacts of Atmospheric Aerosols
Simulating Hydroclimate Change in Southwest North America at 21,000 Years Ago
Implementation and Use of a Global Nonhydrostatic Model for Extended Range Weather Prediction during the RELAMPAGO Field Campaign
Simulating Large California Earthquakes Before They Occur
Materials Simulations in Geophysics
Simulating Aerosol Impacts on Climate. One Particle at a Time: A Regional-Scale, Particle-Resolved Aerosol Model to Quantify and Reduce Uncertainties in Aerosol–Atmosphere Interactions
Evolving Air Quality Under the Changing Climate
Sensitivity of Arctic Sea Ice Thickness Distribution to Sea Ice Internal Dynamics in a Changing Climate
IMAGE PROCESSING TO BUILD A MULTITEMPORAL VEGETATION ELEVATION ECOSYSTEM MODEL OF THE GREAT LAKES BASIN

Allocation: GLCPC/495 Kish
PI: Jennifer Corcoran
Co-PIs: Brian Huberty, James Klaseen, Keith Pelletier
Collaborators: Paul Morel, Joe Knight, Laura Bouguessa-Chavez

1University of Minnesota, Twin Cities
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3SharedGeo
4University of Minnesota
5Michigan Tech Research Institute

EXECUTIVE SUMMARY

Over a period of two-and-a-half years, the research team has acquired, processed, and created high-resolution, multitemporal vegetation elevation ecosystem models (MTVEEM) across the entire Great Lakes Basin (GLB) using stereo submeter, optical satellite imagery, and derived surface vegetation models can be used to better characterize these features and their changes over time, with the added dimension of height.

High-resolution vegetation surface mapping over large geographic regions such as the Great Lakes Basin (GLB) has never been obtained from either aerial or satellite surveys. Additionally, the binational management by Canada and the United States of the GLB limits consistent, repeatable coverage by either country working independently. While a few scattered vegetation surface models exist from expensive airborne active laser sensors within the GLB, these data sets represent single time points and were not planned as continuous, basinwide acquisitions. Having high-resolution multitemporal information in three dimensions enables planned as continuous, basinwide acquisitions. Having high-resolution, multitemporal vegetation elevation ecosystem models across the entire GLB will vastly improve. The amount of data processed and analyzed in the GLB is well beyond the capacity of most academic, private, and government systems; the team could not have done this work without a leading-edge petascale resource such as Blue Waters.

RESEARCH CHALLENGE

Ecosystem management requires knowing the type, size, structure, and density of vegetation over time. These important features need to be mapped repeatedly. Stereo submeter, optical satellite imagery, and derived surface vegetation models can be used to better characterize these features and their changes over time, with the added dimension of height.

RESULTS & IMPACT

As the data are processed, the resulting surface canopy models will be openly available in 2019 initially through the University of Minnesota. Other partners online distribution systems, such as the National Oceanic and Atmospheric Administration’s Digital Coast and the Great Lakes Observing System, will also be used. The final product, a seamless and registered surface vegetation elevation ecosystem model (MTVEEM) of the GLB will enable a large range of science activities at substantially higher resolution than currently available (current status shown in Fig. 1). These canopy maps and change detection products will provide positional accuracies of less than a couple meters with the added ground control points. The team is assessing semicentennial changes in prior-

WHY BLUE WATERS

Stereo satellite imagery allows for the generation of highly accurate surface elevation models; the researchers have already tasked stereo-mode acquisition through Digital Globe over the entire GLB. Each stereo pair is about 1.25 GB; the total number of pairs processed to date is about 120,000 and soon will exceed 150,000. The amount of stereo imagery in a study area the size of the GLB and the computational burden to process each of these image pairs is well beyond those resources available from standard academic, private, and government systems. This is precisely why this project requires a leading-edge petascale resource such as Blue Waters.
PETASCALE PROCESSING OF SATELLITE EARTH OBSERVATIONS

Allocation: Blue Waters Professor/187 Knh
PI: Larry Di Girolamo
Collaborators: Matias Carrasco Kind, Gregory Daues, Yulan Hong, Ralph Kahr, Lusheng Liang, Donald Petrucci, John Towne, Keni Yang, Ping Yang, Yehe Zhan, Guangyu Zhao

1University of Illinois at Urbana–Champaign
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3NASA Goddard Space Flight Center
4NASA Langley Research Center/Science Systems and Applications, Inc.
5The HDF Group
6Texas A&M University

EXECUTIVE SUMMARY

Through collaborative efforts among NASA, HDF Group, and NCSA, the research team fully validated and enhanced the open source tool that resamples Terra satellite data into a common grid with a Python interface to make it applicable beyond Terra to any Earth observation data. The Terra satellite, launched in 1999, continues to collect Earth science data using five instruments: the Moderate-resolution Imaging Spectroradiometer (MODIS), the Multi-angle Imaging SpectroRadiometer (MISR), the Advanced Spaceborne Thermal Emission and Reflection Radiometer, the Clouds and the Earth’s Radiant Energy System (CERES), and the Measurements of Pollution in the Troposphere. Terra data not only serve the scientific community but also the governmental, commercial, and educational communities.

The researchers further used the Terra data set to: (1) characterize the ice crystal roughness of cirrus clouds for a better understanding of ice cloud optical properties; (2) correct biases in the MODIS cloud effective radius retrievals through MISR and MODIS fusion; (3) evaluate MISR and CERES Arctic cloud albedo retrievals, indicating excellent consistency for certain solar zenith angles; and, (4) examine decadal changes in the Earth’s radiance fields, revealing little cloud change in the global mean beyond calibration (Fig. 1) but large changes in certain regions. The research group extended the study by processing observations from spaceborne active sensors, showing a strong correlation between cloud occurrence frequency and climate regimes (Fig. 2).

RESULTS & IMPACT

The research team explored archiving and distributing Terra fusion products through existing NASA and commercial cloud services. They tested accessing and processing the basic fusion data on the Amazon cloud and found its processing time was slightly more than Blue Waters for the same settings but that costs to investigators’ grants by using commercial clouds for a data-intensive project can be prohibitive. The team also fully validated and enhanced the open source tool that resamples or reprojects the radiance fields into a common grid with a Python interface to make the tool applicable beyond Terra to any Earth observation data. Scientific investigation using the fusion data set was carried out primarily in four study areas. (1) The team characterized biases in the MODIS standard product of cloud drop effective radius (Re) and further examined the underlying causes. The results paint a radically different picture of the distributions of Re from what the original MODIS product provided. The bias-corrected cloud drop sizes are now in line with spot measurements from field campaigns and outputs from climate models. (2) The team retrieved ice cloud microphysical properties through MISR–MODIS fusion, showing regional dependence on ice crystal structure. Results have been published in an open access journal, Remote Sensing. (3) The group evaluated the MISR and CERES Arctic cloud albedo retrievals, showing excellent consistency between the instruments for solar zenith angles of less than 70°. These results were also published in Remote Sensing. (4) The team extended a global and regional radiance and texture trend study previously performed on Blue Waters [3] by using additional instruments: MODIS and CERES. The time series of the deseasonalized scaled anomalies of the monthly global mean spectral radiance and texture are shown in Fig. 1. The global blueing shown in the researchers’ previous study [3] mainly results from a calibration drift in the MISR red band. There is no significant global trend in the Earth’s reflected radiation field, but local regional changes were found.

WHY BLUE WATERS

The key advantages of using Blue Waters for access, usage, and distribution of Terra fusion products are that the Terra data and processing are local, whereas access and sharing are global. The research team demonstrated that having the Terra data local, with processing tuned to a massively parallel system with excellent sharing services on Blue Waters, provides an optimum framework for large-scale processing, analytics, and mining of the entire Terra record. In addition, the project staff provide expertise critically needed to optimize workflows.

PUBLICATIONS & DATA SETS


RESULTS & IMPACT

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PUBLICATIONS & DATA SETS

LARGE-SCALE REMOTE MONITORING OF INVASIVE SPECIES DYNAMICS THROUGH A PETASCALE HIGH-PERFORMANCE COMPUTING SYSTEM

EXECUTIVE SUMMARY
The rapid expansion of exotic saltcedar along riparian corridors has drastically altered landscape structures and ecosystem functions throughout the United States. Conducting the large-scale monitoring of spatio-temporal dynamics of this invasive species over the past 40 years is essentially critical to understanding its invasion mechanism. Previous studies indicated that the leaf senescence stage is the optimal time window to remotely monitor saltcedar distributions. However, the computational complexity in predicting the leaf senescence timing, along with the massive volume of satellite data in both spatial and temporal dimensions, makes large-scale invasive species monitoring prohibitive. Instead, the research team developed a parallel computational network model on Blue Waters that can accommodate the spatio-temporal variation in plant phenology to facilitate the large-scale monitoring of invasive species dynamics. Blue Waters provides unprecedented opportunities to achieve region-wide monitoring of saltcedar distribution to revolutionize scientific understanding of saltcedar invasion processes.

RESEARCH CHALLENGE
Remote monitoring of invasive saltcedar dynamics is essential for conservation agencies to develop cost-effective control strategies [1,2]. Acquiring satellite imagery during the leaf senescence stage of saltcedar is necessarily crucial to facilitate the large-scale repetitive mapping of this invasive species [3–5]. However, owing to climate variability and anthropogenic forcing, the timing of saltcedar leaf senescence varies over space and time [6]. Given that the leaf senescence stage of saltcedar lasts only for three to four weeks, it is challenging to pinpoint the appropriate satellite imagery that can accommodate this spatial and interannual variation over wide geographical regions [7]. The dearth of high-performance computational systems that can tackle this phenological issue makes the large-scale saltcedar mapping prohibitive and hinders the understanding of its invasion mechanism.

METHODS & CODES
To accommodate the spatio-temporal variation in plant phenology, the research team developed a complex network-based phenological model using satellite time series. The network-based phenological model constructs an undirected network for each pixel based on its spectral reflectances along the phenological trajectory. Specifically, the spectral reflectance of the pixel obtained on each day is represented as a node. Those nodes that share similar spectral similarity are connected by edges. The network model groups the spectral reflectances along the trajectory into three clusters: a “pretransition cluster,” a “transition cluster,” and a “posttransition cluster” (Fig. 1). Further, the team developed several network measures to accommodate the spatio-temporal variation in invasive species phenology. To overcome the computational limits, the research group proposed an innovative pixel-based remote sensing parallel computational system for large-scale saltcedar monitoring. The parallel system adopts hybrid computation models, including a core-level computation model and a node-level data distribution model. In the core-level computation model, a computing node stores the information of a number of pixels and processes them using OpenMP. The node-level data distribution model includes a two-level data decomposition strategy. The first level uses a pixel-based remote sensing parallel computation model in monitoring the fall foliage transition date for peak chlorophyll content. The second level uses a two-level data decomposition strategy. The first level uses a small number of pixels to process at the large-scale. The second level uses a large number of pixels to process at the large-scale.

RESULTS & IMPACT
The network-based phenological model presents a new representation of the complex phenological process of vegetation. This representation characterizes the vegetation’s phenological status through tracking the continuously changing signatures of vegetation along the temporal trajectory. The network results revealed a gradual phenological shift from north to south along the latitudinal gradient, following the Hopkins bioclimatic law. It suggested that temperature decreased with increasing latitude and would likely be an important force driving the phenological variations in vegetation over wide geographic regions. Along the latitudinal gradient, the interannual variation in the estimated average timing of leaf senescence was generally less than 10 days.

The team has successfully implemented this parallel computational system on Blue Waters and analyzed the massive amount of data and I/O operations are needed to run the model on Blue Waters. This could dramatically reduce the time of I/O operations of the massive imagery involved in this project, and hence reduce the total computation time.

PUBLICATIONS & DATA SETS

Figure 1: Complex network of phenological progress of invasive species with three clusters.
DEFORESTATION OF THE AMAZON FOREST: UNDERSTANDING HYDROCLIMATE IMPACTS BY TRACING THE WATER THAT EVAPORATES FROM THE FOREST

EXECUTIVE SUMMARY

The Amazon Forest has undergone significant deforestation in the past decades with natural forests being replaced by agriculture and pasturelands. In this work, the research team evaluated the impacts of continued deforestation on the hydroclimate of the South American continent. They initiated 10-year climatological simulations created with the Weather Research and Forecasting model (WRF) with added water vapor tracers (WRF–WVT). The water vapor tracers track the water that originates from the Amazonian forest and follow it in space and time as the moisture is advected and contributes to precipitation. In the water-limit ed southern Amazon, the researchers found that the effects of deforestation are locally strong with distinct changes in the deforested areas. Although area-averaged precipitation decreases, the team also found regions with increased precipitation owing to changes in the atmospheric circulation from changes in land cover. This reveals both positive and negative feedback from deforestation and complex land–atmosphere interactions in the hydroclimate of South America.

RESEARCH CHALLENGE

Deforestation of the Amazon Forest in the past decades has seen natural forests being replaced by agriculture and pasturelands (see mapbiomas.org for the evolution of land cover since 1985). A very high rate of deforestation in the year 2005 (19,000 km²) was followed by a sharp decline in 2012; unfortunately, the rate has since increased again to almost 8,000 km² in 2018 [2].

The Amazon is the largest tropical rainforest on Earth. Up to 50% of Amazonian precipitation originates as evapotranspiration from the forest [7,9]. Furthermore, downwind regions in the La Plata and Orinoco Basins are dependent on Amazonian moisture for their precipitation [4,8]. The critical question is how continued deforestation of the Amazon Forest will affect the hydroclimate of the South American continent.

METHODS & CODES

The researchers incorporated Water Vapor Tracers (WVT) into the Weather Research and Forecasting model (WRF) [3,5]. This allows users to trace moisture that originates as evapotranspiration from a tagged Amazon region. Evapotranspiration that originates from the Amazon is numerically "tagged" as it undergoes the same physical processes as total moisture such as advection, convection, phase change, and the like. In addition, WRF–WVT saves tracer moisture-related variables. In particular, tracer moisture advection and horizontal diffusion follow the exact same transport equations in WRF for scalar variables, including water vapor and all micrometeors. Tracer moisture changes phase and is converted to precipitation in the same proportion as full moisture in all cases. All tracer moisture species are generated or converted from one to another and to precipitation, mimicking their full-moisture counterparts.

The research team performed two 10-year continuous simulations for the period 2004–2013 over the domain shown in Fig. 1 using lateral boundary conditions from the ERA–Interim reanalysis data set [1]. The simulation has a horizontal resolution of 20 km and 40 levels in the vertical direction (see Yang and Dominguez, listed under “Publications & Data Sets” for details).

RESULTS & IMPACT

The research team has focused its results on the Southern Amazon Forest (dashed black box in Fig. 2a). This region is characterized by transitional forests where precipitation is less than in the northern tropical forests, and there is a marked dry season [10].

In conclusion, when focusing on the transitional forests of the southern Amazon, the research team has found contrasting behavior during the wet and dry seasons. During the wet season, the main control on ET is through radiation as there is still an ample supply of moisture. During the dry season, the region is water-limited and ET decreases significantly. Precipitation during the wet season is clearly decreased over the deforested areas, but precipitation downwind of the deforested areas is actually increased owing to increased moisture transport. During the dry season, there is very little change in precipitation. These results show the complex behavior of land–atmosphere interactions when changes in land cover occur.

WHY BLUE WATERS

Blue Waters was critical to performing the simulations owing to their very high computational expense. The research team would not have been able to perform them on their local cluster.

PUBLICATIONS & DATA SETS

FORECASTING VOLCANIC UNREST AND ERUPTION POTENTIAL USING STATISTICAL DATA ASSIMILATION

EXECUTIVE SUMMARY
A primary motivation for investigating volcanic systems is developing the ability to predict eruptions and mitigate disaster for vulnerable populations. Over the past three years, the Gregg Lab has been developing approaches for forecasting the evolution of volcanic systems in collaboration with the National Center for Supercomputing Applications (NCSA). The research team has implemented a high-performance computing (HPC) workflow using COMSOL Multiphysics finite-element software that links multiphysics model outputs with geophysical monitoring data for volcanic forecasting. This project focuses on conducting large system-scale numerical experiments to investigate eruption potential and triggering mechanisms for three volcano targets utilizing the unique computational configuration of Blue Waters. In addition to the scientific outcomes of this effort, the experiment marks the largest distributed implementations of COMSOL Multiphysics. This achievement is of great practical importance for finite-element applications and provides benchmarking for future efforts in other fields, such as engineering, in addition to earth sciences.

RESEARCH CHALLENGE
Currently, 500 million people worldwide live on or near active volcanoes. The team’s current efforts on Blue Waters are focused on developing strategies for rapid assimilation of volcano monitoring data sets into evolving geodynamic models to provide near-real-time forecasts and assessment of volcanic unrest. To that end, the group is adapting data assimilation strategies developed in other fields to combine observations of volcanic unrest with geophysical finite-element models to calculate volcanic evolution. By combining multiphysics finite-element models with volcanic monitoring data, the team is able to track the stress evolution of a magma system and provide probability forecasts of volcanic stability during periods of unrest. Utilizing ensemble-based methods, hundreds to thousands of models are run simultaneously to track the evolution of volcanic systems. This method allows the team to evaluate stress accumulation and faulting in the lead-up to volcanic eruptions and to test for potential eruption-triggering mechanisms to provide a framework for early warning probability forecasts for monitoring agencies. The ultimate goal of this work is to provide a transformable data assimilation approach that can be utilized by volcano monitors worldwide.

The volcanic unrest targets were chosen for this study owing to their excellent, real-time geophysical monitoring data sets and past eruption records: (1) Sierra Negra Volcano, Galápagos, Ecuador; (2) Laguna del Maule Volcano, Chile; and (3) Axial Volcano, Juan de Fuca Ridge—a submarine volcano located off the coast of Oregon, U.S.A. Each volcano application provides unique computational and data challenges to allow the team to evaluate potential roadblocks in transferability of the data assimilation approach.

METHODS & CODES
The research team has developed an HPC workflow using Python to efficiently distribute COMSOL Multiphysics models across Blue Waters’ compute nodes and compile model outputs for Ensemble Kalman Filter (EnKF) data assimilation at each timestep. The main computational task is evaluating hundreds of large multiphysics, mechanical fine-element models at each timestep and compiling the model data to provide a probabilistic forecast of volcanic unrest.

RESULTS & IMPACT
The team has applied its Blue Waters allocation to investigate three active volcanic systems. In 2018, the researchers had the opportunity to track the unrest of Sierra Negra Volcano, Galápagos.

PUBLICATIONS & DATA SETS
P. M. Gregg et al., “Forecasting the June 26, 2018, eruption of Sierra Negra Volcano, Galapagos, Ecuador” presented at the 27th IUGG General Assembly, Montréal, Québec, Canada, Jul. 8–18, 2019.

Preliminary version of this paper presented at the 2019 Blue Waters Annual Report, 2019.
**EXECUTIVE SUMMARY**

High-spatiotemporal-resolution evapotranspiration (ET) products with reliable accuracy have many potential applications in agriculture. The research team developed BESS–STAIR, a new framework to estimate high-spatiotemporal-resolution ET that can be used for field-level precision water resources management. BESS–STAIR couples a satellite-driven water–energy–carbon-coupled biophysical model (BESS) with a generic and fully automated fusion algorithm (STAIR) to generate gap-free 30-m-resolution daily ET estimations. Comprehensive evaluation of BESS–STAIR ET estimations revealed: (1) reliable performance over 12 flux tower sites across the U.S. Corn Belt and (2) reasonable spatial patterns, seasonal cycles, and interannual dynamics. The proposed BESS–STAIR framework has demonstrated its ability to provide significant advancements with regard to daily field-level estimations of ET at regional and decadal scales. When scaled up, which is in process, BESS–STAIR ET products could be very useful for precision water resources management and other precision agriculture applications for the U.S. Corn Belt and elsewhere.

**METHODS & CODES**

To address the above two issues, the research team developed a new high-spatiotemporal-resolution ET mapping framework, BESS–STAIR, that integrates the satellite-driven water–carbon–energy-coupled biophysical model BESS (Breathing Earth System Simulator) [1,2] with a generic and fully automated fusion algorithm STAIR (SaTallite dAta IntegRation) [3]. In this framework, STAIR provides daily 30-m multispectral surface reflectance by fusing Landsat and MODIS satellite data to derive fine-resolution leaf area index and visible/near-infrared albedo, all of which, along with coarse-resolution meteorological and CO₂ data, are used to drive BESS to estimate gap-free 30-m-resolution daily ET. The team applied BESS–STAIR from 2000 through 2017 in six areas across the U.S. Corn Belt and validated BESS–STAIR ET estimations using flux tower measurements over 12 sites (85 site-years). Results showed that BESS–STAIR daily ET achieved an overall $R^2 = 0.74$, with RMSE = 0.96 mm d⁻¹ and relative error = 28.6%. In addition, BESS–STAIR ET estimations captured the spatial patterns, seasonal cycles, and interannual dynamics of ET well when benchmarked with the flux measurements. The high performance of the BESS–STAIR framework primarily resulted from: (1) the implementation of coupled constraints on water, carbon, and energy in BESS; (2) high-quality daily 30-m data from STAIR fusion algorithm; and (3) BESS’s applicability under all-sky conditions. BESS–STAIR has great potential to be a reliable tool for water resources management and precision agriculture applications for the U.S. Corn Belt, and even for other agricultural regions worldwide, given the global coverage of its input data.

**RESULTS & IMPACT**

This project represents the first attempt to couple a satellite-driven, physical-process-based model with data fusion techniques to provide daily 30-m-resolution ET estimations at regional and decadal scales. To the research team’s knowledge, there is no explicit bottom-up, biophysically-based high-spatiotemporal resolution, long time series, and regional level methodological framework to estimate daily ET at a 30-m resolution. Other existing methodologies such as ALEXI–STARFM and SEBS–ESTARFM are LST (land surface temperature)-based models, and thus suffer from gap-filling and spatial-sharpening issues. Moreover, validation results from the project show that the BESS–STAIR framework can actually outperform those existing LST-based ET estimations.

**WHY BLUE WATERS**

Blue Waters is essential for this research since other resources, such as those available from XSEDE, are not suitable for the project, considering the petabyte-level storage demand, data availability, intensive I/O, and computation demands.

**PUBLICATIONS & DATA SETS**

BUILDING AN OBJECTIVE SEASONAL FORECASTING SYSTEM FOR U.S. CORN AND SOYBEAN YIELDS

Allocation: Blue Waters Professor/250 Koh
PI: Kaiyu Guan
Co-PIs: Jun Peng, Chongya Jiang, Bin Peng, Sibo Wang
1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

Despite significant advances in both seasonal climate prediction and satellite remote sensing, the produced data have not been fully used in crop yield forecasting at the regional scale, compared to survey-based approaches. In this project, the research team built a seasonal forecasting system for U.S. corn (maize) and soybean yield by bridging the most advanced seasonal climate prediction products from the National Centers for Environmental Prediction (NCEP) and satellite remote sensing within a statistical crop modeling framework. The researchers then evaluated the benefits of using seasonal climate prediction and satellite remote sensing data in forecasting U.S. corn and soybean yield at both national and county levels. They found they could not achieve a better forecasting performance than the official survey-based forecast from the United States Department of Agriculture (USDA) until they used both climate and remote sensing observations in their model. Compared with using historical climate information for the unknown future in each growing season, using climate predictions from NCEP gave better forecasting performance once the team corrected the bias in the seasonal climate prediction products. Using the climate–remote sensing combined model and bias-corrected climate prediction from NCEP, the researchers achieved a better forecasting performance than the USDA forecast. The team’s system will be useful for stakeholders in the agriculture industry and commodity markets.

RESEARCH CHALLENGE

More frequent extreme events and ongoing climate change puts food production at a higher risk [1–4]. Seasonal forecast of agricultural production thus becomes increasingly more important for early warning of food security issues, supply chain planning for the agriculture industry, and market prediction [5–7]. Although many countries and regions around the world have their own operational crop yield forecasting systems with various modeling and data configurations, using combined seasonal climate prediction and remote-sensing data for crop yield prediction at large scales is still rare.

METHODS & CODES

The research team built a seasonal forecasting system for U.S. corn and soybean yield by bridging the North American multi-model ensemble (NMME) seasonal climate prediction products [8] and satellite remote sensing within a statistical crop modeling framework. The seasonal climate prediction products were first bias-corrected and spatially downscaled to 4 km using the percentile mapping algorithm and then aggregated to the county level. Multiple remote-sensing products were used in this system, including the MODIS NDVI, EVI, NIRv, LST, and OCO-2/TROPOMI SIF products. Both traditional statistical regression and machine learning algorithms were used to build the yield prediction models. The model performances were evaluated using the out-of-sample validation method. The crop yield forecasting performances were benchmarked with that from USDA World Agricultural Supply and Demand Estimates (WASDE) reports.

RESULTS & IMPACT

The research group demonstrated that incorporating satellite information significantly improved the yield forecasting performance, compared with other climate-only models using monthly air temperature, precipitation, and vapor pressure deficit. The bias-corrected climate prediction from NMME showed better yield forecasting performance than the historical climate ensemble. Among the remote-sensing features, using NIRv and EVI can generally have better yield prediction performances. The multi-model ensemble approach can lead to the best yield prediction performance. Finally, the team’s yield forecast outperformed the WASDE reports released by the USDA.

WHY BLUE WATERS

Blue Waters was essential for this research because of the need to run ensemble models (more than 200 ensembles for prediction at each time) at a regular updating frequency. The computational and storage requirements can only be fulfilled by using Blue Waters.

PUBLICATIONS & DATA SETS


Figure 1: (a) Temporal correlation between actual yield and yield predicted by the “Best Climate + EVI” model and (b) its median prediction root mean square error (RMSE) from 2003 to 2016 at each county. Counties with yield observations of fewer than five years over the evaluation period are not shown.
EXECUTIVE SUMMARY

“Entrainment” describes how clouds and storms bring dry air from outside the cloud inward by their own turbulent motions. Its effects can limit storm development, longevity, and precipitation. The understanding of entrainment has been limited by inadequate model resolution in past studies. Therefore, the research team is running high-resolution 3D storm simulations on Blue Waters to quantify the interactions among entrainment, precipitation, and the generation of new storms.

The latest results suggest that: (1) The entrainment occurring in developing storms shows a dependency on grid resolution, at least down to scales of 100 meters (m); (2) mature, rotating storms do in fact continue to entrain dry air but intermittently, by features that ascend within the cores of the storms; and (3) the maintenance of thunderstorm outflows is most dependent upon the amount of large ice particles called graupel, but their speed, depth, and strength are more correlated with the amount of evaporating rain beneath the storm.

RESULTS & IMPACT

The latest results are providing new quantitative information that can assist atmospheric scientists researching ways to represent thunderstorm entrainment, precipitation, and outflows in larger-scale weather and climate prediction models. They will also be of use to weather forecasters. The results suggest:

• The entrainment quantified in developing thunderstorms growing in an environment where the winds increase strongly with height is indeed resolution-dependent (Fig. 1), and the team’s calculations suggest that grid spacing of at least 100 m is required for accuracy.

• Although the common thinking is that mature, rotating thunderstorms do not entrain much dry air, the results are showing that they do indeed continue to entrain air (i.e., past the developing stage), but that these main entrainment events are transient in time and space (Fig. 2). This is a unique finding, and the team continues to explore the origin of these signatures and to quantify their overall importance to the total amount of air entrained into the storm as well as their possible effect on precipitation.

• Calculations of the contribution of different kinds of precipitation to the storm outflows have revealed that the amount of large ice particles called graupel that fall from the storm appears to be most important in maintaining them, but that characteristics of the outflow (speed, depth, strength) are more influenced by the evaporation of rain beneath the storm bases. This suggests that certain aspects of precipitation production in storms may be critical to forcing thunderstorm outbreaks.

WHY BLUE WATERS

This Blue Waters allocation has been essential for achieving the high resolution required within a given simulation to properly represent the smaller cloud motions that are important for entrainment and precipitation development over the larger spatial and temporal domains required for thunderstorms and their outflows. As a result of its huge number of nodes, its high speed, large memory, and its large storage capability for high-resolution model output and analysis, Blue Waters enables detailed calculations to be conducted over millions of grid points. The hardware needed to run these kinds of simulations quickly supersedes the limits of most computers.

PUBLICATIONS & DATA SETS


PETASCALE POLAR TOPOGRAPHY PRODUCTION

Allocation: NSF PRAC/6,900 Keh
PI: Paul Morin1
Co-PIs: Claire Porter2, Ian Howat3, Myoung-Jong Noh3
Collaborators: Charles Nguyen; Cathleen Williamson; Charles Crettenden

1University of Minnesota
2Polar Geospatial Center
3The Ohio State University
4National Geospatial–Intelligence Agency

EXECUTIVE SUMMARY

Surface topography is among the most fundamental earth science data sets, essential to a wide range of research activities that include hazard assessment and mitigation, hydrologic modeling, solid-earth dynamics, and many others. Change in surface topography provides critical information about surface processes such as plate tectonics, erosion and subsidence, glacier mass balance, and mass balance of woody vegetation. Over most areas of the globe, however, the spatial resolution (tens of meters) and accuracy (greater than 10 meters) of openly available topographic data sets are insufficient for many of these research activities. Even fewer areas have repeated high-precision elevation measurements for observing change. Methods & Codes

The research team has spent seven years developing an efficient algorithm for constructing photogrammetric DEMs from satellite imagery with the objective of creating a fully automated pipeline capable of handling large amounts of data. The Surface Extraction from TIN-based Search-space Minimization (SETSM) algorithm, initially designed to extract elevation data over ice sheets, has been refined and optimized to handle stereo imagery over any land cover [1,2]. Unlike other DEM extraction algorithms, SETSM’s structure eliminates the need for an existing (i.e., “seed”) DEM for a priori constraints or any data-specific, user-defined search parameters, making it a truly automated algorithm. After an initial preprocessing step that corrects the source imagery for sensor-specific detector alignment artifacts, SETSM takes the two source images and derives increasingly detailed elevation models using its pyramid-based approach. The DEM extraction workflow runs on a single node for efficiency, and several thousands of these single-node tasks are bundled together using the Swift workflow management package to efficiently submit jobs in 100- to 1,000-node batches. Results & Impact

Thus far, the research team has processed the stereo imagery into topography for the poles for all of 2018 as well as the first half of 2019. In addition, they have produced DEMs for 126,000,000 km² of the land surface of the Earth from 60°N to 60°S with additional focus on North America, Australia, Western/Northern Africa, and Central Asia. On average, the poles are covered eight to ten times, with some areas having several hundred unique DEMs for a given location. These data are also processed into continuous mosaics for over 99% of the 20,000,000 km² Arctic and the 15,000,000 km² Antarctic. The polar data have been released to the science community and the public through ArcticDEM.org, and Exo has developed web services and an interactive viewer. These data are now being used by scientists, national institutions, and regional and local governments for a broad range of scientific, civil engineering, and mapping applications. Three hundred scientific publications have used ArcticDEM and 27 of the Reference Elevation Model of Antarctica data sets since the data were first released.

WHY BLUE WATERS

Currently, no other academic computer has comparable capacity or large allocations. Over 1.5 billion hours were required to process the archive of stereo images over the life of the Arctic, Antarctic, and nontropical elevation projects. Additionally, the Blue Waters’ staff were invaluable in adapting the system to handle the single-node, high-throughput ArcticDEM workflow. With their help, the researchers adopted a strategy that enabled ArcticDEM jobs to use primarily backfill nodes on a low-priority basis, increasing overall system utilization and minimizing impact on other projects.

PUBLICATIONS & DATA SETS


The research team is conducting quasi-idealized simulations of convection initiation using Cloud Model 1 (CM1) [1] to enhance the understanding of the physical processes involved. CM1 is a three-dimensional, nonhydrostatic, nonlinear numerical model used for idealized studies of atmospheric flows. It contains several physics packages for parameterizing subgrid turbulence, radiation, cloud microphysics, and the like. The preconvective thermodynamic and kinematic environment for these simulations was taken from one of the Intensive Observation Periods (IOP) of the RELAMPAGO–CACTI field experiment, which was conducted in November–December 2018. This IOP involved complex interactions among the northerly South American low-level jet, thermally driven upslope flows, outflow boundaries from previous convection, and the SDC terrain. The team has conducted simulations of increasing complexity to parse the contributions of various physical processes to convection initiation. The researchers are also using data collected during RELAMPAGO to validate these model runs.

The results and impact of these simulations indicate that the background winds advect the heat and moisture fluxes away from the terrain, causing a smaller increase in convective available potential energy and a smaller decrease in convective inhibition when compared to the simulation with no winds. As shown in Fig. 2, convergence lines and convective cells develop along the high terrain in the simulation with no winds. In the simulation with background winds, a convergence line develops to the south of the main SDC ridge, initiating convection upon interacting with the terrain. In the third simulation, no convection developed at the boundary of the cold pool.

Future simulations will involve parameterizing the effect of synoptic-scale heat and moisture advection and imposing it on the thermodynamic environment in the simulation.

**METHODS & CODES**

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**WHY BLUE WATERS**

Blue Waters has the capacity to provide the sheer amount of computational power required to conduct these simulations. Additionally, the high-resolution model output needs tens of terabytes of space, which Blue Waters has provided. Further, the Blue Waters staff was very prompt in responding to all queries. The research team had some issues compiling the code on Blue Waters, but the staff helped the team through the process.

**PUBLICATIONS & DATA SETS**


**EXECUTIVE SUMMARY**

Previous studies using satellite and radar data show that some of the most intense convective storms initiate over and near the Sierras de Córdoba (SDC) mountain range in Argentina. However, gaps in data and knowledge exist as to how these storms initiate, which contribute to poor predictability of these storms. This study aims to understand the mesoscale processes involved in the initiation of deep moist convection in the region. The study uses quasi-idealized numerical modeling of a real case along with data obtained during the RELAMPAGO–CACTI field experiments in Argentina.

**RESULTS & IMPACT**

The research team carried out three simulations: (1) with no background winds to isolate the contribution of daytime upslope flows to Convective Initiation; (2) with background winds; and, (3) with background winds with a cold pool. In the third simulation, a cold bubble with a temperature perturbation of -10 K was dropped at the southern end of the SDC to mimic the cold pool generated by a previous thunderstorm. Radiation and surface fluxes were turned on in all the simulations. Preliminary results indicate that the background winds advect the heat and moisture fluxes away from the terrain, causing a smaller increase in convective available potential energy and a smaller decrease in convective inhibition when compared to the simulation with no winds. As shown in Fig. 2, convergence lines and convective cells develop along the high terrain in the simulation with no winds. In the simulation with background winds, a convergence line develops to the south of the main SDC ridge, initiating convection upon interacting with the terrain. In the third simulation, no convection developed at the boundary of the cold pool.

Future simulations will involve parameterizing the effect of synoptic-scale heat and moisture advection and imposing it on the thermodynamic environment in the simulation.
SIMULATIONS OF VIOLENTLY TORNADIC SUPERCELLS AND DAMAGING THUNDERSTORMS

Allocations: NSF PRAC/3630 Kwh (begam)
NSF PRAC/31,000 Kwh (Yoyo)
GLPC/360 Kwh (barn)

PI: Leigh G. Orf (all three projects)
Co-PI: Catherine Findeis (began)
Collaborators: Kolten Halbert (began), Eric Sawyer (began)

1University of Wisconsin–Madison
2University of North Dakota
3University of Western Ontario

EXECUTIVE SUMMARY

Three projects on Blue Waters carried out by PI Leigh G. Orf have led to a better understanding of violently tornadic supercells (began and yoyo) as well as thunderstorms that produce damaging straight-line winds (barn).

Breakthrough simulations of violently tornadic supercells previously conducted on Blue Waters brought to light new features in these simulated storms that directly challenge long-held conceptual models of supercell morphology and tornado formation. A feature the research team dubbed the streamwise vorticity current that occurs in a part of the storm that has been long ignored by field meteorologists has been identified as playing a key role in tornado genesis and maintenance.

In new (began), the research team conducted a simulation study of a violently tornadic supercell, run at unprecedented scale and resolution. The simulation, requiring 20,000 Blue Waters nodes and one-quarter of a trillion grid zones, contains the genesis and maintenance of a long-track EF5-strength tornado exhibiting a multiple vortex structure. Novel techniques of visualization recently developed by the team combine volume-rendered imagery of vorticity and cloud field with the track of the tornado as manifest by ground-relative traces of the vorticity, velocity, and pressure fields. These tracks bear a striking resemblance to damage swaths found in nature, clearly showing the cycloidal paths of rapidly moving suction vortices embedded within the wide, wedge-shaped tornado.

RESEARCH CHALLENGE

Tornadoes are common in the United States, and the strongest tornadoes cause devastating damage and severe loss of life. Understanding the nature of the strongest tornadoes (rated EF4/E5 on the Enhanced Fujita Scale) is of great societal interest. A better understanding of these storms will help improve forecasting of the events and provide accurate, targeted warnings, thereby reducing the false alarm rate of the National Weather Service.

Thunderstorms that produce downbursts are also of interest to atmospheric scientists. While "dry" downbursts are relative-ly understood to be forced by the evaporation of rain in a deep, dry atmospheric boundary layer, "wet" downbursts, which are believed to be forced primarily by drag induced by falling rain and hail, are less understood.

METHODS & CODES

The team used the CM1 model, developed at the National Center for Atmospheric Research, for all three projects. One of the PIs, Leigh Orf, has written an I/O driver for CM1 and a set of tools to read data, called LOFS or the "lack of file system." LOFS is so named because it is a file-based file system that sits upon Lustre. Crucially, LOFS allows very high throughput of saved data; organizes it in an efficient, logical manner; and allows for the use of lossy compression on floating point data using ZFP. In addition, LOFS has a simple application programming interface for reading LOFS data directly as well as for converting it to the popular netCDF format, which can be used to share the data with colleagues as input for visualization tools.

RESULTS & IMPACT

Simulations of violently tornadic supercells (began). These simulations and the hours of high-definition animated video shared in near real time on YouTube have shaken up the field of mesoscale meteorology, directly challenging long-established conceptual models of supercells and tornadoes. The processes the research team has identified are novel, with one direct outcome of this work being a $2.3-million National Science Foundation-sponsored program (TORUS) to search for evidence of these features in the real atmosphere.

Quarter-trillion zone tornadic supercell simulation (began). As this simulation is not yet complete and was only recently integrated to its current state, results are preliminary. Video sequences showing high-definition animations of cloud and vorticity fields from a recent talk, shared on social media, have been viewed hundreds of thousands of times. The severe storms community is very aware of this work on Blue Waters, primarily through less highly resolved simulations covered in another Blue Waters allocation.

This new 10-meter simulation and the features that are resolved will be of significant interest to scientists and to the general public. Owing to its sheer size, it will take years to analyze these data; however, without Blue Waters, the simulation simply could not have been performed. The PIs efforts in data management and compression enable the data to be saved at very high temporal resolution; data will be analyzed using new techniques on GPUs on the next-generation Frontera machine and in-house GPUs.

Why BLUE WATERS

No other nonclassified machine available to U.S. scientists has Blue Waters’ capacity. In addition, NCSEA has been exceptional in terms of staff support, helping the team over seemingly insurmountable hurdles and keeping the machine in a healthy state.

PUBLICATIONS & DATA SETS


The geomagnetic field varies in time, mostly owing to the fluid motion in the Earth's outer core. Geomagnetic data assimilation can provide accurate estimates of the core state for fundamental research into such questions as the Earth's interior structure and its evolution. Geomagnetic data can also provide accurate secular variation (SV) forecasts for global geomagnetic models that are used for industrial and navigational applications. Accurate prediction of SV can be achieved via large-ensemble assimilation of geomagnetic observations and theoretical geodynamo models that investigate the self-sustaining process responsible for maintaining the Earth's magnetic field. However, this requires at least one thousand times more computing resources (in both CPU time and data storage) than those for pure geodynamo simulation, which alone is already computationally challenging. Blue Waters enables this research by reducing the research time from years to weeks and by increasing resolutions for geodynamo simulations with Earthlike parameters.

EXECUTIVE SUMMARY

The main objective of this project is to investigate the convergence of assimilation with different ensemble sizes and simulation resolutions for given physical parameters. In two months of work, the research team found that the ensemble size of approximately 256 is optimal for assimilation, based on the computational needs and the forecast accuracies. This result is very important as it establishes a quantitative correlation among the forecast accuracy requirements, computational resource needs, and time periods for progress. For example, with the spatial resolution of approximately 256 x 256 x 256, a single geodynamo simulation (i.e., an ensemble member of GEMS) could require a one-month (wall-clock) computation time with 256 processors/cores. Optimal ensemble sizes can greatly reduce the computational expense and research time without compromising research objectives. In addition, simultaneous 256-ensemble runs can make accurate forecasts of five-year geomagnetic SVs in one month that would otherwise require 20 years if the ensemble runs were limited to sequential executions (one member at a time).

WHY BLUE WATERS

Blue Waters provides the computing resources needed for the research team’s geomagnetic data assimilation research project. Further, the technical staff provide much-needed knowledge to improve and optimize GEMS.
MACHINE LEARNING FOR ERROR QUANTIFICATION IN SIMULATING THE CLIMATE IMPACTS OF ATMOSPHERIC AEROSOLS

Allocations: Innovation and Exploration/200 Ksh

PI: Nicole Riemer

1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

Atmospheric aerosol particles influence the large-scale dynamics of the atmosphere and climate because they interact with solar radiation, both directly by scattering and absorbing sunlight and indirectly by forming clouds. Current climate simulations use highly approximate aerosol models with large and unquantified errors.

To address this uncertainty, the PI applied a new ultra-high-detail spatially resolved and particle-resolved aerosol model, WRF–PartMC, which tracks size and composition information on a per-particle basis. The scientists then used its model output to train machine learning models to predict errors owing to a simplified representation of the aerosol. This allows error predictions merely on the basis of output from the simplified model without running a computationally expensive particle-resolved benchmark case. The scientific impact of this work is the development of a new, innovative method that changes the way aerosol impacts on climate are quantified in current regional and global climate models.

RESEARCH CHALLENGE

One of the largest uncertainties in global climate prediction involves aerosols and their impacts on the radiative budget, a topic of great societal relevance [1]. Aerosol interactions are influenced by both the size and composition of individual particles. Models provide important insights in the study of aerosols but experience a trade-off between the representation of physical and chemical levels. Each simulation models the complex aerosol dynamics and chemistry for on the order of 5 billion individual particles, where each particle is represented as a vector of masses of 20 aerosol species. Simulations of this size were previously unfeasible. Now that such simulations can be conducted, errors owing to aerosol representation can be quantified.

RESULTS & IMPACT

The PI conducted several particle-resolved simulations for the domain of northern California. The output will serve as training data for the machine learning portion of the project. These stochastic simulations utilize realistic source-resolved emissions, capable of modeling different emission sectors such as diesel vehicles, gasoline vehicles, and power plants, which all have complex aerosol composition. Each simulation was initialized for June 17, 2010, and simulated 24 hours, utilizing 6,656 cores and 12 wall-clock hours. Simulations consisted of 5,000 computational particles per grid cell with a domain size of 170 × 160 and 40 vertical levels. Each simulation models the complex aerosol dynamics and chemistry for on the order of 5 billion individual particles, where each particle is represented as a vector of masses of 20 aerosol species. Simulations of this size were previously unfeasible. Now that such simulations can be conducted, errors owing to aerosol representation can be quantified.

The mixing state parameter \( \chi \) varies from 0% to 100%, ranging from all particles containing a single species to 100%, where all particles are identical in composition. Fig. 1 shows relative error in CCN (cloud condensation nuclei) number concentrations as a function of mixing state parameter. Particle populations are projected to fully internally mixed populations, a common representation in other models. When particle populations are further from the model assumption of internally mixed (\( \chi = 100\% \)), models typically overestimate the number of CCN available for cloud formation. This has implications for cloud radiative properties that depend on droplet number and size.

WHY BLUE WATERS

Access to the computational power and storage space on Blue Waters allows for running simulations to produce data for machine learning. Simulations rely on sufficient memory per core to produce statistically powerful particle populations. Working alongside Blue Waters’ staff has alleviated a large portion of the performance issues regarding output by removing tiny writes of data and paying careful attention to what information is output. Reducing the cost of output allows more frequent output, which in turn provides more data for machine learning, as it requires the entire particle state.
EXECUTIVE SUMMARY

How the hydroclimate in Southwest North America will change in the future remains an open question. Although models generally predict an increase in climate extremes in this region with both more severe droughts and more intense precipitation events, large uncertainties remain. By studying the past, we can improve our understanding of the mechanisms driving current and future hydroclimate change in the area.

Records suggest that the hydroclimate of this region was drastically different during much of the last glacial cycle. However, the various mechanisms that produced these signals are difficult to deconvolve and continue to be debated. In this project, the research team employed a high-resolution, water isotope-enabled Earth System model for simulations of the last glacial maximum and preindustrial climates. The combination of water isotope tracers and high resolution allows for more direct comparison of the model outputs with the proxy records.

RESEARCH CHALLENGE

Southwest North America has proven to be climatically sensitive over the observational record. However, confidence in mode projections of that region’s climate is limited by an incomplete understanding of the complex interactions driving regional climate variability and the unprecedented nature of future climate perturbation [1,2]. To better understand the range of possible climates in Southwest North America and provide additional sources of model validation, researchers can look to the past. Fortunately, this region has been particularly well surveyed, with some of the densest and most diverse coverage of paleoclimate proxy records available in the mid-latitudes. Of the many proxy archives gathered in Southwest North America, measurements of δ18O (a measure of the ratio of stable isotopes oxygen-18 and oxygen-16) are particularly useful for understanding past climate variability. However, the various mechanisms that produced these δ18O signals are difficult to deconvolve and continue to be debated.

Comparisons between climate model outputs and cave records are difficult. One common limitation relates to the heterogeneity of the land surface. Many proxy sites, especially those located in Southwest North America, are found in topographically diverse regions that create drastically different microclimates within a few hundred kilometers. In contrast, climate models typically do not resolve such fine spatial scales (Fig. 1), which limits the utility of models for mechanistically understanding this unique climate proxy. Another limitation comes from the indirect comparison of model variables such as temperature and precipitation with the δ18O values found in the cave records. To overcome these common limitations of model–proxy comparison, the research team used a high-resolution, water isotope-enabled Earth system model to simulate the last glacial maximum (21,000 years ago) and preindustrial climates. These experiments shed light on the driving mechanisms behind the dynamic hydroclimatic changes that have been suggested in Southwest North America from more than a century of paleoclimate research.

METHODS & CODES

For this project, the team used the Community Earth System Model (CESM) with prognostic water isotope isotopeograpic tracking. CESM is a widely employed, Intergovernmental Panel on Climate Change-class Earth system model with the ability to accurately simulate preindustrial and present-day climates [3]. This version of CESM, known as cesm, can track 360 and 364 in atmosphere, ocean, land, and sea ice components. Previous studies demonstrated that the 360 and 364 distributions within this version of CESM compare favorably with other isotope-enabled models of similar complexity [4]. Further, this version of CESM can track the transport of water in the atmosphere, allowing for a precise understanding of the mechanisms responsible for changes in isotopic composition of precipitation [5]. Given the topographic heterogeneity of Southwest North America, the team will perform isotope-enabled atmosphere and land-only simulations at approximately 0.25° resolution using prescribed sea surface temperatures.

RESULTS & IMPACT

It is clear that further investigation is necessary to determine the most important mechanisms for driving the pattern of hydroclimatic change at the last glacial maximum. The combination of water isotope-enabled model experiments with speleothem records will allow the team to disentangle the influences of moisture source and transport, temperature, and precipitation amount on speleothem proxy records, an understanding that can be applied broadly to improve proxy interpretations across the region. From the results, the research group will be able to distinguish between several long-standing hypotheses of hydroclimatic change in Southwest North America at the last glacial maximum, including: (1) a southward-displaced Pacific jet stream [6], (2) a strengthening and meridional compression of the storm track [7]; (3) a thermodynamic control arising from a steepened humidity gradient [8]; and (4) an increase in moisture from a subtropical source [9]. Perhaps owing to increased contributions from atmospheric rivers [10]. These global simulations will also prove valuable for a wide range of paleoclimate questions. As the highest-resolution global simulations of the last glacial maximum ever performed, these outputs will be a valuable resource for the paleoclimate community and of particular interest to the paleoclimate model intercomparison project [11].

WHY BLUE WATERS

The large number of compute nodes on Blue Waters is ideal for these simulations. The combination of water isotope tracers and high resolution in CESM requires significant computing resources. Fortunately, CESM throughput scales well with a large number of processors. The research team expects high efficiency when employing well over 1,000 processors simultaneously per simulation. This research would not be possible without the computing power provided by Blue Waters.
IMPLEMENTATION AND USE OF A GLOBAL NONHYDROSTATIC MODEL FOR EXTENDED-RANGE WEATHER PREDICTION DURING THE RELAMPAGO FIELD CAMPAIGN

Allocation: Blue Waters Professor/240 Knh
PI: Robert J. Trapp

EXECUTIVE SUMMARY
The Model for Prediction Across Scales (MPAS) was implemented and then executed on Blue Waters during the RELAMPAGO (Remote sensing of Electrification, Lightning, And Meso-scale/microscale Processes with Adaptive Ground Observations) field campaign in 2018. MPAS is a new, nonhydrostatic weather and climate model that allows for local grid refinement. Because MPAS is also a global model, it is well suited for extended-range predictions, as was demonstrated by the four-day predictions made daily during the campaign. A configuration detail of particular relevance was the specification of 3-km gridpoint spacing over the entirety of South America, with 15-km gridpoint spacing elsewhere around the globe. The 3-km spacing is considered to be “convection permitting,” thus allowing for the explicit representation of thunderstorms over large domains.

Two other models were also employed for separate projects: the Weather Research and Forecasting (WRF) model, for studies of hail and tropical cyclones using a pseudo-global warming approach, and the Cloud Model 1 (CM1), for high-resolution idealized simulations of individual thunderstorms.

RESEARCH CHALLENGE
Thunderstorms and attendant phenomena such as hail, tornadoes, and extreme rainfall have high socioeconomic impact worldwide, thus motivating research to improve not only their predictions but also the understanding of their basic processes. One challenge is that their spatial and temporal scales are small relative to the scales of their meteorological forcing. To accurately predict and represent these storms and phenomena, an approach that can account for temporal scales ranging from days to seconds and spatial scales of thousands of kilometers to hundreds of meters is needed. In other words, very large geospatial domains that have fine gridpoint spacings and long-time integrations with high rates of model output are required. The Blue Waters allocation is providing the research team with the resources needed to achieve this level of simulation.

METHODS & CODES
The team used MPAS with the aforementioned hybrid 3-km/15-km grid configuration and the convection-permitting suites of physics parameterizations. The model was integrated daily for four-day periods, using initial (and lower-boundary) conditions from the Global Forecast System model. This was done for the 45-day duration of the field campaign. The team also employed two other models for separate projects: the WRF model, under a pseudo-global warming approach, and the CM1 model, for high-resolution idealized simulations of individual thunderstorms.

RESULTS & IMPACT
The team concluded, based on the 45-day experiment, that MPAS offers some skill in extended-range, South American forecasts at convection-permitting scales. It would appear that the implied predictability is provided in part by the significant terrain-associated forcing, including that owing to the Andes Mountains and the Sierras de Córdoba Mountains. The researchers did notice, in some cases, that the predictability actually appeared to degrade rather than improve over shorter integration lengths. This could possibly be associated with model spinup; efforts to understand and quantify this are underway.

In the non-MPAS efforts, the team completed the simulation work on tropical cyclones and hailstorms (WRF, pseudo-global warming), and idealized thunderstorm simulations (CM1). The latter simulations were used to examine the strong connections, within storms, between the physical sizes of vertical drafts (“updrafts” and “downdrafts”) and the depth of the pool of cool air generated through these drafts. These physical sizes have impacts on tornado intensity and, more generally, have implications on how convective storms are parameterized in coarse-resolution models.

WHY BLUE WATERS
The project staff provided tremendous assistance in helping to install the model and associated software on Blue Waters. The staff also set up a daily reservation for the model runs. Compared to other high-end high-performance computing resources, Blue Waters is incredibly stable and reliable, which ensured timely delivery of the daily forecasts.

REFERENCES


SIMULATING LARGE CALIFORNIA EARTHQUAKES BEFORE THEY OCCUR

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EXECUTIVE SUMMARY

The Southern California Earthquake Center (SCEC) used Blue Waters to develop the CyberShake probabilistic seismic hazard analysis (PSHA) method and to apply this method to all major urban areas in California. SCEC’s CyberShake [1] hazard models use detailed earthquake fault and seismic velocity models and high-performance software to calculate physics-based probabilistic ground motion forecasts. SCEC is actively collaborating with geo-scientific groups, national seismic hazard map developers [2], and civil engineering groups [3] to verify and validate the CyberShake California seismic hazard models for use in broad impact engineering and public seismic hazard applications and to apply the CyberShake method to other national and international regions.

RESEARCH CHALLENGE

PSHA earthquake forecast models [4] are the scientific basis for many engineering and social applications: performance-based design, seismic retrofitting, resilience engineering, insurance rate setting, disaster preparation and warning, emergency response, and public education. The U.S. Geological Survey (USGS) currently uses PSHA for promoting seismic safety engineering and disaster preparedness across the United States, including California, through its National Seismic Hazard Mapping Project [5]. During the last year, researchers with the SCEC used the high-performance computation capabilities of Blue Waters to calculate physics-based PSHA models for northern California to better understand earthquake hazards and to better inform civil engineering organizations as they develop earthquake-resistant societal infrastructure.

METHODS & CODES

The SCEC earthquake system science program requires a collection of interoperable earth models and open-source scientific applications including OpenSHA [6], UCM [7], Hecules [8], and ANP-ODC [9]. SCEC’s CyberShake seismic hazard model calculations use a workflow system based on HT–Concorde [10] and Pegasus–WMS [11] to perform large regional-scale seismic hazard studies. CyberShake extends existing PSHA methods to produce site-specific seismic hazard curves and other seismic hazard information such as duration of shaking, which is not available from earlier methods. In 2018, SCEC performed CyberShake Study 18.8, which used NCSEAS Blue Waters and OCF’s Titan to calculate PSHA hazard curves up to 1 Hz for 869 locations in central and northern California, producing a physics-based PSHA hazard model for a large Northern California region that includes the San Francisco Bay Area.

RESULTS & IMPACT

Regional PSHA hazard models are used by engineers, seismologists, and governmental organizations in building design, urban planning, community earthquake awareness, and disaster preparedness. During the last year, SCEC completed CyberShake Study 18.8, the first physics-based PSHA model for the San Francisco Bay region. This study used over 3.8 million Blue Waters node hours to calculate a PSHA seismic model for northern California, using deterministic wave propagation simulations in 3D seismic velocity models, combining estimates of hazard curves from 869 locations in California. CyberShake data products show the effects of basin structures and rupture directivity on hazard, improve upon standard attenuation-based methods of calculating seismic hazard, and identify research targets to further improve PSHA estimate accuracy. As a result, the scientific and computational advancements in CyberShake work can help reduce the total uncertainty in long-term hazard models, which has important practical consequences for the seismic provisions in building codes and especially for critical facility operators.

PSHA users including scientific, engineering, and government agencies such as the USGS are evaluating the new information provided by CyberShake results. For seismologists, CyberShake provides a framework to study interseismic physics of earthquakes, seismic ground motions, the interaction of fault geometry, 3D earth structure, ground motion attenuation, and rupture directivity. For governmental agencies responsible for reporting seismic hazard information to the public, CyberShake represents a new source of information that contributes to their understanding of seismic hazards, which they may use to improve the information they report. For building engineers, CyberShake represents a refinement of existing seismic hazard information that reduces some of the uncertainties in current empirical ground motion attenuation models.

CyberShake PSHA estimate simulations for Southern California are under review as inputs to a new Los Angeles urban seismic hazard map under development by the USGS [2]. The SCEC committee for Utilization of Ground Motion Simulations (UGMS) is working within the framework of the Building Seismic Safety Council activities to develop long-period, simulation-based response spectrum acceleration maps for the Los Angeles region. CyberShake acceleration maps are under consideration for inclusion in the National Earthquake Hazards Reduction Program and the American Society of Civil Engineers (ASCE) 7–10 Seismic Provisions, and for the Los Angeles City Building Codes. The UGMS group is using CyberShake simulations to quantify the effects of sedimentary basins and other 3D crustal structures on seismic hazard, information that is difficult to obtain with traditional empirical methods. The SCEC also used the California Earthquake Response Spectra Spectra project, which are being integrated into the ASCE Project 17 recommendations for tall building design [3].

WHY BLUE WATERS

SCEC used Blue Waters to perform large-scale, complex scientific computations involving thousands of large CPU and GPU parallel jobs, hundreds of millions of short-running serial CPU tasks, and hundreds of terabytes of temporary files. SCEC scientists and technical staff have worked closely with the Blue Waters staff to achieve a series of breakthroughs including integration of new physics into wave propagation software [12], optimization of production calculations using GPU code improvements [13], and optimization of the CyberShake runtime performance. Using the well-balanced system capabilities of Blue Waters’ CPUs, GPUs, disks, and system software, together with scientific workflow tools, SCEC’s research staff can now complete CyberShake calculations in weeks rather than months, improvements that were made during years of Blue Waters access and operations.

Blue Waters has enabled SCEC scientists to improve their seismic hazard methodology at a rapid pace.

PUBLICATIONS & DATA SETS


Figure 1: These maps show the CyberShake Study 18.8 model and compare the results to current standard methods based on ground motion prediction equations. This CyberShake seismic hazard model provides multiple layers of information that include hazard maps, hazard curves for selected sites, rupture models, seismic groups, and site-specific seismic intensity and shaking duration measurements.
MATERIALS SIMULATIONS IN GEOPHYSICS

Allocation: Innovation and Exploration/200 Ksh
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EXECUTIVE SUMMARY

Thermodynamics of materials is a fundamental subject for understanding planetary processes and states. The research team has contributed to the development and application of ab initio methods for computing thermal properties of minerals and their aggregates (rocks). Thermodynamic and thermoelastic properties and thermal conductivity are among the main properties needed for modeling thermal convection in and interpreting the seismic tomographic structure of Earth’s interior. Discovery of novel ultramafic and oxide phases at pressures (P) of tens of Mbar and temperatures (T) of approximately 104 K are also advancing understanding of the internal structure of recently discovered terrestrial-type exoplanets. Blue Waters has been used by the research group to perform high-throughput calculations of thermal properties of mineral phases required to model heat transport and interpret the 3D pattern of seismic wave propagation throughout the Earth’s mantle and the inner cores of Earth and terrestrial exoplanets.

RESEARCH CHALLENGE

Ab initio materials simulations for geophysics applications are intrinsically high-throughput calculations since materials properties need to be computed vs. P, T composition (x), strain (ε), atomic configuration, and the like. Such simulations are essentially a “phase space” sampling problem. Mineral phases are structurally and chemically complex, consisting of solid solutions with multiple components, including strongly correlated ones such as FeO, Fe2O3, etc., with primitive cells containing tens of atoms. In addition to properties of single phases, properties of polycrystalline aggregates—rocks—in thermodynamic equilibrium must also be addressed. The thermodynamic equilibrium problem in a multiphase system with multiple components, a challenge of its own, can only be addressed after thermodynamic properties of single phases are accurately obtained. To facilitate these HPC (high-performance computing) calculations, novel methods and workflows have been developed and implemented on Blue Waters for the calculations of single-phase thermal properties.

METHODS & CODES

[Two novel methods based on the phonon quasiparticle concept [1] have been implemented and used on Blue Waters. The first is for computation of lattice thermal conductivity, κlat, and the second for computing thermal properties of anharmonic systems, both in the thermodynamic limit (N → ∞, with N = number of atoms). Molecular dynamics (MD) is first used to obtain phonon quasiparticle properties, i.e., phonon lifetimes (τi) and temperature-dependent phonon frequencies (ωi(T)) at few-phonon wave vectors. Novel interpolation schemes are then used to obtain quasiparticle properties throughout the Brillouin zone (a uniquely defined primitive cell in reciprocal space), which are then used in conjunction with the Boltzmann transport equation (BTE) to compute κlat. Temperature-dependent phonon dispersions are also used to compute thermodynamic properties for weakly or strongly anharmonic systems in the thermodynamic limit. The alternative approach is thermodynamic integration, which carries uncertainties limited to related simulation cell sizes.

RESULTS & IMPACT

Applications of these methods on Blue Waters are illustrated here for two problems. The first is the calculation of κlat in CaSiO3 perovskite (Ca-Pv), an important phase (up to 10 vol%) of the Earth’s lower mantle and a major phase in basaltic crust (approximately 25 vol%). Ca-Pv exists in the cubic structure in Earth’s lower mantle. At low temperatures (T ≈ 700 K) it is mechanically unstable and becomes tetragonal. Calculations and measurements of its properties at relevant conditions (T > 2000 K and P = 23 GPa) have been highly controversial because of its strongly anharmonic nature, preventing calculations of lifetime using perturbation theory and of κ using BTE. Fig. 1 shows calculated (LDA) values compared to a single experimental data point obtained by collaborators (see Fig. 1 caption). Experiment verification of these results, still underway, is important because of the novelty of the approach and because Ca-Pv’s κlat is three times larger than that of Mg-Pv, the mantle major phase. This result will change the estimated values of κlat in the lower mantle by up to 20% to 30%, with profound implications for convection style in the Earth, heat extraction from the core, and the age of Earth’s inner core.

The second problem is the calculation of thermal properties and high-T ab initio equations of state of e-iron, the solid phase of iron expected to exist in planetary cores. These calculations provided T-dependent phonon dispersion, which were subsequently employed to compute thermodynamic properties using a novel method [1] based on the phonon gas model. In metallic e-iron, electron thermal excitations and not anharmonicity are the main source of T-dependent phonon frequencies. These calculations were carried out up to 14 Mbar; a condition achieved only at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory. Temperature in the NIF data (Fig. 2) is expected to follow an adiabat. The research team’s adiabatic equation of state agrees well with the NIF data up to 4 Mbar, deviating at higher pressures. This result suggests the unknown temperature in the NIF data might not quite follow an adiabat, with a cumulative effect causing deviations from adiabaticity in wide pressure ranges.

WHY BLUE WATERS

Such calculations require the execution of large numbers (approximately 103 to 105) of HPC tasks (approximately 10 nodes each). The large number of Blue Waters’ nodes allows the execution of independent tasks simultaneously. This is important for efficient execution of workflows with subsequent stages, each requiring the execution of large numbers of tasks that have dependencies across but are independent within different stages.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

This research aims to reduce key uncertainties in quantifying the impact of atmospheric aerosol particles on the Earth’s climate. Aerosol particles can be brought into the atmosphere by a wide range of anthropogenic activities (resulting from the influence of human beings on nature) or by natural sources. They profoundly impact the large-scale dynamics of the atmosphere because they interact with solar radiation by scattering and absorbing light and by forming clouds. These impacts depend on the composition and size of the particles.

The uncertainties in quantifying these impacts originate from scale interactions and the high computational cost of modeling them. To tackle this problem, the research team developed the particle-resolved 3D model WRF–PartMC, which has the unique ability to track size and composition information at a per-particle level. Particle-resolved simulations require efficient numerical algorithms and a computational resource with the capability to simulate the composition and size of the particles aggregate because they coagulate with each other during transport. For each grid cell in the model domain, it is then possible to construct the full mixing state of the aerosol population as well as the full source apportionment profile.

METHODS & CODES

To overcome the current limitations in representing aerosols and associated uncertainties, the particle-resolved model PartMC–MOADIC [3] was coupled to the state-of-the-art 3D Weather Research and Forecasting (WRF) model [4]. Aspects of these two models complement each other. A box model PartMC–MOADIC is a highly detailed aerosol model that tracks the size and composition of individual particles in the atmosphere but is unable to resolve spatial heterogeneities of aerosol populations. The 3D regional WRF model is an advanced numerical weather model that captures the transport of chemical species in the atmosphere but assumes a crudely simplified aerosol representation. The resulting WRF–PartMC model uses a 3D Eulerian grid for the atmospheric flow, while explicitly resolving the evolution of individual aerosol particles per grid cell.

RESULTS & IMPACT

Aerosol modeling is challenging because of the multiscale nature of the problem: the macroscopic aerosol impact on climate is determined by micrometeorological processes on the particle scale. The innovation of the WRF–PartMC model consists of representing many of these micrometeorological processes explicitly on a per-particle level, which allows for an improved process-level simulation of the key interactions among aerosols, clouds, and radiation. WRF–PartMC is the only model of its kind, and this research is changing the field of aerosol science because it provides the first benchmark for more approximate models commonly used in the field. It also provides a basis for rigorous coarse-graining to develop physically robust parameterizations for use in largescale models. By simulating at a much higher level of detail, particle-resolved models can help close the gap in understanding the effects of modeling choices in global models. Regional-scale particle-resolved simulations allow the quantification of the spatial heterogeneity that determines the conditions where highly detailed aerosol composition is necessary. This next-generation model captures the complex aerosol composition that current-generation models are unable to simulate.

The research team produced findings from a particle-resolved aerosol simulation for a realistic, spatially resolved three-dimensional domain in California, USA. Aerosol and trace gas emissions were taken from the 2011 National Emission Inventory [5], and the meteorology corresponded to June 17, 2010, which coincides with the Carbonaceous Aerosol and Radiative Effects Study field campaign conducted during May–June 2010. On the order of 50 billion computational particles were tracked in this simulation, including their compositional changes owing to gas-to-particle conversion, their coagulation events, and their transport by both the wind and turbulence. The simulation was run over 6.636 cores. Most of the compute time was spent on particle coagulation and dynamic gas-particle partitioning on a per-particle basis.

Fig. 1 shows an example of the level of detail that can be obtained by WRF–PartMC for a simulation in California. In such a model run, the team is simulating the complex aerosol dynamics and chemistry for about five billion individual particles. For any given particle in the simulation, its chemical composition and the sources of the constituent particles that it is composed of (particles aggregate because they coagulate with each other during transport) are stored. Next, the full mixing state of the aerosol population as well as the full source apportionment profile can be constructed for each grid cell in the model domain.

The full aerosol particle state allows for investigating of the spatial and temporal distribution of the mixing state parameter $\chi_{CCN}$ at 06:00 LST (Local Standard Time) and 18:00 LST on June 17, 2010. The mixing state parameter $\chi_{CCN}$ represents the extent that hydrosol (tending to fail to mix with water) and hydrophilic (tending to mix with water) species are internally mixed. At 06:00 LST, these components remain mostly externally mixed with exceptions in the vicinity of urban areas and roadways. At 18:00 LST, $\chi_{CCN}$ increased and is more spatially homogeneous. This indicates that the hydrosol and hydrophilic material is becoming more internally mixed over the course of the day. The WRF–PartMC model allows for the full evolution of the aerosol mixing state, unlike traditional models. WRF–PartMC model results have been used to benchmark these more simplified models and evaluate the error incurred in models owing to simplifying assumptions.

WHY BLUE WATERS

Access to Blue Waters allows for a cutting-edge model formulation that pushes both science and computing by combining the large-scale features of state-of-the-art 3D models with the process-level physical representation of box models. Modeling 3D domains on the order of 100 billion tracked particles creates computationally intensive equations per particle and memory requirements to track high-dimensional and multiscale particle populations. To enable simulations of aerosols at both a high spatial and compositional resolution, there is a need for tens of thousands of cores, fast interconnections among those cores, and sufficient memory per process.

Access to the Blue Waters staff was essential for addressing issues regarding the I/O challenge of outputting billions of particle, their chemical composition, and physical properties. Discussion and suggestions of how to change the model output code led to a two-orders-of-magnitude reduction in the time required to generate output. This reduced output as a bottleneck to code performance.
EXECUTIVE SUMMARY

This study investigates the effects of the changing twenty-first century climate on human health by evaluating projected effects on air quality exceedance events, focusing on particulate matter (PM$_{2.5}$) and ozone (O$_3$). The research team employed fully coupled global climate–chemistry modeling analyses using the Blue Waters system to simulate the historical and future time periods for multiple scenarios. The focus was on the United States, India, and China. The frequency of exceedance events increased in India for both scenarios and the resulting changes in climate, but the United States and China showed improvement in the lower-emissions scenarios. The researchers also examined an ideal clean energy scenario, where mid-century fossil fuel emissions are reduced to zero. By eliminating the burning of fossil fuels, both PM$_{2.5}$ and O$_3$ concentrations reduce by 20% to 60% in high-pollution regions, greatly reducing future health risks.

RESEARCH CHALLENGE

Many studies have shown that projected climate change could affect air quality, but there is little known about the resulting effects on health. One way to look at health effects is to consider exceedances set by environmental policy for upper limits of exposure. The objectives of this study are to better understand how global changes in climate and emissions will affect air quality, focusing on particulate matter and ozone; to project their future trends; to quantify key source contributions; and thus provide actionable information for environmental planners and decision makers to design effective dynamic management strategies, including local controls, domestic regulations and international policies to sustain air quality improvements in a changing world. The research team applied a state-of-the-science dynamic prediction system that couples global climate–chemical transport models to determine the individual and combined impacts of global climate and emissions changes from the present to 2050 under multiple scenarios. The team has conducted three primary experiments using the dynamic prediction system: (1) historical simulations for the period 1990–2015 to establish the credibility of the system and define the process-level understanding of U.S. regional air quality; (2) projections for the period 2030–2060 to quantify individual and combined impacts of global climate and emissions changes under multiple scenarios; and (3) sensitivity analyses to determine future changes in pollution sources and their relative contributions from anthropogenic and natural emissions, long-range pollutant transport, and climate change effects. The advanced state of the prediction system will produce a more complete scientific understanding of the challenges from global climate and emissions changes imposed on air quality management and a more reliable projection of future pollution sources and attribution changes.

METHODS & CODES

The research uses a state-of-the-science approach for advancing quantitative knowledge of the impacts of global changes in climate and emissions on U.S. air quality. The team used CESM1.2 default emissions, which represent surface emissions of approximately 30 species of speciated aerosols. The surface emission of each species is composed of all possible sources of emissions, including those from biomass burning, domestic sources, transportation, waste treatment, ships, industry, fossil fuels, and biofuels, and were composed from POGT, REAS, GFEDv3, and FINN emissions databases [1,2]. The results from the runs done using the current allocation have been presented at scientific conferences.

RESULTS & IMPACT

The research team used the long-term climate chemistry runs done as a part of this project to examine exceedances for surface ozone and particulate matter concentration for two different climate projections using the lower emissions RCP4.5 and the higher emissions RCP8.5 scenarios. The results from two 20-year time periods in the future (2031–2050) were compared with the historical 25-year period (1990–2014). Cumulative distribution functions of surface ozone and particulate matter concentration and trend analysis of exceedance events annually and seasonally were analyzed over three major regions: the United States, India, and China as well as megacities within them. The results show that the frequency of exceedance events for ozone increases significantly at 90% confidence interval in India for both of the climate scenarios and in China for the high climate scenario, but decreases in the future in US especially western US and in China under RCP4.5 scenario. Along with the overall increase in ozone exceedance events, the study also showed a significant shift in seasonality of the events, with the number of episodes increasing during colder months, although ozone has primarily been considered as a summer problem. Unlike ozone, particulate matter concentration showed a significant increasing trend in all the regions in the future, with an overall increase in the number of particulate matter exceedance events annually.

As a part of the project, the research team also looked at a clean energy scenario and its impact on air quality in the mid-century. In this hypothetical scenario, emissions owing to fossil fuel are reduced to zero from 2050 in order to study the impact of a non-fossil fuel-based energy system. The study showed a significant reduction in concentration of both ozone and particulate matter in all the current global hotspots, with a reduction of 20% to 60% in most high-pollution regions.

WHY BLUE WATERS

The computational demand of high-resolution climate models used in this project is extensive, particularly the fully coupled model of the Earth’s climate system with chemistry. Blue Waters, with its petascale-class computational resources, large number of nodes, and storage capability for the output from high-resolution model simulations, was essential for the project. Blue Waters’ staff have been critical in figuring out the various issues arising with the long-term, fully coupled climate chemistry runs using the Community Earth System Model (CESM). Staff members have also helped figure out and resolve various issues with the CESM1.2.2 models. In short, Blue Waters has given the team the computational resources, data management, and staff support to perform this research.

PUBLICATIONS & DATA SETS


SENSITIVITY OF ARCTIC SEA ICE THICKNESS DISTRIBUTION TO SEA ICE INTERNAL DYNAMICS IN A CHANGING CLIMATE

EXECUTIVE SUMMARY

Changes in sea ice are a critical indicator of the climate system state. However, uncertainties exist in understanding, simulating, and predicting sea ice thickness distributions in the Arctic Ocean. In particular, the drastically thinned sea ice and more frequently occurring intense storms might have dramatically changed sea ice dynamic properties and air–ice momentum flux, raising further challenges to reducing the uncertainties. By conducting sensitivity experiments using the coupled sea ice–ocean component of the Community Earth System Model, the research team examined the interactive process between sea ice internal dynamics and thickness distribution. The results suggest that sea ice thickness distribution is highly sensitive to the treatment of its internal force in collaboration with air–ice momentum flux. A decrease in ice strength causes more energy conversion to potential energy, leading to an increase in the ridging process and thickness but a decrease in export via the Fram Strait. A decrease in air–ice momentum flux, however, demonstrates the opposite effect.

