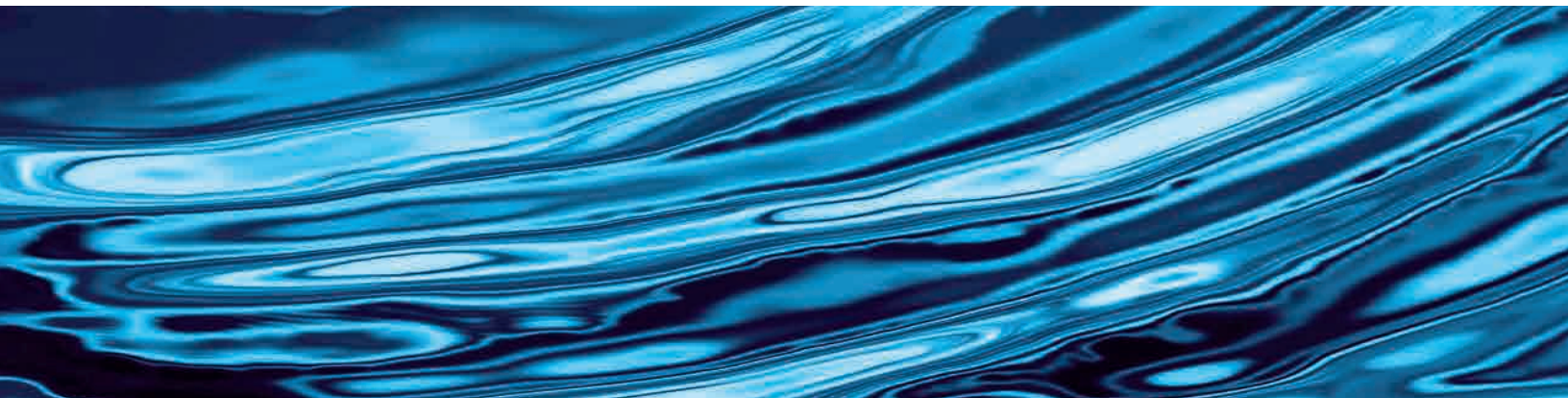
BLUE WATERS

SUSTAINED PETASCALE IN ACTION:
ENABLING TRANSFORMATIVE RESEARCH

2014 ANNUAL REPORT



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2014 ANNUAL REPORT

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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 2014 Blue Waters Symposium presentations.

ISBN 978-0-9908385-1-7

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KB = kilobytes
TB = terabytes
PB = petabytes
I/O = input/output
Mnh = million node hours

Allocations denoted as type/ size in extended abstracts.

A MESSAGE FROM BILL KRAMER

Welcome to the Blue Waters Annual Report for 2014!

This book captures the first year of full production on Blue Waters since the supercomputer started full service on April 2, 2013. We've had a great year, with many researchers transforming knowledge in their respective fields.

As of this writing, we have 124 science teams from well over 50 institutions and organizations using NSF's most powerful system. Many of these teams have worked with our Blue Waters staff to ensure that their research runs as productively as possible, whether that means optimizing the code or implementing new resource or storage management methods.

Blue Waters has provided exceptional service to the nation's science, engineering, and research communities. With a balanced and integrated system with very high sustained computational performance, extraordinary analytical capabilities, very large memory, world-leading storage capacity and performance, leadership-level networking, and an advanced service architecture, the Blue Waters system and staff are empowering teams across all NSF directorates to do breakthrough science that would otherwise be impossible.

In May 2014, science and engineering partners, staff, and others associated with the Blue Waters project met face-to-face at the 2014 Blue Waters Symposium. Not only did the researchers talk about their accomplishments on the already-existing massive machine, but we also discussed how Blue Waters serves as a bridge to even more powerful computers in the future.

Blue Waters continues its commitment to building the next generation of our workforce by recruiting dozens of graduate and undergraduate students into our education programs. For many of these students this is their first exposure to supercomputing, but some, such as our Blue Waters Fellows, have decided to base their entire careers on advanced modeling and simulation or data analytics.

As we compiled this report, the scale of achievement that this project enabled became apparent. We are proud to have been a part of it and look forward to continuing our services for more and bigger science and engineering for years to come.

William C. Kramer
Project Director & Principal Investigator

WHAT IS BLUE WATERS?

Blue Waters is one of the most powerful supercomputers in the world and the fastest supercomputer at a university. It can complete more than 1 quadrillion calculations per second on a sustained basis and more than 13 times that at peak speed. The peak speed is almost 3 million times faster than the average laptop.

The machine architecture balances processing speed with data storage, memory, and communication within itself and to the outside world in order to cater to the widest variety possible of research endeavors. Many of the projects that use Blue Waters would be difficult or impossible to do elsewhere.

Blue Waters is supported by the National Science Foundation (NSF) and the University of Illinois at Urbana-Champaign; the National Center for Supercomputing Applications (NCSA) manages the Blue Waters project and provides expertise to help scientists and engineers take full advantage of the system.

Cray Inc. supplied the hardware: 22,640 Cray XE6 nodes and 4,224 Cray XK7 nodes that include NVIDIA graphics processor acceleration. The XE6 nodes boast 64 GB of memory per node and the XK7s have 32 GB of memory.

Blue Waters' three file systems (home, project, and scratch) provide room for over 26 PB of online storage with a combined 1 TB/s read/write rate for quick access while jobs are running. The three file systems are assembled around Cray's Sonexion Lustre appliances. The scratch file system is the largest and fastest file systems Cray has ever provided.

Compare this to a typical laptop, which has one processor—1/16 of an XE node—with 4 GB of memory and half a terabyte of storage.

To backup or store data from the file systems for longer periods, a nearline tape environment was built using Spectra Logic T-Finity tape libraries, a DDN disk cache, and IBM's HPSS. This system provides over 300 PB of usable storage (380 PB raw).

The supercomputer lives in a 20,000-square-foot machine room, nearly a quarter of the floor space in the 88,000-square-foot National Petascale Computing Facility (NPCF) on the western edge of the University of Illinois at Urbana-Champaign campus.

NPCF achieved Gold Certification in the U.S. Green Building Council's Leadership in Energy and Environmental Design (LEED) rating system, which is the recognized standard for measuring sustainability in construction. The facility uses three on-site cooling towers to provide water chilled by Mother Nature a large part of the year, reducing the amount of energy needed to provide cooling. The facility also reduces power conversion losses by running 480 volt AC power to compute systems, and operates continually at the high end of the American Society of Heating, Refrigerating, and Air-Conditioning Engineers standards for efficiency.

BLUE WATERS SYMPOSIUM 2014

On May 12, 2014, Blue Waters supercomputer users and many of the NCSA staff who support their work converged in Champaign, Illinois, for the second annual Blue Waters Symposium. The ensuing three days were filled with what many of them would later refer to as a wonderful variety of science talks and opportunities for networking and collaboration.

EFFICIENT DISCOVERY THROUGH SUPERCOMPUTING

The science talks ranged from high-energy physics to molecular dynamics to climate science and even political science. Blue Waters enables more efficient progress in science, summarized Paul Woodward, professor of astronomy at the University of Minnesota. Researchers can run simulations quickly and then have more time to draw meaning from the results while someone else runs their simulations. Ed Seidel, director of NCSA, added that big computing and big data will revolutionize science, whether physical or social, by making possible the formerly impossible. Many problems are too complex to solve without such resources.

A few talks touched on social sciences that initially seem incongruous with supercomputing. For example, Shaowen Wang, director of the new CyberGIS Center at the University of Illinois at Urbana-Champaign, is leading an exploration into minimizing bias in voting districts. Later in the same session, Keith Bisset, research scientist at the Network Dynamics & Simulations Science Laboratory at Virginia Tech, said he simulated one scenario of disease propagation for the entire U.S. population for four months in just 12 seconds using 352,000 cores. He estimated that the world population would take 6-10 minutes per scenario, though he emphasized that a realistic assessment of disease threat would require many such runs.

SHARED EVENINGS, COMMON GOALS

The most popular speaker of the symposium was Irene Qualters, the director of the NSF Division of Advanced Cyberinfrastructure. She spoke Thursday morning about the future of supercomputing at NSF and encouraged users to work with NSF to ensure that the future of supercomputing met their needs. The symposium and NCSA's Private Sector Program (PSP) annual meeting met for dinner Tuesday at Allerton Park and Wednesday at Memorial Stadium, combining the most advanced computational science and industry teams in the country, according to Seidel.

Seidel remarked after Wednesday's dinner that he heard a common need from PSP and Blue Waters partners: an all-around system that not only can run simulations, but also analyze and visualize data.

Science talks throughout the symposium bespoke the advances that Blue Waters enabled. Additionally, researchers envisaged what they could achieve with the next generation of supercomputers, looking toward the future of large-scale computing.

BACKGROUND IMAGE: Paul Woodward gave a talk on his work related to stellar hydrodynamics.

QUICK FACTS: Blue Waters users include: 124 teams and 719 researchers.

Symposium attendees: 187.

COMMUNITY ENGAGEMENT & EDUCATION

The Blue Waters Community Engagement program enlists researchers, educators, HPC center staff, campus staff, and undergraduate and graduate students across all fields of study to participate as consumers and providers of knowledge and expertise. The program proactively promotes the involvement of under-represented groups. Community needs drive these activities and we welcome your recommendations and suggestions (please contact the Blue Waters Project Office at bwpo@ncsa.illinois.edu).

Up to 1.8 million node-hours per year are dedicated to educational use, which includes support of formal courses, workshops, summer schools, and other training designed to prepare the petascale workforce. To date, Blue Waters has supported more than a dozen events.

TRAINING AND WORKSHOPS

Experts in the field provide training opportunities that bring petascale resources, tools, and methods to the science and engineering community. Training is offered in person and through video conferences, webinars, and self-paced online tutorials. Recent and upcoming topics include OpenACC, advanced MPI capabilities, GPGPU programming, data-intensive computing, and scientific visualization.

Specifically for its partners, the Blue Waters project provides hands-on workshops by Blue Waters staff and invited speakers twice a year on subjects that facilitate effective use of system resources. Cray, NVIDIA, Allinea, HDF Group, and INRIA have participated in past workshops. An ongoing monthly teleconference/webinar informs users of recent changes to the system such as software, policy, or significant events as well as upcoming training opportunities. Every other month a guest presenter adds relevant topical content to the monthly user group meeting. Topics have included Globus Online data movement, parallel HDF5, and Lustre best practices.

VIRTUAL SCHOOL OF COMPUTATIONAL SCIENCE AND ENGINEERING

The Blue Waters team conducted a pilot web-based college course in collaboration with professor Wen-mei Hwu from the Department of Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign during the spring of 2013. Two collaborating faculty at Ohio State University and the University of Minnesota hosted the course so students at their home campuses could receive credit. Professor Hwu recorded lectures, and participants on each campus watched the videos on their own schedule and then discussed them with local faculty.

Because of the success of this pilot program, Blue Waters is working with faculty to offer more semester-long online courses to allow students at institutions across the country to participate. Each course includes a syllabus with learning outcomes, 40 hours of instruction, reading assignments, homework and exercises, and assessment of learning progress.

Other courses include Parallel Algorithm Techniques in fall 2014 (Wen-Mei Hwu, University of Illinois at Urbana-Champaign) and High Performance Visualization for Large-Scale Scientific Data Analytics in spring 2015 (Han-Wei Shen, The Ohio State University). Blue Waters welcomes faculty across the nation who are interested in offering courses in this manner.

BLUE WATERS GRADUATE FELLOWSHIP PROGRAM

Fellowships are awarded annually to students in multidisciplinary research projects including computer science, applied mathematics, and computational sciences. Fellows receive a generous stipend, tuition allowance, and an allocation on Blue Waters. A call for applications goes out during late fall for fellowships starting in the next academic year.

Blue Waters selected ten PhD students as Blue Waters Fellows for 2014-2015: Kenza Arraki (New Mexico State University), Matthew Bedford (University of Alabama), Jon Calhoun (University of Illinois at Urbana-Champaign), Alexandra Jones (University of Illinois at Urbana-Champaign), Sara Kokkila (Stanford University), Edwin Mathews (University of Notre Dame), Ariana Minot (Harvard University), George Slota (Penn State University), Derek Vigil-Fowler (University of California, Berkeley), and Varvara Zemskova (University of North Carolina at Chapel Hill). They attended the 2014 Blue Waters Symposium, began their research in the fall of 2014, and will present their findings at the 2015 Blue Waters Symposium. Nine additional students were named Blue Waters Scholars and granted allocations on Blue Waters.

Over three years, this fellowship program will award more than $1 million and more than 72 million integer-core equivalent hours to support graduate research.

BLUE WATERS STUDENT INTERNSHIP PROGRAM

The Blue Waters Student Internship Program is designed to immerse undergraduate and graduate students in research projects associated with Blue Waters and/or the Extreme Science and Engineering Discovery Environment (XSEDE) efforts. Twenty one students were selected for 2014-2015. The students attended a two-week institute in late spring 2014 to ensure they were familiar with parallel and distributed computing tools, techniques, and technologies and with computing environments like Blue Waters and XSEDE prior to the start of their year-long internships. A faculty mentor will guide each intern in their use of HPC resources to solve science and engineering problems.

Applications are accepted during the spring. The selection criteria emphasize the likelihood of success, creating a diverse workforce, and promoting excellence.

REPOSITORY OF EDUCATION AND TRAINING MATERIALS

Blue Waters provides access to education and training materials developed by practitioners to foster the development of a broader, well-educated community able to conduct computational science and engineering research using petascale technologies, resources, and methods. The materials include education and course modules related to petascale computing, materials from training and workshop events, and other resources contributed by the HPC community. Included in the repository are 30 undergraduate course modules developed with Blue Waters support that have been viewed more than 28,000 times, and have each been downloaded approximately 6,000 times.

Training materials can be accessed at the following web addresses:

- undergraduate - https://bluewaters.ncsa.illinois.edu/undergraduate
- graduate - https://bluewaters.ncsa.illinois.edu/graduate
- user community - https://bluewaters.ncsa.illinois.edu/training

MEASURING BLUE WATERS

To assure excellent service, the Blue Waters project tracks multiple metrics of success from usage to downtime to service requests. These metrics aim to ensure that we provide a reliable, high-performance system that accelerates discovery across a variety of disciplines.

Target values for the control metrics have been tightened up after six months of operations as we gained experience with the system. Overall for the first year of operations, the Blue Waters project met or exceeded the expectations for the vast majority of our stringent control metrics.

In reading this report, one must keep in mind that the data can be very complex and can change over the course of the project, so single data points often do not provide a clear message. Rather than metrics that measure activity amounts (e.g., number of users, number of jobs) or rates, the Blue Waters project team works hard to measure quality in addition to activity. For example, the number of service requests submitted by Blue Waters partners—all the institutions, organizations, and companies that support and use the supercomputer—may indicate quality issues with the system, or it may indicate an open and proactive relationship with an increased numbers of partners. Such data often has to be analyzed in detail to understand whether an effort is meeting its mission and whether the quality of service is at the expected level. In the following, we report on the status of a few of the Blue Waters control metrics.

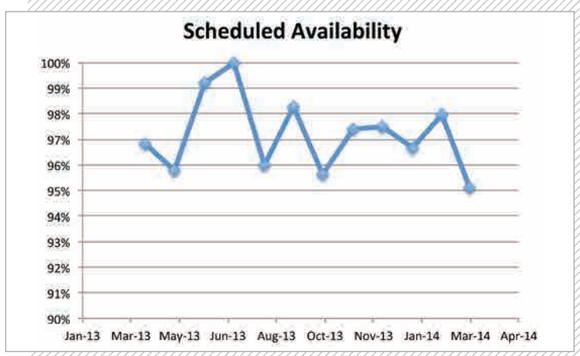


FIGURE 1: Scheduled system availability.

SYSTEM AVAILABILITY

System availability has real value to our partners. When evaluating system availability we use criteria that are more stringent than typical, so one should take care when comparing.

For example, for Blue Waters a service interruption is any event or failure (hardware, software, human, environment) that disrupts the specified service level to the partner base for a specified time period. We call it unscheduled if we give less than 24 hours' notice of an interruption, though we aim for at least seven days' notice. The duration of an outage is calculated as the time during which full functionality of the system is unavailable to users, from first discovery to full

return to service. Partial or degraded service is counted as part of the total outage.

Scheduled availability gives an indication of how reliable the system is for science partners during the time the system is planned to be available (table 1). In all quarters, we have exceeded our required overall goal of 90-92% availability, sometimes substantially. On a monthly basis, the availability looks excellent, falling into a range of 95-98% (fig. 1).

Mean time between system-wide failure (MTBF) is computed by dividing the number of hours the system was available in a month by the number of system-wide interrupts (or one if there are no interrupts) and then converting to days. Since full service began, the goal for MTBF has been greater than or equal to five days. Once again, we exceeded our goals on a quarterly basis. Taking a monthly view, the measured MTBF was above the target for 10 of the 12 months in Blue Waters' first year of service (fig. 2), which is remarkable for a system that is 50% larger than any other system Cray has delivered. Overall the largest impact to science teams is unscheduled outages and thus reducing that type of outage remains a key focus of the NCSA and Cray teams.

A node interrupt is defined as a node failure that results in a partner job failure or serious impact to a job. The interrupt rates are relatively stable and generally below three node interrupts per day. Given the node count of the Blue Waters system, this value is well below projected interrupt rates and translates to served decades of MTBF per individual node.

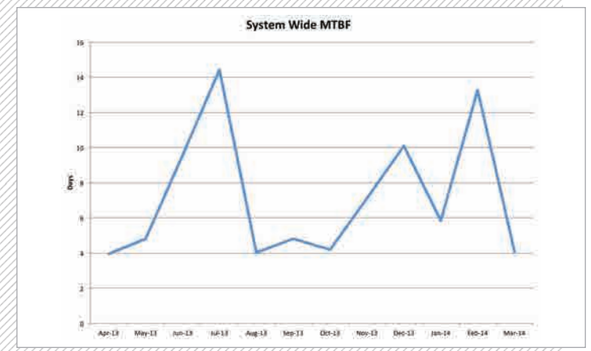


FIGURE 2: System-wide mean time between failures for the entire Blue Waters system.

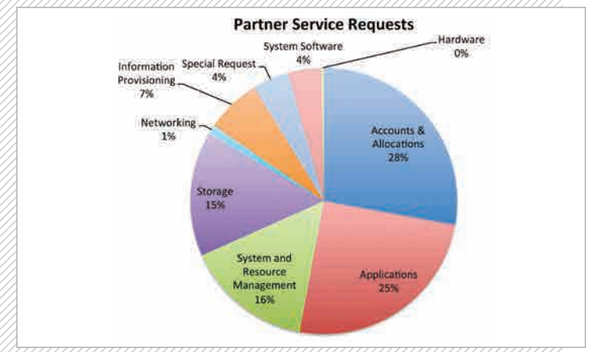


FIGURE 3: Breakdown of partner service requests by type.

SERVICE REQUESTS

Helping our partners effectively use a very complex system is a key role of Blue Waters staff. Obviously, correctly resolving an issue in a short time indicates a good quality of service and, most importantly, a higher degree of productivity for science partners. Table 1 shows measures of our response time to partner service requests (which are "trouble tickets" plus requests for advanced support, special processing, etc.) for the first quarter of 2014 (other quarters are similar). In all areas except giving at least seven days' notice for major upgrades and planned system changes, we consistently met or exceeded our goals. For all the announcements that missed the seven days' notice mark, only one had less than six

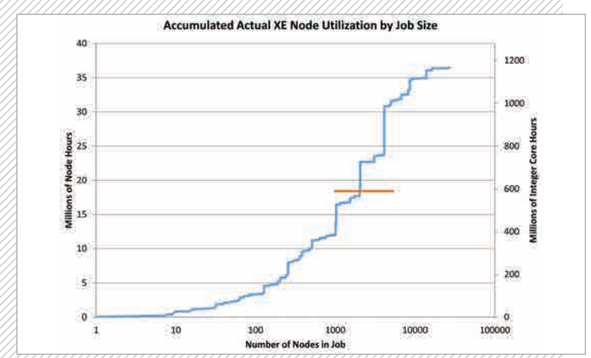


FIGURE 4: Accumulated usage of XE nodes by job size. Red line indicates that 50% of the actual usage comes from jobs using ≥2,048 nodes (65,536 integer-core equivalents).

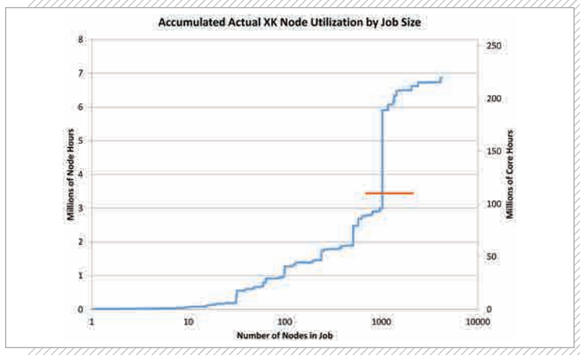


FIGURE 5: Accumulated usage of XK nodes by job size. Red line indicates that 50% of the actual XK usage comes from jobs using ≥1,024 nodes.

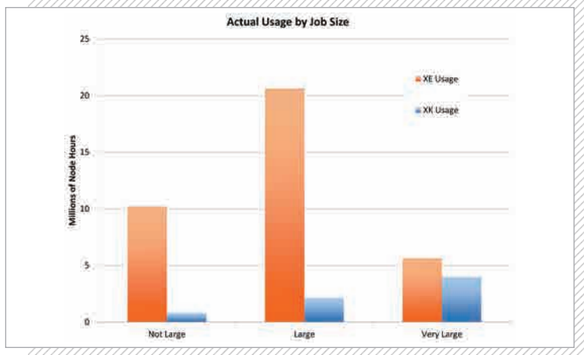


FIGURE 6: Usage per job size category in terms of absolute millions of actual node hours. Orange is XE node hours, blue is XK node hours.

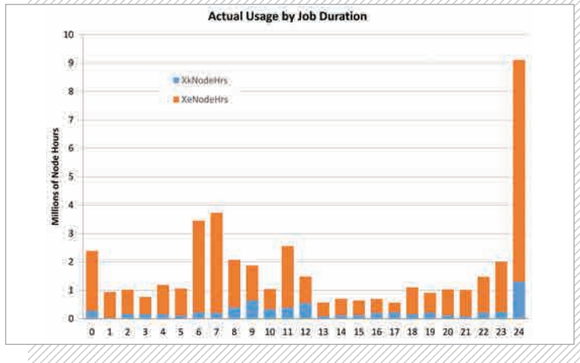


FIGURE 7: Distribution of actual usage by job duration. Orange is XE node hours, blue is XK node hours.

days' notice. That lone event was a security-related update performed the same day it was announced and was transparent to those using the system. It was deemed important enough not to wait for seven days. We treated it as less than 24-hour notice.

Service requests do much more than just report trouble. They also include requests for advanced support, expanded assistance, added services, and suggestions. Fig. 3 shows the relative frequencies of different types of partner service requests in the first quarter of 2014. The total number of service request during the quarter was 388. Accounts & Allocations and Applications, the two largest categories, each made up about a quarter of the requests. All accounts were installed within one business day following the receipt of all required information. Eighty percent of all other service requests were resolved in less than three business days. Some requests will always take longer than three days to resolve, such as requests for additional software or for help with code optimization; the average time to resolution for these more time-consuming requests was 8.2 business days.

PROCESSOR USAGE

From April 1, 2013, through March 31, 2014, partners used more than 135 million node hours on Blue Waters (more than 4.3 billion integer core equivalent hours).

The job size corresponding to 50% of the actual usage is 2,048 nodes (65,536 integer cores) for the XE portion and 1,024 nodes for the XK portion of the Blue Waters system, marked using horizontal lines in fig. 4 and fig. 5, respectively. Note that the horizontal scale on both of these figures is logarithmic. Overall the XK nodes delivered 15.9% of the node-hours, which is only slightly higher than their relative fraction of the overall compute node count.

Fig. 6 presents another view of the usage per job size, where jobs have been categorized by their size (hereafter referred to as "not large", "large", and "very large"). Large jobs are defined as those using from 1-2% up to 20% of the system size for the respective node types, with not large and very large below and above those cutoffs.

Note that a not large job on Blue Waters is actually larger than a full system job on many other systems. Very few systems in the world have more than 20% the number of nodes on Blue Waters, and almost all of them have slower processors.

As a percentage of their respective totals, XE very large jobs accounted for 15.4% and XK very large jobs accounted for 57.7% of the node hours used.

Expansion factor is an indication of the responsiveness of the resource management to work submitted by the science and engineering teams. Expansion factor is defined as the time the job waits in the queue plus the requested wall time of the job divided by the requested wall time of the job. On many systems, larger jobs are typically more difficult for the system to schedule. However, on Blue Waters the emphasis is on offering an environment where the partners can take full advantage of the size and unique capabilities of the system. For example, the scheduler has been configured to prioritize large and very large jobs, thus making it easy for the partners to run their applications at scale. Not large jobs wait in the queue for less time than the requested wall time, on average, independent of the node type. Large jobs take about one to two times the requested wall time to start running, with jobs on XE nodes starting sooner than those on XK nodes. Very large jobs wait in the queue for four to six times the requested wall time while Blue Waters collects the resources needed for such a massive job. All in all, Blue Waters is very responsive and provides exceptional turnaround to the teams for all job sizes.

As might be expected, the most common run time is the current queue maximum of 24 hours (fig. 7). XE jobs have a larger distribution of run times, likely due in part to their much larger node counts. Long run times are generally beneficial to partners since it reduces the overhead cost of job startup and teardown.

Comparing the breakdown of Blue Waters node-hours usage by science discipline, Biology & Biophysics and Particle Physics each consume slightly more than a quarter of the node hours (fig. 8). Astronomy and Astrophysics is next in line with 17% of the node hours, followed by Atmospheric & Climate Science, Fluid Systems, and Chemistry, each of which use 6-7% of system time.

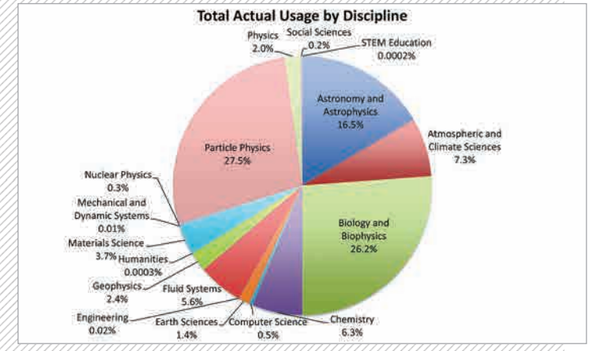


FIGURE 8: Distribution of annual actual usage per discipline area across all allocated projects.

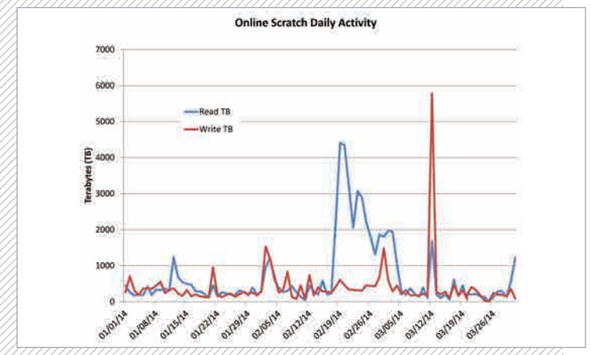


FIGURE 9: Scratch file system daily activity. Blue is read, red is write activity.

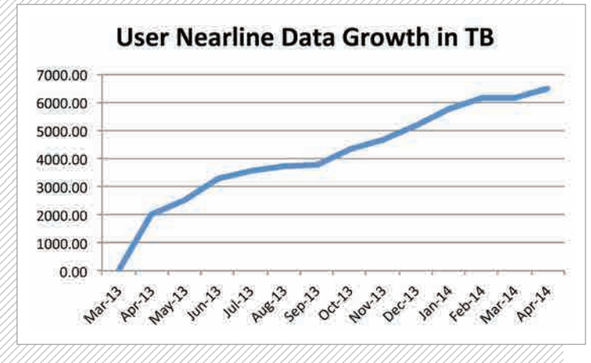


FIGURE 10: User data storage growth in the Blue Waters nearline storage.

STORAGE USAGE

The Blue Waters system has three separate file systems totaling 35 raw PB (~26 usable PB): /home, /project, and /scratch. Home directories default to 1 TB and project directories default to 5 TB for each project. Both are managed with user/group quotas and neither is purged. Partners/Projects can request more space in their project directory as needed. Additionally the partners have access to the world's largest nearline tape storage system.

The /scratch file system consists of 21 PB of useable space. Files are purged if they have not been accessed within 30 days. This allows for very large quotas for many teams. The default quota for the scratch directory is 500 TB per project; many teams and partners are granted increases to the default limits for specified time periods by special request.

Fig. 9 shows an example of /scratch file system activity January-March of 2014. The /project and /home file systems show similar variability with much lower activity levels on the order of tens of terabytes in the home directories and hundreds of terabytes in the project directories, as expected.