RESEARCH CHALLENGE

Arctic sea ice thickness is nonuniformly distributed in space, resulting from the complex interactive processes of dynamic and thermodynamic forcings across atmosphere, sea ice, and ocean interfaces and within sea ice itself. The realistic simulation and understanding of sea ice thickness distribution have been longstanding challenges. Along with amplified warming in the Arctic Ocean, dynamic and thermodynamic forcings across the atmosphere and sea ice interfaces have experienced pronounced changes. In particular, intense storms have more frequently occurred in the Arctic Ocean [3], causing even larger fluctuations or changes of atmospheric forcings on underlying sea ice. All of these further complications of how sea ice internal dynamics influence sea ice thickness distribution in the context of a changing climate and, in turn, contribute to the large-scale Arctic sea ice and climate system changes.

METHODS & CODES

The coupled sea ice–ocean component model of the National Center for Atmospheric Research's Community Earth System Model was employed to conduct 25 sensitivity experiments with prescribed different sea ice strengths. The model experiments were initialized using the Polar Science Center hydrographic climatology data [2] and forced by the monthly mean climatological forcing data constructed from the ERA-Interim reanalysis data set [1]. Each experiment covered a period of 100 years, allowing the sea ice and upper ocean to reach a quasi-equilibrium state.

RESULTS & IMPACT

Through examination and comparison of the results from the sensitivity experiments, the PI found that sea ice thickness distribution and sea ice motion are highly sensitive to perturbed sea ice strength prescribed in the model in collaboration with different air–ice momentum fluxes. Using a default sea ice strength defined as the ratio between total sea ice energy loss and total energy changes, thick sea ice occurs along the Canadian Archipelago and greatly decreases toward the central Arctic Ocean and Eurasian Arctic shelf seas. As a result, there is an increase in total sea ice volume for the entire Arctic Ocean throughout the year. All of these changes can be attributed to an enhanced conversion of kinetic energy to potential energy to build up sea ice ridges instead of frictional loss and a decreased sea ice export via the Fram Strait. When sea ice strength decreases, sea ice thickness largely increases from the Canadian Archipelago to the Eurasian Arctic shelf seas. As a result, there is an increase in total sea ice volume for the entire Arctic Ocean throughout the year.

To further investigate the upscaling impacts of the small-scale sea ice internal dynamics on shaping basinwide sea ice thickness distribution, the PI implemented tracers at the beginning of the model experiments with two of them in the Beaufort Sea: one in the East Siberian Sea and the other in the Laptev Sea. The PI then identified the pathways of the tracers, showing the origins of the tracked sea ice and its variation along the paths. The results indicate that decreased sea ice strength or increased air–ice momentum flux cause a clockwise rotation of the ice transpolar drift, resulting in a decrease in sea ice export via the Fram Strait and, therefore, an increase in the basinwide sea ice thickness. In contrast, counterclockwise rotation of the sea ice transpolar drift leads to less sea ice circulation and accumulation in the central/western Arctic, increasing sea ice export via the Fram Strait.

WHY BLUE WATERS

Blue Waters provided a unique opportunity to conduct model experiments at an ultrahigh resolution. Dynamic processes associated with sea ice thickness occur at small spatial and temporal scales. The only way to solve these problems with higher accuracy is through model simulation at superhigh resolutions. Furthermore, high resolution simulations also improve the understanding of upscaling impacts on basin scale sea ice thickness distribution. In addition, synoptic-scale intense storms and the resulting large fluctuation of forcings occur at small spatial and temporal scales. The state-of-the-art climate modeling studies generally do not take this into account. The Blue Waters system and staff paved the way for successful implementation of these model experiments.

PUBLICATIONS & DATA SETS


L. Peng and X. Zhang, “Modeling study on sensitivities of Arctic sea ice thickness distribution to momentum flux and ice strength,” to be submitted, 2019.
PHYSICS & ENGINEERING

FLUIDS

MATERIALS

NANOTECHNOLOGY

NUCLEAR ENGINEERING

NUCLEAR PHYSICS

PARTICLE PHYSICS

QUANTUM PHYSICS

SOLIDS & STRUCTURES

120 The Mechanism of Proton Diffusion in ABO₃ Perovskite Oxides
122 Identification of Amino Acids with Sensitive Nanoporous Mem, Toward Machine Learning-Based Prediction
124 Transfer-Learning-Based Coarse-Graining Method for Simple Fluids, Toward Deep Inverse Liquid-State Theory
126 High-End Visualization of Coherent Structures and Turbulent Events in Wall-Bounded Flows with a Passive Scalar
128 Design of Atomically Precise Nanoscale Negative Differential Resistance Devices
130 Using OpenMP Offloading to Run Code on Blue Waters’ GPU Nodes
132 Numerical Investigation of Turbulence Suppression in Rotating Flows
134 An Efficient Method for Hypersonic Laminar–Turbulent Transition Prediction
136 Quantum Simulations: Properties of Dense Hydrogen
138 Role of Interfaces on the Shear Strength and Bonding Properties of van der Waals Two-Dimensional Materials
140 Atypically Entangled Phases and New Methods for the Quantum Many-Body Problem
142 Direct Numerical Simulation of Pressure Fluctuations Induced by Supersonic Turbulent Boundary Layers
144 The Anomalous Magnetic Moment of the Muon: An Improved Ab Initio Calculation of the Hadronic Vacuum Polarization Contribution
146 Accelerating Thermoelectric Materials Discovery via Dopability Predictions
148 Machine-Learning Turbulence Models for Simulations of Turbulent Combustion
150 Turbulence-Resolved Modeling of Oscillatory Boundary Layer Flows
152 Machine Learning for Particle Physics: Employing Deep Learning for Particle Identification and Measurements at Colliders
154 Molten-Salt Reactors and Their Fuel Cycles
156 A Novel Crystal Structure with Spin-Protected Surface Electronic Conduction
158 Inertial Collapse of Individual Bubbles near Solid-Free Boundaries
160 Electronic Structure of Microscale Dielectric Barrier Discharges
162 Accelerating Virtual Prototyping and Certification in the Aerospace Industry with Scalable Finite-Element Analysis
164 Graphene Nanopore Transistor for DNA-Nick Detection
166 Compressibility Effects on Spatially Developing Plane Free Shear Layer
168 Outwardly Propagating Turbulent Flames
170 Deep Learning for Higgs Boson Identification and Searches for New Physics at the Large Hadron Collider
172 Designing Quantum Logic Gates on Silicon Chips with Large-Scale Multiphysics Simulations
174 Simulation of Rotating Detonation Engines
176 Mapping Proton Quark Structure: Looking Inside the Proton—How Do Quarks Spin?
178 Electron Dynamics of Ion-Irradiated Two-Dimensional Materials
180 Discovery of New Planar Materials via High-Throughput Machine Learning
184 Investigation of Sediment Transport Through Aquatic Vegetation Using Large-Scale High-Fidelity Turbulence Simulations
186 Machine Learning-Assisted High-Throughput Computational Design of Solvents for Liquid-Exfoliation
188 High-Throughput Materials Modeling Optimization
190 Detecting Neurotransmitters with DNA-Wrapped Nanotube Sensors
192 Accurate Effective Interactions in Quantum Materials
194 Supersonic Jet Noise Prediction Using High-Order Large Eddy Simulation
196 Spin Spirals in Multiferroic Bismuth Ferrite and at Metal Surface: From Fully First Principles
198 Numerical Simulations of a Collapsing Caviation Bubble Near an Elastically Deformable Object
200 Numerical Study on Shock Wave–Boundary Layer Interaction and Its Control
202 Free-Surface Flow Modeling of Multiple Tidal Turbines
204 New Insights on Intermittency and Circulation Statistics Obtained from a Massive Turbulence Simulation Database
206 Effects of Surface Defects on Hydrophobicity at Rare-Earth Oxide Interfaces Using Molecular Dynamics Simulations Driven by Ab Initio-Based Deep Neural Network Potentials
208 Constraining the Properties and Interactions of Dark Matter
THE MECHANISM OF PROTON DIFFUSION IN ABO₃ PEROVSKITE OXIDES

EXECUTIVE SUMMARY

Perovskite oxides (ABO₃) are well-known proton conductors. However, the role of the A-site ion on proton diffusion in perovskite oxides is not clear. By performing detailed density functional theory (DFT) calculations, the PI investigated the effect of A ion vacancy on proton transfer in yttrium-doped BaZrO₃, which is one of the widely studied perovskite oxides.

The study showed that the presence of A ions reduces the barrier for local lattice deformations and proton transfer from one oxygen to another. Both these motions are strongly coupled to lattice deformations. The PI identified the key physical mechanisms and the energy barriers associated with both hydroxide rotation and proton transfer by performing nudged elastic band (NEB) calculations. Finally, the PI calculated the bond strength instead of, for example, the BO₃ structure with BO₆-octahedrons.

Clear insights may be obtained by analyzing the role of A-site ions on the origin of activation energy of proton diffusion in perovskite oxides. The study showed that the presence of A ions reduces the bond strength between O and B ions, thereby reducing the energy barrier for local lattice deformations.

RESEARCH CHALLENGE

Although the proton transport mechanisms in perovskite oxides have been explored [1–5], the mechanisms governing the lower activation energy of proton diffusion in perovskite oxides remain unclear. Therefore, the design and development of novel proton-conducting solid oxide electrolytes with high conductivity remain a significant challenge. In addition, another key question that has not been addressed regarding proton transport in perovskite oxides is the role of A-site ions on proton diffusion; i.e., why do good proton conductors have the ABO₃ perovskite structure instead of, for example, the BO₃ structure with BO₆-octahedrons?

Based on DFT calculations, the origin of activation energy of proton transfer and hydroxide ion rotation were revealed. Specifically, the outward O–B–O bending and A ion motions and hydroxide ion reorientation govern the hydroxide ion rotation process while the inward O–B–O bending motion and donor oxygen—proton—acceptor oxygen interactions govern the proton transfer process. The presence of A ions reduces the bond strength between O and B ions, thereby reducing the energy barrier for local lattice deformations such as the O–B–O bending motion. In addition, the presence of A ions decreases the bonding strength of protons with acceptor oxygen and increases the bonding strength of protons with donor oxygen, promoting proton motion from donor oxygen to acceptor oxygen. This work provides a thorough atomistic understanding of the role of A-site ions on proton diffusion in perovskite oxides and the results can enable design and discovery of novel materials with improved proton diffusion properties.

METHODS & CODES

All DFT calculations were performed using the Vienna Ab initio Simulation Package [7–9]. The Perdew–Burke–Ernzerhof [10] exchange-correlation functional was employed based on the projector augmented-wave method [9]. The cutoff energy for the plane-wave basis set was 500 eV for all calculations, which were nonspin polarized. The migration energy barriers were calculated using the climbing-image nudged elastic band method [11].

RESULTS & IMPACT

Based on DFT calculations, the origin of the activation energy of proton transfer and hydroxide ion rotation were revealed. Specifically, the outward O–B–O bending and A ion motions and hydroxide ion reorientation govern the hydroxide ion rotation process while the inward O–B–O bending motion and donor oxygen—proton—acceptor oxygen interactions govern the proton transfer process. The presence of A ions reduces the bond strength between O and B ions, thereby reducing the energy barrier for local lattice deformations such as the O–B–O bending motion. In addition, the presence of A ions decreases the bonding strength of protons with acceptor oxygen and increases the bonding strength of protons with donor oxygen, promoting proton motion from donor oxygen to acceptor oxygen. This work provides a thorough atomistic understanding of the role of A-site ions on proton diffusion in perovskite oxides and the results can enable design and discovery of novel materials with improved proton diffusion properties.

WHY BLUE WATERS

This project required large-scale ab initio simulations to obtain the origin of activation energy of proton diffusion in solid oxides. For the DFT calculations, using eight to 10 nodes (256 to 320 cores) for each job can achieve the best performance, which is attributed to the power of Blue Waters and the support of project staff. Thus, running ab initio simulations on Blue Waters was easy and quick, speeding up the research greatly.

PUBLICATIONS & DATA SETS

IDENTIFICATION OF AMINO ACIDS WITH SENSITIVE NANOPOROUS MoS$_2$: TOWARD MACHINE LEARNING-BASED PREDICTION

EXECUTIVE SUMMARY

Identifying a chain of amino acids can enable breakthrough advances in early diagnosis of disease and the health status of the human body. Many diseases, including cancer, diabetes, and digestive disorders, are caused by malfunctioning ribosomes leading to defective proteins. Therefore, sequencing an amino acid chain helps diagnose diseases at early stages.

In this study using petascale-based molecular simulations with a total aggregate simulation time of 66 microseconds ($\mu$s), the researcher demonstrated that a nanoporous single-layer molybdenum disulfide (MoS$_2$) can detect individual amino acids in a polypeptide chain with high accuracy and distinguishability. With the aid of machine learning techniques, the PI featurized and clustered the ionic current and residence time of the 20 amino acids and identified the fingerprints of the signals. In addition, using advanced machine learning classification techniques, the PI was able to predict the amino acid type of over 2.8 million hypothetical sensors.

METHODS & CODES

Molecular dynamics (MD) simulations were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS). LAMMPS is an open source classical MD code for simulation of liquid, solid, and gas phases. The LAMMPS-based simulations involved three different interatomic potentials: Tersoff potential, Lennard–Jones potential, and long-range Coulombic via particle–particle particle–mesh. Each simulation box contained about 32,000 atoms consisting of a monolayer MoS$_2$, an amino acid chain, water molecules, and ions. The amino acid chain was pulled through the nanopore using an external force. Fig. 1 shows a polypeptide chain translocating through the nanopore of MoS$_2$.

RESULTS & IMPACT

This study has shown that a single-layer MoS$_2$ nanopore can detect individual amino acids in a polypeptide chain with high accuracy and distinguishability. Using extensive MD simulations (with a total aggregate simulation time of 66 $\mu$s) the ionic current and residence times of each residue of amino acid types was characterized and featurized. The amino acids were clustered into different groups based on their physical properties (e.g., size, polarity, and hydrophobicity). In addition, the type of amino acid was classified using machine learning techniques for any future ionic current and residence time sensor readings. Logistic regression, nearest neighbor, and random forest machine learning classifiers resulted in the prediction of amino acid types with an accuracy of 72.45%, 94.55% and 99.6%, respectively.

WHY BLUE WATERS

This project involved 4,103 extensive MD simulations with up to 50,000 atoms and an aggregate simulation time of 66 $\mu$s. These expensive computations would not have been possible without a petascale supercomputer. Also, the LAMMPS MD package scales almost linearly with the number of cores up to 100 on Blue Waters.

PUBLICATIONS & DATA SETS


Figure 1: A snapshot of proline polypeptide translocation through the MoS$_2$ nanopore.
EXECUTIVE SUMMARY

Machine learning is an intriguing method to circumvent difficulties faced with the development and optimization of force field parameters. In this project, a deep neural network (DNN) was used to solve the inverse problem of the liquid-state theory—particularly, to find the relationship between the radial distribution function (RDF) and the Lennard–Jones (LJ) parameters at various thermodynamic states. Using molecular dynamics (MD), many observables, including RDF, are uniquely determined by specifying the interatomic potentials. However, the inverse problem (e.g., determining the potential using a specific RDF) is not feasible through MD simulations unless it is combined with a complementary method.

In this project, the PI developed a framework integrating DNN with 1.5-terabyte MD trajectories (26,000 distinct systems and a total simulation time of 52 microseconds) to predict LJ parameters. The results show that DNN was successful not only in parameterization of the atomic LJ liquids but also in parameterizing the potentials for coarse-grained models of multiamolecule molecules.

RESEARCH CHALLENGE

The Lennard–Jones (LJ) potential form is one of the widely used interatomic potentials to study atomistic systems [1]. By specifying the potential parameters and the thermodynamic state, MD can compute various quantities of interest such as the radial distribution function (RDF). However, given a specific RDF, MD cannot directly predict the potential parameters; i.e., the inverse problem is considered a difficult task [2]. As per Henderson’s theorem [3], the relationship between the pair potential and RDF is unique at a given thermodynamic state, implying that the potential parameters can be determined uniquely based on the RDF.

In this work, the PI explored the feasibility of force field development based on Henderson’s theorem with a data-driven and deep learning-based approach. This inverse problem can also be viewed as a coarse-graining problem where the objective is to develop a pair-potential between coarse-grained particles such that the RDF of the original system is reproduced. While different frameworks such as the fundamental measure theory and integral equations have been developed to address this problem, both accuracy and generalizability to more complex systems are still issues. Alternatively, reproducing a given RDF relies on MD to refine the potential parameters. For example, MD data are either integrated with a theoretical framework (e.g., iterative Boltzmann inversion) or used to optimize statistical errors with given RDFs (e.g., simplex and relative entropy). These approaches require thousands of simulations for a specific system and the data are often not reused.

The main bottleneck in reusing data to parameterize a new system originates from the complexity of physics-based model development and long-term storage of the data. To overcome these issues, recent data-driven approaches, known as the physics of data, have emerged. Machine learning is one of the key physical inverses, primarily due to access to parallel resources and parallelization. However, the efficiency of machine learning relies on access to the XK nodes on Blue Waters. Similarly, deep learning is a good coarse-graining strategy as it performs well in the total variation of the RDF), the PI concluded that deep learning is a good coarse-graining strategy as it performs well on both metrics.

WHY BLUE WATERS

This project involved 40,000 MD simulations of up to 10,000 atoms with a total simulation time of 52 microseconds. The feasibility of such computations is a result of the petascale resources and GROMACS’ linear scaling on Blue Waters. Similarly, deep learning training using the TensorFlow module of Python relies heavily on access to the XK nodes on Blue Waters. Various neural network architectures were tried on Blue Waters (over 10 million training iterations) to select the optimized network and to avoid overfitting and underfitting.

METHODS & CODES

The PI performed MD simulations using the GROMACS package (GROMACS). GROMACS uses the well-known LJ potentials with the Verlet algorithm. The deep learning model development was performed using TensorFlow on Blue Waters. Fig. 1 shows the workflow of the data generation, training, inference, and assessment phases.

RESULTS & IMPACT

The PI assessed the performance of DNN by considering two cases. First, he investigated the generalizability and transferability of the interatomic potential for LJ particles (development of atomistic force fields for single-atom particles). Second, he considered transfer learning for coarse-grained (CG) force-field development. Generalizability points to using DNN to predict potential parameters for LJ particles for a given thermodynamic data set. Transferability refers to using DNN to estimate potential parameters with thermodynamic states outside the training data set. Transfer learning refers to the use of DNN to estimate potential parameters for CG representation of simple multiamolecule molecules.

Fig. 2 compares the predicted DNN and the ground truth potential parameters used in the MD simulations. All the points are distributed almost uniformly around the one-to-one mapping line (the line on which the ground truth and DNN parameters match exactly). While the thermodynamic states and RDFs vary for each point, the DNN is able to relate them correctly to the underlying potential parameters. The DNN results for the LJ particles exhibit no more than 4.4% mean absolute percentile error in the total variation of the RDF), the PI concluded that deep learning is a good coarse-graining strategy as it performs well on both metrics.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Despite the chaotic behavior of turbulence, investigations performed during the last six decades have conclusively demonstrated the presence of organized motions called “coherent structures” in turbulent boundary layers, which are responsible for transporting most of the turbulent kinetic energy. Investigations have also elucidated passive scalars, which are defined as diffusive contaminants that exist in a low concentration but sufficiently enough to provoke a significant impact on energy expenditures, heat transfer, and air pollution. Research has also found that the transport phenomenon in real-situation flows usually occurs under complicated external conditions such as favorable/adverse pressure gradients, local flow perturbations, and spatially developing boundary-layer flows. Therefore, computational investigation through Direct Numerical Simulation (DNS) with millions of “flow and thermal sensors” and high temporal resolution may shed light on the unknown aspects of transport phenomena in accelerated/decelerated boundary layers. In addition, coherent structures in such a complex environment and their interactions (turbulent events) can be better identified and visualized by DNS.

RESEARCH CHALLENGE

These research efforts make use of tremendous computational resources, not only during the running stage but also in the visualization—animation stage. Therefore, state-of-the-art parallel computing and graphics processing unit (GPU) programming are essential. Furthermore, the high spatial/temporal resolution of DNS examines the physics behind turbulent events and passive scalar transport in highly accelerated/decelerated boundary layers for potential applications to flow heat/transfer control and turbulence modeling in aerospace applications.

The research team’s DNS study uses thousands of cores in a parallel computational environment. DNS is a numerical tool that aims to resolve all turbulent length and time scales, capturing the whole energy spectrum of the flow field. Consequently, the numerical approach requires high mesh resolution and, thus, very small physical timesteps or high temporal resolution. This results in highly costly numerical predictions with the pay-off of getting the whole “picture” of the problem: no other numerical approach can supply such a level of information and accuracy in turbulent wall-bounded flows. Even experimental approaches fail to measure transport phenomena in the near-wall region of boundary layers. DNS is able to accurately predict flow parameters in regions up to one hundred times closer to the surface than in experiments. Traditionally, DNS has been limited to small computational domains (or low Reynolds numbers); however, the significant growth of petascale computing resources such as Blue Waters has allowed researchers to tackle higher Reynolds number problems in a reasonable time. To the best of the researchers’ knowledge, this project is the first time that numerical predictions of high-Reynolds-number boundary layer subjects to extreme streamwise pressure gradients have been carried out, representing a formidable computational challenge with tremendous importance for the fluid dynamics and scientific visualization communities.

METHODS & CODES

Computationally speaking, it is very challenging to capture the physics of unsteady spatially developing turbulent boundary layers owing to the following requirements: (1) the high resolution necessary to resolve the small scales, (2) a computational box that is large enough to appropriately capture the influence of the large-scale motions, and (3) the realistic time-dependent inflow turbulent conditions that must be prescribed. Therefore, the research team used the inflow generation method devised by Araya et al. [1], which is an improvement on the original rescaling-recycling method of Lund et al. [2]. The seminal idea of the rescaling/recycling method is to extract the flow solution (mean and fluctuating components of the velocity and thermal fields) from a downstream plane (called “recycle”) and after performing a transformation by means of scaling functions, the transformed profiles are reinserted at the inlet plane, as seen in Fig. 1.

To successfully perform the DNS, a highly accurate, efficient, and highly scalable computational fluid dynamics solver is required. PHASTA is an open-source, parallel, hierarchical (second- to fifth-order accurate), adaptive, stabilized (finite-element) transient analysis tool for the solution of compressible [3] or incompressible flows [4]. Combining minimal dissipation numerics and adaptive unstructured meshes, PHASTA has been applied to flows ranging from validation on DNS and large-eddy simulation benchmarks such as channel flow and decay of isotropic turbulence to cases of practical interest including incompressible and compressible boundary-layer flow control. PHASTA has been carefully constructed for parallel performance and scaling to 786,432 cores (on one, two, and four processes per core, which exceeds three million processes) in Mira (Argonne’s 10 petaflop supercomputer). PHASTA has also been ported and scaled well on GPU-based and Intel “Xeon Phi”-based architectures.

RESULTS & IMPACT

This project, based on DNS big data, contributed to a better understanding of coherent structures, turbulent events, and passive scalar transport in boundary layers subject to streamwise pressure gradients and vertical jets, and pushed the boundaries in terms of high-end visualization. It has also led to the improvement of flow control tools for mixing enhancement, drag reduction, and heat-transfer augmentation in aerospace applications such as the fuel cooling technique. Fig. 1 depicts iso-contours of the Q-criterion [5] in order to visualize coherent structures emanating from the crossflow jet. It has been observed that the counter-rotating vortex pair system experienced a quick attenuation owing to the strong flow acceleration prescribed (Favorable Pressure Gradient). Furthermore, DNS of high Reynolds number-zero-pressure gradient flows has been performed in large-scale systems (approximately 52 million grid points). Fig. 2 shows iso-contours of a λ2 eigenvalue for coherent structure visualization in low and high Reynolds number flows. The presence of vortex loops in low Reynolds number flows (horseshoes) is evident, while the turbulence structure seems finer and more isotropic in high Reynolds number flows (hairpins). Since the lead institution of this project is the University of Puerto Rico at Mayaguez, the research impact has involved underrepresented minorities: six undergraduate students, two graduate students, and one early-career faculty.

WHY BLUE WATERS

This project makes use of state-of-the-art DNS, which supplies the highest possible level of flow information but at a high computational cost. This endeavor would not be possible without the invaluable contribution and support of the Blue Waters resources.

PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY

Downsizing device dimensions to the nanometer range raises significant challenges to traditional device design owing to potential current leakage across nanoscale dimensions and the need to maintain reproducibility while dealing with atomic-scale components. The research team has investigated negative differential resistance (NDR) devices based on atomically precise graphene nanoribbons. This computational evaluation of the traditional double-barrier resonant tunneling diode NDR structure uncovers important issues at the atomic scale concerning the need to minimize the tunneling current between the leads while achieving high peak current.

The team has proposed a new device structure consisting of multiple short segments that enables high current by the alignment of electronic levels across the segments while enlarging the tunneling distance between the leads. The proposed structure can be built with atomic precision using a scanning tunneling microscope (STM) tip during the intermediate stage of the synthesis of an armchair nanoribbon. In addition, the team has conducted an experimental evaluation of the band alignment at the interfaces and an STM image of the fabricated active part of the device.

RESEARCH CHALLENGE

Designing band alignment to manipulate electronic transport behaviors across an interface is the key to achieving novel functionalities in semiconductor junctions and heterostructures (HSs). The recent development of graphene and graphene nanoribbons (GNRs) offers new opportunities to design nanoscale devices and to test NDR at the atomic scale. Following the bottom-up synthesis of graphene and graphene nanoribbons (GNRs) offers new opportunities to design nanoscale devices and to test NDR at the atomic scale. Taking this into account, the team has conducted an experimental evaluation of the band alignment at the interfaces and an STM image of the fabricated active part of the device.

RESULTS & IMPACT

In this work, the research team has demonstrated a practical device structure based on armchair GNRs to deliver a strong NDR effect. The proposed GNR-based HSs consist of seven-carbon-atom-wide armchair GNRs (7–aGNRs) and an intermediate structure appearing in GNR synthesis. This intermediate structure consists of partially converted GNRs with one side of the poly-anthrylene precursors and STM manipulations, ensuring an atomically precise graphene nanoribbon fabrication. This intermediate/GNR double-barrier structure, two segments of the 7–aGNR, each with a length of four anthrylene units, approximately 17.0 Å, as barriers, and they are directly connected to the bulk graphene leads. An intermediate structure of the same length, acting as a quantum dot, is sandwiched between the barriers, giving a structure labeled as a 4–4–4–4 HS. No obvious NDR is found, because direct tunneling can occur for this very short device. When much longer segments are used, NDR does occur, but the current decreases to the pA level, which is much too small to be used in devices.

To enlarge the magnitude of the current while enhancing the favorable NDR characteristics, the research team has proposed a new device design based on five short segments (Fig. 1). The team uses two 7–aGNR barriers and three intermediate parts, sandwiched between two graphene leads. Instead of connecting the 7–aGNR barriers directly to the graphene leads, the researchers inserted intermediate segments between the barriers and the leads to better align the energy levels on the opposite sides of the barriers. The use of five segments extends the active region of the device, preventing direct tunneling between the leads while allowing the barriers to be short, thereby enhancing the current. In the paradigmatic example, the team chose each segment to have the length of four anthrylene units, giving a 4–4–4–4–4–4 HS active region. In the calculated I–V curve in Fig. 1, the NDR appears at a relatively small bias with a large peak-to-valley ratio, which well satisfies the practical requirement for electronic circuit applications.
EXECUTIVE SUMMARY

Heterogeneous systems containing a CPU+GPU pair on a single node (such as Blue Waters’ XK nodes) are becoming more common. Programming such systems effectively is a difficult challenge, especially for applications that have not been developed from the ground up to support such systems. In this context, OpenMP has emerged recently as an interesting solution, by leveraging OpenMP offloading capabilities in existing code. In this work, OpenMP offloading was added to PlasCom2, a multiphysics simulation application, with the Hydra framework. Hydra enables concurrent execution of application code on a CPU+GPU pair, resulting in efficient resource usage and high-performance portability. Performance results on Blue Waters show gains of up to three times on a single XK7 node [2,3].

RESEARCH CHALLENGE

Programming heterogeneous systems is a challenging task, as few programming models support executing code on accelerators, leading to the use of specialized solutions such as CUDA, OpenCL, Legion, or Kokkos for these devices. Such specialized languages have the advantage of being able to provide the best performance in many cases since they can often provide support for special device features and offer good code generation for specific device types. However, existing application code can often not be reused and must be rewritten in a new language. Code is often not portable between devices (for example, between CPUs and GPUs), such that distinct devices may require different implementations, leading to duplicated code and an increased difficulty of code maintenance.

METHODS & CODES

Based on the offloading support available in recent OpenMP versions, the team developed Hydra, which is a library to support concurrent execution on host and accelerator devices. For PlasCom2, Hydra [1–3] measures the relative performance of the host and accelerator at startup and determines the best workload distribution based on these data. During execution, Hydra handles the data movement between host and offloading device as well as the actual code execution [2,3]. Hydra requires an OpenMP 4.5 compiler and runtime but has no additional dependencies [1].

RESULTS & IMPACT

OpenMP offloading enables simple and efficient execution of a single code base on different types of devices, with minimal changes to existing code. Hydra builds on top of OpenMP offloading to add support for fully heterogeneous execution; that is, running parts of the problem concurrently on different device types. Using Hydra with PlasCom2 resulted in a speedup of three times compared to CPU-only execution on a Blue Waters XK7 node. Compared to running only on the GPU, performance from heterogeneous execution was improved by 17%. Some of the computationally intensive kernels of PlasCom2 showed a speedup of up to four times (Fig. 1). OpenMP offloading and Hydra show that existing codes can be enabled to run on heterogeneous systems with a low number of changes and high performance efficiency.

WHY BLUE WATERS

Blue Waters was essential to the research by providing a stable, high-performance platform with easy access to modern accelerators. Hydra and its integration into PlasCom2 could be developed directly on Blue Waters, allowing the team to evaluate and compare different implementation possibilities on a real system.

For PlasCom2, the research team needed an approach that was able to use the existing code (in C++ and Fortran) on several types of accelerators without having separate implementations for different device types. Furthermore, the team wanted to be able to support different hardware and software environments with this approach, and run concurrently on the host and offloading devices to use all available computing resources efficiently.
**EXECUTIVE SUMMARY**

In past experiments, simulations, and theoretical analyses, rotation has been shown to dramatically affect the characteristics of turbulent flows, such as by causing the mean velocity profile to move radially outward leading to an overall drag reduction, as well as by affecting the Reynolds stress tensor (the total stress tensor in a fluid). The axially rotating pipe is an exemplary prototypical model problem that exhibits these complex turbulent flow physics. For this flow, the rotation of the pipe causes a region of turbulence suppression that is particularly sensitive to the rotation rate and Reynolds number (the ratio of inertial forces to viscous forces within a fluid). The physical mechanisms causing turbulence suppression are currently not well understood, and a deeper understanding of these mechanisms would be of great value for many practical applications involving swirling or rotating flows, such as swirl generators, wing-tips, axial compressors, jet engines, and the like.

The research team conducted direct numerical simulations (DNS) of rotating turbulent pipe flows at different Reynolds and rotation numbers. The main objectives of this work were to analyze the effects of rotation on turbulence considering turbulence as being suppressed may not appropriately describe the characteristics of this flow at these conditions. In summary, turbulence suppression is occurring (for large enough rotation numbers) for all three Reynolds numbers used in this study. The results for the turbulent kinetic energy also seemingly display a change in trends at N = 1 for all three Reynolds numbers, which is discussed in more detail in [12,13].

**RESULTS & IMPACT**

The current research is concerned with axially rotating flow pipe flow in the axial direction and, therefore, for the laminar case the axial mean flow is not directly affected by the rotation. Hence, the parabolic mean flow profile observed in laminar nonrotating pipes also describes the axial (laminar) velocity profile for the rotating case. The axially rotating pipe can be described by two nondimensional parameters: the Reynolds number Re = U/D, based on the mean bulk flow velocity U, the pipe diameter D, and the kinematic viscosity ν as well as the rotation number N = Vθ/R of the pipe, which is sometimes also referred to as swirl rate. The rotation number characterises the angular velocity through the azimuthal velocity v of the pipe inner wall, Vθ = (ΩD/2) (in nonrotating reference frame).

While models such as Reynolds-averaged Navier–Stokes (RANS) and wall-resolved large-eddy simulation fail to accurately reproduce the flow physics involved in turbulence suppression, DNS can be used to effectively study rotation effects on turbulent structures. Ashraf et al. [8] demonstrate some of the severe limitations of several advanced RANS models when compared to the DNS data presented here. Existing DNS studies of rotating pipe flows have been restricted to relatively low Reynolds numbers (Re < 10,000), and a strong dependence on rotation number has been observed. Thus, one of the goals of the current work is to provide detailed DNS data at large Reynolds numbers.

The streamwise velocity profiles (not shown here) illustrate how the turbulent flow is affected by rotation in the mean. The velocity profiles are plotted versus the distance from the wall y = 1–r/R, where r is the local radius and R is the total radius of the pipe. It can be seen that the streamwise velocity profile tends to widen the laminar profile as the rotation number N is increased. Near the wall, the wall-normal velocity gradient is reduced, which leads to a reduction in skin friction and a speed-up of the flow toward the center of the pipe.

In summary, turbulence suppression is occurring (for large enough rotation numbers) for all three Reynolds numbers versus rotation number is illustrated in Fig. 1b, and a reduction in turbulent kinetic energy was obtained for all rotation numbers at Reynolds numbers of Re = 11,700 and 19,000. Interestingly, an initial increase in turbulent kinetic energy can still be observed until N = 1 for Re = 5,300 and, thus, considering turbulence as being suppressed may not appropriately describe the characteristics of this flow at these conditions.
AN EFFICIENT METHOD FOR HYPersonic LAMINAR–Turbulent Transition PREDICTION

Allocation: Innovation and Exploration/140 Knh
PI: Oliver M. F. Browne
Collaborator: Christoph Brehm

EXECUTIVE SUMMARY

A thorough understanding of the laminar–turbulent transition process of high-speed boundary layers is of paramount importance when designing supersonic or hypersonic vehicles. These high-speed vehicles are among the most difficult and challenging to design owing to significant aerothermal loads experienced on the vehicle during the transition to turbulence. An accurate prediction of the boundary-layer state can help reduce design margins and, ultimately, guide the development of novel, innovative, high-speed vehicles.

In this project, the research team has developed and validated a new efficient stability and transition prediction method for hypersonic boundary layers; namely, the AMR–WPT (adaptive mesh refinement wavepacket tracking) method, which was up to 10 times more efficient when compared with static mesh approaches. The AMR–WPT method was validated against conventional stability and transition methods (LST—linear stability theory, DNS—direct numerical simulation, etc.).

RESEARCH CHALLENGE

Conducting numerical transition prediction investigations for complex geometries is either generally too computationally expensive (e.g., DNS) or unable to capture all flow physics (e.g., nonlinear receptivity, nonlinear instability mechanisms, nonlinear breakdown, and the like). The latter is due to the assumptions that these conventional methods rely upon (e.g., LST—linear and parallel flow assumptions, parabolized stability equations—mostly linear, although they can be weakly nonlinear, etc.) The AMR–WPT method attempts to capture all flow physics as DNS can but also to be competitive with LST in terms of computational efficiency.

In many cases, the instabilities in high-speed boundary layers are convectively unstable and appear as localized convecting wavepackets. This inherent nature of the wavepacket can be exploited with AMR, which can be employed to track the wavepacket as it convects downstream and ultimately reduce the number of grid points that are required for the simulation.

METHODS & CODES

The governing equations of the AMR–WPT method are the disturbance flow formulation of the 3D compressible Navier–Stokes equations. This formulation decomposes the flow state vector and fluxes in the Navier–Stokes equations into steady base flow (or mean flow) components and unsteady disturbance components. From the disturbance flow equations, the higher-order terms can either be dropped to solve the linear disturbance flow equations or included to solve for the nonlinear disturbance flow equations—this research considered both. The base flow terms are computed by interpolating from a base flow solution on a base flow mesh. The disturbance is introduced into the flow field via wall forcing (blowing/section) [1,4], which subsequently develops into a wavepacket. Disturbance generation via particulate collision was also investigated [3]. At predefined intervals, a refinement/derefinement step is performed to redistribute the grid points to track the wavepacket as it convects downstream (Fig. 1).

The AMR is handled by the external library PARAMESH [5]. Higher-order prolongation and restriction operators are employed for transferring the information between different refinement levels in the block-structured Cartesian mesh. Dynamic load balancing and Morton ordering is used to redistribute the loads among the different processors after each refinement/derefinement step is performed.

RESULTS & IMPACT

The AMR–WPT method has been validated against a number of test cases including: (1) a 2D M = 5.35 (M is Mach number) flat-plate boundary layer [1,2]; (2) an axisymmetric M = 10 7° straight cone [1,2]; (3) a 3D M = 5.35 flat-plate boundary layer [4]; and (4) a 3D M = 4.14 straight wedge [3]. Fig. 2 shows an example of the AMR–WPT method for a particulate collision.

The AMR algorithms were able to successfully track the wavepackets in all cases and significantly reduce the number of grid points that were required when compared with static mesh methods. In static mesh approaches, the computational cost scales with the size of the domain whereas with the AMR–WPT method the cost scales with the size of the wavepacket. Different criteria were tested to determine the most appropriate parameter(s) for tracking the wavepackets (i.e., refining/derefining the mesh). This ultimately comes down to a compromise between efficiency and accuracy [1–4]. The next step will be to examine more complex geometries.

WHY BLUE WATERS

The Blue Waters supercomputer and its staff were essential for this research. The large amount of computational resources and storage facilities available on the system played a considerable part in enabling this research to move forward at the pace it did. The expertise of the project staff allowed the research team to maximize the efficiency of its code and parallelization capacity on the Blue Waters system.

PUBLICATIONS & DATA SETS


QUANTUM SIMULATIONS: PROPERTIES OF DENSE HYDROGEN

EXECUTIVE SUMMARY

The research in this project on Blue Waters is related to the Materials Genome Initiative, the federally supported cross-agency program to develop computational tools for designing new materials. In the past year, the research group has been running calculations for dense hydrogen and lithium in order to make predictions that have been tested experimentally. In particular, the team performed coupled electron–ion quantum Monte Carlo calculations of the transition between molecular and atomic hydrogen to determine the changes in optical properties across the transition. During the past year, their prediction of a transition was verified by a new experiment.

RESEARCH CHALLENGE

The phase diagram of high-pressure hydrogen is of great interest both for fundamental research, such as in astrophysics, and for energy applications such as high-temperature superconductivity in hydrides.

METHODS & CODES

The team employs quantum Monte Carlo calculations that provide nearly exact information on quantum many-body systems. This is the most accurate general method capable of treating electronic correlation; thus, it needs to be in the kernel of any materials design initiative. The method is able to use Blue Waters effectively because there are several pathways to find parallel performance.

RESULTS & IMPACT

The research group’s recent computations on Blue Waters included the following two projects:

- Liquid–liquid phase transition in hydrogen by coupled electron–ion Monte Carlo simulations. The phase diagram of high-pressure hydrogen is of great interest both for fundamental research, such as in planetary physics, and for energy applications. The existence and precise location of a phase transition in the liquid phase between a molecular insulating fluid and a monatomic metallic fluid is relevant for planetary models. Recent experiments reported contrasting results about the location of the phase transition. Theoretical results based on density functional theory are also very scattered. Before 2018, the research team performed highly accurate coupled electron–ion Monte Carlo calculations of this transition, finding results that lay between the two experimental predictions, close to that measured in Diamond Anvil Cell experiments but at 25–30 gigapascal higher pressure. The transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity, and in electron localization. During 2016–17, the research team’s prediction of a transition was verified by three separate experiments. In particular, a new experiment [1] verified the results of the team’s calculation, which was covered by The New York Times [2].

- Recently, the team has continued the calculations to control various computational approximations and quantify their errors. In the papers listed below, the researchers published additional information about dense hydrogen as the system changes from a molecular liquid to an atomic liquid. These findings are valuable in understanding and reconciling the different experiments. More accurate predictions of the Compton profile in liquid and solid lithium. The research group has performed very accurate calculations of the momentum distribution of electrons in liquid and solid lithium to compare with new scattering experiments done on the latest experimental light source. These calculations removed many of the assumptions and approximations of earlier calculations. For example, the team simulated both solid and liquid lithium at the experimental conditions of temperature and specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity, and in electron localization. During 2016–17, the research team’s prediction of a transition was verified by a new experiment. In particular, a new experiment [1] verified the results of the team’s calculation, which was covered by The New York Times [2].

WHY BLUE WATERS

Access to Blue Waters was necessary because of the computational demands of the calculation involving hydrogen and lithium. The systems typically had more than one hundred electrons and core electrons in the simulation. They were able to agree with experiment on an order of magnitude better than previous calculations. The work will be published in 2019 together with the experimental data.

PUBLICATIONS & DATA SETS


ROLE OF INTERFACES ON THE SHEAR STRENGTH AND BENDING PROPERTIES OF VAN DER WAALS TWO-DIMENSIONAL MATERIALS

EXECUTIVE SUMMARY

Two-dimensional van der Waals materials such as graphene and hexagonal boron nitride (h-BN) are of significant technological importance owing to their unconventional properties at the nanoscale. Using Blue Waters’ computational resources, detailed theoretical calculations and molecular static simulations were used to quantify the interfacial strength properties of graphene–titanium (Ti) and graphene–aluminium (Al) nanocomposites, as well as the bending rigidity of layered graphene and hexagonal boron nitride nanostructures. The results show that the strongly chemisorbed graphene–Ti interface is drastically weakened by the formation of a metal oxide phase, while the weakly physisorbed graphene–Al interface is significantly strengthened through metal oxide formation. The research team’s simulations for the bending rigidity of two- to six-layered boron nitride nanostructures show substantially higher bending stiffness than that of multilayered graphene. These computational results are in excellent agreement with recent experiments.

RESEARCH CHALLENGE

Single-atom sheet nanostructures such as graphene and hexagonal boron nitride offer interesting design capabilities owing to their unique strong in-plane covalent binding, with highly tunable but weak van der Waals interactions at the interfaces. For example, graphene or its rolled counterpart, carbon nanotube, can be used as reinforcements in lightweight metal matrix composites (e.g., Ti and Al), leading to high stiffness and strength as well as stability at high temperatures. This makes them ideal candidates for manufacturing lightweight damage-tolerant structures relevant for the aerospace and automobile industries. Such a unique combination of properties relies on effective bonding along the graphene–metal interface. The local binding properties of surface oxidized metals can differ profoundly from those on bare metals, and the associated mechanisms can affect the overall strength of the nanocomposite. On the other hand, the bending rigidity of monolayer 2D materials is simply governed by the underlying chemical bond stretching/compression/rotation behaviors of atoms within the single atomic sheet. However, for multilayer 2D materials, the bending rigidity becomes more complicated owing to the added contributions of interlayer interactions. While monolayer h-BN and graphene have bending rigidities of a similar order of magnitude, the stronger interlayer interaction at h-BN interfaces suggests a potentially different modulus for their multilayer counterparts. Simulations of such local behavior with atomistic details can uncover key mechanisms that are otherwise inaccessible through state-of-art experiments.

METHODS & CODES

The research team performed density functional theory (DFT) calculations for graphene–metal interfaces using the Vienna Ab initio Simulation Package. They used Projector Augmented Wave-based pseudopotentials to represent the interaction between ionic cores and valence electrons, while the local density approximation was adopted for exchange and correlation. Electronic energy of the structures was minimized by the conjugate gradient method. The team determined the binding properties at the interfaces of graphene–metals, with and without oxidation, by computing electron localization functions that describe the probability of finding one electron in the neighborhood of another electron. Interfacial shear strength was extracted by computing the sliding potential energy surface as a function of relative interfacial displacements. To investigate the bending and interlayer shear rigidities of h-BN and graphene nanosheets, the research team conducted molecular static simulations using the classical molecular dynamics code LAMMPS. The team adopted a recently developed Tersoff parametrization to represent the intralayer interactions in h-BN. The intralayer atomistic interactions between C atoms in graphene were governed by a second-generation reactive empirical bond order potential. The interlayer interactions for both graphene and h-BN were described by registry-dependent Kolmogorov-Crespi-type force fields. The group performed stiffness calculations of folded h-BN and graphene sheets with varying numbers of interlayers by first constructing sinusoidally modulated initial geometries and minimizing their energies by the conjugate gradient method.

RESULTS & IMPACT

In Fig. 1, the DFT simulations suggest opposite changes to the binding and shear strength properties of graphene on these two types of metals when surface oxidized [1]. The researchers observed distinctly higher electron localization function values of approximately 0.3 across Ti–graphene versus approximately 0.1 across Al–graphene because of hybridization of the unoccupied d-orbitals in transition Ti metal with the 2p-orbitals of C atoms in graphene. For graphene on Ti–O and Al–O substrates, the Ti–C and Al–C interactions are weakened by O atoms on the metal surface. The high interfacial shear strength of approximately 5 GPa of pure Ti/graphene is reduced by two orders of magnitude to approximately 20 MPa along Ti–O/graphene, while the interfacial shear strength of approximately 10 MPa along pure Al/graphene remains similar in magnitude along Al–O/graphene. These fundamental insights on graphene–metal interfaces have important implications for graphene–reinforced metal matrix composites and the fabrication of graphene–metal contacts in graphene transistors, as well as the transfer printing and epitaxial growth of graphene on metallic substrates.

The research group’s simulations showed that the bending properties of multilayer h-BN and graphene are significantly different from their monolayer counterparts [2]. While the bending stiffness of monolayer h-BN and graphene is associated with pure bending of the single atomic layer, the stiffness of folded two- to six-layered h-BN and graphene has added contributions from interlayer sliding and out-of-plane deformation. The research team developed models for the bending and interlayer shear moduli of ultrathin boron nitride nanosheet, as viewed from the top, in inset (a) at locations of maximum normal and shear separations indicated by red dashed lines, pink, grey, and blue denote boron, nitrogen, and carbon atoms, respectively.

PUBLICATIONS & DATA SETS

**EXECUTIVE SUMMARY**

This work focuses on: (1) developing new machine-learning approaches to simulate the quantum many-body problem, and (2) elucidating novel phenomena in atypically entangled phases. The many-body problem, in brief, involves understanding the collective behavior of large numbers of interacting particles. Entanglement deals with the phenomenon of particles that remain correlated even when separated by great distances. One new machine-learning approach simulates difficult quantum many-body electronic systems by combining deep neural networks with ideas originally developed by Feynman about backflow. Using this new approach, the research team extrapolated to near exact energies on difficult quantum many-body systems and competed favorably with other state-of-the-art methods. One important entangled phase is the spin-liquid; the team has discovered an expanded spin-liquid regime in the phase diagram of the stuffed honeycomb model.

**RESEARCH CHALLENGE**

Entanglement makes quantum mechanics both interesting and difficult to simulate. Einstein once described entanglement in quantum mechanics as “spooky action at a distance,” and phases of matter ranging from spin-liquids to eigenstate phases have exotic properties because of their atypical entanglement. Entanglement is also responsible for causing the exact solution of quantum many-body systems to scale exponentially with system size; every two years researchers can simulate one more electron.

The research team's problem is twofold: to identify, classify, and find phases with interesting entanglement, as well as to develop new methodologies based on ideas from machine learning to overcome the barriers to efficient simulation. The two phases of atypical entanglement - the group is most interested in - are spin-liquids and eigenstate phases. Spin-liquids are phases of matter whose entanglement is so complicated that they can't be constructed with short quantum circuits. In spin-liquid materials, the electron 'fractionalizes,' splitting into multiple pieces. Spin-liquids support anyons, which are important for constructing quantum memories and quantum computers. While the theory of spin-liquids is well established, the key question is to bring these spin-liquids into the real world by finding physical systems that support them. Eigenstate phases of matter are a recently discovered class of physical systems whose eigenstates have atypical entanglement. The entanglement of a typical eigenstate is boring; all particles are uniformly entangled with each other. On the other hand, in eigenstate phases, the entanglement in each eigenstate is highly structured. In addition to weird entanglement, these states of matter never equilibrate—the equivalent of a never-cooling cup of coffee. Eigenstate phases might be the key to allowing quantum computers to run at higher temperatures. The key question the team is addressing here is to increase the number of known eigenstate phases.

The research team has developed two algorithms to identify, classify, and find phases with interesting entanglement. In one case, the researchers have mapped out a very general phase diagram of the stuffed honeycomb lattice that interpolates between a triangular and honeycomb lattice. To accomplish this, they find the lowest eigenvector of matrices, which are 68 billion by 68 billion using a parallel exact diagonalization code the team developed. In an alternative approach, they have searched for a numerical Hamiltonian that best fits the collaborators' experimental data on a spin-ice material. The team has approached better quantum mechanical simulations in two ways: by using deep neural networks and also by using an inverse approach. In the first case, they use deep neural networks to represent the quantum wave function. Wave functions map electron positions to scalar amplitudes. To generate this amplitude, they take a configuration and have a deep neural network generate a matrix whose determinant is then evaluated. This builds on other approaches that have neural networks generate the amplitude. In the second case, the research team has tackled the quantum many-body problem using an inverse approach that avoids the exponential cost of the forward method. The team's algorithm takes a targeted set of properties encoded as a wave function and outputs the Hamiltonians that might have generated it. This turns out to be extremely useful because it is easy to write down wave functions with interesting and exotic physics.

**RESULTS & IMPACT**

The research group has determined that the phase diagram of the stuffed honeycomb lattice supports nine different phases. One of these phases is a spin-liquid phase that significantly expands the known spin-liquid regime on the triangular lattice. This increases the chance that experimentalists might be able to find spin-liquid behavior in real materials. In eigenstate phases, the team has discovered an entirely new type of eigenstate phase [10], making it the second nontrivial concrete example of this type of phase. This phase has eigenstates with two different types of intersected eigenstates; some of the eigenstates have entanglement that grows logarithmically with system size, and some are constant. The implications of this discovery are that the system equilibrates (i.e., the coffee cup cools) depending sensitively on the starting conditions of the system. The two algorithms the team has developed have significantly improved the regime of simulatable systems. The machine learning methodology extrapolates to the correct answer on difficult Hubbard systems in the regime where the researchers believe superconductivity exists and competes favorably with other state-of-the-art methods including the density matrix renormalization group. The inverse approach the team has developed has allowed them to find a whole class of Hamiltonians that support a spin-liquid-like state.
EXECUTIVE SUMMARY

When air flows over solid surfaces at high speeds, the very thin region near the surface that is referred to as the boundary layer can become chaotic and turbulent; these turbulent motions can then generate intense, outward-propagating sound waves. In particular, for fast flows inside a supersonic wind tunnel, the turbulent boundary layer over the tunnel wall radiates outward-propagating sound waves and causes the generation of freestream acoustic noise in the wind tunnel. This research exploited the cutting-edge computational power of the Blue Waters to advance fundamental understanding of the generic statistical and spectral features of acoustic radiation from high-speed turbulent boundary layers. Such an understanding helps define the freestream disturbance environment in supersonic/hypersonic wind tunnels and allows more accurate extrapolation of experimental measurements from noisy wind tunnels to free flight.

RESEARCH CHALLENGE

Testing in conventional (noisy) wind tunnels has been an important means of characterizing and understanding when, where, and how a high-speed boundary layer flowing over an aerodynamic body transitions to turbulence, which causes a large increase in skin-friction drag and surface heating. Because the existing low-disturbance (i.e., quiet) facilities operate only at Mach 6, moderate Reynolds numbers (the ratio of inertial forces to viscous forces within a fluid), fairly small sizes, and low freestream enthalpy (total heat content of a system), conventional facilities will continue to be employed for testing and evaluation of high-speed vehicles, especially for ground testing involving other Mach numbers, higher freestream enthalpies, and larger models. To enable better use of transition data from conventional facilities and more accurate extrapolation of wind tunnel results to flight, one needs an in-depth knowledge of the broadband disturbance environment in those facilities, which is dominated by acoustic radiation from tunnel wall turbulent boundary layers.

METHODS & CODES

Direct numerical simulations (DNS) were conducted using HyperWENO, an in-house high-order finite-difference solver that solves the compressible Navier–Stokes equations describing the evolution of the density, momentum, and total energy of the flow. The governing equations can be described and solved in either general curvilinear coordinates or cylindrical coordinates, depending on the flow configuration. The inviscid fluxes of the governing equations were computed using a seventh-order weighted essentially nonoscillatory (WENO) scheme. Compared with the original finite-difference WENO introduced by Jiang and Shu [1], the present scheme is optimized by means of limiters [2] to reduce the numerical dissipation. WENO adaptation was limited to the boundary-layer region for maintaining numerical stability while the optimal stencil of WENO was used outside the boundary layer for optimal resolution of the radiated acoustic field. A fourth-order central difference scheme was used for the viscous flux terms, and a third-order low-storage Runge–Kutta scheme [3] was employed for time integration, which significantly relieved the memory requirement and is well suited for time-accurate simulations such as DNS. The turbulent inflow can be generated using either a recycling/rescaling method [4] or a digital filtering method [5]. On the wall, no-slip conditions were applied for the three velocity components and an isothermal condition was used for the temperature. At the top and outlet boundaries, unsteady nonreflecting boundary conditions were imposed. Periodic boundary conditions were used in the spanwise or azimuthal direction.

RESULTS & IMPACT

The current work advanced the state-of-the-art knowledge of the global pressure field induced by supersonic turbulent boundary layers across a wide range of Mach numbers. The study represents the first-ever attempt to exploit the advances in high-performance computing to overcome the difficulties in experimental measurements and to provide access to both flow and acoustic quantities that are difficult to obtain otherwise. In particular, the study led to an unprecedented simulation of a full-scale nozzle of a hypersonic wind tunnel (Fig. 1) and allowed the first successful comparison between numerical predictions and measurements of pressure fluctuations over the nozzle wall. The simulations also captured all major features of the freestream disturbance spectra and structures (Fig. 2) and helped clarify the physics of the noise generation process in supersonic/hypersonic wind tunnels. The characterization of wind tunnel freestream disturbances paved the way for extrapolation to flight from the boundary-layer transition data obtained in noisy wind tunnels.

WHY BLUE WATERS

DNS are used to capture both the broadband turbulence field within the boundary layer and the near-field acoustic disturbances radiated by the boundary layer. In such simulations, extremely fine meshes are required to fully resolve all the turbulence scales in order to obtain the pressure spectra in the high-frequency/large-wave-number range. In the meantime, the simulations need large domain sizes to locate very-large-scale coherent structures in the pressure field as well as to accommodate the eddy decorrelation length and to minimize inlet transience as a result of inflow boundary conditions. A large number of timesteps are also required for the study of the low-frequency behavior of the pressure spectrum. As such, the proposed computational efforts cannot be conducted without the world-class computing capabilities of Blue Waters.
**THE ANOMALOUS MAGNETIC MOMENT OF THE MUON: AN IMPROVED AB INITIO CALCULATION OF THE HADRONIC VACUUM POLARIZATION CONTRIBUTION**

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**EXECUTIVE SUMMARY**

A central goal of high-energy physics is to search for new particles and forces beyond the Standard Model of particle physics. The muon anomalous magnetic moment is sensitive to contributions from new particles and is also one of the most precisely measured quantities in particle physics, with an experimental uncertainty of 0.54 parts per million. At present, the measurement disagreement with Standard Model theory expectations by more than three standard deviations. The Fermilab Muon g–2 Experiment will ultimately reduce the experimental error by a factor of four; first results are expected in the fall of 2019. To identify definitively whether any deviation observed is due to new particles or forces, the theory error must be reduced to a commensurate level. An ongoing project by this collaboration uses numerical lattice quantum chromodynamics (QCD) to target the hadronic vacuum polarization contribution, which becomes important at large Euclidean times. While the ensemble to be used in this project is relatively small, the large number of propagator inversions needed to compute the additional correlation functions requires a petascale machine such as Blue Waters.

**RESEARCH CHALLENGE**

The muon anomalous magnetic moment (g–2) enables a very precise test of the Standard Model of particle physics and a probe of new particles and forces beyond. In the Standard Model, the anomaly arises owing to quantum–mechanical loop contributions. Virtual contributions from new particles could therefore lead to an observable deviation between measurements and the Standard Model prediction. The most recent measurement of the muon g–2 has a precision of 0.54 parts per million and disagrees with Standard Model theory expectations by more than three standard deviations. The Muon g–2 Experiment at Fermilab (with team members from the University of Illinois at Urbana–Champaign) began running in 2019, and expects to reduce the experimental error by a factor of four. To leverage the anticipated reduction in experimental errors and determine unambiguously whether or not the present disagreement is due to effects from new particles or forces, the theoretical errors on the Standard Model prediction must be brought to a commensurate precision on the experimental timescale. The dominant source of uncertainty in the Standard Model prediction of the muon g–2 is from the hadronic vacuum polarization contribution owing to virtual quarks and gluons [3] (see Fig. 1), which is the target of this work. Numerical lattice–QCD simulations provide the only method for calculating the nonperturbative hadronic contributions to the muon g–2 with controlled uncertainties that are systematically improvable. The basic quantity from which the hadronic vacuum polarization correction is calculated is a two–point function with vector–current operators at the source and sink. The hadronic vacuum polarization is obtained from integrals of this correlation function over Euclidean time. However, at large Euclidean time the vector–current correlation function receives contributions from two–pion states that cannot be resolved from a statistical analysis of the vector–current correlation function alone, because its statistical errors increase rapidly with the Euclidean time. In the joint project described above, these contributions are currently estimated phenomenologically from a scalar quantum electrodynamics calculation.

**RESULTS & IMPACT**

The project was carried out using the MIMD lattice computation (MILC) collaboration code [5], which has been in production use on a wide variety of massively parallel computers for over 20 years, with continual improvements to address the community’s evolving science goals and to accommodate changing hardware. The MILC code, which currently consists of about 300,000 lines, makes extensive use of the libraries of the U.S. Lattice–QCD collaboration’s QCD applications programming interface for CPUs [6] and the QUDA framework for lattice–QCD on GPUs [7,8]. It was part of the Blue Waters acceptance test and one of the applications launched at its dedication and has been running on Blue Waters for over five years with significant improvement in performance over this period. Porting the MILC code to Blue Waters’ XE nodes was straightforward, and with the integration of the QUDA libraries, the MILC code also runs efficiently on the XK nodes.

**WHY BLUE WATERS**

This project requires the computation of a large (approximately 100) number of propagators on each available configuration in order to obtain the desired correlation functions. While the small ensemble the research team used in this project allowed them to compute each propagator on only three or four nodes, performing all the propagator inversions needed on each of the 10,000 configurations in the ensemble required a petascale resource such as Blue Waters. Another essential aspect is that the code used in this project had already been adapted and optimized to Blue Waters (with the help of Blue Waters’ staff) in the course of prior projects funded under PRAC allocations.

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**Figure 1:** Hadronic vacuum polarization contribution to the muon’s anomalous magnetic moment.

**Figure 2:** A representative subset of the correlation functions to be computed in this work. A single square at the source or sink indicates a fermion bilinear vector–current operator, while two circles with (without) a red line represent connected (disconnected) two–pion operators. The temporal locations are labeled \( t_{\text{src}} \) and \( t_{\text{sink}} \) and the thick lines indicate propagation in time.
ACCELERATING THERMOELECTRIC MATERIALS DISCOVERY VIA DOPABILITY PREDICTIONS

EXECUTIVE SUMMARY

Nowadays, the experimental realization of new thermoelectric materials—which convert wasted heat to usable electricity—still requires considerable effort and resources, often accelerated through computational guidance, with use of first-principles calculations providing relevant materials properties such as electronic and phonon transport and thermodynamic stability. Semiconductors are called semiconductors because they exhibit intermediate electrical conductivity (better than typical insulators but not as good as metals). For thermoelectric materials, researchers need to improve their electrical conductivity by “doping” the semiconductor. Doping refers to the intentional introduction of defects in the material that help to improve the electrical conductivity—typically by several orders of magnitude.

The current bottleneck in the discovery of new thermoelectric materials, however, is that greater than 90% of the materials identified as promising on a computer cannot be doped in the laboratory. To overcome this, the research team uses Blue Waters, which to date has allowed the calculation of full density functional theory, which approximates the Schrödinger equation to determine the defect formation energy, which governs how readily the defect may form. For this, the team used first-principles quantum mechanical methods based on the framework of density functional theory, which approximates the Schrödinger equation to make it solvable.

As the new candidate materials being considered are structurally complex ternary and quaternary semiconductors, a large number of intrinsic defects are possible, requiring a large set of quantum mechanical simulations to accurately predict dopability and the laboratory growth environments that will maximize it.

The large computational costs historically had limited dopability calculations to case-by-case studies in which one material was considered at a time in a serial manner. Harnessing the predictive power of computation to model dopability on a large scale is critical in accelerating the transition from novel semiconductors to functional devices. Only Blue Waters offers the large-scale computational resources that are essential to the research team’s integrated simulation/experimental approach to the discovery of new thermoelectric materials.

METHODS & CODES

To overcome the bottleneck of identifying high-electrical conductivity semiconductors as candidate thermoelectrics, the research team used Blue Waters to carry out high-throughput quantum mechanical calculations of semiconductor dopability and predict the best candidate materials before they are even synthesized in the laboratory. The dopability of a semiconductor is a result of its defect chemistry: some semiconductors resist doping via formation of intrinsic defects that counteract the effect of the dopant whereas others do not. Therefore, assessing dopability requires a comprehensive analysis of the possible intrinsic defects that could form in a material in response to any attempts to dope it. Identifying low-energy defects requires solving the quantum mechanical Schrödinger equation to determine the defect formation energy, which governs how readily the defect may form. For this, the team used first-principles quantum mechanical methods based on the framework of density functional theory, which approximates the Schrödinger equation to make it solvable.

The as‐new candidate materials being considered are structurally complex ternary and quaternary semiconductors, a large number of intrinsic defects are possible, requiring a large set of quantum mechanical simulations to accurately predict dopability and the laboratory growth environments that will maximize it. To streamline the simulation process, the team has developed an automated simulation workflow and protocol on Blue Waters to facilitate the large-scale analysis. This has enabled us to establish a closed feedback loop between simulations and experimental validation, enabling rapid screening of candidate materials in a manner not previously demonstrated.

RESULTS & IMPACT

To date, using Blue Waters the team has carried out systematic investigations of a set of approximately 30 new candidate thermoelectric materials. The group has helped to predict several new ternary and quaternary materials that exhibit the desired degree of dopability, which have subsequently been synthesized in the laboratory and are soon to be synthesized. Over the course of this project, the researchers expect this work to create the largest data set of semiconductor dopability focused on complex ternary and quaternary thermoelectric materials. Selected results highlighting some new materials identified using this approach are shown in Fig. 1b.

WHY BLUE WATERS

Practically, the key hurdle to this computation-driven approach is the need to calculate a large number of intrinsic and extrinsic point defects to directly assess dopability of semiconductors. The large computational costs historically had limited dopability calculations to case-by-case studies in which one material was considered at a time in a serial manner. Harnessing the predictive power of computation to model dopability on a large scale is critical in accelerating the transition from novel semiconductors to functional devices. Only Blue Waters offers the large-scale computational resources that are essential to the research team’s integrated simulation/experimental approach to the discovery of new thermoelectric materials.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Predictive simulations of turbulent combustion are crucial to the design of energy-conversion systems in the transportation, power, and defense sectors, among others. Due to their multiscale, multiphysics nature, these systems are typically intractable to simulation at full resolution. Lower-resolution simulations are possible but require closure models; currently, state-of-the-art turbulence models have the potential to supplant traditional turbulence models utilizing machine learning (ML) techniques and large-scale, fully resolved computational data sets. The team trains and refines neural network-based models across the problematic regimes, then refines the models using an adjoint solution, which is analogous to an on-the-fly error-control procedure. The resulting ML-based models are more accurate than the most commonly used models and can be generalized to different applications. Alternatively, the deep learning model can be harnessed to produce predictions of similar accuracy to those of existing models at reduced computational cost.

RESEARCH CHALLENGE

Turbulent combustion is an inherently multiscale, multiphysics phenomenon relevant to virtually every sector in which chemical energy is converted to mechanical energy. Modern combustors for gas turbines, internal combustion engines, rocket propulsion, and hypersonic flight all require turbulent flow to enhance fuel–oxidizer mixing and to increase burning rates. Accurate prediction of the performance, efficiency, and emissions of these devices is an essential aspect of the engineering design and test cycle. However, the most common closure models used to make these predictions computationally tractable are based on nonreacting turbulence theory and are known to fail in regimes relevant to the next generation of clean combustors. One key challenge is the prediction of turbulence–combustion interactions in premixed flames. These interactions are necessarily precluded by the use of nonreacting turbulence models [1–3]. Linearly coupled reacting-turbulence models have been developed [3,4] but are of limited use owing to their exclusion of nonlinear interactions. The research team therefore focuses on developing nonlinear models that are capable of capturing such interactions.

METHODS & CODES

The researchers have developed a machine learning approach to turbulent combustion model development with a focus on predicting nonlinear turbulence–combustion interactions. Numerical databases from fully resolved direct numerical simulations (DNS) of turbulent combustion form the basis of these model-development efforts. The team generates DNS databases across a range of turbulent combustion regimes using the semi-implicit, second-order, energy-conservative code NGA [5,6]. These databases are subsequently downsampled using a low-pass filter to obtain flow fields comparable to those obtained from a large-eddy simulation (LES, i.e., modeled) calculation. Because the filtered fields originate from full-resolution data, the “true” model outputs are also available. Using deep neural networks as a nonlinear statistical model, the team approximates these “true” outputs from input variables that are available in LES. The resulting models are trained a priori using out-of-sample DNS data and a posteriori by implementation in analogous LES calculations. As a novel approach to model development, they have developed a new DNS/LES code, PyFlow, that is capable of refining the model during the a posteriori step using an adjoint solution. This code is GPU-accelerated and has potential to address modeling challenges over a wide range of flows.

RESULTS & IMPACT

The initial results show an encouraging ability of the machine learning-based models to predict turbulence–combustion interactions more accurately than traditional turbulence models. These findings are obtained from a priori testing and demonstrate that ML-based models have the potential to supplant traditional turbulence models in LES. However, in a posteriori testing, the researchers found that numerical errors (including finite-difference errors) owing to the reduced LES resolution accumulate in neural network inputs and reduce the models’ predictive accuracy. The issue of numerical error is unavoidable in LES but can potentially be mitigated using the team’s a posteriori model refinement step. By training in situ, models can be developed that are less sensitive to numerical error, for example, by reducing weights associated with error-prone inputs and hidden parameters. The a posteriori training step, therefore, represents a potentially significant contribution to ML-based model development and LES of turbulent combustion. WHY BLUE WATERS

This research relies on both CPU-only and GPU-accelerated compute nodes for different tasks. Because Blue Waters offers both types of nodes on a common file system, data access and sharing are greatly streamlined among tasks and project members. Additionally, the team utilizes Blue Waters-specific Python installations and packages that are supported by NCDA project staff. These installations are optimized for Blue Waters and offer substantially improved application performance compared to user-installed libraries.

Figure 1: Illustration of a direct numerical simulation (DNS) of an expanding hydrogen–air premixed flame kernel (colored surfaces) in isotropic turbulence (grayscale background). The simulation is discretized using LGW grid points and utilizes up to 16,384 cores. Machine learning models trained on many DNS databases are tested in analogous large-eddy simulations (LES).
EXECUTIVE SUMMARY

Oscillatory boundary layer flows play an important role in coastal engineering, offshore engineering, and coastal sediment transport. However, current state-of-the-art models fail to accurately predict the complex interaction of turbulent oscillatory flow with sediment transport, highlighting the existing knowledge gaps regarding the complex interactions among the oceanic flow, the coastal bottom, and sedimentation processes. Recent experimental and numerical studies conducted by the research team indicate the presence of a phase-lag between the time instant when the maximum bed shear stress occurs with respect to the maximum free-stream velocity in transitional oscillatory boundary layer flows. However, the effect of turbulent coherent structures and turbulence modulation under severe acceleration remain unknown. The current work is the first computational effort to simulate the effect of flow coherent structures and turbulent events such as sweeps and ejections on the maximum bed shear stress phase difference compared to the maximum free-stream velocity value.

RESEARCH CHALLENGE

Recent experimental studies conducted in the Large Oscillatory Water-Sediment Tunnel at the Ven Te Chow Hydrosystems Laboratory at the University of Illinois at Urbana-Champaign examine the transition between the laminar and turbulent flow regimes with a smooth bed. The results indicate a significant change in the widely used phase difference diagram between the maximum bed shear stress and the maximum free-stream velocity [1]. This observation is extremely important for the field of environmental fluid mechanics and coastal sediment transport. Nevertheless, due to the limitation of the applied pointwise experimental technique (Laser Doppler Velocimetry), it was not possible to explicitly associate this finding with the development of three-dimensional flow turbulence structures usually referred to as turbulence coherent structures.

This work is the first computational effort to quantify the effect of the three-dimensional turbulent flow structures on the phase difference between the maximum bed shear stress and the maximum free-stream velocity. Also, it will be the first numerical study that will quantify the effects of flow regime and bed characteristics on the turbulent characteristics and quadrant analysis under oscillatory flow conditions. It will also be among the first studies that will study the momentum exchange between the free-stream oscillatory flow and the seabed unsteady flow conditions.

METHODS & CODES

In this work, the research team developed a direct numerical simulation (DNS) model capable of simulating the complex oscillatory boundary layer flow using the spectral element method framework provided by the highly scalable open-source code Nek5000 [2]. Except for the analysis of turbulence characteristics of oscillatory boundary layer flow over different flow conditions, the present work requires use of a proper model for the simulation of the suspended sediment using an Eulerian approach and proper boundary conditions for the sediment mass exchange between the coastal bed and the free-stream flow (e.g., [3-4]).

Due to the data-rich outputs of our simulations, the team is collaborating with the Data Analytics and Visualization (DAV) group of the National Center for Supercomputing Applications in an effort to find an efficient way to visualize the coherent flow structures and the numerical results. The team plans to apply high-performance, data-intensive visualization and analysis techniques by means of producing high-quality, interactive visualizations of simulation results in an effort to uncover new knowledge through the efficient analysis of the information-rich data. Special attention will be given to the application of efficient methods for the estimation of the geometric characteristics of coherent flow structures as well as the quantification of their effect on flow behavior.

RESULTS & IMPACT

DNS results for mean flow and turbulent statistics were compared against previous experimental and numerical observations [1,2] and the comparison agrees well both qualitatively and quantitatively. Quadrant analysis shows that turbulent events such as sweeps and ejections dominate for most of the period. Phase difference results agree well with the previous experimental findings.

This work is the first in the literature that explores the effect of turbulence characteristics of the flow—and particularly the turbulent flow structures, such as turbulent spots (Fig. 1)—on the phase difference between maximum bed shear stress and free-stream velocity. The team identified hairpin vortices for the first time in the oscillatory boundary layer in addition to other flow structures previously reported in the literature (vortex tubes and turbulent spots). They studied the effect of these structures on the turbulence statistics and found that vortex tubes seem to have minimal effect. On the contrary, turbulent spots, which are spatially and temporarily sporadic, lambda-shaped, highly energetic structures, have a significant effect on turbulence characteristics.

WHY BLUE WATERS

The present work pushes the limit of the turbulent-resolving flow modeling of oscillatory flows. The dimensions of the computational domain were chosen based on the prior knowledge of experimental observation of turbulent spots [6,7] to ensure that the computational domain is big enough to allow these turbulent structures to develop. This size is larger than any of the previous domains reported in the literature, and together with the increased number of computational points (on the order of 0.8 billion) make this study the first of its kind in terms of the computational resources and the high-performance computing facilities it requires. Thus, it can be materialized only on a petascale supercomputer such as Blue Waters.
MACHINE LEARNING FOR PARTICLE PHYSICS: EMPLOYING DEEP LEARNING FOR PARTICLE IDENTIFICATION AND MEASUREMENT AT COLLIDERS

Executive Summary

The Large Hadron Collider (LHC) at CERN, in Switzerland, is the world’s most powerful particle accelerator. The LHC recreates the conditions of the Universe a tenth of a second after the Big Bang by colliding together high-energy protons. In 2012, the Higgs boson was discovered in LHC data, completing the Standard Model of physics and leading to the Nobel Prize in Physics in 2013. This discovery transformed our understanding of the building blocks of matter and the fundamental forces by explaining the origin of the masses of subatomic particles.

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Research Challenge

The research team employed DNNs and CNNs to distinguish among signals from electrons and photons and hadronic backgrounds and measure particle energies. The team simulated samples of individual electron, photon, charged hadron, and neutral hadron images in a simple high-granularity calorimeter detector implemented with the Geant4 simulation toolkit. These images were used to train NNs, using PyTorch, that distinguish between electrons vs. charged hadrons and photons vs. neutral hadrons, and to measure the energies of the four particle species. To optimize the network architectures, the scientists varied the NN hyperparameters, including the number of NN layers, number of neurons per layer, and the learning and dropout rates.

Results & Impact

The research team evaluated the performance of DNNs and CNNs trained on particle images and compared the results to the current state-of-the-art algorithms widely used in particle physics. These algorithms employ NNs and boosted decision trees (BDTs) to analyze a precomputed set of particle features such as the calorimeter shower depth and width. For both classification and energy measurement at the LHC.