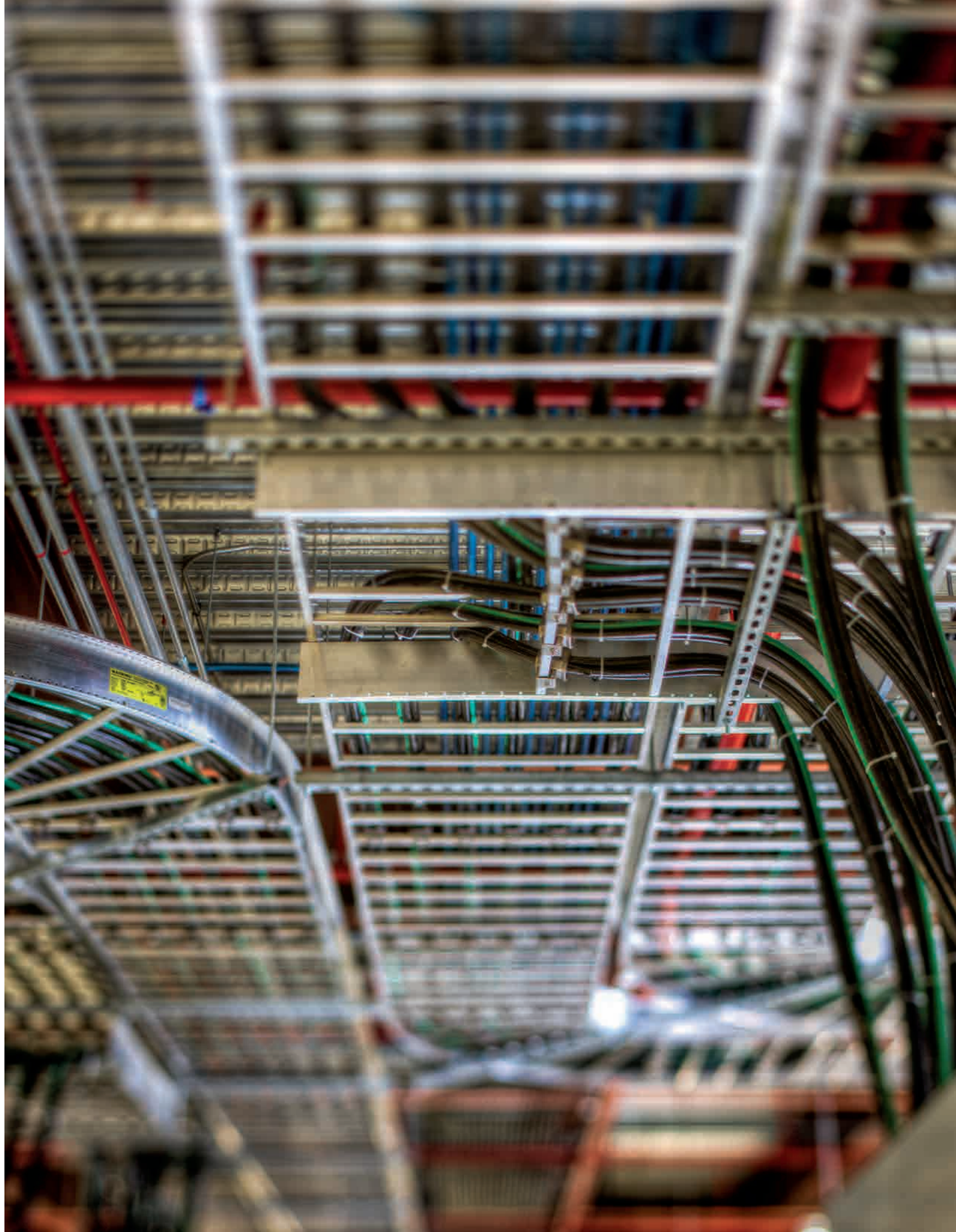
At the time of this writing, there are 55 partners in 26 projects actively storing data in the Blue Waters nearline tape subsystem for a total of 6.5 PB of data and more than 44 million files by the end of the first year of production (fig. 10). Two very large projects have stored more than 1.2 PB each.

WRAP UP

The metrics presented for the first year of service are high level and very brief. Blue Waters may be the most instrumented system in the world, as we collect more than 7.7 billion monitoring data points every day to help us understand, assess, and improve how well Blue Waters is serving our partners. As discussed above, Blue Waters users, stakeholders, and reviewers believe our quality of service is exceeding expectations.

METRIC	TARGET	DATA FOR 1/1/2014-3/31/2014
Service requests are recorded and acknowledged in a timely manner	95% of partner service requests are acknowledged by a human-generated response within four working hours of submission	96% of partner service tickets had a human-generated response within four business hours **EXCEEDS EXPECTATIONS**
Most problems are solved within a reasonable time	80% of partner service requests are addressed within three working days, either by - resolving them to the partner's satisfaction within three working days, or, - for problems that will take longer, by informing the partner how the problem will be handled within three working days (and providing periodic updates on the expected resolution)	80% of partner service requests were resolved within three business days **MEETS EXPECTATIONS**
Accounts are installed in a timely manner	95% of accounts requests are installed within one working day of receiving all necessary information from the partner/project leader.	100% of account requests were resolved within one business day of receiving all the required information from the partner. **EXCEEDS EXPECTATIONS**
Providing timely and accurate information	All planned system outages announced at least 24 hours in advance.	100% of planned system outages were announced at least 24 hours in advance. **MEETS EXPECTATIONS**
	All major upgrades and planned system changes announced at least seven days in advance.	50% - One security related update was performed the same day as the announcement. **BELOW EXPECTATIONS** Two planned outages had less than seven days' notice, one six days 20 hours, the other six days and 8 hours.

TABLE 1: Metrics for service request response and resolution time.



SYMPOSIUM WORKING GROUP REPORTS

DATA @SCALE

Two group discussions were organized at the 2014 Blue Waters Symposium by taking an application-driven approach to addressing application characteristics tied to technical requirements for current and future scenarios in data @scale. The discussions focused on addressing full life cycles of data @scale innovation; data archiving and sharing; algorithms, software and tools; education and workforce development; and challenges and opportunities.

Discussion questions
The following discussion questions were posed to the group participants.

General:
- What are the major challenges of data handling for your applications?
- What new architecture, software, and tools will likely improve your data @scale practices?
- What should the National Science Foundation, the University of Illinois at Urbana-Champaign, and the National Center for Supercomputing Applications be doing to help your projects achieve desirable data handling?

Data Movement:
- How easy and practical is it to move your datasets today?
- Is it sufficiently fast and simple?
- Are today's software and tools adequate for your data movement needs? If not, what are your recommendations for addressing the inadequacies?

Data Sharing:
- What are your requirements for sharing your data within your community? What about publicly?
- What obstacles do you face that complicate your data sharing?
- How could today's software and tools be improved to advance data sharing capabilities?
- What is missing from today's capabilities?

Analysis, Software, and Tools:
- What are major limitations of current software and tools for your data handling?
- How do these limitations affect your projects?
- Do you have any suggestions for eliminating these shortcomings?
- Do you need any software and tools for data handling that are important to your projects but currently missing?

With the wide range of domains represented, data handling requirements are significantly different with regard to data I/O patterns (e.g., from one file per process to single shared file per application), file sizes (e.g., from a few kilobytes to a terabyte or more), software, and tools (e.g., MPI-IO, NetCDF, HDF, BoxLib). Furthermore, data analytics is diverse across domains. For example, for simulation-centric applications, pre- and post-processing still represent typical scenarios while there is an increasing trend toward enabling *in situ* analytics and using visualization as a key input for steering simulations.

Specific requirements for data @scale capabilities include management of not only data but also metadata. Both data and metadata are expected to grow explosively in nearly every domain due to continuing improvements of observational technologies and data-intensive scientific practices as well as the anticipated increase in computing power in the foreseeable future. A major challenge in scalable management of data and metadata is validation and verification, especially considering the related challenges of fault tolerance on the computing side.

Another major requirement addressed was data archiving, sharing, and movement. Generally speaking, data archiving, sharing, and movement facilitate scientific data analysis that sometimes takes longer than the length of a project allocation on Blue Waters. Meeting the requirements for scientific analysis of massive simulation datasets by pertinent communities therefore demands innovative mechanisms and services for data archiving, sharing, and movement.

Recommendations
The following key recommendations were synthesized based on the group discussions.

Address the full life cycle of data:
- Avoid the need to move data for analysis and visualization
- Support data access beyond allocations to maximize scientific analysis and impact
- Enable analytics where data are located
- Provide dedicated resources for data analysis

Data archiving and sharing:
- Provide data repository with efficient access
- Enable easy and secure data sharing
- Minimize impact on computational work (i.e., decouple file systems from compute nodes such that post-processing does not impact simulations and vice-versa)

Algorithms, analysis, software, and tools:
- Provide common libraries and utilities for data manipulation @scale
- Use machine learning to extract data out of large generated datasets
- Support data compression for efficient storage and transfer
- Extend access to nearline storage for analysis
- Provide software-as-a-service support for data analytics @scale
- Build fault tolerance capabilities into applications

Education and workforce development:
- Improve education of application scientists regarding the capabilities for the state-of-art data management, analysis, and visualization
- Foster synergistic education efforts on data science and HPC capabilities

A number of science scenarios were discussed to elucidate these recommendations.

Donald J. Wuebbles, a climate scientist at the University of Illinois at Urbana-Champaign, described a scenario in which petabytes are easily generated on Blue Waters by running 30 different climate models. How can we manage and quickly sift through such data @scale while enabling pertinent scientific communities to access related data and metadata? Furthermore, data size and complexity will continue to increase significantly as climate models pursue high spatiotemporal resolutions with improved assimilation of observation data. Several scientists also mentioned that their current simulations easily generate terabytes or even petabytes of data. These datasets are often too big to be moved anywhere else. Generally, scientific communities need and would benefit from have long-term access to examine such massive simulation datasets, which naturally leads to increased data searching, publishing, sharing, and movement requirements. The National Data Service initiative led by NCSA was brought up as a fundamental solution to meet such requirements.

While computational simulation represents a major source of big data on Blue Waters, the ability to handle other sources of big data has become increasingly important. Scott Althaus, a political scientist at Illinois, described a scenario in which his project needs to move multiple terabytes of text data onto Blue Waters to develop scalable data analytics and suggested there should

be opportunities to implement fast, easy to use, and secure data transfer services for long-tail scientists who might not be familiar with related high-performance computer tools.

Multiple discussions emphasized that data analysis workflows typically require interactive access to computational resources, for which the job queue management approach does not work well. The allocation of data @scale resources also needs to consider both computing and storage requirements, coupled with software capabilities and customized to application characteristics in a cloud fashion. It is important to understand how to support data-centric computational resources such as those based on Apache Hadoop for enabling data-intensive analysis workflows that need to be integrated with Blue Waters.

The participants of the working group were asked to envision grand science drivers for data @scale innovation. Larry Di Girolamo, an atmospheric scientist at Illinois, posed the question: How do we fuse petascale (or beyond) data from multiple geographically distributed sites to generate new scientific data products? Patrick Reed, a professor of civil and environmental engineering at Cornell University, asked the question: How do we perform interactive data analytics @scale for steering simulations? These questions suggest that the convergence of computational and data sciences is both desirable and synergistic. Such convergence is expected to fuel innovative integration of computing, data, and visualization capabilities. A great example of this is a typical workflow in CyberGIS (geographic information science and systems based on advanced cyberinfrastructure), where geospatial scientists from many domains focus on scientific problem solving with seamlessly integrated compute-, data-, and visualization-driven capabilities provided through CyberGIS software and tools.

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MANY-CORE COMPUTING

Science teams that use accelerators code close to the hardware for the most part (CUDA, or custom code generators). A couple of teams opt for a portable approach to accelerators so that they can leverage PHI and NVIDIA architecture with a single code base using OpenCL or a portable library like Thrust. The cost of porting to accelerators is seen as high (approx. one year's effort for a good programmer) and that's been a barrier to uptake by smaller teams. Going forward, there is hope that the next generation of accelerators will be on the motherboard, which is anticipated to improve memory performance issues experience with the current PCI-based approach. There is a strong desire for a portable language (OpenMP 4 or OpenACC), but at this time it is not clear which of those will endure.

The state of many-core

Hwu opened the first day of discussion with a review of the hardware differences between Blue Waters and Titan. Several of the known challenges were listed (small DRAM, programming, experience in production, etc.) and he described early success stories like NAMD, Chroma, and QMCPACK. While accelerator usage is high, the number of teams using them and the diversity of applications on the XK nodes is less than we hoped.

We then covered a handful of broad questions about accelerator usage to get feedback from the teams.

1. How portable is accelerator code and what is being done to address issues of portability?
Most teams believe this is a big issue and a challenge they need to address as they look into adapting code for use on accelerators. Beyond that, the response of the science teams varies. Some teams are still waiting for a winning standard (perhaps OpenACC?) or cannot justify the porting expense at this time. With CUDA, you are locked into a vendor (NVIDIA). OpenMP 4 has "Open" in the name, but so far only Intel supports it well. Other groups have engineered code generators into their build and can target specifically X86, NVIDIA, or another core architecture effectively. Two software technologies that are portable between different architectures today—OpenCL and the Thrust C++ Cuda library—revealed a ray of hope. A few teams are using those now to generate code across all architectures.

2. What issues prevent you from porting your work to many-core accelerators and what would make it more viable?
Answers to this question reflected some of the same themes from those for question one but with a few twists. Hardware limitations and perceived performance gains are big factors. There were several performance horror stories about MPI on Xeon PHI; OpenMP threads or Intel libraries are currently the ways forward on Xeon PHI. On the software side, getting started in CUDA is still perceived as a bit of a barrier, and one team requested more sample codes and how-to style programming guides to get up and running.

The porting process is seen as a cost to the teams. In some cases, the low memory-to-core ratio compared to general purpose CPU cores requires significant algorithm changes. Science teams may not consider adding a computer science staffer to their project as furthering their science, especially if the payoff cannot be quantified up front. They perceive a significant risk that performance gains may not be realized even if they invest time and resources in porting their code to the accelerators.

3. Which tools do you find most (or least) useful with accelerators (profiling, counters, debuggers, etc.)?
There was universal agreement that vendors should focus on Linux and HPC as well as Windows (or perhaps instead of Windows). Many times, a tool waits an entire release cycle or more before it is ready for Linux. Science teams are less interested than HPC center or vendor staff in vendor tools. Most teams that are serious about performance are timing their own codes and are proud of that work. If this is the preferred approach, a possible path forward is to focus on more timing APIs and libraries that are open, performant (high resolution), and portable. TAU (Sameer Shende, University of Oregon), for example, is widely regarded and respected as a great all-purpose tool that is portable, but its learning curve is not trivial.

4. Are you planning algorithm changes that would lead to better use of accelerators?
Teams that have not done so need to resolve the lower memory-to-core ratio they would have available on many-core devices. One brave person asked the question we all consider when starting a move to accelerators: Will the time I spend working on algorithm improvement be worth it if I realize just a 1.5 or 2.0 x speedup?

Many-core in the future

On the second day of the working group, we discussed Intel's (Arnold) and NVIDIA's (Hwu) hardware and software roadmaps.

- The PCI bus is a limiting factor for both brands of accelerators and the future seems likely to bring the accelerators to the motherboard. Intel's Knight's Landing version of the Xeon PHI is reported to support that capability, and NVIDIA is moving ARM processors (running Linux) closer to the accelerator (see the NVIDIA Jetson board). We can expect more progress from NVIDIA in closing the physical gap between processors and accelerators as we have seen with the PHI.

- Memory bandwidth and size are both increasing in next-generation hardware. As nodes become more compute capable (more threads and cores via many-core), the network bandwidth is not expected to keep pace and system balance is probably going to suffer. We may have to all learn to program like Paul Woodward.

- Teams greatly desire access to device memory, similar to GPUDirect from NVIDIA and Infiniband available through Intel and others. Lowering the latency by copying data only once (or not at all for upcoming motherboard socket-based accelerators) is a big performance boon.

- We discussed the topic of weak vs. strong scaling. Not all codes behave the same way and science teams require widely varying algorithms for their science. It is difficult to build one system that handles both types of codes equally well.

- Whatever the next generation brings, it should come with hardware performance counters and support for tools that report the single-core performance in a straightforward way. Scaling starts with core 0 (well, 1 for Fortran). There is no motivation to do better if you cannot tell how you are doing right now.

- The teams on Blue Waters get their network performance metrics by direct observation. Many teams have detected torus issues via variations in the wall clock time per simulation time step. The next machine should have more bandwidth and a better scheduler that can optimize geographic placement (topology) of jobs to fully benefit from the communication architecture.

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TRACK-1 SYSTEMS: TRENDS AND NEEDS

After just one year of service, the current NSF Track-1 supercomputing system, Blue Waters, supports over 120 science teams and almost 600 of the country's leading scientists. It has enabled transformative and wide-ranging impacts across a broad range of science and engineering (S&E) disciplines.

Though Blue Waters has years of grand challenge science exploration remaining, now is the critical time to identify the needs and desires of the nation's science, engineering, and research communities for large-scale systems to follow Blue Waters, wherever they are deployed. As one S&E team PI stated, the "first Track-1 system available to the community has set in motion a significant rethinking by NSF investigations of what is possible and what is practical. It would be a very bad idea to nip this flowering of very large-scale computation in the bud" by not having a path forward beyond the useful life of the first Track-1 system.

While all teams indicated the need for more computational and analytical resources and more networking, the needs of S&E communities are diversifying as large instruments generate huge quantities of data that must also be processed and analyzed, and as multiple communities will need to work together to address modern grand challenges with multiple computing modalities. Hence, a Track-1 level system—the most powerful class of computation and analysis system available—will need to be embedded more deeply in a diverse ecosystem of instruments, data archives, smaller Track-2 systems, clouds, and digital services to support the diverse needs of the communities NSF serves.

Key trends

The trends derived from the working group at the 2014 Blue Waters Symposium and other sources may be evident first in best-of-breed implementations (aka, breakthrough, hero, grand challenge) calculations. Best-of-breed applications typically address a scientific discipline's very important yet previously infeasible problems; Track-1 systems enable solutions. Community standard practices advance as other science teams adopt the best-of-breed techniques to solve different, new problems. These are the trends that emerged as we move to the second generation of Track-1 systems:

1. Changing workflow methods to accommodate computational methodologies. When size prohibits saving entire large datasets, the use of *in situ* visualization and analysis to reduce data movement and speed time to solution becomes necessary. This trend also involves the integration of some high-throughput work to analyze and reduce large-scale simulation results.
   a. Support of data streaming pipelines for deadline-driven analysis for experimental and observational systems such as LSST, LIGO, and genomic sequencing. These could be primary support for experimental projects or back-end expansion and will require more integration of workflow and resource management methods.
   b. Use of visualization to interpret and understand the simulation and analysis results, whether *in situ* with simulations or after the simulation or analysis.
   c. Malleable/elastic resource management for application load balancing and resiliency.
   d. Automation through workflows to support repeatability of computational/analytical solutions.
   e. Use of data model programming methods, often combined with more traditional math model programming methods in a single application or workflow.

2. Increased integration with data sources and increased use of simulation data products.
   a. Using data from multiple experiments and observations to set up the initial conditions for simulation is common in many fields. For example, in computational biology the interpretation of multiple experimental inputs requires computation of atomic-level models of very large macromolecular systems, like the capsid of the AIDS virus, that are consistent with all experimental data types.
   b. Assimilating observation data, steering during simulations, and/or extensive post analysis and validation (e.g., weather, climate, solar physics).
   c. Many traditional best-of-breed modeling and simulation teams are realizing that using Track-1 systems enables them to produce community datasets that are then useful for others to analyze in different ways.

3. The need to dramatically increase fidelity* in models and simulations to improve insights and address new problems. Fidelity increases tend to be domain specific, but lead to more accurate predictions and increases in the scope of the problems that can be simulated.
   a. Increasing use of multi-scale and multi-physics. These are needed to accurately explore simulated phenomena.
   b. Increasing resolution. Many areas require orders-of-magnitude increases in resolution to provide better insights. This is realized by finer grids, more elements or atoms, more particles, etc., and by increased resolution in observations. A key example is modeling turbulence of complex flows and chemistries.
   c. Increasing complexity. Increased understanding in physical models and simulation studies, combined with increased detail in experiments and observations, drives the development of more complex models and simulations with more attributes, more physical sub-processes, and higher degrees of precision. Examples include the use of full-cloud models in weather and climate rather than parameterizations, direct calculation of turbulence in fluids, and complete treatment of fluids, magnetic fields, nuclear equations of state, and radiation transport for multiple particle species in relativistic astrophysics.
   d. Increased number of ensemble† trials. Ensembles provide statistical or other information for uncertainty quantification and probability analysis. For example, weather predictions may have up to 50 to 75 ensemble members for a single prediction. Materials, structures, biophysics, and astrophysics also use ensembles. Note that this does not imply smaller-scale runs, but rather more runs at scale (32,000 to 320,000 core equivalents).

4. Longer simulated time periods are often required to accurately simulate the system of interest. Sometimes long simulated time periods are the result of increases in fidelity. However, simulations of larger systems often require longer periods of time to stabilize, and in many problems the time scales of natural processes are longer than current simulations (e.g., in the magnetosphere, global effects can occur on scales of days whereas kinetic simulations currently can only simulate several hours).

5. A long-range investment program for computational and analytical resources is required to go beyond the S&E of today and be competitive in the world. To make major improvements in the capability of S&E applications often requires development, testing, and optimization at scale before production S&E investigations can be performed. The time line for NSF-related facilities, such as LIGO and LSST, extend well beyond any planned funding for Track-1 and Track-2 resources. Until there is a sustainable investment program that is as long as or longer than the lifecycles of NSF-related facilities, the facilities will continue to create stand-alone and redundant cyberinfrastructure, which in the long run is more expensive for the community.

6. Increased number of problems to address. As it becomes possible for new best-of-breed simulations to study complex systems, the solution of many other important problems also becomes possible, thereby quickly elevating this level of simulation to community standard practice. For instance, the first 100 million all-atom simulations were completed in 2013. By 2020 there will be tens to hundreds of teams doing hundreds to thousands of 100 million atom simulations to solve outstanding problems in biology. Similar situations exist in aircraft and engine design, drug discovery, weather and climate prediction, and many other fields.

7. Changing algorithmic methods. S&E teams will substantially improve their algorithmic methods to reach new research goals over the next five to ten years—not just to address new computer architectures, but also to improve the time to solution independent of hardware changes and to develop the algorithms needed for multi-physics and multi-scale simulations. This is a continuing re-engineering practice that is typically motivated by trying to use new technologies or trying to get better results in the same or less time.

a. Going forward, most S&E teams will change their algorithms to adjust to new system architectures that require more concurrency within and across nodes, less I/O and communication bandwidth, and less memory per core. Additionally, teams will upgrade their algorithms and work methods to improve the quality and efficiency of their science output. An example is replacing particle mesh Ewald (PME) calculation with multi-level summation and higher order PME interpolation in all-atom simulations.
b. Use of adaptive gridding and malleable/elastic resource management will expand for applications load balancing and resiliency. Improving load balancing is critical to overcoming both Amdahl's law limits and the increasing variation in system component performance, while resiliency is needed to address the number of single-point failures in systems with millions to billions of discrete components.

Future systems

The working group estimated possible Track-1 system capabilities and characteristics for three time frames approximately four years apart to show the feasibility of systems that would be able to support the evolving science requirements for the equivalent Track-1 investment level (see table at right). Because of the complexities, costs, and challenges to S&E team productivity involved in managing and moving @scale datasets, it is most effective to have a single system that has a single, integrated communication fabric that can support multiple workflows and modes of computing and analysis. For simplicity of the examples, the characteristics of the alternatives discussed below are based on a single system with homogeneous computational node types. The best value choice for an actual Track-1 system could be a combination of node choices connected with a common interconnect sub-system, a uniform storage name space, and a common, secure software environment, where multiple node types can efficiently run different workloads in a single overall system.

The alternatives presented here are developed based on interpreting vendor and technology roadmaps. Consistent with the NSF Track-1 program goals, a key metric for the Track-1 follow-on is sustained performance for a wide range of S&E applications. Here, sustained performance is defined as time to solution for real science, engineering, and research problems. The optimization target that represents sustained performance in a meaningful manner for evaluation is the Sustained Petascale Performance (SPP)[†] Metric developed as part of the current Track-1 acceptance process.

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DEPLOYMENT TIME FRAME	SYSTEM TYPE	PEAK (PF)	NODES	AGGREGATE MEMORY (PB)	ESTIMATED RUNNING POWER (MW)	BW SPP ESTIMATE (PF)	ONLINE STORAGE CAPACITY (PB)
2012/2013	Reference: current Track-1 – Blue Waters	~13	27,648	1.66	9-11	1.3	36
2016/2017	X86 General Purpose CPU (Based on Intel Skylake Processor)	~55	~19,200	~3.5	9-10	7-9	~200
2016/2017	Intel Many Core (Based on Intel's Knight Landing Processor)	~100	~26,500	~2.3	8-10	6-10	~200
2016/2017	X86 CPU with NVIDIA GPU (Based on Intel Skylake Processor with NVIDIA GPU)	~100	~21,000	~1.2	9-11	7-11	~200
2020/2021	General Purpose CPU System	~200	~30,000	~10	12-14	40-50	~400
2020/2021	Accelerated, Many Core System	~500	~30,000	~4.0-10	8-10	40-50	~400
2024/2025	Accelerated, Many Core System	~1,200	~30,000	~15-30	15-20	100-200	~1,000

* In this document *fidelity* means "accuracy in details" of the science problem.

† In this document *ensemble* means running the same application and basic problem but with different initial conditions and/or system parameters in order to obtain high-confidence results and provide new insights. It may also mean running the same problem using different applications. It does not mean running different problems.

‡ Kramer, W., How to Measure Useful, Sustained Performance. *Supercomputing 2011 Conference (SC11)*, Seattle, Wash., November 12-18, 2011.

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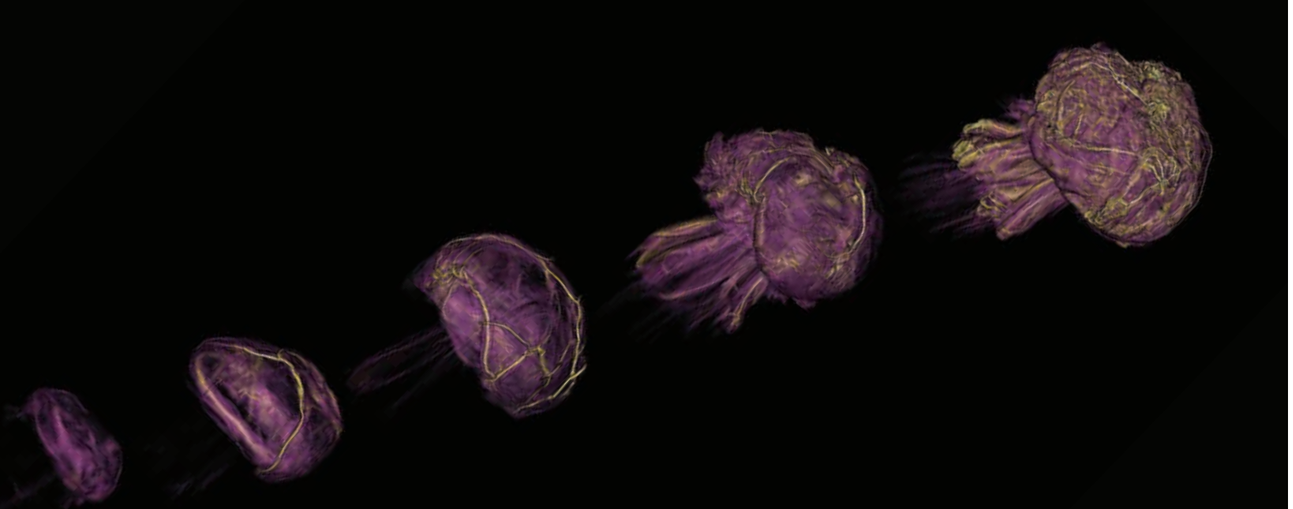

THE DEFLAGRATION PHASE OF CHANDRASEKHAR-MASS MODELS OF TYPE IA SUPERNOVAE

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EXECUTIVE SUMMARY:

The unique resources of Blue Waters are used to address an important unsolved problem in computational astrophysics: the propagation of turbulent nuclear combustion inside a Type Ia supernova. Adaptive mesh refinement allows the burning front to be modeled with an unprecedented effective resolution of $36{,}864^3$ zones (~136 m/zone; compare to typical 1 km/zone found in the literature). The initial rise and expansion of the deflagration front are tracked until burning reaches the star's edge (~0.8 seconds). Pre-existing turbulence affects the propagation only at the earliest times and, even then, only for nearly central ignition. Even central ignition—in the presence of a background convective flow field—is rapidly carried off center as the flame is carried by the flow field. Overall, very little mass is burned in our models, resulting in very little expansion of the star; any subsequent detonation will therefore produce an exceptionally bright supernova.

INTRODUCTION

Type Ia supernovae (SNe Ia) are thermonuclear explosions of white dwarf stars made unstable by accretion of matter from a binary companion. Once the burning is underway, a subsonic flame burns through the star in about a second, turning carbon and oxygen fuel into mostly radioactive ^{56}Ni ash. The amount of fuel that burns, and hence the energy and brightness of the supernova, is very sensitive to details of the flame propagation. This is a complicated problem because prior convection made the fuel turbulent and the burning itself creates more turbulence.

Understanding exactly how SNe Ia explode has been a challenge of astrophysics for several decades. However, SNe Ia have been used as standardizable candles—objects of inferred intrinsic brightness that can be used to measure cosmological distances. Using SNe Ia in this way lead to the discovery of the accelerated expansion of the universe.

In the Chandrasekhar-mass (MCh) model, a single white dwarf accretes material from its companion, slowly compressing and heating the core of the white dwarf until it is hot enough to enable carbon fusion and drive convection. This simmering phase lasts a century before the burning triggers a thermonuclear runaway near the center of the star, producing a flame

(deflagration) in the turbulent interior of the white dwarf.

At its birth, the flame is less than a millimeter in thickness. Full-star calculations attempting to resolve the initial flame while simulating the entire star would need to cover length scales spanning more than ten orders of magnitude. This is not feasible with current supercomputers without approximations. However, modeling the effects of the turbulence is very important for flame propagation as the small-scale turbulent eddies can wrinkle the otherwise smooth flame, subsequently increasing its propagation speed.

METHODS AND RESULTS

There have been few highly resolved studies of nuclear combustion inside stars and none at this resolution. Several novel results emerged.

One was a better understanding of how the burning spreads. Five distinctive phases were observed: (1) nearly isotropic spread by laminar burning; (2) early floatation and the emergence of a single "vortex ring"; (3) fracturing of that ring and the development of more isotropic turbulence; (4) nearly constant-angle floatation with burning by entrainment; and (5) spreading by a lateral pressure gradient as the flame neared the surface. Each phase was successfully compared to analytic approximations.

Another aspect was exploring the effect on the burning of the turbulence initially present on the grid from prior simmering. We directly mapped the results of our previous simmering calculations (done elsewhere) directly into Castro for further evolution. For a typical ignition location (about 40 km off center) the background turbulent flow field had only a minor effect on flame propagation and nucleosynthesis. If one artificially chooses a more centrally located ignition point where the flame floats slowly, then the flame has more time to interact with the turbulent field, leading to more distortion of the flame and larger changes in nucleosynthesis. In the limiting case of central ignition, the presence of a turbulent field causes the flame to be pushed to one side and possibly entirely off center; the MCh model for SNe Ia produces asymmetric explosions, even in the fortuitous case of igniting a sphere at the white dwarf's center.

Our initial conditions used a single, 2 km radius ignition point. Previous studies in the literature have used ignition "points" 50 to 200 km in radius. Others have (unrealistically) used tens to hundreds of smaller (10 or 20 km in radius) ignition kernels distributed about or near the center of the white dwarf. One consequence of using our small ignition point is that less material burns and the white dwarf expands less than in other studies. This implies that if the flame turns into a detonation, the detonation will burn through relatively high-density material, producing copious amounts of ^{56}Ni and an extremely bright supernova. On the other hand, if a detonation does not occur the amount of ^{56}Ni produced solely during the deflagration will yield an extremely faint supernova. The results of our simulations thus have important implications for the viability of the MCh model to explain the typical SN Ia.

WHY BLUE WATERS

Our prior simulations of the simmering phase in the MCh model showed that ignition occurred in a single zone of roughly (4 km)^3 in size. The requirement to resolve this hot spot with several tens of zones led to an initial fine-level resolution of about 100 m/zone, using adaptive mesh refinement.