WHY BLUE WATERS

Optimizing the network performance using hyperparameter scans requires retraining NNs hundreds or thousands of times, which is especially challenging for memory-intensive networks such as GoogLeNet or ResNet. The 4,228 GPU-enabled XK nodes with 25 TB of GPU accelerator memory available on Blue Waters enables training and optimization of neural networks beyond what has previously been achievable, allowing for detailed investigations of their behavior for both particle physics and general machine learning.

Publications & Data Sets


Figure 1: The relative energy resolution of true types of particles vs. the true particle energy for a (dashed line) simple linear fit to the total calorimeter energies vs. a (solid line) convolutional neural network.

Figure 2: Signal vs. background efficiency receiver operating characteristic (ROC) curves for (left) photons vs. neutral pions and (right) electrons vs. charged pions discrimination, using a boosted decision tree and a cell-based or feature-based deep neural network.
MOLTEN-SALT REACTORS AND THEIR FUEL CYCLES

EXECUTIVE SUMMARY
The Advanced Reactors and Fuel Cycles Group (ARFC) at the University of Illinois at Urbana-Champaign models and simulates nuclear reactors and fuel cycles with a goal of improving the safety and sustainability of nuclear power. In the context of high-performance computing, this work couples multiple physics at multiple scales to improve the design, safety, and performance of advanced nuclear reactors. In particular, thermal–hydraulic phenomena, neutron transport, and fuel reprocessing couple tightly in nuclear reactors. Detailed spatially and temporally resolved neutron flux, temperature distributions, and isotopic compositions can improve designs, characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for these unique physics. In this work conducted on Blue Waters, ARFC has demonstrated the capability to simulate coupled, transient neutronics, thermal hydraulics, and fuel reprocessing in multiple advanced, molten-salt-fueled nuclear reactor designs.

RESEARCH CHALLENGE
Nuclear power is an emissions-free, safe source of electricity with unparalleled energy density, baseload capacity, and land-use efficiency, so the world’s energy future increasingly depends on improved safety and sustainability of nuclear reactor designs and fuel cycle strategies. The current state of the art in advanced nuclear reactor simulation focuses primarily on traditional light-water reactor designs. ARFC’s work extends that state of the art by enabling better understanding of the dynamics in these reactors.

METHODS & CODES
Blue Waters has enabled ARFC to develop and test two new significant software solutions: Moltres and SaltProc. Moltres is a first-of-its-kind finite-element application simulating the transient neutronics and thermal hydraulics in a liquid-fueled molten-salt reactor design [1–4]. SaltProc is a highly capable Python tool for fuel reprocessing simulation [5–7].

RESULTS & IMPACT
Current interest in advanced nuclear energy systems and molten-salt reactor (MSR) concepts has illuminated a need for tools that model these systems. By developing such applications in the open, ARFC enables both transparency and distributed collaboration on promising nuclear reactor concepts. Detailed spatially and temporally resolved neutron fluxes, temperature distributions, and changing isotopic compositions can improve designs, help characterize performance, inform reactor safety margins, and enable validation of numerical modeling techniques for unique physics. ARFC has demonstrated multiphysics simulations of multiple molten-salt reactor designs. Steady state, transient, and fuel cycle analysis simulations have been run in 2D as well as 3D by leveraging the Moltres and SaltProc tools developed in the research group.

Finally, recent fuel cycle dynamics were obtained from depletion and SaltProc reprocessing simulations for a 60-year time frame. A molten-salt breeder reactor full-core safety analysis was performed at the initial and equilibrium fuel salt compositions for various reactor safety parameters such as effective multiplication factor (shown in Fig. 2), neutron flux distributions, temperature coefficients, rod worths, power, and breeding distributions [5–7].

WHY BLUE WATERS
Simulations that faithfully capture this coupling at realistic spatial and temporal resolution are only possible with the aid of high-performance computing resources. To assess nuclear reactor performance under a variety of conditions and dynamic transients, the ARFC group must conduct myriad 2D and 3D finite element simulations using the MOOSE framework and their in-house-developed modules. Such simulations commonly occupy tens of thousands of CPU cores at a time and vary in computational time. The MOOSE framework has been shown to scale very well up to 10,000 cores. The ARFC group has demonstrated appropriate scaling for MSR simulation above 20,000 CPU cores (600 Blue Waters nodes). Transient and multiscale simulations, which require greater capability per simulation, are on the horizon for this work. They may occupy up to 100,000 CPU cores at a time. Only a few of these larger simulations will be necessary to enable better understanding of the dynamics in these reactor systems.
A NOVEL CRYSTAL STRUCTURE WITH SPIN-PROTECTED SURFACE ELECTRONIC CONDUCTION

Allocation: Illinois/40 Knh
PI: Prashant K. Jain1
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1University of Illinois at Urbana–Champaign
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EXECUTIVE SUMMARY

Newly discovered nanostructures can fill the need for materials in energy and optoelectronic technologies. Using a kinetically driven method of nanostructure synthesis, the research team accesses novel crystal structures of ionic semiconductors. For example, the group synthesized mercury selenide (HgSe) nanocrystals with a wurtzite structure quite unlike the natural zincblende form. The scientists computed the bulk band structure of the wurtzite form, which showed a finite band-gap and band inversion—prerequisites for a 3D topological insulator (TI) property. To determine if wurtzite HgSe is indeed a 3D TI, the team needed to elucidate the surface electronic structure. Using the current allocation, the researchers determined band structures of wurtzite HgSe slabs with specific surface facets. These computations showed the spin-protected nature of surface states in wurtzite HgSe, allowing its conclusive designation as a 3D TI. Spin-protection allows resistanceless electron transport along the surface. Thus, the newly discovered HgSe crystal structure can lead to logic devices capable of operating efficiently with minimal heat dissipation.

RESEARCH CHALLENGE

Engineered nanocrystals are often utilized for making new functional electronic and optical materials such as superionic solids and battery electrodes. The research team makes use of unconventional methods that enable manipulation of the chemical composition and crystal structure of nanocrystals. These techniques often produce novel compositions and crystal phases that are often not found in the bulk phase diagram. Further, computational electronic structure investigations allow the researchers to explore the properties of these new, unconventional materials. In addition, the team is also elucidating chemical trends in heterostructures and alloys and developing solid-state principles from these trends. The results from these investigations will enable the rational design of new phases and compositions with targeted applications for resolving longstanding challenges of energy storage and device efficiency.

With advances in nanotechnology and chemical synthesis, materials are becoming ever more complex. Computations can uncover chemical principles that will ultimately allow prediction of the properties of tomorrow’s indispensable materials—an existing Grand Challenge. However, these studies require extensive calculations spanning a range of physicochemical parameters. As opposed to a single large and expensive calculation, this work requires a library of moderately expensive calculations. The net cost for generating such a library of data is feasible only with a resource such as Blue Waters, with considerable payoff for future scientific advances. When solid-state principles such as those resulting from this project become known, the rate at which new materials can be discovered or designed will be greatly expedited, because the community is no longer limited to a time- and energy-consuming trial-and-error approach.

METHODS & CODES

The research group used the open source Quantum Espresso software suite [1] to run density functional theory calculations of the electronic band structure. To study the effects of chemical composition, crystal structure, and crystallite size on the electronic properties, numerous calculations must be run. Each calculation is distinguished from the others by the crystal structure, chemical formula, or crystallite size. Through analysis of orbital energies, electronic character (orbital and spin), and band structures, the nature of surface electronic states and topology can be determined.

RESULTS & IMPACT

Prior electronic structure calculations by the research team demonstrated that bond elongation in a novel wurtzite polymorph of mercury selenide (HgSe) and mercury–cadmium selenide (HgCd1/2Se1/2) is responsible for the opening of a band gap. Combined with the inverted band structure of HgSe, it was thought that these polymorphs would exhibit 3D topological insulator (TI) behavior [2]. Three-dimensional TIs are of interest because electrons at their surface states are spin-protected from back scattering. This protection allows 3D TI materials to conduct electrons along their surface without resistance. For this reason, 3D TIs are of interest as components of energy-efficient logic devices that can operate at high capacity with minimal heat dissipation. While the team’s past work suggested the possibility of the wurtzite phase being a 3D TI, a definitive conclusion was not possible without a well-defined exposed surface facets. As compared to electronic structure calculations of fully periodic bulk crystals, calculations of slab geometries are more expensive; but the latter system allows access to information of surface electronic states, which is missing in bulk crystal calculations.

The most recent spin-resolved calculations of the surface band structures of faceted slabs has shown the existence of spin-protected electronic states on a wurtzite HgSe surface (Fig. 1). Spin protection, however, is missing from analogous wurtzite CdSe surfaces. These calculations now provide a firm basis for designating wurtzite HgSe as a 3D TI material.

In addition, the research team performed all-atom calculations of nanocrystals. While computationally expensive, this work was undertaken to understand how crystallite size and nanoscale confinement influence surface electronic structure and topology. Unlike slab geometries, which are periodic in x and y directions, the nanocrystal geometries are finite in all dimensions. Nanocrystals of wurtzite-structure HgSe and CdSe of different size (2 nm, 2.5 nm, and 3 nm) were studied. The team identified nanocrystal surface states based on the spatial character of the electronic states. This systematic set of calculations shows that surface states have a much richer character in these nanoscale-confined geometries as compared to that in the bulk.

WHY BLUE WATERS

Single calculations of a slab and even all-atom calculations of a nanocrystal may be accomplished using computational resources other than Blue Waters. However, a large number of single calculations of these geometries with varying elemental composition and crystal dimensions are required for the research team’s study of size effects and chemical trends. The computational expense of such an effort would be prohibitive were it not for a Blue Waters allocation. Furthermore, the specialized hardware of Blue Waters allows the Quantum Espresso code to run even more efficiently. This is because Quantum Espresso’s parallelization schemes involve sizable and frequent communication among CPUs, which rely on the speed of the Blue Waters communication hardware.

PUBLICATIONS & DATA SETS

INERTIAL COLLAPSE OF INDIVIDUAL BUBBLES NEAR SOLID/FREE Boundaries

EXECUTIVE SUMMARY

Inertial collapse of cavitation bubbles is a particularly complicated multi-scale (ranging from micro- to macro-bubbles in space, and microseconds to hours in time) and multiphysics (compressible fluid mechanics, multiphase flows, heat transfer, and solid mechanics) problem with a range of applications from naval hydrodynamics to biomedical ultrasound.

One of the main consequences of cavitation is structural damage to nearby objects. Collapse of cavitation bubbles can concentrate energy into a small volume, produce high pressures and temperatures, and generate shock waves. When they are adjacent to a neighboring interface such as another bubble, a solid object, or a free surface, the collapse becomes asymmetric and a re-entrant liquid jet penetrates the bubble. This jet hits the opposite side of the bubble and generates a radiating propagating water hammer shock.

To investigate this phenomenon, the research team carried out high-resolution numerical simulations of the collapse of: (1) a single bubble near an interface, and (2) multiple bubbles near a solid surface. These simulations yielded the detailed nonspherical bubble morphology as well as the pressure and temperature fields based on the relevant nondimensional parameters entering the problem. These simulations will be used to model the collapse of bubble clouds, to comprehend the damage mechanisms, and potentially to mitigate erosion.

RESEARCH CHALLENGE

Cavitation research is essential to a variety of applications ranging from naval hydrodynamics to medicine and the energy sciences. Vapor cavities can grow from submicron-sized nuclei to a small volume, can produce high pressures and temperatures, and generate strong shock waves. When they are adjacent to a neighboring interface such as another bubble, a solid object, or a free surface, the collapse becomes asymmetric and a re-entrant liquid jet penetrates the bubble. This jet hits the opposite side of the bubble and generates a radiating propagating water hammer shock.

To carry out the simulations, the team developed a novel numerical framework to solve the compressible Navier–Stokes equations for a binary, gas–liquid system [6,7]. This numerical approach prevents spurious pressure and temperature oscillations across the material interfaces. For discretization, the group developed a solution-adaptive central-differencing/discontinuity-capturing approach. The basic idea is to use a high-order accurate, nonlinearly dissipative central discontinuity scheme in smooth regions, and to apply a more dissipative, computationally expensive, high-order accurate, shock- and interface-capturing approach only to the regions with discontinuities. For this purpose, a discontinuity sensor discriminates between smooth and discontinuous (shocks, contacts, and interfaces) regions. The time marching is handled with a third-order accurate TVD Runge–Kutta scheme. To perform the three-dimensional numerical simulations of the problems of interest, an in-house code was developed in C++, which was parallelized using the MPI library and implemented the parallel HDF5 library for I/O. The code was verified and validated against a series of theoretical and experimental data. To better understand the detailed collapse dynamics, as well as to comprehend the damage mechanisms and potentially mitigate erosion, the team studied the collapse of individual bubbles near solid/free boundaries.

RESULTS & IMPACT

When a cavitation bubble collapses near an interface, the collapse becomes nonspherical, leading to the formation of a high-velocity re-entrant liquid jet (Fig. 1). The impact of the jet on the opposite side of the bubble can generate a water-hammer shock wave that propagates in the surrounding media and thus can create high-pressure regions on the surface of neighboring solids (Fig. 2). Simulating the collapse of a single bubble near an interface delves into the details of the re-entrant jet formation and the corresponding shock propagation. The results will be used to provide scaling laws for important collapse parameters (e.g., jet velocity, bubble non-sphericity, collapse time, and shock pressure) that can be used to predict the single-bubble dynamics. However, the disruptive effects of cavitation erosion in real flow problems are generally caused by the collapse of bubble clouds that include thousands of bubbles. To simulate such flows where resolving every bubble is numerically impossible, a robust cloud model is required. Current models are typically based on spherical bubble dynamics, and thus neglect the nonspherical effects of the collapse owing to bubble–bubble/bubble–boundary interactions [8], which leads to an inaccurate estimation of the impact loads on nearby surfaces. To address this, the team simulated the collapse of a bubble pair near a solid surface to investigate and quantify the bubble–bubble/bubble–boundary interactions and their effects on the collapse dynamics. The simulation showed that such interactions significantly influence the collapse and potentially mitigate erosion.

WHY BLUE WATERS

Performing three-dimensional high-resolution simulations of up to 3.6 billion gridpoints that can effectively resolve the small-scale features of the flow, as well as handling postprocessing and visualizations of large data files, requires substantial computational power. A petascale computing resource such as Blue Waters makes these simulations possible and has been essential for the success of the present study. This project will help researchers to gain valuable insights and understanding of these complex flows, which was not previously possible.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

The research team conducted high-throughput simulations to predict rates of electron emission from dielectric surfaces under AC voltage. By spanning a large range of dielectric barrier discharge (DBD) operating conditions, the team produced a data set that is the first of its kind for DBD plasma generators. The work relies on a method the researchers developed previously for the accurate simulation of material systems containing up to ten million atoms and their electrons. The study also tested the feasibility of numerical integrators for slow, nonperturbative electron dynamics and showed that adaptive numerical integrators perform better than expected. This observation demonstrates that it is possible to leverage numerical engineering methods to optimize or design dynamic electron systems such as DBD plasma generators.

RESEARCH CHALLENGE

The research aims to extend the length and timescales of atomistic, quantum-mechanical materials simulation, particularly of systems containing millions and tens of millions of atoms, under slow, nonperturbative, realistic AC voltages. Materials and phenomena in these temporal and spatial domains are important in many different technologies, from microelectronics to medical science to energy technologies. Traditional electronic structure calculations at this scale are constrained by memory and communication overheads, as they were designed to minimize the number of FLOPS. The research team’s approach prioritizes memory and communication constraints as more limiting, and that is the reason they can simulate ten-million-atom systems on 100 nodes within a few minutes. The team has also taken a similar approach toward extending simulated timescales of electronic systems, with promising results. As a tested application, the researchers have chosen to investigate dielectric surfaces in dielectric barrier discharge plasma generators, which are important in combustion, materials processing, and catalysis.

METHODS & CODES

The simulations use density-functional-based tight-binding, which is a semiempirical electronic structure method. The main computational workflow is to read the atomic coordinates, construct the Hamiltonian, and compute the required eigenspace that denotes the ground state of electrons.

Extending system size. In order to simulate million-atom systems, the team implemented its algorithm [1] using the PETSc distributed matrix library [2]. They used the code they developed to compute the density matrix, which is a fundamental electronic structure quantity for a system of atoms and their electrons. This computational method [1] combines the advantages of two existing linear scaling methods—the kernel polynomial expansion (KPE) [3] and second-order spectral projection purification (SP2) [4] methods. The KPE method is computationally efficient and can be easily expressed in terms of sparse matrix–vector multiplications (SpMVs) but cannot satisfy one of the required constraints on its own. On the other hand, the SP2 method is highly accurate but can be prohibitively costly in terms of memory and communication when expressed in terms of sparse matrix–matrix multiplications. When expressed in terms of SpMVs, the SP2 method scales exponentially with the number of iterations required to converge. An advantage of SP2, however, is that the method converges quadratically near the correct solution P [4]. Thus, the researchers have constructed a hybrid method that takes the inexpensive KPE solution and purifies $P_n$ with a few SP2 iterations that are more expensive.

Extending timescales. The research team tested implicit-explicit time-step integrators based on [5] within PETSc and found them to be appropriate for simulating 400-site electronic systems driven by slow, nonperturbative AC fields. This is significant because quantum-mechanical forward-time simulations are usually done using specialized explicit integrators [6–8]. Numerically, the team found that appropriately tuned implicit–explicit time-steppers conserve the invariants of electronic motion given in [9]. However, these temporal simulations currently scale quadratically with the number of sites, and future algorithmic work will be necessary to improve performance.

High-throughput simulations of small systems. The researchers built upon their electronic structure code, producing a data set for physical systems corresponding to pressures ranging from 10 Pa to 10 GPa and for electric fields between 10 V/m to 1 MV/m. The main computational bottleneck here was the size of data generated as well as constraints on wall-time. The constraint on wall-time was not prohibitive, but it limited the number of physical AC cycles that were averaged to produce the data set.

RESULTS & IMPACT

The team’s recent work expands the scope of atomistic electronic structure simulations, extending the boundaries of the realm of feasible simulations. This allows researchers to simulate larger, more heterogeneous systems that are essential to understanding, designing, and optimizing complex devices and phenomena, directly affecting research on surface and dielectric properties for combustion, catalysis, and materials processing.

WHY BLUE WATERS

Access to the Blue Waters system made this work possible by permitting studies on a single platform that offered both large parallelism and resources for memory-intensive computations. Depending on the tuning of the method, it is possible to either carry out the entire computation on a single node, in a very memory-intensive approach, or, by distributing the computation over many processors, to perform the algorithm in a massively parallel way. The Blue Waters system allowed the team to study these approaches and to plan for future studies with more optimized tuning. The scale of Blue Waters also allowed them to extend the boundaries of possible electronic systems and phenomena that can be simulated in the future. In addition, they benefited from the smooth, transparent, and dependable access to various system modules, as well as helpful and timely responses from Blue Waters staff.

PUBLICATIONS & DATA SETS


ACCELERATING VIRTUAL PROTOTYPING AND CERTIFICATION IN THE AEROSPACE INDUSTRY WITH SCALABLE FINITE-ELEMENT ANALYSIS

University of Illinois at Urbana-Champaign Livermore Software Technology Corp. National Center for Supercomputing Applications

EXECUTIVE SUMMARY

The aerospace industry increasingly relies on physics-based modeling and simulation for the design and analysis of systems in complex engineering products. Advanced modeling and simulation techniques such as finite element analysis (FEA) are being used to replace physical testing with virtual testing and mitigate the costs and risks of certification. Improved fidelity in simulation models generally requires explicit modeling of smaller geometric formations in computational structural models. LS–DYNA is a prominent FEA code used widely in the industry. This research provides the feasibility of efficiently solving extreme-size real-world multiphysics problems at petascale and potentially exascale scales, thus adding novel value to engineering research by enabling the creation of high-fidelity models that yield detailed insight into the performance and safety of proposed engine designs.

METHODS & CODES

The aerospace industry relies on advanced commercial FEA codes that are used for nonlinear, quasistatic, and dynamic deformations in computational structural models. LS–DYNA is a prominent FEA code used widely in the industry. This research has been performed with LS–DYNA and with modules of the LS–DYNA code, including a graph-partitioning scheme and the factorization kernel used in the direct solver. The aerospace community uses LS–DYNA for extreme-event modeling for gas-turbine engines such as bird-strikes, fan-blade-off, and whole-engine failure. The computational time of implicit FEA is dominated by the assembly, constraint processing, matrix reordering, symbolic factorization, numerics factorization, and triangularization. Because they have different parallel efficiencies, each step consumes a varying fraction of the wall-clock time as the processor count grows. A remarkable increase in efficiency (Fig. 2b) has been achieved since the beginning of this multiaxial effort, to the point where LS–DYNA can successfully run the largest engine models on tens of thousands of cores on Blue Waters. The effort includes application–hardware-level profiling, creation of novel scalable algorithms, memory management improvements, computational workflow modifications, and improvements to reduce previously unknown Amdahl (i.e., serial) fractions. The computational complexity of the numerical pipeline is centered on the sparse matrix factorization step.

The team's previous research proved for the first time that a sparse matrix factorization algorithm can scale on tens of thousands of computational cores [1]. Floating-point arithmetic throughput rate and memory utilization are two major metrics that characterize performance scaling of factorization. Fig. 2a shows strong scaling results for the multiaxial solver’s factorization kernel, when factoring symmetric indefinite sparse matrices. An increase in computing operations rate and reduction in memory storage needed per Message-Passing Interface rank has been observed for up to 33,000 OpenMP threads. This sustained performance increase indicates potential for more performance growth. This work constitutes, to the best of the researches' knowledge, the largest implicit LS–DYNA calculations to date, and the results have been presented in technical conferences [2–4].

WHY BLUE WATERS

Blue Waters—with large amounts of distributed memory, thousands of multicores processors, a low-latency file system, and increased bandwidth of advanced interconnect technologies—enabled the research team to address parallel processing challenges and to demonstrate that implicit FEA of large-scale models could be performed in a timely manner using large-scale computing systems. This research on Blue Waters has allowed computer-aided engineering to have a greater impact on the design cycle for new engines, and is a step toward using simulation of digital twins, i.e., computer-generated representations of complex engineering systems.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Significant effort has been placed on advancing new generations of single-molecule detection technologies. Unlike other existing platforms, solid-state nanopores have the versatility to perform tasks that go beyond DNA sequencing, such as detecting epigenetic modifications, RNA and protein sequencing, and folding patterns. In such settings, it is crucial to develop computational tools that enable the identification of optimal solid-state membranes and pore geometries for the problems at hand. In this regard, the research team studies the implementation of innovative 2D solid-state nanopore devices to detect and map minute structural damages in the backbone of the double-strand DNA molecule, which have been suggested as a cause of cancer. The team’s two-step objectives will be achieved through, first, understanding the physics behind the interactions of damaged DNA with 2D solid-state membranes and, second, detecting the variations in ionic current through the pore and the transverse electronic current across the membrane caused by such interactions.

RESEARCH CHALLENGE

A normal human cell is subjected to approximately 70,000 lesions per day. Of these, single-strand DNA (ssDNA) breaks, which have been suggested as a cause of cancer. The team’s two-step objectives will be achieved through, first, understanding the physics behind the interactions of damaged DNA with 2D solid-state membranes and, second, detecting the variations in ionic current through the pore and the transverse electronic current across the membrane caused by such interactions.

METHODS & CODES

This research consists of a two-step process that first includes molecular dynamics (MD) simulations with the latest NAMD version and, second, the exploitation of MD data to calculate the current variations owing to DNA translocation through the nanopore via electronic transport modeling. The system is built, visualized, and analyzed using VMD [2]. The DNA is described by the CHARMM27 force field [3]. An external electric field is applied to the system to drive the DNA nicks through nanopores. For each frame of the trajectory files obtained from the MD simulations, the ionic current blockade is calculated instantaneously [4]. Further, the electrostatic potential induced by the biomolecule around the pore is obtained by using the self-consistent Poisson–Boltzmann equation (PBE) formalism. The PBE is solved numerically using the multigrid method until the convergence criterion is met. Once the electrostatic potential calculated planar to the membrane is obtained, the transverse conductance of the DNA backbone as miniscule as ssDNA breaks using electronic sheet currents obtained across the membrane.

RESULTS & IMPACT

Real-time detection of damaged-DNA strands is nearly impossible and has not been reported by anyone using existing technologies. Fig. 1 illustrates the nanopore setup used for simultaneous calculation of the ionic and transverse sheet currents. Resolving the duration and magnitude of each dip of the ionic current signal gives an insight into the structure of part of the biomolecule inside the pore. Simultaneously, the variations in the electronic sheet current flowing from source to drain across the 2D membrane detect the change of the electric potential induced on the edge of the nanopore by the translocating DNA, revealing the position of the damaged backbone.

The results obtained using this methodology are highly encouraging. In all the simulation runs, the molecule is halted in the pore at the nicked site owing to strong attraction between the graphene membrane and the damaged backbone. This behavior can be explained by the fact that the cleaved backbone of the dsDNA molecule is arrested in the pore owing to higher hydrophobic interactions between the DNA and the graphene membrane.

To validate this theory, the research team calculated the van der Waals energies between the normal DNA with graphene and the damaged DNA with graphene (Fig. 2a). It is clear that there is higher attraction at the nicked-site with the graphene atoms resulting in the molecule being arrested in the pore. The ionic currents calculated for the translocation of 20 base-pair dsDNA with a break in the backbone show no distinct feature contributed by the nicked site on the signal. However, a clear dip is seen in the transverse sheet current signal corresponding to the location of the breakage, enabling the electronic detection of damages (Fig. 2b).

The research team has validated the methodology outlined above by detecting other sequence-specific dsDNA breaks along a randomly sequenced strand. This technique can be easily scaled to have a dense array of multiple g-QPC nanopores implemented on a complementary metal–oxide–semiconductor chip to detect multiple damaged DNA strands in a massively parallel scheme [7]. The researchers strongly believe such a detection mechanism can enable the development of versatile semiconductor electronics for early cancer detection caused by structural modification of the genome.

WHY BLUE WATERS

It is only possible to investigate the interactions of biomolecules with solid-state materials, to characterize the stochastic structural fluctuations of the DNA with nicks translocating through solid-state nanopores, and to further obtain the electronic response using all-atom MD simulations coupled with electronic transport calculations with peta-scale computing resources such as Blue Waters. The research team’s systems consist of about 500,000 atoms, each requiring multiple MD simulation (NAMD) runs. With NAMD code efficiently deployed on XE/XK nodes to run highly parallel simulations of large biomolecular systems, Blue Waters is well-suited for the requirements of this research.

PUBLICATIONS & DATA SETS

COMPRESSIBILITY EFFECTS ON SPATIALLY DEVELOPING PLANE FREE SHEAR LAYER

Allocation: Innovation and Exploration/190 Keh
PI: Fared Farzad Mashayek
Co-PIs: Jonathan Komperda, Dongru Li, Ahmad Peyvan

EXECUTIVE SUMMARY

Compressible turbulent free shear flows have a wide variety of applications in modern technology and commonly occur in engineering systems such as gas turbines, scramjet engines, rocket exhausts, and the like. However, a fundamental understanding of the physics of such flows is limited by a lack of detailed information about the turbulent transition process and the turbulent quantities under the influence of compressibility. This work is the first computational effort to investigate the compressibility effects on the transition to turbulence and the turbulent energy exchange mechanisms in a three-dimensional, spatially developing turbulent plane free shear layer, via data produced by direct numerical simulation (DNS). The DNS was performed using a high-order discontinuous spectral element method for different convective Mach numbers with a naturally developing inflow condition. The location of the transition zone was predicted by the analyses of vorticities and the turbulent viscous dissipation rate. The energy exchange was examined via the analyses of the budget terms of turbulent kinetic, mean kinetic, and mean internal energy transport equations.

METHODS & CODES

The research team performed DNS on Blue Waters using a high-order DSEM [1–3]. The DSEM used hexahedral nonoverlapping elements in an unstructured grid. A high-order local basis function with a different polynomial order within each element in order to change the grid resolution during simulation. The method introduces negligible diffusion and dispersion errors and is spectrally convergent for smooth solutions [1,2]. In the current work, the grid consists of 1,368,260 elements with a polynomial order of p = 5, resulting in a total of 395,544,160 solution ordinates. The storage of these variables was necessary both on computation and storage of 47 variables for fluctuations, nine for averages, five for instantaneous variables, and three for coordinates. The storage of these variables was necessary both on disk as well as in memory at runtime, which exceeds the available storage space and memory available per core on many supercomputers. Thus, this combination of computation and data storage is ideal for performing the simulations, considering that the efficiency is relatively high (82%) on Blue Waters.

RESULTS & IMPACT

This work presents the first DNS results for a spatially developing, 3D compressible turbulent FSL with a naturally developing inflow condition for different convective Mach numbers. It shows a 3D representation of the instantaneous turbulent structures via iso-surface of the second invariant of velocity gradient tensor for convective Mach numbers of 0.3, 0.5, and 0.7 (Fig. 1). Further, it demonstrates the vortex stretching mechanism in the spanwise direction, such as the formation of secondary streamwise vortices and the breakdown of primary spanwise vortices, which are responsible for the onset of turbulence transition. Also, the contours of the instantaneous spanwise vorticity (Fig. 2) indicate the location of the turbulence transition region under the influence of compressibility for each case. The spiral-type rolls ups can only be observed in the flow with the highest convective Mach number, 0.7. The instantaneous variables and their statistics were used to investigate the compressibility effects on turbulence transition and turbulent energy exchange and to calibrate turbulence models.

This work conducts the DNS of an FSL to generate detailed data for all flow field variables in both the transition and self-similar turbulent regions for different convective Mach numbers. It identifies the location of the turbulence transition zone under the influence of compressibility. It determines the energy exchange mechanisms responsible for energy redistribution among turbulent kinetic energy, mean kinetic energy, and mean internal energy and examines the influence of compressibility on such mechanisms. It provides calibrations for turbulent models.

WHY BLUE WATERS

To resolve all relevant scales of turbulent structures, the grid used in this work consisted of roughly 0.3 billion solution points. Also, the generation of full statistics for the cases required the computation and storage of 47 variables for fluctuations, nine for averages, five for instantaneous variables, and three for coordinates. The storage of these variables was necessary both on disk as well as in memory at runtime, which exceeds the available storage space and memory available per core on many supercomputers. Thus, this combination of computation and data storage is well suited for a leading-edge petascale high-performance computing system such as Blue Waters.

PUBLICATIONS & DATA SETS

OUTWARDLY PROPAGATING TURBULENT FLAMES

Allocations: illinois/80 Kish
PI: Moshe Matalon1
Co-PI: Shikhar Mehra1

1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

The research team’s objective is to simulate the evolution of centrally ignited flames in order to assess the roles played in their propagation of hydrodynamic and thermo-diffusive instabilities as well as background turbulence. The simulations were conducted within the framework of the hydrodynamic theory, which has been systematically derived using a multiscale asymptotic technique [1] and is thus free of turbulence-modelling assumptions and/or ad hoc adjustment parameters. The flame devolves into a well-defined moving interface that separates the burned products from the unburned mixture. The flame propagation relative to the flow depends on the local stretch rate, which combines the effects of surface geometry and hydrodynamic strain rate. The stretch rate is modulated by a mixture-sensitive parameter known as the Markstein number, which mimics the effects of diffusion and chemical reactions occurring inside the thin-flame zone. This eliminates the necessity for explicit reaction-chemistry modeling, thereby alleviating mesh size and timestep restrictions that render direct numerical simulation studies impractical.

RESEARCH CHALLENGE

Combustion and well in the foreseeable future remain the primary mode of power generation. The process is inherently complex, involving the interdiffusion of a large number of chemical species (nearly 5,000 for real fuels) that interact chemically as well as the generation of heat that affects the density of the mixture and modifies the underlying flow field.

Flames encountered in most applications are turbulent in nature. Turbulence adds a stochastic, time-dependent, three-dimensional aspect to this intricate problem. While fundamentally processes such as reaction chemistry, molecular, and energy transport are reasonably well known, it is still a major challenge to integrate these components with a highly turbulent flow field to produce practical computational results for the description of turbulent combustion. Additionally, complexity arises from intrinsic flame instabilities associated with thermal expansion and/or the disparity between the diffusion rates of the different species and of mass and energy, which are known to distort the flame even under laminar conditions.

The hydrodynamic theory adopted in this work is formulated in an intrinsic coordinate system [2] that requires a parametric description of the flame surface. The flame's evolution is described in terms of surface differential operators. The numerical solution of such an equation on an arbitrary, time-dependent surface is still an active area of research. Constructing an intrinsic coordinate system is nontrivial and computationally expensive, particularly for an evolving highly corrugated surface. The frequent need for remeshing renders this problem computationally intractable.

The research team uses a new class of embedding methods to extend the surface differential equation into Cartesian space such that when the solution is restricted to the surface, the solution to the original problem is recovered. This embedding method also allows the researchers to solve the partial differential equations using Cartesian operators instead of surface differential operators, further reducing execution time. The implementation appropriates concepts from computational geometry and has been used to study a diverse array of applications including image-processing.

METHODS & CODES

The computations were made possible by coupling the embedded manifold approach with an adaptive mesh, variable-density incompressible Navier–Stokes solver. It is built on AMReX, an open source framework, to write massively parallel, block-structured adaptive mesh refinement applications [3]. The code underwent restructuring to improve efficiency and reduce memory demands for the nearly 30 million particles that constitute the turbulent spherical flame surface. Sample calculations illustrating a wrinkled flame front interacting with eddies of different sizes are depicted in Fig. 1.

RESULTS & IMPACT

The major contribution of this work was to develop a scalable, hybrid partial differential equation-based Cartesian embedding method for moving surfaces. This method is capable of handling multivalued and disjointed flame surfaces to simulate a complex, turbulent premixed flame. The methodology was used to investigate the effects of the hydrodynamic, or Darrieus–Landau, instability on early and long-time flame kernel development in turbulent flows. The hydrodynamic instability resulting from the gas expansion is responsible for the corrugated appearance of the flame surface even in the absence of significant perturbations such as boundaries, obstacles, and/or turbulence. The instability is known to induce acceleration and enhance the flame propagation speed. The most practical outcome of this work includes the derivation of scaling laws for the turbulent flame speed in terms of flow and physicochemical characteristics. Its importance is in estimating fuel-burning rates in internal combustion engines and other similar applications.

WHY BLUE WATERS

Access to the Blue Waters system has been instrumental to this study; not only did it afford the research team access to extensive computing power, it also made available large memory nodes that were capable of processing the large number of particles on the flame surface.

PUBLICATIONS & DATA SETS

DEEP LEARNING FOR HIGGS BOSON IDENTIFICATION AND SEARCHES FOR NEW PHYSICS AT THE LARGE HADRON COLLIDER

EXECUTIVE SUMMARY

The Large Hadron Collider (LHC) is the world’s most powerful particle accelerator, designed to study the fundamental nature of matter and the forces that govern its interactions by colliding beams of protons at the highest-available energies. The research team is using Blue Waters to process, simulate, and analyze high-energy proton–proton collision data produced by the ATLAS experiment at the LHC and to improve researchers’ sensitivities to new phenomena by developing novel approaches to identifying Higgs bosons produced with high momentum at the LHC by using machine learning techniques.

RESEARCH CHALLENGE

The goal of particle physics is to understand the universe at its most fundamental level, including the constituents of matter, their interactions, and the nature of space and time itself. This quest is one of the most ambitious and enduring of human endeavors.

The Standard Model (SM) of particle physics describes all known fundamental particles and their interactions, including the Higgs boson, which was discovered at the LHC in 2012 with significant contributions by the Illinois (Neubauer) Group. The discovery led to François Englert and Peter W. Higgs receiving the 2013 Nobel Prize in Physics. The SM has withstood the last 40 years of experimental scrutiny, with important exceptions being neutrino mass, dark matter, and dark energy. Recent developments in particle physics and cosmology raise the exciting prospect that we are on the threshold of a major step forward in our understanding.

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RESEARCH CHALLENGE

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The research team is working to extend this approach to the single-lepton channel, which brings additional challenges, and to develop it as a general W+W⁻ → hS tagger for ATLAS that can be applied to searches involving boosted dibosons and not limited to the semileptonic Higgs + scalar searches described here. The team is using Blue Waters to implement this approach as a jet-mass decorrelated tagger to avoid learning the mass and tracking DNNs using both calorimeter and tracking information.

RESULTS & IMPACT

Fig. 2 shows a particular one-month period in 2018 in which 35,000 Blue Waters cores were utilized to process 35 million collision events. The top panel of this figure shows that this approach is cost-effective, boosting cluster utilization, and has no adverse effect on other high-performance computing workloads. The job output was made available to the rest of the ATLAS collaboration for use in analysis of the LHC data to improve SM measurements and to search for new physics beyond the SM. Fig. 2b shows the Higgs boson identification accuracy as a function of the number of training epochs for a variety of DNN configurations and hyperparameter settings. The team is also using Hyperopt, a convenience wrapper using Hyperopt with Keras models, on Blue Waters to automate the scanning of hyperparameters in a variety of machine and deep learning approaches to improve the Higgs boson identification over backgrounds. The techniques show promise in addressing the challenges of boosted Higgs boson identification and improving the sensitivity of new physics searches at the LHC.

Why Blue Waters

Blue Waters, as a large CPU and GPU resource with high data-throughput capabilities, greatly facilitated this research. The strong support for containers allowed the research team to deploy their science application on Blue Waters’ nodes. Also, Blue Waters provided a means for a highly parallelized and automated scanning of free parameters in the team’s machine learning configurations and, therefore, rapid optimization of the researchers’ boosted Higgs boson identifier.

PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY

Quantum computing is a revolutionary method of information processing that takes advantage of the quantum mechanical principles of superposition and entanglement. It is theoretically proven to provide a massive improvement of the complexity of certain algorithms used in cryptography, database search, and modeling correlated quantum systems such as atoms, molecules, and superconductors.

One of the most scalable designs of quantum information processing chips is based on the interactions between a few electrons trapped in silicon chips under metallic electrodes. These trapped electrons can be selectively manipulated in a crystal containing hundreds of millions of other electrons and nuclei, defects, magnetic and electrical noise, and mechanical vibrations [1]. In this project, the research team developed a method for computing the interactions between the trapped electrons in a realistic environment and studied the effect of variations in the environment on the interactions. This study will help in accelerating the experimental and chip design processes of quantum computing systems.

RESEARCH CHALLENGE

The team computed the interaction between two electrons trapped under positively charged electrodes occupying an area of 25 nanometers (nm) x 25 nm and separated by 10 nm. The efficient working of these chips requires the interaction strength to be designed accurately. The interaction strength depends on multiple factors such as device geometry, electrode voltages, neighboring crystal atoms, proximity to other charged defects, electrical noise, and crystal strain. The biggest challenge is to efficiently address the impact of all these factors to provide insight and guidance into the design of quantum logic gates.

METHODS & CODES

The factors that determine interaction strength can be grouped by the physics that efficiently describe them, i.e., continuum, atomistic, and correlated. The team has developed three different modeling tools to address each of these: (1) finite-element method-based software for continuum physics, (2) large-scale atomistic tight binding software for atomic and solid-state physics, and (3) full configuration interaction method-based software for correlated physics. The tools consecutively process data to arrive at the final results. The methods are embedded in the NEMO package.

RESULTS & IMPACT

The research team has shown the impact of gate lengths, gate spacings, and voltages on the quantum mechanical interaction strength between two qubits (the basic unit of quantum information). This “exchange” interaction has been shown to be sensitive to the design. The researchers have proposed the use of a special “exchange gate” for efficient control of two qubits. They also have shown that nonideal factors such as defects and strain can cause electrical distortions in the device. However, in most cases electrical tuning of gate voltages can be used to overcome nonideal behavior.

WHY BLUE WATERS

All three methods used in this project require large processing power, memory, and storage facilities. Furthermore, the methods are often run sequentially with data being translated from one form to another. Blue Waters provided all the needed resources. Access to a large number of nodes and storage disks was particularly critical. Furthermore, the support staff constantly monitored the system and helped with libraries and compilation, which enabled the research team to focus on the science.

PUBLICATIONS & DATA SETS

SIMULATION OF ROTATING DETONATION ENGINES

Allocation type: GLCPC/480 Knh
PI: Venkat Raman

1University of Michigan

EXECUTIVE SUMMARY

Rotating detonation engines (RDEs) have received increased attention as possible replacements for conventional gas turbine systems owing to their expected high thermal efficiency. The compression across the detonation wavefront driven by chemical reactions induces additional pressure gain. Although extensive research has been performed by both the experimental and numerical communities to realize these devices, they are limited to hydrogen/air chemistry because of its high detonability and relatively simple reaction mechanism. To make RDEs more practical and applicable, simulations of the detailed physics with hydrocarbon chemistry need to be conducted. With the allocated time on Blue Waters in 2019, the researcher has performed a series of full-system simulations with ethylene/air chemistry. These simulations reveal that the slow wave propagation observed in experiments is due to a wave aided by the deflagration mode, with wave speeds within 5% of the experimental results.

RESEARCH CHALLENGE

Although RDEs are increasingly being studied, the concept originates from the 1960s. Recent advancements in materials science and a better understanding of detonative combustion enable the RDE system to be operable. Extensive research has been performed through experiments and simulations to understand and optimize the operation of RDEs [1–3]. However, most of the research has been conducted with hydrogen/air mixtures, while hydrocarbon chemistry is the more practical fuel [2,3]. Several experiments with ethylene/air mixtures reveal that the wave speed is drastically slower than hydrogen/air mixtures, at nearly 50% of the ideal case [1]. Furthermore, the flame front is thicker than that of hydrogen/air chemistry. To understand the detailed physics of combustion in RDEs, simulations of the full system are necessary.

Full-system RDE simulations with ethylene/air chemistry raise three primary challenges owing to their unique geometry and dynamics. First, the fuel and oxidizer are separately injected using a nonpremixed injection scheme, which requires the use of unstructured grids. Secondly, ethylene/air chemistry is more complex and stiffer than hydrogen/air chemistry. In other words, the number of species being transported will increase the computational cost. Lastly, a finer resolution is necessary to resolve the reaction induced by the shock wave at the wavefront. Since the geometry is complex and three-dimensional, a finer resolution exponentially increases the computational cost. To perform the full-system simulation, a highly scalable solver and a large amount of allocation time on high-performance computing resources are necessary.

METHODS & CODES

The University of Michigan detonation solver, UMdetFoam, is based on OpenFOAM and Cantera. OpenFOAM provides the finite-volume tools, which are widely used in the turbulent combustion community. UMdetFoam implements a MUSCL-based Harten–Lax–van Leer-contact scheme for space and second-order Runge–Kutta scheme for time integration. Diffusion terms are discretized by the Kurganov, Noelle, and Petrova method. In order to handle chemistry integration, this finite-volume method was coupled with Cantera, an open-source framework for chemical kinetics, thermodynamics, and transport processes. UMdetFoam has MPI-based parallelism with linear scalability demonstrated up to 60,000 cores, with support for GPUs. For this study, a reduced-order two-step mechanism was employed to reduce the computational cost.

RESULTS & IMPACT

In this study, the ethylene/air RDE facility at the Air Force Research Laboratory was simulated. The channel width was 22.86 mm, and the dimensionless area ratio between the oxidizer inlet and the detonation chamber was 0.059.

The full-system simulation enabled extraction of extensive data on the physics in the combustion facility. Fig. 1 shows the general behavior of the system. The pressure wave propagates in the azimuthal direction, aided by the reaction. The wavefront of this RDE is thicker than that of hydrogen/air, as reported in the 2018 Blue Waters Annual Report. Furthermore, oblique shock waves are not created with ethylene/air mixtures, and the product gases appear at some distance from the chamber bottom. This wave standoff behavior is also observed in the experiment. Analysis suggests that the wave is not in the detonation mode but is in a deflagration mode strong enough to sustain the wave. The incomplete mixing and low detonability of the mixture cause this deflagration-dominant mode of operation. The simulation captures the slow wave speed within 5% of the experimental data, which is almost 50% of the ideal condition. The fuel and oxidizer injection behavior are extracted from the simulation as well. The fuel stream is pushed to the outer wall by the oxidizer stream, as shown in Fig. 2. In other words, the mixing is not enhanced near the chamber bottom, causing the standoff of the flame.

The simulation also shows that the injection velocity was almost constant during RDE operation because the wave is too weak to affect the injection dynamics. This result can help researchers to optimize the design of RDEs and to understand the effect of low detonability and fuel-oxidizer stratification on the wave structure. Design improvements resulting from high-fidelity simulations and experiments bring RDE systems closer to realization.

WHY BLUE WATERS

The Blue Waters high-performance computing resource greatly accelerated this research for three primary reasons: (1) users are provided with a large number of cores to run cases and exploit the parallelizability of the solver, which is necessary to simulate full-system RDEs; (2) the working directory allows users to store the large amounts of data (50 TB) generated by numerical simulations without concerns over exceeding a storage quota; and (3) helpful support staff are available to professionally and promptly reply to user questions and concerns. In this study, nearly 10,000 cores were parallelized to perform full-system RDE simulations. The computing resources allowed the project to quickly implement, test, and deploy computational tools and to achieve the desired results.

PUBLICATIONS & DATA SETS

MAPPING PROTON QUARK STRUCTURE: LOOKING INSIDE THE PROTON—HOW DO QUARKS SPIN?

Allocation: NSF PRAC/9,440 Knh
1University of Illinois at Urbana–Champaign
2ETH Zürich
3INFN Torino
4JINR Dubna
5University of Novosibirsk
6LIP Lisbon
7University of Munich
8University of Bonn
9CERN
10University of Ioannina
11Technical University of Denmark
Collaborators: Marco Meyer1,2, Robert Heitz1, April Futch1, Charles Naim2, Angela Maggiora3, Andrei Gridin4, Nicolas Pierre2, Anatolii Koval5, Celso Franco5, Yu–Chin Liu, Florian Kooper5, Heer Pekela5, Babak Parsamyan5

EXECUTIVE SUMMARY

COMPASS (the Common Muon and Proton Apparatus for Structure and Spectroscopy experiment) probes proton substructures scattering high-energy pion and muon beams off nuclear targets at CERN. The experiment explores the momentum and coordinate phase space of quarks inside the proton. Observing correlations between proton spin and the transverse momentum of quarks will shed light on the quark dynamics inside the proton and will provide a critical test of fundamental predictions derived from quantum chromodynamics, the quantum field theory describing the nuclear force. The measurements produced 4.5 petabytes of experimental and simulated data. Raw COMPASS data of the 2018 Drell–Yan campaign with the nuclear physics community about one year earlier than usual. This fast turnaround time for the analysis was unprecedented.

RESEARCH CHALLENGE

Observation of the sign change of the Sivers function (“Sivers functions”) in Drell–Yan scattering compared to existing measurements in semi-inclusive deep-inelastic scattering (SIDIS) is one of the few performance Nuclear Science Advisory Committee [1] milestones for DOE- and NSF-funded research in nuclear physics. The 2015 and 2018 Drell–Yan campaigns of the COMPASS experiment at CERN constitute the first measurements addressing this question [2]: the negative pion beam from the Super Proton Synchrotron was impinged on a target of transversely polarized protons. Sivers functions arise from correlations between proton spin and quark transverse momentum and thus appear connected to quark orbital motion inside the proton.

RESULTS & IMPACT

Blue Waters allowed the research team to analyze the physics results of the 2018 COMPASS run with the nuclear physics community about one year earlier than usual. This fast turnaround time for the analysis was unprecedented.

METHODS & CODES

The team used Blue Waters (BW) for four major tasks: experimental data production to convert raw data into a format for physics-level analysis; extraction of detector efficiency maps from raw data as input to realistic simulations; Monte–Carlo simulations; and physics-level analysis. The various work flows are sketched in Fig. 1.

Three petabytes of raw COMPASS data collected at CERN were transferred to BW using the File Transfer System FTS3 [3], a bulk data mover created to globally distribute CERN–LHC data. The data were packed into tar files of 100 GB on BW Lustre and then stored on BW tape. Upon production request by the COMPASS analysis coordinator, they were then retrieved from tape. For each triggered event in COMPASS, the information of the detectors was recorded by the Data AcQuisition (DAQ) system. The COMPASS Reconstruction Analysis Library (CORAL) software performed the conversion of raw data information to physical quantities. CORAL’s function was to reconstruct particle trajectories and momenta, and the position of vertices. The reconstructed information was stored in the form of Data Summary Trees (DSTs), which were used and analyzed using the COMPASS Physics Analysis Software Tools (PHAST). CORAL and PHAST jobs were submitted to the BW node using the production framework ESCALADE, which allows for a detailed bookkeeping of job status, failure, and output. Detector efficiencies were extracted from a sampled fraction of the experimental data. They required separate submissions to the BW grid for each of the 240 detector planes, which made the efficiency maps about a factor of seven more CPU-expensive compared to the standard data productions.

The production of Monte–Carlo data began with the generation of signal and background events with event generator packages. For the simulation of the detector response to the physics event, a GEANT4 [4] toolkit was then used based on the description of the COMPASS apparatus. Lastly, simulated hits were subjected to the same reconstruction CORAL and PHAST codes as experimental data.
ELECTRON DYNAMICS OF ION-IRRADIATED TWO-DIMENSIONAL MATERIALS

Executive Summary

Exploiting the unique properties of two-dimensional materials for next-generation electronic devices and other novel technologies depends on high-resolution techniques for nanoscale imaging and structure manipulation, which often employ focused ion beams. Along with radiation-induced degradation of thin materials and materials’ surfaces in space and nuclear applications, solving this technological challenge demands a detailed understanding of the response of thin materials to ion irradiation. In order to accurately study the subfemtosecond electron–ion dynamics in thin materials under ion irradiation, the research team performed first-principles simulations of few-layer graphene irradiated by charged particles ranging from protons to xenon ions. This research lays the groundwork for a predictive computational framework capable of determining optimal ion beam parameters for a desired imaging or patterning application and of indicating a material’s susceptibility to radiation-induced defects.

Research Challenge

Two-dimensional materials have a variety of remarkable properties, making them promising candidates for a wide range of potential applications including flexible electronics, solar cells, nanoscale sensors, and other electronic devices [1]. However, the properties of atomically thin materials are often sensitive to defects, nanopores, functionalization, and other types of nanostructure, which can either degrade performance when undesirable or enable an application when intentional [2,3]. Thus, precise techniques for imaging and patterning 2D materials, likely reliant on focused beams of energetic ions, are necessary for scalable and reliable manufacturing of devices based on 2D materials. In addition, materials for space and nuclear applications must withstand constant bombardment by energetic ions, and mitigating erosion of nuclear cladding or radiation shielding materials fundamentally involves controlling surface behavior. Overcoming these engineering challenges requires a thorough understanding of the response of 2D materials and materials’ surfaces to ion radiation.

However, the vast majority of current knowledge about ion-irradiated materials pertains to bulk materials, leaving surface effects largely unknown. The research team’s first-principles approach provides unprecedented insight into electron dynamics in ion-irradiated materials, which is critical for developing both novel devices based on 2D materials and radiation-resistant materials for space and nuclear applications (see Fig. 1).

Methods & Codes

The research team used Qbox/Qb@ll [4], their highly parallel implementation of real-time time-dependent density functional theory [5], to perform accurate first-principles simulations of excited-electron dynamics. This approach treats nuclei as classical point charges interacting electrostatically with electrons. Electrons are treated quantum-mechanically; their quantum orbitals, represented in a plane-wave basis, are governed by the time-dependent Schrödinger equation (TDSE) equations, a system of coupled partial differential equations. The team used the common adiabatic (without transfer of heat or mass) local-density approximation for the exchange–correlation potential describing the quantum correction to the electron–electron interaction.

Starting with the lowest energy configuration of the material as the initial condition, the electronic orbitals were propagated in time by numerically integrating the TDSE equations. The simulations generated a time-dependent electron density that was further analyzed to extract the secondary electron yield and the charge captured by the projectile, among other quantities.

Results & Impact

First, the team explored new numerical methods that could accelerate first-principles simulations of excited-electron dynamics, enabling study of longer timescales and larger systems. Specifically, the researchers interfaced Qb@ll with the PETSc library [6,7], allowing rapid testing of different numerical integration algorithms for propagating the electronic states over time. Thus far, the team has concluded that enforced time-reversal symmetry outperforms all available Range–Kutta schemes in terms of stability and time-to-solution. Identifying an integrator that reduces computational cost while sacrificing accuracy would help make feasible extremely accurate simulations of defect formation in materials. This capability would deepen the understanding of defect formation mechanisms, provide transformative insight for nanostructure engineering techniques, and expedite the development of novel electronic devices for the benefit of society.

The team also implemented and applied new analysis techniques to extract the projectile charge state and the kinetic energy spectrum of emitted electrons. These methods provide additional information about the charge dynamics and energy dissipation mechanisms occurring as the ion interacts with the material, allowing more detailed insight into surface effects and predictions of projectile parameters most likely to induce defects. While models for bulk materials typically assume an equilibrated projectile charge and do not consider energy lost to electron emission, the team found that a highly charged projectile’s effective charge varies dynamically as it traverses graphene and does not reach an equilibrium value within a few-layer sample (see Fig. 2). Furthermore, the initial charge of a heavy projectile strongly influences both energy transfer and electron emission, and accounting for electron emission can change the projectile parameters that maximize energy deposited in the material. These findings not only demonstrate the disparity in behavior between few-layer material and bulk materials but also establish the need for further study of ion-irradiated 2D materials and special tuning of ion beam parameters for imaging and processing 2D materials.

Why Blue Waters

Blue Waters enabled the research team to conduct the long simulations of large systems involved in this project. In order to accurately model a few-layer material or a material surface under irradiation, scientists must evolve hundreds or thousands of electrons over thousands of timesteps in an elongated simulation cell containing a large vacuum outside the material. These aspects make the simulations computationally expensive and are only possible with a massively parallel implementation of the first-principles approach and a high-performance supercomputer.

Publications & Data Sets


Figure 1: The first-principles simulations of ion-irradiated few-layer materials provide information about secondary electron emission, energy transfer, and excited electron dynamics. Understanding these processes will advance radiation tolerance and improve ion beam imaging and patterning techniques needed to create novel electronic devices based on 2D materials.
DISCOVERY OF NEW PLASMONIC MATERIALS VIA HIGH-THROUGHPUT MACHINE LEARNING

EXECUTIVE SUMMARY
Plasmonics aims to manipulate light through choice of materials and nanoscale structure. Finding materials that exhibit low-loss responses to applied optical fields while remaining feasible for widespread use is an outstanding challenge. Online databases have compiled computational data for numerous properties of tens of thousands of materials. Owing to the large number of materials and high computational cost, it is not viable to compute optical properties for all materials from first principles. For this project, plasmonic quality factors for a training set of 1,000 metals and 2,000 semiconductors were computed using density functional theory (DFT) and the Drude model. The research team trained regressors to rapidly screen the Materials Project (MP) database to identify potential new plasmonic metals. Descriptors were limited to symmetry and quantities obtained using the chemical formula. The machine learning models filtered through 7,445 metals in the MP database. From this, the team predicted AlCu3, ZnCu, and ZnGa3 as candidates and verified their quality factors with DFT.

RESEARCH CHALLENGE
As mentioned before, the field of plasmonics seeks to manipulate light at the nanoscale. Precise control over plasmon response enables many applications including subwavelength waveguides [1], nanooptics [2], superlenses [3], subwavelength imaging [4], nanochemistry [5], and biosensors [6]. Currently used plasmonic materials consist of noble metals and electron-doped semiconductors with high electrical conductivity [7]. Unfortunately, noble metals suffer from large losses in the visible spectrum owing to absorption while semiconductors require high electron doping concentrations. Further advances of plasmon-based technology require finding new high-performance materials.

METHODS & CODES
To quantify the response of a material to an applied electrical field, the team computed its dielectric function. Two dominant contributions to the dielectric function were considered: interband transitions of electrons from valence states to conduction states near the Fermi energy. This imposes challenging requirements for CPU hours that cannot be met by a system such as the Campus Cluster. The computational cost of DFT scales as the cube of the number of electrons; for large system sizes such as the Materials Project database with the pymatgen open source library [9,10].

RESULTS & IMPACT
We have used DFT calculations of materials’ dielectric functions to train and validate machine learning models which predict plasma frequencies and plasmonic quality factors for metals and semiconductors in the Materials Project database. The constructed models allow for rapid calculation of the optical properties necessary to predict the suitability of a material for plasmonic applications. By applying the models to a large database, we have been able to search for predicted high-quality factor metals and semiconductors without requiring explicit DFT calculations for all materials in the database, significantly reducing the computational cost. From the database metals, we have identified three potential new metals, AlCu3, ZnCu, and ZnGa3, as candidates and predicted high-quality factors for all available materials. For the 200 materials with the largest predicted quality factors, the dielectric functions and quality factors were explicitly calculated with DFT.

WHY BLUE WATERS
The present research requires DFT simulations for thousands of materials with up to dozens of atoms. The computational cost for DFT calculations is further increased by the need for accurately mapping the electronic energies near the Fermi surface. Dense 33 x 33 x 31 point meshes to sample momentum space are required to obtain converged calculations of the electronic properties near the Fermi energy. This imposes challenging requirements for CPU hours that cannot be met by a system such as the Campus Cluster. The computational cost of DFT scales as the cube of the number of electrons; for large system sizes such as in this project, available computing power can quickly become a limiting factor. Efficiently carrying out electronic structure DFT calculations for this work requires nodes with fast communication. In addition, this research requires multiple of these runs and, hence, it needs a machine such as Blue Waters that allows the research team to routinely carry out this work.
TURBULENT MULTIPHASE THERMAL FLOW MODELING OF DEFECT FORMATION MECHANISMS AND ELECTROMAGNETIC FORCE EFFECTS IN CONTINUOUS STEEL CASTING

Allocation: Illinois/TS Kibb

RESULTS & IMPACT

Turbulent fluid flow, surface slag/molten steel interface instability, liquid-level fluctuations at the meniscus, slag entrainment, and entrainment were computed from the multiphysics model simulations. This enables understanding of slag defect formation mechanisms, especially the slag entrapment owing to sudden level drops near meniscus regions. From the validated EEDPM model [4,5] simulations, argon bubble behavior and size distributions in the turbulent molten steel flow inside a slide-gate nozzle of the real caster [6] were revealed in detail. This calculation is expected to contribute to more accurate particle-capture results by being coupled with the advanced particle capture model [7]. In addition, the study investigated initial solidification-related defects such as meniscus freezing, hook formation [9,10], and longitudinal crack formation near the meniscus with the further aid of the coupled heat-transfer model. For example, in mega-thick slab casting, as shown in Fig. 1, the distribution of superheat flux around the meniscus is very nonuniform with the use of high-precision, customized mold flow pattern. In particular, superheat was unable to reach the meniscus corner, leading to deep hooks and/or longitudinal crack formation. In addition, the effect of the M–EMS on mold flow pattern, temperature, and superheat distribution was quantified from the magnetic-induction MHD model simulations. With M–EMS, the superheat flux at the shell front became more uniform owing to the rotating flow around the perimeter of the mold, resulting in higher superheat flux to the corners, as shown in Fig. 2. This effect is expected to lessen initial solidification defects so long as the magnetic field strength is within an optimal range.

WHY BLUE WATERS

The high-resolution models used to more accurately simulate and better understand defect formation mechanisms in continuous steel casting are very computationally intensive. The many coupled governing equations need to be solved for turbulent flow, particle transport and capture, temperature, and MHD fields. Moreover, many computational cells are required to capture these complex and interrelated phenomena on micron and millisecond scale in the huge domain. Blue Waters enables such high-resolution simulations in a reasonable time frame by speeding up ANSYS Fluent HPC calculations by more than 3,000 times and CUFLOW calculations by 50 times. Furthermore, the Blue Waters parallel computing environment enables numerous cases to be calculated simultaneously with different process conditions for parametric studies essential to optimize this complex process. Thus, the Blue Waters supercomputer provides a great contribution to obtaining deep insights into complicated defect-related phenomena with high resolution in order to improve this important commercial process.

PUBLICATIONS & DATA SETS

INVESTIGATION OF SEDIMENT TRANSPORT THROUGH AQUATIC VEGETATION USING LARGE-SCALE HIGH-FIDELITY TURBULENCE SIMULATIONS

Allocation: Illinois/680 Knh
PI: Rafael Tinoco Lopez
Co-PI: Paul Fischer
Collaborators: Som Dutta, Pallav Ranjan

University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

Turbulence generated by aquatic vegetation in fluvial and coastal systems drives changes in the hydrodynamics and sediment mechanics within aquatic ecosystems. It is expected that plants extract energy from the flow, reducing near-bed flow velocities, thus damping erosion. However, turbulence generated by vegetation patches can actually enhance resuspension and transport under the right conditions. This study uses direct numerical simulations (DNS) and large-eddy simulations (LES) through various arrays of idealized vegetation, represented as cylinders, to increase the understanding of the interactions among vegetation, flow, and sediment. Simulations are conducted using the high-order spectral element-based computational fluid dynamics (CFD) solver Nek5000. Staggered arrangement of cylinders mimicking an actual experimental setup have been simulated to shed light on the details of flow features and suspended sediment distribution as a function of flow, plant, and patch characteristics, thus increasing the understanding of different hydro- and morphodynamic processes.

RESEARCH CHALLENGE

Vegetation patches in rivers and coastal areas act as ecosystem engineers to modify various aspects of their own ecosystem [1]. Aquatic vegetation provides a wide range of ecosystem services [2], from nutrient uptake and oxygen production to habitat creation to bed stabilization and even carbon sequestration and nutrient farming. Owing to computational limitations, past computational studies have mostly focused on using CFD models based on Reynolds averaged Navier–Stokes equations, which only provide an averaged approximation of the flow field. The few studies that have used high-fidelity LES have been limited by the number of vegetation elements that can be modeled. Further, the number of both experimental and numerical studies investigating vegetation–flow–sediment interactions is still very limited. Most of the existing data in this area come from laboratory experiments [3] that simulate conditions closer to nature but often lack the spatial and temporal resolution required to capture some fundamental processes in detail.

This study is coupled with experimental research currently being conducted at the Van Te Chow Hydrosystems Laboratory and the Ecohydraulics and Ecomorphodynamics Laboratory at the University of Illinois at Urbana–Champaign. The study conducts numerical simulations at an unprecedented scale, resolving details that in conjunction with the experiments will provide as yet unknown insights into the fundamental dynamics of flow and transport in the presence of aquatic vegetation [4]. These large-scale computations will help improve lower-order models of the processes while also informing better experimental design and measurement practices. The number of computation points required to model the whole domain is near 1.2 billion, making the study a unique opportunity because of the scale and complexity of the processes investigated. While such simulations are still tractable on a petascale platform such as Blue Waters, the computational cost is too high, resulting in a reduced number of modeled scenarios, which constrains the insights that a broader range of parameters could yield.

METHODS & CODES

The research team conducted high-resolution LES and DNS of the flow at different configurations of the idealized vegetation using the open source, spectral element-based high-order incompressible Navier–Stokes solver Nek5000 [5,6]. Sediment transport was modeled under the Eulerian framework using the advection–diffusion equation [7], making this study one of the first to look at the complex interaction among sediment–flow–vegetation using high-fidelity CFD simulations.

RESULTS & IMPACT

The research team conducted three-dimensional LES for a range of Reynolds numbers between 8,000 and 20,000 for a staggered array of rigid cylinders. The first part of the study focused on understanding hydrodynamic changes to the flow field owing to the presence of an emergent vegetation array compared to existing experimental data. To allow for access of measuring probes in laboratory experiments, a section of a vegetation patch is often cleared out, resulting in a small gap where the measurements are taken. The team has proven that measurements within such a gap may not be representative of flow within the patch (Fig. 1). An optimal dimension of a gap in the vegetation can be found such that experimental measurements of flow statistics within it are representative of the flow field within the array. Simulations focused on suspended sediment concentration highlighted that turbulent kinetic energy is the governing factor in erosion, resuspension, and transport of suspended sediments in vegetated flows. This suggests that the equilibrium boundary condition used for simulating suspended sediment transport in nonvegetated channel flows should be modified to account for local erosion and deposition based on turbulent kinetic energy rather than mean shear stress (Fig. 2).

These findings will improve the estimates of sediment transport in natural water bodies, allowing for better sediment management strategies for rivers, ports, and harbors. Simulations were conducted using up to 90 million computational points, running on 8,196 processors at a time, which would be unaffordable without the use of a petascale supercomputing facility such as Blue Waters.

WHY BLUE WATERS

The study pushes the limit of the scale at which high-resolution simulations are used to study complex multiphase flow in environmental fluid mechanics, requiring computational resources with sustained computing power at an unprecedented scale such as Blue Waters. Simulations have been conducted for up to 296 million computational points, with the code scaling strongly up to 32,768 Message-Passing Interface ranks. Without access to petascale high-performance computing resources, completing the study within a realistic timeframe would be impossible. In addition, since visualization of a phenomenon is an effective way to understand and explain its mechanics, the team will continue to work with Blue Waters project staff to create animations using data from the simulations.

PUBLICATIONS & DATA SETS


MACHINE LEARNING-ASSISTED HIGH-THROUGHPUT COMPUTATIONAL DESIGN OF SOLVENTS FOR LIQUID-EXFOLIATION

EXECUTIVE SUMMARY

Computational study and machine learning are two advanced tools of scientific discovery. In this project, the research team performed high-throughput computational studies to understand and obtain data on the liquid-phase exfoliation (LPE) process with various solvents. Then, the team analyzed the data using various machine learning algorithms to obtain optimal solvent composition, which facilitates the LPE process. Considering the nanoscale of phenomena occurring in the LPE process, the combination of computational physics and machine learning is one of the best methods to optimize the solvent to further improve the LPE process. This can then guide experimentalists in initial steps by reducing the number of expensive experimental attempts, especially since commonly used solvents in the LPE process are room temperature ionic liquids (RTILs) that have up to several million possible solvents.

RESEARCH CHALLENGE

LPE is an advanced mass production method for 2D materials with applications in various technologies such as water desalination, energy storage, optoelectronic devices, DNA sequencing, and energy generation. Compared with other 2D material production methods such as mechanical exfoliation or chemical vapor deposition, LPE produces higher yields with lower costs. LPE is also a simple method that uses an external ultrasonic force on a bulk material immersed in a solvent [1,2]. The bottleneck of the LPE process is the design of a solvent that optimizes the yield, stability, and quality of produced 2D materials.

Because the LPE process occurs in the interface of a bulk material and a solvent, it has a nanoscale nature (Fig. 1). Therefore, knowledge of macroscopic properties of the solvent and bulk material does not allow experimentalists to select the optimal solvent. However, recent computational studies using molecular dynamics (MD) simulations have provided insight into LPE [3].

Even though these studies are crucial in understanding the key parameters of the LPE process, they do not contribute directly to the design and screening of all possible solvents. In this project, the research team combined high-throughput computational studies of various solvents with machine learning algorithms to relate interactions between 2D nanosheets with the composition of the solvents. Based on the applied machine learning algorithm, the team predicted the best solvent composition for the LPE process. The study, therefore, can significantly improve 2D material production, particularly since one of the objectives is to release a computational tool for users in industry and academia.

METHODS & CODES

The research team performed MD simulations using the GROMACS package. GROMACS is an open-source classical MD code for simulation of various physiochemical and biological systems. The GROMACS package supports various potential forms used in the MD simulation of both solvents (RTILs) and 2D materials. The machine learning model development was performed using the TensorFlow and scikit-learn packages, both of which are accessible through Python (bwpy) on Blue Waters. Fig. 2 shows the workflow of the current study, in terms of both data generation and training as well as the inference and design phases.

RESULTS & IMPACT

The current study uses MD simulations and machine learning methods to help users with computational or experimental background with the selection of an optimal solvent for 2D materials production with the LPE process. The most commonly used solvents for the LPE process are RTILs, also known as “designer solvents,” so named because more than a million RTILs could theoretically be synthesized. Considering the number of possible solvents and the costs and risks associated with carrying out experiments, it is necessary to guide experimentalists, especially in the initial steps. Even though MD simulations provide physically consistent and realistic data on the LPE process with a resolution impossible to obtain in experiments, MD data are used to understand the LPE process at the molecular level; the design of solvents requires further development. To make good use of the MD data, the team applied a machine learning algorithm with a high predictive capability to relate solvent composition with MD data, with the objective of facilitating solvent design. The machine learning models can then be used later to optimize solvent compositions, narrowing the number of possible solvents and guiding experimentalists toward the most promising ones.

WHY BLUE WATERS

Increasing the accuracy of machine learning models requires a huge amount of data. Each specific solvent simulation must go through energy minimization, equilibrium in the NVT ensemble and, in the NPT ensemble, peeling and umbrella sampling, followed by data analysis. Such MD simulations are computationally expensive; Blue Waters makes such simulations possible.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Empirical potentials are “coarse-grained” models of atomic interactions and are fundamental to materials modeling. They allow molecular dynamics simulations of processes involving 10^10 atoms and timescales of nano- to microseconds or longer, and are necessary for both length- and time-bridging methods that span orders of magnitude in scale. Their optimization to reproduce computationally demanding quantum mechanics-based simulation methods is a significantly challenging problem.

Recently, the researchers developed a new approach that relies on a combination of Bayesian sampling of potential parameters [1] with the optimization of the fitting database [2]. The team’s algorithm optimizes the target structures and properties, as well as their “weights,” to guide the optimization of a potential to make accurate predictions [3]. This automated approach can work both for predictions where experimental or theoretical guidance is missing by including related structures and also to determine when an empirical potential form may be too limited to capture the predictions of interest.

RESEARCH CHALLENGE

The algorithm to optimize a coarse-grained empirical potential (Fig. 1) has recently been demonstrated in the team’s publications. Recently, the team achieved the next step to reach increased complexity and, hence, significantly greater impact across materials science, physics, chemistry, and biology: improved parallelization of the algorithm to reach large scale. The algorithm relies on Bayesian sampling of parameter space to determine optimal parameters along with error estimates for predictions from the model. The parameters are optimized against a “fitting database”: a selection of structures with density functional theory (DFT) energies and forces, and with relative weights capturing the importance of each entry. The database is optimized by using a genetic algorithm over the weights. At the center of this algorithm is their massively parallel architecture with a worker–manager structure; their algorithm has been on Blue Waters.

METHODS & CODES

This project uses the research team’s newly developed parallel evaluation engine, implemented in Python. The code continues to be in active development and is available through Github (https://github.com/TrinkleGroup/s-meam). The underlying parallel algorithm is worker–manager, where individual workers are tasked with evaluating forces or energies for a specific structure; sets of parameters can be passed to a given worker and the forces or energies sent back to the manager. At the beginning of a run, each worker analyzes its structure to convert the spline calculation into vector-matrix operations for efficient evaluation. This helps to keep each worker’s evaluation for one parameter set efficient but also permits even faster evaluation of sets of parameters through vectorized operations. The code uses NumPy and SciPy along with Message-Passing Interface for communication. Current runs of up to 512 cores have shown that the computational problem is related, but distinct, from the evaluation typically needed for molecular dynamics calculations where a single parameter set is evaluated against a very large number of structures. The computational engine will be used to take advantage of genetic algorithms for parameter optimization, Monte Carlo evaluation of Bayesian estimates of uncertainty, and cyclic improvement of databases, but other optimization schemes (such as Paresco optimization) could be considered as well.

RESULTS & IMPACT

Generating a highly efficient and massively parallel materials modeling optimization engine will enable new approaches to the development of empirical potentials that leverage machines at Blue Waters’ scale. The research team is designing a general framework that is maximally efficient for large sets of parameters to be evaluated against a fixed set of candidate structures. This computational problem is related, but distinct, from the evaluation typically needed for molecular dynamics calculations where a single parameter set is evaluated against a very large number of structures. The computational engine will be used to take advantage of genetic algorithms for parameter optimization, Monte Carlo evaluation of Bayesian estimates of uncertainty, and cyclic improvement of databases, but other optimization schemes (such as Pareto optimization) could be considered as well.

WHY BLUE WATERS

The computational engine is designed specifically to leverage massively parallel architecture with a worker–manager structure; access to Blue Waters has been instrumental for the implementation and testing of the code as well as preliminary runs. This work would have been impossible otherwise.
EXECUTIVE SUMMARY

The rapid and efficient detection of modulatory neurotransmitters is critical in understanding the functional mechanisms of novel sensors of neurotransmitters. This project's computational systems and developed a quantum model of an exciton at the CNT surface in the electrostatic environment generated by the DNA polymers, solvent, and neurotransmitter analytes. With the help of the simulations performed, the research team proposed the mechanisms behind the low optical signal of the ring-DNA-wrapped CNTs, and how the adsorbed dopamine neurotransmitter molecules distort ring-conformations of short DNAs and increase the optical signal of CNTs. Furthermore, the team has been screening short DNA polymers of different sequences, wrapping (9,4) and (6,5) carbon nanotube surfaces to disclose mechanisms responsible for a strongly quenched optical signal.

RESULTS & IMPACT

In this study, the research team performed multiscale simulations of short and long DNA polymers (12 to 30 nucleotides) with different sequences, wrapping (9,4) DNA polymers remained in helical conformations in molecular dynamics (MD) simulations, shorter 12-nucleotide (GT)6 DNA polymers rearranged from initial helical conformations into ring-like conformations in each of the five independent trajectories performed. To confirm that the ring-like conformation is a favorable adsorbed state of a (GT)6 DNA on the (9,4) CNT, the team calculated the free energy landscape of the DNA (Fig. 1) on the (9,4) CNT surface at room temperature (T = 300K), using replica exchange MD. The landscape revealed two distinct stable conformations for (GT)6: a left-handed helix and a nonhelical ring-like conformation. The team next performed quantum calculations of the systems and developed a quantum model of an exciton at the CNT surface in the electrostatic environment generated by the DNA polymers, solvent, and neurotransmitter analytes. With the help of the simulations performed, the research team proposed the mechanisms behind the low optical signal of the ring-DNA-wrapped CNTs, and how the adsorbed dopamine neurotransmitter molecules distort ring-conformations of short DNAs and increase the optical signal of CNTs.

WHY BLUE WATERS

To overcome the computational timescale limitations, the project required the use of replica exchange MD simulations, which can usually be performed only with access to the large resources of a petascale machine such as the Blue Waters supercomputer.

PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY
In this project, the research team developed multiscale quantum models from first-principles (ab initio) calculations that explicitly consider the subatomic physics of electrons and nuclei. The work represents a new level in connection between the subatomic scale and up to nanometer- and micrometer-scale quantum effects. The research is enabled by a combination of high-performance computing to gather data and advanced data science techniques to analyze the resultant data. The ensuing multiscale-effective models may then be used to predict the behavior of materials at those length scales and to understand quantum materials, for which quantum effects are starkly visible in their behavior.

RESEARCH CHALLENGE
All materials that we deal with day to day are made up of the same ingredients—nuclei and electrons. The variety of different objects and devices emerges from the many-particle behavior of these systems. How that actually occurs is still not well understood in many cases. Part of the challenge is that the electrons and nuclei behave according to quantum mechanics, whose equations are notoriously difficult to solve for more than just a few particles. Researchers use the concept of effective models to describe the behavior without having to explicitly consider the details of the fundamental particles. These effective models are used to design devices and otherwise describe how the materials behave. However, for new and emergent materials, it is often not known how to connect these effective models to the underlying dynamics of electrons and how to predict the correct effective model without appealing to experiment.

METHODS & CODES
The research group has recently developed a way of exploring the quantum solution space, which in turn allows them to derive effective models from high-accuracy first-principles calculations. The method involves performing many Monte Carlo calculations to simulate the electrons, which can run in parallel on thousands of nodes, and to analyze their results. The team uses the open-source QWalk [1] code, which was developed at the University of Illinois at Urbana–Champaign.

RESULTS & IMPACT
Fig. 1 shows the application of the effective model ideas to real materials. The question the research group is trying to answer in this study is ultimately why some materials (called unconventional superconductors) superconductor at high temperatures while some do not, which has been an open question in the field for decades. One of the leading explanations is that the motion of charge in the system is coupled to the motion of small magnetic moments that surrounds each atom, called spin. In this study, the team explored the coupling between charge and spin by finding the lowest energy charge configuration while fixing the spin to different configurations. If they are coupled, then the charge configuration changes with the spin configuration. Using Blue Waters, the team performed a large-scale study of dozens of materials and found that all the unconventional superconductors have coupling between spin and charge. This advance may be useful in finding new similar materials using high-performance computation.

WHY BLUE WATERS
Blue Waters was critical for the performance of this work. The quick turnaround of the calculations enabled the research team to accelerate the development of challenging methods by a large, difficult-to-quantify amount. In fact, some of these problems would have been unapproachable without the power of the Blue Waters system.

PUBLICATIONS & DATA SETS
EXECUTIVE SUMMARY

The environmental impact of aviation is measured in emissions and noise. The communities in the vicinity of airports bear the brunt of aircraft noise during takeoffs, climbs, flyovers, approaches, and landings. Research has shown that exposure to loud noise is harmful to human physiological and psychological health and welfare.

The research team at the University of Kansas has identified a novel and powerful means of mitigating jet noise by inducing shear layer swirl through embedded vanes near the nozzle exit lip. The team has employed a newly developed high-order (up to sixth order) Navier–Stokes solver capable of handling mixed unstructured meshes to perform computational predictions of the aero-acoustic noise using implicit large-eddy simulations. Blue Waters enables the team to accurately compute the near- and far-field supersonic jet noise. As a result, the research group can perform computational evaluations of a new concept in supersonic jet noise mitigation, which has the potential to significantly reduce the jet noise generated by military aircraft.

RESEARCH CHALLENGE

The noise generated by supersonic aircraft is deafening. The communities in the vicinity of airports bear the brunt of the noise during their takeoff, climb, flyover, approach, and landing. Human physiological and psychological health and welfare are negatively affected by exposure to this noise. The problem in the military is even greater since there are servicemen and women working near advanced supersonic jets during takeoffs and landings. The long-term health risk has created a huge problem for the Department of Defense (DOD). However, finding a solution has been a challenge. This project evaluates a promising new concept to reduce such noise.

METHODS & CODES

The research team used swirl-generating vanes placed inside the nozzle to enhance mixing in order to reduce noise [1]. The team employed a state-of-the-art unstructured mesh-based high-order Navier–Stokes solver (up to sixth order in space and fourth order in time) called hpMusic [2] in combination with large-eddy simulation to directly compute the near- and far-field jet noise. The near-field simulation was coupled with the Lighthill acoustic analogy [3] to compute the far-field jet noise.

hpMusic has been developed with support from AFOSR (Air Force Office of Scientific Research), NASA (National Aeronautics and Space Administration), and ARO (Army Research Office), and has been used to perform Implicit Large-Eddy Simulations for real-world complex configurations. The solver is based on the flux reconstruction/correction procedure via reconstruction method [4] on mixed unstructured meshes [5]. In addition, hpMusic has both explicit and implicit time-marching algorithms such as the explicit SSP Runge–Kutta scheme, an optimized second-order backward difference formula. The solver has been successfully implemented on massively parallel supercomputers such as the petascale Blue Waters. A scalability study demonstrated excellent parallel efficiency with over 10,000 cores.

RESULTS & IMPACT

The research team has completed the simulations of one baseline supersonic nozzle and one model with vanes to generate swirls to enhance turbulent mixing and mitigate jet noise. In addition, the team has performed mesh refinement and p-refinement studies to assess the sensitivity of the mesh resolution and the order of the simulation.

Based on the results of simulations and data analysis, the group will design more refined vane configurations to reduce jet noise. The team anticipates multiple iterations will be required to arrive at a nearly optimal design configuration. Extensive data analysis and comparison with other simulations and experimental data is currently being performed. So far, the computational results are very promising.

WHY BLUE WATERS

Jet noise computations using large-eddy simulation are very computationally expensive even on supercomputers because the acoustic magnitude is several orders smaller than the mean flow scales [6]. The use of Blue Waters increases the computation speed by at least a factor of 20 compared with the team’s local cluster, thus enabling these very complex simulations to be carried out in a timely fashion. The DOD-funded jet noise mitigation project lasts for only one year. Access to Blue Waters is essential for the team to achieve its goals for this project along with the professional and timely support provided by the Blue Waters staff.

Figure 1: Key flow structures and acoustic waves captured in a large-eddy simulation of a supersonic jet (iso-surfaces of the Q-criterion colored by the streamwise velocity, with acoustic waves shown on the symmetry plane).
EXECUTIVE SUMMARY
This work explores the long-ranged noncollinear magnetic textures, called spin spirals, in the multiferroic material BFO, as well as the BiFeO3/metal interface. These spin spirals are of prime importance for technological applications owing to their potential for spintronics and low-power magnetoelectric devices. The presence of spin spirals is induced by the Dzyaloshinskii–Moriya interaction (DMI), originating from spin-orbit coupling. This research investigates the magnetic interaction, and especially the DMI, in multiferroic materials and the interface between multiferroics and metals. With the computational resources of Blue Waters, the research team carried out fully first-principles or ab initio calculations in BFO, to reveal the stability of spin cycloids (the precession of spins along a propagation direction with a perpendicular rotational axis) under various strain conditions and to obtain the accurate magnetic interaction parameters that will be used to construct an effective Hamiltonian for combining Monte–Carlo simulations to study finite-temperature properties.

RESEARCH CHALLENGE
BiFeO3 (BFO) is a multiferroic magnetoelectric material at room temperature. This means that a magnetic field can change its polarization and an electric field can change its magnetization. This property is very rare in nature, which explains the strong interest in BFO and why it is called the “holy grail of multiferroic physics.” BFO is also non-collinear and antiferromagnetic (AFM) material, exhibiting a magnetic cycle at room temperature. Although this spin spiral is well characterized experimentally, several questions remain, such as the stabilization mechanism(s) of the different spin spirals and their interplay with structural distortion. For instance, the type of cycle in bulk BFO in the R3c phase is well characterized as being propagated along one of the [1–10] directions. However, a few recent experimental studies proposed that a type-II cycle (such as propagated along [11̅–2]) may be favored in BFO thin films that are moderately strained, but the measurements could also be explained as a mixture of different types of cycles. Further, when BFO is deposited on a substrate with a large compressive strain (more than 4.5% in magnitude), it undergoes a phase transition toward the so-called super-tetragonal phase, which is of great interest because of its very large polarization. This phase may host exotic noncollinear magnetic structures. In addition, one of the challenges in spintronics is to understand the interfacial DMI in patterned films, which are commonly used in industry. In that case, the difficulty is to model the polycrystalline sample of the DMI. Only a few such techniques such as bubble expansion or via Brillouin light scattering (BLS) in the latter, only the averaged DMI over the entire sample can be measured. It is therefore of prime importance to understand the origin of the different contributions to the DMI. To that end, the research team has explored the magnetic exchange interaction and the DMI in Fe1-xCox/Pt in collaboration with experimentalists.

METHODS & CODES
The research team used first-principles calculations based on density functional theory (DFT) in order to study the magnetic spin spirals in BFO. They applied the full potential linearized augmented plane wave (FLAPW) method [1,2] as implemented in the FLEUR code (www.flapw.de). This method is one of the most accurate implementations within DFT, owing to the self-consistent treatment of all the involved electrons (core and valence) and the precise and “natural” expansion of the wave functions (i.e., in spherical harmonics around the nuclei and in plane waves in the interstitial region). The choice of an accurate all-electron full-potential code was motivated by the fact that this project requires the treatment of noncollinear magnetism and spin-orbit coupling on the same footing as well as a highly accurate description of eigenfunctions and eigenenergies (leading to the need for an extremely good basis set). Therefore, the simulations of complex magnetic states in the presence of spin-orbit coupling (SOC) represent a cutting-edge problem in supercomputing. FLEUR is to date the only existing code containing all of the above-mentioned features and that is, therefore, capable of calculating SOC effects in noncollinear systems fully ab initio.

Further, the team computed the total energies at various reciprocal-space points based on the generalized Bloch’s theorem. The ground-state magnetic configuration was determined and compared with experiments. Remarkably, this approach allowed the team to extract the exchange and DMI interaction coefficients by considering neighboring interactions over a long range.

RESULTS & IMPACT
The research team explored for the first time different spin spirals in BFO at an ab initio level. The study revealed that the competition between the first- and second-nearest neighbor exchange interactions leads to a flat energy landscape near the G-type antiferromagnetic state. Slightly favoring a spin cycloid propagating in the [1–10] direction. Its stability is enhanced by the polarization but suppressed by the antiphase oxygen octahedral tiltings. Surprisingly, such a trend is found for the DMI energy, which further lowers the energy of the cycloidal state and reduces the cycloidal period. The predicted period is in good agreement with experiment. For the super-tetragonal phase of BFO, the calculated energy dispersion of the G-AFM state suggests that cycloid formation is strongly favored. As illustrated in Fig. 1, the cycloid is likely to propagate along the [10̅0] direction, as it has a noticeably lower energy than that of propagation along [1–10]. To our knowledge, this is the first work that predicts the existence of type-I cycle in T–BFO, which can then be verified by future experiment and may lead to promising spintronic applications.

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SPIN SPIRALS IN MULTIFERROIC BISMUTH FERRITE AND AT METAL SURFACE: FROM FULLY FIRST PRINCIPLES

Figure 1: Spin spiral energy dispersion curves near the G-type antiferromagnetic state of BFO in the Planes or super-tetragonal plane. (a) Cycloid propagation along the [1–10] direction. (b) Cycloid propagation along the [10̅0] direction.
NUMERICAL SIMULATIONS OF A COLLAPSING CAVITATION BUBBLE NEAR AN ELASTICALLY DEFORMABLE OBJECT

Allocation: Innovation and Exploration (220 K)
PL: Zhen Xu
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EXECUTIVE SUMMARY

The aim of this work is to understand the structural damage to nearby objects as a result of cavitation (the formation of small vapor-filled cavities). In extreme cases, cavitation gas bubbles collapse into small volumes that produce high pressures and temperatures and generate strong shock waves that interact with the surroundings. When adjacent to a neighboring elastically deformable object, the collapse becomes asymmetric and a re-entrant liquid jet forms within the bubble. The jet hits the opposite side of the bubble and generates an outwardly propagating water-hammer shock wave that interacts with the surroundings. The high pressures and temperatures as well as the corresponding shock waves produced by the collapse of cavitation bubbles can damage nearby objects [1–4]. This damage is recognized as one of the main consequences of cavitation and is an essential research topic in a variety of hydrodynamic and aero-thermo/biomedical applications. In naval applications, engineers still struggle to cope with the deleterious effects of cavitation erosion on surfaces and hydraulic machinery, which lead to degradation in performance and need for repair and/or replacement. In the context of therapeutic ultrasound, the pressure pulses from the collapse of cavitation bubbles are employed to fragment kidney stones and pathogenic tissues.

RESEARCH CHALLENGE

Cavitation bubble dynamics appear in a wide range of hydraulic applications such as turbomachinery, naval structures, biomedical ultrasound, and combustion. Cavitation happens owing to the reduction in local pressure beyond the tensile threshold in the surrounding liquid, thereby incurring a mechanically driven phase change in the liquid and leading to the formation of vapor bubbles. Vapor bubbles collapsing near surfaces/objects form a re-entrant jet that impacts the distal bubble wall, generating a water-hammer shock wave that interacts with the surroundings. The high pressures and temperatures as well as the corresponding shock waves produced by the collapse of cavitation bubbles can damage nearby objects [1–4]. This damage is recognized as one of the main consequences of cavitation and is an essential research topic in a variety of hydrodynamic and aero-thermo/biomedical applications. In naval applications, engineers still struggle to cope with the deleterious effects of cavitation erosion on surfaces and hydraulic machinery, which lead to degradation in performance and need for repair and/or replacement. In the context of therapeutic ultrasound, the pressure pulses from the collapse of cavitation bubbles are employed to fragment kidney stones and pathogenic tissues.

Understanding the collapse dynamics and the associated damage mechanisms will enable researchers to develop techniques to control (either by mitigation or enhancement) cavitation erosion. However, the wide range of temporal and spatial scales of these flows significantly limits the ability to obtain precise experimental measurements. As a result, numerical simulations serve as a valuable complementary tool to further our understanding of the physics, alongside analytical and experimental efforts. For this reason, the research team has developed a novel numerical framework to investigate the detailed dynamics of nonspherical bubble collapse near viscoelastic objects using high-resolution simulations based on MPI. This code solves the three-dimensional compressible Navier–Stokes equations with thermodynamically consistent evolution equations for the elastic contribution of the stress to represent multiple gases, liquids, and viscoelastic solids [5–8]. The code is based on high-order accurate (in smooth regions), non dissipative schemes with discontinuity detectors to apply high-order numerical dissipation at shock wave and material interfaces. Thus, the code can accurately solve problems involving broadband features, e.g., turbulence, and discontinuous features such as material interfaces, shock, and shear waves. To perform the three-dimensional numerical simulations of the problems of interest, an in-house code was developed in C++, which was parallelized using the MPI library and implemented the parallel HDF5 library for I/O. The code has been verified and validated against a series of theoretical and experimental results.

METHODS & CODES

The team used its in-house petascale production code for the large-scale simulations based on MPI. This code solves the three-dimensional compressible Navier–Stokes equations with thermodynamically consistent evolution equations for the elastic context of therapeutic ultrasound, the pressure pulses from the collapse of cavitation bubbles are employed to fragment kidney stones and pathogenic tissues.

RESULTS & IMPACT

To better understand the detailed bubble collapse dynamics near an elastically deformable object or in confinement, two problems configurations were considered: (1) shock-induced collapse of a single bubble near a finite-sized (spherical) calcium stone, and (2) collapse of a single bubble in a confined channel. When a cavitation bubble collapses in these configurations, the collapse becomes nonspherical, leading to the formation of a high-velocity re-entrant liquid jet(s) (Fig. 1). The impact of the jet upon the opposite side of the bubble generates a water-hammer outwardly propagating shock wave, and thus can create high-pressure regions on the surface of the neighboring surfaces/objects (Fig. 2). Scaling laws of the maximum pressures (and resulting impact loads) exhibited on these surfaces based on important collapse parameters (e.g., driving pressure, bubble location) were developed to predict the single-bubble dynamics. In the first study, the synchronization of the shock wave with the bubble collapsing near the stone depends on the initial bubble size–stone size ratio for maximizing the tension inside the stone that could lead to its comminution. These results will enable further optimization and development of ultrasound therapy tools used to fractionate elastic stones. Scaling results from the second study showed that for significant confinement, the bubble collapse jet formation dynamics change with the re-entrant jet forming in the direction parallel to the channel. This then further strengthens the collapse of the remaining bubble remnants. As a result, the channel-scaling relationship deviates from the scaling for a single bubble collapsing near a single wall. These results enable the team to predict and quantify the damage mechanisms involving the nonspherical bubble collapse near a finite-sized elastic object in confined geometries to develop cavitation mitigation/enhancement strategies.

WHY BLUE WATERS

The three-dimensional high-resolution simulations (requiring more than one billion grid points) that can effectively resolve the necessary small-scale features of the flow for high-fidelity results for over 36-hour simulation wall-times, as well as postprocessing and visualizations of large data files, require substantial computational power and resources. The Blue Waters petascale computing and simulation wall-time capabilities make such simulations possible and were essential for the success of this study.

PUBLICATIONS & DATA SETS


EXECUTIVE SUMMARY

The overarching objective of this project is to study and improve the numerical modeling of ramp-induced shock wave–boundary layer interaction (SWBLI) control by micro-vortex generators (MVGs) in high-speed flows. The research team utilizes high-order large-eddy simulation (LES) with a large grid system to study the correlation between SWBLI low-frequency and vortex motion. SWBLI, which causes boundary layer separation and adverse pressure gradients, is a prominent problem faced by the air-breathing propulsion systems of high-speed aero vehicles. The consequences of the interaction include degraded engine performance and decreased overall propulsive efficiency of a high-speed vehicle. MVGs can alleviate or overcome the adverse effects of SWBLI and, therefore, improve the “health” of the boundary layer. An improved physical understanding of how MVGs reduce shock-induced boundary layer separation will contribute significantly to the understanding of the complex viscous–inviscid interactions that dominate high-speed aerodynamics.

RESEARCH CHALLENGE

SWBLI, which causes boundary layer separation and adverse pressure gradients, is the prominent problem faced by the air-breathing propulsion systems of high-speed aero vehicles. Particularly, SWBLI in high-speed inlets can significantly reduce the quality of the flow field by inducing large-scale separation, causing total pressure loss, flow distortions, localized heating and peak pressures, and unsteadiness. The consequences of the interaction are generally degraded engine performance and also the decreased overall propulsive efficiency of a high-speed vehicle. An improved understanding of SWBLI and flow-control technologies will directly benefit aeronautics research.

METHODS & CODES

As a result of advances in computer and code capability, high-order and high-resolution LES has become an important tool to study flow mechanisms. To capture details of instantaneous flow structure and reveal the mechanism of interaction between the vortices and the shock wave, large-scale LES was carried out. The research team used body-fitted grids for discretizing the domain. In order to obtain high-order accuracy, an elliptic grid generation with orthogonal and smoothness requirements was adopted to generate the grids [3]. The three-dimensional, time-dependent, conservative Navier–Stokes equations in a curvilinear coordinate were applied as the governing system. A fully developed turbulent inflow was generated by high-order direct numerical simulation (DNS) on a flat plate with flow transition from laminar to turbulent [6]. A million inflow files were recorded as a time-dependent turbulent inflow. Adiabatic and no-slip conditions were enforced at the wall boundary on the flat plate. Periodic boundary conditions were assumed for the spanwise direction. On the inflow (the inflow could be supersonic in the lower part of the boundary layer) and the outflow boundaries, nonreflecting boundary conditions [7] were applied.

RESULTS & IMPACT

The research team collected MVG-controlled ramp flow data at two different Mach numbers (2.0 and 2.5). More data (at Mach numbers 3.0, 3.5, and higher) will be collected in the future. The study of supersonic ramp flow controlled by MVG array is ongoing and data are being collected. A series of ringlike vortices generated behind an MVG array was discovered by high-order and high-resolution LES (Fig. 1). The mechanism of the evolution and interaction of these vortices will be investigated both numerically and analytically. The numerical results obtained through this project will lead to a better understanding of the driving source of low-frequency unsteadiness of the SWBLI and thus may aid in developing methods to improve flow control in high-speed flows. The methods presented in this study as well as the resulting numerical solutions and mathematical model can pave the way for fully understanding the mechanisms of SWBLI.

WHY BLUE WATERS

Computational fluid dynamics is one of the best techniques to study complicated flows. The major scientific challenge in this study is to capture numerous small-scale vortices and the detailed process of the vortex–shock wave interaction in such a complex system with the existence of the turbulent boundary layer and flow separation. This requires very powerful massively parallel processing systems along with large memory and a very large amount of storage. As one of the most powerful supercomputers in the world, Blue Waters is the best choice for this project.
EXECUTIVE SUMMARY
In this project, the PI simulated two back-to-back, full-scale, complex-geometry tidal turbines in free-surface flows using an in-house computational free-surface flow framework and the Blue Waters supercomputer. In addition, the PI investigated the wake and free-surface effects on tidal turbine performance in the downstream turbine through a case study. To quantify the free-surface effect, the researcher performed a pure hydrodynamics simulation and a free-surface simulation. He observed a significant drop in the thrust coefficient and production coefficient between the upstream and downstream turbines owing to the velocity deficit. Further, both simulations predicted almost the same thrust and production coefficients for the upstream turbine, while the pure hydrodynamics simulation predicted a noticeably higher thrust coefficient and production coefficient for the downstream turbine.

RESEARCH CHALLENGE
Although computational fluid dynamics simulations are widely used in the research and development of tidal energy, few of them consider the free-surface effect, which has been proven in experiments to have a significant influence on tidal turbine performance. In this project, the PI developed a computational framework that is able to simulate multiple tidal turbines in turbulent free-surface flows. This framework will ultimately facilitate the research and development of tidal energy farms.

METHODS & CODES
The PI developed an in-house MPI-based parallel free-surface flow simulation framework. In the computational framework, the level-set method was adopted to track the evolution of the air–water interface. The aerodynamics and hydrodynamics were governed by a unified two-phase incompressible Navier–Stokes equation in which the fluid density and viscosity are defined by means of the level-set function. The finite-element-based Arbitrary Lagrangian Eulerian Variational Multiscale formulation enhanced with weak enforcement of essential boundary conditions was employed to discretize the free-surface flow equations. The sliding-interface formulation was used to account for the presence of the tower and nacelle, thus enabling the so-called full-machine simulation. The sliding-interface formulation was also augmented to include level-set redistancing.

RESULTS & IMPACT
In this project, a computational free-surface flow framework was used to simulate two back-to-back tidal turbines in free-surface flows. The simulations were carried out at full scale and with the full complexity of tidal turbine component geometry. Without any empiricism, the simulations were able to accurately capture the effect of the free surface on the rotor hydrodynamic loading and the interaction between the upstream and downstream turbines. For the deep-immersion operating conditions considered in this work, the free-surface simulation predicted a drop in the thrust coefficient of 70% and a drop in the production coefficient of 38.7% between the upstream and downstream turbines. By comparing the results of the pure hydrodynamics simulation and the free-surface simulation, the team found that the free surface does not affect the upstream turbine but does significantly change the performance of the downstream turbine.

This work is a first step toward using free-surface flow simulations of multiple full-scale tidal turbines with complex geometry. The proposed framework will help improve the efficiency of tidal farms by better understanding the combined wake and free-surface effects on turbines. In the future, the PI will conduct a parametric study of the distance between the upstream turbine and downstream turbine. He also plans to extend the current methodology to simulate multiple tidal turbines arranged in arrays and will consider both the fluid–structure interaction effect and cavitation.
EXECUTIVE SUMMARY

Substantial advances in both domain science and computing for fluid turbulence have continued in this work on Blue Waters. A recent focus is in the study of intermittency, which is most likely characterized by multipoint descriptors of turbulence structure, whose multifractal characteristics have in turn led to significant difficulties in analyses. However, the research team has found that the circulation of velocity around a closed contour or loop (equivalent to a two-dimensional area average of a vorticity component) has much simpler (“bifractal”) properties. In particular, if all sides of a rectangular loop are within the inertial range of scale separations then the circulation, at least to a very close approximation, only on the size of the loop but not its shape. The study of circulation also demonstrates how a massive high-resolution turbulence database at high Reynolds numbers can provide much clearer answers than previously feasible in the literature.

RESEARCH CHALLENGE

Since turbulence is characterized by fluctuations arising over a wide range of scales, many research strategies focused on fundamental understanding have been formulated in the context of a search for scale similarity (or departures therefrom). For example, moments of the instantaneous energy dissipation rate averaged over spatial regions of linear size varying over a substantial range provide a telling indicator of flow structure (Fig. 1) as well as playing an important role in corrections of classical similarity theory to account for the effects of intermittency [1]. However, researchers have also learned that [2] as a result of demanding resolution requirements [3], precise and reliable results are (whether experimentally or numerically) very difficult to obtain, which is especially the case for high-order statistics at high Reynolds numbers.

In fluid dynamics, circulation is defined as the line integral of the velocity vector around a closed loop, or, equivalently, the integral of a vorticity vector component over the area enclosed. This concept is important in the occurrence of aerodynamic lift, oceanic transport, mantle convection inside the core of the Earth, and other contexts. In principle, the statistics of circulation will depend on both the size and shape of the loop, but a theory known since the 1990s [4] suggests that only the size matters, provided that length scales on every side are within the inertial range. A wide inertial range is necessary for this theory to be tested properly. As a result, it is not surprising that several studies in the past [5,6] were not conclusive. However, since computations using machines such as Blue Waters [7] have reached resolution levels some 4,000 times larger (in terms of total number of grid points) than the state of the art of the 1990s, there is reason for new optimism.

METHODS & CODES

The research team integrated the Navier–Stokes equations over a large number of timesteps, using Fourier pseudo-spectral methods in space and finite differences in time. Circulation was computed via postprocessing of a substantial number of instantaneous snapshots of the velocity field saved during the simulations. While investigators can use either the line integral or area integral definitions as noted above, the area integration approach is more convenient. It also has the advantage of providing a more intuitive connection to the vorticity vector, which characterizes the tendency of local fluid elements to rotate on their own axes as a result of deformation by the turbulent flow. The required code development mainly resides in implementing a two-dimensional system decomposition used to perform the simulations.

RESULTS & IMPACT

In [8], the research team reported on a detailed study of the statistical properties of circulation using a large database in isotropic turbulence over a range of Reynolds numbers. The highest grid resolution analyzed involved over four billion grid points (16,384 in each of the three Cartesian coordinate directions). The team primarily studied circulation computed as area integrals of the vorticity over rectangular loops. The simulation results (Fig. 2) provide strong support for the theoretical prediction (noted above) that the statistics of circulation depend only on size but not the shape of the loop, provided the entire loop is all constrained within the inertial range. The probability density function of the circulation appears to scale in a manner consistent with the classical Kolmogorov 1941 hypothesis without significant effects of intermittency. Furthermore, the circulation is shown to exhibit, to excellent accuracy, a bifractal behavior at the higher Reynolds number considered: space-filling for low-order moments, following the paradigm of Kolmogorov 1941 [9,10], and a monofractal with a dimension of about two for higher orders. This change in character, occurring roughly at the fourth moment for the highest Reynolds number considered, is reminiscent of a phase transition encountered in other branches of physics.

The evidence obtained in this study points to a reduction in complexity when considering averaged vorticity over loops, which may provide a route to circumventing the spatial complexities involving velocity differences and gradients in turbulence [11]. This conclusion suggests that a great simplification, in principle, of the intermittency problem in three-dimensional turbulence may be possible when viewed through the lens of vorticity correlators in loop spaces. This great simplification may, in turn, have the impact of invigorating the use of similar loop formulations in tackling turbulence.

WHY BLUE WATERS

The 8,1923-grid resolution of the research team’s production simulations requires access to a world-class machine such as Blue Waters. The machine capacity on Blue Waters has also proven sufficient to allow the team to obtain data at even higher resolution, i.e., 12,2883 and even 16,3843 (although only for short periods of time), which is the highest known worldwide in the turbulence community. Indeed, 16,3843 data, although short in time span, have been the focus of analysis presented in [8].

PUBLICATIONS & DATA SETS

Hydrophobic and superhydrophobic surfaces that are robust to harsh environments have immense potential to enhance the performance of a plethora of applications. However, the successful widespread commercialization of hydrophobic surfaces has been fraught with many challenges. The biggest challenge is the lack of mechanical, chemical, and thermal robustness.

Recent studies show that rare-earth oxides (REOs) are intrinsically hydrophobic and durable owing to their unique electronic structure. However, surface defects such as adatoms (single atoms lying on surfaces) and vacancies are ubiquitous and may change the wettability of REOs. Thus, in this project, the research team investigated the influence of the defects on hydrophobicity and elucidated the mechanism governing wettability by employing first-principle neural network potentials combined with molecular dynamics (MD) simulation. This work is significant for simulating and understanding the hydrophobicity of REOs at the molecular level and providing insights to identify ideal candidates with strong hydrophobicity when considering the presence of defects.

Starting from bulk water, a specific bulk REO such as ceria (CeO$_2$), and a wide range of REO–water interfaces, the team carried out DFT reference calculations using VASP [2]. Projector augmented waves with a plane wave energy cutoff of 700 eV to converge the results were used to describe the electron-core interaction in the DFT calculations. Furthermore, more uncorrelated structures for DFT calculations were generated by taking snapshots of ab initio MD simulation trajectories. The calculated energy and force were related with a vector of atom-centered symmetry functions defined by atomic environment. For each atom, the symmetry function vector was fed into an individual atomic neural network and the network was constrained to have the same architecture and parameters for each element in the system. Using these symmetry functions related to each kind of atom and energy, the reference data were split into training sets to determine the fitting parameters for each type of atom and test sets to verify the transferability of those parameters. An iterative gradient-based fitting process was used to determine the fitting parameters by minimizing the error function until a set of parameters could accurately reproduce the reference energies and forces and a converged neural network potential energy surface was obtained. Using the generated potentials, the research team performed MD simulations to collect trajectories to quantify the level of hydrophobicity.

RESULTS & IMPACT

By performing MD simulations with constructed neural network potentials (NNPs) based on density functional theory (DFT) data have the ability to enable efficient classical MD with accuracy close to ab initio MD. By combining classical MD with NNPs, the research team was able to perform long-timescale simulations with high accuracy.
CONSTRAINING THE PROPERTIES AND INTERACTIONS OF DARK MATTER

Allocation: NSF FRAC/14,000 Knh
PI: Phiala Shanahan1
Collaborators: Balint Joo2, David Murphy1, William Detmold1, Michael Wagman1
1Massachusetts Institute of Technology
2Thomas Jefferson National Accelerator Facility

EXECUTIVE SUMMARY

This project addresses the Grand Challenge research problem of understanding the nature of the mysterious dark matter that permeates the universe. In particular, to interpret the results of direct experimental searches for dark matter it is necessary to quantify the interaction of potential dark matter particles with the nuclei used as targets in the detectors. This is a hugely demanding computational task that requires significant resources.

RESEARCH CHALLENGE

Understanding the nature of dark matter is a defining challenge for contemporary particle and nuclear physics. This project will provide necessary theoretical input for interpreting dark matter searches that are currently being undertaken at laboratories around the world, and will allow optimal design of the next generation of such experiments. The interaction of a broad class of dark matter candidates with the nuclei used in direct detection experiments is governed by nuclear scalar matrix elements. In recent work, the research team determined the scalar matrix elements of light nuclei via first-principles calculations of the underlying interactions with the Standard Model, albeit with larger-than-physical values of the quark masses used in the study (allowing computationally cheaper calculations). These calculations revealed significant, and unexpected, order 10% nuclear effects in the scalar interactions in light nuclei. These significant effects in small nuclei potentially indicate even larger effects and uncertainties in the scalar matrix elements of the much larger nuclei, for example xenon, typically used in direct detection experiments. If these effects persist in a controlled study at the physical values of the quark masses, it will have significant implications for the interpretation of the results of current and future dark matter direct detection experiments around the world.

METHODS & CODES

This study has been undertaken within the framework of lattice QCD (quantum chromodynamics), which is a first-principles method of calculating strong interaction matrix elements numerically on a discrete four-dimensional spacetime. In this approach, Monte Carlo techniques are used to create a representative set, known as an ensemble, of configurations of the background gluon fields on the links defined between points on the spacetime lattice. This ensemble is then used to perform calculations of quantities of physical interest. As the only known direct method of studying QCD at the low energies relevant for hadronic and nuclear interactions, lattice QCD is an important source of information for tests of the Standard Model, and it provides results for various hadronic and nuclear matrix elements that are systematically improvable and model-independent. As such, it is the necessary tool for the calculations undertaken.

RESULTS & IMPACT

This project began in mid-2019. The codebase has been successfully implemented on Blue Waters and production runs have begun. The calculations that are running are producing the time series data that will allow the determination of the nuclear quantities that govern the interactions of dark matter with light nuclei. Additionally, data structures are being generated that form the first step in calculations of nucleon–nucleon scattering and studies of light nuclear spectroscopy. Once the calculations are complete, they will enable understanding of nuclear effects in dark matter interactions with nuclei that will have far-reaching impacts on current and future terrestrial searches for dark matter. The research team anticipates that the precision they will achieve with the runs that are in progress will be sufficient to influence the design of future experiments searching for dark matter.

WHY BLUE WATERS

Undertaking a controlled calculation of the interactions of dark matter with nuclei is a hugely demanding computational task that requires significant resources that would not otherwise be available to the project team.
<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMPUTER SCIENCE &amp; ENGINEERING</td>
<td></td>
</tr>
<tr>
<td>ENGINEERING &amp; FINANCE</td>
<td></td>
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<tr>
<td>NETWORK CONGESTION</td>
<td></td>
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<tr>
<td>PARALLEL FUNCTIONALITY</td>
<td></td>
</tr>
<tr>
<td>RESILIENCE</td>
<td></td>
</tr>
<tr>
<td>SCALABILITY</td>
<td></td>
</tr>
<tr>
<td>VISUALIZATION</td>
<td></td>
</tr>
</tbody>
</table>

**212** Cinematic Scientific Data Visualization for CADENS

**214** The Structure and Statistics of Reed–Muller Codes

**216** A Parallel Framework for Scaling Phylogeny Estimation Methods to Large Genomic Data Sets

**218** Algorithms for Extreme-Scale Systems

**220** Kaleidoscope: Live Forensics for Large-Scale Data Center Storage Systems

**222** Extensible and Scalable Adaptive Sampling to Fold Proteins on Supercomputers

**224** Improved Scalability Through Node-Aware Communicators

**226** Scalable Line and Plane Solvers

**228** Detection of Silent Data Corruptions Using Machine Learning

**230** Pushing the Boundaries of Large-Scale Tensor Computations

**232** Algorithms for Large-Scale Evolutionary Tree Construction: Improving Scalability and Accuracy through Divide and Conquer

**234** HPC Development of Deep Learning Models in Scientific Computing and Finance

**236** Optimization of a Field Data Parallel Output Library
EXECUTIVE SUMMARY

The Advanced Visualization Lab (AVL) at the University of Illinois at Urbana–Champaign (Illinois) has continued to work on the National Science Foundation–funded CADENS project (Center for Advanced Digitally Enabled Science, ACI-1445176). The AVL coproduced and rendered visualization scenes for two full-dome planetarium shows, Birth of Planet Earth and Imagine the Moon. The research team has used Blue Waters for processing data as well as rendering scenes in 4K monoscopic, 4K stereoscopic, and full-dome formats. The researchers also rendered visualizations for the Earth’s Call climate change event in Aspen, CO, U.S.A., May 17–19, 2019.

RESEARCH CHALLENGE

Drawing on data from scientists involved in high-performance computing-based research, the AVL creates visualizations in cinematic style intended for public outreach, through flat-screen science documentaries, films, and full-dome planetarium shows.

METHODS & CODES

The team’s Blue Waters visualization work depends on several externally provided packages: Houdini, commercial visual effects software from SideFX; yt, the data analysis and visualization package (yt-project.org) for ingesting and regidding some types of data; VMD, the Visual Molecular Dynamics package from John Stone of the Theoretical Biophysics group at Illinois (www.ks.uiuc.edu); and Python with numpy and scipy for many types of data preprocessing from the forms provided by the scientists into forms usable by Houdini. The team has also developed their own software tools, including Ytini for yt-Houdini integration, and Rhude to organize the Houdini rendering workflow for Blue Waters’ environment.

Visualizing energy harvesting in a photosynthetic purple bacterium [1] involved combining structural models from atomic, protein, organelle, and cell scales using multiple software tools [2]. The construction of structural models [3] was performed with VMD [2] and Mathematica, which was also used for the determination of relevant energy conversion steps [1]. Multiple copies of a static chromatophore model [3] were assembled in Houdini to emulate the interior of a low-light-adapted purple bacterial cell. Dynamic elements—photons, electronic excitations, protons, quinols/quinones, and ATP—were choreographed using Houdini to illustrate energy conversion processes for a lay viewer. Since the timescales for these conversion processes span almost 12 orders of magnitude (femtoseconds to milliseconds) [1], the animations deliberately represent a simplified visual narrative rather than the results of a specific simulation at one timescale. Some visual elements were rendered using Houdini, others with VMD. In addition, the researchers relied on Blue Waters’ capability to create a high-quality visualization of Sarah T. Stewart’s Moon-forming collision [4], as explained below.

RESULTS & IMPACT

Blue Waters enabled the research group to create and refine two data-driven cinematic animations for two full-dome planetarium shows released in 2019:

• Visualizing Energy Harvesting in a Photosynthetic Purple Bacterium [1–3]—Birth of Planet Earth
• Formation of the Moon [4]—Imagine the Moon

Full-dome shows have a lifespan of about 10 years, and though it has only been several months, Birth of Planet Earth has already received two awards and is being shown internationally. To suggest potential public impact for this work, it can be compared with another full-dome planetarium show in the CADENS series, Solar Superstorms, for which AVL also relied on Blue Waters for data visualization. Since its 2015 release, it has been booked by over 70 planetaria and science museums in 15 countries, and translated into at least 10 languages.

The research team also used Blue Waters to create data-driven graphics for the Earth’s Call climate change event in 2019, which was viewed by more than one million people globally. The group visualized a total of 12 data sets for this event, five of which [5–9] were rendered using Blue Waters owing to the length of time required to render each frame.

WHY BLUE WATERS

Access to Blue Waters has allowed the team to iterate quickly and to meet deadlines. They were able over the course of a single weekend to render a Houdini scene involving a chromatophore model [3] and its surrounding environment that was made up of six separate render layers and totaled 20,870 image frames. The capability to render a large amount of images in a short period of time has allowed the team to make several iterations of the scene before finalizing a video shown during the International planetary Society 2018 conference. This would not have been possible on the team’s local cluster.

Furthermore, Blue Waters has made it possible to not sacrifice visual quality for render speed. One approximately 200-frame segment of the visualization of a planetary collision [4] was taking as many as 20 hours per frame to render. Blue Waters made it possible to render these images despite the long render time. Without Blue Waters, the team would have had to either change many render settings and significantly decrease the render quality, to change the camera position and lose the dramatic effect of having an arm of disk material pass closely overhead, or to spend many days trying to come up with a different data representation of the simulation to make the render more manageable on the local cluster.

PUBLICATIONS & DATA SETS

Birth of Planet Earth, full-dome planetarium show, directed by Thomas Lucas, distributed by Spitz, Inc., 2019.


THE STRUCTURE AND STATISTICS OF REED–MULLER CODES

Allocation: Exploratory/20 Knh
PI: Iwan Duursma
Collaborator: Hsin-Po Wang

1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

This project focuses on computing the Tutte polynomial of the Reed–Muller (RM) codes of block length 64. RM codes are among the earliest linear block codes whose construction is easy to describe, and yet their properties have not been fully understood. They are related to polar codes, a class of codes that was introduced in the last 10 years and that is known to have good asymptotic properties. It is conjectured that RM codes also share those properties. The Tutte polynomial is an invariant of linear block codes that captures the probability of error when correcting erasures in codewords. The Tutte polynomial is used more generally in graph theory, knot theory, and physics.

RESEARCH CHALLENGE

The Tutte polynomial is a two-variable generating function for the corank-nullity distribution over all subsets of columns of a given matrix. It can be computed exhaustively or recursively using a sequence of deletion–restriction operations. It is known that computing the Tutte polynomial for general block codes is #P-hard (the quantitative version of nonpolynomial hardness). For Reed–Muller codes, Tutte polynomials are known up to length 32. The research team extended this to length 64 and, moreover, computed a newly defined invariant that provides more detailed information than the Tutte polynomial.

METHODS & CODES

The reduction that essentially brings this problem within a feasible scope is the Plotkin structure of RM codes. The fact that the construction of RM codes is recursive suggests that an invariant can be computed along the recursion. However, this fact only reduces the time cost by a factor of 60,000. The remaining work still costs Blue Waters 2,000 node-hours to complete. All the codes employed were produced by the team.

RESULTS & IMPACT

The researchers computed the Tutte polynomial along with extra data that allow followers to double-check whether the computation is correct. The exact polynomial may be found at https://github.com/Symbol1/BlueWaters-RM64/blob/master/rm64tutte.txt. The extra data with a full explanation of how they were computed and how they can be verified may be found at https://github.com/Symbol1/BlueWaters-RM64.

WHY BLUE WATERS

The role of Blue Waters is twofold. First, this computation is CPU-intensive, with a great deal of conditional branching and bitwise operators, and Blue Waters provides a parallel context to accelerate the computation using all 32 cores in a node. Second, the team generated an abundance of intermediate data that should be kept in RAM to avoid the hard disk’s I/O, because otherwise the I/O becomes the bottleneck. The team expected more, but the given 64 GB of memory per node barely fits. (The researchers tailored the MPI reduce function to save space.) In addition, the computation does not write any error-handling codes, but apparently Blue Waters was all green when this job was running, thanks to its sustainable design.

PUBLICATIONS & DATA SETS

Computation of Reed–Muller codes of length 64 on Blue Waters. [Online]. Available: https://github.com/Symbol1/BlueWaters-RM64
 Phylogenetic trees are graphical models of evolution that can be used to study how species evolve and adapt to their environment. Recent advances in sequencing technology have resulted in an explosion of data and the creation of ultra-large data sets. Today, scientists need to estimate highly accurate phylogenetic trees from these data sets; however, this process is computationally challenging. Many of the best methods are not easily parallelizable and have large computational footprints (memory and running time).

The research team’s main result is a parallel framework for scaling phylogeny estimation methods to large data sets while maintaining accuracy. By running their preferred method within the team’s parallel framework, scientists will be able to estimate evolutionary trees using reduced computational resources. Thus, these computational tools will be useful for researchers attempting to build the Tree of Life, a scientific and computational grand challenge, as well as for conservation biologists and agriculture, and other domains.

RESEARCH CHALLENGE

Phylogenetic trees are graphical models of evolution that can be used to study evolutionary processes such as how species evolve and adapt to their environments. Such models are useful in a variety of applications, including the prediction of protein function or the classification of molecular sequences of unknown origin. Recent advances in sequencing technologies have resulted in an explosion of data, including genome-scale data sets for very large numbers of species. Today, scientists need to estimate highly accurate phylogenetic trees from such data sets; however, building those evolutionary trees from genome-scale data sets is challenging. For example, genome-scale data sets can be more heterogeneous owing to incomplete lineage sorting (ILS) and other biological processes that result in different regions of the genome having different evolutionary histories. In addition, many of the best methods for phylogeny estimation are heuristics for solving NP-hard optimization problems and the solution space for these problems grows exponentially with the number of species. In order to overcome this challenge, the research team introduced a new divide-and-conquer approach that divides the species into pairwise disjoint subsets and combines subset trees together by solving the disjoint tree merger (DTM) problem, which can be solved in polynomial time.

RESULTS IMPACT

The team implemented the divide-and-conquer approach (using TreeMerge to combine subset trees) as a parallel framework and performed a benchmarking study on Blue Waters. They compared running methods within the parallel framework (in order to estimate subset trees) versus running methods to estimate a tree on the full data set. The researchers found that running methods within the parallel framework dramatically reduced running time and maintained accuracy for two leading species tree estimation methods: ASTRAL-III [1] (Fig. 1) and RAxML [2] (not shown). Novel species tree methods are continually being developed, and many of these new methods are computationally intensive (for example, new Bayesian inference methods). Because researchers can specify that the method be run on subsets, the research team’s parallel framework will be useful in the rapidly progressing field of computational biology and will further research efforts toward building the Tree of Life, a scientific and computational grand challenge.

WHY BLUE WATERS

Method development is an iterative process that requires testing any new method on many large data sets. This process also requires that the new method be compared in terms of accuracy to the best existing methods; running the existing methods on large data sets can take months of CPU time. Without the Blue Waters system, the research team would have been unable to efficiently develop and improve upon novel methods.

PUBLICATIONS & DATA SETS


Figure 1: Communication performance for a 3D halo exchange on Blue Waters using the vendor-provided implementation of MPI_Cart_create (dotted lines) and the researchers' alternative implementations for highly scalable Krylov methods for process mapping in regular Cartesian topologies, "in Proc. 25th Eur. MPI Users' Group Meeting, Barcelona, Spain, Sept. 23–26, 2018, pp. 1–9.


Both zchunk and zlines are available at https://github.com/oshkosher/zlines.

MeshIO is available at https://github.com/oshkosher/meshio.

The improved implementation of MPI_Cart_create is part of basemm and is available from wgropp@illinois.edu.

WHY BLUE WATERS
Scalability research relies on the ability to run experiments at large scale, requiring tens of thousands of nodes and hundreds of thousands of processes and cores. Blue Waters provides one of the few available environments where such large-scale experiments can be run. In addition, Blue Waters provides a highly capable I/O system, which the research team used in developing improved approaches to extreme-scale I/O.

PUBLICATIONS & DATA SETS


Both zchunk and zlines are available at https://github.com/oshkosher/zlines.

MeshIO is available at https://github.com/oshkosher/meshio.

The improved implementation of MPI_Cart_create is part of basemm and is available from wgropp@illinois.edu.

RESEARCH CHALLENGE
This work directly targets current barriers to effective use of extreme-scale systems by applications. For example, Krylov methods such as Conjugate Gradient are used in many applications currently being run on Blue Waters and other large-scale systems. These methods depend both on high-performance matrix–vector products, which are communication intensive, and on collective all-reduce operations, which introduce synchronization that can limit scalability. Developing and demonstrating a more scalable version of this algorithm would immediately benefit these applications. The research team’s approach begins with developing a performance model that captures the key aspects of the intra- and inter-node communication costs and uses that model to inform the development of new algorithms. This approach has also yielded improved parallel I/O routines and a better implementation of a process placement operation that can improve the performance of applications.

METHODS & CODES
To address these challenges, the research team has developed several performance models that address limitations in off-node communication bandwidth, message matching costs, network contention, and the effect of system “noise.” Benchmarks to test these performance models have been developed, and experiments have been conducted with some applications. These performance models have led to new algorithms for providing good and efficient implementation of process mapping for regular meshes. Some of the codes are open source and available; the routines for process mapping in regular Cartesian topologies are under consideration for inclusion in the MPICH implementation of the Message-Passing Interface (MPI).

RESULTS & IMPACT
Paul Eller, working with PI William Gropp, has been using Blue Waters over the last year for an investigation into performance modeling of scalable Krylov solvers for structured grid problems. This includes developing code for measuring and processing parallel runtime and network performance counters, developing a collection of kernels relevant to structured grid problems, exploring their use in several applications, and developing performance models with penalty terms that accurately model parallel performance at scale. He has run experiments to determine parameters for the performance models and performed scaling studies for the various parallel communication kernels and scalable conjugate gradient solvers. These results have led to a paper submitted to the 2019 Association for Computing Machinery International Conference on Supercomputing. These experiments have helped to better understand Krylov solver performance at scale, to develop more accurate performance models, and to optimize the solvers to obtain better performance. Ed Karrels, also working with William Gropp, has continued to explore parallel I/O performance, including exploring the sensitivity of several parameters for I/O operations, such as stripe count and size, and the number of processes per node performing I/O operations. The goal is to provide better guidance for users in choosing I/O parameters and to develop more automatic methods for selecting these parameters within parallel I/O libraries. The libraries that he developed in the previous year—MeshIO, zlines, and zchunk—remain available for use by applications.

In addition, William Gropp has developed a new algorithm for implementing process mapping for Cartesian grids, which is needed for many applications that use structured grids. MPI provides a convenient routine for this operation, but few MPI libraries provide a good implementation of this operation. As a result, applications must either forgo the performance or use ad hoc, nonportable techniques to achieve a good mapping. Such tools do exist for Blue Waters, but these are not portable to other systems and often fail to provide good process mappings in practice. Applications should be able to rely on the features in MPI and not need to use nonstandard, nonportable methods. Finally, by using insight gained from the team’s new performance model, they developed an alternative implementation of MPI_Cart_create that provides a significant performance benefit compared to the vendor-supplied implementation, as shown in Fig. 1.
KALEIDOSCOPE: LIVE FORENSICS FOR LARGE-SCALE DATA CENTER STORAGE SYSTEMS

Allocation: Exploratory/50 Ksh
PI: Rekilin kans hyn
Collaborators: Saurabh Jha, Shenglan Cui, Tianyin Xu, Jeremy Enos, Mike Showman, Greg Bauer, Mark Dalton, Zbigniew Kalbarczyk, Bill Kramer

EXECUTIVE SUMMARY

The research team has developed Kaleidoscope, an innovative system that supports live forensics for application performance problems caused by either individual component failures or resource contention issues in large-scale distributed storage systems. The design of Kaleidoscope was driven by the team’s study of I/O failures observed in a petascale storage system. Kaleidoscope is built on three key features: (1) using temporal and spatial differential observability for end-to-end performance monitoring of I/O requests, (2) modeling the health of storage components as a stochastic process using domain-guided functions that account for path redundancy and uncertainty in measurements, and (3) observing differences in reliability and performance metrics among similar types of healthy and unhealthy components to attribute the most likely root causes.

The research team deployed Kaleidoscope on the Cray® Sonexion®, an evaluation showed that Kaleidoscope can run live forensics at five-minute intervals and pinpoint the root causes of 95.8% of real-world performance issues, with negligible monitoring overhead.

RESEARCH CHALLENGE

Large-scale storage services are typically implemented on top of clusters of servers and disk arrays to provide high performance (e.g., load balancers and congestion control) as well as high availability (e.g., RAID, and active-active high-availability server pairs). Component failures and resource contention are chronic problems that lead to I/O timeouts and slowdowns in such systems. State-of-the-art solutions focus on reliability failures and, hence, do not attempt to distinguish between resource contention and component failures in storage systems, as highlighted in Fig. 1. Knowing whether a problem is due to resource contention or component/node/subsystem failure is critical in effectively coordinating a recovery strategy.

A combination of component failures and contention issues significantly degrades application performance in production settings. This project uses a mixture of proactive monitoring and machine learning to jointly address the above issues. The team has incorporated the proposed techniques into an automated tool called Kaleidoscope. This tool has been demonstrated in live traffic on a production system to: (1) locate components such as data servers and RAID devices causing I/O bottlenecks such as I/O slowdowns or timeouts, (2) differentiate between a reliability failure and a resource contention issue, and (3) quantify the negligible impact on system performance while delivering high precision and recall.

METHODS & CODES

The research team used two years of production data in excess of one terabyte from Blue Waters including system-generated storage error logs and store read/write latency logs collected intelligently using Kaleidoscope. Kaleidoscope is a generic framework for supporting runtime detection and diagnosis of large-scale storage systems. The key components of the tools are:

- Proactive monitoring. Kaleidoscope monitors the end-to-end performance of a storage system using Store-Pings, a set of monitor primitives that covers all the storage operations involved in serving a client’s I/O requests (e.g., creating, reading, writing, and deleting files). Store-Ping monitors are strategically placed to provide both spatial and temporal differential observability in real time (steps 1–3 in Fig. 2).

- Modeling and inferring component health. The health of a component in a storage system such as a metadata server or a RAID device is modeled as a stochastic process that accounts for uncertainty (owing to performance variability and asynchrony) as well as nondeterminism in distributed storage systems. The research group built a system model by using the factor graph (FG) formalization, which infers component health by ingesting the monitoring data collected by Store-Pings. The inference on the model allows Kaleidoscope to localize unhealthy components in near real time (step 4 in Fig. 2).

- Methods to determine the cause of I/O failures. A set of statistical methods (including a local outlier factor algorithm run using data on server load, disk load, and disk bandwidth utilization) and clustering of storage system error logs are used to distinguish between component failures and resource overloads. The statistical methods are based on a comparison of reliability and performance metrics (such as the number of active processes on a data server) as they are collected for healthy and unhealthy components. Note that the distinction between healthy and unhealthy components is provided by the FG-based model (Step 5 in Fig. 2).

RESULTS & IMPACT

Deployment. Kaleidoscope has been deployed on Blue Waters’ Cray® Sonexion®, a 36-petabyte production system that employs the Lustre file system. Lustre is used by more than 70% of the top 100 supercomputers and is offered by cloud service vendors such as Amazon and Azure. Its design resembles that of many other object-based POSIX storage systems such as the IBM GPFS, BeeGFS, Ceph, and GlusterFS. The team measured the overhead introduced by Store-Ping monitors on the production system and found the overhead to be less than 0.01% on the peak I/O throughput of the Cray® Sonexion®.

Performance effectiveness. The evaluation was based on 843 production issues identified and resolved by Blue Waters system managers in a two-year period as the ground truth. Overall, Kaleidoscope correctly localized the component failures and resource overloads for 99.3% of the cases. In addition, Kaleidoscope accurately identified the likely root cause for 95.8% of the cases, i.e., disambiguation between resource contention and component failures.

Figure 2: An overview of Kaleidoscope. Kaleidoscope consists of three components for identifying failure localization and failure diagnosis (marked in gray).

WHY BLUE WATERS

Blue Waters is one of the few open-science capacity systems that provides a testbed for scaling computations to tens or hundreds of thousands of cores on CPUs and GPUs. It also enables the study of failures and performance degradations of applications in production petascale systems, thereby allowing researchers to understand the performance–fault–tolerance continuum in high-performance computing systems.

PUBLICATIONS & DATA SETS


Figure 1: Common patterns of I/O failures. Notations: “HB” is heartbeat process, “sys” is service process, each box represents the storage component (e.g., data servers).
The previous version of ExTASY was developed to reduce the complexity of adaptive sampling and was used by the research team to show in [1] that ExTASY can scale complex workflows on supercomputers. The next step for ExTASY was to demonstrate an end-to-end execution of adaptive sampling for reference proteins. By comparison with reference results, the research team confirmed that adaptive sampling delivers accurate results for protein folding and protein dynamics and that the sampling could be investigated. The achieved speed-up for three proteins—Chignolin, BBA, and Villin, with 10, 28, and 35 residues, respectively—the employed protein dynamics. Further comparison of adaptive sampling strategies is discussed in [2]. By utilizing different adaptive sampling strategies, the research team has shown that this workflow can be easily adapted to different exploration strategies.

**RESULTS & IMPACT**

The new version of the ExTASY workflow holds proteins with a shorter time-to-solution than brute-force MD. Fig. 2 shows that adaptive sampling utilizing ExTASY is about one order of magnitude faster than brute-force MD. Additional results confirming the accuracy of protein folding and protein dynamics may be found in [3]. By utilizing different adaptive sampling strategies than in previous versions of ExTASY, the research team has shown that this workflow can be easily adapted to different exploration strategies.

**PROTEIN FOLDING SIMULATIONS**

Protein folding simulations require large numbers of GPU node-hours despite the speed-up achieved by ExTASY. Blue Waters is essential to deliver these computational resources. The investigated proteins are relatively small and undergo fast folding; larger proteins would require even larger computational resources.

**PUBLICATIONS & DATA SETS**


IMPROVED SCALABILITY THROUGH NODE-AWARE COMMUNICATORS

Executive Summary

Sparse matrix operations abound in numerical simulations and represent significant costs at scale. As researchers anticipate future machine networks and compute units, these communication-bound operations will continue to incur significant cost. The focus of this work is on reducing communication at scale, particularly in settings where machine layout and multiple compute units can be exploited. Blue Waters is an ideal setting for developing these methods since the research team can expose node-level (as well as socket-level) parallelism. The work has identified new methods for organizing communication to reduce the overall time-to-solution.

Research Challenge

Sparse matrix operations such as sparse matrix–vector multiplication and sparse matrix–matrix multiplication are key kernels in many iteration and preconditioning techniques. Yet, these operations incur a significant communication penalty in situations where the matrix patterns are highly unstructured. The goal of this work is to identify metrics for predicting communication overhead and to construct communication routines that can significantly reduce cost by utilizing certain aspects of the machine such as the node and socket layout.

Methods & Codes

This work has led to the development of scalable solvers within the RAPtor package [1] and has helped to shape the development of a node-aware library [2] that can be used easily by application codes from a range of scientific disciplines. Both software packages rely on node-aware MPI communication, which reroutes standard internode communication to reduce the total cost of sending data through the network.

There are two variations of this work, both aggregating data at the node level to reduce the number and size of messages being sent through the interconnect. Two-step node-aware communication consists of each process gathering all data to be sent between two nodes on a single message on the node of origin. These data are then sent as a single message between nodes, after which it is redistributed locally to any process on the receiving node that needs it.

Three-step node-aware communication adds another layer of aggregation, agglomerating all data to be sent to a single node and sending these data directly to the corresponding process on the destination node. The receiving process then distributes these data to all on-node processes that need it. Alternatively, three-step communication adds another layer of aggregation, agglomerating all data to be sent between two nodes on a single process on the node of origin. These data are then sent as a single message between nodes, after which it is redistributed locally to any process on the receiving node that needs it.

Results & Impact

The optimal method of communication varies with communication pattern as well as network topology. Therefore, optimizing communication costs throughout the algebraic multigrid (AMG) requires different strategies based on the system being solved. There are several factors that impact communication costs, including the sparsity pattern on a particular level of the AMG hierarchy, the amount of data being communicated on each level, and the number of active processes. Fig. 1 displays the cost of each strategy for matrix–matrix multiplication on each level of an AMG hierarchy, a dominating kernel in the AMG setup phase. The results show that standard communication outperforms node-aware on fine levels where communication is regular and structured, while node-aware strategies are optimal on coarse levels. Similarly, while three-step communication is often optimal, two-step node-aware communication often outperforms on the first few coarse levels when messages are large.

One goal of this work on Blue Waters is to develop a method to automatically select the communication strategy. RAPtor includes a predictive performance model that identifies the optimal communication strategy for each operation. Fig. 2 shows the cost of standard AMG versus node-aware AMG where performance models select the optimal communication strategy for each operation. Communication costs can vary widely for different computational kernels and machine settings—this work automates the communication strategy leading to significant speedups and reduced time-to-solution.

Why Blue Waters

Blue Waters was central to this work, providing a large scale of resources to test the models and routines developed by the research team. The node-level layout of Blue Waters provided the initial inspiration for the algorithms the team developed, and the consistency of the compute environment was a central component in reproducible testing at scale.

Publications & Data Sets

SCALABLE LINE AND PLANE SOLVERS

Allocation: Illinois/75 Knh
PI: Luke Olson*
Co-PI: Amanda Bierer*
Collaborator: Andrew Reisner*
*University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY

Structured elliptic solvers play an important role in a range of applications, from plasmas to solid mechanics. However, their scalability is limited owing to the global nature of the problem. Multigrid methods have been effective at solving this class of problems; however, structured multigrid solvers rely on sweeps over lines and planes in the mesh in order to yield an effective method, which severely limits scalability. Through this work, the research team has developed scalable kernels for line and plane relaxation methods.

RESEARCH CHALLENGE

Sparse matrix problems arising from elliptic partial differential equations present a significant computational challenge in many applications at scale. Iterative approaches such as multigrid preconditioned conjugate gradient methods have proven to be cost effective. Yet, in situations with high mesh anisotropy or variable problem coefficients, multigrid solvers require the use of more robust components. Point relaxation techniques such as the Jacobi method are insufficient, thus requiring the use of line and plane forms of these methods.

METHODS & CODES

Line relaxation (and in 3D, plane relaxation) plays an important role in preconditioning structured elliptic problems. Fig. 1 highlights the importance of line relaxation in comparison to a standard weighted Jacobi (pointwise) relaxation solver in multigrid for the case of an annulus with moderate 10:1 stretching of the grid. There is a significant reduction in total iterations, yet each pass of line relaxation requires a distributed tridiagonal solver. The key bottleneck in a tridiagonal (or banded solver) is the limited work per processor. Fig. 2 highlights the \( O(p) \) effect, with \( p \) cores increasing in one dimension. A straightforward implementation of the tridiagonal solver results in a linear relationship. This work focuses on a multilevel form of the problem where a new tridiagonal problem is formed in the communication overlap, resulting in a \( O(\log p) \) dependence and significantly reducing cost. The current approach centers on two interrelated aspects to further advance the solver. First is the development of a scalable and accelerator-aware halo exchange library, called Tausch [1], which can be used in a variety of structured codes. Second is the extension of the structured solver Cedar [2] to accelerators, such as the XK portion of Blue Waters.

Figure 1: Point and line relaxation convergence for a Poisson problem on an annulus.

Figure 2: Scalability of sequential line relaxation versus multilevel line relaxation as the core count \( p \) increases.

RESULTS & IMPACT

This work has directly contributed to the algorithms, testing, and development of the Tausch [1], Cedar [2], and RAPtor [3] software packages. Each of these targets general use in a wide range of scientific applications.

WHY BLUE WATERS

Blue Waters has played a key role in testing structured solvers at scale, for example in [4]. Access to large core counts and consistent testing has been instrumental in developing scalable algorithms and accurate performance models that form the core of this work.
DETECTION OF SILENT DATA CORRUPTIONS USING MACHINE LEARNING

Allocation: Exploratory/40 Knh
PI: Marc Snir
Collaborator: Franck Cappello

1University of Illinois at Urbana–Champaign
2Argonne National Laboratory

EXECUTIVE SUMMARY

Future supercomputers are expected to encounter more frequent bit-flips as the number of devices increases and their size shrinks; furthermore, one could reduce power consumption by tolerating more frequent errors. Some errors may escape the notice of the error detection mechanisms provided in hardware. To handle those, it may be necessary to detect errors in software. One promising approach is to periodically test the state of a long-running computation and identify “anomalous” states indicating that a bit-flip occurred.

The research team is using a convolutional neural network (CNN) as a detector. The CNN is trained with multiple examples of correct and incorrect computation states, next used as a classifier. Using this method, the team achieved a high detection rate, with an acceptable overhead. The method is practical and could be used on future systems should their rate of undetected bit-flips require software detection.

RESEARCH CHALLENGE

Future supercomputers are expected to encounter more frequent hardware errors, owing to the increase in the number of devices and the decrease in their size. Furthermore, one can decrease power consumption of supercomputers by tolerating more frequent errors. Some of these errors may not be detected and could corrupt the computation output. The research group’s goal is to detect silent data corruptions by periodically running tests on the state of an ongoing computation.

METHODS & CODES

A single bit-flip in one variable of a large simulation can result in an error that propagates through the entire data set over time. Figs. 1 and 2 illustrate error propagation for two different iterative simulations. The research team’s hypothesis is that machine learning can be used to detect such error patterns. The problem is that these error patterns are superimposed onto the correct computation state.

The team is treating the correct simulation as “noise” and is looking for the signal of a propagating error added to the noise. This is done by training a convolutional neural network (CNN) with multiple examples of correct and faulty simulations and then using the network as a detector. The training needs to be repeated once for each code, but the training procedure does not depend on the code.

RESULTS & IMPACT

Using this technique, the researchers have achieved a much higher detection rate than was previously achieved [1]. Furthermore, unlike previous methods, errors can be detected multiple iterations after they occurred so that the error detector need not be run at each iteration. The recall rate is around 90% and the overhead for running the detector could be as low as 1%. Follow-up work, to be published, aims at better understanding which errors do lead to a noticeable corruption of the final result, as only those need to be detected; and to extend these methods to work on 3D data sets. This research indicates that it will be possible to use future supercomputers efficiently, even if undetected bit-flips become common.
PUSHING THE BOUNDARIES OF LARGE-SCALE TENSOR COMPUTATIONS

Allocation: Illinois/20 Kiib
PI: Edgar Solomonik

Executive Summary

This project seeks to develop new parallel algorithms and scalable productive software for matrix and tensor computations. Over the past year, the research team has made significant advances in software infrastructure of the Cyclops library for tensor computations. This library provides a productive algebraic programming interface in Python and C++ that performs numerical and combinatorial operations in a data-distributed manner. The team has developed software for hypersparse matrix representations, automatic optimization of contraction order, parallel tensor-times-tensor-product kernels, and has significantly extended capabilities at the Python level. The team currently is benchmarking tensor completion algorithms on Blue Waters using the new Python interface layer and has obtained preliminary benchmarking results for new Cyclops application in genomic analysis. Separately, the researchers have developed a new practical communication-avoiding parallel algorithm for QR factorization, evaluating its performance via large-scale runs on Blue Waters.

Research Challenge

Tensor computations are a growing area in computational science, with applications in quantum chemistry and physics, quantum circuit simulation, machine learning, optimization, and numerical PDEs (partial differential equations). They also push the boundaries of numerical linear algebra technologies, requiring algebra on large, extremely sparse, and in some cases unstructured matrices, as well as redistribution of their data. These applications create a demand for better algorithms and software for distributed-memory tensor computations.

Methods & Codes

The research group led the development of Cyclops, a distributed-memory library for tensor computations, which is likely the most widely used distributed tensor algebra library. Cyclops uses MPI, OpenMPS, CUDA, and HPTT (High-Performance Tensor Transpose). It interoperates with ScaLAPACK and makes use of advanced sparse matrix routines in MLK. Cyclops provides a much simpler and more intuitive interface for both that is almost entirely agnostic to sparsity. It also provides a wide range of further functionality, including sparse and dense tensor contractions and generalized elementwise operations that enable graph and combinatorial algorithms. Additionally, it provides an interface to Python and a wide variety of functionality in a style similar to the NumPy library of mathematical functions.

The group has also developed standalone codes for parallel numerical linear algebra kernels. The researchers have developed and maintained suites of algorithms for tensor completion and tensor decomposition, which employ variants of alternating least squares, coordinate descent, and stochastic gradient descent methods, all parallelized using Cyclops. The team planned to benchmark the newly developed tensor decomposition and tensor completion kernels on Blue Waters in the summer of 2019.

Aside from tensor computations, the group also works on improving basic numerical linear algebra operations, such as computation of dense QR and eigenvalue decomposition of symmetric matrices. Edward Hutter, a Ph.D. student at the University of Illinois at Urbana-Champaign (Illinois), developed and maintains a new QR algorithm and library that achieves asymptotic improvements in communication efficiency by a new parallelization for the Cholesky--QR2 algorithm. One application of such large rectangular QR factorizations is in computing the Tucker decomposition of tensors.

Results & Impact

The team's work on Cyclops has a leading role in parallel infrastructure for numerical tensor algebra. Their library enables distributed-memory parallelism in leading quantum chemistry codes, including QChem, PySCF, and CCAS. The library has been used to execute methods for quantum chemistry at near one petaflops and was used by a group of IBM and Lawrence Livermore National Laboratory researchers to perform a 49-qubit quantum circuit simulation, a central result in the field of quantum supremacy testing.

The research team is currently collaborating with researchers in the physics department at Illinois and chemistry department at Caltech to develop the first massively parallel versions of tensor network codes. One-dimensional and two-dimensional tensor networks (namely DMRG and PEPS, two methods for computing properties such as ground state energy of quantum systems, which represent the quantum many-body state via 1-D and 2-D tensor networks, respectively) provide highly accurate results for ground and excited state properties of highly correlated quantum systems. Researchers in the Illinois physics group (led by Bryan Clark) are currently prototyping initial versions of DMRG on Blue Waters.

A major impact on applications provided by Cyclops is the ability to rapidly develop massively parallel code via tensor algebra. A very recent example of this is the research group's collaboration with a team of bioinformatics researchers who are interested in computing a Jaccard similarity matrix from the data of a large set of genomes, the first calculation of this type. Using Cyclops primitives for general sparse matrix multiplication, the team implemented the necessary kernels for logical (bitwise) operations within a week and are seeing good weak and strong scaling in small-scale initial tests on Blue Waters (Fig. 1). These results should pave the way for the bioinformatics team to apply for resources to perform a full-scale computation.

The team has obtained large-scale results for the new Cholesky--QR2 parallel algorithm, which achieves better parallel scaling trends than ScaLAPACK's QR owing to needing less communication, but it is slightly behind in absolute performance because it requires more FLOPS (Fig. 2). The team has also obtained results on more compute-intensive architectures, where the new Cholesky--QR2 algorithm outperforms ScaLAPACK significantly on large node-counts. The researchers are currently developing a GPU-accelerated version of the Cholesky--QR2 algorithm that they believe will be effective on the GPU nodes of Blue Waters as well as on future architectures. QR is one of the most widely used dense linear algebra primitives, so this work has the potential to impact many applications. These results will appear in the proceedings of the 2019 International Parallel and Distributed Processing Symposium.

Why Blue Waters

As Illinois researchers, the team takes pride in using and showcasing results from the Blue Waters high-performance computing infrastructure. They also generally aim to test new algorithms and software on multiple supercomputing architectures, and Blue Waters is both unique and is itself diverse (providing large infrastructure for both GPU and pure-CPU runs). Using Blue Waters provided the team with a better understanding of the dependency of the performance of Cholesky--QR2 for architectures with different ratios of bandwidth and compute rate. In a number of applications areas of interest, including quantum chemistry, quantum circuit simulation, tensor decomposition, and bioinformatics, the capability of calculations is often bounded by memory, making Blue Waters the architecture of choice.

Publications & Data Sets

EXECUTIVE SUMMARY

Evolutionary trees are used to advance the understanding of how life evolved on Earth, how species adapt to their environments, and to predict the structure and function of proteins. However, despite large numbers of whole genomes and increasing amounts of biomolecular sequence data available for use, the inference of a Tree of Life is beyond the reach of current methods, as even relatively small data sets can require many CPU years for analysis. This project aimed to develop new algorithms for large-scale evolutionary tree estimation, focusing on conditions with large numbers of species and/or whole genomes. Specific contributions of this work include new algorithmic strategies that greatly improve the scalability and accuracy of powerful statistical methods so they can be used to construct phylogenies on ultralarge data sets of importance to biologists.

METHODS & CODES

Biologists use evolutionary trees to improve the understanding of how species evolve and adapt to their environments, to predict protein structure and function, to explore the early origins of life and how humans moved across the globe, and the like. The advances in whole genome assembly have suggested that the accurate inference of a Tree of Life may be achievable. However, despite large numbers of whole genomes and increasing amounts of biomolecular sequence data available for use, the inference of a Tree of Life is much more challenging than was expected. The main issues impeding this are: (1) the inference of these evolutionary trees is computationally challenging, as the most accurate methods are based on attempts to solve hard optimization problems (such as maximum likelihood) and current optimization methods do not scale to large data sets with good accuracy; and (2) standard approaches to phylogeny estimation, which make strong assumptions about the homogeneity of the statistical process underlying the molecular sequence data, do not have good accuracy in the presence of heterogeneity across genomes and across time, and yet substantial heterogeneity is now well established [1–3]. While some methods have been developed to enable phylogeny estimation in the presence of heterogeneity across genomes, these methods are computationally intensive, even on just moderately large data sets. Hence, current approaches to phylogeny estimation either do not provide good accuracy on large data sets or cannot even run on large data sets within reasonable timeframes.