This configuration required a couple billion zones. As the flame grew, so too did the number of fine zones required to resolve the flame. This is definitely a large-scale, Blue Waters-class problem. The zones were spread over 4,096 MPI tasks, each with 16 threads for a total of 65,536 cores. Checkpoint files made every couple of wallclock hours were between 150 GB and 250 GB in size and made use of Blue Waters' high performance I/O. Being able to quickly dump this data to archival storage via the Globus Online interface made managing the several tens of terabytes of data extremely pleasant.

PUBLICATIONS

Malone, C. M., A. Nonaka, S. E. Woosley, A. S. Almgren, J. B. Bell, S. Dong, and M. Zingale, The Deflagration Stage of Chandrasekhar Mass Models for Type Ia Supernovae. I. Early Evolution. *Astrophys. J.*, 782:11 (2014), doi:10.1088/0004-637X/782/1/11.

FIGURE 1 (BACKGROUND): The color map shows the magnitude of vorticity, with white/yellow being regions of large vorticity and, therefore, relatively strong turbulence. The burning flame initially has a shape similar to a torus or smoke ring. As the burning bubble makes its way towards the surface of the star, the smoke ring shape breaks apart due to the turbulent flow, which pushes strong vortex tubes to the flame's surface. Unlike a smoke ring, however, our flame is continuously powered by thermonuclear reactions and does not dissipate within the star. Eventually, the vortex tubes penetrate the whole of the flame and the bulk flow inside the flame becomes turbulent. This leads to an accelerated entrainment of fresh fuel and increased burning.

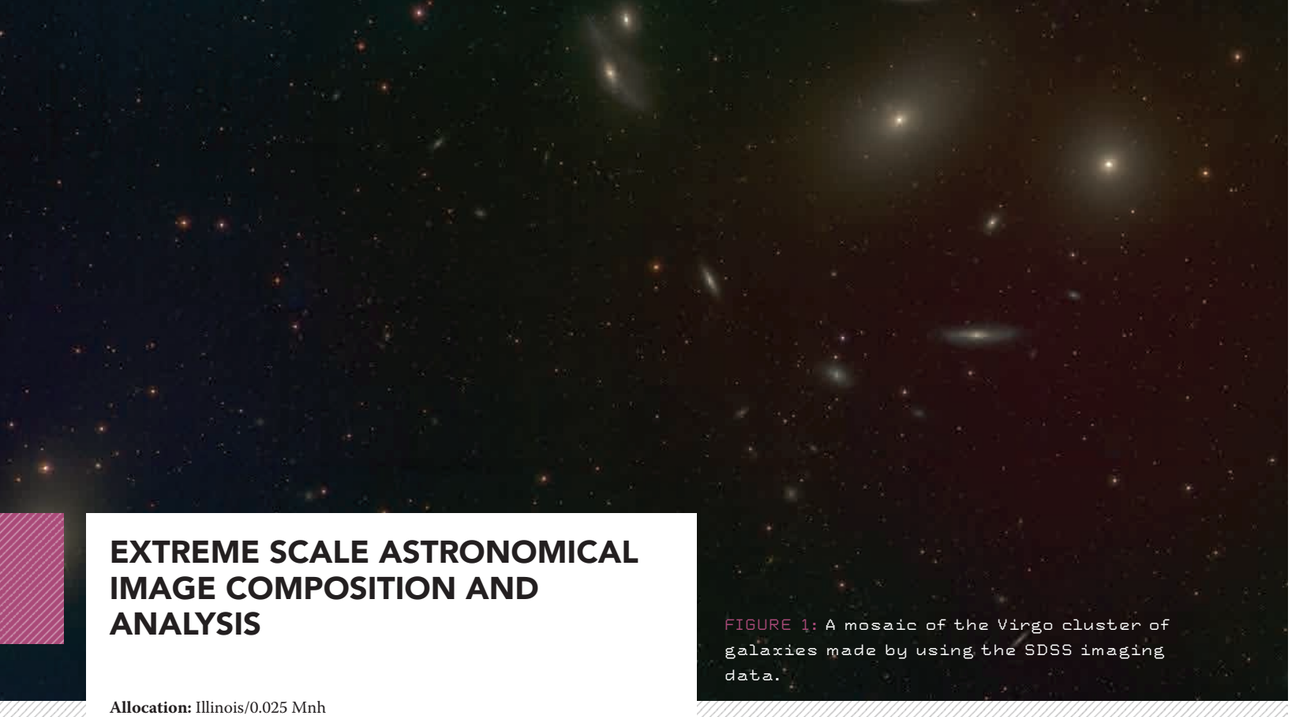


FIGURE 1: A mosaic of the Virgo cluster of galaxies made by using the SDSS imaging data.

EXTREME SCALE ASTRONOMICAL IMAGE COMPOSITION AND ANALYSIS

Allocation: Illinois/0.025 Mnh
PI: Robert J. Brunner[1,2]
Collaborators: Britton Jeter[2]; Harshil Kamdar[2]; Eric Shaffer[2]; John C. Hart[2]

[1]National Center for Supercomputing Applications
[2]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

We are using Blue Waters to create large-scale images from ground-based sky surveys. Projects like the recently completed Sloan Digital Sky Survey and the ongoing Dark Energy Survey obtain images by using charge-coupled devices (CCDs). These projects built large mosaic cameras by combining many CCDs to tile the focal plane of a telescope. By leveraging an open-source image composition tool, we are taking the individual calibrated images from each CCD and combining them to make large-area mosaic images. In addition, we can use other open source tools to combine large-area mosaics that were taken through different filters to make pseudo-color images of the universe. These images will be used for both public outreach and scientific exploration of the nearby universe.

INTRODUCTION

A standard cosmological model, the so-called Lambda Cold Dark Matter Cosmology (LCDM) [1], posits that we live in a spatially flat universe that is dominated by two controlling parameters: dark energy, which drives the expansion of space, and dark matter, which drives the formation of structure in the universe. Together, dark matter and dark energy account for ~96% of the total matter-energy content of the universe; the other 4% is normal baryonic matter (e.g., protons and neutrons). While quantifying the relative contributions of these dark components is a significant scientific achievement—it was Science magazine's "Scientific Breakthrough of the Year" in 2003 and resulted in the 2011 Nobel Prize in Physics—it also highlights the fact that we know very little about either of them.

A number of major projects are underway to acquire data that can expand our knowledge, like the Sloan Digital Sky Survey (SDSS) [2] and Dark Energy Survey (DES). The petascale Large Synoptic Survey Telescope (LSST) will begin later this decade and was recently deemed the most important ground-based astronomy project by a National Research Council committee in 2010. All of these projects (and others not listed) try to detect stars and galaxies in small image subsets in order to rapidly process the large data volumes. These search techniques find fewer nearby galaxies than the standard cosmological model predicts [3].

To improve detection, we are stitching together the small, calibrated images from the SDSS (and soon from the DES). By creating large, science-grade image mosaics, we can look for new galaxies or coherent streams of stars that are difficult or impossible to identify in the standard image frames.

METHODS AND RESULTS

The SDSS survey has archived over one million images 10 arcminutes by 13 arcminutes, covering 14,000 square degrees across five wavelength bands, and calibrated both astrometrically and photometrically.

For our research, we are porting and optimizing the open-source Montage software to Blue Waters [4]. Currently we are using MPI, although we hope to explore adding OpenMP or OpenACC to capitalize on Blue Waters' capabilities more fully. Initially we used the XE6 nodes, which more closely match our proof-of-concept. Our ultimate goal is to make a single image of the entire SDSS survey in each band. We also plan to incorporate DES imagery.

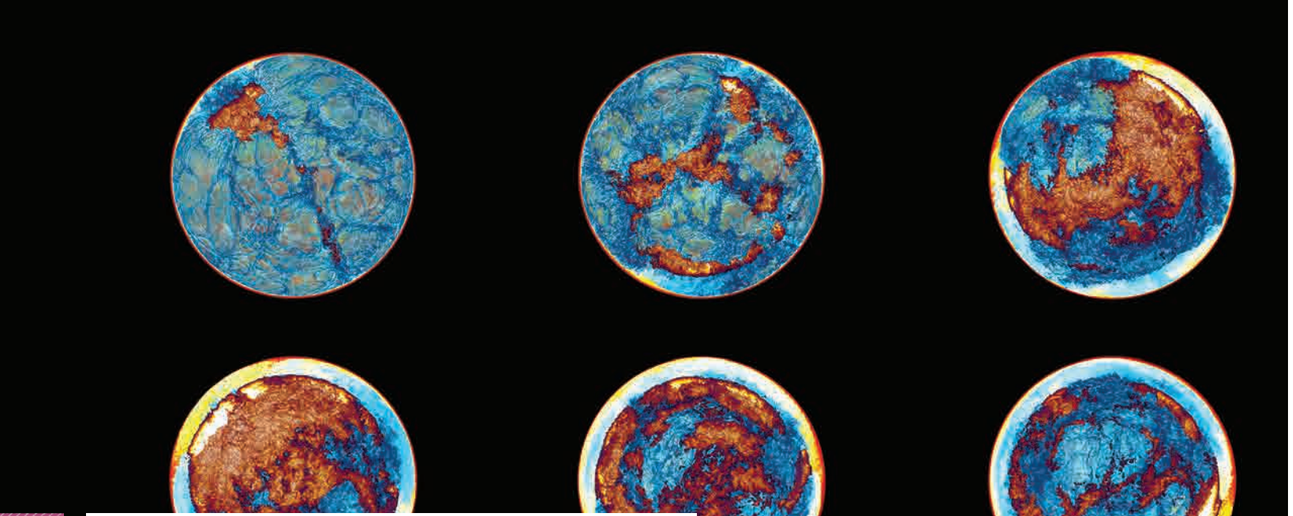
A one-degree square image routinely takes around an hour to create for each of the five SDSS bands (u, g, r, i, and z). Each resulting mosaic is approximately 400 MB, assuming 4 bytes per pixel, and consists of over 100 individual field images (figs. 2-3 shows RGB composites of three different bands). However, intermediate storage needs reach 10 GB per one-degree block because Montage aligns, registers, and stitches the images iteratively for each filter, which requires closer to 2 GB per filter for projection, background correction, and intermediate storage.

Once we finish developing our image-stitching pipeline on Blue Waters, we will extend this software stack to develop hierarchically larger images. (This approach underlies Google Earth and Google Sky.) We keep all data live on the disks to speed up subsequent reprocessing. By building these images, we will support object detection at a variety of levels as well as publish outreach tools and images that allow rapid panning and zooming. We also can use a separate tool called STIFF [5] to convert images taken through different filters into a color composite image for public viewing (as in figs. 2-3). Finally, we will use SExtractor [6], a standard source detection and extraction program in astronomy, to explore SDSS and DES data to look for previously unknown nearby galaxies and tidal streams.

WHY BLUE WATERS

We plan to complete our goal to create a single image of the entire SDSS in each band, each of which would exceed one terapixel, by the end of summer in 2014. The creation and subsequent analysis of each of these images is an extremely large computational challenge that is ideally suited to Blue Waters' large disks system, large memory nodes, and on-board GPU processors.

FIGURES 2 + 3 (RIGHT): One-degree square images made by combining nearly one thousand calibrated images from the Sloan Digital Sky Survey: (top) M51, the Whirlpool Galaxy, and (bottom) the Coma Cluster of galaxies. Each of these images is four times the size of the full moon.



PETASCALE SIMULATION OF TURBULENT STELLAR HYDRODYNAMICS

Allocation: NSF/3.88 Mnh
PI: Paul R. Woodward[1]
Co-PI: Pen-Chung Yew[1]
Collaborators: Falk Herwig[2]; Chris Fryer[3]; William Dai[3]; Michael Knox[1]; Jagan Jayaraj[4]; Pei-Hung Lin[5]; Marco Pignatari[6]; Ted Wetherbee[7]

[1]University of Minnesota
[2]University of Victoria, B. C.
[3]Los Alamos National Laboratory
[4]Sandia National Laboratory
[5]Lawrence Livermore National Laboratory
[6]University of Basel
[7]Fond du Lac Tribal and Community College

EXECUTIVE SUMMARY:

We are exploiting the scale and speed of Blue Waters to enable 3D simulations of brief events in the evolution of stars that can profoundly impact their production of heavy elements. We are focusing on hydrogen ingestion flash events because these are potential sites for the origin of observed, strongly anomalous abundance signatures in stars that formed in the early universe. Hydrogen that is pulled down into a ^{12}C-rich helium-burning convection zone would produce ^{13}C, which is, via the ^{13}C(α,n)^{16}O reaction, a very strong neutron source for the production of heavy elements. These flash events, as well as many properties of how pre-supernova stars evolve, critically depend on convective boundary mixing, which demands a 3D treatment. We simulated H ingestion in a very late thermal pulse star, Sakurai's object, for which detailed observational data is available to validate our simulation methodology.

INTRODUCTION

We are interested in understanding the origin of the elements in the developing universe. Elements heavier than hydrogen and helium were manufactured within stars and later expelled into the interstellar gas to become incorporated in later generations of stars and planets. The first generations of stars played a particularly important role. The late stages of evolution of these stars can be strongly affected by hydrogen ingestion events. The products of nucleosynthesis are later expelled along with the outer envelopes of these stars, contributing to the gradual build-up of the chemical inventory that we find now in our solar system.

The H-ingestion events occur, for example, when a convection zone above a helium-burning shell reaches unprocessed hydrogen-helium gas above it in the asymptotic giant branch (AGB) stage of evolution of such stars. In order to understand the H-ingestion flashes, as well as the evolution of many other types of stars such as the pre-supernova evolution of stars that eventually explode, it is critical to be able to quantitatively simulate convective boundary mixing between the hydrogen-helium gas and the helium-carbon mixture below it.

METHODS AND RESULTS

The simulation of this process, if it is to yield accurate estimates of the elements that are produced, must be carried out in 3D. The entrainment of hydrogen-rich gas at the top of the convection zone is the result of complex, nonlinear shear instabilities which act against the stable stratification of the more buoyant hydrogen-rich gas. To accurately simulate this process we must resolve these unstable waves and also the thin layer in which the composition of the gas changes from the helium-carbon mixture of the convection zone to the hydrogen-helium mixture above. We require a fine grid and a numerical method capable of producing accurate results for modes that are only several cells in wavelength.

When the growing convection zone encounters the hydrogen-rich layers, it is deep in the sense that the ratio of the radii of its top and bottom boundaries is significant (i.e., about two or more). The depth of the convection zone implies that the convection cells that develop within it will be very large, so that only a few of the largest convection cells will fill the entire convection zone volume. Thus, we also require that our problem domain contain the entire convection zone, not just a small sector of it. Finally, we must carry the simulation through many turn-over times of the largest eddies in the convection zone so that entrainment of hydrogen-rich gas can react back on the flow to accelerate entrainment through burning of ingested hydrogen. This process is slow because the initial entrainment is small.

The above challenges to computation are met in this work by the combination of our PPMstar simulation code and the Blue Waters system. Our studies show that grids of $1{,}536^3$ cells are sufficient to deliver accurate simulation of the entrainment of hydrogen-rich gas at the top of the helium-shell flash-convection zone, using the piecewise-parabolic method gas dynamics method and the piecewise-parabolic Boltzmann advection scheme to follow the multi-fluid volume fraction. The result of this work-in-progress is that we have discovered a previously unknown global oscillation of shell hydrogen ingestion (GOSH). The GOSH is shown in fig. 1.