RESULTS & IMPACT

Figure 1: The result of using TreeMerge (a divide-and-conquer strategy) with the leading maximum likelihood method, RAxML, as a species tree constructed on 1,000 species with 1,000 genes when there is gene tree heterogeneity owing to incomplete lineage sorting [5]. The plots explored results for two types of genetic cases: exons and introns. The number of replicates for which RAxML returns a tree is given by N; when run by itself, RAxML cannot complete on some data sets within 60 hours on Blue Waters, but when run within the divide-and-conquer framework, it completes on all data sets. (“ILS” refers to incomplete lineage sorting.)
HPC DEVELOPMENT OF DEEP LEARNING MODELS IN SCIENTIFIC COMPUTING AND FINANCE

EXECUTIVE SUMMARY

This allocation was used to support several deep learning proj-
ects across a variety of applications. The three applications were:
(1) scientific computing, (2) modeling high-frequency financial
data, and (3) image recognition. The first application develops and
evaluates deep learning closure models for large eddy simulation
(LES) models of turbulent flows. The deep learning LES models
are trained on direct numerical simulation (DNS) data from the
Navier–Stokes equation. The DNS data sets are generated using
Blue Waters and the deep learning LES models are trained using
Blue Waters’ GPU nodes. In the second application, deep learn-
ing models are trained and evaluated on massive high-frequen-
cy data sets. In the third application, which only used a small
amount of the overall allocation, the asymptotics of deep learn-
ing models were analyzed on image data sets such as the Medi-
fied National Institute of Standards and Technology and Cana-
dian Institute for Advanced Research 10 data sets.

RESEARCH CHALLENGE

Deep learning has revolutionized fields such as image, text,
and speech recognition. Owing to this success, there is growing interest in applying deep learning to other fields in science, en-
gineering, medicine, and finance. Blue Waters was used to devel-
oped and test deep learning methods and models for important ap-
lications in scientific computing and quantitative finance. The
research team developed deep learning models for turbulence, which has been a longstanding challenge in computational sci-
ence and engineering. The preliminary results demonstrate the
ability of the machine learning-based models to predict turbu-
ent flow energy spectra more accurately than traditional tur-
bulence models. In another project, the team developed a deep
learning model for high-frequency financial data. Financial in-
itations have a strong interest in developing and using machine
learning methods in scientific modeling has the potential to advance simulation and design in engineering.

WHY BLUE WATERS

Deep learning uses multilayer neural networks (deep neural
networks) to build statistical models of data. This training of the
deep learning model can be computationally intensive owing to
both the large number of parameters and the large amounts of
data. GPUs can be used to accelerate training of deep learning
models. The researchers leveraged Blue Waters’ large amount of
GPU resources to develop deep learning models for applications
in engineering and finance. Blue Waters' XE nodes were also ex-
tensively used to generate DNS data sets, which was extremely
computationally expensive and required parallelization over thou-
sands of cores. The Blue Waters technical staff provided invaluable help throughout the project, including solving a number of
technical issues related to deep learning computational frame-
works such as PyTorch.

METHODS & CODES

In the scientific computing project, the team developed a deep
learning closure model for LES and generated DNS data sets. These
DNS data sets were filtered and downsampled to yield appropri-
ate data sets for training the deep learning LES model, which was
parallelized across 24 GPU nodes. Synchronous gradient descent
was used to train the deep learning model.

As part of this project, the research team also developed a new
DNS/LES code, PyFlow, for training and simulation of the
deep learning LES model. This code is GPU-accelerated and has
potential to address modeling challenges over a wide range of
flows. Similarly, the high-frequency financial data project used
synchronous gradient descent (distributed across multiple com-
pute nodes) to train deep learning models.

RESULTS & IMPACT

In the scientific computing project, the deep learning LES mod-
el is able to more accurately predict the filtered DNS data than
traditional LES models. For example, in out-of-sample tests, the
deep learning LES model more accurately reproduces the energy
decay and energy spectrum as compared to traditional LES models
such as Smagorinsky and Dynamic Smagorinsky. The use of deep
learning and machine learning methods in scientific modeling has
the potential to advance simulation and design in engineering.

OPTIMIZATION OF A FIELD DATA PARALLEL OUTPUT LIBRARY

Executive Summary

TecIO-MPI is Tecplot, Inc.’s parallel data output library. It is designed to output to Tecplot’s native file format the field data re-
results of numerical simulations, such as those produced by com-
putational fluid dynamics (CFD). Its initial implementation suf-
fered from unacceptable parallel performance in some cases. In
this work, the profiling software tools available on Blue Waters
were used to identify and remedy the sources of this unacceptable
performance. The researchers then ran test cases, scaling up to
912 nodes, to confirm acceptable performance and scaling. The
results confirm order-of-magnitude reductions in output time
and indicate that output times scale linearly with output file size.

Research Challenge

Parallel simulation codes break large problems into smaller
pieces and solve these smaller pieces simultaneously by using
many CPU cores. At the end of the solution (and perhaps peri-
odurally during the solution), each core’s portion of the overall
solution must be written to disk, perhaps all to a single file. This
parallel file output must be fast enough to not hinder the over-
all solution progress significantly. Thus, any code that performs
this output must be optimized for parallel performance. But par-
allel optimization requires tools that can not only examine the
execution time of blocks of code but can also identify wait states
caused by communication delays among the multiple processes
that run together to produce the solution or output. Further, to
optimize a massively parallel code requires testing that code on
hardware representative of the hardware on which it is intend-
ed to run. Blue Waters provided the answer to these challenges.

Methods & Codes

The research team ran the TecIO-MPI library with a test har-
ness that loaded data previously serialized to disk and then called
into TecIO-MPI to output the data. The test harness was a stand-
in for the sort of simulation code with which TecIO-MPI is de-
signed to run. This allowed repeated tests of the software with-
out the overhead of an actual CFD-type solver. The researchers
performed parallel profiling with Cray’s Performance and Analy-
ysis Tools, and data were written to a single file on Blue Waters’
 Lustre file system. Hotspots that were identified were record-
ed to improve performance, and the software was retested to en-
sure the fixes were effective.

Results & Impact

The performance of TecIO-MPI was improved to the point that
CFD-solver authors should find it acceptable—roughly the
cost of a single solver iteration—and measured wall-clock output
times appear to scale linearly with output file size. The file format
the library outputs enables Tecplot to visualize on typical desktop
workstations—via contour flooding, streamline generation, slic-
ing, etc.—much larger files than can typically be handled on such
machines by loading from disk only the data required to produce
the artifacts. The more expensive in this postprocessing scales with the number of solution cells raised to the two-thirds power,
such that its advantage grows exponentially with larger file sizes.

Why Blue Waters

Blue Waters provided access to both hardware and software
required for this project to be successful. Its ability to scale prob-
lems to many CPU cores, and its use of the popular Lustre file
system, ensured that the software was being tested in a represen-
tative environment, such that performance improvements seen
in this work would also be seen by the intended users of this soft-
ware. Blue Waters’ Cray performance-measuring tools were indis-
 pensable in identifying performance bottlenecks and confirming
their removal. And the technical support staff were very helpful
with identifying the appropriate configuration of the compilers
and profiling software required for this work.
RESOLVING THE STRUCTURE OF BACTERIOPHAGE HK97 WITH ATOMISTIC RESOLUTION

Allocation: Illinois/450 Knob
PI: Aleksei Aksimentiev1
Collaborators: Kush Coshic1, Christopher M. Maffeo1, David Winogradoff2
1University of Illinois at Urbana–Champaign
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EXECUTIVE SUMMARY

Viruses are omnipresent, diverse, and potentially lethal biological systems that our bodies encounter every day in copious quantities without us taking notice. The essence of each virus is its genome, a biological program written using letters of the genetic alphabet. The genome is protected from the outside world by a protein shell (a viral capsid) until the conditions are met for viral invasion, at which point the genome is released from its protective shell into a host cell, initiating a new cycle of infection. The ongoing adaptation of viruses to antiviral drugs currently in use necessitates development of the next generation of drugs that target viruses from a physical standpoint. By carrying out large-scale molecular dynamics simulations on Blue Waters, the research team has constructed the first atomically resolved model of a complete virus particle, including the 3D structure of its genome, an untapped resource of potential drug targets. The modeling approach demonstrated by this proof-of-principle simulation may be applied in the future to develop new antiviral drugs.

RESEARCH CHALLENGE

Atomistic structures of protein capsids have been resolved for many viral species, but the structural organization of their genomes still remains largely unclear. One such viral species is the HK97 bacteriophage, for which experiments have characterized the packaging mechanism and resolved its protein capsid with atomistic resolution [1]. Previous cryogenic electron microscopies such as HK97 [6], yielding a fully atomistic model of the HK97 bacteriophage genome, for which experiments have characterized the packaging mechanism and resolved its protein capsid with atomistic resolution [1]. Previous cryogenic electron microscopy and Small-Angle X-Ray Scattering experiments [2] have not yet elucidated the precise organization of the genome in individual virus particles. Previous computational efforts have addressed the dynamic behavior of the capsid [3,4], matrix [1], or the outer envelope, but the structural assignment of nucleic acids inside viral capsids has not been explored comprehensively. Using Blue Waters, the research team has met the challenge of reconstructing the 3D structure of the HK97 bacteriophage genome, a double-stranded DNA molecule containing 39,732 base pairs.

METHODS & CODES

To obtain microscopically correct structures of DNA inside viral capsids, the researchers employed a multiscale approach whereby the results of computationally inexpensive coarse-grained (i.e., with reduced representation) molecular dynamics (MD) simulations were used to set initial conditions for fully atomistic all-atom simulations of a virus particle loaded with DNA. With four base pairs of DNA represented as one coarse-grained particle, the 39,732-base-pair-long genome was packaged into a grid-based implicit protein capsid through a narrow portal that exerted a physiological packaging force [5]. Starting from the final packaged conformation, the team obtained an atomistic model of the genome from a series of simulations gradually increasing in resolution. Subsequently, water and ions were added to mimic conditions at DNA densities typical of pressurized viruses such as HK97 [6], yielding a fully atomistic model of the HK97 genome submerged in explicit solvent. The DNA structure was then placed inside the all-atom capsid through a set of all-atom simulations carried out in the presence of a confining potential. The final atomistic system was comprised of roughly 27 million atoms. All MD simulations were carried out using NAMD [7].

RESULTS & IMPACT

The research team validated the results of the coarse-grained simulations by comparing experimentally determined internal pressure inside a viral capsid [8] to the pressure exerted by the DNA genome on the confining potential. Small-Angle X-ray Scattering profiles generated from the atomic model of the genome were found to be in quantitative agreement with experimental data [2]. The team performed further simulations to characterize the effect of different packaging mechanisms and to determine the contribution of bending stress (attributed to confining a stiff polymer, DNA) to the internal pressure. For quantifying the geometry of the DNA inside the capsid, the scientists evaluated a toroidal order parameter that indicated a preferential ordering of the packaged DNA about the axis along which the DNA was packaged into the capsid. Overall, the team found the outcome of the simulations matched experimental data extremely well, which validates the obtained structures of the HK97 genome. The simulation protocol developed through this project can now be applied to other viruses to predict their genomic structures, offering exciting avenues for designing new antiviral drugs.
EXECUTIVE SUMMARY

Single-molecule protein sequencing would provide unprecedented insights into cellular processes and the diseases that arise from protein malfunction. As compared to nucleic acid sequencing, there are no robust methods that can read the protein sequence without any challenges. In collaboration with the Ouldali Lab at the University of Cergy–Pontoise and the Behrends Lab at the University of Freiburg, the research team is developing a nanopore system that can identify the type of amino acids that pass through the nanopore from a modulation of the nanopore ionic current—a crucial first step toward realizing nanopore protein sequencing. The researchers have already shown that a biological nanopore aerolysin can identify thirteen out of the 20 different amino acids. Using atomistic molecular dynamics (MD) simulations, the team aims to further engineer the aerolysin nanopore to enable identification of all 20 amino acids and to increase the identification fidelity by extending the time that amino acids spend within the nanopore. Successful outcome of this project will pave the way toward the first single-molecule protein sequencing method.

RESEARCH CHALLENGE

Cells express many thousands of proteins to perform a diverse set of complex tasks that are essential to the health of a living organism. A technology providing inexpensive yet sensitive and quantitative identification of the proteins in a cell will help numerous researchers elucidate biological processes, including the molecular origins of many diseases [1]. Existing protein binding and precipitation assays are relatively low-throughput, and their application is typically limited to detection of a few predetermined protein species [2,3]. However, protein sequencing methods aim to identify and quantify proteins and posttranslational modifications have shown that the nanopore volume confined by the two entrances and exit of the aerolysin nanopore. Importantly, the simulations of protein systems.

WHY BLUE WATERS

To get an accurate estimate of the ionic current and fast convergence of the free-energy landscape, the team needs explicit-solvent all-atom MD simulations that are run in parallel for exchange of structure information between different windows. Because of the long timescales and parallel MD simulations of a 0.5-million-atom system, this project is computationally demanding. The Blue Waters petascale system is one of a few supercomputers in the world with the computational power sufficient to carry out fully atomistic enhanced sampling simulations of peptide translocation through a nanopore. The large number of XK nodes on Blue Waters with graphics processing unit accelerators connected by the fast Gemini interconnect makes it one of the best publicly available systems for performing large-scale parallel MD simulations of protein systems.

PUBLICATIONS & DATA SETS

DYNAMIC INTERACTIONS BETWEEN LIPID-TETHERED DNA AND PHOSPHOLIPID MEMBRANES

**Allocation:** Blue Waters Professor/240 Koh

**PI:** Aleksei Aksimentiev

**Collaborators:** Patrick M. Arnott, Himanshu Joshi, Stefan Howorka

**1University of Illinois at Urbana-Champaign**

**2University College London**

**EXECUTIVE SUMMARY**

Lipid-anchored DNA can attach functional cargo to bilayer membranes; this has applications in DNA nanotechnology, synthetic biology, and cell biology research. An understanding of DNA membrane-binding strength and structural dynamics at the nanoscale is required to optimize the DNA anchoring for these applications. Using simulations performed on the Blue Waters supercomputer, the research team elucidated how membrane binding of cholesterol-modified DNA depends on electrostatic and steric factors involving the size and charge of the lipid headgroup, duplexed or single-stranded DNA, and the buffer composition. Atomistic molecular dynamics (MD) simulations explain the experimental findings and elucidate the dynamic nature of anchored DNA, such as the mushroom-like conformation of single-stranded DNA hovering over the bilayer surface in contrast to a straight-up conformation of double-stranded DNA. The information from this study is expected to facilitate the development of biomimetic DNA versions of natural nanopores and cytoskeletons for research and nanobiotechnology.

**RESEARCH CHALLENGE**

A lipid molecule attached to the end of a DNA strand can anchor the strand to a lipid bilayer membrane. This simple principle has been applied to design lipid-spanning DNA nanoparticles [1,2] for applications in the fields of nanobiotechnology [3], biosensing [4], and synthetic biology [5]. Controlling the interactions between anchored DNA and a bilayer membrane is critical to attaining the desired performance of such lipid-spanning DNA nanoparticles. There are numerous unanswered questions about the nature of such interactions; in particular, about the affinity and the conformation of the tethered DNA strands to and near the bilayer membrane and how those are affected by the charge and size of the lipid headgroup.

**METHODS & CODES**

The research team performed explicit-solvent all-atom MD simulations of several lipid-conjugated DNA systems using the latest version of NAMD2 [6]; the CHARMM36 [7] forcefield to describe the bonded and nonbonded interactions among DNA, lipid bilayer membranes, water, and ions; and the team's custom NBFIX corrections for nonbonded interactions [8]. The analysis and postprocessing of the simulation trajectories were performed using VMD and CPPTRAJ [9,10].

**RESULTS & IMPACT**

Complementing the gel-shift experiments carried out by the collaborators in the Howorka group at the University College London, the researchers at the University of Illinois at Urbana-Champaign built and simulated several all-atom models of DNA–lipid systems that differed from one another by the composition of the lipid membrane, the type of DNA molecules, and the buffer conditions. The lipids were chosen on the basis of their widespread usage of cholesterol-conjugated DNA for sculpting and assembling lipid-anchored DNA strands interact with lipid bilayer membranes. Based on the titration results from the gel-shift assay, this study for the first time quantified the binding affinity of cholesterol-conjugated DNA to lipid membranes in terms of their equilibrium dissociation constant. The quantitative insights into the binding affinity and molecular accessibility of DNA will facilitate rational design of membrane-spanning DNA nanoparticles and broaden the usage of cholesterol-conjugated DNA for sculpting and assembling lipid bilayer membranes into functional biomimetic systems.

**WHY BLUE WATERS**

Explicit-solvent all-atom MD simulations were needed to examine the fine details of lipid-tethered DNA interactions with the bilayer membrane and to accurately characterize the effect of various factors such as the charge and the size of the lipid headgroups as well as the type of the DNA constructs (single- or double-stranded DNA). Because of the long timescale needed to decipher these details, such MD simulations are computationally demanding. The large number of XK nodes on Blue Waters with graphics processing unit accelerators connected by the fast Gemini interconnect makes it one of the best publicly available systems for performing simulations studying DNA–lipid interactions in atomistic detail. Over the past several years, the research team has used Blue Waters to carry out a set of landmark simulations in the area of nucleosomes and DNA dynamics, bringing high-performance simulations to the forefront of this research field.

**PUBLICATIONS & DATA SETS**

INFLUENCE VIRULENCE AND TRANSMISSIBILITY THROUGH THE COMPUTATIONAL MICROSCOPE

RESEARCH CHALLENGE

IAV causes severe illness and thousands of deaths every year. The virus can undergo random reassembly of its segmented genome that may result in devastating worldwide pandemics. In this concerning scenario, the most critical mutations are usually found in two membrane glycoproteins: hemagglutinin (HA) and neuraminidase (NA), characterized by a wide population of carbohydrate structures located on their surface. Glycans are implicated in numerous viral processes, such as infectivity, pathogenicity, transmissibility, protein cooperativity, and small-molecule binding, thus deeply affecting IAV biology [1]. The number of glycosites exposed by HA and NA changes at regular temporal intervals and alters IAV antigenic properties [2], providing one explanation for why IAV represents a relentless health threat requiring vaccines to be updated every few years.

Experiments aimed at deciphering how minute modifications in glycoproteins can impact IAV functions are strongly hampered by glycans’ high variability, flexibility, and small size. Computer simulations and modeling techniques, assisted by a continual growth of hardware and software technologies, constitute a viable alternative approach [3,4]. With access to Blue Waters’ high-performance resources, the research team was able to build and simulate a realistic all-atom viral coat model of the currently circulating A/Michigan/45/2015 (H1N1) virus, crossing multiple spatial and temporal scales. Mutations that occurred within the antigenic site located on the HA head of this pathogen were so dramatic that in 2017 the World Health Organization decided to change the vaccine composition to target this specific strain. The research team seeks to elucidate the key roles of glycans in IAV biology and their impact on immune response escape.

METHODS & CODES

The preparation of the glycosylated A/Michigan/45/2015 (H1N1) system was based on the pandemic 2009 H1N1 viral coat built by Durrant et al. [4], which was in turn shaped upon cryoelectron tomography structural data [5]. This model, including NA, HA, and M2 proton channels embedded in a lipid bilayer, was overall ameliorated and upgraded with the addition of glycans on the glycoproteins’ spikes, thus notably increasing its complexity. After setting the glycosylation profiles and detecting all the N- and O-linked glycans and model refinement, the resulting 161-million-atom system was ready to undergo MD simulations in explicit water and isothermal–isobaric conditions (NPT), using the molecular dynamics package GROMACS [6] integrated with in-house scripts. After the addition of glycans and model refinement, the resulting 161-million-atom system was ready to undergo MD simulations in explicit water and isothermal–isobaric conditions (NPT), using the memory-optimized version of the NAMD code specifically tweaked for XK and XE nodes and suitable for running MD simulations of multiamillion-atom systems.

Results & Impact

In this work, the research team has dramatically increased the level of accuracy of its previous IAV construct [4] by adding a total of 1,791 glycans on the HA and NA spikes. The extreme variability of the glycoproteins exhibited by NA and HA has often discouraged investigators from modeling the glycans in computer simulations, thus neglecting their critical functional and structural contributions. By incorporating information from collaborators, bioinformatics, and experimental data into this computational approach, the research team has given rise to an even more realistic system crossing different spatial scales, from the atomic/molecular level of single glycans and proteins to the subcellular scale of the viral coat as a whole. MD simulations were conducted on Blue Waters using 6,096 XK nodes, which allowed us to collect an average of 15 nanoseconds (ns)/day, for a total of 420 ns and 18 terabytes of generated data. Although this research is still in progress, preliminary inspection and analyses have revealed an exceptional interplay among the glycoproteins co-adjutated by the attached glycans (Fig. 1). The observation of similar behavior with this level of accuracy and statistics, and the same biological significance, could have not been ascertained from single glycoprotein simulations. This work, embracing a multiscale computational protocol without losing the atomic detail, represents a cutting-edge attempt to bridge some gaps in the understanding of the IAV biology deriving from the current experimental limitations.

WHY BLUE WATERS

Having access to a platform such as Blue Waters was absolutely crucial in order to perform MD simulations of such a massive system and to achieve a relevant amount of sampling. Carrying out the research on lesser supercomputers would have been beyond the bounds of possibility. Blue Waters’ efficient parallelism and tremendous scale provided outstanding performance in a time-efficient manner, enabled by using a memory-optimized version of the NAMD code specifically tweaked for XK and XE nodes and suitable for running MD simulations of multimillion-atom systems.

EXECUTIVE SUMMARY

This work explores Influenza A Virus (IAV) biology using the "computational microscope"; a powerful, continually improving tool capable of disclosing moving pictures of the unseen atomic world of biological systems, including viruses. The team has integrated experimental structural data to push the boundaries of computer simulations toward larger scales while increasing the complexity and realism of the modeled constructs. This allowed the team to build a mesoscale IAV model of the currently circulating A/Michigan/45/2015 (H1N1) strain, and to perform all-atom molecular dynamics (MD) simulations of the massive (161-million-atom) system. MD provided unique insights on viral dynamics and glycoprotein interplay that is otherwise not accessible through individual protein simulations, which will shed light on the role played by glycans in modulating IAV virulence and transmissibility.

Allocation: NSF PRAC/850,000 Koh
PI: Rommie Amaro1
Collaborator: Lorenzo Casalino

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Figure 1: Snapshot after 420 nanoseconds of all-atom molecular dynamics simulation on the whole Influenza A/Michigan/45/2015 (H1N1) viral coat. Glycans (colored using the symbol nomenclature for Glycogen standard) have been added on the two fundamental glycoproteins, neuraminidase and hemagglutinin (shown in red and blue, respectively), deeply affecting their dynamics and interplay. Credit: Dr. Lorenzo Casalino.

In this work, the research team was able to build and simulate a realistic all-atom viral coat model of the currently circulating A/Michigan/45/2015 (H1N1) virus, crossing multiple spatial and temporal scales. Mutations that occurred within the antigenic site located on the HA head of this pathogen were so dramatic that in 2017 the World Health Organization decided to change the vaccine composition to target this specific strain. The research team seeks to elucidate the key roles of glycans in IAV biology and their impact on immune response escape.

METHODS & CODES

The preparation of the glycosylated A/Michigan/45/2015 (H1N1) system was based on the pandemic 2009 H1N1 viral coat built by Durrant et al. [4], which was in turn shaped upon cryoelectron tomography structural data [5]. This model, including NA, HA, and M2 proton channels embedded in a lipid bilayer, was overall ameliorated and upgraded with the addition of glycans on the glycoproteins’ spikes, thus notably increasing its complexity. After setting the glycosylation profiles and detecting all the N- and O-linked glycans and model refinement, the resulting 161-million-atom system was ready to undergo MD simulations in explicit water and isothermal–isobaric conditions (NPT), using the memory-optimized version of NAMD 2.13 [7] and the CHARMM36 all-additive force field [8].

RESULTS & IMPACT

In this work, the research team has dramatically increased the level of accuracy of its previous IAV construct [4] by adding a total of 1,791 glycans on the HA and NA spikes. The extreme variability of the glycoproteins exhibited by NA and HA has often discouraged investigators from modeling the glycans in computer simulations, thus neglecting their critical functional and structural contributions. By incorporating information from collaborators, bioinformatics, and experimental data into this computational approach, the research team has given rise to an even more realistic system crossing different spatial scales, from the atomic/molecular level of single glycans and proteins to the subcellular scale of the viral coat as a whole. MD simulations were conducted on Blue Waters using 6,096 XK nodes, which allowed us to collect an average of 15 nanoseconds (ns)/day, for a total of 420 ns and 18 terabytes of generated data. Although this research is still in progress, preliminary inspection and analyses have revealed an exceptional interplay among the glycoproteins co-adjutated by the attached glycans (Fig. 1). The observation of similar behavior with this level of accuracy and statistics, and the same biological significance, could have not been ascertained from single glycoprotein simulations. This work, embracing a multiscale computational protocol without losing the atomic detail, represents a cutting-edge attempt to bridge some gaps in the understanding of the IAV biology deriving from the current experimental limitations.

WHY BLUE WATERS

Having access to a platform such as Blue Waters was absolutely crucial in order to perform MD simulations of such a massive system and to achieve a relevant amount of sampling. Carrying out the research on lesser supercomputers would have been beyond the bounds of possibility. Blue Waters’ efficient parallelism and tremendous scale provided outstanding performance in a time-efficient manner, enabled by using a memory-optimized version of the NAMD code specifically tweaked for XK and XE nodes and suitable for running MD simulations of multimillion-atom systems.
HOW BLUE WATERS IS AIDING THE FIGHT AGAINST SEPSIS

Owing to their high occurrence in ever more common hospital-acquired infections, studying the mechanisms of infection by *Staphylococcus epidermidis* and *Staphylococcus aureus* is of broad interest. These pathogens can frequently form biofilms on implants and medical devices and are commonly involved in sepsis—the human body’s often deadly response to infections.

Central to the formation of biofilms is very close interaction between microbial surface proteins called adhesins and components of the extracellular matrix of the host. The research team uses Blue Waters to explore how the bond between staphylococcal adhesin and its human target can withstand forces that so far have only been seen in covalent bonds. The team uses a synergistic combination of computational and experimental methods. This approach is essential to elucidating the mechanism by which an intricate network of hydrogen bonds makes the staphylococcal adhesion ultrastable, revealing possible routes for the development of antimicrobial strategies.

**RESEARCH CHALLENGE**

Antibiotics are increasingly powerless against a growing number of “super bacteria” that have evolved to survive humankind’s pharmacological offensive. The shortage of new medicines to treat what the U.S. Centers for Disease Control calls “nightmare bacteria” is evident. Public health agencies across the world have begun warning of the consequences of a postantibiotic era in which a common infection could, once again, become a death sentence.

The fight against sepsis, the human body’s often deadly response to bacterial infections, has become the topic of nationwide campaigns in the United States. Exploring the mechanism by which bacteria initiate infections is, therefore, key to developing new antimicrobial therapies. Investigations at the molecular level of the mechanism of adhesion between *Staphylococcus epidermidis* and *Staphylococcus aureus* and the extracellular matrix of their human hosts could lead to a detailed understanding of adhesion, one of the first steps of staph infections. This understanding may, in turn, allow researchers to develop possible competitors for their interaction with humans, stopping infection at its early stages.

**METHODS & CODES**

The research uses single-molecule force spectroscopy along with all-atom steered molecular dynamics (SMD) simulations to investigate with exquisite precision the mechanics of interaction between SdrG and Fgβ. SdrG is an SD-repeat protein G and is one of the adhesion proteins of *Staphylococcus epidermidis*. Fgβ is the human fibrinogen β chain and is a short peptide that is part of the human extracellular matrix.

For SMD molecular dynamics simulations, the team uses Blue Waters’ GPU nodes (XK) and the GPU-accelerated NAMD package. In a wide-sampling strategy, the team carried out hundreds of SMD runs for a total of over 50 microseconds of simulation. To characterize the coupling between the bacterial SdrG protein and the Fgβ peptide, the team conducts SMD simulations with constant velocity stretching at multiple pulling speeds. The SMD procedure is inspired by experimental approaches and is equivalent to attaching one end of a harmonic spring to the end of a SdrG protein and pulling on the Fgβ peptide. To quantify the strength of interaction between the two molecules, the force applied to the harmonic spring is recorded at regular intervals.

**RESULTS & IMPACT**

The steered molecular dynamics simulations performed on Blue Waters revealed, and single-molecule force spectroscopy experiments confirmed, the mechanism by which this complex withstands forces previously only associated with the strength of a covalent bond. The target human peptide (Fgβ), confined in a screwlike manner in the binding pocket of the bacterial adhesin protein (SdrG), distributes forces mainly toward the peptide backbone through an intricate hydrogen bond network. This behavior allows SdrG to attach to Fgβ with exceptionally resilient mechanoactivity, virtually independent of the peptide’s side chains.

This unexpected mechanism expands the understanding of why pathogen adhesion is so resilient, which may open new ways to inhibit staphylococcal invasion. The development of anti-adhesion therapy could block the first steps of biofilm formation by staph bacteria, facilitating bacterial clearance. Understanding the mechanism of staph infection at the atomic level may also open new avenues for an intelligent design of antimicrobial therapies.

The research team’s initial findings were published in *Science* in 2018 [1]. Currently, the team is working on developing a new protocol for finding peptides with a higher affinity for staphylococcal adhesins. The initial results are promising, and a peptide sequence with a slightly higher affinity has already been identified.

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**Figure 1**

Staph bacteria (shown as colored rods) adhere to their human hosts (surface at the bottom) with exceptional mechanical resilience. By combining experimental and computational approaches, the research team is deciphering the physical mechanisms that underlie the persistent stickiness of these bacterial adhesins (transparent purple structure), a major step in combating such invaders.

**WHY BLUE WATERS**

The research group’s work depends on obtaining multiple simulation replicas with a fast turnaround time. This approach allows the team to quickly test any and all hypotheses both computationally and experimentally. For this work, the team uses Blue Waters GPU (XX) nodes and CUDA-accelerated molecular dynamics software NAMD.
**A PHYLOGENOMIC HISTORY OF PROTEIN FUNCTION AND DYNAMICS**

### EXECUTIVE SUMMARY

Studying the evolution of protein function is important for synthetic biology and translational medicine. The ability of proteins to undergo motions that perform a certain function depends on their molecular dynamics (MD) simulations, generating dynamics networks that capture topological features of protein structures, and constructing a three-dimensional network morphospace to trace the evolutionary emergence of protein function.

### RESEARCH CHALLENGE

Proteins perform a multitude of functions that sustain life on our planet. Understanding their evolution can impact agriculture, biotechnology, and biomedicine. Protein loops play an important role in protein function and dynamics by virtue of their structural and functional flexibility [1]. Conservation of protein dynamics and flexibility [2] suggest the existence of signature motions corresponding to higher and lower levels of cellular organization may provide evidence of modularity in protein dynamics. Previous work from the research group has demonstrated the utility of networks to model evolutionary interaction at the organizational level of protein domains and loops [3].

### METHODS & CODES

The research team extended its previous data set of 116 loops from protein domains belonging to metaconsensus enzymes [4] by including 58 additional structures. This augmented the group's structural data set with previously underrepresented functional categories. The all-atom MD simulations were performed using an isobaric–isotemperature ensemble (NPT) in the TIP3P (transferable intermolecular potential with three points) water. We applied harmonic restraints of 2 kCal/mol Å² to the resulting structure. The peptide's sodium and chloride ion concentration of 100 mM was used to mimic near-physiological conditions. Depending on the number of atoms in the system, the researchers performed 50 to 70 ns (nanosecond) production runs with 1 ns of minimization using NAMD and the CHARMM36 force field. They generated networks based on the dynamic cross-correlation matrices computed from the simulations, from which they calculated network metrics for cohesion and centralities using the R package bio3D and graph, respectively [5, 6]. The researchers performed community structure detection on these networks that in turn generated trees for which they computed imbalance metrics using the R package phyloTop [7]. Other than network metrics, variables capturing the biological properties of the structure and corresponding movements were directly measured using principal component analyses, radius of gyration, and root mean square deviation. The protein structures were annotated with evolutionary age (nd) derived from phylogenetic timelines developed in the research team's lab [8].

### RESULTS & IMPACT

To illustrate the potential of networks to discern modularity, the researchers leveraged comparative genomics to assess whether protein loop structures held significant evolutionary signal. Nearly 2,100 proteomes belonging to Archaea, Bacteria, and Eukarya along with 6,046 viral proteomes were downloaded from the RefSeq database [9]. The team included proteomes from representative and reference categories with chromosome or complete genome assembly in the study, as well as all viral proteomes listed in the National Center for Biotechnology Information viral genomes project [10]. The final set of proteomes was scanned against HHM profiles of structural domains using HMMER [11]. This genomics survey of protein domains provided degenerate feature matrices to construct maximum parsimony trees of domains, following the protocol established by Kim et al. [12]. The resulting tree of domains with protein loops as characters are being compared against trees of domains with protein loop architectures as characters. The congruence of both the trees will help in establishing the presence (or absence) or phylogenetic signal embedded in loop architectures carried by the protein domain.

### WHY BLUE WATERS

The computational heavy lifting of Blue Waters facilitated the completion of time-intensive research endeavors, including the scanning of the proteomes of approximately 2,000 organisms and thousands of viruses with sophisticated hidden Markov models of protein domain recognition. Other computational experiments involved MD simulations of 300 all-atom explicit water peptide systems. Access to Blue Waters helped the research team to complete these studies in a reasonable time period. Blue Waters support staff were knowledgeable in supercomputing matters and comprised domain experts. They were extremely helpful in answering both technical and field-specific queries.

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**Figure 1:** The maximum modularity scores (y-axis) for 170 of the 174 dynamic networks across the evolutionary timeline of protein domains (x-axis) spread across 3.84 billion years of evolution. Violin plots describe measures of central tendency with box-and-whisker depictions of medians, quartiles, and data spread, all of them embedded within density plots of the data. Modularity is high at the beginning of the timeline, and decreases with time with episodic up-down fluctuations.

**Figure 2:** The average ladder size (y-axis) for trees based on community network structures for 170 of the 174 MD simulations distributed across the evolutionary timeline (x-axis). Box-and-whisker plots describe how average ladder size stayed mostly consistent and close to the mean for each age (nd) bin. However, a biphasic pattern was evident with average ladder sizes positively skewed in evolution (especially at nd bins > 0.6). Sizes indicate higher values than the median for the red bins. Rhomboid symbols represent outliers.
EXECUTIVE SUMMARY

Induction of potentially deadly abnormal cardiac rhythms is one of the most common and dangerous risks of drugs in development and clinical use. Induction has been tightly associated with the loss of function of the cardiac ion channel protein hERG, which is responsible for transporting potassium ions out of the cell and restoring resting electric potential at the end of a heartbeat. This leads to the prolongation of the QT interval (the time of ventricular activity) on the ECG. The problem, however, is that not all hERG-blocking and QT-prolonging drugs cause cardiac arrhythmias resulting in withdrawal of safe and efficient pharmaceuticals. The research team has developed a computational pipeline encompassing atomic and tissue scales that lets us estimate drug proclivity for arrhythmogenesis from its chemical structure. All-atom enhanced sampling molecular dynamics simulations of hERG–drug interactions simultaneously running on multiple Blue Waters nodes allowed the team to compute drug binding affinities and rates, which were used to predict emergent arrhythmias on a cardiac tissue scale.

RESULTS & IMPACT

Small-molecule pharmaceuticals form the basis of common-use treatments for the majority of human ailments, and development of new safe and efficient drugs is a cornerstone of modern biomedical research. A challenging and yet unaddressed problem plaguing these efforts is the lack of a robust and accurate method for the prediction of drug cardiotoxicity in the form of deadly heart rhythm disturbances. Such cardiac arrhythmias are often caused by a drug-induced blockade of potassium channel hERG, a major cardiac membrane-embedded ion transport protein [1]. hERG blockade leads to an increased duration of cardiac cell membrane voltage perturbation (so-called action potential), often manifesting as a prolongation of the QT interval on the ECG. The problem, however, is that not all hERG-blocking and QT-prolonging drugs cause arrhythmias, and currently there is no methodology that can predict drug proclivity for arrhythmogenesis from its chemical structure [2]. This has led to the withdrawal from development of potentially safe pharmaceuticals. To avoid this, the research team aims to develop a multiscale computational pipeline starting from state-dependent atomistic structural models of hERG–drug interactions all the way to functional kinetic models of cardiac cells and tissues, which would allow researchers to make such predictions. The enhanced sampling all-atom molecular dynamics (MD) simulations on Blue Waters are an integral part of this pipeline and allow the computation of drug affinities and rates, which are used as functional model parameters.

METHODS & CODES

The project's molecular systems of approximately 128,000 atoms consisted of the hERG protein built from a cryo-electron microscopy (cryo-EM) structure (PDB ID 5VA2) and embedded in a hydrated POPC (a phosphatidylcholine) lipid bilayer. The systems were assembled using CHARMM-GUI and simulated using NAMD with CUDA support on Blue Waters' XK nodes. After staged equilibration, umbrella sampling (US) and US–Hamilto- nian-tempering replica exchange (US/H-RE) [3] MD simulations with 91 windows were used to study drug binding along the channel pore using 30 or 10 nanosecond-long production runs for each. Drug binding affinities were computed from free energy profiles, whereas drug ingress ("on") and egress ("off") rates were calculated based on diffusion coefficient profiles and from the ratio of "on" rates and affinities, respectively.

REFERENCES

First, the team established that a cryo-EM hERG structure [4] likely represents an open conducting channel. The researchers also developed an inactivated hERG model by enforcing previously measured crystallographic S62D, extracellular hydrogen bonds [5] in restrained MD simulations, which also led to a distorted hERG selectivity filter configuration (Fig. 1b) thought to be important for inactivation [6]. In addition, the team developed atomistic CHARMM force field models of charged (+) and neutral (0) dofetilide [1]. Free energy profiles in Fig. 1c indicate more favorable binding for neutral dofetilide to the open hERG model compared to dofetilide (+) as well as inactivated state binding of both drug forms (compared to ΔGbind in Fig. 1d). Both US/MD and US/H-REMD provided similar results (Fig. 1c and 1d) but at a fraction of computational cost for the latter. For open hERG, the team obtained a good agreement between experimental 3.5–11 μM [7–9] and the team's computed (25±12 μM) drug affinities, Kd accounting for drug form ratios at physiological pH. For inactivated hERG, experimental data suggest dofetilide binding in nanomolar range [7], but a much weaker affinity of 200±140 μM was computed. Thus, the inactivated hERG model likely is not representative of a channel state with high-affinity drug binding, and alternative models are actively being developed.

Impotantly, the team computed "on" and "off" dofetilide rates for the open hERG model and directly used these values as parameters for their functional kinetic model of hERG–dofetilide interactions [10]. It was in turn integrated into the functional cardiac cell and tissue models, used to directly predict emergent arrhythmia indicators such as early afterdepolarizations in action potential profiles and beat-to-beat instabilities in computed pseudo-ECGs. The researchers' MD simulation-informed multiscale model provided excellent agreement for a range of experimental and clinical data, including a dose-dependent high pro-arrhythmia risk of dofetilide [10]. The team is working to utilize this pipeline for other hERG blocking drugs with different proclivities for arrhythmogenesis and, more importantly, suggest drug chemical modifications, which can alter its hERG interactions to ameliorate pro-arrhythmia risks but maintain their efficacy. Thus, the atomistic MD studies on Blue Waters helped the research group to develop and test a computational transferable protocol for robust prediction of drug cardiotoxicity based on its chemical structure, which can lead to faster and cost-effective development of safe and efficient pharmaceuticals and thus save human lives.

WHY BLUE WATERS

Access to Blue Waters' petascale architecture was indispensable for the success of these studies, since it allowed the team to efficiently conduct ~300 or more US/MD and US/H-REMD runs on GPU-equipped XK nodes at once, greatly reducing the total wall simulation time to just a few days and also permitting robust evaluation of simulation convergence.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Genes perform multiple functions, in part owing to their multiple messenger RNA isoforms. Messenger RNA (mRNA) is a large family of RNA molecules that conveys genetic information from DNA to the ribosome, where they specify the amino acid sequence of the protein products of gene expression. Alternative splicing produces multiple mRNA isoforms of genes that have important diverse roles such as regulation of gene expression, human heritable diseases, and response to environmental stresses. Alternative splicing is one mechanism that allows genes to perform multiple functions. Despite the diverse role of alternative splicing, very little has been done to assign functions at the mRNA isoform level. Therefore, differentiating the functions of mRNA isoforms is vital for understanding the underlying mechanisms of biological processes.

The goal of this study is to develop a functional network and recommendation (recommender) system to predict tissue-specific mRNA isoform function and understand implications of such alternative isoforms on metabolic pathways for the mouse and Arabidopsis thaliana model systems. (Arabidopsis is a small flowering plant that is widely used as a model organism in plant biology.)

Highlights from the research team’s outcomes include: (1) the processing of over 100 tissue-specific Arabidopsis RNA-Seq data sets as well as mRNA and protein sequence characterizations; (2) developing a random forest-based framework for mRNA-level functional network prediction; and (3) optimizing hyperparameters for the recommender system.

RESEARCH CHALLENGE

This research considered three major challenges in mRNA isoform function prediction. The first is the unavailability of mRNA isoform-level functional data, which is required to develop machine learning tools. However, the available data, even at the gene level, does not include all genes, further complicating the matter. The second challenge is the lack of information about tissue specificity in functional databases such as Gene Ontology, Kyoto Encyclopedia of Genes and Genomes, and UniProt. The third challenge is the lack of mRNA isoform-level “ground truth” functional annotation data. Therefore, the research team’s work includes using mRNA isoform and protein sequences, high-throughput RNA-sequencing data, and functional annotations at the gene level to develop computational methods for predicting functions for alternative spliced mRNA isoforms.

Some limitations of previous studies that have been overcome in the current work include: (1) predicting novel mRNA isoform interactions with no gene-level interaction information in current biological databases, (2) predicting tissue-specific mRNA isoform-level functional networks and mRNA isoform function, (3) limiting bias in the machine learning model by using a more biologically sound way of defining nonfunctional (negative pairs) mRNA isoform pairs, (4) formulating the task of mRNA isoform-level functional network prediction as a simple supervised learning task and formulating the task of mRNA isoform function prediction as a recommendation system, and (5) incorporating the relations between the Gene Ontology terms apart from the obvious hierarchical relations.

METHODS & CODES

The team has used STAR [1] and StringTie [2], which are codes for high-performance alignment and assembly of RNA-Seq reads and expression analysis for transcripts, without compromising mapping accuracy. These scale almost linearly with an increasing number of processing cores with a minimal increase in the memory requirement. Both tools are written entirely in C++ for higher efficiency and faster performance. All mRNA and protein sequence properties were calculated using R Bioconductor packages. These provide the means to calculate several diverse types of sequence properties. In addition, the team used TensorFlow and scikit-learn to build the machine learning systems.

RESULTS & IMPACT

One of the outcomes of this project was the evaluation and validation of the team’s supervised learning-based machine learning framework for predicting tissue-specific mRNA isoform functional networks in Arabidopsis. Tissue-specific mRNA isoform functional Networks (TENSION) makes use of single mRNA producing gene annotations and gene annotations tagged with “NOT” to create high-quality mRNA isoform-level functional data. The team used those to train random forest algorithms to develop mRNA isoform functional network prediction models. By using a leave-one-tissue-out approach and incorporating tissue-specific mRNA isoform-level predictors along with those obtained from mRNA isoform and protein sequences, the team has developed mRNA isoform-level functional networks for Arabidopsis tissues. Another outcome is the evaluation of different combinations of hyperparameters of the mRNA function recommendation system (mFRecSys) for making tissue-specific function recommendations for mRNA isoforms. In mFRecSys, the team considers mRNA isoforms as “users” and Gene Ontology biological process terms as “items.” By using explicit contexts for mRNA isoforms, Gene Ontology biological process terms, and tissue-specific mRNA isoform expression, mFRecSys is able to make tissue-specific mRNA isoform function recommendations.

This work emphasizes the significance of incorporating diverse biological context to develop better machine learning tools for biology. It also highlights the use of simplified supervised learning methods for biological network prediction. The machine learning models and recommendation systems developed as part of this work also draw attention to the power of simple mRNA isoform sequence-based predictors to improve mRNA isoform function prediction. The methods developed have potential practical applications, for instance, as predictive models for distinguishing the functions of different mRNA isoforms of the same gene or identifying tissue-specific functions of mRNA isoforms.

WHY BLUE WATERS

Blue Waters was essential to the two research outcomes of this project, as they both involved extensive validation and optimization. The computational resources of Blue Waters allowed the research team to perform these experiments at scale, enabling the optimization of many different experimental settings. Furthermore, conversations with the staff have been instrumental in improving job efficiency.

PUBLICATIONS & DATA SETS


**EXECUTIVE SUMMARY**

The research team applies physics-based molecular dynamics computations to protein modeling by leveraging external information through the team’s Modeling Limited Data (MELD) accelerator method. MELD runs on GPUs and is able to harness sparse, noisy, and ambiguous information using “sub-bay” stacking Bayesian inference. It can lead to orders-of-magnitude speedups in protein folding and protein–protein docking over traditional molecular dynamics (MD) methods.

MELD x MD was ranked first in last summer’s Critical Assessment of Structure Prediction (CASP) protein structure prediction competition in the experimental NMR data-assisted predictions category. This event tests how well computations can utilize real-world NMR data to determine high-resolution protein structures. This is an important blind test that shows that molecular simulations to matters of protein structure and complex, and determining the structures of amyloid aggregates, such as those that are problematic across the spectrum of neurodegenerative diseases.

### RESULTS & IMPACT

High-performance computing (HPC) on Blue Waters has been essential to this work in two ways: (1) the invention and development of the MELD method, and its application to proteins, has been very costly computationally and could not have been done without these national HPC resources; and (2) the princip-

### RESEARCH CHALLENGE

A central step in understanding how proteins perform their biological actions and how to design drugs to inhibit or activate them is to know a protein’s 3D atomic structure. Experimental methods, such as X-ray crystallography, nuclear magnetic resonance spectroscopy (NMR), and cryo-electron microscopy (cryo-EM) provide the underlying data, but such methods require a computational means of converting that data into a meaningful structure. Different experiments have different limitations: data can be sparse, or ambiguous, or noisy and combinatorial. Researchers need computational approaches that can handle these limitations. The best would be physics-based simulations, properly sampled, to provide proper Boltzmann populations and free energies.

This is the challenge the research team is addressing with its MELD-accelerated molecular dynamics (MELD x MD) [1,2]. MELD x MD is a substantial enhancement of traditional MD in biomolecular simulations because it allows for the exploration of more limited data in determining protein structures or larger proteins [3] and larger motions in all the applications of physical molecular simulations to matters of protein structure and mechanism [4].

### METHODS & CODES

The team developed a plugin (MELD) to the MD package OpenMM [5]. MELD consists of a Hamiltonian and Temperature replica exchange MD protocol in which the Hamiltonian varies according to external information coming from experiment, general knowledge, or bioinformatics. What is unique about MELD is that the information is expected to be unreliable. Hence, rather than enforcing all of it, only a fraction is enforced. The part to be enforced changes at every timestep and is chosen in a deterministic way.

### RESULTS & IMPACT

High-performance computing (HPC) on Blue Waters has been essential to this work in two ways: (1) the invention and development of the MELD method, and its application to proteins, has been very costly computationally and could not have been done without these national HPC resources; and (2) the principle way that researchers measure success of their methods, and compare them to other methods in the field, is through blind competitions, such as the biennial CASP event. Physics-based methods have been too computationally slow to enter these many-protein-time-limited events in the past. CASP13 in 2018 involved 100 protein challenges, each with a three-week computational deadline. MELD x MD now brings physical methods into the realm of these real-world competitive tests.

We believe that MELD x MD is potentially field-changing [1–4]. It can bring orders-of-magnitude greater speedups to MD simulations of a broad range of protein properties. From the NMR event and other such CASP tests, we are learning that the forcefields [7] and solvent models are quite good [8] and are often now better than many bioinformatics and database-driven approaches [9], with the added important power that they provide proper populations and free energies [10,11]. We are learning that MELD x MD can succeed in many venues—assisting in structure determination [3,6], ab initio protein folding [1,2,9], ligand binding, protein–protein docking [13], and others. Going forward, we believe the method will have additional niches important to scientists working to understand structures, dynamics, mechanisms, and to improve drug discovery. Two such applications currently in progress are assisting with cryo-EM to determine large protein structures and complexes, and determining the structures of amyloid aggregates, such as those that are problematic across the spectrum of neurodegenerative diseases.

### WHY BLUE WATERS

Blue Waters is the only system in the United States that has enough GPUs for the research team to compete in CASP and allows many jobs using a relatively low number of GPUs (30 each) to run up for 48 hours. Compilation of both Amber and OpenMM/MELD have not been trivial to optimize, and support from project staff has been invaluable, especially during the deployment of the new Python standard libraries. Furthermore, conversations with the staff have been invaluable to set up ways to run jobs efficiently during the CASP competition.

### PUBLICATIONS & DATA SETS


Figure 2: MELD x MD was the highest-ranked group in NMR data-assisted CASP13. a) The MELD x MD method (group code 431) had the highest Z-score of all groups that competed in NMR data-assisted CASP13. b) MELD x MD predictions are aligned to reference structures.
EXECUTIVE SUMMARY

Slow modes discovery is an important topic in molecular simulation because it can help extract meaningful kinetic information for the analysis of dynamic processes and can serve as good collective variables for enhanced sampling. In this project, the researcher developed a new deep learning-based method called "state-free reversible VAMPnets" that is able to discover hierarchical nonlinear slow modes accurately with much lower computational cost than its predecessors. Moreover, this method can be well integrated with the powerful Markov model to improve its kinetic resolution significantly. This method is expected to be very helpful for understanding dominant kinetic transitions in biomolecular processes and to be useful for drug discovery.

RESEARCH CHALLENGE

Identifying the collective motions governing the longtime behaviors of biomolecules such as DNA and proteins is vital in understanding and engineering the behavior of these molecules of relevance to industrial catalysis, human health, and clean energy. This work establishes new basic science techniques combining applied mathematics and deep learning to "harness the data revolution" and perform data-driven inference of collective motions from molecular dynamics simulation trajectories. Existing methods for slow mode recovery such as time-lagged independent component analysis, or TICA, are only able to discover linear slow modes. Further, they require expert knowledge and hyperparameter tuning (e.g., kernel TICA) or fail to discover multiple hierarchical slow modes (e.g., time-lagged autoencoders or variational dynamics encoders). It is an outstanding challenge to develop a simple, robust, flexible, accurate, and efficient method to extract nonlinear hierarchical slow modes from simulation data.

METHODS & CODES

Recent advances in deep learning have made it a powerful tool to solve problems in many different fields. A variational principle developed for slow mode recovery such as time-lagged independent component analysis, or TICA, is only able to discover linear slow modes. Further, they require expert knowledge and hyperparameter tuning (e.g., kernel TICA) or fail to discover multiple hierarchical slow modes (e.g., time-lagged autoencoders or variational dynamics encoders). It is an outstanding challenge to develop a simple, robust, flexible, accurate, and efficient method to extract nonlinear hierarchical slow modes from simulation data.

RESULTS & IMPACT

The method has been tested on four different systems, including two toy models and two realistic molecular systems. Where available, the results show excellent agreement with theoretical analysis or previous calculations. This approach led to the development of kinetic models for protein folding at unprecedented time resolution and the establishment of highly efficient molecular simulators that, once trained, can perform molecular simulations at a six orders of magnitude lower cost than conventional approaches. These advances are valuable for better understanding and engineering of molecular machines for clean energy production as well as drugs and vaccines to improve human health.

WHY BLUE WATERS

This research requires running many long, large simulations; performing computationally intensive data processing; and training large numbers of machine-learning models with different training parameters. Access to Blue Waters allowed these computations to be performed at the scale and parallelism necessary to support this research. The Blue Waters staff were also invaluable in helping to improve the efficiency, performance, and workflow of the computations.

PUBLICATIONS & DATA SETS


Figure 1: The molecular structure of alanine dipeptide and its three leading slowest kinetic modes: These three collective variables capture dominant transitions between the metastable basins marked in the image to providing molecular understanding of folding. The timescale associated with each transition is listed alongside each panel.

Figure 3: The molecular structure of alanine dipeptide and its three leading slowest kinetic modes: These three collective variables capture dominant transitions between the metastable basins marked in the image to providing molecular understanding of folding. The timescale associated with each transition is listed alongside each panel.
EXECUTIVE SUMMARY

Demonstrations of artificial and biohybrid (partly synthetic, partly biological) miniaturized swimming robots have underscored their potential as diagnostic and therapeutic vehicles, as well as the lack of and need for rigorous engineering methods for design and flow control. A brief survey reveals that most prototypes operate in flow regimes where viscous streaming can be leveraged. Streaming generates rectified flows in response to body-fluid oscillations and offers powerful control options for transport, mixing, drug delivery, and assembly. Thus, although streaming is not currently being exploited, it aligns well with mini-bots’ intended applications. One reason for this is that although streaming phenomena are well understood for simple bodies of uniform curvature, little is known in the case of complex, active geometries. Therefore, this project brings together modeling, simulations, and experiments to understand how viscous streaming relates to body morphology and aims to connect this understanding to biology and robotics to enhance the capabilities of current minibots.

RESEARCH CHALLENGE

The long-term goal of this work is to enable the rational design of miniaturized robots capable of operating in uncertain flow environments, of navigating the bloodstream, and of delivering localized treatment. The researcher is motivated by recent proof-of-concept demonstrations of artificial and living minibots in fluids and, by the potential as diagnostic and therapeutic vectors, and by the lack of and need for rigorous engineering methods for design and flow control.

Toward this vision, the PI has revisited a well-known fluid dynamic effect: viscous streaming. This fluid mechanism takes place when an immersed body oscillates within specific size–frequency ratios (which happen to overlap with minibots’ operating conditions), and is responsible for the emergence of characteristic transport, mixing, and flow control. A brief survey reveals that most prototypes operate in flow regimes where viscous streaming can be leveraged. Streaming generates rectified flows in response to body-fluid oscillations and offers powerful control options for transport, mixing, drug delivery, and assembly. Thus, although streaming is not currently being exploited, it aligns well with mini-bots’ intended applications. One reason for this is this that although streaming phenomena are well understood for simple bodies of uniform curvature, little is known in the case of complex, active geometries. Therefore, this project brings together modeling, simulations, and experiments to understand how viscous streaming relates to body morphology and aims to connect this understanding to biology and robotics to enhance the capabilities of current minibots.

RESULTS & IMPACT

This research has shown that oscillations can be utilized to improve transport robustly in an idealized two-dimensional master–slave setting across intermediate Reynolds numbers (1 ≤ Re ≤ 100). The analysis of flow features identifies viscous streaming as the catalyst for this improvement. In order to leverage this information, the PI designed geometries exhibiting more favorable streaming patterns, which resulted in improved slave transport. To that extent, this project demonstrated a rational design approach by modifying the classic circular cylinder via the introduction of multiple curvatures and fore–aft symmetry breaking. Moreover, the work showed that similar concepts extend to three dimensions even though favorable streaming effects are actuated differently.

Concurrently, the PI has developed Elastica [3], a software that captures the dynamic response of complex musculoskeletal architectures through assemblies of Cosserat rods [3,5]. In particular, the PI employed Elastica to computationally design, simulate, and optimize the structure of a biohybrid walking bot [6] and a biohybrid swimmer that combines neurons and muscles [7]. In collaboration with experimentalists, these designs were fabricated and tested, confirming the predictive capacity. These results illustrate the biophysical accuracy of the PI’s solvers, rendering them powerful tools for the engineering design, optimization, and synthesis of micro-robots operating in fluids.

WHY BLUE WATERS

Blue Waters’ sheer size and cutting-edge technology enables optimization processes that entail thousands of simulations. This allows the design of unprecedented biological architectures, bringing within reach novel high-impact applications, from soft robotics and biomedicine to precision manipulation and fabrication.

PUBLICATIONS & DATA SETS


Figure 1: Goal—understand/exploit the nexus (body shape)–(viscous streaming) in 2D, 3D, and biohybrid bots for drug delivery.
MOLECULAR DYNAMICS SIMULATIONS OF THE HBV CAPSID

**Allocation:** Innovation and Exploration 199, 261 Kish

**PI:** Jason A. Hadden–Perilla

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1. University of Delaware
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**EXECUTIVE SUMMARY**

The hepatitis B virus (HBV) is a major cause of liver disease. The World Health Organization estimates that more than 250 million persons currently suffer from chronic infection, with no cure available. Researchers aim to develop new treatments targeting HBV’s capsid, the protein shell that encloses its viral genome. The research team has been leveraging Blue Waters since 2015 as a computational microscope to study the capsid, employing all-atom molecular dynamics simulations to reveal details of structure and function that are inaccessible to experiments. Currently, the team is investigating the capsid’s response to mutations and drug compounds, probing its mechanics to uncover capabilities and potential vulnerabilities. The researchers have learned that amino acids aspartate-78 and threonine-109 each play important but heretofore, unrealized roles in capsid assembly, and the team has implicated threonine-109 in drug resistance. Heteroreactive hydrophobicity (HAP) compounds disrupt the capsid’s shape, volume, and solvent transport properties. Importantly, simulation of the multimillion-atom capsid system is only possible on a petascale supercomputer such as Blue Waters.

**RESEARCH CHALLENGE**

The HBV capsid is a complex molecular machine. It self-assembles from 120 capsid-protein dimers to package RNA, facilitating the maturation of the RNA to DNA, and hijacks various components of the host cell’s own machinery to transport its genomic cargo throughout the viral infection cycle. Drugs that disrupt the capsid have been identified but have not been approved for human use. The ability to produce new treatments that target the capsid depends heavily on understanding its inner workings and the mechanisms by which it carries out its function; by determining how the capsid works, researchers can also determine how best to inhibit it.

**METHODS & CODES**

Molecular dynamics simulations provide a powerful tool to investigate virus capsids such as that of HBV [1]. This project has demonstrated that when performed at all-atom resolution, simulations can capture remarkably subtle details of capsid structure and dynamics, including changes induced by bound drugs [2]. The simulations employed NAMD [3], a highly scalable bio-molecular simulation code with a long and successful track record of deployment on Blue Waters. While all-atom simulations of the intact HBV capsid come at a great computational expense, access to NAMD on Blue Waters has enabled the research team to reveal critical new insights into its function and suggest strategies for targeting it with novel therapeutics [4,5].

**RESULTS & IMPACT**

Aspartate-78. The surface of the HBV capsid exhibits 120 spikes (Fig. 1). One of the most incorporated capsid-protein dimers. The tips of the spikes contain four negatively charged amino acids: two copies each of glutamate-77 and aspartate-78 (Fig. 2a). The research team’s collaborators hypothesized that mutation of aspartate-78 to an uncharged amino acid would promote capsid assembly by decreasing electrostatic repulsion; however, experiments indicated that substitution of aspartate with serine was detrimental to the formation of capsids.

Aspartate-78. The surface of the HBV capsid exhibits 120 spikes (Fig. 1). The research team used Blue Waters to simulate the intact HBV capsid on the microsecond timescale [4], producing an ensemble of 12 million samples that characterized the dynamical behavior of threonine-109. The team’s analyses showed that threonine-109 plays a significant amount of time mediating contact among neighboring dimers within the capsid (Fig. 2b), revealing why mutation of this amino acid can alter the ability of the proteins to interact and assemble. Furthermore, the team found that the interdimer contact formed by threonine-109 can occlude a hydrophobic pocket recognized by capsid-disrupting drugs (Fig. 2b). Threonine-109’s ability to physically block the binding of such compounds confers some native drug resistance to HBV. Mutation of threonine-109 to larger, more hydrophobic amino acids enhances the rate of capsid assembly and also increases drug resistance.

HAP compounds. Drugs from the heteroreactive hydrophobicity (HAP) family (Fig. 2b) can misdirect HBV capsid assembly and disrupt intact capsids. The research team previously used Blue Waters to simulate a HAP-bound capsid and observed that the compounds induced changes in the capsid’s shape [2] consistent with experimental observations. Now, the team has extended the drug-bound capsid investigation to the microsecond timescale, treating HAP as a small-molecule probe to test the capsid’s mechanics. The results indicate that saturation with HAP compounds increases the capsid’s volume and alters its solvent transport properties, revealing insight into the mechanism by which HAPs induce disruption. The team’s analyses were enabled by a novel method in which the researchers collaborated that uses ray-casting to accurately detect the interior versus exterior space of biomolecular containers, including virus capsids. The methods are highly parallelizable and take advantage of Blue Waters’ Lustre filesystem.

The research team used Blue Waters to simulate multiple copies of wild type and mutant HBV capsid–protein dimers, obtaining conformational sampling totaling six microseconds. The team’s analyses showed that together, glutamate-77 and aspartate-78 induce sodium localization within their vicinity and transiently coordinate individual sodium ions within the spike tip (Fig. 2a). Substitution of aspartate-78 with serine caused the spike interface to open, dramatically reducing sodium localization and coordination. Both simulations and cryo-electron microscopy data showed that the mutation increased disorder in the spikes, demonstrating that aspartate-78 and its ion-mediated interactions are important for maintaining spike secondary structure and conformation conducive to productive capsid assembly.

Threonine-109. A number of drugs that target the HBV capsid are known to interfere with its assembly process. Experiments by the research team’s collaborators indicated that mutation of the amino acid threonine-109 (Fig. 2b) could increase both the rate of capsid assembly and the capsid’s resistance to assembly-disrupting drugs; however, no explanation for threonine-109’s role in either aspect was apparent from high-resolution crystal or cryo-electron microscopy structures of the capsid.

The research team used Blue Waters to simulate the intact HBV capsid on the microsecond timescale [4], producing an ensemble of 12 million samples that characterized the dynamical behavior of threonine-109. The team’s analyses showed that threonine-109 plays a significant amount of time mediating contact among neighboring dimers within the capsid (Fig. 2b), revealing why mutation of this amino acid can alter the ability of the proteins to interact and assemble. Furthermore, the team found that the interdimer contact formed by threonine-109 can occlude a hydrophobic pocket recognized by capsid-disrupting drugs (Fig. 2b). Threonine-109’s ability to physically block the binding of such compounds confers some native drug resistance to HBV. Mutation of threonine-109 to larger, more hydrophobic amino acids enhances the rate of capsid assembly and also increases drug resistance.

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**WHY BLUE WATERS**

Simulations of the intact HBV capsid are only feasible on a petascale supercomputer such as Blue Waters because of their computational expense. Investigating the capsid under physiological conditions at full chemical resolution requires calculations involving the interactions of millions of atoms. Simulations exploring the microsecond timescale can take months, even on thousands of processors. The exciting discoveries revealed by this work underscore the essential role for leadership-class computing resources in supporting basic science research toward gaining an understanding of viruses and developing new antiviral treatments.

**PUBLICATIONS & DATA SETS**


MOLECULAR DYNAMICS SIMULATIONS OF THE HBV CAPSID AS A DRUG TARGET

EXECUTIVE SUMMARY

Hepatitis B virus (HBV) is a major cause of liver disease. The World Health Organization estimates that more than 250 million people worldwide suffer from this chronic infection, with no cure available. Researchers aim to develop new treatments targeting HBV's capsid, the protein shell that encloses its viral genome (Fig. 1a). The research team has been leveraging Blue Waters since 2015 as a computational microscope to study the capsid, employing all-atom molecular dynamics simulations to reveal details of structure and function that are inaccessible to experiments. Currently, the team is endeavoring to further characterize the capsid as a drug target by investigating morphological disruption by heteroaryldihydroxyimidine (HAP) compounds, cooperativity in HAP uptake, and the structural and statistical details of HAP binding modes under physiological conditions. The team's findings go far beyond conclusions that can be drawn from static models derived with crystallography or cryo-electron microscopy. Importantly, simulation of the multimillion-atom capsid system is only possible on a petascale supercomputer such as Blue Waters.

RESEARCH CHALLENGE

The HBV capsid is a complex molecular machine that self-assembles from 120 capsid-protein dimers to package RNA. In addition, it facilitates the maturation of RNA to DNA and hijacks various components of the host cell's own machinery to transport the capsid's genomic cargo throughout the viral infection cycle. Drugs that disrupt the capsid have been identified but have not been approved for human use. Researchers' ability to produce new treatments that target the capsid depends heavily on understanding the capsid's inner workings and the mechanisms by which known drug compounds disrupt it; by determining how the capsid works, researchers can also determine how best to inhibit it.

METHODS & CODES

Molecular dynamics simulations provide a powerful tool to investigate virus capsids such as HBV [1]. The research team's work has demonstrated that when performed at all-atom resolution, simulations are capable of capturing remarkably subtle details of capsid structure and dynamics, including changes induced by bound drugs [2]. These simulations employ NAMD [3], a highly scalable biomolecular simulation code that boasts a long and successful track record of deployment on Blue Waters. While all-atom simulations of the intact HBV capsid come at a great computational expense, access to NAMD on Blue Waters has enabled the team to reveal critical new insights into the capsid's function and to suggest strategies for targeting it with novel therapeutics [4,5].

RESULTS & IMPACT

The HBV capsid is composed of 120 capsid-protein dimers, arranged according to icosahedral symmetry (Fig. 1a). There are two possible orientations that dimers can occupy within the capsid structure, which are referred to as AB and CD. Drugs known to target the capsid recognize hydrophobic pockets found at the interfaces of B/C and C/D subunits, referred to as B sites and C sites (Fig. 1b). Previously, the research team used Blue Waters to simulate the apo (unbound) form of the HBV capsid on the microsecond timescale [4] and observed differences in the structure and dynamics of B sites versus C sites, despite symmetry [5]. Now, the team has used Blue Waters to study the capsid's response to drug binding in each of these quasi-equivalent locations, furthering characterization of the capsid as a drug target. The simulations of the intact capsid with drugs from the HAP family complexed in B sites, C sites, or both B and C sites reach the microsecond timescale.

Morphology. Preliminary work on HAP-bound capsids demonstrated that the compounds induce changes in the capsid's shape [2] consistent with experimental observations. The presence of drugs causes the capsid to adopt a faceted morphology similar to that of a regular geometric icosahedron (Fig. 2). Recent results reveal that drug binding in C sites leads to more pronounced faceting than drug binding in B sites. Saturation of the capsid with drugs in B and C sites leads to intermediate faceting and increased particle size. Importantly, these findings underscore the capsid's resilience and ability to make structural adjustments to accommodate drug uptake.

Cooperativity. Experiments by the team's collaborators suggest that drug uptake in the capsid is cooperative, meaning that the binding of one drug molecule makes the binding of a second more likely. The research team's findings indicate that within the apo-form capsid, B sites remain mostly open, while C sites spend a significant portion of the time closed and occluded. As such, initial drug binding is most probable in B sites. Using the new simulation data, the team has learned that the presence of drugs in B sites causes C sites to become occluded less often, confirming the existence of a cooperativity mechanism. Further, the presence of drugs in C sites causes B sites to be occluded more often, reducing the likelihood of drugs binding there. Similar to the faceting effect, cooperativity between drug binding sites arises from shifts in interdimer orientations as the capsid makes structural adjustments to accommodate drug uptake.

Binding modes. The research team's simulations of drug-bound capsids have provided the unique opportunity to expand characterization of drug binding modes far beyond what was previously determined from static crystal structures. Using Blue Waters, the researchers have produced ensembles of six-millibin samples for B and C quasi-equivalent binding sites, which capture the dynamical interactions of HAPs with the capsid under native physiological conditions at full chemical resolution. The structural and statistical details revealed by these data sets are invaluable toward the design and optimization of new drug compounds that target the capsid and have the potential to support the discovery of new therapeutics.

WHY BLUE WATERS

Owing to computational expense, simulations of the intact HBV capsid are only feasible on a petascale supercomputer such as Blue Waters. Investigating the capsid under physiological conditions at full chemical resolution requires calculations involving the interactions of millions of atoms. Simulations exploring the microsecond timescale can take months, even on thousands of processors. The exciting discoveries revealed by this work underscore the essential role for leadership-class computing resources in supporting basic science research toward understanding viruses and developing novel antiviral treatments.

PUBLICATIONS & DATA SETS


TOWARD PREDICTIVE COMPUTATIONAL DESIGN OF PRECISION MOLECULAR OPTOELECTRONICS

EXECUTIVE SUMMARY

The research team introduced and fully developed novel scalable algorithms and software for predictively accurate (ab initio) electronic-structure calculations for the key electronic parameters of precision organic optoelectronic devices such as solar cells, light-emitting diodes, field-effect transistors, smart windows, etc. The team transformed the usual non-scalable sum-of-products expressions of many-body Green's function theories into a few high-dimensional integrals, which were then evaluated by a highly scalable Metropolis Monte Carlo algorithm. The algorithm efficiently computes energy differences (including quasi-particle energy bands) directly without a sign problem on many CPUs or GPUs.

RESEARCH CHALLENGE

The world is entering an exciting new era of chemical technology in which synthetic chemists can now fabricate complex solid-state materials made of organic components with precise dimensions so that the fabricated materials display predicted/desired functions and performance as optoelectronic devices. Research into such technology may be assisted powerfully by computational methods that can predict the key optoelectronic parameters of the component conjugated organic molecules, such as electron binding energies, charge mobility, exciton binding, air stability, etc. A systematically accurate series of approximations for these properties in a molecule and solid exists as many-body Green's function theory [1]. However, as compared with either ab initio theories, many-body Green's function theory is less well understood or developed both theoretically and algorithmically. The research group aims to address this issue with the assistance of Blue Waters.

METHODS & CODES

The team mathematically transformed the usual sum-of-products expressions of second- and third-order many-body Green's function—GF2 [2] and GF3 [3]—theories, and their complete-basis set correction by explicitly correlated ansätze [4] into single high-dimensional integrals by a Laplace transform. Specifically, in the last funding cycle, 84 Feynman diagrams defining GF3 (Fig. 1) [1] were automatically generated by symbolic computing software and transformed into algebraic formulas consisting of integrals over 20-dimensional coordinates of three coupled electron pairs and over two imaginary time coordinates. These were then evaluated by a Metropolis Monte Carlo method with judiciously chosen weight functions. The resulting stochastic GF2 and GF3 methods can directly compute energy differences (electron detachment/attachment energies) without a sign problem on thousands of CPUs [5] or hundreds of GPUs [6] with an unprecedented efficiency.

RESULTS & IMPACT

Supercomputers of the size and style of Blue Waters are changing the way chemical computing is being designed and performed. Conventional deterministic and matrix-algebra-based algorithms have given way to stochastic algorithms because of their superior parallel scalability on CPUs and GPUs; cost performance for high dimensions at the expense of having stochastic errors; naturally fault-tolerant and indefinitely restartable algorithms; and, finally and importantly, their relatively low human cost of code development. What the research team has achieved in this project is a paradigm of such changes in chemical computing.

WHY BLUE WATERS

The stability and ease of use as well as the balanced deployment of CPUs and GPUs are all essential for the rapid coding/profiling of new scalable algorithms from scratch and their capacity testing.

PUBLICATIONS & DATA SETS


IMPACT OF BATCH EFFECT AND STUDY DESIGN BIASES ON IDENTIFICATION OF GENETIC RISK FACTORS IN SEQUENCING DATA

Allocation: Illinois/280 Kobi
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Co-PIs: Yan W. Asmann, Liudmila Sergeevna Mainzer

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Mayo Clinic

EXECUTIVE SUMMARY

To explore how systematic biases within a genomic data set can impact downstream statistical analysis of genetic variants, the research team conducted stratified association analysis on Alzheimer’s disease genomic data. The researchers profiled a set of variants with highly significant, novel associations with Alzheimer’s disease that were impacted by heterogeneity in subcohort composition and exome capture. The team identified genotype quality, age, and population stratification as likely contributing factors to vastly different minor allele frequencies as well as a batch effect across sequencing center cohorts. These findings highlight important considerations for analysis of this data set and for the design of future studies.

RESEARCH CHALLENGE

The large-scale samples required to identify disease-associated variants in genomic sequencing data often introduce batch effects and other confounding variables or biases from study design. If not adequately addressed in the analysis, batch effects will reduce statistical power and increase false associations, and bias findings highlight important considerations for analysis of this data set.

RESULTS & IMPACT

The research team identified 30 novel Alzheimer’s-associated genomic variants with exome-wide significance. Further examination showed that the significance of these variants originated entirely from samples processed at Broad, which used the Illumina capture kit. To investigate the cause of the Broad-exclusive significance, the researchers compared multiple variant quality parameters including genotype quality, sequencing depth, and alternative allele concentration, and identified significant batch differences in genotype quality values of the variants from Broad (Illumina kit) compared to Washington University and Baylor (Nimblegen kits). The team also found several age-related differences between Broad and the other two centers. First, the Broad samples had higher minor allele frequency in both cases and controls, possibly indicating population stratification. Second, the Broad cohort consisted of a disproportionately large number of younger cases. Finally, the minor allele frequencies of the 30 variants declined with age in both Broad cases and controls, suggesting that the variants are associated with age.

WHY BLUE WATERS

The Alzheimer’s Disease Sequencing Project data set used in this study consists of over 9,000 whole-exome sequencing samples. Processing this immense quantity of genomic data and conducting the downstream analysis required 250,000 node hours on Blue Waters. By parallelizing computational jobs across thousands of nodes, the research group was able to achieve what would take over 100 years on a single server in months. In addition, Blue Waters is one of the few systems that allows users to keep hundreds of terabytes of data in active storage for simultaneous processing, an important step in data integration across genomic workflows.

PUBLICATIONS & DATA SETS

MICROSCOPIC IDENTIFICATION OF PIP2 BINDING SITES ON A CA2+-ACTIVATED CL CHANNEL

EXECUTIVE SUMMARY
Membrane proteins dwell in a sea of phospholipids that not only structurally stabilize the proteins by providing a hydrophobic environment but also dynamically regulate protein function. While many cation channels are known to be regulated by the negatively charged phosphatidylinositol 4,5-bisphosphate (PIP2), relatively little is known about anion channel regulation by phosphoinositides. Using atomistic molecular dynamics simulations on Blue Waters combined with experimental patch clamp electrophysiology, the research team has identified several PIP2 binding sites in TMEM16A, a CT (chloride) channel that performs myriad physiological functions ranging from epithelial fluid secretion to regulation of electrical excitability. These PIP2 binding sites form a band at the cytoplasmic interface of the membrane that the team proposes constitutes a network to dynamically regulate this extensively allosterically regulated protein. The microscopic description of the PIP2–TMEM16A interactions provided by this research adds a crucial layer of information for understanding the regulation mechanisms of ion channels by specific lipids.

METHODS & CODES
To gain insight into the binding of PIP2 to TMEM16A, extended molecular dynamics (MD) simulations were performed on the atomic model of the ion channel [11] using the highly mobile membrane mimetic model (HMMM) [12]. The HMMM model was introduced to accelerate lipid diffusion in atomistic simulations in order to obtain enhanced sampling of the interaction of lipid headgroups with proteins within simulation timescales currently achievable. This model replaces a portion of the membrane hydrophobic core by a more fluid representation using simply carbon solvent ethane (NCS), while employing short-tailed lipids to maintain a full description of the headgroups and the initial part of the tails (Fig. 1). This model provides a more flexible and mobile environment that allows for rapid rearrangement and displacement of the lipid headgroups, thereby facilitating phenomena that might be inaccessible with conventional membrane models owing to the inherently slow dynamics of the lipids. In each of the six independent simulation systems, eight PIP2 molecules were added to the inner leaflet of an otherwise phosphatidylcholine (POPC) lipid bilayer evenly surrounding the protein at the beginning of the simulations. To determine whether binding of PIP2, influenced by full-length acyl chains, after the completion of lipid-binding simulations with HMMM membrane (500 nanoseconds [ns] each), short-tailed lipid molecules were converted back to full-length lipids, and the resulting full systems were subjected to additional equilibrium simulations of 100 ns each. All MD simulations were carried out on Blue Waters using the Nanoscale Molecular Dynamics (NAMD) simulation package [13].

RESULTS & IMPACT
The research team unbiased atomistic MD simulations with approximately 1.4 PIP2 in POPC bilayers revealed spontaneous binding of PIP2 to several potential sites on the surface of the TMEM16A channel (Fig. 1). Three of these sites captured 85% of all PIP2–protein interactions and were validated to be critical for PIP2 regulation through mutagenesis experiments by the collaborators. Simulations showed that PIP2 is stabilized by hydrogen bonding between basic residues and the phosphate/hydroxyl groups on the inositol ring of the lipid headgroup. Binding of PIP2 to different sites produces different conformational effects in the cytoplasmic part of transmembrane helix 6 (TM6), which forms one side of the channel pore and plays a key role in channel gating. The occupation of the major sites is especially shown to induce a dramatic rotation of the cytoplasmic end of TM6 away from the pore (Fig. 2). This pore dilation increases the accessibility of the inner vestibule of the channel to the cytosolic ions and resulted in spontaneous penetration of Cl– ions into the pore (Fig. 2). Based on this observation, the research team proposed that a network of PIP2 binding sites at the cytosolic face of the membrane allosterically regulates channel gating. The data provided by these simulations add to a growing body of knowledge showing that TMEM16A is a highly allosteric protein that is gated by a network of interactions involving both Ca2+ and PIP2.

WHY BLUE WATERS
The state-of-the-art architecture of Blue Waters makes it an excellent computing resource for this scientific research. The GPU-optimized simulation package NAMD has been extensively tested and optimized for Blue Waters. The large number of GPUs available on the XK nodes significantly increased the overall productivity. In addition, the technical support provided by the experts and scientists of the Blue Waters team has contributed to the accomplishment of the research goals by smoothing out technical issues that have arisen during the allocation.

PUBLICATIONS & DATA SETS
PARACELLULAR ION TRANSPORT

Allocation: GLPC/590 Keh
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Collaborator: Christopher Weber

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EXECUTIVE SUMMARY

Permeation of water, ions, and small molecules through the space between neighboring cells is controlled by macromolecular structures known as tight junctions. Tight junctions seal the paracellular space and act as barriers that limit diffusion of molecules down their electrochemical gradient. Claudins are one of the major components of tight junctions and play a key role in determining paracellular permeability. Little is known about the assembly of claudins and the architecture of tight junction pores. The research team built an atomic model of claudin pores and verified its function using molecular dynamics (MD) simulations. The team then used the MD simulations to build a simple model of tight junction networks and simulate their transport properties. However, the architecture of tight junctions at the cellular level is still unknown.

RESEARCH CHALLENGE

Claudin pores are one of the major components of the tight junctions that control the transport of ions and small molecules in paracellular space between neighboring cells [1,2]. Little is known about the molecular architecture of tight junctions and the assembly of components into ion channels. The research team used all-atom MD simulations to determine: (1) the structure of claudin pores and their functional mechanism, and (2) the mechanical properties of tight junction strands at the cellular level.

The simulations carried out in this project are among the largest simulations of ion channels to date. The tight junction network consists of a few hundred ion channels assembled into linear strands of tiny pores in two parallel lipid membranes.

METHODS & CODES

The researchers ran atomic-scale MD simulations of claudin pores in two parallel lipid membranes. The highly scalable MD program NAMD was used to build and refine the model and to simulate its ion transport function. Moreover, to investigate the macroscopic properties of tight junctions at relevant length scales (micrometers), the team ran simulations of the system using a hybrid resolution representation using the PACE force field, in which the protein was represented atomically and its environment, including lipid membranes and solvent, were coarse-grained. The size of the systems simulated in this project range from 350,000 atoms to two million particles.

RESULTS & IMPACT

In this project, the team developed the first atomic model of a new class of ion channels: claudin pores. They used MD simulations to build and refine an atomic model based on a recently proposed architectural model [3,4] and to assess its stability. Furthermore, they verified this structural model by simulating its ion transport function. The simulations verified functional characteristics of claudin pores such as their charge and size selectivity and predicted mutations that reversed the charge selectivity of the channel. These mutations were further verified in electrophysiology experiments in the collaborator’s laboratory. In addition, these simulations identified the molecular nature of ion selectivity in paracellular pores, which was again verified by experiments [5].

To investigate ion transport across tight junctions—the parallel networks of claudin pores that span the cell membrane—the team developed systems consisting of more than 180 claudins (44 pores) in two parallel membranes. Initial simulations of the system at equilibrium indicate that claudins form flexible strands with persistence lengths comparable to those obtained experimentally (approximately 200 nm). Furthermore, the simulations determined the origin of this flexibility and pairwise protein–protein interactions that are responsible for the formation of strands and their shape.

These are the first simulations of ion transport in paracellular pores ever conducted, and they have opened up new opportunities for studying the functional mechanism of these channels as well as the physical properties of tight junctions at the cellular level. Future studies could result in the development of possible inhibitors for this class of ion channel in the small intestines or kidneys, or enable the delivery of drugs across the blood–brain barrier.

WHY BLUE WATERS

Access to Blue Waters was essential in running simulations consisting of the assembly of several hundreds of proteins into functional ion channels. These simulations, which reached a few micrometers in length, were only possible through access to the large number of nodes available on Blue Waters. Equally important was the knowledge of the Blue Waters staff in compiling the codes and helping the research team to identify performance issues.

PUBLICATIONS & DATA SETS

TERRA–REF is collecting automated high-throughput remote sensor data on diverse varieties of sorghum and wheat. Remote sensors mounted in a field scanner instrument box scan over one acre of plants, producing thousands of daily measurements with high spatiotemporal resolution. Sensor data types range from hyperspectral imaging to 3D reconstructions and thermal profiles, all at 1-mm resolution. The program is making the data available for researchers not only to study the plants but also the sensors themselves in order to learn what new information these sensors provide.

METHODS & CODES
Data from the sensors is streamed from the field scanner to the National Center for Supercomputing Applications, where it is calibrated and processed. Blue Waters’ nearline tape storage is used both for backup and for staging of data for reprocessing. The data is then organized, annotated, and processed. This process uses RabbitMQ to recognize and handle each data set as it arrives or is created. Clowder extractors created using novel predictive models and algorithms process the raw data into high-resolution images, point clouds, and time series, and then extract features related to plant growth, chemistry, and physiological efficiency. Clowder stores metadata and tracks provenance for derived data sets.

RESULTS & IMPACT
All software used in the processing pipeline is available on GitHub with permissive open-source licenses. Similarly, curated data sets generated by this platform will be published and placed in the public domain to maximize the impact of these unprecedented data.

WHY BLUE WATERS
The Blue Waters nearline system provides TERRA–REF with a quickly accessible and reliable storage system for both data backup and staging data for reprocessing. Having reliable storage for backup allows the research team to focus on the data processing and delivery infrastructure.

PUBLICATIONS & DATA SETS

QUANTUM–CLASSICAL PATH INTEGRAL SIMULATION OF PROTON TRANSLOCATION IN BIOLOGICAL CHANNELS

Allocation: Illinois/75 Knh
PI: Nancy Makri
1University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY
The PI uses the quantum–classical path integral (QCPI) methodology, along with the modular decomposition of the path integral, to perform highly accurate simulations of proton translocation dynamics in water chains embedded in biological channels. These methods allow an accurate treatment of important quantum mechanical effects, accounting for the effects of the protein environment in full atomistic detail.

RESEARCH CHALLENGE
Understanding the mechanism of the proton translocation along water chains embedded in biological channels continues to attract much theoretical and experimental effort. An interesting question is related to whether the dynamic is sequential or concerted. The accurate treatment of quantum effects, along with a faithful treatment of phase interference in the interaction of the protons with the environment, is critically important for reaching definitive conclusions in this regard. Unfortunately, quantum mechanical calculations scale exponentially with the number of coupled degrees of freedom.

METHODS & CODES
The PI’s initial calculations on a protonated water dimer are based on the QCPI [1–7] methodology she developed, with several recent advances to her code. Specifically, its ability to describe solvents has been increased with the addition of a molecular dynamics package, developed by her for QCPI, that contains an implementation of the CHARMM force field for protein environments along with accurate potentials for water clusters as well as the ability to simulate various subsystems, each with its own force field. Another development of the methods is the flexibility of augmenting the system Hamiltonian with matrix elements that depend on time through select solvent coordinates. The extension of this work to treat longer chains with multiple transferring protons will utilize the modular decomposition of the path integral [8–10] developed recently by the PI.

RESULTS & IMPACT
This project involves the simulation of the dynamics of the protonated water dimer in the gramicidin A protein channel. The problem of the translocation of a proton along a water chain has fascinated scientists for decades. Since the discovery of water chains in protein channels, such a system has been considered a model for a proton pump that helps maintain osmotic pressure between a cell and its environment. The diffusivity of the proton is in fact a fast process that can be accounted for if one considers not only quantum tunneling but also its interplay with the thermal fluctuations of the oxygen atoms of the chain and the coupling to the protein that surrounds it.

Using the QCPI code, the PI has simulated the transfer dynamics of the excess proton injected in a neutral water dimer, from which she estimates a population decay on a timescale of shorter than 0.1 picosecond. This process is driven in great part by the strengthening of the hydrogen bond that pulls the oxygen atoms closer. This picture becomes more complicated in longer chains, where the motion of the oxygen atoms is correlated, and there are more reaction pathways for the proton diffusion that may correspond to a shuttling motion or a concerted displacement of multiple hydrogen atoms. The researcher plans to address these questions by simulating the dynamics of proton translocation in longer chains, taking into account the quantum mechanical character of multiple transferring protons using the modular decomposition of the path integral methodology.

WHY BLUE WATERS
The QCPI calculations require a multilevel parallelism. Blue Waters provides the ideal platform for the implementation of the algorithm.
A NEW STABILIZED FLUID–STRUCTURE INTERACTION METHOD: COUPLED SYSTEM OF ANISOTROPIC VISCOELASTIC MODEL FOR ARTERY AND NON-NEWTONIAN MODEL FOR BLOOD

EXECUTIVE SUMMARY

Fluid–structure interaction (FSI) is a class of multiphysics problems that combines fluids and solids in a single-pass simulation to capture the interactive and integrated behavior of the system. Because of the instabilities that are unique to nonlinear material models, especially in the presence of moving interfaces, a comprehensive strategy for FSI requires mathematical formulations with enhanced stability properties and coupled solution algorithms that preserve the dissipative structure of the underlying coupled continuum problem.

The research team has developed a stabilized monolithic method for coupling incompressible non-Newtonian fluids [1,3,4] with anisotropic (having a physical property that has a different value when measured in different directions) viscoelastic (materials that exhibit both viscous and elastic characteristics when undergoing deformation) models of artery walls. The method is applied to an idealized curved artery to investigate the mathematical attributes of the models as well as that of the coupled solution algorithm. The algorithm and codes have been optimized on the XE nodes of Blue Waters.

RESEARCH CHALLENGE

Realistic, patient-specific models help not only to simulate preoperative diseased configurations but also to analyze postoperative outcomes. This has evolved into the concept of computational medicine, a form of personalized medicine in which patient-specific computer modeling and engineering analysis methodologies are used to noninvasively diagnose and evaluate the efficacy of various possible treatments and to plan and design the optimal intervention based on prediction of outcomes. However, creating spatial discretizations for FSI problems that satisfy nodal compatibility is not always an easy task and, therefore, considerable effort has been devoted to numerical methods that accommodate nonmatching interfaces [2]. Flexibility to accommodate nonmatching meshes is of great practical value in problems of industrial strength that invariably have complex geometric configurations. Relaxing the nodal continuity requirements necessitates techniques for enforcing the conditions on the continuity of the fields across the interface. The research team followed the ideas proposed in Truster and Masud [5,7] and developed an interface-stabilized method with least-squares-type terms that enforce continuity of traction at the nonmatching meshes along the fluid–solid interface. Accurate prediction of stress and deformation in the arterial wall in patient-specific applications requires that physiologically relevant constitutive models [6] are employed for the artery wall, which is comprised of soft tissue with embedded collagen fibers. Anisotropy caused by embedded fibers in soft biological tissues is a more difficult numerical problem, and it becomes a challenge for numerical methods when large deformations are involved in an FSI simulation. In the present work, multiple layers of artery wall, intima (the innermost layer of an artery or vein), media, and adventitia (the outermost layer of the wall of a blood vessel) are modeled via a hyperelastic energy functional that accounts for finite stretching of the soft tissue as well as anisotropy induced by the directionally oriented collagen fibers. The reinforcing fibers are laid helically around the artery wall with alternate layers placed orthogonally to one another to form a network of directionally oriented layers.

\[ F \left( \mathbf{u} \right) = \frac{2}{3} \rho - 2 \bar{\mathbf{C}}_{ij} \mathbf{E}_{ij} = 2 \left( \rho \mathbf{u} \mathbf{u}^T - \mathbf{I} \right) \]

where \( \rho \) are the material parameters of a neo-Hookean type solid; \( \alpha_1 \) and \( \alpha_2 \) are material parameters for a neo-Hookean type solid; and \( \mathbf{u} \) and \( \mathbf{a} \) are material parameters for reinforcing fibers.

METHODS & CODES

Numerical methods, which are not constrained by node-on-node matching, provide great advantage in developing patient-specific computational models. The researchers have employed a variational multiscale framework to develop advanced numerical techniques with enhanced stability and accuracy properties for this class of problems. The team’s emphasis has been on the development of a unified mathematical framework that can have wider application both in the domain of fluids as well as in solids. The enhanced stability facilitated by the mathematical construction results in a robust FSI algorithm that has been applied to the blood–artery interaction problem. The method is implemented in the context of a finite-element method using low-order Lagrangian elements and has been optimized on the XE nodes of Blue Waters.

RESULTS & IMPACT

Fig. 1 shows the stress–strain response for a representative material volume of the artery wall to illustrate its anisotropic response under axial stretching. A parametric study was carried out over biologically relevant values of the material coefficients, and the nonlinear stress-strain response is presented in Fig. 1. The sample was first loaded in the axial direction that is aligned with the direction of the fibers and a gradual softening response was observed. Subsequently, the unit cube was loaded in the lateral direction and the stress-carrying capacity was reduced by five times. In addition, a gradual softening response was observed, as shown in Fig. 1b.

Fig. 2 shows the curved geometric configuration of the blood–artery model. The unidirectional collagen model was put in layers to create a network that is shown by the red and blue fibers in Fig. 2a. The mesh was comprised of hexahedral elements where the red region represents the fluid subdomain. The researchers simulated a few cardiac cycles and Fig. 2c presents an instantaneous snapshot of the deformation of the artery wall along with the streamlines of the blood flow. The team also projected the arterial wall shear stress (WSS) on the artery wall, which is one of the most significant factors affecting the progression of arterial disease. Since it is difficult to obtain spatiotemporal WSS data via in vivo experiments, advanced FSI simulations with appropriate constitutive models provide a virtual platform to facilitate important and insightful information for the diagnosis and treatment of arterial disease. Such information can also be critical at the planning stage for developing patient-specific strategies for surgical intervention.

WHY BLUE WATERS

The coupled solution algorithm for nonmatching FSI meshes was implemented on the Blue Waters Platform and tested on XE nodes. Since element-level developments are all local to individual elements both in fluids and in solids, this part is easily and efficiently parallelized. However, the interface coupling terms need special attention as they require information from both fluid and solid subdomains across the interface. This implementation takes advantage of the local memory on the processing node, thereby exploiting the calculation of element-level matrices and vectors. Preliminary tests confirm the robustness of the method for highly nonlinear problems. This model will now be applied to patient-specific geometry to see the scalability of the FSI method with nonmatching meshes to problems of clinical relevance.

PUBLICATIONS & DATA SETS


ATOMIC SCALE SIMULATION OF AMYLOID BETA WITH DISMANTLING PEPTIDE-BASED INHIBITORS

Allocation: Illinois/715 Kohl
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Co-PIs: Giuseppe Licari, Xing Jiang, Andres Arango, Jimmy Do
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EXECUTIVE SUMMARY

Aggregation of amyloid beta (AB) proteins plays a fundamental role in Alzheimer’s disease. Several inhibitors of AB aggregation have been proposed in the literature, but no effective treatment is yet available. In this work, the research team introduced novel multivalent polymer–peptide conjugates (mPPCs) that can dis-aggregate or inhibit AB formation. Moreover, the team recently evaluated new macrocyclic peptidomimetic (MP) libraries that can also hinder AB aggregation.

The researchers used all-atom molecular dynamics (MD) simulations to investigate how mPPCs and MPs bind AB fibrils and alter their stability. Simulations of mPPCs alone or in the presence of AB show that mPPCs self-aggregate in solution, but in the presence of AB they strongly interact with AB through both their peptide and backbone moieties. Furthermore, a docking analysis based on the simulation results reveals that inhibitors may destabilize AB through introducing defects in the fibril.

RESEARCH CHALLENGE

Protein aggregation is implicated in major pathophysiological conditions including Alzheimer’s and Parkinson’s disease. The occurrence of Alzheimer’s disease, in particular, has been linked to the formation of toxic aggregates of amyloid beta (AB) peptides. Although several inhibitors have been developed, the aggregation mechanism is still poorly understood. The research team has recently developed a novel class of hydrophilic, high molecular weight polymers, mPPCs, that bear multiple copies of peptides and can inhibit AB fibril formation (Fig. 1) [2,3]. This multivalency strategy uses multiple simultaneous interactions of the ligand with AB to enhance the affinity. Another strategy involves the use of MP that are stable under physiological conditions and favor interactions with AB owing to their preorganized structures. However, little is known about how these molecular architectures interact with the target protein and what can be done to enhance their effect and increase their specificity.

METHODS & CODES

All MD simulations were performed using NAMD [4], a GPU-accelerated code that has been optimized to run on Blue Waters. In-house scripts using VMD generated mPPC models with different compositions, molecular weights, and peptide loadings [5]. The latter software can also be used to remotely visualize trajectories on Blue Waters. The AB oligomer was obtained from the Protein Data Bank (code: 2LMN).

RESULTS & IMPACT

The simulations of mPPC polymers in solution highlighted that all polymers form pseudospherical self-aggregates within a few hundreds of nanoseconds (Fig. 2a). This self-aggregation resulted from hydrophobic and hydrogen bond interactions among components of the polymers. In particular, the size of mPPC aggregates did not increase monotonously with the peptide loading but rather decreased at high values. The size contraction of mPPC was ascribed to the increase of hydrophobic contacts as the number of peptides grafted onto the polymer increased, causing a more tightly packed aggregate. Interestingly, in the presence of AB, mPPCs wrap around the protein and form a stable complex. From the analysis of contacts and hydrogen bonds, the research team concluded that stabilization of this complex was significantly enhanced by the mPPC-backbone interaction with AB, confirming the effectiveness of the multivalent design of the polymers. These analyses also revealed that proline residues of MP-PCs contribute the most to interactions with AB.

MD simulations performed on an AB oligomer provided multiple conformations of the protein. Molecular docking of an MP performed on these conformations (Fig. 2b) showed that the inhibitors can intercalate inside defects generated owing to thermal fluctuations, as captured during the simulation, in the AB secondary structure. Perturbed beta-sheet structures of AB can allow the insertion of inhibitors, which in turn will weaken and eventually dismantle the fibril structure.

Overall, the insights obtained from these simulations provide a molecular-level mechanism associated with the inhibition of AB aggregation and will support the design of new inhibitors.

WHY BLUE WATERS

The resources provided by Blue Waters in terms of computational power and network performance were essential to carrying out this project because of the need for simulation of a large data set. The large computer allocation allowed for the simulation of multiple systems, some of which were replicated multiple times with varying initial conditions to enhance sampling.

PUBLICATIONS & DATA SETS


Figure 1: Molecular model of a potato inhibitory mechanism of a polymer inhibitor (backbone in cyan and active peptides in multicolor) wrapping around the proteic strain. (b) Docking poses (red) of a macrocyclic peptidomimetic for two different conformations of an amyloid beta oligomer.
Transport Mechanism of Pot Transporters: Employing Loosely Coupled Molecular Dynamics Simulations to Characterize Protein Structural Dynamics

Executive Summary

Protein-coupled oligopeptide transporters (POTs) use the inwardly directed proton flow to uptake small peptides and peptide-like molecules. The human POT transporters Pept1 and Pept2 provide the main route through which the body absorbs and retains dietary proteins. Human POTs also recognize several important families of peptidlike drug compounds such as β-lactam antibiotics. POTs undergo large-scale conformational changes that are the key in understanding the transport mechanism of these proteins. Despite many experimental and computational efforts, however, the inward-(IF) to outward-facing (OF) structural transition of POTs has remained elusive owing to limitations in methodology. Therefore, the researcher has employed novel molecular dynamics (MD)-based enhanced sampling techniques to characterize the large-scale conformational changes of a bacterial POT transporter, namely GkPOT. With the help of petascale supercomputing, these MD-based techniques provide a detailed description of GkPOT’s conformational landscape, which sheds light on the structure–function relationship in POT transporters.

Research Challenge

Membrane transporters provide the machinery to couple active transport of materials to various forms of cellular energy. POT transporters couple energy from proton flow to the transport of small peptides and peptidlike molecules. Key features of POTs are their substrate promiscuity, which is of great interest from a biomedical perspective. Human POT transporters Pept1 and Pept2, which play a key role in absorbing and retaining dietary proteins, recognize several important families of peptidlike drugs such as β-lactam antibiotics. These proteins can uptake poorly absorbed/retained drugs when attached to amino acids or dipeptides as in prodrugs. Proteins can uptake poorly absorbed/retained drugs when attached to amino acids or dipeptides as in prodrugs. The human POT transporters PepT1 and PepT2, which play a key role in absorbing and retaining dietary proteins, recognize several important families of peptidlike drugs such as β-lactam antibiotics. These proteins can uptake poorly absorbed/retained drugs when attached to amino acids or dipeptides as in prodrugs.

Methods & Codes

The PI has used a novel ensemble-based simulation approach (12–15) to reconstruct the entire transport cycle of GkPOT. Bi-exchange umbrella sampling (BEUS) and string method with swarms of trajectories (SMwST) are both loosely coupled MD-based algorithms that require parallel execution of hundreds of MD simulations (14) and have recently been modified within a Riemannian geometry framework (15). The methodology is specific based on applying orientation-based forces on protein transmembrane helices in order to speed up the exploration of protein conformational space.

The software engine used for the simulations is NAMD, a highly scalable MD code implemented in Charm++, an object-based message-driven execution system based on C++. NAMD has been enhanced to support extremely scalable loosely coupled multiple-copy algorithms. Multiple concurrent NAMD instances are launched with internal partitions of Charm++ and located continuously within a single communication world. Messages between NAMD instances are passed by low-level point-to-point communication functions, which are accessible through NAMD’s Tcl scripting interface.

Results & Impact

The OF structure shown in Fig. 1 represents the first OF model of POT transporters and was generated using the researcher’s all-atom MD simulations in combination with orientation-based BEUS/SmwST algorithms (16). The model is verifiably a stable OF structure since the subsequent equilibrium simulations show a water accessibility consistent with an OF state (Fig. 1). The simulations also suggest that the full IF–OF transition requires the binding of both proton and substrate. The pathways generated reveal that the proton-bound GkPOT cannot transition to the OF state (16). Unlike previous simulation studies, which had relied on either unbiased equilibrium simulations or simple representations (e.g., coarse-graining), this new approach combines the accuracy of all-atom MD with the accessibility of long timescales provided by enhanced sampling techniques. The successful employment of these multiple-copy algorithms using Blue Waters resources opens a new window to the structural biology of membrane transporters that bypasses the limitations of computational approaches to studying structure–function relationships in these proteins.

Why Blue Waters

This work has explicitly shown that the unbiased all-atom MD, which is routinely used in the field, could be quite misleading in deciphering mechanistic features of membrane transporters owing to the great gap in the timescales associated with the conventional simulations and the function of these proteins (11). On the other hand, loosely coupled multiple-copy algorithms such as BEUS and SmwST (14,15) can be used to reconstruct unknown conformational transitions of membrane transport proteins. Unlike the conventional all-atom or coarse-grained MD that can be performed on subpetascale machines, BEUS/SmwST simulations of membrane transporters are well-suited for large petascale computational resources such as Blue Waters since they require hundreds of nodes for a single job. The “weak scaling” of these algorithms makes them particularly attractive for large petascale machines, as they can utilize hundreds of compute nodes with almost perfect efficiency.

Publications & Data Sets


ACTIVATION MECHANISMS OF THE MECHANOSENSITIVE CHANNEL OF LARGE CONDUCTANCE: EMPLOYING LOOSELY COUPLED MOLECULAR DYNAMICS SIMULATIONS TO CHARACTERIZE PROTEIN STRUCTURAL DYNAMICS

EXECUTIVE SUMMARY

The mechanosensitive channel of large conductance (MscL) is a model system for the study of mechanosensation. Understanding MscL’s conformational dynamics has specific biomedical applications. The high level of conservation of MscL in bacteria and its absence from the human and animal genomes make it an attractive drug target for novel antibiotics. In addition, MscL has been proposed as a liposomal drug delivery nanovalue. For example, through engineering MscL can become pH-activated to release drugs when it senses the low pH of the tumor microenvironment.

The PI employed all-atom molecular dynamics (MD) simulations along with novel enhanced sampling techniques to characterize the large-scale conformational changes of MscL and its interactions with its candidate modulators. These simulations elucidate the conformational landscape of MscL at the molecular level, providing a rational design framework for designing more efficient modulators for MscL.

RESEARCH CHALLENGE

The mechanosensitive channel of large conductance (MscL) [1] is a bacterial membrane transport protein that serves as a model system for the study of mechanosensation, a process involved in hearing, touch, balance, and cardiovascular and kidney regulation [2,3]. Owing to its unique properties, MscL has also been proposed for use in various biomedical applications, both as a drug target for novel antibiotics [4] and as a stimulus-triggered nanovalue for drug delivery liposomes [5–8]. Unfortunately, MscL structure is only known in its inactive, closed state [9]. If the molecular basis of MscL activation were understood, researchers could engineer more efficient functional nanovales and design more potent antibiotics targeting MscL.

It is vital to model the active, open state of MscL as well as the entire opening/closing process in order to characterize the MscL activation mechanism. The timescales involved in this process are beyond the currently accessible limits of traditional all-atom MD. The tilting of transmembrane helices is the main rate-limiting step required to form the open pore [10]. While many MD studies have been conducted to study MscL activation, the techniques used in these studies rely on simplifications such as coarse-graining [11]. The main challenge in characterizing the large-scale conformational changes of proteins such as those associated with MscL is to reach the functionally relevant timescales without compromising the chemical details.

METHODS & CODES

The PI used a novel ensemble-based simulation approach [12–15] to simulate the activation process of wild-type and engineered MscL. Bias-exchange umbrella sampling (BEUS) and string methods with swarms of trajectories (SMwST) are both loosely coupled MD-based algorithms that require parallel execution of hundreds of MD simulations [14] and have been recently modified within a Riemannian geometry framework [15]. The methodology is specifically centered on applying orientation-based forces and string methods to construct unknown conformations on protein transmembrane helices in order to speed up the exploration of protein conformational space.

In the software engine used for the simulations is NAMD, a high-performance molecular dynamics application that bypasses the limitations of computational approaches to studying structure–function relationships in these proteins.

WHY BLUE WATERS

The PI has explicitly shown that unbiased all-atom MD, which is routinely used in the field, could be quite misleading in deciphering mechanistic features of membrane transporters owing to the great gap in the timescales associated with the conventional simulations and the function of these proteins. On the other hand, loosely coupled multiple-copy algorithms such as BEUS and SMwST [14,15] can be used to reconstruct unknown conformational transitions of membrane transport proteins. Unlike the conventional all-atom or coarse-grained MD that can be performed on subpetascale machines, BEUS/SMwST simulations of membrane transporters are well-suited for large petascale computational resources such as Blue Waters as they require hundreds of nodes for a single job. The “weak scaling” of these algorithms in particular makes them attractive for large petascale machines, as they can utilize hundreds of compute nodes with almost perfect efficiency.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

The most common sexually transmitted bacterium, Chlamydia trachomatis, is an intracellular pathogen responsible for a swath of debilitating conditions including blinding trachoma, which afflicts roughly 84 million people worldwide and has led to total blindness in eight million people. Despite what is well understood about C. trachomatis, important aspects remain mysterious, particularly, how this organism accomplishes membrane fusion. Postinfection, cellular inclusions undergo this critical step whereby separate inclusions are fused together inside the host cell before maturation and expulsion. In 2016, it was shown that the virulence of C. trachomatis is wholly dependent on this stage of its lifecycle, and completion thereof was traced to one protein known as IncA. With the structure of IncA provided by experimental collaborators and with access to Blue Waters, the PI performed studies that could be accomplished with no other scientific instrument: simulating the dynamics of IncA over microseconds to uncover key structural and conformational factors of this important cell machinery.

MOLECULAR MECHANISMS OF INFECTION BY CHLAMYDIA

RESULTS & IMPACT

Using a high-resolution crystal structure of wild-type IncA provided by experimental collaborators—IncA87–246—the PI aimed to assess if the coordinates represented a thermodynamic minimum or a metastable intermediate capable of reorganizing into a fusion-competent state. For comparison, two other constructs identified experimentally were tested: a truncated mutant IncA87–237 and a point-mutant IncA87–246(G144A). Without understanding the dynamics of C. trachomatis’ key fusion protein, and what conformation might be assumed to initiate fusion, no conclusions leading to drug targets may be formed. In a world where classic antibiotic treatments are leading to super-resistant pathogens, the need for new drug targets cannot be overstated.

METHODS & CODES

The simulations used the NAMD molecular dynamics engine, which is optimized to take full advantage of high-performance distributed-memory architectures. Using NAMD, the PI sampled all three systems for an aggregate of twelve microseconds. These trajectories provided invaluable insights into the dynamics of IncA variants and will be used in further in-depth analyses. Blue Waters not only made collecting these data practical but enabled the researcher to efficiently gather evidence identifying key structural features of IncA that help regulate its overall structure and flexibility. Similarly, parallel I/O capabilities of Blue Waters’ Lustre file system enabled the high-throughput postprocessing of the obtained trajectories feasible.

RESULTS & IMPACT

The simulations showed that the crystal structure of IncA87–246 represents a thermodynamic minimum that is not likely to unfold to initiate fusion. Analysis of obtained trajectories showed that the C-terminal domain of the fusion peptide is essential to regulating global structural flexibility, particularly in the region known as the Hclamp, which was shown in simulations to have a much higher mobility than the rest of the structure (Fig. 1a). Importantly, because IncA is thought to recognize a conspecific or separate regulatory protein before fusion, the high mobility of Hclamp hints at its significance in the fusion process. Truncated mutant IncA87–237—which does not have C-terminal domain—showed a wildly fluctuating Hclamp region as well as a poorly maintained globular structure (Fig. 3a, b), explaining the experimentally observed inability of this truncated construct to even initiate fusion. Additionally, when the distance between the C-terminal domain and Hclamp is narrowed down, as was tested with the point-mutant IncA87–246(G144A), overall structural stability increases. Increased stability, observed as decreased root-mean-square fluctuation (RMSF), is most apparent in the Hclamp region of IncA87–246(G144A) (Fig. 1a). Consequently, this prevented the Hclamp from forming any lasting hydrogen bonds with helix A, which were observed in the other constructs (Fig. 1c). This finding supports the idea that the Hclamp region and its interactions with the C-terminal domain are critical determinants of structure and dynamics. Moreover, it provides insights into why the G144A construct could not form a homodimer in solution experiments.

PUBLICATIONS & DATA SETS


CALIBRATING THE SIMBIOSYS TUMORSCOPE FOR THE FIGHT ON CANCER: A SCENARIO ANALYSIS ENGINE FOR DETERMINING OPTIMAL THERAPY CHOICE

EXECUTIVE SUMMARY

Use of the most toxic drugs in a “scorched earth strategy” is common in the treatment of breast cancer, even though less toxic drugs have only single-digit lower rates of success. To address this issue, the TumorScope software was calibrated to accurately predict the response of breast cancer to the various drugs commonly used for treatment. Calibration resulted in high correlation between predicted and actual outcomes for nearly 200 patients spanning all types of breast cancer. More pertinent to treatment planning, TumorScope was able to improve the accuracy of identifying patient/drug combinations that will achieve pathological complete response (PCR) after treatment by two to three times that of the current state-of-the-art method. PCR is the strongest predictor of long-term survival for breast cancer patients and the desired outcome for all drug-based therapies. Physicians can thus use the computational analysis of different therapies produced by TumorScope to weigh likelihood of therapy success versus drug toxicity.

RESEARCH CHALLENGE

Despite significant advances in cancer treatment in both the number and efficacy of therapies, success rates of any individual therapy remain low. This is especially true in breast cancer where, while overall five-year survival rates tend to be greater than 70%, the efficacy rates of any individual therapy range from 20% to 40%. Critically missing is a way for physicians to distinguish which therapy will be most effective for each patient, or whether or not the available therapies will work. As a consequence, many patients are prescribed a therapy, often at high physical, mental, and monetary cost, that is either too extreme or completely ineffective.

What is needed is a method of predicting the likelihood of success for different therapies that does not increase the number or cost of laboratory tests. SimBioSys set out to solve this problem by developing TumorScope, a personalized medicine approach that constructs realistic, 3D models of patients’ tumors that, when coupled with novel simulation algorithms, can be used to perform scenario analysis (Fig. 1a).

METHODS & CODES

Simulations were performed using a proprietary simulation engine known as TumorScope. Data from nearly 200 breast cancer patients who underwent neoadjuvant (presurgery) chemother-apy [1–3] were used to construct initial conditions for the simulations. The data set represents patients of all common breast cancer types as well as drugs, including chemotherapy and immunotherapy. At several times throughout the course of therapy, clinical outcomes such as tumor volume, tumor longest dimension, and overall pathological response were used to assess the accuracy and applicability of a particular parameter set. Parameter sets were varied systematically for each drug to minimize the deviation between predicted results and clinically measured results.

RESULTS & IMPACT

Simulations included a 3D representation of the local environment with the various tissues found around the breast tumor (Fig. 1a). The TumorScope software simulated the interactions among the tissues along with their biology, the drug perfusion (Fig. 1b), and resulting response of the tumor to different drug regimens (Fig. 1c). Depending on the drug regimen—that is, the combination of drugs chosen and frequency of administration—a patient’s tumor response might be drastically different. As demonstrated in Fig. 1c, a patient given the same combination of drugs every three weeks (e.g., a “standard regimen”; Fig. 1c, left) or every two weeks (e.g., a “dose-dense regimen”; Fig. 1c, right) can lead to either progression or regression of the tumor mass. Empowered with this information, the physician and patient may opt for the more toxic dose-dense regimen.

As with every predictive model, TumorScope had freely tunable parameters. To make accurate predictions, model parameters were systematically tuned to match predictions with clinical outcomes. The research team leveraged the large number of

WHY BLUE WATERS

The Blue Waters system has been critical for the calibration of the TumorScope prediction engine. Calibration required simulating the response of hundreds of patients to various therapies while varying a number of parameters. Even with the fast time-to-solution of the predictive engine (one prediction per hour), a calibration process of this scale would have required months to years of computer time to complete. By leveraging the large number of GPUs available on Blue Waters, these calibration processes could be performed in just a few days. The computer allocation during the 2018–2019 year effectively allowed for the complete tuning of the TumorScope software for breast cancer.
INVESTIGATING THE CLIMATE-RELEVANT IMPACTS OF CHEMICAL COMPLEXITY IN MARINE AEROSOLS

EXECUTIVE SUMMARY

Marine atmospheric aerosols make up a significant portion of the planetary aerosol budget and represent one of the largest sources of uncertainty in current climate models. Aerosols impact climate through cloud seeding and multiphase heterochemistry. However, understanding of the structure and morphology of marine aerosols and the resulting impacts on atmospheric processes is extremely limited. Given the difficulty of experimental single-particle analysis techniques and the high complexity of individual particles, computational methods are used to explore how particle size and chemical composition impact climate-relevant physical and chemical properties of marine aerosols. Model sea spray aerosols are generated based on experimentally determined aerosol lipidomic and proteomic information, then simulated using Blue Waters, with the goal of understanding how chemical complexity modulates aerosol dynamics.

RESEARCH CHALLENGE

Marine aerosols impact the climate by interacting with incoming solar radiation, serving as nuclei for cloud formation and providing interfaces for heterogeneous and multiphase atmospheric chemistry. Individual aerosols vary widely in their size, chemical profile, and internal mixing states; however, current single-particle analysis techniques in the laboratory are not able to access the nanosecond to millisecond timescale dynamics within these aerosols, which ultimately guide their climate-relevant properties. These simulations allow the researchers to understand how aerosol chemistry ultimately impacts the dynamics and interactions within aerosols at the microscale, including protein and lipid partitioning, diffusion, and water transport across the interface, allowing the team to make predictions about macroscale aerosol behavior. The variation in lipid, protein, and saccharide (carbohydrates such as simple sugars or polymers) concentration—strongly mediated by the biochemistry at the ocean surface—allows the research team to connect ocean microbiology to aerosol properties. Integrating computational methods with experimental techniques advances the capacity to accurately model marine aerosols, inching scientists closer to unraveling the complexity of marine aerosol chemistry and how it shapes our climate.

METHODS & CODES

While marine aerosols have yet to be fully characterized in terms of their chemical composition and structural morphology, and though they exhibit a wide variety of types and variation based on relative humidity, ocean conditions, geographic origin, etc., the team based their aerosol models on the recipe derived by Bertram et al. [1] for submicron particles at 70% relative humidity. The researchers’ models were constructed with PACKMOL [2] and parameterized using the CHARMM36 [3] force field and TIP3P [4] water. All simulations were carried out with GPU-accelerated NAMD [5].

To investigate the impacts of chemical complexity on nanoaerosol molecular dynamics, the team simulated three aerosol systems and increased the number of components at each step. The three aerosol systems were simulated in triplicate for up to 500 nanoseconds each. System I contains a base level of complexity, and includes four fatty acids at experimentally determined ratios, protein (Burkholderia cepacia lipase), and sodium chloride. In system II, the team added lipopolysaccharides from E. coli and increased the diversity of cation types to include magnesium, calcium, and potassium in addition to sodium. System III is the most chemically complex and includes a neutral polysaccharide (laminarin) as well as glucose monomers.

RESULTS & IMPACT

Although work only began in early 2019, the team hopes the results will lend a more complete understanding of nascent sea spray aerosol morphology. Microscopy data show that sea spray aerosol morphology will challenge the current understanding of marine aerosol morphology, and could have impacts on how scientists model multiphase atmospheric aerosol chemistry.

WHY BLUE WATERS

The Blue Waters system has enabled the research team to explore molecular dynamics on systems of real physical and chemical relevance to the climate, which includes simulating particle sizes up to 100 nanometers in diameter, containing millions of atoms, for microsecond timescales. The Blue Waters staff has been integral to the success of this work. Their expertise in GPU-accelerated NAMD has allowed the team to get their simulations up and running quickly, with minimal setbacks.
MOLECULAR DYNAMICS BINDING FREE ENERGY CALCULATIONS OFFER A WINDOW TO UNDERSTAND PROTEIN–PROTEIN BINDING SPECIFICITY

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EXECUTIVE SUMMARY

Extracellular domains of cell surface receptors and ligands mediate cell–cell communication, adhesion, and initiation of signaling events. In order to understand highly organized cellular systems, it is necessary to study how intricate dynamical networks arise from specific protein–protein interactions. Thus, the research team has used a free energy computational methodology to quantitatively examine the basis for protein binding specificity in two subfamilies of recently identified genes within the immunoglobulin superfamily found in the model organism Drosophila melanogaster (the common fruit fly).

RESEARCH CHALLENGE

The living cell can be pictured as a collection of macromolecules that are carrying out a number of well-defined tasks. Thanks to tremendous progress made in X-ray crystallography, our knowledge of the three-dimensional structure of individual proteins present in the cell has been greatly expanded in the last decades. However, as scientists seek to comprehend the function of highly organized cellular systems, it is becoming increasingly clear that this will not be possible without understanding how intricate dynamical networks arise from specific protein–protein interactions. For example, the intercellular communications needed for the morphogenesis of the central nervous system is essentially mediated by protein–protein interactions and recognition processes involving cell surface receptors and ligands.

Some of the most intriguing of such interactions are presented by the set of recently identified Dpr–DIP complexes in the common fruit fly (Drosophila melanogaster), which has a total of 20 Dpr genes. The Dpr (defective proboscis extension response) and DIP (Dpr-interacting proteins) genes belong to the immunoglobulin superfamily and associate to form a molecular complex (Fig. 1). Most members of the DIP subfamily cross-react with several members of the Dprs and vice versa.

The Dpr–DIP binding specificity plays a critical role in neuronal development and synaptogenesis. The research team’s objective is to use a free energy computational methodology to quantitatively explain the basis for Dpr–DIP protein binding specificity. To understand how cell surface receptors control development, the researchers need to answer questions such as how the distinct structural features of cell adhesion complexes, including possible sets of highly homologous proteins, instruct the formation of synaptic networks. In other words, scientists must decipher the molecular code that governs the specific association of these proteins and understand why some of them bind together but not others despite their high structural similarities.

Predicting with quantitative accuracy when and why proteins can specifically associate and bind must begin with the statistical mechanics concept of binding free energy. For a binary protein complex, the binding affinity is determined by the equilibrium dissociation constant and the binding free energy. Based on insight gained by categorizing and observing many known protein–protein complexes, several models have been proposed to predict the experimental binding affinities using the features discussed above. Although some have been very successful on small training sets, the published models have performed considerably less well on larger sets and their predictive value remains poor. From this point of view, a computational approach based on atomic molecular dynamics (MD) simulation and free energy methodology is advantageous because it does not rely on any particular empirical assumptions about the binding; the approach is applicable to any protein complex and does not suffer from the limitations displayed by empirical bioinformatics/evolution or docking/scoring methods, which often perform poorly in large-scale benchmark testing. But this raises several important issues, such as whether the atomic force fields used in the simulations are sufficiently accurate, or whether one can design an efficient computational strategy to overcome the challenges presented by conformational sampling. Another important question is whether one can truly design an effective and scalable computational strategy to tackle the processes occurring over long timescales that is well adapted for a leadership-class computer such as Blue Waters. Unbiased MD trajectories, while very valuable, can be limited. However, advanced free energy methodologies can help overcome these limitations.

METHODS & CODES

The solution to this computational problem proposed by the research group is to break down the binding process into a large number of physically meaningful steps and express the binding free energy as a sum of free energies associated with each step. This requires carrying out a large number of simulations with different biasing restraints acting on the system. The biased data are harvested from a large collection of copies or replicas of the molecular system via a replica-exchange algorithm. Such multiple-copy algorithms (MCAs) offer a general and powerful strategy to enhance the sampling efficiency of conventional MD simulations.

Further, the simulation program NAMD fully supports extremely scalable and efficient parallel active messaging interface-level parallel algorithms (MCAs) offer a general and powerful strategy to enhance the sampling efficiency of conventional MD simulations. The MCAs on leadership computers. This makes it possible to carry out extremely scalable MD simulations on Blue Waters using the team’s MD replica-exchange free energy strategy.

RESULTS & IMPACT

The research team has developed and tested a novel theoretical framework for binding free energy calculations, leveraging on the optimal curvilinear minimum free energy path determined from the string method. Fundamentally, this curvilinear pathway strategy is based on the reversible spatial separation of two binding macromolecules, which is clearly the method of choice to quantitatively characterize the affinity of large molecular complexes in solution. Nonetheless, previous implementations based on the potential of mean force for the separation of two proteins along a predefined rectilinear path led to MD calculations that converged too slowly. The proposed methodology was validated by comparing the results obtained using both rectilinear and curvilinear pathways for a prototypical host–guest complex formed by cucurbituril binding benzene and for the barnase–barstar protein complex. The researchers found that the calculations following the traditional rectilinear pathway and the string-based curvilinear separation pathway agree quantitatively, but convergence is faster with the latter.

WHY BLUE WATERS

The multiple-copy algorithms require a very large number of nodes to be effective. Blue Waters is a unique platform that makes it possible to fully exploit the power of this advanced sampling methodology.
MOLECULAR BASIS OF THE NITRATE TRANSPORT MECHANISM IN PLANTS

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EXECUTIVE SUMMARY
Growing evidence suggests that efficient use of nitrogen is required to improve crop productivity. The gene NRT1.1 has been identified as a nitrate transporter that enables nitrogen uptake by plants. NRT acts as a nitrate sensor and transports substrate molecules across the membrane. It belongs to the major facilitator family whose function relies on the alternate access mechanism where the substrate binding site of the transporter protein alternately opens and closes at either side of the membrane. The crystal structure of NRT1.1 was determined in the inward-facing (IF) state as a homodimer and provided the first glimpse of structure information on this class of proteins. These proteins undergo intrinsic conformational changes; the dynamics among the functionally important intermediate states remain elusive. In this project, the research team investigated the conformational dynamics and structural transport mechanism of NRT1.1 using molecular dynamics simulations.

RESEARCH CHALLENGE
Nitrogen is an essential nutrient required for plant growth and development. Plants uptake nitrogen as nitrate ions through the nitrate transporter (NRT1.1), which actively mediates the transport of nitrate ions from the soil into cells. NRT1.1 exhibits a dual affinity transporter (LAT) and at high nitrate concentration, NRT1.1 acts as a low-affinity transporter (LAT) and at high concentration, it is phosphorylated at Thr101, resulting in a high-affinity transporter [1,2]. Recently, the crystal structure of NRT1.1 bound to a nitrate ion (NO3−) was obtained as a homodimer in the IF state [3,4]. NRT1.1 belongs to the major facilitator superfamily that contains 12 transmembrane helices and functions based on an alternate access mechanism to transport signaling molecules. NO3− was bound to the protonated His356 and Thr360 on TM7 in the binding site, and biochemical studies show that the mutation of these residues results in a loss of ion transport [3,4]. The phosphorylation of Thr101, the phosphorylation site residue, increases the affinity of the nitrate ions. However, the conformational dynamics and mechanistic basis of NO3− uptake remain elusive. In this project, the research team performed long microsecond simulations to understand the functional dynamics of NRT1.1 and characterize the NO3− transport mechanism. The results will provide molecular-level understanding of the phosphorylation-mediated increased affinity switch mechanism of NRT1.1.

METHODS & CODES
The simulations were performed with AMBER14 [5]. The simulations produced massive amounts of data (several TB), the Python package MDTraj was used for data processing and analysis [6,7]. The MD data were featureized to biologically relevant reaction coordinates and Markov state models (MSM) were constructed using MSMBuilder [8]. MSM is a statistical model constructed to explore the kinetics of the biological events. MD simulation data will be clustered based on kinetically relevant microstates and the transition matrix that was constructed. Using the transition matrix, the rate of probability of transition to the different states were obtained. The state population are easily converted to free energies using Boltzmann distribution. The obtained free energies of individual states are called the “MSM weighted free energy” of populations.

RESULTS & IMPACT
Conformational dynamics of unphosphorylated (UnpNRT) and phosphorylated (pNRT) ensembles. The IF-state crystal structure of NRT1.1 (Protein Data Bank ID: 4CH1) [5] was the starting structure of the simulations. The research team performed extensive simulations to explore the conformational dynamics and nitrate transport mechanism of UnpNRT (~110 µs) and pNRT (~45 µs). The high-dimensional simulation data were converted to the slowest process and clustered to kinetically relevant states. MSM were constructed to gain insights into the thermodynamics and kinetics of UnpNRT and pNRT conformational ensembles. An MSM-weighted free energy landscape plot was shown by projecting the MD data obtained on the minimum helical tip distance of the pore channel radius on the extracellular and intracellular region (Fig. 1). The free energy barrier for one complete conversion cycle of IF to outward-facing (OF) structures was estimated to be approximately 2.5 kcal/mol in UnpNRT and approximately 1 kcal/mol in pNRT. The phosphorylation at Thr101 results in a conformationally driven ion-coupled transport mechanism and results in a canonical L-shaped landscape. However, UnpNRT samples more intermediate states and may result in a low-affinity transporter.

Nitrate ion transport mechanism in NRT. The nitrate ion is recognized by the group of polar and positively charged residues at the extracellular part of the transporter in the OF state (Fig. 2); the distances between the periplasmic and cytoplasmic gating residues are approximately 2.5 Å and 3 Å, respectively. The ion diffuses in the pore and interacts with Thr360. Nitrate ions escape from the intermediate interaction and bind to protonated His356 on TM7, in accord with the experimental finding that crucial interaction mediates the nitrate transport. The sidechain conformation of His356 is further favored by polar contacts of Gha476 and Tyr388. The tight binding of nitrate ions at the center of the transporter facilitates the conformational change from the OF to the occluded (OC) state. The breakage of polar contacts between Lys164 and Tyr480 leads to the opening of the intracellular gate and the release of nitrate to the cytoplasmic side. This study reveals the molecular level detail of functionally important intermediate states and the nitrate ion transport mechanism using extensive simulation. In this work, the PI has also determined the key residues that drive the nitrate transport as well as the conformational switches. His future work will be focused on engineering NRT to improve the nitrate transport to increase the crop yield.

WHY BLUE WATERS
Biologically important conformational transitions are slow processes that are difficult to observe by running simulations on local hardware. Powerful resources like Blue Waters are required to study such complex biological processes in full atomistic detail and over long timescales. Blue Waters provides thousands of GPUs that are used for parallel molecular dynamics simulations to perform MSM-based adaptive sampling of the conformational energy landscape of proteins. Blue Waters increases the overall compute performance by several orders of magnitude in terms of the real time required for simulation.

PUBLICATIONS & DATA SETS
SIMULATIONS UNCOVER THE MECHANISM OF SEROTONIN TRANSPORT IN THE BRAIN

EXECUTIVE SUMMARY

The serotonin transporter (SERT) is a member of the neurotransporter-sodium symporters (NSS) family that transports neurotransmitters in conjunction with an electrochemical gradient of ions. SERT initiates the reuptake of extracellular serotonin in the synapse to terminate neurotransmission in the nervous system. Recent cryogenic electron microscopy structures have revealed structural insights into functional conformations of SERT dynamics. However, despite being a major molecular drug target, knowledge of how serotonin is recognized, bound, and transported remains unclear. In this study, the research team performed extensive molecular dynamics (MD) simulations of the human SERT to investigate the structural transition to various states and determined the complete transport pathway in SERT. Further, the team provided a comprehensive approach for characterizing the thermodynamics of key states and critical residues involved in the substrate transport process.

RESEARCH CHALLENGE

The neurotransmitter serotonin (5HT) regulates many physiological processes in the body with implications for cognitive function, mood, and behavior [1]. In neurons, SERT signaling is terminated through the reuptake of 5HT from the synaptic cleft [2]. The lack of knowledge of the dynamics of these transporters has led to a lack of understanding of the molecular basis of selectivity for designing effective anti-depressants and therapeutic molecules.

METHODS & CODES

Obtaining sufficient sampling is a recurring challenge in simulating complex biological processes. To overcome this issue, the research team adopted a Markov state model (MSM)-based adaptive sampling methodology to efficiently explore the conformational landscape. In each round of adaptive sampling, multi-short MD simulations were conducted in parallel. The simulation data were clustered using the K-means algorithm based on a designated metric and starting structures were chosen from the least populated states to seed the subsequent rounds of simulation. The simulations were employed using the AMBER v18 suite [3]. The highly parallelized framework implemented in AMBER offers enhanced scaling on GPU nodes to massively accelerate complex biomolecular simulations.

RESULTS & IMPACT

Conformational dynamics of human SERT. To understand the effects of substrate-induced protein dynamics, the entire import process of serotonin was studied using MD simulations. Simulations were initiated from the outward-facing (OF) SERT crystal structure (Protein Data Bank: 57/3). An aggregated total of approximately 290 microseconds (μs) of SERT simulations were obtained and analyzed using MSM, which parses the simulation data into kinetically relevant states and calculates the transition probabilities between the states. MSM-weighted simulation data were projected onto a coordinate system defined by distances between the extracellular and intracellular gating residues (Fig. 1). The conformational landscape plots reveal that despite the absence of serotonin binding, apo-SERT may undergo transitions from the OF state to the inward-facing (IF) state (Fig. 1a). Extracellular gating residues Arg104 (TM1b) and Glu493 (TM10) can extend to 10 Å, enlarging the extracellular entrance tunnel. The apo states are relatively stable, with a free energy of approximately 0.5 kcal/mol. The distance between gating residues Arg104–Glu493 decreases to 3 Å and is associated with electrostatic interactions, forming occluded (OC) conformations that are more stable than the OF state (Fig. 2). Closure of the extracellular entrance tunnel in the OF state weakens contacts on the intracellular side of the transporter, creating an energetically accessible pathway toward the IF state. The free energy barrier for transition from the OC–IF state in apo-SERT is estimated as approximately 3 kcal/mol, which is higher compared to the OF–OC transition (approximately 2 kcal/mol).

Serotonin transport in SERT. The substrate-bound conformational landscape plots depict deviations in the relative free energies of conformational states and reduced the free energy barriers in between states (Fig. 1b). Binding of serotonin in the entrance tunnel stabilizes the OF states. The gating residues interact with Glu332 (TM4) and Lys490 (TM10) and widens the extracellular vestibule (Fig. 2). The diffusion of 5HT to the S1 site via the allosteric site (S2) leads to the closure of the extracellular cavity to obtain the OC state. The OF–OC transition has a free energy barrier of approximately 1.5 kcal/mol, which is similar to apo-SERT. The downward movement of SHT facilitates the opening of the intracellular gate and leads to the IF state. The free energy barrier for the structural transition to the IF state is estimated as approximately 1.5 kcal/mol. The presence of SHT in the intracellular pathway stabilizes SERT in the IF state, with a free energy of approximately 1 kcal/mol as compared to approximately 3 kcal/mol in apo-SERT.

This study reveals an atomistic-level perspective into the elusive mechanism of substrate transport in SERT. Using MSM, the research team has identified the free energy barriers associated with the transport process and key interactions that drive transport. The results provide an extensive understanding into the molecular recognition of serotonin in SERT and can serve as a model to study other closely related neurotransmitter transporters.

WHY BLUE WATERS

Simulation of complex biological processes requires multiple parallel nodes to reach relevant timescales. The unique architecture of Blue Waters provides hybrid CPU and GPU frameworks to conduct large-scale simulations. These computations would not be achievable within a reasonable time without Blue Waters’ petascale computing capability.

PUBLICATIONS & DATA SETS


ELUCIDATING THE LIGAND SELECTIVITY AND ACTIVATION MECHANISMS OF CANNABINOID RECEPTORS

EXECUTIVE SUMMARY

Cannabinoid receptor 1 (CB1) is a therapeutically relevant drug target for controlling obesity, pain, and central nervous system disorders. However, owing to the harmful side effects of full agonists (molecules that activate CB1) and antagonists (molecules that deactivates CB1), no clinical drug that targets CB1 is currently available. A deeper mechanistic understanding of CB1 selectivity and activation mechanisms with respect to homologous protein cannabinoid receptor 2 (CB2) remains elusive. To understand selectivity and partial agonism, the research team performed extensive simulations using Blue Waters to investigate the conformational dynamics of CB1 and CB2 as well as ligand binding to CB1.

RESULTS & IMPACT

Despite belonging to the same endocannabinoid system and sharing a 42% sequence identity, the selectivity of ligands for CB1 and CB2 can vary by several orders of magnitude. Understanding the selectivity of these two similar proteins has significant implications for designing new selective drugs. The recent discovery of the crystal structure reveals interesting differences between inactive structures of CB1 and CB2. The extracellular part of inactive CB2 matches with the active part of CB1, while the intracellular part matches with the inactive part of CB1. A study on cardiovascular diseases reveals that inactive CB1 (or antagonist-bound) and active CB2 (or agonist-bound) protected against antipsychotic clozapine-induced carboxylic acid [3]. This opposing effect leads the research team to hypothesize that the inverse movement of the extracellular helix could be observed during CB2 activation. MD simulation shows that the extracellular helix I and the intracellular helix VI move outward (Fig. 1b). This movement could lead to the formation of the active state for CB2.

To understand the molecular mechanism of partial agonism exhibited by Δ^9-THC, the researchers performed simulations of Δ^9-THC binding to CB1 (Fig. 2a). They observed a gradual movement of Δ^9-THC toward the binding pocket via the opening between helices I and II [2]. This movement leads to the formation of an energetically separable microstate and calculated the transition probability between these states. The bulkiest aromatic portion of the ligand faces the maximum barrier between the N-loops and helix I as the hydroxylic group of the ligand forms hydrogen bonds with polar residues, which leads to the formation of intermediate state 1 (Fig. 2b). Overcoming this resistance, the ligand moves further toward the binding pocket of the receptor and is stabilized in the antagonist bound pose of CB1 (Fig. 2c). Steric hindrance from the MET 103 residue blocks the Δ^9-THC from going inside the binding pocket.

Discerning the atomistic details of CB1 and CB2 selectivity and partial agonism will aid selective drug design for CB1. The conformational space of CB1 reveals the generation of the intermediate state during activation by toggle switch pair movement (TRP 356 and PHE 200 residues moving toward the intracellular and extracellular side, respectively). Additionally, the Δ^9-THC binding simulation reveals the initial binding pathway for partial agonists and important residues that can be responsible for selectivity.

WHY BLUE WATERS

Observing the activation and ligand binding mechanism of a protein receptor is a computationally expensive process. The computer architecture of Blue Waters allowed the research team to perform hundreds of microseconds of MD simulations to understand the necessary conformational changes of these proteins. The adaptive sampling method helped the team to utilize the GPU power of Blue Waters very efficiently. The current project would not have been possible without Blue Waters’ computational facility.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

This is the first attempt to fully understand how memories are formed in the brain by means of a detailed computational model of each neuron in the hippocampus, a brain area important for learning and memory. The computational capacity of Blue Waters allows the research team to rapidly conduct simulations of brain function at 1:1 scale, to observe and record the behavior of millions of model neurons, and to compare the results with experimental data. The researchers’ model is capable of representing spatial location via the activation of a small number of neurons sensitive to a specific location, closely approximating the navigational system used by the brain. Further, the software infrastructure developed for this project is now allowing the team to explore several hypotheses about the formation of neural sequences as part of the process necessary for storing memory traces.

METHODS & CODES

The principal simulation environment the researchers use is NEURON [1], http://www.neuron.yale.edu/neuron/, which describes neurons in terms of membrane properties and geometric structure [2] and networks in terms of connections between neurons [3]. The biophysical dynamics of the neuronal membrane are described by differential-algebraic equations solved by an implicit integrator optimized for branched structures [1]. NEURON can be fully parallelized via message passing interface with near-linear scaling [3].

The representation of the geometric structure of neurons and their connectivity requires hundreds of gigabytes for each of the models, which has necessitated a parallel computational infrastructure for data management. Thanks to the Petascale Application Improvement Discovery program, the research team has developed a parallel 1/O software substrate based on the HDF5 file format that allows the rapid generation and analysis of neuronal morphology and connectivity data according to user-specified rules about neuronal structure and distribution of connectivity in a 3D volume.

The construction of biophysical models of neurons involves tuning a set of parameters in order to make the model neuron dynamics closely match experimental recordings of real neurons. Because of complex dendritic geometry and nonlinear ion channel dynamics, the model parameter space is enormous. The team has devised a multiobjective evolutionary optimization algorithm that varies ion channel distributions in order to fit the experimentally obtained electrophysiological properties of the target neuron type. This optimization method can be applied not only to models of diverse neuron types but also to a number of other problems ranging from the study of information processing in microcircuits to parameter tuning of large-scale network dynamics.

RESULTS & IMPACT

The research team has made significant progress in developing a biophysically detailed, full-scale model of the rodent hippocampus comprised of realistically diverse cell types, cell-type-specific connectivity, and nonuniform distributions of synaptic input strengths. The researchers have constructed a full-scale model of the input layer to the hippocampus, the dentate gyrus (DG), to generate sparse, selective, and sequential population activity that matches in vivo experimental data [4,5]. The DG model has also served as the prototype to develop general software infrastructure to specify, simulate, optimize, and analyze large-scale biophysically detailed neuronal network models and is scalable across tens of thousands of processors. The team is extending the DG model to include CA3 and CA1 [6] and will release their modeling framework as a general open-source tool to construct models of any brain region at any level of scale and detail.

The DG model now contains over 1.2 million model cells and receives its principal input from stimulus patterns designed to mimic the spatial information content provided to the hippocampus by the entorhinal cortex. The neuronal synapses include NMDA receptors, which have a characteristic nonlinear transfer function. The researchers have found this biophysical property to be critical for a highly sparse subset of granule cells to fire at high rates within their place fields while maintaining essentially zero firing rate out of field, despite receiving a constant barrage of excitatory inputs. The team has been able to use their model to test a prominent theory that a log-normal distribution of synaptic weights combined with lateral inhibition is sufficient to generate singly peaked place fields when being driven by multiply peaked gridfield inputs from the medial entorhinal cortex [7].

The model now also contains a back-projection from CA3 pyramidal cells to DG, which is the first step toward creating an interconnected model of the hippocampus. The back-projection will enable testing of a theory of SWR-related memory replay that posits that interactions between CA3 and DG are required for proper sequence generation [8].

WHY BLUE WATERS

The brain is one of the most complex systems studied by science. Computational modeling of the brain presents challenges in terms of both the mathematical complexity of neuronal dynamics and the large number of neurons and other cells that are part of the nervous system. This project requires the simulation of behaviorally relevant activity of approximately 2% of the total number of neurons in the rodent brain; but even then, such simulations have only been possible on Blue Waters, where producing seconds of simulated brain activity currently takes tens of hours on thousands of processors. Blue Waters has been indispensable in enabling the research team to simulate the brain at a biologically realistic anatomical scale and a behaviorally relevant timescale.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

A seminal event in the history of life on Earth is the transition from single-celled organisms to multicellular life, which required the ability to form strong yet dynamic cell–cell contacts. Among the many classes of molecules that fulfill this role, the cadherin superfamily of cell adhesion proteins is one of the most prominent. Two members of the classical cadherin family, desmoglein (DSG) and desmocollin (DSC), form the robust cell–cell contacts known as the desmosomes, which provide mechanical strength to skin epithelial and cardiac tissues in the face of constant stress, normal stretching, and which protect them from cuts and abrasions. Using the molecular dynamics engine NAMD on Blue Waters, the PI was able to perform simulations on an atomistic model of the desmosome. These simulations provided insight into how this essential cellular junction may function and respond to forces, both in its wild type form and with the addition of disease-causing mutations.

RESEARCH CHALLENGE

Skin epithelial and cardiac tissues are subject to constant stress. The skin epithelium must withstand stretching and shearing forces as well as abrasions, while cardiac tissue must remain viable despite continuous contraction and expansion. To maintain the integrity of these tissues, the cells that comprise them have developed strong and mechanically robust contacts with one another, including the apical adherens junction and the more basally situated desmosome. The desmosome is found in skin epithelial and cardiac tissues and is formed through interactions of the desmosomal proteins DSG and DSC. However, the stoichiometry and three-dimensional arrangement of these proteins in the junction remain largely unknown.

The architecture of the adherens junction is believed to be a well-ordered array of molecules, forming a zippelike pattern in which both trans-interactions (those formed from opposite cells through the strand-swap mechanism) and cis-interactions (those between molecules from the same cell) are present in the lattice structure [1]. The molecular arrangement in three-dimensional space has been more difficult to identify in desmosomes, however. While it is known that both DSG and DSC are required for the formation of the mature desmosome [2,3], the stoichiometry relationship between DSG and DSC and the arrangement of molecules in the junction is a question that remains to be descriptively answered. Models from cryo-electron tomographic imaging and those based on the structure of E-cadherin lattices have been suggested, however, and with the deposition of high-resolution crystal structures of DSG and DSC, further information can be extracted from these models [4–7].

Lattices of DSG and DSC, constructed based on the crystallographic lattice of C-cadherin, offer insight into how these proteins may be arranged in the desmosome and how their interactions contribute to desmosome function. In addition, these models can offer molecular explanations for skin epithelial and cardiac diseases. Several missense mutations known to cause cardiomyopathies have been mapped to the extracellular domain of DSG and DSC, suggesting that adhesive or mechanical properties are compromised. However, the molecular mechanism underlying this often fatal disease remains unknown. Simulations on these models offer a unique ability to bridge the gap between genetics and cell biology, and this power is leveraged in these simulations to propose a model of desmosomal dysfunction in arrhythmogenic cardiomyopathy.

METHODS & CODES

Models were constructed using high-resolution crystal structures of DSG and DSC [1,7]. Lattices for the desmosome were assembled based on the crystallographic lattices present in the solution of classical cadherins and contain four DSG and four DSC molecules. This was done both in a ‘polarized’ fashion, with all DSG on one side and all DSC on the other. To replicate the physiological conditions located in the extracellular space in which the desmosome is found, models were solvated in explicit water and ions. Models were constructed using VMD (Visual Molecular Dynamics) [8] and simulated using NAMD [9], both of which are developed at the University of Illinois at Urbana–Champaign. In addition to the wild-type systems, two separate systems were built by introducing mutations to the DSG molecules in the lattice, both of which cause the inherited and often fatal disease arrhythmogenic cardiomyopathy. All systems consist of approximately 1.8 million atoms.

RESULTS & IMPACT

The wild-type lattice was simulated in equilibrium for 20 nanoseconds (ns), and was subsequently subjected to stretching to reveal molecular dynamics simulations at 10, 1, and 0.1 nanometer (nm)/ns. Additionally, creep tests were performed in which a constant force was applied to one face of the lattice with the other held fixed, allowing the viscoelastic behavior of the junction to be studied. The resultant elastic response and mechanical properties of the complexes were analyzed, providing a glimpse of how these essential cellular junctions may respond to force in vivo. Such modeling and simulation efforts offer unique insights into how these molecules may arrange physiologically and may guide future experimental efforts. Simulations have revealed the formation of cis-interactions that persist throughout equilibrium and stretching, suggesting a possible lateral contact that may have relevance in desmosome function. Creep tests revealed differing viscoelastic behavior in these proteins in the lattice as opposed to individual dimers. In particular, the damping coefficient for each individual protomer was increased when it was tested in the lattice compared to the dimer alone, suggesting the lattice acts as a shock absorber to distribute force across the junction. This property would be vital to maintain desmosomal integrity as it is subject to very rapid and often violent perturbations.

WHY BLUE WATERS

Atomistic simulations as large as those performed on these models of the desmosome, which are composed of up to 1.8 million atoms, require significant computational resources. Such simulations need a fast networked and massively parallel system such as Blue Waters. With the slowest stretching speed, at 0.1 nm/ns, the PI was able to sample hundreds of nanoseconds, a timescale that would be unfeasible for such a large system without the capabilities provided by Blue Waters.
SIMULATION OF VIRAL INFECTION PROPAGATION DURING AIR TRAVEL

Allocation: NSF PRAC/25 Ksh
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EXECUTIVE SUMMARY

There is direct evidence of the spread of infection during commercial air travel for common infectious diseases including influenza, Severe Acute Respiratory Syndrome (SARS), tuberculosis, and measles. This has motivated calls for restrictions on air travel, for example during the 2014 Ebola outbreak. However, such restrictions carry considerable economic and human costs. Ideally, decision-makers ought to take steps to mitigate the likelihood of an epidemic without imposing restrictions. Towards that end, science-based policy analysis can yield useful insight to decision-makers.

The effectiveness of any policy depends on the human response to it. Given the inherent uncertainties in human behavior, the research team simulated a variety of scenarios and identified the vulnerability of policies under those potential scenarios. Supercomputing was used to deal with the large number of scenarios and the need for a short response time in case of national emergencies. The results identified new boarding procedures that, if implemented, can result in a substantial reduction in the risk of the spread of infectious diseases.

RESEARCH CHALLENGE

The research team modeled pedestrian movements during air travel as particles using the force-field approach proposed by Helbing et al. [1]. Both pedestrian density and the speed of the immediate neighbor in a pedestrian line determine pedestrian speed and trajectory [2,3]. The team’s modifications incorporated these aspects into the pedestrian movement model. The pedestrian trajectory information was then integrated with a discrete-time stochastic susceptible-infected model for infection transmission that accounts for demographic stochasticity and variations in susceptibility of the population. This approach provides insight into the consequences of policy choices that change passenger behavior at individual levels. The team input this information into a global phylogeography model to assess the impact of these policies at a global scale.

Inherent uncertainties in human behavior and insufficient data during the initial stages of an epidemic make accurate predictions difficult. The team parameterized the sources of uncertainty and evaluated vulnerability under different possible scenarios. The researchers used Blue Waters to deal with the computational load that arises from a large parameter space, as well as a low discrepancy parameter sweep to explore the space of uncertainties efficiently.

Phylogeography (the study of the historical processes that may be responsible for the contemporary geographic distributions of individuals) uses genetic mutation information and geographic locations of viruses to model the spread of epidemics across large geographic scales. The team used Blue Waters to analyze 264 full-genome Ebola sequences from Guinea, Liberia, Sierra Leone, Italy, the United Kingdom, and the United States. The research group also used the BEAST software installed on Blue Waters to implement the phylogeography model.

METHODS & CODES

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RESULTS & IMPACT

In prior work, the research team used the above approach with Ebola. They studied the impact of different procedures for boarding, disembarkation, and seat assignment on infection spread. That work showed that on a 182-passenger Boeing 757 airplane, random boarding can lead to a substantial reduction in infection transmission compared with the current zone-based boarding. The team also obtained similar results showing the potential for changes in in-plane movement, deplaning procedure, seating arrangement, and plane sizes to reduce the likelihood of infection transmission. The improvements obtained for individual flights by these policy changes can bring substantial benefits over the course of an epidemic. In fact, based on transportation data from 2013, if unrestricted air travel were to have occurred during the 2014 Ebola epidemic, then the probability of generating 20 infectives per month from air travel could have been reduced from 67% to 40% using better pedestrian movement strategies. This could further be reduced to 13% by exclusively using smaller 50-seat airplanes.

The researchers have extended their approach to other directly transmitted diseases including SARS and influenza. This required changes to include aerosol and fomite transmission mechanisms, while pedestrian movement accounts for the proximity between infectious and susceptible individuals. The team has successfully extended the application to other high-density areas such as airport security-check areas and a generic airport gate. The research group also found that different queuing strategies can generate a decrease in infection risk of up to an order of magnitude.

The team also developed a low discrepancy parameter sweep, which reduced the number of parameter combinations that ought to be tried by one to three orders of magnitude over the conventional lattice-based sweep. Using the number-theoretic properties of a low discrepancy sequence helped balance the load on the Blue Waters machine [4].

WHY BLUE WATERS

In an emergency, scientists usually need to model a variety of scenarios owing to a lack of data. This leads to a large parameter space of uncertainties, which requires a large computational effort. In addition, the models typically need fine-tuning, which leads to an iterative process where the model is repeatedly tuned based on results from the previous validation step. Consequently, rapid turnaround time is critical, which requires massive parallelism. Such parallelism becomes even more crucial during the course of a decision-making process, where results are typically needed in a short time span. The Blue Waters support team helped optimize parallel I/O in the code to reduce simulation time by a factor of two.