WHY BLUE WATERS

We need to carry our simulations forward for about 6 million time steps, so it is fortunate that our code runs at 10% to 11% of the 64-bit peak performance on Blue Waters when we run such a problem on 443,232 CPU cores in parallel. We see 0.42 to 0.44 Pflop/s sustained performance running in this mode, depending upon the mapping of our job to the machine's toroidal communications fabric. At this rate, it takes about three minutes (~26 time steps per second) to simulate one minute for the star. The hydrogen ingestion flash lasts for about one day, and the simulation shown in fig. 1 simulated 20 hours. It was carried out on the machine in a single four-day interval. Blue Waters is unique in enabling such a large and detailed simulation to be performed in so short a time.

PUBLICATIONS

Woodward, P. R., F. Herwig, and P. H. Lin, Hydrodynamic Simulations of H Entrainment at the Top of He-Shell Flash Convection. *Astrophys. J.*, (submitted) arXiv:1307.3821.

Herwig, F., P. R. Woodward, P.-H. Lin, M. Knox, and C. L. Fryer, Global Non-Spherical Oscillations in 3 D 4π Simulations of the H-Ingestion Flash. *Astrophys. J. Lett.*, (accepted) arXiv:1310.4584.

FIGURE 1 (BACKGROUND): Entrainment of hydrogen-rich gas into the helium-shell flash-convection zone of the very late thermal pulse star called Sakurai's object and the subsequent development of the Global Oscillation of Shell Hydrogen ingestion (GOSH) at problem times 251, 626, 963, 970, 976, and 982 minutes (left to right, top to bottom) since the beginning of the simulation.

Concentrations of entrained helium gas from large to small range in color from red (1.6×10^{-2}) to yellow (1×10^{-3}), white (1.6×10^{-4}), aqua (2.5×10^{-5}), and finally dark blue (3×10^{-6}). Superposed on this image of the entrained gas concentration is the rate of energy release from burning the entrained hydrogen (slowest to fastest combustion: dark blue, red, yellow, white). As combustion causes the entrainment rate to increase, hydrogen ingestion ultimately leads to global oscillations of shell hydrogen ingestion and burning, or GOSH. A movie can be found at www.lcse.umn.edu/MOVIES.

AB INITIO MODELS OF SOLAR ACTIVITY

Allocation: NSF/6.5 Mnh
PI: Robert Stein[1]
Collaborators: Aake Nordlund[2]; Mats Carlsson[3]; William Abbett[4]; Bart De Pontieu[5]; Viggo Hansteen[3]; Jesper Schou[6]

[1]Michigan State University
[2]University of Copenhagen
[3]University of Oslo
[4]University of California, Berkeley
[5]Lockheed-Martin Solar & Astrophysics Laboratory
[6]Göttingen University

EXECUTIVE SUMMARY:

The objective of this project is to understand how solar magneto-convection powers the Sun's activity, heats the chromosphere and corona, and accelerates charged particles. To achieve this we have begun modeling the generation of magnetic fields by dynamo action and their emergence through the solar surface. The first step is to relax a model of solar magneto-convection from the top of the photosphere to a depth of 30 Mm in order to use results from deep convection zone dynamo and flux emergence calculations as boundary conditions for the surface magneto-convection simulations. Simultaneously, we investigate the role of surface dynamo action in the development of active regions.

FIGURE 1 (TOP RIGHT): Horizontally averaged (solid) and minimum and maximum entropy for the calculation relaxing the 30 Mm deep model, as a function of the depth grid number. The entropy at depth has become nearly constant already.

FIGURE 2 (BOTTOM RIGHT): Vertical magnetic field volume visualization with superimposed fluid streamlines looking downward from above. This magnetic concentration has a vortical fluid flow around its surface.

INTRODUCTION

Earth's weather and space weather is controlled by our Sun—by its radiation, by coronal mass ejections into the solar wind, and by energetic particles originating from solar active regions. These, in turn, are controlled by the interaction of magnetic fields, convection, and radiation. How magnetic fields emerge through the photosphere and are shuffled around by the convective motions governs chromospheric and coronal heating and determines the generation of flares and coronal mass ejections. The behavior of magnetic fields at the solar surface is controlled by the solar convective dynamo. New magnetic flux emerging in active regions interacts with existing fields to release huge amounts of energy when the fields reconnect. This heats the local coronal environment to many millions Kelvin and can produce flares and coronal mass ejections. Our project attempts to model this chain of events.

METHODS AND RESULTS

The formation and emergence of solar active regions is modeled by coupling simulations of dynamo-produced magnetic flux rising through the deep solar convection zone using the anelastic code ANMHD with the compressible radiation-dynamics code STAGGER and a chromosphere and corona simulation code called BIFROST. Each calculation provides boundary conditions for the model above it. To couple ANMHD and STAGGER we are extending the surface magneto-convection model downward to a depth of 30 Mm. The roll of dynamo action near the solar surface to emerging magnetic flux and atmospheric heating is also being modeled using STAGGER.

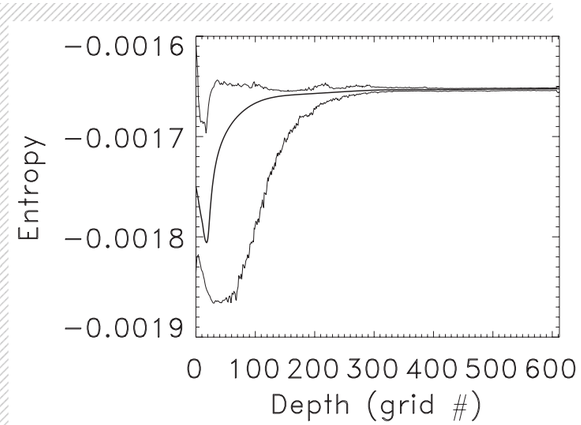
Radiation transfer using STAGGER still takes a significant portion of the time (25%), mostly due to communication. In its current version, which is the result of several months of work by Nordlund, STAGGER runs half as fast on Blue Waters as on NASA's Pleiades supercomputer, but we are able to use 4-8 times as many processors, resulting in a significant speedup. We are working on schemes to run STAGGER on different processors, simultaneously with the magneto-hydrodynamics, in order to further speed up the simulation.

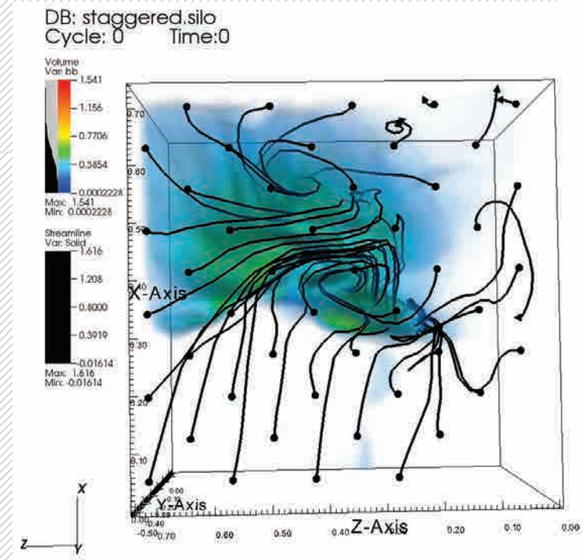
30 Mm extension

The 96 Mm wide by 20 Mm deep extension to 30 Mm depth has completed 5.5 solar hours of simulation so far. The entropy in the extended region is nearly constant and equal to that in the original 20 Mm simulation (fig. 1). The convective and kinetic energy fluxes, however, are several times too large and are decreasing slowly with time. The convective cell structure and temperature-velocity correlations are still in the process of relaxing to their statistically steady-state form. Once this extension is relaxed, ANMHD and BIFROST are ready to couple to it and complete the chain.

Surface Dynamo

The dynamo calculation has a domain 96 Mm wide by 20 Mm deep. Thus far, it has run for 59 solar hours (about 1.25 turnover times) with the most recent 10 hours on Blue Waters at a resolution of 48 km horizontally and 12-78 km vertically on a grid 4032x4032x500. The total magnetic energy has reached 2.7% of the kinetic energy and is increasing slightly slower than exponentially. The magnetic energy is roughly the same fraction of the kinetic energy at all depths (except in the photosphere) and both are power laws in the density.





Subsurface Structure of Sunspots

In our simulations, mini active regions are spontaneously produced by the magneto-convection and downflows without being inserted arbitrarily as initial conditions. As a result we can analyze the subsurface structure of the pores (small sunspots but without penumbra because of the upper boundary condition of a potential magnetic field that we impose at the top of the photosphere). Fig. 2 shows a case of magnetic field lines twisted around a magnetic concentration that penetrates nearly vertically through the surface in one of the pores. Other cases of subsurface braiding of magnetic field lines are found.

Data for Analyzing Solar Observations

As an additional benefit, the datasets produced in the dynamo simulation have been useful for understanding solar observations [e.g., 1]. This data is also being used for analyzing local helioseismic inversion procedures. The data from the flux emergence calculations is being used to analyze Stokes spectra inversion procedures.

WHY BLUE WATERS

To model the emergence of magnetic flux through the solar surface requires simulating the time evolution of magneto-convection for many hours of solar time. To obtain results in a reasonable time requires as many processors as possible. Currently, only Blue Waters provides a substantial number of useable processors. The relaxation of magneto-convection down to a depth of 30 Mm is running on 64,000 processors on Blue Waters. The modeling of dynamo action in the top two-thirds of convective scale heights is running on 32,000 processors.

PUBLICATIONS

Nagashima, K., et al., Interpreting the Helioseismic and Magnetic Imager (HMI) Multi-Height Velocity Measurements. *Solar Physics*, (2014), doi: 10.1007/s11207-014-0543-5.

EVOLUTION OF THE SMALL GALAXY POPULATION FROM HIGH REDSHIFT TO THE PRESENT

Allocation: NSF/9.38 Mnh
PI: Thomas Quinn[1]
Collaborators: Fabio Governato[1]; Lauren Anderson[1]; Michael Tremmel[1]; Charlotte Christensen[2]; Sanjay Kale[3]; Lucasz Weslowski[3]; Harshitha Menon[3]

[1]University of Washington
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FIGURE 1 (RIGHT): Gas distribution for our pathfinder simulation. This simulation represents a uniform cosmological volume that is 80 million light years on a side, contains ~2 billion particles, and is capable of resolving scales down to ~1000 light years. This resolves the morphologies of galaxies down to very small masses and gives us a large statistical sample of interesting objects. We evolved the simulation for ~1.5 billion years, creating a dataset of ~5 TB, which we will use to understand the formation and evolution of galaxies in the early universe.

EXECUTIVE SUMMARY:

Creating robust models of the formation and evolution of galaxies requires the simulation of a cosmologically significant volume with sufficient resolution and subgrid physics to model individual star-forming regions within galaxies. This project aims to do this with the specific goal of interpreting Hubble Space Telescope observations of high redshift galaxies. We are using the highly scalable N-body/Smooth Particle Hydrodynamics modeling code, ChaNGa, based on the Charm++ runtime system on Blue Waters to simulate a 25 Mpc cubed volume of the universe with a physically motivated star formation/supernovae feedback model. This past year's accomplishments include running a pathfinding simulation at one-tenth the needed resolution, which we will use to study overall star formation histories and luminosity functions. We also significantly improved the parallel scaling of the ChaNGa simulation code and demonstrated strong scaling out to 524,000 cores.

INTRODUCTION

Understanding galaxy formation and morphology within a cosmologically significant survey requires the incorporation of parsec-scale physics in simulations that cover a gigaparsec or more. Recent work by our group has shown that with physically motivated subgrid models at roughly the 100 parsec scale, many of the morphological properties of galaxies based on star formation and feedback can be reproduced.

The Cold Dark Matter (CDM) paradigm for structure formation has had many successes over a large range of scales, from Cosmic Microwave Background fluctuations on the scale of the horizon to the formation and clustering of individual galaxies. However, at the low end of the galaxy luminosity function, the CDM theory and observations are somewhat at odds. In particular, the existence of bulgeless, cored small galaxies is not a natural prediction of CDM.

METHODS AND RESULTS

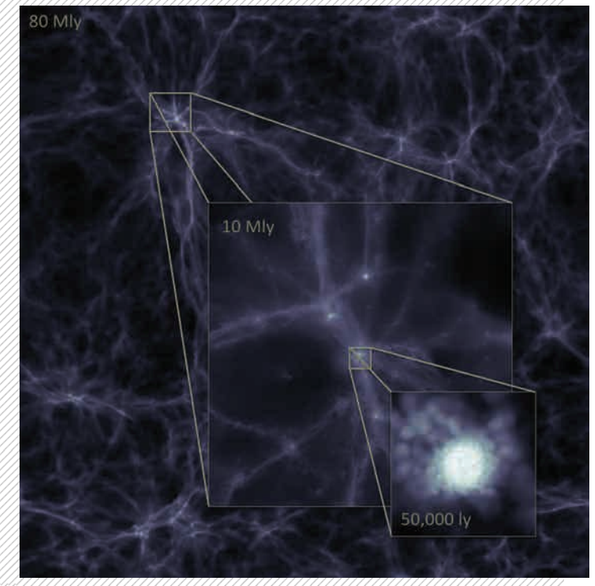
In our previous cosmology work, we used a "zoom-in" technique in which we selected halos from a large dark matter simulation and resimulated those halos with high resolution and gas dynamics. However, this technique has the serious shortcoming that the conclusions can be extremely biased by our selection of halos. Hence a simulation is needed in which all halos within a representative volume of the universe are simulated with high-resolution gas dynamics. Such a simulation is computationally challenging, but it will allow us to answer a number of outstanding questions that are difficult or impossible to answer with simulations of individual galaxies.

For this project, our simulations will model recent Hubble Space Telescope (HST) survey volumes from high redshift to the present with sufficient resolution to make robust predictions of the luminosity function, star formation rate, and morphologies appropriate for these surveys. These results can be directly compared with results from observational programs. We can therefore address some basic issues of the CDM model:

- How are dark matter dynamics and galaxy morphology connected?
- Does the standard ΛCDM model produce the correct number densities of galaxies as a function of mass or luminosity?
- What is the overall star formation history of the universe?

We have improved the scaling of our simulation code by identifying and addressing a number of bottlenecks that only became apparent when scaling beyond 16,000 processors. In particular, we addressed bottlenecks in the load balancing, the domain decomposition, and the tree building phase of our computation. We have moved to a hierarchical load balancer where decisions are distributed among subvolumes. Domain decomposition was both optimized in its serial performance and its communication requirements by reusing information. Treebuilding originally required an "all-to-all" to identify where off-processor tree nodes where located, which has been replaced by a more dynamic algorithm.

We have run a "pathfinding" simulation at one-tenth the mass resolution of our proposed simulation. While this simulation does not have sufficient resolution to study the detailed morphology of individual galaxies, it can tell us about gross morphology and the star formation and merger history of these galaxies. This simulation is now being analyzed to make predictions about the luminosity function and star formation history of high redshift galaxies.



WHY BLUE WATERS

The mass and spatial resolution requirements for reliably modeling galaxy morphology have been set by our published resolution tests. Therefore the size of the simulation we will perform is set by the subvolume of the universe we wish to model. The HST observing program to survey star-forming galaxies in the Hubble ultra-deep field, "Did Galaxies Reionize the Universe?", was awarded hundreds of observation hours to determine the number, nature, and evolution of star-forming galaxies in the Hubble ultra-deep field. The approximate volume of this survey is equivalent to our proposed simulation volume. This volume will not only allow us to make direct comparisons with the survey, but also enhance its scientific return by understanding how those surveyed galaxies will evolve to the present.

This volume size and our required resolution give a total of 12 billion particles of gas and an equal number of dark matter particles. This is just over an order of magnitude larger than simulations that we could run on other resources to which we have access. Hence a sustained petascale facility like Blue Waters is essential for this simulation.

PUBLICATIONS

Menon, H., L. Wesolowski, G. Zheng, P. Jetley, L. Kale, and T. Quinn, ChaNGa: Adaptive Techniques for Scalable Uniform and Non-Uniform N-Body Cosmology Simulation. *Supercomputing 2014*, New Orleans, La., November 16-21, 2014. (submitted)

Quinn, T., Pathways to Exascale N-body Simulations. *Exascale Comput. Astrophys.*, Ascona, Switzerland, September 8-13, 2013.

Quinn, T., ChaNGa: a Charm++ N-body Treecode. *11th Ann. Charm++ Wksp.*, Urbana, Ill., April 15-16, 2013.

MODELING HELIOPHYSICS AND ASTROPHYSICS PHENOMENA WITH A MULTI-SCALE FLUID-KINETIC SIMULATION SUITE

Allocation: NSF/0.78 Mnh
PI: Nikolai V. Pogorelov[1]
Co-PIs: Sergey Borovikov[1]; Jacob Heerikhuisen[1]

[1]University of Alabama in Huntsville

EXECUTIVE SUMMARY:

Plasma flows in space and astrophysical environments are usually characterized by a substantial disparity of scales, which can only be addressed with adaptive mesh refinement techniques in numerical simulations and efficient dynamic load balancing among computing cores. Multi-Scale Fluid-Kinetic Simulation Suite is a collection of codes developed by our team to solve self-consistently the magnetohydrodynamics, gas dynamics Euler, and kinetic Boltzmann equations. This suite is built on the Chombo framework and allows us to perform simulations on both Cartesian and spherical grids. We have implemented a hybrid parallelization strategy and performed simulations with excellent scalability up to 160,000 cores. We present the results of our newest simulations of the heliopause and its stability, which explain the Voyager 1 "early" penetration into the local interstellar medium and help constrain its properties.

INTRODUCTION

Flows of partially ionized plasma are frequently characterized by the presence of both thermal and nonthermal populations of ions and neutral atoms. This occurs, for example, in the outer heliosphere—the part of interstellar space beyond the solar system whose properties are determined by the solar wind interaction with the local interstellar medium (LISM). Understanding the behavior of such flows requires that we investigate a variety of physical phenomena: charge exchange processes between neutral and charged particles, the birth of pick-up ions, the origin of energetic neutral atoms (ENAs), and solar wind turbulence, among others. Collisions between atoms and ions in the heliospheric plasma are so rare that they should be modeled kinetically. As a result, one needs a tool for self-consistent numerical solution of the magnetohydrodynamics (MHD), gas dynamics Euler, and kinetic Boltzmann equations.

METHODS AND RESULTS

Our Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS) solves these equations using an adaptive-mesh refinement (AMR) technology [1]. The grid generation and dynamic load balancing are ensured by the Chombo package, which also helps preserve conservation laws at the boundaries of grid patches. To analyze the stability of the heliopause and investigate the flow in the heliotail, the local resolution of our simulations must be five to six orders of magnitude smaller than in our typical computational region.

We focus on the two latest numerical results obtained on Blue Waters: (1) MHD-kinetic simulations of the plasma flow in a long heliotail, and (2) the heliopause instability as an explanation of the deep penetration of the LISM plasma into the heliosphere [2]. The interstellar magnetic field (ISMF) is draped around the heliotail in Fig. 1. Fig. 2 shows the plasma density distribution in our solar wind-LISM interaction simulations that revealed that solar cycle effects help destabilize the surface of the heliopause and allow deep penetration of the LISM plasma into the heliosphere, which agrees with Voyager 1 observations as it crossed the heliopause in mid-2012 at 121 AU from the Sun. Plasma and magnetic field distributions were used to model ENA fluxes [3] and cosmic ray transport [4]. Our kinetic neutral atom model turned out to be uniquely suited to investigate the structure of the heliospheric bow shock modified by charge exchange [5].

The behavior of plasma and magnetic fields in the vicinity of the heliospheric termination shock and the heliopause is of major importance for the interpretation of data from the Voyager 1 and 2 spacecraft, the only *in situ* space missions intended to investigate the boundary of the solar system. Our team proposed a quantitative explanation to the sky-spanning "ribbon" of unexpectedly intense flux of ENAs detected by the Interstellar Boundary Explorer. Our physical model allowed us to constrain the direction and strength of the ISMF in the near vicinity of the global heliosphere [6,7]. With realistic boundary conditions in the LISM, we simulated the solar wind-LISM interaction and explained the sunward solar wind flow near Voyager 1, penetration of the LISM plasma into the heliosphere, and other phenomena [8,9].

WHY BLUE WATERS

We used new possibilities provided by NSF PRAC award on Blue Waters to model challenging space physics and astrophysics problems. We ported MS-FLUKSS to Blue Waters and used it to solve the Boltzmann equation for ENAs and ideal MHD equations for plasma using a global iteration approach. We implemented the following improvements: (1) plasma data and arrays storing the source terms for the MHD code are now shared among the cores of a single node (this was done by using a hybrid MPI+OpenMP parallelization); (2) load balancing is now a two-level algorithm that guarantees even workload between nodes and threads within a single node; (3) we use parallel PFD5 for in/out operations; (4) full 64-bit support was implemented to allow the code to handle more than 2 billion particles. As a result of these improvements, the code scales well to 160,000 cores [10]. A 650 GB data file containing 10 billion particles can be written in 32 seconds.

PUBLICATIONS

Borovikov, S. N., and N. V. Pogorelov, Voyager 1 near the Heliopause. *Astrophys. J. Lett.*, 783 (2014), L16.

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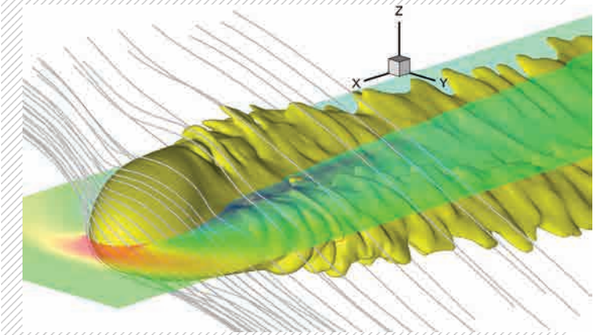


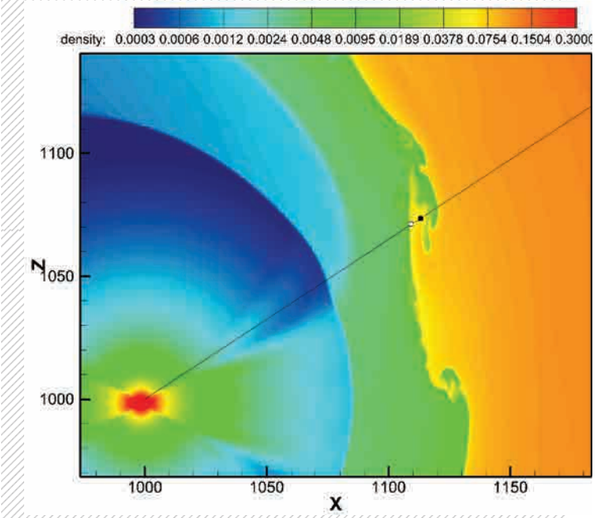
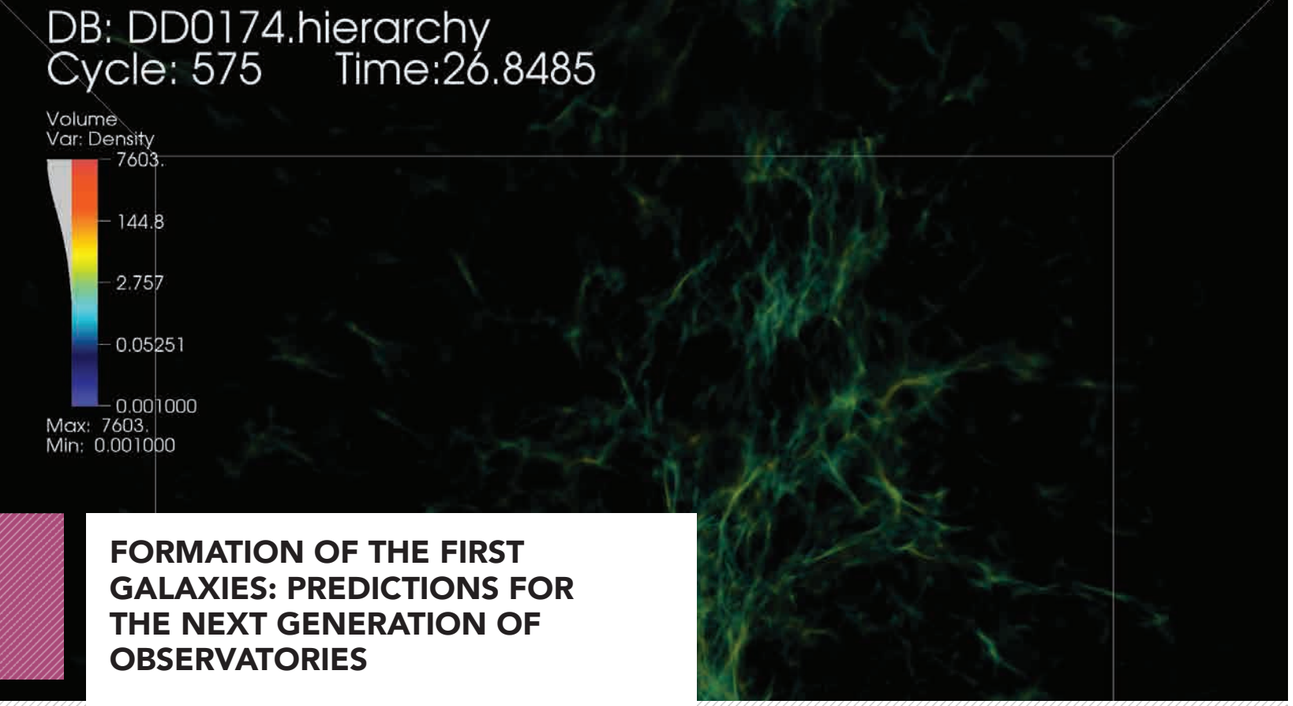


FIGURE 2 (BOTTOM): Plasma density distribution in the meridional plane as defined by the solar rotation axis (vertical in this figure, with the Sun located at the point (1000, 1000) in this plane) and the vector of the LISM velocity at large distances from the heliosphere. The straight black line shows the current Voyager 1 trajectory. The two points on the line show positions of Voyager 1 with an interval of 2 years. One can see the termination shock and the heliopause, which is unstable near Voyager 1 due to a Rayleigh-Taylor instability caused by charge exchange.

FIGURE 1 (TOP RIGHT): Interstellar magnetic field lines draped around the heliopause exhibits violent Kelvin-Helmholtz instability at distances above 1,000 AU in the tailward direction. The heliopause is shaped by the interstellar magnetic field. Also shown is the distribution of plasma density on the solar equatorial plane. The computational grid is a cube with 5,000 AU per side. It extends 5,000 AU into the tail. It is shown that the flow becomes superfast magnetosonic at about 4,000 AU.



FORMATION OF THE FIRST GALAXIES: PREDICTIONS FOR THE NEXT GENERATION OF OBSERVATORIES

Allocation: NSF/7.8 Mnh
PIs: Brian O'Shea[1]; Michael Norman[2,3]
Collaborators: James Bordner[3]; Dan Reynolds[4]; Devin Silvia[5]; Sam Skillman[6,7]; Britton Smith[8]; Matthew Turk[9]; John Wise[10]; Hao Xu[2]; Pengfei Chen[2]

[1]Michigan State University
[2]University of California, San Diego
[3]San Diego Supercomputing Center
[4]Southern Methodist University
[5]Michigan State University
[6]Stanford University
[7]SLAC National Accelerator Laboratory
[8]University of Edinburgh
[9]Columbia University
[10]Georgia Institute of Technology

EXECUTIVE SUMMARY:

We are investigating the earliest stages of cosmological structure formation—namely, the transition of the universe from a dark, empty place to one filled with stars, galaxies, and the cosmic web. In investigating the "cosmic Dark Ages," we focus on three specific topics: (1) the transition between metal-free and metal-enriched star formation, which marks a fundamental milestone in the early epochs of galaxy formation; (2) the evolution of the populations of high-redshift galaxies that will form Milky Way-like objects by the present day; and (3) the reionization of the universe by these populations of galaxies. Using Blue Waters, we have successfully modeled the formation of the first generation of metal-enriched stars in the universe.

INTRODUCTION

The mechanisms that control the formation and evolution of galaxies are poorly understood. This is doubly true for the earliest and most distant galaxies, where observations are limited and often indirect. It is critical to understand the properties of the first generations of galaxies because they reionized the universe, dispensed large quantities of metal into the low-density intergalactic medium, and served as the sites of formation and early growth for the supermassive black holes that are found at the center of every present-day massive galaxy.

METHODS AND RESULTS

In this PRAC project, we are investigating the earliest stages of cosmological structure formation—namely, the transition of the universe from a dark, empty place to one filled with stars, galaxies, and the cosmic web. In investigating the "cosmic Dark Ages," we focus on three specific topics: (1) the transition between metal-free and metal-enriched star formation, which marks a fundamental milestone in the early epochs of galaxy formation; (2) the evolution of the populations of high-redshift galaxies that will form Milky Way-like objects by the present day; and (3) the reionization of the universe by these populations of galaxies. All of these problems require simulations with extremely high dynamic range in space and time, complex physics that include radiation transport and non-equilibrium gas chemistry, and large simulation volumes. We are using the Enzo code [1], which has been modified to scale to a large number of cores on Blue Waters, the only machine that can satisfy the heavy data and communication needs.

Using Blue Waters, we have successfully modeled the formation of the first generation of metal-enriched stars in the universe and have shown that the strength of the primordial supernova (and the total quantity of metal produced) do not directly correlate to the properties of these first metal-enriched stars. In addition, the presence of dust (which may form in the ejecta of the first supernovae) can have a critical effect on metal-enriched star formation, directly resulting in additional cooling and the formation of additional molecular hydrogen that further increases cooling rates. This may cause additional fragmentation and lower mass stars. We also find that if these Population III stars form massive black hole/stellar binary systems, they are likely to be prodigious emitters of X-ray radiation. This radiation both heats and ionizes the intergalactic medium, in some cases to 104 Kelvin! This may be important for predicting the topology of the 21 cm neutral hydrogen signal, which low-wavelength radio arrays will detect in the coming years.

WHY BLUE WATERS

The simulations required to properly model the earliest galaxies require extremely high spatial and temporal dynamic range, complex physics, and, most importantly, radiation transport and non-equilibrium gas chemistry. Furthermore, large simulation volumes, and thus many resolution elements, are needed in order to model enough galaxies to be able to adequately compare theory to observations in a statistically meaningful way. Taken together, these require a supercomputer with large memory and disk space to accommodate huge datasets, 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

Xu, H., K. Ahn, J. Wise, M. L. Norman, and B. W. O'Shea, Heating the IGM by X-rays from Population III binaries in high redshift galaxies. *Astrophys. J.*, (submitted) arXiv:1404.6555v2.

Wise, J. H., B. D. Smith, B. W. O'Shea, and M. L. Norman, The formation of metal-enriched stars from Population III supernovae: differences in enrichment history due to explosion energy. (submitted).