PUBLICATIONS & DATA SETS

EXECUTIVE SUMMARY

Age-associated diseases are increasing along with the aging of the world’s population. This includes diseases that affect the brain such as Alzheimer’s disease (AD). AD annually costs $290 billion and contributes to more than 500,000 deaths yearly in the United States [1]. Leveraging advanced Magnetic Resonance Imaging (MRI) acquisitions and high-performance GPU-enabled computing, the research team has developed a method to investigate properties of the brain blood supply that were not previously measurable. Acquiring high-resolution MRI data of the brain while correcting for small motions of the brain during the scan delivers information on the density and microstructure of the vessels during a noninvasive MRI scan. Previously, these properties of the vessels have only been observable after death but have correlated with disease progression. The current study will enable monitoring these blood vessel characteristics over the lifespan.

RESEARCH CHALLENGE

MRI is a noninvasive, nonionizing tomographic imaging technique that enables imaging of the human brain with a variety of functional and structural contrasts, all with no more than minimal risk to the participants. For research in the basic sciences involving human subjects, MRI can measure quantities that are difficult to measure or otherwise inaccessible, such as blood flow, vascular density, and the microstructure of blood vessels in the brain. However, the MRI techniques to obtain these measures of the properties of blood vessels have lacked sufficient signal-to-noise ratio and spatial resolution to enable the monitoring of those biomarkers of health and disease. In the current work, the team leverages advanced 3D acquisitions along with a complete signal model for image reconstruction from the acquired data in order to increase the available signal and spatial resolution [2,3]. Image reconstruction can be computationally expensive for large data sets when the research team needs to incorporate compensation for physical effects in the MRI scanner along with motion of the brain during data acquisition. This can result in reconstruction times of a month or more per data set when using a single workstation, severely limiting application of these techniques.

METHODS & CODES

The team uses a GPU-accelerated image reconstruction package called PowerGrid [4] to implement 3D, field-corrected, non-Cartesian image reconstruction with nonlinear motion correction. To speed the algorithm, the researchers use GPUs to achieve high performance via OpenACC. Specifically, the team uses an implementation of the nonuniform Fast Fourier Transform (NUFFT) [5] that has been GPU-accelerated via OpenACC.

RESULTS & IMPACT

The use of OpenACC on a high-performance computing platform such as Blue Waters is not without its challenges, and the interoperability of packages and compilers needs to be addressed to more efficiently leverage the large number of GPU nodes. However, large data sets such as the one in this project are not feasible to reconstruct without utilizing massive multicore strategies. The team focused on increasing the multicore utilization for NUFFT, which is the main kernel in their code, expanding the portable parallelization to use either CPUs or GPUs depending on the environment. With only one hardware-specific library (that handles efficient Cartesian FFTs), researchers can swap CPUs or GPUs for these libraries using the latest OpenACC-capable compilers. This enables transitions to future computing platforms and more widespread adoption of this approach by enabling the code to perform either on hardware accelerators or CPU cores.

WHY BLUE WATERS

Blue Waters provides an ideal environment for the highly parallel task of image reconstruction in MRI. Each participant’s data requires reconstruction of many images, each with a different image contrast reflecting different properties of the brain blood flow. Utilizing multiple GPUs enables the acceleration of each image’s reconstruction and the availability of a large number of GPU-enabled nodes allows the simultaneous reconstruction of all the images from several subjects’ data.
**EXECUTIVE SUMMARY**

At the heart of many cellular processes, mechanosensitive proteins are required for converting mechanical cues into biochemical signals. Protein mechanics are also crucial in holding large macromolecular complexes together during mechanical stress, while permitting assembly and disassembly of these complexes to continue to take place at physiologically needed rates. Employing state-of-the-art computational tools and in a close collaboration with experimentalists, the research team has shown how specific protein complexes can be "activated" under shear force to withstand high mechanical loads. They have discovered that protein mechanostability is highly dependent on the direction of the force application. They have also shown that mechanical stability can be achieved by a protein architecture that directs molecular deformation along paths that run perpendicular to the pulling axis. These mechanisms of mechanical protein stabilization have potential applications for the engineering of systems exhibiting shear-enhanced adhesion or tunable mechanics.

**RESEARCH CHALLENGE**

Interfacing biology, physics, and engineering, mechanobiology studies how mechanosensitive proteins sense and respond to mechanical cues in different ways. Guided by advances in single-molecule force spectroscopy, researchers are acquiring a new level of understanding of mechanosensitive proteins. However, protein mechanics is a challenging topic to study experimentally because molecular-level mechanical properties remain hidden to ensemble-averaging methods. They require techniques such as molecular dynamics that offer simultaneous high spatial and temporal resolution. The research team employed Blue Waters to investigate how cellulosomes, large molecular machines that can efficiently degrade plant fibers, can be mechanically activated to withstand high mechanical loads. Understanding how cellulosomes work can have a considerable impact on rational design of more efficient enzyme complexes for biotechnology and bioreactors. Also, cellulosome-containing bacteria were recently found in the human gut, a paradigm-shifting discovery that shows at least some humans are able to fully digest plant fibers.

**METHODS & CODES**

The research team has employed a combination of in silico and in vitro single-molecule force spectroscopy to elucidate, with atomic resolution, protein mechanics at high-force loads. Using a wide sampling approach, steered molecular dynamics simulations were performed with many replicas, allowing the team to analyze experiments and simulations in the same statistical framework. Wide sampling combined with dynamic network analysis allowed them to visualize most probable deformation pathways through the protein architecture and understand how resistance to mechanical stress arises at the level of individual protein complexes. Simulation results were validated using single-molecule force spectroscopy experiments carried out with an atomic force microscope over a range of loading rates. By recording the force required to break the protein complexes for thousands of individual interactions, the team collected sufficient statistics to analyze the interactions and unfolding pathways thoroughly. They achieved remarkable agreement between simulations and experiments, demonstrating that they probe fundamentally the same molecular mechanics.

**RESULTS & IMPACT**

The chemistry at the interface between biomolecules affected by mechanical forces is still largely unexplored. Even the best-studied mechanically stable biomolecular complexes, namely the streptavidin/biotin complex, has mechanical properties that have only recently been revealed. By using Blue Waters, the research team has shown that a wide range of rupture forces previously reported for the separation of the complex are due to unspecific tethering of streptavidin [1]. In fact, different anchoring points in the same protein can lead to unspecific or specific binding of the complex [2]. In cellulosomes, which are usually found in harsh environments, mechanical stability at specific pulling geometries is crucial for their high efficiency. The team had previously shown that a cohesin:dockerin (two major components of a cellulosome) complex could withstand forces up to four times that of the streptavidin/biotin complex [3], which was previously considered to be the strongest protein complex.

In this project, the team has discovered a cohesin:dockerin complex that is significantly stronger than the one they previously reported [4]. The scaffold (ScaB) is found within the same cellulosome that was previously reported. The role of the ScaB complex is to connect the large protein machinery of the cellulosome to the cell wall via high-affinity binding to the same cohesin of the ScaB complex. This cohesin is itself covalently linked to the peptidoglycan cell wall (Fig. 1). The team's single-molecule experiments show that there are limitations in the most mechanically stable complexes [4], with forces up to a nanomechanon. The team's simulation results reveal that the mechanical stability is achieved by an architecture that directs the force along pathways running perpendicular to the pulling axis (Fig. 2). Taking advantage of Blue Waters' size and power, the team has also investigated how different cohesin domains found in a single cellulosome scaffold withstand shear forces. The results show that in the same scaffold, different cohesins can have a large (up to a factor of four) difference in mechanical stability, depending on the cohesin's position in that scaffold [5]. Remarkably, all seven cohesins in the same scaffold share high sequence identity. A striking agreement was observed between simulation and experiment, motivating the researchers to computationally explore how point mutations could affect the mechanical stability of cohesins. In an intelligent design strategy, simulations revealed that a single mutation in an alanine residue, replacing it by a glycine residue, could make one of the weaker cohesins much stronger. The experiments also revealed that this mutation, which replaces a methyl group by a single H, was responsible for a 2.6-fold increase in the mechanical stability of that cohesin [5]. The team's results show the vast potential offered by large supercomputers for molecular engineering and biotechnology.

**WHY BLUE WATERS**

Fast turnover time is fundamental when working synergistically with experimentalists. Blue Waters' sheer size allowed the researchers to simulate many experiment replicates at about the same speed experiments can be performed. Without Blue Waters, testing new hypotheses computationally would not have been feasible.

**PUBLICATIONS & DATA SETS**


W. Yang et al., "In situ conformational changes of the Escher- chia coli serine chemoreceptor in different signaling states", mBio, vol. 10, no. 4, July 2019.


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ATOMIC SIMULATION OF A PROTOCELL

EXECUTIVE SUMMARY

Computational biology has been critical in achieving a molecular understanding of the dynamics and function of proteins, nucleic acids, and biological membranes. Most research in this field has been limited to single-protein characterization owing to limitations in computational power and analytical methods. However, to truly understand the mechanisms of biological systems, proteins need to be studied in the broader context of a cell. This project aims to address this emerging challenge that remains to be addressed and, therefore, out of the cell [2,3].

Modeling membranes at cellular scales is also relevant to understanding the movement of materials within the cell and between different compartments within the cell. Diverse in form, structure, and lipid composition, they are highly heterogeneous environments containing lipids and proteins that act in concert to regulate the flow of information and materials into and out of the cell [2,3]. Modeling membranes at cellular scales is an emerging challenge that remains to be addressed and, therefore, is one of the critical steps in modeling the cell. The research team has a long tradition in modeling and simulating membranes and membrane proteins, particularly emphasizing their importance for including the natural environment in the simulations [4–8].

RESEARCH CHALLENGE

The living cell represents a spatially complex and highly regulated arrangement of molecules whose coordinated motions and activities underlie all the processes that allow it to grow, reproduce, and carry out a wide spectrum of cellular functions. Recent advances in experimental techniques have targeted the identification of the positions of subcellular organelles, ribosomes, and macromolecules such as proteins, messenger RNA, and DNA at high resolution [1]. This has in turn fed a growing demand for next-generation computational tools that allow researchers to construct realistic, cellular-scale structural models at a range of resolutions; to resolve molecular functional states; and to simulate their stochastic, time-dependent behavior.

Biological membranes constitute the most fundamental component of cellular and subcellular structures, defining the active boundaries not only between the cell and its environment but also between different compartments within the cell. Diverse in form, structure, and lipid composition, they are highly heterogeneous environments containing lipids and proteins that act in concert to regulate the flow of information and materials into and out of the cell [2,3]. Modeling membranes at cellular scales is an emerging challenge that remains to be addressed and, therefore, is one of the critical steps in modeling the cell. The research team has a long tradition in modeling and simulating membranes and membrane proteins, particularly emphasizing the importance of including the natural environment in the simulations [4–8].

METHODS & CODES

The MD simulations were performed with NAMD [9], a highly parallelized, GPU-accelerated, publicly available MD program with demonstrated scalability to hundreds of thousands of processors for both single- and multiple-replica simulations. All-atom MD simulations rely on the accurate integration of the equations of motion for all atoms of the system. The total potential energy of the system was described by the CHARMM36m force field [10,11]. Periodic boundary conditions were used to avoid surface effects at the simulated system's boundaries, allowing the efficient computation of nontruncated electrostatic interactions by the fast Fourier transform-based particle-mesh Ewald method [12].

RESULTS & IMPACT

The research team designed, developed, and tested a protocol for the construction of spherical cellular envelopes of any lipid/protein composition, which can be divided into three stages. The first step in the designed workflow was to use experimentally derived or user-specified cell diameters to directly determine the surface area of the inner and outer leaflet of the cell envelope and to accurately calculate the number of lipids needed to construct both leaflets. The membrane shell was then generated using the Fibonacci sphere algorithm [13] to approximately solve the Tammes problem [14,15] for the thousands of lipids required to create a micrometer-scaled membranous protocell. Next, each protein was assigned a unique position on the spherical surface. In order to do this, coarse-grain approximations of each protein were generated using a hierarchical clustering algorithm. These were then simulated using a force field that properly orients and localizes them to the intended membrane surface. Lastly, the membrane and the proteins were merged, which involved removal of requisite lipids from both the inner- and outer-membrane leaflets to ensure conservation of surface area and avoid clashes between lipid and protein molecules.

The number of lipids that each protein displaced was carefully derived from conventional (smaller) protein-embedded lipid bilayer simulations and dictated how many lipids were removed from the spherical membrane. Lipids were hierarchically eliminated based on their degree of impingement into the intended protein volume and any remaining potential protein–lipid clashes were resolved via a brief grid-steered simulation of the membrane that forces any offending lipids from the protein space. This procedure ensured that the exact number of lipids matching the cross-sectional area of the protein (calculated independently for the inner and outer leaflets) were removed. Finally, the membrane and proteins were merged together and solvated, and the final system was used for MD simulations.

The simulations performed on Blue Waters for this project informed areas of refinement for the research team's assembly protocol, particularly for the removal of lipids during the incorporation of proteins and solvation procedures. The final simulations indicated the constructed protocell systems are stable and that the assembly protocols are adequate. The project presents the most carefully crafted and stable protocol at full atomic detail (Fig. 1).

WHY BLUE WATERS

For this project, the researchers performed MD simulations with NAMD of systems measuring one billion atoms in size, which can only be achieved on a petascale computing platform such as Blue Waters. The GPU accelerators on Blue Waters confer a significant boost to simulation speed (two to three times) versus the non-accelerated CPU-only nodes. NAMD has been extensively tested and optimized for Blue Waters, making use of the high-speed node interconnect and showing sustained petascale performance across hundreds, even thousands, of nodes. The team's benchmarks demonstrated an efficient scaling performance (greater than 80%) while using up to 2,048 Blue Waters GPU (XK7) nodes for a one-billion-atom system.
EXECUTIVE SUMMARY

In 2015, a rampant epidemic of Zika virus infection spread from Brazil to the rest of the Americas. The responsible pathogen, the Zika virus, continues to pose a major health concern. Infections have been linked to the development of Guillain–Barre syndrome in adults and microencephaly in infants. The dangers posed by the Zika virus and other flaviviruses such as the West Nile and Dengue viruses call for a better understanding of their structures and infection mechanisms.

Enhanced knowledge about such viruses can allow scientists to design effective drugs and vaccines to combat future outbreaks. The goal of this project is to provide an atomic-level description of the structure and dynamics of the Zika virus envelope—the outer shell of the virus particle made of protein and lipid—via modeling and molecular dynamics simulations. The team also explored how the stability of the viral envelope depends on the presence of a lipid bilayer and its composition.

RESEARCH CHALLENGE

Zika virus, a flavivirus, is a 40-nm-diameter particle consisting of an envelope and a nucleocapsid. The viral envelope of a mature Zika virus has three components: E proteins, M proteins, and a lipid bilayer (Fig. 1). Recent cryo-electron microscopy [1,2] studies have shown that 180 copies of each E and M protein are icosahedrally arranged in the viral envelope. Both E and M proteins are embedded (either fully or perpendicularly) into a lipid bilayer lining the inner shell of the Zika virus envelope.

The modeling of E and M proteins anchored into the lipid vesicle with proper lipid packing density is the most challenging part of this project. The number of lipid molecules needs to be as accurate as possible to assemble a reliable and structurally stable viral envelope with correct “breathing” dynamics. The goal is to develop a model for the Zika virus envelope with full atomistic detail in explicit aqueous medium (20 million atoms) and to thereby gain dynamic information on the particle.

METHODS & CODES

The research team developed and simulated three different systems: (1) a viral protein envelope in the absence of lipids, to serve as a control; (2) a viral protein envelope enclosing a lipid membrane composed of only neutral lipids, to study how lipids contribute to the stability of the shell; and (3) a viral protein envelope enclosing a lipid membrane with a native composition, to examine the effect of specific lipids.

The molecular dynamics (MD) simulations were performed with NAMD [3], a highly parallelized, GPU-accelerated, publicly available MD program with demonstrated scalability to hundreds of thousands of processors for both single- and multiple-replica MD simulations. All-atom MD simulations rely on the accurate integration of the equations of motion for all atoms of the system. The total potential energy of the system was described with the CHARMMGem force field [4,5]. Periodic boundary conditions were used to avoid surface effects at the simulated system’s boundary, allowing the efficient computation of nontruncated electrostatic interactions by the fast Fourier transform-based particle-mesh Ewald method [6].

RESULTS & IMPACT

To develop a structural model for the whole Zika virus envelope, the researchers first placed a single icosahedral asymmetric unit [2] containing three E and M proteins in a lipid bilayer with a native composition. They relied on lipidomic analysis of other flaviviruses [7,8] for the composition of the lipid bilayer. A short, 50-nanosecond simulation (Fig. 2a) showed some clear curvature generated in the lipid bilayer by the envelope proteins, which might be indicative of specific lipid–protein interactions leading to the budding process. The next step was to create a boundary defining the maximum spread of the single icosahedral asymmetric unit using a convex hull algorithm and to select a lipid patch that is covered by the proteins. This single protein–lipid patch is replicated 60 times to form the entire Zika virus envelope (Fig. 2b). Since the team’s current model is still imperfect in terms of lipid packing density, they focused on estimating the number of lipid molecules as correctly as possible by measuring the volume in the lipid layer excluded by the stem and transmembrane helices of the proteins. To overcome the lipid–protein overlap, the team is now designing a grid-force-based simulation protocol.

This project will have a great impact in the modeling of complete virus systems, which can then be used to study the viral infection mechanism.
MULTISCALE SIMULATIONS OF COMPLEX SELF-ASSEMBLING BIOMOLECULES: TARGETING HIV-1

Allocation: NSF PRAC/200 Keb
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EXECUTIVE SUMMARY

Biomolecular proteins are capable of performing extraordinary multiscale processes that are used to accomplish the useful macroscopic biological functions of the cell. From changing conformations (shape) to self-assembling into large microcompartments, these nanomachines are at the heart of the cellular machinery that underlies all living activity. The research team’s overarching research goal is to develop advances in theoretical and computational methodology that couple multiscale–scale phenomena to higher-scale descriptions. A key element of the team’s strategy is to systematically coarse-grain or reduce the representations of atomic-scale systems in a manner that is rigorously consistent within the framework of statistical mechanics. The team applies the computational tools it developed to understand biophysical phenomena that pose major public health risks. In the present research, the research team unraveled the mechanisms by which innate immune sensors assemble to block the human immunodeficiency virus type-1 (HIV-1) infection and how capsid inhibitor drugs might perturb capsid assembly processes.

RESEARCH CHALLENGE

HIV-1 is the causative agent of autoimmune deficiency syndrome (AIDS), which has affected millions of individuals worldwide and resulted in approximately one million AIDS-related deaths in 2017. Understanding the molecular-scale mechanisms and physical principles that govern viral processes such as the self-assembly of HIV-1 capsids is critical to the effective treatment of the disease. Retroviruses subvert normal cellular processes in order to replicate viral genetic information and assemble the viral capsid, “in preparation, 2019.” Innate immune sensors target the viral capsid, “in preparation, 2019.” Viral Capsid Restriction. Innate immune sensors target the viral capsid to restrict viral activity. These results show how the coupling between two interaction sites of TRIM5α can give rise to self-assembling behavior, in which a critical balance of interaction strengths must be maintained. These advances in multiscale simulation have opened up remarkable opportunities to study the dynamics of biomedically relevant problems that were largely intractable until now. Methodological advances in computational methods that increase the accuracy, predictive power, and range of phenomena under study contribute directly to public health by elucidating the fundamental chemistry underlying infectious diseases.

WHY BLUE WATERS

Multiscale simulations of viral processes are inherently computationally expensive, requiring the evaluation of interactions among many proteins and millions of particles. An immediate advantage of CG models is that their reduced representations are very computationally efficient, allowing leadership petascale resources such as Blue Waters to probe the dynamics of molecular systems that are many orders of magnitude in both length and time scales and would otherwise be inaccessible to conventional molecular simulations. The team’s highly scalable, custom molecular dynamics software was developed with the expertise of Blue Waters staff to perform CG simulations across thousands of computer processors and has been made available to the broader scientific community. The researchers’ atomic-scale and coarse-grained simulations were made possible thanks to the massively parallel computing infrastructure of Blue Waters. These exciting advances in fundamental simulation methodology and novel discoveries in self-assembly phenomena highlight an essential role for access to state-of-the-art leadership-class computing resources.

PUBLICATIONS & DATA SETS

IMPROVING THE AGREEMENT OF AMBER SIMULATION OF CRYSTALS OF NUCLEIC ACID BASES WITH EXPERIMENTAL DATA

Allocation: Innovation and Exploration/100 Ksh
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Co-PIs: Valery Poltev2, Thomas E. Cheatham III3, Jerry Bernholc4
Collaborator: Rodrigo Galindo–Nurillo5

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2Autonomous University of Puebla
3University of Utah
4North Carolina State University
5North Carolina State University

EXECUTIVE SUMMARY

Classical molecular dynamics is a ubiquitous tool in the bio-pharmaceutical, chemical, and material sciences. Thousands of research teams nationwide and across the globe depend on the AMBER force field to conduct computer simulations of important practical applications. The present work extends the AMBER parameter optimization protocol to reproduce structure and thermodynamic properties of 12 crystals of five nucleobases. The target training data include enthalpies of sublimation at various temperatures, crystal volume, position of the atoms in the crystal, and key intermolecular distances. Further extending that data set, the project employs an unprecedented database of 161 base–base interaction energies to fine-tune the parameters to improve the agreement with experimental data.

RESULTS & IMPACT

The optimized parameters improved the agreement with the reference data set. On that set, the derived parameters scored above the existing CHARMM and AMBER force fields for nucleic acid bases.

WHY BLUE WATERS

The ability to run hundreds of small jobs that span to a thousand of nodes in the aggregate node allocation in backfill with high job turnaround is unique to Blue Waters.

RESEARCH CHALLENGE

The utility of molecular dynamics simulations depends on the accuracy of their underlying parameters. Improving the predictive ability of molecular dynamics requires training the method against a large number of experimental data.

METHODS & CODES

The computational methodology involves running molecular dynamics simulations of crystals of nucleic acids with the CHARMM package and performing grid searches for the optimal value of parameters to improve the agreement with experimental data.

ALGORITHMS FOR CANCER PHYLOGENETICS

Allocation: Director Discourtiory/50 Ksh
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EXECUTIVE SUMMARY

Cancer is a genetic disease characterized by intratumor heterogeneity, or the presence of multiple cellular populations with different sets of mutations. Cellular heterogeneity gives cancer the ability to resist treatment, and quantifying the extent of heterogeneity is key to improving our understanding of tumor genesis (the production or formation of a tumor or tumors). In this project, the research team developed and employed novel phylogenetic techniques (the use of information on the historical relationships of lineages to test evolutionary hypotheses) to reconstruct the evolutionary histories of individual tumors from DNA and RNA sequencing data. Typically, these data are obtained from shotgun sequencing of tumor biopsies using bulk sequencing technology. Highlights of this project's research outcomes include a novel method to jointly infer a phylogeny and to estimate clone-specific expression profiles from matched RNA and DNA bulk sequencing samples.

RESULTS & IMPACT

Simulation experiments showed that this method is capable of prioritizing the true underlying phylogeny with high accuracy. The method can also accurately deconvolve the cis- and trans-effects of gene regulation at the clonal level. The research team analyzed matched single-sample DNA and RNA breast cancer data from TCGA and found that the method is able to differentiate between linear and branching phylogenies.

WHY BLUE WATERS

Blue Waters was essential to the research outcome of this project because it involved extensive benchmarking and validation using simulated data. The computational resources of Blue Waters allowed the research team to perform these experiments at scale, enabling the study of the performance of the algorithms and the underlying problem statements in many different experimental settings. This is something that would not have been possible on other platforms.

PUBLICATIONS & DATA SETS

AMPHOTERICIN-DRIVEN STEROL EXTRACTION: PROBING THE MECHANISM

Allocation: Illinois/200 Koh
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Co-PIs: Chad Rienstra1, Martin Burke1
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EXECUTIVE SUMMARY

The need for effective and nontoxic antifungal drugs is ever-present. By utilizing the petascale computing capabilities of Blue Waters, the research team aims to corroborate the experimental observation of the extraction of sterols from a membrane by an extramembranous amphotericin (AmB) sponge. The detail provided by all-atom molecular dynamics simulations will shed light on the nature of the AmB–sterol interactions and characterize the mechanism of extraction. Current simulations demonstrate AmB sponge–membrane surface interactions. Full characterization of the sterol extraction mechanism will open new directions for antifungal and antimicrobial drug design.

RESEARCH CHALLENGE

Life-threatening systemic fungal infections are on the rise, and their effect is particularly severe for immunocompromised patients [1]. AmB is a potent antifungal drug with a remarkably low incidence of resistance development [2]. Unfortunately, AmB is toxic not only to fungal cells but also to human cells through cholesterol extraction [3], which limits the drug’s use. Understanding the mechanism of sterol extraction is the first step in the modification of AmB such that it becomes less toxic to humans.

METHODS & CODES

Molecular dynamics (MD) is a versatile and powerful technique that allows for the study of large membrane systems at atomistic detail. The research team’s simulations employed NAMD [3], a publicly available and highly scalable MD program that has demonstrated scalability on Blue Waters [4,5].

In preparation for simulations on Blue Waters, molecular systems were constructed using the highly mobile membrane mimetic model (HMMM), which reduces lipid tail lengths and fills the resulting inner leaflet space with a hydrophobic solvent [6,7]. The benefit of using this type of system in the preparation stage is that it accelerates the dynamics of the lipid headgroups by eliminating the steric bulk and hindrance caused by long lipid tails while simultaneously maintaining the atomistic detail of the headgroups. Accelerating lipid dynamics decreases the amount of simulation time necessary for sampling while maintaining the atomistic detail of the headgroups, which allows for the capture and characterization of lipid membrane interactions [8–10]. After the preparation phase, full lipid tails were grown on the lipids using the HMMM Builder [10]. The full-tail systems were then submitted to replica exchange MD (REMD), which allows for the system to be simulated at different temperatures in parallel. REMD simulations are available in the NAMD software on Blue Waters.

RESULTS & IMPACT

The researchers assembled two systems incorporating the extramembranous AmB sponge: one with a phosphatidylcholine (POPC) and cholesterol membrane and a second with a POPC and ergosterol membrane. (POPC is a lipid that is prevalent in human cells.) The team’s MD simulations of the full-tail membrane systems revealed spontaneous movement of the sponge toward the membrane and the formation of an encounter complex. The stable orientations of the sponge and membrane demonstrate the existence of favorable AmB–membrane surface interactions. The researchers expect to observe AmB–sterol-specific interactions and eventually sterol extraction from the membrane into the sponge with longer simulation timescales conducted as part of the team’s ongoing study.

The mechanism by which AmB kills fungal and human cells has not been determined. Recent studies have shed some light on that mechanism by demonstrating that the extramembraneous sponge efficiently extracts ergosterol from yeast cells [11]. Using the petascale computing power of Blue Waters with MD to simulate the extraction of sterols by the AmB sponge will allow the team to more completely characterize the mechanism of sterol removal. Understanding this mechanism will enable new directions in the constant and time-demanding battle of pharmaceutical chemistry in the development of new antifungal drugs.

WHY BLUE WATERS

To complete the proper sampling for the large membrane and extramembranous AmB sponge systems, the petascale computing power of Blue Waters is essential. These systems contain hundreds of thousands of atoms and require long simulation timescales of hundreds of connected replicas, each using hundreds of compute cores to observe AmB sponge–membrane interactions and, ultimately, sterol extraction. The goal of this project highlights the need for Blue Waters and future petascale resources for researchers to advance the development not only of less toxic antifungal medications but also the entire process of drug design.
SOCIAL SCIENCE, ECONOMICS, & HUMANITIES

ECONOMICS

320 Climate Policy in a Dynamic Stochastic Economy

322 Characterizing Descriptivity in Writing through Text Analysis of Books from the HathiTrust Digital Library

324 High-Frequency Trading in Nanoseconds: Analysis, Modeling, and Policy Implications

HUMANITIES
CLIMATE POLICY IN A DYNAMIC STOCHASTIC ECONOMY

EXECUTIVE SUMMARY

There are significant uncertainties in both the climate and economic systems. Integrated Assessment Models (IAMs) of the climate and economy aim to analyze the impact and efficacies of policy responses to climate change. The research team developed and solved new computational IAMs, with more than 10-dimensional continuous state space, that incorporate a spatial temperature system, climate tipping points, economic risks, carbon capture and storage, and/or regional economic activities. The team then analyzed the optimal policy under uncertainty and risks and how such a policy impacts economic activities. They found that tipping points and sea level rise significantly increase the social cost of carbon (SCC), but efficient adaptation and carbon capture and storage can significantly decrease SCC, while ignoring spatial heat transfer leads to nonnegligible bias. Moreover, they have solved dynamic stochastic cooperative and noncooperative equilibria and find that noncooperation leads to much lower carbon taxes and then to a much higher temperature in the future.

RESEARCH CHALLENGE

A major characteristic of leading IAMs is that their geophysical sector determines the mean surface temperature, which in turn determines the damage function, and then damages are related to the mean surface temperature of the planet. However, climate science shows that under global warming, the temperature at the latitudes closer to the poles will increase faster than at latitudes nearer to the Equator. This effect is called polar amplification (PA). Moreover, most countries in the tropic area are poorer and more vulnerable to climate change than rich countries in the higher-latitude regions. Furthermore, PA will accelerate the loss of Arctic sea ice, leading to a potential meltdown of the Greenland and West Antarctica ice sheets, which then could cause serious irreversible sea level rise. All of these factors call for a more realistic and regionalized IAM.

Most existing IAMs are perfect foresight forward-looking models, assuming one knows all of the future information. However, there are significant uncertainties in the climate and economic systems. For example, PA will increase the likelihood of tipping points that may significantly change the Earth system and economic productivity. On the other hand, technological progress such as carbon capture and storage as well as more efficient adaptation may reduce potential climate damage significantly. International cooperation or noncooperation will lead to significantly different solutions. All of these uncertainties call for a richer and more dynamic stochastic IAM, which is computationally challenging.

METHODS & CODES

Cai, Brock, Xepapadeas, and Judd [1] developed a model of dynamic integration of regional economy and spatial climate under uncertainty (DIRESCU) that includes spatial heat and moisture transport from low latitudes to high latitudes, sea level rise, permafrost thaw, and tipping points. To model spatial heat and moisture transport, they disaggregated the globe into two regions: region 1 is the region north of latitude 30°N to 90°N (called the North), while region 2 is the region from latitude 90°S (the South Pole) to 30°N (called the Tropic South). The research team adapted the computational method in DSICE [2], developed by Cai and Judd in past years using Blue Waters, to solve DIRESCU in a cooperative world. They also studied the regional climate policy under noncooperation between the North and the Tropic South by developing an iterative method to find feedback Nash equilibrium in DIRESCU.

Cai and Judd [4] extended DSICE to study the impact of carbon capture and storage on climate policy in the face of economic risks and also with a climate target constraint. If the global average surface temperature increase is above 2° or 1.5°Celsius, then the Earth likely will incur significantly larger damages. The researchers adapted the computational method in DSICE again to solve this constrained model.

These computational methods are parallelized using the master–worker structure and needs frequent communication between the master and workers. The problems are large. For example, DIRESCU has 10 continuous state variables and one binary state variable as well as eight continuous decision variables and a horizon of over 500 years. It corresponds to solving a Hamilton–Jacobi–Bellman (HJB) partial differential equation with 10 or 11 state variables in a cooperative world, or a system of two HJB equations in a noncooperative world. Blue Waters allows the researchers to solve these large problems efficiently.

RESULTS & IMPACT

In the past year, the DSICE paper [2] was accepted by the Journal of Political Economy and has been cited more than 190 times according to Google Scholar. The paper demonstrates that economic output caused by carbon emissions—i.e., the social cost of carbon (SCC)—is substantially affected by both economic and climate risks. Moreover, SCC is itself a stochastic process with significant variation.

DIRESCU [1] and Cai and Judd [4] are two research projects continuing from last year’s Blue Waters project. This year, the team made significant revisions. In DIRESCU, they developed a computational method to solve the feedback Nash equilibrium, which is well known to be computationally challenging, particularly for high-dimensional dynamic stochastic games. The researchers studied many cases in DIRESCU [1] and Cai and Judd [4], where each case used thousands of node hours of Blue Waters.

WHY BLUE WATERS

The research team’s parallel computational package requires low-latency communications because it uses the master–worker structure and needs frequent communication between the master and workers. The problems are large. For example, DIRESCU has 10 continuous state variables and one binary state variable as well as eight continuous decision variables and a horizon of over 500 years. It corresponds to solving a Hamilton–Jacobi–Bellman (HJB) partial differential equation with 10 or 11 state variables in a cooperative world, or a system of two HJB equations in a noncooperative world. Blue Waters allows the researchers to solve these large problems efficiently.

PUBLICATIONS & DATA SETS

CHARACTERIZING DESCRIPTIVITY IN WRITING THROUGH TEXT ANALYSIS OF BOOKS FROM THE HATHITRUST DIGITAL LIBRARY

Allocation: Exploratory/10Kish
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Co-Pi: Syam Bhattacharyya1, José Eduardo González1
Collaborators: Bois Captains1, Craig Wills1, Peter Organisciak1
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EXECUTIVE SUMMARY

This project approaches quantifying the notion of descriptivity in text. The immediate objective was to explore descriptivity in forms of writing that have been characterized as exemplifying different writing styles and genres. Digital text analysis offers an opportunity to operationalize the anecdotal notion of descriptivity by developing quantified metrics for descriptivity. This work leveraged the resource represented by the HathiTrust Digital Library repository. The requested allocation was used to create an updated data set of preprocessed, extracted features from the HathiTrust corpus with exploratory methods to support the research. These extracted “features” were quantifiable facts about the pages of the books, most usefully counts of words (unigrams) or strings of words (bigrams).

RESEARCH CHALLENGE

There is a belief that writing has, since World War II, taken an overall turn away from “tell” toward “show”; this suggests that writers are becoming increasingly more interested in description. However, estimating descriptivity is difficult. This is useful not only for literary and historical studies (the research team’s immediate focus of interest) but also for researchers from beyond these areas. Characterizing books or pages in books by such a metric in the form of user-generated metadata is helpful for the use of a text corpus resource because users of the resource may want to find more descriptive or less descriptive books, depending on their needs, especially since treating text as data opens up new experiences of reading [2].

The notion of description has been the topic of a longstanding discussion in literary and historical studies. In his influential 1956 essay “Narrate or Describe?” György Lukács distinguished, in the case of fiction, between a dynamic concept of “narration” in which verbal description of material objects is intertwined with the progression of the protagonists’ character development through action, and mere “description,” in which description is static and isolated from the flow of action [3]. Such a distinction becomes easy to operationalize in terms of the research team’s metric. Theorists from literary studies and historiography, such as Hayden White, have, likewise, associated description without narrativity with lack of meaning [4]—a notion that could similarly be operationalized to engage with ongoing debates in the humanities [5,6] and in cultural analytics [7]. In particular, bigrams are useful in several ways. In certain circumstances (such as when queries can be explicitly identified as good candidates for bigram use), greater improvements in information retrieval tasks are obtained from using bigrams as queries rather than other queries [8]. The inclusion of bigrams provides consistent gains in sentiment analysis tasks [9].

METHODS & CODES

The research team developed code to compute a simple proxy metric for “descriptiveness” with part-of-speech-tagged unigrams (tagged with Penn Treebank part of speech categories). The script counts the total count of two “per-page co-occurring” parts of speech for any volume. When using HathiTrust Research Center unigrams, “per-page co-occurring” simply means min(x,y), where x is the number of occurrences on a page of the part-of-speech-tag X, and y is the number of occurrences on a page of the part-of-speech-tag Y. This estimation using unigrams, however, typically produces an overcount, as the count generated is not restricted only to contiguous tokens among the equal number of paired tokens but also includes tokens from within the page that are not contingously paired; this can be rectified by the use of bigrams.

RESULTS & IMPACT

The useful impact of this work is the presentation of the demonstration that as more computational power is becoming available, more complex and fine-grained analysis (such as that using bigrams) can be undertaken to approach the problem at progressively deeper levels. The research team has used this continuing work in teaching an undergraduate independent/directed study offered through the English Department of the University of Pennsylvania in 2018 and in a digital humanities seminar in Singapore in September 2019.

WHY BLUE WATERS

The short size of the data set and the embarrassingly parallel computational nature of generating the needed features made Blue Waters an ideal environment for conducting this exploratory analysis. Using advanced features such as bigrams allowed for a better estimation of co-occurrence. This has allowed the team to use adjectives and nouns as well as adverbs and verbs in the form of actual pairs in the per-page-co-occurring parts of speech used in computing the metric to measure descriptiveness. For extracting these advanced features, the team created 100 partitions of approximately equal size from the 5.4-million input volumes of text and ran 100 jobs, with each job using 100 nodes and each node processing the text from twenty books (volumes) simultaneously. The average number of volumes per partition was 54,200, and the total number of nodes used was 10,000 (100 x 100). The total number of cores used was 200,000 (100 x 2,000), and the average time taken to process one partition was one hour, 45 minutes. The output produced was 6.25 terabytes (TB), consisting of 55 gigabytes of entities, 2.11 TB of bigrams, and 4.08 TB of trigrams.

PRESENTATIONS & DATA SETS


Figure 1: “Data” usage of words (developer’s view). The content-eligible text made available after crunching in the form of actual pairs in the per-page co-occurring parts of speech used in computing the metric to measure descriptiveness.
EXECUTIVE SUMMARY
This interdisciplinary project involves economics and computer science and examines how to analyze and understand financial trading and its effects on the stock market. It fosters research on the financial ecosystem by hosting a series of collaborative workshops with financial economists and data scientists. The goal is to create new metrics and data for the discipline of finance in economics and inform public policy in the era of big data.

RESEARCH CHALLENGE
The advent of big data has reshaped not only the methodological challenges and opportunities facing financial economics but also the phenomena studied in the field. However, traditional academic research in finance emphasizes economic explanations to such an extent that, in the words of the prominent economist Susan Athey, "If you said that an economist was data mining, that was an insult." Consequently, big data techniques have as yet gained little traction in academic research.

Existing studies in financial economics focus mostly on the economic behavior of humans. Advances in computing technology and machine-learning techniques have introduced cyber players, which use computer algorithms to make trading decisions. Existing U.S. Security and Exchange Commission (SEC) regulations, however, are designed for human traders. This project lays the groundwork for public policy for cyber traders in the era of big data. The research aims to understand the origin and impact of these cyber players in financial markets. The focus is on high-frequency traders (HFTs), which are cyber players that operate at exceptional speed, measurable in nanoseconds.

METHODS & CODES
The NASDAQ exchange provided more than 15 TB of raw data consisting of 10 years of records consisting of all the orders submitted, executed, and canceled in the NASDAQ market during that time period. The team combined all of these messages and generated snapshots of the market at the resolution of nanoseconds using the computational power of Blue Waters. The financial data could easily be sliced to the granularity of stock-days, and the biggest stock-day (May 6, 2010, the so-called flash crash day) is only a matter of hundreds of MB.

To balance the CPU loading, the researchers distributed larger jobs to CPUs first and then filled in smaller jobs when larger jobs were completed. Aggregation of outputs was easy and could be done with a single node.

RESULTS & IMPACT
The research team discovered an important driver of high-frequency trading: discrete prices. The SEC’s Rule 612 imposes a minimum price variation for stock trading called a tick size. The prevailing one-cent tick size constrains price competition. The first-come, first-served rule at the same price then generates queuing, or early arrival to the market, to beat rivals.

Yao and Ye [1] found that HFTs are more active in securities with lower prices because a one-cent uniform tick size implies a larger relative tick size. Further, they showed that the current policy initiative to reduce HFTs by increasing the tick size would only encourage HFTs. Li, Wang, and Ye [2] incorporated a discrete tick size and allowed non-high-frequency traders (non-HFTs) to supply liquidity.

The findings show that the increase in tick size reduces stock market liquidity and that firms that face tick-size constraints reduce their share repurchase by 45%. Further, the Ye, Zheng, and Zhu [4] findings show that after the tick size pilot, treated firms’ investment-sensitivity increases, resulting from an increase in stock price information and managers incorporating the information from the stock price into investment decisions.

This project has stimulated collaborations among financial economists, computer scientists, and experts on high-performance computing (HPC). The PI has organized three conferences in collaboration with the National Bureau of Economic Research, the National Center for Supercomputing Applications (NCSA), and top finance journals to jump-start big data research in finance. NCSA Director William Gropp and several experts on supercomputing from XSEDE (https://www.xsede.org) gave lectures during the conferences. SEC Chief Economist S. P. Kothari spoke about policy challenges and research opportunities in the era of big data (https://bit.ly/3iUxKk). The co-editor of The Journal of Financial Economics, Toni Whited, gave a speech about HPC for structural estimation. The PI spoke about big data in finance. A website has been created for the collaborative workshops, including videos of the two keynotes (https://bit.ly/2MyldAg). The PI will organize five more collaborative conferences in the future.
A Massively Parallel Evolutionary Markov Chain Monte Carlo Algorithm for Sampling Spatial State Spaces
A MASSIVELY PARALLEL EVOLUTIONARY MARKOV CHAIN MONTE CARLO ALGORITHM FOR SAMPLING SPATIAL STATE SPACES

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1University of Illinois at Urbana–Champaign
3National Center for Supercomputing Applications
2Euler Circle

EXECUTIVE SUMMARY

The research team has developed an Evolutionary Markov chain Monte Carlo algorithm for sampling from large, idiosyncratic, and multimodal state spaces. This algorithm combines the advantages of evolutionary algorithms (EA) as optimization heuristics for state space traversal and the theoretical convergence properties of Markov chain Monte Carlo algorithms for sampling from unknown distributions. The team encompassed two of these algorithms within the framework of a multiple-try Metropolis Markov chain with a generalized Metropolis–Hastings ratio. Further, the group harnessed the computational power of massively parallel architecture by integrating a parallel EA framework that guides Markov chains running in parallel. Because the algorithm is a sampling algorithm, it is applicable to any field that samples, which is essentially all fields of science.

RESEARCH CHALLENGE

The challenge is to create a method that randomly samples from unstructured spatial data with stringent spatial constraints.

METHODS & CODES

The researchers’ approach is two-pronged. The first prong involves developing an optimization algorithm that explores the solution landscape in a spatially aware manner. The second prong involves integrating the optimization algorithm into the sampling framework of a Markov chain Monte Carlo (MCMC) technique. The algorithm is implemented in ANSYS C and can be compiled on Linux and OS X as a standard multithreaded process. It uses MPI non-blocking functions for asynchronous migration for load balancing and efficiency. In addition, the C SPRING 2.0 library provides a unique random number sequence for each MPI process, which is necessary for running a large number of parallel MCMC chains.

RESULTS & IMPACT

MCMC methods are used to sample from unknown distributions. While the theory ensures sampling from unknown distributions, this theoretical result is asymptotic (approaching a value or curve arbitrarily closely). For large applications, the time required before the theoretical convergence is realized may be prohibitively long. Hence, while MCMC methods are theoretically attractive, successful implementation for complex applications can be quite challenging.

A common MCMC strategy is to define a Markov transition function that amounts to a small or local random change in the current state. Small local changes are attractive for two reasons. First, they are conceptually and operationally simple. Second, the Metropolis–Hastings ratio needs to lead regularly to accepted transition proposals. Since a small change likely results in a large Metropolis–Hastings ratio, the movement of the Markov chain is then fairly fluid. At the same time, because these are small movements in a very large state space, the resulting Markov chain converges slowly and is, moreover, likely to become trapped in localized regions. Hence, for large or complex applications, it is not likely to converge rapidly enough to be practically useful.

To improve performance and hasten convergence, one strategy is to define larger steps for the Markov chain. If designed well, larger moves have the ability to more efficiently and effectively traverse a large state space, leading to faster convergence of the chain. At the same time, devising large and effective movements intelligently is not straightforward. "Large" movements often result in small Metropolis–Hastings ratios, which lead to rejected proposals, and thus to a nonfluid and ineffective Markov chain. To devise a chain that is able to traverse the state space in both an effective and efficient manner, the team integrated movements from optimization heuristics. A central task in marrying these two techniques is to fit the mechanics of the optimization search within the theoretical framework that enables sampling in an MCMC algorithm. One cannot use optimization operators directly, but one can adapt the operators to an MCMC framework to provide the proposal set for directional sampling according to the structure of the multiple-try Metropolis Markov chain model.

In short, the project has resulted in an evolutionary Markov chain Monte Carlo that uses evolutionary algorithm operators to guide a large number of parallel Markov chains. Statistical evidence generated by this algorithm was used in a lawsuit filed in federal court in Ohio that resulted in a three-judge panel finding that the current congressional map in that state was a partisan gerrymander [1].

WHY BLUE WATERS:

These methods scale to all of the processor cores on Blue Waters through nonblocking MPI communication calls. The computational approach the team implemented in their solution requires generating a very large number of solutions that can be used as a representative sample. Generating a large number of statistically independent draws is only feasible on a leadership-class supercomputer such as Blue Waters.

PUBLICATIONS & DATA SETS


Figure 1: Performance of the spatial path relinking crossover operator. This operator was designed in the context of an evolutionary algorithm framework. It has been adopted via a multiple-try framework for a Markov chain Monte Carlo crossover. It has been adapted via a multiple-in-the context of an evolutionary algorithm operator. This operator was designed for state space traversal and the theoretical convergence properties of Markov chain Monte Carlo algorithms for sampling from unknown distributions. The team encompassed two of these algorithms within the framework of a multiple-try Metropolis Markov chain with a generalized Metropolis–Hastings ratio. Further, the group harnessed the computational power of massively parallel architecture by integrating a parallel EA framework that guides Markov chains running in parallel. Because the algorithm is a sampling algorithm, it is applicable to any field that samples, which is essentially all fields of science.

Figure 2: The algorithm produced over three million electoral maps for the State of Ohio by partitioning voter tabulation units into 16 districts. These maps were produced for the partisan gerrymandering case, APRI v. Householder. A three-judge panel found the evidence compelling and ordered a redrawing of the Ohio congressional map [1].
322 The Contributions of Root Systems to Drought Response in the Amazon Rainforest
324 Star Formation in Dwarf Galaxies: Using Simulations to Identify Key Observables to Test Models
326 Improving Convectionally Induced Turbulence Forecast Parameters Through Bulk Numerical Simulations for Aviation Safety
328 Modeling Nonlinear Physical–Biological Interactions: Inertia and Sargassum in the North Atlantic
330 Predictions About the Invisible Gas in Galaxy Clusters
332 Computational Fluid Dynamics Investigation into Pulmonary Airflow Patterns in Monitor Lizards (Varanidae)
334 The Early Instability Scenario for Planet Formation in the Solar System
336 The Distribution of Shear Stress and Nutrients in a Tidally Energetic Estuary: The Role of Numerical Resolution and Vegetation
338 Exascale Astrophysics with Enzo–E: Development of Physics Modules for Galaxy-Scale and Cosmological Simulations
340 Magnetohydrodynamic Simulation: Galaxies
342 GPU-Accelerated Interstellar Chemistry with WIND: A General Ordinary Differential Equation Solver
344 Improved Trumpet Initial Lapse and Shift for Binary Black Hole Simulations
346 Using Spectroscopic Data and Molecular Simulations to Estimate Heterogeneous Ensembles: How to Study Complicated, Flexible Proteins When Experimental Data Are Limited
348 Electron Density-Based Machine Learning for Accelerating Quantum Calculations
350 Improving Trumpet Initial Lapse and Shift for Binary Black Hole Simulations
352 Extending the Longevity of Produced Water Disposal Wells: Evaluation Using Reactive Transport Simulation
354 The Impacts of Hydrometeor Centrifuging on Tornado Dynamics: Improving the Realism of Tornado Simulations
356 The Transport and Dynamics of Wave-Driven Reef Jets Under the Influence of Rotation and Bottom Friction
358 Simulation of Bluff Body Stabilized Flames with PelaC: Adaptively Resolving Turbulence–Combustion Interactions in Real-World Engineering Problems
THE CONTRIBUTIONS OF ROOT SYSTEMS TO DROUGHT RESPONSE IN THE AMAZON RAINFOREST

Elizabeth Agee, University of Michigan
2016–2017 Graduate Fellow

EXECUTIVE SUMMARY

Rising global temperatures and changing patterns of precipitation are highlighting the vulnerability of tropical forests to heat- and drought-induced stress. As a critical global ecosystem, tropical forests sequester carbon, mediate weather patterns, and have impacts far beyond their regions. This research explores the role of tree root systems in mediating the impact of strong drought events. Model simulations of tree water uptake show that different combinations of tree traits will confer different degrees of resilience to water limitation. Results from this work may be used to more effectively direct future measurement efforts and to improve predictions of tropical forest response.

RESEARCH CHALLENGE

Tropical forests cover less than 7% of the earth’s surface but play a significant role in global water, energy, and carbon cycles. Rapid changes in forest structure owing to anthropogenic activities and changing climate may have significant imprints that extend far beyond the tropical regions. Current model projections of forest response are beset by uncertainties associated with tree water uptake under water limitation. Improvements in the representation of tree response to water limitation will help refine projections and inform conservation and policy actions.

METHODS & CODES

The computational complexity of single-plant models has previously limited incorporation of root systems’ hydrological models at the forest plot or ecosystem scale. Over the past decade, developments in micro- and macroscale hybridization schemes have opened the door for highly scalable models of three-dimensional root water uptake and soil water physics.

In this work, root architectures that represent the structural and spatial distribution of roots were modeled using the open source RootBox model [1]. Each tree system was assigned hydraulic parameterization (e.g., root hydraulic conductivity, water potential thresholds) based on statistically generated water usage strategies. These strategies may range from risky, which favors carbon assimilation over hydraulic integrity, to conservative, which will limit carbon assimilation and therefore water uptake to protect hydraulic pathways from damage. Root water uptake has been coupled with the massively parallel flow and transport model, PFLOTRAN [2], using hybridization techniques from [3].

Using these tools, the PI explored how tree roots contributed to forest drought resilience in areas of the Amazon rainforest during the 2015–2016 El Niño drought event. To tease apart the contributions of various ecophysiological properties, ensemble modeling approaches were employed that test a multitude of risk configurations and root distributions. Each of these approaches uses spatial distributions from the field site in the Tapajós National Forest (K67) located in the eastern Amazon River Basin in Brazil and is validated with data collected from the same region.

RESULTS & IMPACT

High stem density and functional diversity present large challenges for representing individual water uptake processes. Different scenarios of root functional diversity, largely tested through rooting depth, displayed significant differences in the onset of water limitation. Partitioning of roots into different depth classes dependent on size helped to alleviate the impacts of water limitation by allowing individuals to tap into separate soil water reserves, reducing the overall hydraulic stress of the system as monitored by root collar potential.

WHY BLUE WATERS

Advances in computational platforms such as Blue Waters allow for increased model fidelity, presenting an opportunity to model forests at higher degrees of detail at the scale of individual trees. In data-scarce spaces, systems like Blue Waters provide the resources needed to run many simulations. The high number of simulations allows for understanding sources of uncertainty and targeting future measurement campaigns, saving resources and increasing the impact of difficult fieldwork.

Elizabeth Agee completed a Ph.D. in environmental engineering from the University of Michigan in 2019, having worked under the direction of Valeriy Ivanov. Agee currently is a postdoctoral associate at the Oak Ridge National Laboratory.
EXECUTIVE SUMMARY
Modern cosmological hydrodynamic simulations self-consistently model the evolution of segments of the universe under the influence of gravity and hydrodynamics. To model how gas turns into stars, these codes use analytic prescriptions taking place below the resolution of the simulation. Though implementation details differ, in large galaxies the results tend to converge.

These prescriptions, however, have not been tested in the low-mass limit. In new simulations at cutting-edge resolution capable of resolving the faintest known galaxies, the PI tested how different star formation recipes affected the resulting galaxy distributions. These tests included running different models on Blue Waters and then comparing galaxies across simulations. The research found that the robustness of the models depends on the galaxy environment, with results being model-dependent in isolated regions but converged in dense environments. These results, paired with observations, can help constrain the underlying small-scale physics of how gas forms into stars. Additionally, they highlight the need for simulators to further investigate these trends to ensure accuracy in interpreting their results in faint galaxies.

RESEARCH CHALLENGE
When running cosmological hydrodynamic simulations of galaxy formation, scientists simulate the evolution of galaxies within large volumes of space. Despite strategies to maximize the already enormous range of spatial and time scales relevant to galaxy formation, it is impossible to resolve the scales in which stars form. Including realistic star formation is crucial to modeling conditions gas turns into stars. These subresolution prescriptions, which are analytic prescriptions that determine under what conditions gas turns into stars, are model-dependent in isolated regions but converged in dense environments. These results, paired with observations, can help constrain the underlying small-scale physics of how gas forms into stars. Additionally, they highlight the need for simulators to further investigate these trends to ensure accuracy in interpreting their results in faint galaxies.

RESULTS & IMPACT
The results suggest that in the environment far from the Milky Way, the change in one model to another led to the existence of half as many galaxies because of the greater difficulty of gas collapsing into stars, as shown in [5]. In a region such as the Milky Way, however, there is little difference because the environment is different and better able to form stars regardless of the subresolution recipe.

With upcoming large surveys such as the Legacy Survey of Space and Time, researchers expect the discovery of up to hundreds of new galaxies very close to the Milky Way. It is unknown what the properties of these galaxies will be, and theoretical work will be necessary to understand the upcoming observations. This project is a first step in constraining the uncertainty in simulations. Furthermore, the differences among the star formation models present us with differences that are testable with future observations. Pairing the simulations with observations can therefore greatly increase the understanding of how the first star formation proceeded in the early universe.

WHY BLUE WATERS
Cosmological galaxy simulations involve enormous dynamic ranges in both space and time, and include many different computationally intensive processes relevant to galaxy formation. Additionally, modeling the faintest galaxies requires incredibly high resolution, greatly increasing the computational requirements for running these simulations. Therefore, the advanced computational capabilities of Blue Waters make it the best machine for accomplishing this work.

PUBLICATIONS & DATA SETS

Elaad Applebaum, a fourth-year Ph.D. student in physics at Rutgers University, is working under the supervision of Alyson Brooks. He expects to receive his degree in 2021.
EXECUTIVE SUMMARY

The number of global flight routes is projected to increase over the next five years, increasing the likelihood of airplanes being influenced by hazards associated with thunderstorms. While turbulence diagnostics are available to pilots and flight dispatchers, many of these predictions have been verified for midlatitude clear-air turbulence only. Current thunderstorm avoidance guidelines do not account for the stage of convection that influences turbulence probability.

For the first time, aviation encounters of convectively induced turbulence in both the midlatitudes and tropics were simulated at high spatial and temporal resolution to identify biases in current turbulence diagnostics and to investigate the influence of storm stage on turbulence probability. This research has found significant disagreement among the turbulence diagnostics for all cases. The probability of turbulence near developing convection was found to be greater than near mature convection, especially in tropical environments, supporting the need for storm stage and region-specific avoidance guidelines.

RESEARCH CHALLENGE

Out-of-cloud convectively induced turbulence (CIT) is a hazard to aviation operations because it can occur vast distances away from convective sources [1] and is nearly impossible to detect using on-board radar systems. CIT is a prediction challenge owing to the spatial (10 to 1000 meters) [2] and temporal scales (seconds to minutes) on which it occurs. Meteorological variables from forecasting systems can be used to calculate large-scale turbulence diagnostics, but generally these modeling systems are too course to resolve the numerous CIT generation mechanisms and turbulence propagation. While progress has been made in understanding CIT potential in the midlatitudes through field campaigns, modeling studies, and statistical examinations of pilot reports—all of which have been used to develop avoidance guidelines for aviation [3]—little is known about CIT potential in the tropics. The lack of research on tropical CIT increases the risk of turbulence encounters for tropical flight routes. As new flight routes and air traffic continue to increase, aviation will be more susceptible to convective hazards in both the midlatitudes and tropics.

High-resolution simulations of convection in the midlatitudes and tropics allow for analysis of turbulence potential for various convective regimes by capturing the majority of turbulence generation mechanisms. These simulations also help identify the limitations of popular turbulence diagnostics and motivate the development of new diagnostics. Understanding the variations of turbulence potential with convective type, stage, and region allows for the adaptation of thunderstorm guidelines that are more specific and efficient for aviation operations, reducing aviation turbulence incidents.

METHODS & CODES

The Weather Research and Forecasting (WRF) model [4] was used to simulate six cases of CIT on Blue Waters at 500-meter horizontal resolution and 10-minute output. Each case was a real aviation encounter that caused passenger injuries structural damage and was associated with convection. Midlatitude turbulence cases were paired with tropical turbulence cases where the convective morphology and cause of turbulence were similar. For example, on June 28, 2018, a commercial aircraft was flying out of cloud in North Dakota in the vicinity of severe convection and encountered severe turbulence. This case was paired with a tropical case that occurred on June 20, 2017, where a commercial aircraft experienced severe turbulence while navigating out of cloud near convection [5]. Turbulence diagnostics including the Richardson number [6], eddy dissipation rate [7], and second-order structure functions [8] were computed in cloud and out of cloud (0.1 g kg-1 threshold) [9]. Convective stage (i.e., developing and mature) was differentiated by tracking convective objects and their vertical velocities with time [10]. Environmental static stability and vertical wind shear were examined near developing and mature convection related to turbulence potential.

RESULTS & IMPACT

Six simulations of convection in the midlatitudes and tropics using high spatial and temporal resolution were performed using WRF. Simulated convective properties including morphology, strength, and location compared well against observations. The accuracy of the turbulence diagnostics for intensity and location varied drastically but had the most agreement for the midlatitude cases (Fig. 1). The eddy dissipation rate frequently underpredicted the areal coverage and intensity of out-of-cloud turbulence. Richardson number and structure functions most reproduced accurate turbulence probabilities with similar areal coverages and locations.

The examination of convective stage for the six cases illustrated the variation of turbulence probability for convective type and region (Fig. 2). The greatest probability of turbulence near mature convection occurred in the midlatitudes. Turbulence probability was found to significantly increase near developing convection in both the midlatitudes and tropics, with the greatest increases occurring in the tropics. This result highlights the increased risk for tropical aviation routes where real-time observations are limited.

The environmental static stability and vertical wind shear near developing and mature convection was found to have regional dependencies but not always storm-type dependencies. Static stability near tropical convection was not influenced by convective stage, but near-midlatitude convection was influenced by convective stage. Vertical wind shear was found to be influenced by region, storm type, and storm stage. Vertical wind shear increased significantly around developing convection for both regions and could be an indicator of turbulence potential. For all six cases there was a positive correlation between vertical wind shear and turbulence intensity.

This work motivates the need for more high-resolution simulations of convection to address the shortcomings of turbulence prediction and avoidance for aviation operations. More examination of turbulence diagnostics and turbulence potential in various environments is vitally needed to reduce turbulence encounters.

WHY BLUE WATERS

Blue Waters was necessary for this project because high-resolution (spatial and temporal) simulations of convection require computational resources not available on local systems. Blue Waters allowed for thorough analysis of CIT for large domains and over long temporal periods to capture storm evolution, which required thousands of computing cores. Storage of high-resolution simulations of convection is an additional challenge that was adequately addressed through Blue Waters’ resources.

A fourth-year Ph.D. student in atmospheric sciences at the University of North Dakota, Katelyn Barber is working under the direction of Gretchen Mullendore. Wiebke Deierling of the National Center for Atmospheric Research served as a collaborator on this study.
EXECUTIVE SUMMARY

The floating seaweed of the genus Sargassum serves as a critical habitat in the open Atlantic but causes economic harm to coastal communities when it washes ashore in large aggregations. This study links Sargassum dispersal and growth to underlying ocean circulation features. A model framework and satellite observations were used to determine how Sargassum responds to inertial forces, and the implications for its basinwide distribution. The resources of Blue Waters facilitated model development and allowed implementation at high resolution over the entire Sargassum habitat, covering over 4 x 107 km2. This enabled the calculation of Sargassum’s inertial parameters. Accounting for inertia leads to an increase in export from the Sargasso Sea, providing a return pathway to the tropics. It also leads to increased retention in the Gulf of Mexico and Caribbean Sea, where the retention can cause management challenges. Including inertial effects in models of Sargassum could improve forecasting of coastal inundation events.

RESEARCH CHALLENGE

Floating Sargassum supports a diverse ecosystem in an otherwise nutrient-poor region of the ocean, supporting invertebrates, fish, and even sea turtles [1]. However, changes in Sargassum abundance and distribution over the past decade have resulted in millions of dollars in economic harm when it washes ashore [2]. Accurate predictions of these beaching events require an understanding of both the ocean currents that transport Sargassum and how much it grows along the way. Understanding the effects of inertia is particularly important because that can alter trajectories and potentially change the rate of entrainment in eddies, where growth conditions can differ from the surrounding water. Cyclonic eddies tend to propagate westward and northward in the North Atlantic, which could potentially drive more Sargassum to vulnerable coastal areas, while anticyclonic eddies would tend to carry Sargassum south toward the equator. The strength of inertial effects determines which of these two scenarios is more likely. Modeling inertial effects on Sargassum is difficult because it requires estimates of density and radius, yet Sargassum rafts are highly nonpherical. While density can be determined directly from field samples, estimating radius requires a novel approach.

METHODS & CODES

This research uses a system of four coupled models to simulate Sargassum growth and transport. A Hybrid Coordinate Ocean Model (HYCOM) [3] domain was implemented at 1/12th (< 10 m) resolution with 28 hybrid vertical layers, encompassing the known Sargassum distribution from 15°S to 64°N and 100°W to 15°E. Coupled to this is a biogeochemical model adapted from the work of Fennel [4], which includes nitrogen and phosphorus, phytoplankton, zooplankton, and detritus to effectively capture the dynamics of biologically mediated nutrient cycling in the upper ocean. Sargassum rafts are modeled using an individual-based physiology model embedded within a Lagrangian particle model. The particle model is modified from the HYCOM Lagrangian particle package to allow for Sargassum buoyancy, inertial effects, reproduction (particle splitting), and sampling of the underlying nutrient availability to allow for growth. The effective radius of a modeled Sargassum raft was determined via an inverse method. Lines of visible Sargassum from satellite remote sensing [5] were compared with the finite-size Lyapunov exponent field to determine the deflection angle. A total of 91 Sargassum lines were measured from four dates in 2018 when there was high abundance. These angles were compared with angles calculated from model simulations with varying particle radius. An Anderson–Darling k-sample test was used to compare model and observed probability density functions and determine the Sargassum effective radius. This parameter was then applied to the Sargassum particles in the coupled model system to examine the effects of inertia on growth and distribution.

RESULTS & IMPACT

This multiscale modeling project provides the first estimates of Sargassum parameters for implementing inertial effects. Although the size of Sargassum rafts can vary from centimeters up to aggregations spanning kilometers, they respond to inertial forces differently than a sphere with a radius of 0.95 m and a density of 92% of ambient sea water (Fig. 1). Accounting for these inertial properties changes how Sargassum moves and grows. Inertial Sargassum is entrained in eddies much more frequently, with 61% entrainment compared to 12% entrainment of noninertial rafts. Sargassum is 48% more likely to be retained in the Western Gulf of Mexico and 36% more likely to be retained in the Caribbean Sea than noninertial particles. Finally, there is a seasonal increase in export of up to 20% off the Sargasso Sea, which helps explain how the seasonal pattern of Sargassum distribution can restart every year. These inertial effects and changes in trajectories also have implications for Sargassum growth. Although simulations did not show significant differences in growth for Sargassum inside versus outside of eddies, there were differences in overall growth between inertial and noninertial Sargassum particles. The annual mean biomass is 8% higher when inertia is accounted for, growth rates more frequently approach their theoretical maximum, and survival time is increased. This is owing to higher transport into and retention within regions with optimal growing conditions. Accounting for these physical and biological consequences of inertia can help improve predictions of Sargassum beaching events and allow coastal communities to better mitigate their harmful effects.

WHY BLUE WATERS

The resources of Blue Waters have made the scale and scope of this project possible. High-resolution ocean circulation modeling alone has a high computational cost. By utilizing Blue Waters, this was accomplished along with coupling it with ocean biogeochemistry, Lagrangian particles, and individual organism physiology at temporal and spatial scales that span orders of magnitude. The NCSA staff has also been key to the success of this project. Their responsiveness and expertise was critical to implementing and running this code on Blue Waters.

PUBLICATIONS & DATA SETS


Maureen T. Brooks received a Ph.D. in marine-estuarine-environmental sciences in 2019, working under the direction of Victoria Coles at the University of Maryland Center for Environmental Science Horn Point Laboratory.

Figure 1: Deflection angle derived from the inertial equations (shading). Density ratio is indicated by the effective radius and density ratio of Sargassum determined in this study.
PREDICTIONS ABOUT THE INVISIBLE GAS IN GALAXY CLUSTERS
Iryna Butsky, University of Washington
2016–2017 Graduate Fellow

EXECUTIVE SUMMARY
Quasar absorption-line studies in the ultraviolet (UV) can uniquely probe the nature of the multiphase cool–warm gas in and around galaxy clusters, promising to provide unprecedented insights into the interactions between infalling galaxies and the hot X-ray-emitting intracluster medium (ICM). This work resulted in a high-resolution simulation of a galaxy cluster used to study the physical properties and observable signatures of the cool ICM gas. The PI extracted synthetic spectra to demonstrate the feasibility of detecting and characterizing the thermal, kinematic, and chemical composition of this cool gas and demonstrated the feasibility of observations with the existing Cosmic Origins Spectrograph aboard the Hubble Space Telescope.

RESEARCH CHALLENGE
Galaxy clusters are the largest structures in the universe, composed of thousands of galaxies that are gravitationally bound to a massive central galaxy. Compared to isolated galaxies, cluster galaxies are more likely to have stopped forming stars—becoming “quenched.” The cluster environment plays a critical role in governing the gas cycle that fuels star formation in galaxies.

There are several ways in which the cluster environment can deprive galaxies of gas, causing them to quench. For example, galaxies in a crowded cluster environment can lose gas during galaxy mergers or owing to tidal forces from close encounters. Additionally, the space between galaxies in a galaxy cluster is composed of a hot, dense gas known as the intracluster medium (ICM). Galaxies simply moving through the cluster experience a headwind force from the ICM that can be strong enough to remove all of the gas’s all the gas. The gas that has been stripped from galaxies enriches the ICM with heavy elements and contributes to its unique density, temperature, and chemical structure. Therefore, studying the structure of the ICM in detail places stringent constraints on the mechanisms responsible for quenching galaxies.

Traditionally, galaxy clusters have been observed directly through X-ray emission. Although this method is ideal for studying the hot (T > 106K) and dense inner ICM, it cannot detect the diffuse, cool (T = 104-6K) gas that makes up a large fraction of the ICM at the cluster outskirts. Although the diffuse, cool ICM gas is virtually invisible to X-rays, it can be observed indirectly through UV absorption. This research uses an extremely high-resolution simulation of a galaxy cluster, RomulusC (Fig. 1; [1]) to perform a detailed characterization of the properties of the cool ICM gas and to make predictions for its observational signature using existing and future UV telescopes.

METHODS & CODES
The RomulusC cluster simulation was run on Blue Waters using the modern astrophysical hydrodynamics simulation code, ChaNGa [2]. ChaNGa is parallelized through the Charm++ parallel infrastructure framework [3] and scales up to 500,000 cores on Blue Waters. Postprocessing of the simulation was done using the Python analysis tool, yt [4]. The PI generated realistic, instrument-specific synthetic absorption spectra from the simulation using TriDent [5]. The synthetic spectra were then analyzed in an analysis pipeline developed for observers, using the Veeper software [6]. The unique combination of state-of-the-art simulations with observational analysis techniques is the key strength of this work.

RESULTS & IMPACT
Using the extremely high-resolution RomulusC simulation, the PI found that the cool ICM phase comprised a significant fraction of the total gas mass at the cluster outskirts. This cool gas (observable through UV absorption) traces a highly complementary structure to that traced by the hot ICM gas that is traditionally studied through X-ray emission. Furthermore, the results found that although the hot phase of the ICM has a uniform distribution of heavy elements, the cool phase of the ICM has a more clustered distribution of “metals” that traces gas stripping from cluster galaxies.

The use of synthetic spectroscopy allowed for detailed predictions for the observational signature of this cool ICM gas in clusters using the currently available Cosmic Origins Spectrograph on board the Hubble Space Telescope (Fig. 2). The results showed that random sightlines throughout a galaxy cluster should have a 40% chance of detecting cool gas (traced by hydrogen I absorption) and a 15% chance of detecting warm gas (traced by oxygen VI absorption). Future UV space telescopes such as LUVOIR will increase both the probability of detecting absorption features and the number of possible sightlines probing each galaxy cluster to revolutionize our understanding of galaxy evolution.

WHY BLUE WATERS
While galaxy clusters span several million parsecs in size, their structure is dictated by star formation and feedback processes that happens on subparsec scales. Capturing this large span of physical scales requires detailed subgrid models and significant computational resources. Therefore, these simulations require the use of massively parallel, high-performance supercomputers such as Blue Waters.

PUBLICATIONS & DATA SETS

A fourth-year Ph.D. candidate in astronomy at the University of Washington, Iryna Butsky works under the direction of Tom Quinn and Jessica Werk, and plans to graduate in June 2021.
This research used computational fluid dynamics modeling to simulate how air flows through the lungs of monitor lizards in order to investigate why there are different types of lung airflow patterns among various types of animals (e.g., birds, mammals, reptiles). The PI found that monitor lizard lungs have a unique net-unidirectional airflow pattern where, although air moves in multiple directions through each part of the lung during breathing, each part transports more air in a certain direction over the whole breath cycle. This fascinating airflow pattern has features in common with both bird lungs (fully unidirectional) and mammal lungs (fully tidal).

RESEARCH CHALLENGE

An important open question in comparative physiology concerns a functional explanation for the variety of lung designs in vertebrates: Why are the lungs so diverse? Unidirectionally pulmonary airflow, a condition where certain lung gases travel in a consistent direction during both inspiration and expiration, was long thought to be found only in birds and to have been a requirement for the high metabolic demands of powered flight [3]. Recent work, however, discovered unidirectional flow patterns in alligators, monitor lizards, and iguanas, which are animals very small, delicate, and complex, so determining how air flows through the lungs can be point-validated to reconstruct the diversity of pulmonary flow patterns in vertebrates. This project seeks to investigate these patterns in monitor lizards, an extremely diverse group of lizards [8] that nonetheless have a conserved body plan and unidirectional pulmonary airflow [6].

METHODS & CODES

CFD simulations were run in OpenFOAM, an open source continuum mechanics library using a custom moving-boundary code based on the SIMPLE algorithm (transientSimpleDyMFoam). Model geometry was segmented from computed tomography scans of a live, anesthetized lizard. Simulation data were visualized in ParaView. Simulations were validated by means of visualization of aerosolized lipids through a microendoscope placed in the distal portion of the IPB and toward the front of the lung. Figure 1: Different types of airflow patterns in animal lungs. Mammals (top left) have a total airway pattern where air moves to and fro through a ramifying network of bronchi. Birds (top right) have looping bronchi and air moves in the same direction during both inspiration and expiration. Invertebrates (bottom) have a ramifying network of bronchi. Monitor lizards (bottom) have a net-unidirectional air pattern where air moves to and fro through the whole ventilatory cycle in each part of the lung. (Top images from [1]; bottom image from [2]).
The THE SOLAR SYSTEM

The solar system's outer planets (Jupiter, Saturn, Uranus, and Neptune) formed rapidly, while gas was still present in the infant solar system [1]. While the outer planets' evolutionary history is rather well understood by theorists [2,3], the leading models seem to be incompatible with the solar system's terrestrial system (Mercury, Venus, Earth, and Mars) [4]. The research team has used large suites of N-body simulations of the solar system's earliest epochs of formation and growth to develop a new, robust model for the solar system that explains both its inner and outer regimes. Additionally, the team conducted the largest-evolutionary history simulations using a realistic code that accounts for the effects of fragmentation as bodies collide [5]. The team also used GPU acceleration [6] to accurately model dynamics down to realistic mass resolutions during the solar system's earliest epochs, and in the young asteroid belt. Finally, the team performed a detailed investigation into the origin of the solar system's most peculiar planet, Mercury.

RESEARCH CHALLENGE

Accurately modeling the late stages of planet accretion is subject to numerical limitations and simplifications. In particular, to keep the calculation tractable, most authors [7,8] employ integration schemes that neglect collisional fragmentation. The initial planet-forming disk, which in reality contained millions of solid objects with a range of masses, must be approximated with just over a thousand bodies (the majority of which are assumed not to interact gravitationally with one another). Nevertheless, such studies have proved successful at replicating the general orbits of the inner planets.

However, explaining Mars' small mass (just 10% that of Earth) and rapid formation (about 10 times faster than Earth, as inferred from isotopic dating [9]) requires substantial modification to the standard theory of planet formation [8,10]. Furthermore, the asteroid belt's low total mass (only a few percent that of the Moon) and unique dynamical structure are still largely unexplained [7,8,10]. Earth and Mars are both in the Sun's "potentially habitable" zone, yet Mars is small, barren, and unable to support a robust atmosphere. Understanding the dynamical mechanisms that prevented Mars from growing into an Earth-like planet will give us insight into how special our own world really is.

METHODS & CODES

For the fragmentation simulations, the team used a modified version of the Mercuhy hybrid integrator, written in fortran [11,13]. The simulations of terrestrial accretion begin with the simplest initial conditions, consistent with observations of pro-to-planets disks [1,7,8]. To systematically test the effects of a giant planet instability, the team performed several batches of integrations and triggered the instability during different epochs of terrestrial growth. To investigate the effect on the asteroid belt, the researchers used a GPU code written in CUDA C (GENGA, [6]) to reperform successful integrations with a larger number of objects in the belt region. Because gas–disk interactions are complex, the exact mass and planetesimal size distributions that emerge from the primordial gas (and go on to form the inner planets) are not well known. Therefore, "simple" initial conditions might not be representative of physical reality. The team investigated this problem using GPU acceleration as well. Further, they employed a forcing function to mimic the effects of gas drag, and utilized a multi-annulus approach to track the accretion of millions of small objects in the infant terrestrial disk.

RESULTS & IMPACT

This work offers a simple and elegant explanation for Mars' small size and rapid growth (Fig. 1). The instability simulations consistently outperform the control run when measured against a variety of success criteria. In successful simulations, Mars undergoes no further accretion events after the instability, while Earth and Venus continue to grow (thus matching their relative geological formation times [9]). Additionally, the team found that accounting for collisional fragmentation results in fully grown systems of terrestrial planets that are better matches to the actual solar system in terms of their orbital excitation (eccentricities and inclinations; Fig. 2) and planet spacing (particularly that of Earth and Venus). Furthermore, the instability proves successful at depleting a primordially massive asteroid belt (consistent with disk models [8]) at the 99.9% level. Thus, an early dynamical instabilty among the giant planets can simultaneously explain the structure of both the inner and outer solar system.

WHY BLUE WATERS

Blue Waters boosts state-of-the-art resources that were unavailable to the success of this project. The research relied on GPU accelerators on XK nodes almost exclusively. Having the ability to efficiently run large suites of GPU-accelerated jobs led the PI to seek out a Blue Waters allocation.

PUBLICATIONS & DATA SETS

THE DISTRIBUTION OF SHEAR STRESS AND NUTRIENTS IN A TIDALLY ENERGETIC ESTUARY: THE ROLE OF NUMERICAL RESOLUTION AND VEGETATION

Salme Cook, University of New Hampshire
2017–2018 Graduate Fellow

EXECUTIVE SUMMARY

Oceans tides represent a major forcing mechanism in many coastal environments, responsible for the transport of salt, temperature, sediment, nutrients, and pollutants. Increases in population density and associated anthropogenic impacts have altered the productivity of estuarine environments, resulting in increased nutrient loading and amplified suspended sediment that reduces water quality. To accurately predict sediment transport, a good understanding of the bed shear stress that drives the sediment erosion, suspension, and deposition is essential. In this work, a high-resolution three-dimensional coupled hydrodynamic–wave–sediment transport numerical model (COAWST) was implemented and verified in a tidally dominated estuary located in the Gulf of Maine. The model was used in conjunction with available observational data sets to predict the shear stress distribution from the tidal channels across the mudflat.

RESEARCH CHALLENGE

The coastal ocean includes diverse ecosystems encompassing both terrestrial and marine habitats that support approximately one-third of the world’s population [1]. We are only beginning to understand the economic and environmental value of these resources and how to protect them in the face of climate change, sea level rise, extreme storm events, and increased human impact and pollution associated with population growth. These highly nonlinear systems are difficult to observe; however, the advent of numerical models and increased computational resources has made predicting the dynamics of these systems more accessible. Coastal managers and decision-makers rely on data to understand how to protect them for future generations. Coastal currents and waves and their interactions with vegetation are complex and until recently, researchers have relied on sparse observations and theory alone. With the increase in numerical modeling formulations and computing power, the predictive capability of managers to help create more resilient coastal communities has increased. Better management of human impact and better understanding of the complex biogeochemical interactions and physical properties of these systems can help us sustainably interact and rely on them.

An open question this research addressed is the resolution required to capture the shallow water dynamics and how to couple these higher-resolution models to coarser regional and global models. In this work, the PI employed a validated high-resolution numerical model of a New Hampshire estuary (Fig. 1) to estimate the nutrient loading from sediments in the estuary to the coastal ocean.

METHODS & CODES

This research was unique in that it relied on both collecting observational data in the estuary and the use of numerical model data sets. The observations were used to validate the model for currents and estimated shear stress in several locations. This provided fidelity in the overall distribution of shear stress in currents temporally and spatially within the estuary. The numerical model used was the COAWST modeling system. The 10-meter and 30-meter grid models were forced on the ocean side with four stages of the tide. The model runs (not shown) included the effects of vegetation and resolution and found that incorporating vegetation was an important improvement to the model, whereas the higher-resolution 10-meter model vs. the coarser-resolution 30-meter model had little effect on estimates. This provides a significant savings in computational resources when considering this issue. Future work looking at the distribution of waves or sediment types might require the higher-resolution model.

The distributions of shear stress were then used to estimate internal nutrient loading from sediments for a typical tidal cycle, spring, and neap cycle, and averaged over a month. When compared with rivers, model results suggest that internal sources of nutrient loads from sediment are on the same order as rivers for at least half of the year. These results indicate that when eelgrass populations are healthy and abundant, they lower the availability of sediment for resuspension and subsequent release of nutrients. This study demonstrates that a coupled hydrodynamic–vegetation model is capable of estimating the distribution of shear stress for a tidally dominant estuary.

RESULTS & IMPACT

The results of this study present an estimate of spatial distribution of shear stress in a tidally dominant estuary using a verified numerical model and compared with stress estimates from observed currents at several locations. The spatial distribution of depth averaged velocities and shear stress are presented in Fig. 2 for four stages of the tide. The model runs (not shown) included the effects of vegetation and resolution and found that incorporating vegetation was an important improvement to the model, whereas the higher-resolution 10-meter model vs. the coarser-resolution 30-meter model had little effect on estimates. This provides a significant savings in computational resources when considering this issue. Future work looking at the distribution of waves or sediment types might require the higher-resolution model.

Although nutrient loading from sediments is considered an internal load to the system, estuarine managers do not incorporate it into current nutrient loading estimates. This is not a process that can be mitigated; therefore, greater attention must be placed on those processes that can be controlled in terms of previous surface cover, fertilizer use in residential and agricultural lands, industrial outputs of nitrogen and phosphorus, and wastewater treatment plants.

WHY BLUE WATERS

The Blue Waters system and associated project staff were incredibly reliable and provided a powerful tool that was integral for this research, whereas the other machines the PI has used were incapable. The professionalism and efficient nature of the project staff were and are simply unparalleled, and have created a new standard in high-performance computing scientific support.

PUBLICATIONS & DATA SETS


Salme Cook received a Ph.D. in oceanography from the University of New Hampshire in May 2019, having worked under the direction of Tom Lippmann.
EXASCALE ASTROPHYSICS WITH ENZO–E: DEVELOPMENT OF PHYSICS MODULES FOR GALAXY-SCALE AND COSMOLOGICAL SIMULATIONS

Andrew Emerick, Columbia University

2018–2019 Graduate Fellow

EXECUTIVE SUMMARY

The Enzo–E/Cello project involves a new astrophysical hydrodynamics code written to take advantage of the next generation of exascale computing systems currently under construction. This research has been under development for several years, during which time the code has demonstrated impressive scaling capabilities on test problems utilizing the entire Blue Waters system. In addition, the PI worked to implement key physics modules into Enzo–E/Cello that are required for its use on production-level science runs studying the evolution of individual galaxies and large, cosmological volumes of the universe. This code development is necessary to enable cutting-edge astrophysics research on upcoming next-generation systems.

RESEARCH CHALLENGE

Advancements in our understanding of the universe over the past several decades have largely been due to an investment in ever-improving high-performance computational resources and the development of computational codes to model astrophysical phenomena on those machines. However, much of the current generation of astrophysical hydrodynamics codes—used to study everything from planet formation, star formation, stellar evolution, galaxies, and cosmology—were first written in the 1990s, when scaling to hundreds or thousands of concurrent tasks was the newest technology. Many of these codes are not well suited to take full advantage of the next generation of exascale computing systems that will allow for millions (or more) of concurrent tasks. In particular, Enzo, a grid-based adaptive mesh refinement (AMR) code and one of the most widely used astrophysical hydrodynamics codes, has multiple design shortcomings that prevent it from making efficient use of next-generation computing systems. While continued optimization has improved Enzo’s performance over the years, a complete refactoring is required. For this reason, the Enzo–E/Cello project began with the aim of completely redesigning the AMR hierarchy control system (Cello) to scale well to large systems while layering on modern physics modules and algorithms (Enzo–E). Like its predecessor, Enzo, this is an open-source code project that will be available to the astrophysical community for use in a broad range of contexts to tackle new challenging open questions in astronomy. In this project, the PI worked to develop and port the physics modules necessary to conduct the first set of science/production simulations with Enzo–E/Cello, including models for star formation, chemistry, radiative cooling and heating, stellar feedback, analytic gravitational potentials, and isolated galaxy initial conditions.

METHODS & CODES

This project utilized both the well-established AMR, cosmological, hydrodynamics code Enzo and the newly developed code project Enzo–E/Cello. Both codes are written predominantly in C++, with some underlying routines written in Fortran. While Enzo uses MPI for communication across processors/nodes, Enzo–E/Cello uses Charm++, a parallel programming library developed at the University of Illinois at Urbana–Champaign. The change means that Enzo–E/Cello utilizes task-based parallelism rather than domain decomposition or data parallelism.

RESULTS & IMPACT

The Enzo–E/Cello project has made significant strides over the past few years in developing a powerful, scalable AMR hydrodynamics code by demonstrating nearly ideal scaling using the entire Blue Waters computing system on a handful of simple test problems. In this project, the PI successfully implemented physics modules for star formation, stellar feedback, chemistry, radiative cooling and heating, analytic gravitational potentials, and isolated galaxy initial conditions. In addition, he helped improve the code with additional documentation, bug fixes, and error testing. This work has enabled researchers to begin planning in detail the types of simulations possible with this new code and to conduct a variety of scaling and performance tests. This petascale machine and its support of large simulation runs with large node counts has enabled the PI to explore the limits of Enzo–E/Cello to better target future development and optimization.

WHY BLUE WATERS

Blue Waters has provided the computing environment and technical support needed to develop the new code and to conduct a variety of scaling and performance tests. This petascale machine and its support of large simulation runs with large node counts has enabled the PI to explore the limits of Enzo–E/Cello to better target future development and optimization.

As a sixth-year Ph.D. student in astronomy at Columbia University, Andrew Emerick successfully defended his dissertation in May 2019, having worked under the direction of Greg Bryan and Mordecai–Mark Mac Low.

of the universe, and the formation of the first- and second-generation of stars in the early universe. Finally, the code is entirely open source and well documented, allowing for its use by the broader astrophysical community.
MAGNETOHYDRODYNAMIC SIMULATION: GALAXIES

Forest Glines, Michigan State University
2019–2020 Graduate Fellow

EXECUTIVE SUMMARY

Magnitized plasmas contribute to many phenomena in the universe, from stars and black hole jets to galaxy clusters. However, computational models of these plasmas require efficient use of vast computational resources. Implementing these models is further complicated by the growing number of architectures of upcoming machines. Most of these machines use different accelerators from different manufacturers, each with a different programming environment that normally requires a rewrite of the simulation code. In order to prepare for future supercomputers, the PI developed K-Athena, a conversion of the magnetohydrodynamics code Athena++ using kokkos, a performance portability library, which allows one codebase that runs efficiently on many computer architectures. In this work, the researcher used K-Athena on the GPUs on Blue Waters to study the transference between kinetic and magnetic energies in the magnetic turbulence by modeling the Taylor–Green vortex. The next step will be to develop physics-rich galaxy cluster simulations with magnetic fields, cosmic ray physics, and active galactic nuclei feedback.

RESEARCH CHALLENGE

Plasmas dominated by magnetic fields are ubiquitous in the universe. Scientists know from observations of synchrotron radiation that galaxy clusters, the largest gravitationally bound structures in the universe, host large-scale magnetic fields. Although the precise coupling of these fields and larger clusters is not yet understood, researchers know they influence cluster evolution. Magnetic fields generated within the active galactic nuclei (AGN), the supermassive black holes at the center of galaxy clusters, drive jets that carry energy out into the cluster, playing a key role in the transport of small-scale kinetic energy into magnetic energy [3]. Cosmic rays, charged particles with relativistic velocities, stream along the magnetic fields and drive winds, carrying metals from stars and providing pressure support in the cluster [2]. Magnetic fields also couple to turbulence within the cluster gas through the small-scale dynamo effect, where small turbulent eddies wind up and grow magnetic fields, transporting small-scale kinetic energy into magnetic energy [3].

Although these effects have been observed, it is unclear how important they are in the evolution of galaxy clusters. Researchers can explore this, however, through simulation. Galaxy cluster simulations modeling the dark matter, gas dynamics, magnetic fields, and aforementioned effects would advance our understanding of galaxy clusters. However, such accurate models require the computational resources of next-generation supercomputers. Most upcoming supercomputers, though, are moving to new hardware such as the GPUs on Blue Waters and other accelerators instead of the traditional CPUs. These accelerators use unique application programming interfaces (APIs), requiring codes to be rewritten for each API. To circumvent writing multiple codes, new tools such as RAJA, Kokkos, and additions to OpenMP allow for writing performance-portable code that executes efficiently across many hardware platforms. Taking advantage of these tools, the PI investigated creating a magnetohydrodynamics code that will be able to run on these upcoming accelerators. This led to the development of K-Athena, a conversion of the astrophysical magnetohydrodynamics code Athena++ [4] using Kokkos [5], a performance portability library, which attains high performance on CPUs and GPUs using thousands of nodes. For this fellowship, the PI is using K-Athena on Blue Waters to study magnetic turbulence in the magnetized Taylor–Green vortex as the first application of K-Athena. The magnetized Taylor–Green vortex is a periodic initial field that decays into a turbulent flow. By modeling the vortex at high resolution, its energy spectrum can be measured to create simplified magnetic turbulence models. These models can be inserted into other simulations to account for turbulence below the simulation resolution. The next effort will be to add additional physics to K-Athena such as cosmic rays and AGN to do state-of-the-art galaxy cluster simulations on Blue Waters.

METHODS & CODES

Magnitized plasmas are expensive to evolve, requiring high resolution to accurately model many phenomena. Efficient usage of hardware is required to achieve these resolutions. To meet this challenge, the PI converted the existing Athena++ code using the Kokkos library [4] to enable high-performance runs on both CPUs and accelerators. Kokkos allows a single kernel to be compiled with OpenMP for CPUs, CUDA for NVIDIA GPUs, and other APIs for future machines.

The coding began using the plasma code Athena++ owing to its well-written structure and extremely efficient performance on CPUs [5]. The simple kernel design and robust data structures in Athena++ took minimal effort to incorporate Kokkos. The resulting K-Athena code runs near peak performance on state-of-the-art CPU and GPU machines using thousands of nodes.

RESULTS & IMPACT

This research using Blue Waters is just beginning. Results have already shown K-Athena performs on a variety of supercomputers, but simulating the Taylor–Green vortex on Blue Waters will be its first scientific application. By simulating magnetized turbulent flows with high resolution, this research will capture enough of the energy spectra to be able to extrapolate the effects of turbulent flows far below the simulated resolution in magnetized plasma simulations. Accounting for the turbulent cascade and small-scale dynamo effect will be crucial for modeling accurate galaxies and galaxy clusters with magnetic fields. These turbulence models will be used in next-generation astrophysical and cosmological simulations, consequently helping constrain the properties of dark matter and dark energy.

WHY BLUE WATERS

These magnetic turbulence simulations and idealized galaxy cluster simulations using the GPU-accelerated K-Athena code are well served by Blue Waters (BW). The resolution and scale of the simulations require large computational resources that are only available on a few supercomputers, including BW. The large number of GPU nodes on the BW system allows the simulations to use less energy and fewer resources. Additionally, the BW staff were very helpful in providing suggestions for compiling code to run at the best performance.

As a fourth-year Ph.D. student in astrophysics, Forest Glines works under the direction of Brian O’Shea at Michigan State University. He expects to receive his degree in April 2021.
GPU-ACCELERATED INTERSTELLAR CHEMISTRY WITH WIND: A GENERAL ORDINARY DIFFERENTIAL EQUATION SOLVER

Alexander Gurvich, Northwestern University
2018–2019 Graduate Fellow

EXECUTIVE SUMMARY

Radiative cooling owing to interstellar chemistry is an important component of modern cosmological simulations, but the fully time-dependent calculation is often too computationally expensive to include for large-volume and high-resolution simulations. To address this limitation, the PI created WIND, a general GPU-accelerated ODE (ordinary differential equation) solver that supports systems that are coupled and stiff. After a naïve first implementation, we have seen a speedup by a factor of three for our problem. In addition, we have identified a number of bottlenecks whose mitigation can improve the code substantially, with the goal of making WIND a public code that is applicable to a wide variety of problems.

RESEARCH CHALLENGE

Many simulations of radiative cooling approximate the processes of interstellar chemistry by assuming that the gas in the simulation is in chemical equilibrium; however, comparisons with time-dependent interstellar chemistry in the FIRE simulations show that there is a significant difference. Including time-dependent chemistry results in more accurate cooling processes during the course of the simulation also enhances the predictive power and applicability of the simulation to interpreting real-life observations. Nevertheless, it is computationally expensive—taking up to 98% of the computational cost of the simulation when enabled, which has restricted the volume and resolution of the simulations we have been able to run.

METHODS & CODES

We developed WIND, a brand-new GPU-accelerated code, to address the challenge of simulating radiative cooling so that we can apply our time-dependent chemistry model in a new regime of simulation. WIND is a general ODE solver and can be applied to any system of ODEs, either coupled or independent. WIND also includes two numerical methods for integrating ODEs, one of which is an "implicit method" that allows WIND to efficiently solve stiff systems of ODEs (ones that involve many very different timescales). We have implemented these algorithms for both GPUs in CUDA and for CPUs in C, allowing users to take advantage of GPUs when they are available but switch to the CPU version if they are not.

RESULTS & IMPACT

We have preliminarily found that our new ODE solver is three times faster on GPUs than when run on CPUs, with increasing speed as the system of equations is made larger. Additionally, there are at least three concrete targets for improving this result where naïve first-attempt implementations were used. Future work will be focused on these hotspots to improve the speed of WIND so that it can be made public and applicable to a wide variety of problems.

WHY BLUE WATERS

Blue Waters gave me access to GPUs when I had none; the XK nodes on Blue Waters were absolutely critical to the development and testing of WIND.

Alexander Gurvich is a third-year Ph.D. candidate in astronomy and astrophysics at Northwestern University. There, he works under the direction of Claude–André Faucher–Giguère. He hopes to graduate in 2023.
EXECUTIVE SUMMARY
Flexible proteins play critical roles in cellular transport but are extremely challenging to model at high resolution. Experimental techniques such as double electron–electron resonance (DEER) report on conformational heterogeneity but are sparse over atom coordinates. The PI developed a methodology, Bias-Resampling Ensemble Refinement (BRER), to incorporate multimodal DEER data into molecular dynamics (MD) simulations to obtain high-resolution, experimentally validated models of flexible proteins. The results from ensemble simulations of unbound syntaxin-1a, a protein involved in the formation of SNARE complexes, which drive neuronal vesicle fusion, show that the PI’s method better reproduces experimental data than current state-of-the-art methods. Specifically, the methodology promotes sampling of significant backbone conformational change, unlike any other existing methods. In addition, BRER simulations of the soluble domain of syntaxin-1a revealed a previously unresolved open conformation of syntaxin-1a.

RESEARCH CHALLENGE
It is difficult to study flexible proteins that play critical roles in infectious disease and cellular transport because so many states contribute to their conformational ensembles. High-resolution models of these systems are important for innovation in drug development and for answering fundamental questions in biophysics. It is challenging to develop atomic-resolution models using experiments alone because experimental techniques that report on heterogeneity often do so for only a few atomic degrees of freedom. Therefore, new hybrid methods are needed that include experimental and computational approaches to understand these systems.

METHODS & CODES
The PI developed a new method for incorporating distributional data into MD simulations (Hays, Cafiso, and Kasson, 2019; see Publications & Data Sets below). This was done using the software package gmuxpi, a Python interface for the GROMACS MD engine. The Python package for BRER simulations is freely available at https://github.com/jmhays/run_brer and the gmxapi code is at https://github.com/kassonlab/gmxapi.

RESULTS & IMPACT
The PI developed both a method and an open source software package to integrate sparse experimental data using MD simulation to better understand flexible proteins. This will enable scientists, specifically spectroscopists, to study systems that would be too heterogeneous and complicated for standard refinement methods.

WHY BLUE WATERS
The researcher has run multiple sets of ensemble simulations on Blue Waters to test the novel method and accompanying software package. A petascale, multi-GPU resource like Blue Waters was absolutely essential for completing both testing and production of all-atom ensemble simulations, which demanded over 200K node-hours over the course of the Graduate Fellowship. The Blue Waters staff were also critical both in terms of the software development and in professional development. The PI learned to compile and run complicated software packages on CRAY systems. Further, she learned a great deal about general high-performance computing through the online and NCSA Symposium workshops, including how to utilize singularity containers, which have become an essential part of the researcher’s laboratory workflow development.

PUBLICATIONS & DATA SETS

Jennifer M. Hays obtained her Ph.D. in biomedical engineering from the University of Virginia in November 2019 and worked under the direction of Peter M. Kasson.

Figure 1: Ensemble MD simulations refined using BRER better reproduce these experimental distributions (52/210, 105/216, 196/228) than two other prevailing refinement methods: EBMetaD and restrained-ensemble MD.
EXECUTIVE SUMMARY
This project aims to develop a machine learning (ML) algorithm that can be used to generate catalytic reaction mechanisms and kinetic models at reduced computational cost. The ML-based model will be trained to electron density to accelerate the three most computationally intensive components of the reaction energy profile: transition states, global minima, and entropy. The work will fill for the first time combine structural and density data to enhance ML convergence. The representation of the molecular systems will be invariant to rotations, translations, and reordering of atoms. Because it will use distances, partial charges, and bond orders, it should be generalizable to any size system. All generated surface data will be made available to the public upon publication of the work. On Blue Waters, the PI has computed electron density for local minima of carbon monoxide platinum nanoparticles; these data will also serve as the input for the data generation necessary for entropy predictions.

RESEARCH CHALLENGE
A vast array of materials properties can be computed using quantum chemical calculations that cannot be identified with even the best experiments available today. Machine learning (ML) algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster. For bulk materials properties, training algorithms can emulate these calculations at speeds that are orders of magnitude faster.

METHODS & CODES
The electronic density distribution completely specifies the energy of a chemical system’s state and can be calculated using density functional theory (DFT) based on the Kohn–Sham equations [3]. With ML, descriptors of input data are mapped to density Functional Theory (DFT) based on the Kohn–Sham energy of a chemical system’s state and can be calculated using DFT. Without an infinitely large training set, however, relying only on atomic positions does not allow extrapolation. Combining geometric and electronic density information will help alleviate this issue and is an innovation of this project.

The method for accelerating quantum-based calculations used in this work includes electronic density as input for ML and should significantly accelerate transition state, energy minima, and entropic calculations. This representation will also enable the extrapolation of the algorithms to systems that include atom types not found in the original training set. This method will combine structural and three-dimensional electron density data to accelerate calculations of molecular reactions on catalyst surfaces. Partial charges, atomic dipoles, and possibly effective bond orders can represent the electron density; as partial charges represent the density at local minima specific to atoms, atomic dipoles represent the asymmetry of the charge, and bond orders represent the density in the space between atoms. This representation of electron density is easily combined with geometric information and can be made invariant to translations, rotations, and reindexing of atoms.

The PI uses the Vienna Ab initio Simulation Package (VASP) [8] for generating electron densities of the ground state and CHARGEMOL [9] for integrating those densities. In addition, he uses his own code for calculating frequencies and spectral intensities used in the physics- and data-based surrogate models.

RESULTS & IMPACT
This project has generated thousands of DFT calculations already and the PI has implemented parallel versions of VASP and CHARGEMOL on Blue Waters, which are generating data. These calculations serve as the basis of the modeling. Previous work, which the PI has submitted for publication, provides evidence that the calculated electronic densities are accurate and can be used in surrogate modeling. That work used the electron density and physics-based surrogate models to generate complex infrared spectra that were then used to learn the mapping from spectra to local structure via multinomial regression. The PI plans to implement this electron density-based machine learning algorithm to speed up the calculations of spectra for this model and to aid automatic structure generation. Further plans are to learn the forces and electron asymmetry directly to compute vibrational frequencies and spectral intensities. This approach should also drastically reduce the number of calculations needed to relax a structure to its local optimum. A training set of local optima will be used to identify global optima and identify transition states. Upon completion of this work, a database of all DFT calculations will be freely available to research groups studying surface science and catalysis.

WHY BLUE WATERS
Blue Waters provides the necessary computational power to generate massive data. In the first week of the fellowship, the PI had already used several thousand node hours. The highly parallel architecture is necessary to train neural networks on large amounts of data with many features.

Joshua Lansford is in the fourth year of a Ph.D. program in chemical engineering at the University of Delaware and expects to graduate in 2020. His advisor is Dionisios G. Vlachos.
EXECUTIVE SUMMARY
For every barrel of oil an average of seven barrels of water is produced [1]; disposal of this produced water adds significantly to the cost of domestic oil and gas development and is one of the largest problems facing the industry today. Reactive transport simulations investigate treating produced water before deep well disposal in the Permian Basin, Texas, U.S.A. This study found that a reduction of HCO₃⁻ and Ca²⁺ concentrations led to increases in well lifetime of more than 13 years. Increasing the lifetime of a produced water disposal well near a producing well lowers the cost of transporting each barrel of produced water. These cost savings have the potential to create an increase in the number of economically viable oil and gas plays in the United States.

RESEARCH CHALLENGE
Produced water management is one of the biggest challenges associated with oil and gas development [2]. It is estimated that onshore wells in the United States generate 14 to 21 billion barrels of produced water every year [1,3]. Of that total, 92% is managed using injection [1]. Disposal of produced water can be expensive, with the use of disposal wells costing between $0.05 and $2.65 per barrel [4]. With each barrel of extracted oil creating multiple barrels of produced water, disposal costs can add significantly to the cost of oil.

The interaction between produced water and the water in the disposal formation can create mineral precipitation, which impacts the continued disposal of water in that formation and eventually leads to the sealing and abandonment of the well. Reduction of mineral precipitation through produced water treatment can increase the lifetime of disposal wells, thereby saving transportation costs.

METHODS & CODES
PFLOTRAN, a massively parallel, multistage, multicomponent reactive transport code [5] is used to create simulations of a control produced water injection in the Permian Basin, TX, U.S.A. This control water simulation was generated from the Permian Basin Brine Database [6] as a synthetic water that is representative of an amalgamation of brines present in the basin. Dolomite, anhydrite, and calcite minerals precipitate in the Permian Basin from four ions: Ca²⁺, Mg²⁺, HCO₃⁻, SO₄²⁻. In this study, we created simulations that reduced each of these ions in the control water by 25%, 50% and 75%, for a total of 12 simulations. In each simulation, produced water is injected at 20,000 gallons/day from a center point into a 100 m x 100 m x 100 m observation area. The grid is variable, with higher-discretization 1-m cells concentrated around the injection zone. The injected produced water mixes with the formation water already present in the matrix, a median of the Permian Basin Brine Database. Each simulation runs until porosity reaches zero, which we consider the end of the well lifetime.

RESULTS & IMPACT
The results show that reducing calcium, magnesium, or bicarbonate increases injection time: our measure of increased well lifetime. The control simulation mineral volume results show calcite and dolomite as the dominant minerals controlling precipitation volume, while only a small amount of anhydrite precipitation was observed. A calcium concentration reduction of 75% increases the well lifetime by over 5,000 days owing to a decrease in anhydrite, calcite, and dolomite. Reducing bicarbonate concentration by 75% increases the well lifetime by over 4,500 years by decreasing the volume of calcite and dolomite precipitated. Reducing magnesium concentration by 75% leads to an increase in well lifetime of over 300 days owing to the reduction of dolomite precipitation. Reducing sulfate concentration by 75% actually decreases injection time by 50 days. Reducing the concentration of sulfate only affects anhydrite, the mineral with the lowest volume. When anhydrite is not formed, there is more Ca²⁺ available in the water. This calcium forms calcite, leading to the precipitation of more calcite more quickly than the control simulation, and thus shows a decrease in well lifetime.

These results indicate that in the Permian Basin, oil and gas companies should pursue the treatment of calcium or bicarbonate in produced water to extend the lifetime of produced water disposal wells. This pursuit of treatment should come in the form of funding research of calcium and bicarbonate treatment for Permian Basin produced waters. By increasing the lifetime of a disposal well near the producing well, companies save money on transporting produced water. These cost savings can lead to cheaper oil and gas and create more economically viable hydrocarbon plays in the United States, assisting in the development of domestic assets.

WHY BLUE WATERS:
Blue Waters is essential for this research owing to the timescales of the simulations and the amount of output data. These simulations represent thousands of days of time; without the power of parallelization of Blue Waters, running each simulation could take months. Over the course of each simulation more than 6,000 output files can be printed, totaling over 600 GB of data. Blue Waters allows us to process such large data volumes.

PUBLICATIONS & DATA SETS

Kara Marsac graduated in May 2019 with a Ph.D. in hydrology from the Colorado School of Mines, having worked under the direction of Alexis Navarre–Sitchler.
EXECUTIVE SUMMARY
This research project focuses on reducing error in simulations of merging pairs of black holes in order to better study the gravitational wave emission at merger. It currently takes months of supercomputer time to perform difficult simulations (for example, where the black holes are spinning quickly or are very differently sized), and increasing the accuracy of these simulations translates to an increase in required computational resources. We would like to change the initial values given to the gauge equations to be closer to their settled shape, allowing the gauge to settle more quickly and reducing error in the simulations.

RESEARCH CHALLENGE
The challenge of this research is to gain accuracy in the most challenging binary black hole simulations without increasing computational cost. The low mass-ratio and high-spin areas of parameter space are very sparsely covered; we hope this project will fill out that parameter space so that researchers have waveforms to compare to potential detections from the Laser Interferometer Gravitational-Wave Observatory.

METHODS & CODES
To perform numerical relativity simulations, we use the Einstein Toolkit and specifically modify the Rochester Institute of Technology TwoPunctures initial data thorn. We are constructing new initial data values for the gauge based on their expected settled shape.

RESULTS & IMPACT
We are seeing a reduction in error using these new initial data, and therefore are gaining accuracy without actually having to use more computational resources.

WHY BLUE WATERS
These simulations require the use of large-scale computing resources due to computational intensity. The staff itself is knowledgeable about both the system and about the software I use.

Nicole Rosato is in the second year of a doctoral program in mathematical modeling at the Rochester Institute of Technology. She is working under the direction of Carlos Lousto and hopes to graduate in 2021.

Figure 1: A visualization of gravitational radiation emitted 7 milliseconds after the merger of binary black hole system GW150914, detected by the Laser Interferometer Gravitational-Wave Observatory on September 14, 2015.
ESCAPING FROM AN ULTRACOLD INFERNO: THE ULTRACOLD KRb DIMER REACTION

Micheline Soley, Harvard University
2019–2020 Graduate Fellow

EXECUTIVE SUMMARY

Ultracold chemistry, the study of reactions at temperatures below one millikelvin, offers an unprecedented opportunity for control over the outcomes of chemical reactions [1], and the ultracold molecules formed in these reactions have applications ranging from quantum computers [2] to investigations of fundamental constants of nature [3]. In this project, computational simulations of product formation in the ultracold potassium–rubidium (KRb) dimer reaction ($\text{K}_2\text{Rb}_2$) were performed. Although ultracold reactions would typically be studied with quantum mechanics, computational simulation of time-dependent quantum mechanics is currently beyond reach for ultracold systems. Therefore, a combination of semiclassical and quantum mechanics have been employed on Blue Waters to bring simulation of ultracold chemical reactions within reach.

RESEARCH CHALLENGE

Several properties of the ultracold KRb dimer reaction make it computationally intractable with state-of-the-art quantum techniques. Cold systems entail simulation of long length scales, which require larger memory allocations and more computational operations. Furthermore, although the incoming and outgoing molecules in the ultracold KRb dimer reaction are cold, the reaction passes through a hot intermediate phase (Fig. 1) that entails simulation of short length scales. Simulation of both long and short length scales demands multiscale and multiphysics techniques. These issues are compounded by the chaotic behavior of the molecules shown in Fig. 2, which is expensive to simulate. These concerns must be addressed in order to gain an understanding of ultracold reactions, which is vital to theorists and experimentalists in ultracold chemistry as well as physicists and chemists developing ultracold technologies.

METHODS & CODES

To bring simulation of the ultracold KRb dimer reaction within reach, we make use of the fact that the reaction behaves like an ultracold inferno [4]. Although quantum mechanics is required to study the cold products, semiclassical mechanics can be used to study the extremely hot intermediate complex. Therefore, we combined quantum and semiclassical techniques to make investigation of the reaction possible. Blue Waters is then used to accelerate this research. To study the hot intermediate complex, Monte Carlo integration was performed with up to quintillions ($1,000,000,000,000,000,000$) of sampling points on Blue Waters. Parallelized random matrix and R-matrix theory code was then used on Blue Waters to predict the final distribution and rate of formation of the cold products.

RESULTS & IMPACT

Preliminary results help confirm that parallelized semiclassical mechanics can be used to calculate the number of configurations efficiently in place of costly quantum mechanics. Analysis of the results of the ultracold KRb dimer reaction will directly inform ongoing experiments on the reaction, which will provide a deeper understanding of how chemical reactions occur at ultracold temperatures. This study is at the frontier of the field as it seeks to make simulation of reactions possible that are computationally intractable with existing time-dependent quantum mechanical techniques. These techniques can be applied more generally to other chemical systems to help push the limits of reactions that can be studied in the field of computational chemistry. In collaboration with the results of the experimental Kang-Kuen Ni group, these computational results will help expedite development of key technologies such as quantum computers.

WHY BLUE WATERS

The Monte Carlo integration and statistical R-matrix theory codes are computationally intensive. The Blue Waters supercomputer can significantly reduce the amount of time it takes to run these calculations and provide an opportunity to perform many tests simultaneously. This speed and flexibility make calculation of statistical R-matrix theory codes practical. In addition, the Blue Waters support staff will help show that it is possible to simulate ultracold chemical reactions efficiently with a combination of semiclassical and quantum mechanics.

Micheline Soley, a fifth-year doctoral candidate in chemical physics at Harvard University, works under the direction of Eric J. Heller and expects to graduate in May 2020.

Figure 1: The ultracold KRb dimer reaction can be thought of as an ultracold inferno. In the reaction, a hot four-atom complex ($4,000\,\text{K}$) breaks apart into two cold molecules ($14\,\text{K}$). Magnification (10x) is shown to scale.

Figure 2: Computational simulation of the chaotic path of the molecules (multicolor line).
THE IMPACTS OF HYDROMETEORIC CENTRIFUGING ON TORNADO DYNAMICS: IMPROVING THE REALISM OF TORNADO SIMULATIONS

Ronald Stenz, University of North Dakota
2016–2017 Graduate Fellow

EXECUTIVE SUMMARY

Continued population growth in regions prone to tornadoes makes enhancing the understanding of these violent weather phenomena increasingly important. This research project attempts to improve the understanding of tornadoes by making simulations used to study these destructive and dangerous weather events more physically realistic. For the first time, the impacts that centrifuging of precipitation has on the vorticity budgets of these numerically simulated tornadoes will be quantified. Preliminary findings so far have been consistent with radar observations of tornadoes by removing an unrealistic buildup of precipitation in the vortex center (widely seen in current tornado simulations) of simulated vortices and tornadoes. Ongoing work uses numerous tornado simulations to evaluate the significance of the inclusion of precipitation centrifuging in tornado dynamics, as well as more generally studying how a tornado acquires its vorticity, or spin, in different environmental conditions.

RESEARCH CHALLENGE

The primary research challenge being addressed is the lack of precipitation centrifuging in numerical simulations of tornadoes. In current simulations, precipitation follows the air flow, creating an unrealistic buildup of precipitation in the vortex center, which in turn creates a source of negative buoyancy that potentially limits the stretching of vorticity. In nature, as precipitation moves around a circulation such as a tornado, there is no force strong enough to keep the precipitation from moving outward, or being centrifuged, away from the circulation center. Observed tornadoes have a minimum of precipitation in the vortex center, while simulated tornadoes often have a relative maximum of precipitation in the vortex center. Addressing this challenge in improving the model’s realism requires the efficient calculation of millions of trajectories during a simulation and a solution that is numerically stable with other components of the model physics. Creating a centrifuging code that can work consistently with many different microphysical parameterizations is one of the challenging goals of this project.

With millions and sometimes billions of dollars of damage caused by tornadoes every year, along with the risk of fatalities or serious injuries from each tornado, a better understanding of these destructive weather events is needed to improve forecasting, preparedness, and mitigation of their impacts. By including the centrifuging of precipitation into the model used to learn about tornadoes, simulations become more consistent with what is observed in nature. Research findings have shaped and will continue to shape forecasting methods and plans for preparedness and damage mitigation. Therefore, continued improvement in the understanding of tornadoes will provide results that can be used in operational settings, ultimately aiding those living in regions prone to tornadoes.

METHODS & CODES

The widely used Cloud Model 1, which was designed for studying small-scale atmospheric phenomena such as thunderstorms [1] and has also been designed to run efficiently on supercomputers such as Blue Waters, was used for this research. To quantify the impacts of centrifuging on tornado dynamics, simulations were first performed without centrifuging. Just prior to the formation of a tornado, a checkpoint was employed, allowing the model to be run both with and without centrifuging from that point to determine the impact of the centrifuging of precipitation on tornado dynamics. To determine the magnitude of the centrifuging occurring, a centrifuging algorithm based on [2] used trajectories released within the simulation to calculate the curvature of the flow and ultimately how quickly precipitation will be centrifuged outward from the tornadic circulation. To quantify these impacts over a large sample size, atmospheric profiles of temperature, moisture, and wind from atmospheric soundings that were in close proximity to observed supercells [3] were used as the environmental conditions for our simulations of storms and their resulting tornadoes. A subset of these environments known to produce simulated tornadoes in previous research has been used for this study.

RESULTS & IMPACT

Idealized simulations and full-scale storm simulations (with a resulting tornado) have been completed with and without centrifuging. In simulations without centrifuging, an unrealistic maximum of precipitation developed within the vortex core. However, after adding centrifuging, the precipitation in the vortex center was removed and a physically realistic precipitation minimum formed in the vortex center for both the idealized and full-scale tornado simulations. Similar to radar observations of tornadoes, the removal of precipitation from the vortex center was completed within several minutes in both types of simulations. Optimization of this centrifuging algorithm is in progress, with the goal of sharing the findings and eventually the centrifuging code to allow future research to benefit from the improved realism of tornado simulations. The work on the algorithm includes producing a centrifuging code that will work consistently with all microphysical parameterizations. Potential findings from this study on both the importance of centrifuging and also more general findings about how tornadoes work have the potential to improve future forecasting of tornadoes and also facilitate further research into understanding these deadly and destructive storms.

WHY BLUE WATERS

Blue Waters was critical to this project because tornado simulations require thousands of computing cores and produce large amounts of data that must be stored and analyzed. Data generated in a typical simulation are in the order of tens and sometimes even hundreds of gigabytes per node. The computing power of Blue Waters, along with the available storage for the data, was a perfect match for this project. In addition, the technical and visualization support available greatly facilitated the accomplishment of our research goals.

Ronald Stenz, a sixth-year doctoral candidate in atmospheric sciences at the University of North Dakota, works under the direction of Matthew Gilmore. He expects to receive his degree in 2020.
UNRAVELING FUNCTIONAL HOLE HOPPING PATHWAYS IN THE [Fe₄S₄]‑CONTAINING DNA PRIMASE

Darion Teo, Duke University

EXECUTIVE SUMMARY

This work has resulted in a Python module (EHPath.py) for characterizing charge hopping pathways in proteins and nucleic acids, which is the first computational tool that maps and ranks hopping pathways according to their mean residence time. The functionality of the module has been evaluated in several proteins including the oxygen-utilizing model enzyme cytochrome p450. Force field parameters that describe the high-potential iron–sulfur cluster have also been developed for molecular dynamics (MD) simulations. These two advances will enable the investigation of the role of an amino acid mutation found in gastric tumors in attenuating primase–DNA charge transfer and, in turn, primer handoff to polymerase α in DNA replication.

METHODS & CODES

This work has resulted in a Python module (EHPath.py) that can map and rank charge hopping pathways in proteins/nucleic acids according to the mean residence time detailed in [3]. This code has also been used to evaluate hopping pathways in proteins of interest (manuscript submitted). The Python module is available at https://github.com/etransfer/EHPath. With regard to developing force field parameters to treat [Fe₄S₄]²⁺/³⁺ for MD simulations, this work utilized broken-symmetry [4] density functional theory (BS–DFT) to optimize the geometries of the cluster in the two redox states (with relevant redox layer spin assignments), followed by force constant calculations using Seminario’s methodology [5]. Existing Lennard–Jones 6–12 parameters were used for the MD simulations. Partial atomic charges for the cluster were also derived. The force field parameters were derived and tested for robustness in MD simulations.

RESULTS & IMPACT

High-potential Fe₄S₄ clusters (in the 2+/3+ oxidation states) are important because they are commonly found in enzymes related to DNA replication and repair, including DNA primase and Polα. Investigating the impact of the Y345C mutation in primase will advance the understanding of the primer handoff process driven by charge transfer as well as other cellular redox processes that are paramount in the regulation of major metabolic pathways. In addition, this will help inform the design of inhibitors that target such mutations. Furthermore, the newly developed force field parameters can be widely used by the research community for MD simulations of high-potential iron–sulfur cluster-containing proteins. Similarly, the Python module is available to the community for evaluating charge hopping pathways in proteins/nucleic acids that are relevant to other research areas.

WHY BLUE WATERS

The Blue Waters fellowship has greatly advanced the progress of this research—both in terms of time and computation. The advance in the computational power made it feasible to perform these types of calculations which would have otherwise been computationally prohibitive. Access to the top-notch computational power of the Blue Waters supercomputer has been very useful for running and completing BS–DFT and Hessian DFT calculations efficiently. The Blue Waters Point of Contact has also provided advice and engaged in helpful discussions through email exchanges and in-person meetings.

RESEARCH CHALLENGE

Recent work [1] suggests that primer handoff from the human DNA primase to polymerase α (Polα), as part of the lagging strand synthesis in DNA replication, is driven by charge (electron or hole) transfer and the modulation of the redox states of the high-potential iron–sulfur (i.e., [Fe₄S₄]²⁺/³⁺) clusters housed in the p58c and p180c domains of primase and Polα, respectively. Experiments have investigated the efficiency of charge transfer between [Fe₄S₄]²⁺/³⁺ in wild-type/mutant p58c and the protein-bound RNA/DNA duplex. Both Y345C and Y345F mutations in primase were found to reduce [Fe₄S₄]²⁺/³⁺-RNA/DNA charge transfer by approximately 60 to 95% [1]. The Y345C somatic mutation is of particular interest owing to its presence in gastric tumors [2]. In order to investigate the impact of mutation on charge transfer computationally, two challenges have to be met. First, a computational tool that can map and rank charge hopping pathways in proteins/nucleic acids has to be developed; this module can then be utilized to examine the hopping pathways between the RNA/DNA duplex and [Fe₄S₄]³⁻/²⁺ in both the wild-type and mutant Y345C primase. Second, as there are no current force field parameters that can treat the high-potential [Fe₄S₄]³⁻/²⁺ cluster, new parameters have to be developed. Once these two challenges are overcome, molecular dynamics (MD) simulations of the mutant and wild-type proteins can be performed; the trajectories obtained from these simulations would then help evaluate the possible attenuation of mutant primase binding to nucleic acid through Generalized Born/Poisson–Boltzmann methods, as well as the modulation of charge hopping pathways between the RNA/DNA duplex and [Fe₄S₄]³⁻/²⁺.
THE TRANSPORT AND DYNAMICS OF WAVE-DRIVEN REEF JETS UNDER THE INFLUENCE OF ROTATION AND BOTTOM FRICTION

Walter Torres, Duke University
2018–2019 Graduate Fellow

EXECUTIVE SUMMARY

Predicting the fate of pollutants, heat, nutrients, carbon, and larvae in the coastal ocean is of acute ecological, commercial, and social importance—especially so on coral reef islands and atolls. On many reefs, jets arising from the interaction of reef topography and waves are responsible for exchanging water between the nearshore and open ocean, and so their dynamics are of particular interest.

This project involves a computational fluid dynamics study of an idealized coral reef island and demonstrates how the interaction among small-scale physical forcing (friction due to bottom roughness) and large-scale processes (e.g., the Coriolis force) modulates the behavior of wave-driven reef jets. Preliminary results show that lower bottom frictional regimes that are associated with degraded reef conditions increase the offshore export of the jets, simultaneously attenuating the relative importance of the Coriolis force that facilitates alongshore transport.

RESEARCH CHALLENGE

Coral reefs are hotspots for marine biodiversity. Reefs provide habitat for a panoply of taxa while also providing vital ecosystem services such as food security, economic well-being, coastline protection, and they are also culturally significant heritage sites [1,2]. Unfortunately, coral reefs face global-scale threats such as ocean warming and acidification; reefs worldwide have already experienced significant degradation, so it is paramount to understand how environmental processes affect coral health in order to inform ecological management efforts [3].

The resilience of a coral reef ecosystem to stressors is tightly entwined with the circulation field. Waves and currents replenish nutrients, transport coral and fish larvae between populations, moderate temperatures, and modify the coastal geomorphology [4]. Computational fluid dynamics modeling provides a way to investigate fundamental circulation processes on reefs that are otherwise analytically intractable, allowing us a deeper understanding of the physics underlying this complex multiscale system. This study focuses specifically on the dynamics of wave-driven reef jets, which are common hydrodynamic features on reefs that arise owing to the interaction of reef topography and wave transformation in shallow water [5]. As surface gravity waves shoal and break, there is a vigorous shoreward input of energy, momentum, and mass; this is balanced by the presence of strong oceanward jets that form in the crenellations of the reef topography. These features can remain coherent over several kilometers yet are driven by wave-shoaling processes that happen over short spatial scales (10–100 m) in extremely shallow water (0.1–10 m). And so, this problem is inherently multiscale: a modeling challenge that demands a short timestep and fine spatial resolution.

RESULTS & IMPACT

The results indicate that degraded reefs may be less retentive and experience shorter residence times owing to the decrease in bottom friction associated with the lower structural complexity of unhealthy coral. Preliminary model runs demonstrated that (unsurprisingly) the Coriolis force deflects the trajectory of the reef jets at some distance offshore, while jet centerline velocities’ magnitudes are weaker for healthy rough reefs owing to the large bottom friction. Stronger bottom friction also increased the relative importance of the Coriolis force in modifying the structure of the jet, as well as the size, speed, and coherence of the eddies shed from it. Surface waves also may influence the advection of these eddies, confounding them nearer to shore via the Stokes drift mechanism. It is highly interesting that small-scale frictional processes on the very shallow back reef and reef crest have ramifications for the structure and evolution of kilometer-scale features such as jets and eddies. Future runs carried out over longer integration times along with detailed particle tracking studies will more clearly identify jet–jet interactions and recirculation patterns.

METHODS & CODES

We modeled circulation on an idealized grid representing a coral reef island with a reef crest, inner lagoon, and a series of reef passes and reef flats. This annular domain was constructed in polar coordinates using variable grid spacing to conserve computational time. A uniform shoreward wave forcing was applied symmetrically to the domain on the outer boundary, with a closed inner boundary and periodic lateral boundary conditions. Results shown here are from a series of pilot numerical experiments that were carried out under permutations of bottom roughness and Coriolis force conditions (healthy rough reef vs. degraded smooth reef [0° and 30°S latitude]). Simulations used the Coupled–Ocean–Atmosphere–Wave–Sediment–Transport (COAWST) modeling system [6]. COAWST produces circulation and wave fields by coupling the ocean (Regional Ocean Modeling System) and wave (Simulating Waves in the Neearshore) models, which numerically solve the 3D primitive equations and 2D wave action equation, respectively. The wave-circulation coupling provided in COAWST was critical for simulating wave-driven reef jets.

This research has made progress in understanding fundamental exchange processes between the open ocean and nearshore reef environment, leveraging the high-resolution model simulations made possible by Blue Waters. The work has generated new hypotheses and predictions that will be evaluated in situ on Moenasa, a coral reef island in French Polynesia, and will also aid the interpretation of ecological data being collected through the National Science Foundation’s Long Term Ecological Research (LTER) initiative, especially on factors affecting coral resilience such as larval recruitment, nutrient loading, and organismal behavior.

WHY BLUE WATERS

The Blue Waters supercomputing resource was essential in producing physically representative results; because we were able to achieve high spatial and temporal resolution for a coupled model over long integration times, the model captures the salient physics and time-evolution of barotropic reef jets. In addition, the Blue Waters support team provided outstanding and expedient technical support with software installation and module use.
EXECUTIVE SUMMARY

Gas turbine engines are widely used for propulsion and load-leveling applications, the latter being critical for incorporating intermittent renewable energy sources such as wind on the electrical grid. While efficiency, emissions, and flame stability are central to advances in turbine design, the extreme level of complexity continues to limit the accuracy of high-fidelity models and the control of gas turbine systems. This project uses the state-of-the-art high-performance computing (HPC) resources provided by Blue Waters to perform high-fidelity direct numerical simulations of turbulent premixed flames stabilized on bluff bodies. (By definition, bluff bodies are those that, because of their shape, have separated flow over a substantial part of their surface.) By studying the dynamics of stabilized flames, the researcher analyzed how high-fidelity models should be adapted to strongly turbulent compressible flows with complex chemistry in the presence of strong shear layers and examined mechanisms for enhancing flame stabilization while maintaining high efficiency and low emissions.

RESEARCH CHALLENGE

As researchers and engineers work to improve the understanding and control of gas-engine systems, the complexity and extreme conditions found in these systems pose a significant challenge for computational approaches. To understand the challenges that engineers face and to better understand the interactions among turbulence, combustion, and recirculation zone dynamics that impact stability, the project poses two important questions:

- How should large-eddy simulation (LES) modeling be adapted to highly turbulent compressible flows with complex chemistry in the presence of strong shear layers, where key physics can be left unresolved by the grid?
- What new mechanisms can be applied to better stabilize flames and prevent blowout while maintaining high efficiency and low emissions?

The first question is motivated by the current inability to model gas turbines in a physically accurate yet computationally efficient manner, while the second is central to turbine design and operation. In this project, these questions are addressed by performing high-fidelity direct numerical simulations (DNS) of turbulent premixed flames stabilized on bluff bodies. In particular, data produced by the high-resolution DNS are being used to analyze key dynamics associated with turbulence–flame interactions in bluff body configurations that are not well captured in high-fidelity LES, that also must be included in future low-fidelity models for practical turbine design, and that lead to instability and flame blowout.

METHODS AND CODES

The researcher has adapted the next-generation compressible reacting flow solver PeleC to the Blue Waters HPC architecture. PeleC, under development at Lawrence Berkeley National Laboratory and the National Renewable Energy Laboratory, scales well, is fully parallelizable, and can be run using both the Message Passing Interface and OpenMP paradigms. The PeleC code uses built-in embedded boundary capabilities for structural modeling, which enables accurate implementation of different bluff body configurations for this work. Furthermore, PeleC incorporates Adaptive Mesh Refinement (AMR) via the AMReX suite, allowing different regions of the simulation domain to be resolved at different levels of fidelity. This permits the addition of local refinement on areas of physical interest, fully resolving flame dynamics and turbulence–combustion interactions. Fig. 1 shows an example of AMReX and AMR at work, with refinement on vorticity. This dynamic refinement results in high-resolution simulations running at reduced computational cost when compared with traditional static meshes. This is particularly true for highly dynamical systems such as engines and turbines where the location of flames and vortex structures is often unpredictable and intermittent in time. The research also incorporates multi-step chemistry through Chemkin-type inputs in order to model chemical kinetic effects without loss of fidelity.

RESULTS & IMPACT

This work used the PeleC exascale combustion code to simulate bluff body flow and successfully produced high-resolution simulations of nonreacting bluff body flow using AMR to provide localized resolution in the near-wake region of the bluff body. Localized refinement allows the simulations to physically resolve the recirculation zone dynamics of the target experimental case at a level not previously examined. These simulations help to determine necessary parameters for computational modeling of this bluff body configuration, including simulation domain, boundary conditions, and resolution criteria necessary for accurate and efficient performance. The lessons learned have been used to design and instantiate reacting-flow simulations and, with these, to explore chemistry model performance and stability within the PeleC simulations running on Blue Waters.

WHY BLUE WATERS

Blue Waters has been both formative and essential for this research. The allocation has allowed the researcher to begin using the highly scalable, adaptive PeleC code to tackle engineering challenges that would not otherwise be able to be considered: questions that are directly applicable to power generation, aviation, and the broader community. The staff have been both attentive and responsive, and ultimately were invaluable in getting the PeleC code up and running, helping with system-specific questions and advice for avoiding potential roadblocks along the way.

Samuel Whitman is a third-year Ph.D. candidate in mechanical engineering at the University of Colorado, Boulder. He expects to receive his degree in 2020 and has been working under the direction of Peter Hamlington and James G. Brasseur.

Figure 1: Flow around a triangular prism bluff body, with high-vorticity regions in red. Adaptive meshing provides localized refinement based on the vorticity. Here, each grayscale box shows three-dimensional grids that are between eight and 32 cells on each side. This localized refinement results in higher-resolution simulations at reduced computational cost.
The Science and Engineering Team Advisory Committee (SETAC) brings together a diverse group of scientists and engineers who represent the various science and engineering research teams using Blue Waters and the breadth of research powered by the Blue Waters system. The committee provides guidance and assessment to help the Blue Waters project deliver the best possible performance and services that will in turn assist research teams in achieving breakthrough results.

The SETAC makes recommendations on technical directions, strategies, and management while identifying potential challenges for petascale applications. As users themselves, the SETAC members also provide advice for solving common issues that arise from moving applications to Blue Waters and from system software at scale.

The SETAC members are nominated and the committee convenes three to four times per year and is available to the Blue Waters Project to provide guidance and advice as needed throughout the year.

SETAC Members

PETASCALE COMPUTING RESOURCE TEAMS
- Paul Woodward, Physics and Astrophysics, University of Minnesota (Chair)
- Tom Cheatham, Chemistry, University of Utah
- David Ceperley, Physics and Material Science, University of Illinois Urbana–Champaign
- Tiziana Di Matteo, Physics and Cosmology, Carnegie Mellon University
- Paul Morin, University of Minnesota
- Susan Bates, NCAR
- Brian O’Shea, Michigan State University
- Manuela Campanelli, Rochester Institute of Technology
- Tom Jordan / Philip J. Maechling, University of Southern California
- Said Elghobashi, University of CA Irvine
- Nikolai Pogorelov, University of Alabama, Huntsville

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION TEAMS
- H. Birali Ramesha, University of Chicago

INDUSTRY TEAMS
- Rick Arthur, General Electric Global Research, Advanced Computing

UNIVERSITY OF ILLINOIS AT URBANA–CHAMPAIGN TEAMS
- Athol Kemball, Astronomy, University of Illinois at Urbana–Champaign

OTHER BLUE WATERS PROJECTS

The projects listed here had a Blue Waters allocation during this reporting period but did not submit a report for the project.

Graphical Representation of Objects
John Carusone

Massive Galaxies and their Black Holes
Claude-Andre Faucher-Giguere

CFD Software Development
Paul Fischer

Parallel MLFMA
Levent Gurel

Peptide Mutations Influenza Fusion
Peter Kasson

Core-collapse Supernovae and their Ejecta
Eric Lentz

4-D Earth Simulation
Lijun Liu

Studying Subduction Dynamics
Lijun Liu

Cell Simulations of a Minimal Cell
Zaida Luthey-Schulten

Lipids Control membrane Transporter Dynamics
Mahantshacharyan

Gas & Galaxies in Enzo
Molly Peoples

Neuroimaging with MR Elastography
Hillary Schwartz

Modeling the Earth’s Deep Interior
Xiaodong Song

Modeling the Microbiome in IBD Patients
Rebecca Stumpf

Magnetic Reconnection in Laser-Driven Plasmas:
From Astrophysics to the Laboratory In Silico
Samuel Totorica

Surface Defects on Hydrophobicity
Yang Zhang

Protein Stability under Confinement
Yang Zhang
REFERENCES

Balsara, Dinshaw S.


Huetta, Eli (3)


Levin, Deborah A. (2)


Petzack, Donald


Pogorelov, Nikolai


Shapiro, Stuart L.


Diao, Chunyuan

Di Girolamo, Larry

Domínguez, Francisco
Pavlis, Nikolaos


Nesbitt, Stephen W.


Pavlis, Nikolaos


Riemer, Nicole


Tabor, Clay


Vidalé, John


93

West, Matthew


93

Wuebbles, Donald J.


Aluru, Narayana R. (1)


Aluru, Narayana R. (2)


Bodony, Daniel J.

Breth, Christoph


Mashayek, Farzad


Matalon, Moshe


Riedl, Caroline


Rieppel, Anne

Riordan, Thomas, B. A.


Riordan, Thomas, B. A.


Trikkott, Dallas R.


Timoleon Lopez, Rafael O. A.


Toussaint, Kimani


Xu, Bin


Xu, Zhao


Yeung, Pui–Kuen


Zhang, Yang

Duursma, Iwan M.


Aksamitalev, Aleksi (3)


Carano—Anulito, Gustavo


Clancy, Colleen E.


Moradi, Arif


Metro, Jeffrey S.


Moradi, Mahmoud (inquest)


Martinez, Maria Teresa


Shukla, Diwakar (2)


Prather, Kimberly


Shukla, Ivan


Srinivasan, Ashok


Sutton, Brad P.


Tajhorsheed, Emad (1)


Voith, Gregory A.


Ye, Mao

“Climate policy under spatial heat transport: co-


10.1093/mnras/stw1741.

“Choosing the Right Bigrams for Information Retrieval.” Proc. Meeting Inter.


Applebaum, Eland

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Soley, Micheline

Stenz, Ronald

Teo, Darius
# INDEX

<table>
<thead>
<tr>
<th>Index</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>32</td>
</tr>
<tr>
<td>Agee, Elizabeth</td>
<td>32</td>
</tr>
<tr>
<td>Aksimentiev, Aleksei</td>
<td>123, 240, 242</td>
</tr>
<tr>
<td>Alur, Narayana</td>
<td>120, 122, 124</td>
</tr>
<tr>
<td>Amaro, Romnie</td>
<td>244</td>
</tr>
<tr>
<td>Anisimov, Victor</td>
<td>314</td>
</tr>
<tr>
<td>Applebaum, Elaad</td>
<td>314</td>
</tr>
<tr>
<td>Araya, Guillermo</td>
<td>126</td>
</tr>
<tr>
<td>B</td>
<td>14</td>
</tr>
<tr>
<td>Balsara, Dinshaw</td>
<td>14</td>
</tr>
<tr>
<td>Barber, Kateyn</td>
<td>116</td>
</tr>
<tr>
<td>Bernardi, Rafael</td>
<td>146</td>
</tr>
<tr>
<td>Bershook, Jerry</td>
<td>128</td>
</tr>
<tr>
<td>Bodony, Daniel</td>
<td>130</td>
</tr>
<tr>
<td>Brehm, Christoph</td>
<td>132</td>
</tr>
<tr>
<td>Brooks, Maureen</td>
<td>238</td>
</tr>
<tr>
<td>Browne, Oliver</td>
<td>134</td>
</tr>
<tr>
<td>Burrows, Adam</td>
<td>16</td>
</tr>
<tr>
<td>Butsky, Iryna</td>
<td>340</td>
</tr>
<tr>
<td>C</td>
<td>246</td>
</tr>
<tr>
<td>Caetano-Anolles, Gustavo</td>
<td>246</td>
</tr>
<tr>
<td>Cai, Yongyang</td>
<td>250</td>
</tr>
<tr>
<td>Campenni, Manuela</td>
<td>18, 20</td>
</tr>
<tr>
<td>Carrasco Kind, Matias</td>
<td>22</td>
</tr>
<tr>
<td>Ceperley, David</td>
<td>136</td>
</tr>
<tr>
<td>Chew, Huck Rong</td>
<td>138</td>
</tr>
<tr>
<td>Cho, Wendy</td>
<td>320</td>
</tr>
<tr>
<td>Chu, Shanna</td>
<td>361</td>
</tr>
<tr>
<td>Cieri, Robert</td>
<td>362</td>
</tr>
<tr>
<td>Clancy, Colleen</td>
<td>350</td>
</tr>
<tr>
<td>Clark, Bryan</td>
<td>140</td>
</tr>
<tr>
<td>Clement, Matthew</td>
<td>344</td>
</tr>
<tr>
<td>Cook, Salme</td>
<td>346</td>
</tr>
<tr>
<td>Corcoran, Jennifer</td>
<td>78</td>
</tr>
<tr>
<td>Cox, Donna</td>
<td>312</td>
</tr>
<tr>
<td>D</td>
<td>60</td>
</tr>
<tr>
<td>Di Girolamo, Larry</td>
<td>60</td>
</tr>
<tr>
<td>Di Matteo, Tiziana</td>
<td>24</td>
</tr>
<tr>
<td>Diao, Chunyuan</td>
<td>62</td>
</tr>
<tr>
<td>Dickerson, Julie</td>
<td>152</td>
</tr>
<tr>
<td>Dill, Ken</td>
<td>254</td>
</tr>
<tr>
<td>Dominguez, Fancina</td>
<td>64</td>
</tr>
<tr>
<td>Dovanie, J. Stephen</td>
<td>352</td>
</tr>
<tr>
<td>Draayer, Jerry</td>
<td>26</td>
</tr>
<tr>
<td>Duan, Tian</td>
<td>142</td>
</tr>
<tr>
<td>Duersma, Iwan</td>
<td>214</td>
</tr>
<tr>
<td>E</td>
<td>315</td>
</tr>
<tr>
<td>El-Kebir, Mohammed</td>
<td>315</td>
</tr>
<tr>
<td>El-Khadra, Aida</td>
<td>144</td>
</tr>
<tr>
<td>Emerick, Andrew</td>
<td>340</td>
</tr>
<tr>
<td>Ertelkin, Elif</td>
<td>146</td>
</tr>
<tr>
<td>F</td>
<td>236</td>
</tr>
<tr>
<td>Ferguson, Andrew</td>
<td>236</td>
</tr>
<tr>
<td>Freund, Jonathan</td>
<td>140</td>
</tr>
<tr>
<td>G</td>
<td>150</td>
</tr>
<tr>
<td>Gammie, Charles</td>
<td>28</td>
</tr>
<tr>
<td>Garcia, Marcelo</td>
<td>150</td>
</tr>
<tr>
<td>Gazolla, Mattia</td>
<td>258</td>
</tr>
<tr>
<td>Glines, Forrest</td>
<td>160</td>
</tr>
<tr>
<td>Gnedin, Nickolay</td>
<td>30</td>
</tr>
<tr>
<td>Gregg, Patricia</td>
<td>16</td>
</tr>
<tr>
<td>Gropp, William</td>
<td>216, 218</td>
</tr>
<tr>
<td>Guan, Kaizhu</td>
<td>88, 90</td>
</tr>
<tr>
<td>Gurwich, Alexander</td>
<td>152</td>
</tr>
<tr>
<td>H</td>
<td>262</td>
</tr>
<tr>
<td>Hadden-Perrill, Jodi</td>
<td>260, 262</td>
</tr>
<tr>
<td>Hawley, John</td>
<td>132</td>
</tr>
<tr>
<td>Hays, Jennifer</td>
<td>204</td>
</tr>
<tr>
<td>Hirata, So</td>
<td>266</td>
</tr>
<tr>
<td>Hochberman, Benjamin</td>
<td>152</td>
</tr>
<tr>
<td>Hopkins, Philip</td>
<td>44</td>
</tr>
<tr>
<td>Hudson, Matthew</td>
<td>266</td>
</tr>
<tr>
<td>Huerta Escudero, Elin</td>
<td>38, 38, 40</td>
</tr>
<tr>
<td>Huff, Kathryn</td>
<td>144</td>
</tr>
<tr>
<td>I</td>
<td>220</td>
</tr>
<tr>
<td>Iyer, Ravishankar</td>
<td>220</td>
</tr>
<tr>
<td>J</td>
<td>16</td>
</tr>
<tr>
<td>Jain, Prashant</td>
<td>18</td>
</tr>
<tr>
<td>Jha, Shantenu</td>
<td>222</td>
</tr>
<tr>
<td>Jiang, Tan</td>
<td>208</td>
</tr>
<tr>
<td>Johnson, Eric</td>
<td>158</td>
</tr>
<tr>
<td>Johnson, Harley</td>
<td>160</td>
</tr>
<tr>
<td>K</td>
<td>62</td>
</tr>
<tr>
<td>Kemball, Athol</td>
<td>42</td>
</tr>
<tr>
<td>Khalili-Araghi, Fatemeh</td>
<td>270</td>
</tr>
<tr>
<td>Kostic, Soid</td>
<td>162</td>
</tr>
<tr>
<td>L</td>
<td>256</td>
</tr>
<tr>
<td>Lansford, Joshua</td>
<td>256</td>
</tr>
<tr>
<td>Lasher-Trapp, Sonia</td>
<td>92</td>
</tr>
<tr>
<td>LeBauer, David</td>
<td>272</td>
</tr>
<tr>
<td>Lefebvre, Jean-Pierre</td>
<td>16</td>
</tr>
<tr>
<td>Levin, Deborah</td>
<td>44, 46</td>
</tr>
<tr>
<td>Liu, Yi-Hsin</td>
<td>48</td>
</tr>
<tr>
<td>M</td>
<td>244</td>
</tr>
<tr>
<td>Makri, Nancy</td>
<td>274</td>
</tr>
<tr>
<td>Marsac, Kara</td>
<td>159</td>
</tr>
<tr>
<td>Mashayek, Farzad</td>
<td>166</td>
</tr>
<tr>
<td>Masud, Arif</td>
<td>176</td>
</tr>
<tr>
<td>Matalon, Mouhe</td>
<td>176</td>
</tr>
<tr>
<td>Menanteau, Felipe</td>
<td>50</td>
</tr>
<tr>
<td>Moesta, Philipp</td>
<td>81</td>
</tr>
<tr>
<td>Moore, Jeffery</td>
<td>276</td>
</tr>
<tr>
<td>Moradi, Mahmoud</td>
<td>280, 282</td>
</tr>
<tr>
<td>Morin, Paul</td>
<td>91</td>
</tr>
<tr>
<td>N</td>
<td>54</td>
</tr>
<tr>
<td>Neubauer, Mark</td>
<td>170</td>
</tr>
<tr>
<td>Nesbitt, Stephen</td>
<td>96</td>
</tr>
<tr>
<td>Norman, Michael</td>
<td>54</td>
</tr>
<tr>
<td>O</td>
<td>54</td>
</tr>
<tr>
<td>O’Shea, Brian</td>
<td>56</td>
</tr>
<tr>
<td>Osborn, Luke</td>
<td>224, 226</td>
</tr>
<tr>
<td>Otf, Leigh G.</td>
<td>58</td>
</tr>
<tr>
<td>P</td>
<td>103</td>
</tr>
<tr>
<td>Pavli, Nikolaos</td>
<td>100</td>
</tr>
<tr>
<td>Perilla, Juan</td>
<td>284</td>
</tr>
<tr>
<td>Peterson, Joseph</td>
<td>286</td>
</tr>
<tr>
<td>Petrack, Donald</td>
<td>58</td>
</tr>
<tr>
<td>Pogorelov, Nikolai</td>
<td>60</td>
</tr>
<tr>
<td>Pogorelov, Taras</td>
<td>116</td>
</tr>
<tr>
<td>Prather, Kimberly</td>
<td>288</td>
</tr>
<tr>
<td>Pratt, Jane</td>
<td>62</td>
</tr>
<tr>
<td>Q</td>
<td>64</td>
</tr>
<tr>
<td>Quinn, Thomas</td>
<td>64</td>
</tr>
<tr>
<td>R</td>
<td>172</td>
</tr>
<tr>
<td>Rahman, Rajib</td>
<td>172</td>
</tr>
<tr>
<td>Ramam, Venkat</td>
<td>24</td>
</tr>
<tr>
<td>Ricker, Paul</td>
<td>66</td>
</tr>
<tr>
<td>Riedl, Caroline</td>
<td>176</td>
</tr>
<tr>
<td>Riemer, Nicole</td>
<td>160</td>
</tr>
<tr>
<td>Rosato, Nicole</td>
<td>369</td>
</tr>
<tr>
<td>Roux, Benoit</td>
<td>290</td>
</tr>
<tr>
<td>S</td>
<td>180</td>
</tr>
<tr>
<td>Schleife, André</td>
<td>178, 180</td>
</tr>
<tr>
<td>Shanahan, Phiala</td>
<td>208</td>
</tr>
<tr>
<td>Shapiro, Stuart</td>
<td>88</td>
</tr>
<tr>
<td>Shklover, Dwaikar</td>
<td>292, 294, 296</td>
</tr>
<tr>
<td>Sirignano, Justin</td>
<td>234</td>
</tr>
<tr>
<td>Snir, Marc</td>
<td>238</td>
</tr>
<tr>
<td>Soley, Michelle</td>
<td>362</td>
</tr>
<tr>
<td>Solomonik, Edgar</td>
<td>230</td>
</tr>
<tr>
<td>Sotelsz, Ivan</td>
<td>298</td>
</tr>
<tr>
<td>Sotomayor, Marcos</td>
<td>300</td>
</tr>
<tr>
<td>Sriv Pillai, Ashok</td>
<td>302</td>
</tr>
<tr>
<td>Stenzi, Ronald</td>
<td>306</td>
</tr>
<tr>
<td>Sutton, Brad</td>
<td>304</td>
</tr>
<tr>
<td>T</td>
<td>104</td>
</tr>
<tr>
<td>Tabor, Clay</td>
<td>104</td>
</tr>
<tr>
<td>Taffin, Dave</td>
<td>235</td>
</tr>
<tr>
<td>Tskhovshid, Emad</td>
<td>396, 398, 310</td>
</tr>
<tr>
<td>Tchekhovsky, Alexander</td>
<td>70</td>
</tr>
<tr>
<td>Teo, Darius</td>
<td>166</td>
</tr>
<tr>
<td>T&lt;Selfsky, Saul A.</td>
<td>76</td>
</tr>
<tr>
<td>Thomas, Brian</td>
<td>102</td>
</tr>
<tr>
<td>Tinoco Lopez, Rafael</td>
<td>184</td>
</tr>
<tr>
<td>Torres, Walter</td>
<td>186</td>
</tr>
<tr>
<td>Toth, Gabor</td>
<td>12</td>
</tr>
<tr>
<td>Toussaint, Kimani</td>
<td>186</td>
</tr>
<tr>
<td>Trapp, Robert</td>
<td>106</td>
</tr>
<tr>
<td>Trinkle, Dallas</td>
<td>148</td>
</tr>
<tr>
<td>Turk, Matthew</td>
<td>74</td>
</tr>
<tr>
<td>V</td>
<td>108</td>
</tr>
<tr>
<td>Vidal, John</td>
<td>108</td>
</tr>
<tr>
<td>Vedr, Gregory</td>
<td>312</td>
</tr>
<tr>
<td>Yeković, Lela</td>
<td>390</td>
</tr>
<tr>
<td>W</td>
<td>192</td>
</tr>
<tr>
<td>Wagner, Lucas</td>
<td>192</td>
</tr>
<tr>
<td>Wang, Zhi Jian</td>
<td>194</td>
</tr>
<tr>
<td>Warmow, Tandy</td>
<td>232</td>
</tr>
<tr>
<td>Wentzcovitch, Renata</td>
<td>110</td>
</tr>
<tr>
<td>West, Matthew</td>
<td>112</td>
</tr>
<tr>
<td>Whiteman, Samuel</td>
<td>270</td>
</tr>
<tr>
<td>Wuebbles, Donald J.</td>
<td>114</td>
</tr>
<tr>
<td>X</td>
<td>196</td>
</tr>
<tr>
<td>Xu, Bin</td>
<td>196</td>
</tr>
<tr>
<td>Xu, Zhen</td>
<td>198</td>
</tr>
<tr>
<td>Y</td>
<td>202</td>
</tr>
<tr>
<td>Yan, Jishui</td>
<td>202</td>
</tr>
<tr>
<td>Yang, Guang</td>
<td>200</td>
</tr>
<tr>
<td>Ye, Mao</td>
<td>324</td>
</tr>
<tr>
<td>Yeung, Pui-Kuen</td>
<td>204</td>
</tr>
<tr>
<td>Z</td>
<td>168</td>
</tr>
<tr>
<td>Zhang, Xiadong</td>
<td>166</td>
</tr>
<tr>
<td>Zhang, Yang</td>
<td>206</td>
</tr>
</tbody>
</table>
Blue Waters is supported by the National Science Foundation.