FIGURE 1 (BACKGROUND): Volume rendering of the matter density field from the central region in our "rare peak" simulation, which explores the formation of what will at the present day become a galaxy cluster. At early times, this is simply a large overdensity of small dwarf-like galaxies, but exploring the properties of such objects is critical to understanding how the first stages of structure formation take place.

UNDERSTANDING GALAXY FORMATION WITH THE HELP OF PETASCALE COMPUTING

Allocation: NSF/3.13 Mnh
PI: Kentaro Nagamine[1]
Collaborators: Ludwig Oser[2]; Jeremiah P. Ostriker[2,3]; Greg Bryan[2]; Renyue Cen[3]; Thorsten Naab[4]; Manisha Gajbe[5]

[1]University of Nevada, Las Vegas
[2]Columbia University
[3]Princeton University
[4]Max-Planck-Institut für Astrophysik
[5]National Center for Supercomputing Applications

EXECUTIVE SUMMARY:

Understanding the formation of the present-day galaxy population is an outstanding theoretical challenge that will only be mastered with the help of high-performance computer simulations. This requires a dynamic range of more than ten orders of magnitude and a multitude of resolution elements when computing galaxy populations in huge cosmological volumes. Observational surveys encompass ~10^6 galaxies, whereas contemporary work on high-resolution cosmological zoom-in simulations usually covers less than a hundred objects. We developed a scalable approach to model full galaxy populations with a parallel ensemble of high-resolution simulations. We are also working toward updating the code to utilize the hybrid nature of modern supercomputers and to implement the Fault Tolerance Interface on Blue Waters to reduce checkpointing overhead and to recover jobs from partial node failures.

INTRODUCTION

Understanding the formation of the present-day galaxy population is an outstanding theoretical challenge that will only be mastered with the help of high-performance computer simulations. Embedded in the cosmic web, the structural properties of galaxies can only be predicted when the galactic domains of star formation—molecular clouds—are numerically resolved. This requires a dynamic range of more than ten orders of magnitude and an enormous number of resolution elements when computing galaxy populations in huge cosmological volumes.

Observed galaxies follow surprisingly tight fundamental scaling relations that any successful model of galaxy formation has to reproduce. Since no two galaxies look alike, we need to recover the statistical properties of the overall galaxy population instead of explaining the formation of a single galaxy like the Milky Way. Observational surveys encompass ~10^6 galaxies, whereas contemporary work on high-resolution cosmological zoom-in simulations usually covers less than a hundred objects. We are trying to mitigate this huge discrepancy in the number of galaxies seen in observed versus theoretical results. Larger scale full-box cosmological simulations can simulate thousands of galaxies at the same time; however, they lack the resolution to resolve the internal structure of galaxies.

METHODS AND RESULTS

HECA

Simply using ever larger computer clusters will not alleviate the problem. Once gas dynamic processes become important, smoothed particle hydrodynamics (SPH) as well as grid codes scale poorly to arbitrarily large problem sizes. With an increasing number of compute nodes, the resources lost due to communication overhead and load balancing grows, thereby limiting the problem sizes and/or resolution fineness that can be computed in a reasonable amount of time.

We developed a scalable approach to model full galaxy populations with a parallel ensemble of high-resolution simulations. Instead of simulating the full box at high resolution, we split it into tens of thousands of independent "zoom" calculations, and for each zoom run, only the region of interest is fully resolved while the rest of the cosmological volume is kept at lower resolution to provide proper gravitational tidal forces. The initial conditions of each zoom run are selected such that contaminated boundary regions do not impact the target of interest. We call this method Hierarchical Ensemble Computing Algorithm (HECA). Initial scaling tests demonstrate that running large numbers of individual zoom simulations in parallel outperforms the traditional full-box approach, providing a way to efficiently use supercomputers like Blue Waters with ~10^5 compute nodes to study cosmological galaxy evolution.

Code improvements

We updated the TreeSPH code "GADGET-3" to account for physical processes that are important for forming galaxies with stellar properties that compare well to observed galaxies. The formation and evolution of galaxies from cosmological initial conditions up to the present day is simulated, considering the effects of radiative cooling from primordial gas, as well as gas enriched with metals and star formation. We included recently developed prescriptions for kinetic stellar feedback originating from asymptotic giant branch stars and supernovae of Type I and II [1,2]. Additionally we implemented kinetic feedback from active galactic nuclei [3].

On top of the physical modules, we used a novel implementation of SPH that is able to deal with the known shortcomings of SPH—mainly the inability to sufficiently capture hydrodynamical instabilities. This includes a pressure-entropy formulation of SPH with a Wendland kernel, a higher-order estimate of velocity gradients, a modified artificial viscosity switch with a strong limiter, and artificial conduction of thermal energy [4].

Each of the above-mentioned improvements overcame known problems in individually simulated galaxies (like insufficient angular momentum, overcooling, late quenching of star formation, metal enrichment of the IGM, and hydrodynamical instabilities). We would like to use the full set of improvements to simulate the statistical nature of a significant number of galaxies.

Work in progress

In addition to our algorithmic approach successfully making better use of the available resources, we are currently updating the code to utilize the hybrid nature of modern supercomputers (i.e., to use a shared-memory approach for parallelization on a compute node and distributed memory parallelization for communication between nodes). Furthermore, we are trying to implement the Fault Tolerance Interface on Blue Waters to reduce checkpointing overhead and to recover jobs from partial node failures.

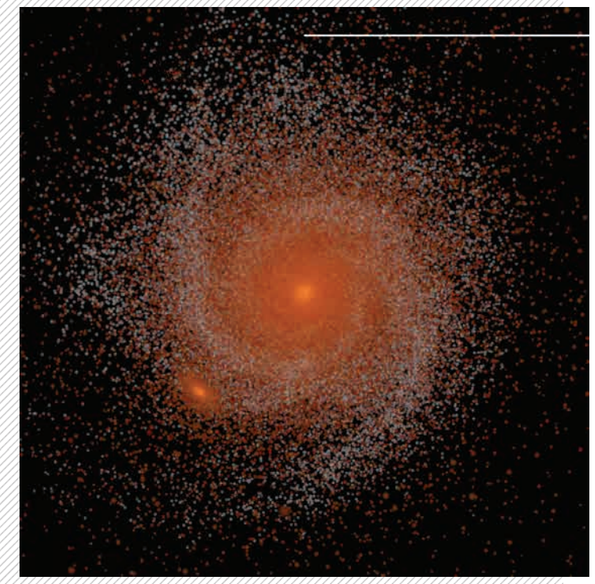


FIGURE 1: Stellar distribution of a simulated Milky Way-size halo at the present day. The young stars (white) form an extended disk (white bar represents a scale of 30 kpc) similar in size to our galaxy, but the simulated galaxy still forms a larger fraction of bulge stars.

FROM BINARY SYSTEMS AND STELLAR CORE COLLAPSE TO GAMMA RAY BURSTS

Allocation: NSF/3.81 Mnh
PI: Peter Diener[1]
Collaborators: Philipp Moesta[2]; Sherwood Richers[2]; Christian D. Ott[3]; Roland Haas[2]; Anthony L. Piro[2]; Kristen Boydstun[2]; Ernazar Abdikamalov[2]; Christian Reisswig[2]; Erik Schnetter[1,4]

[1]Louisiana State University
[2]California Institute of Technology
[3]University of Tokyo
[4]University of Guelph

EXECUTIVE SUMMARY:

We present results of new 3D general-relativistic magnetohydrodynamic simulations of rapidly rotating, strongly magnetized core collapse. These simulations are the first of their kind and include a microphysical finite-temperature equation of state and a leakage neutrino approximation scheme. Our results show that the 3D dynamics of magnetorotational core-collapse supernovae are fundamentally different from what was anticipated based on previous simulations in 2D. A strong bipolar jet that develops in a 2D simulation is crippled by a spiral instability and fizzles in full 3D. Our analysis suggests that the jet is disrupted by an m=1 kink instability of the ultra-strong toroidal field near the rotation axis. Instead of an axially symmetric jet, a completely new flow structure develops. Highly magnetized spiral plasma funnels expelled from the core push out the shock in polar regions, creating wide secularly expanding lobes.

INTRODUCTION

Stellar collapse liberates gravitational energy of order 10^{53} erg/s (100 B). About 99% of that energy is emitted in neutrinos, and the remainder powers a core-collapse supernova (CCSN) explosion. A small fraction of CCSN explosions are hyperenergetic (~10 B) and involve relativistic outflows [e.g., 1,2]. Importantly, all supernova explosions connected with long gamma ray bursts are of Type Ic-BL. Typical explosions may be driven by the neutrino mechanism, in which neutrinos emitted from the collapsed core deposit energy behind the stalled shock, eventually driving it outward. However, the neutrino mechanism appears to lack the efficiency needed to drive hyperenergetic explosions. One possible alternative is the magnetorotational mechanism. In its canonical form, rapid rotation of the collapsed core and magnetar-strength magnetic field with a dominant toroidal component drive a strong bipolar jet-like explosion that could result in a hypernova. A number of recent 2D magnetohydrodynamic (MHD) simulations have found robust and strong jet-driven explosions but only a handful of 3D studies have been carried out with varying degrees of microphysical realism [3-6] and none have compared 2D and 3D dynamics directly.

G means Gauss, a measure of magnetic field B strength.

METHODS AND RESULTS

We have carried out new full, unconstrained 3D dynamical spacetime general-relativistic MHD (GRMHD) simulations of rapidly rotating magnetized CCSN explosions. These are the first to employ a microphysical finite-temperature equation of state, a realistic progenitor model, and an approximate neutrino treatment for collapse and postbounce evolution. We compared the 3D simulations to 2D simulations that used identical initial conditions.

The 3D simulations require fast per-core performance in combination with an efficient communication network. A typical simulation employs nine levels of adaptive mesh refinement (AMR) to increase resolution where needed in the collapsing star and requires 4 TB of memory while producing 500 TB of simulation output. As the shockwave, launched by the sudden halt of the collapse due to the formation of the protoneutron star, expands to greater radii, the entire postshock region needs to be kept at a constant high resolution (~1.5 km) to guarantee stable MHD evolution. The AMR box covering the shocked region alone contains 200 million points and pushed even Blue Waters' computational infrastructure to its current limit.

Our results for a model with an initial poloidal B-field of 10^{12} G indicate that 2D and 3D magnetorotational CCSN explosions are fundamentally different. In 2D, a strong jet-driven explosion occurs. In unconstrained 3D the developing jet is destroyed by non-axisymmetric dynamics, most likely caused by an m=1 MHD kink instability to which the toroidally dominated postbounce magnetic field configuration is prone. The subsequent CCSN evolution leads to two large asymmetric shocked lobes at high latitudes (fig. 1), a completely different flow pattern from 2D. Highly magnetized tubes tangle, twist, and drive the global shock front steadily but not dynamically outward. A runaway explosion does not occur during the ~185 ms of postbounce time covered.

The high precollapse field strength of 10^{12} G yields ~10^{16} G in toroidal field and $\beta=P_{gas}/P_{mag}<1$ within only ~10-15 ms of bounce, creating conditions favorable for jet formation. Yet, the growth time of the kink instability is shorter than the time it takes for the jet to develop. In a short test simulation with an even more unrealistic, ten times stronger initial field, a successful jet is launched promptly after bounce but subsequently also experiences a spiral displacement. Realistic precollapse iron cores are not expected to have magnetic fields in excess of ~10^{8}-10^{9} G, which may be amplified to no more than ~10^{12} G during collapse. The 10^{15}-10^{16} G of large-scale toroidal field required to drive a magnetorotational jet must be built up after bounce. This will likely require tens to hundreds of dynamical times, even if the magnetorotational instability operates in conjunction with a dynamo.

The results of the present and previous full 3D rotating CCSN simulations suggest that MHD and also a variety of non-axisymmetric hydrodynamic instabilities will grow to non-linear regimes on shorter timescales, disrupting any possibly developing axial outflow. This is why we believe that the dynamics and flow structures seen in our full 3D simulation may be generic to the postbounce evolution of rapidly rotating magnetized core collapse that starts from realistic initial conditions.

If the polar lobes eventually accelerate, the resulting explosion will be asymmetric, though probably less so than a jet-driven explosion. The lobes carry neutron-rich (Ye ~0.1-0.2) material of moderate entropy (s ~10-15 k_b baryon^{-1}), which could lead to interesting *r*-process yields, similar to what previous studies have found for their prompt jet-driven explosion. Even if the lobes continue to move outward, accretion in equatorial regions may continue, eventually (after 2-3 s) leading to the collapse of the protoneutron star and black hole formation. In this case, the engine supplying the lobes with low-β plasma is shut off. Unless their material has reached positive total energy, the lobes will fall back onto the black hole, which will subsequently hyperaccrete until material becomes centrifugally supported in an accretion disk. This would set the stage for a subsequent long gamma ray burst and an associated Type Ic-BL CCSN that would be driven by a collapsar central engine [7] rather than by a protomagnetar [8].

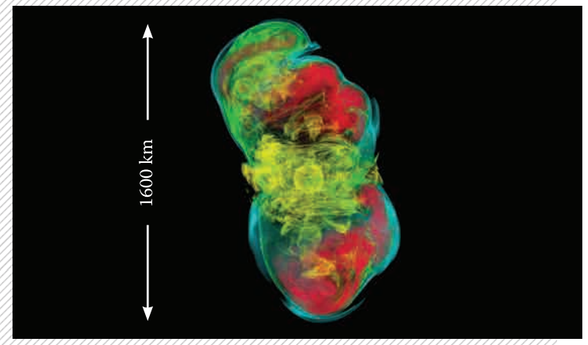


FIGURE 1: Volume rendering of entropy from the simulation in [9] at $t - t_b$=161 ms. The z-axis (vertical) is the spin axis of the protoneutron star and we show 1600 km on a side. The colormap for entropy is chosen such that blue corresponds to s=3.7k_b baryon^{-1}, cyan to s=4.8k_b baryon^{-1} indicating the shock surface, green to s=5.8k_b baryon^{-1}, yellow to s=7.4k_b baryon^{-1}, and red to higher entropy material at s=10k_b baryon^{-1}. The outflows from the protoneutron star (in the center) get severely twisted, resulting in two giant polar lobes.

The results of our study highlight the importance of studying magnetorotational CCSN explosion in 3D. Future work will be necessary to explore later postbounce dynamics, the sensitivity to initial conditions and numerical resolution, and possible nucleosynthetic yields.

Animations and further details on our simulations are available at http://stellarcollapse.org/cc3dgrmhd.

WHY BLUE WATERS

A typical simulation requires 20,000 cores on Blue Waters, and only on Blue Waters was our code able to scale efficiently to such numbers due to the availability of the outstanding interconnect infrastructure.

SIMULATING THE FIRST GALAXIES AND QUASARS: THE BLUETIDE COSMOLOGICAL SIMULATION

Allocation: NSF/2.63 Mnh
PI: Tiziana Di Matteo[1]
Collaborators: Rupert Croft[1]; Yu Feng[1]; Nishikanta Khandai[2]; Nicholas Battaglia[1]

[1]Carnegie Mellon University
[2]Brookhaven National Laboratory

EXECUTIVE SUMMARY:

Computational cosmology—simulating the entire universe—represents one of most challenging applications for petascale computing. We need simulations that cover a vast dynamic range of space and time scales and include the effect of gravitational fields that are generated by (dark matter in) superclusters of galaxies upon the formation of galaxies. These galaxies, in turn, harbor gas that cools and makes stars and is being funneled into supermassive black holes that are of the size of the solar system.

We have started a full-machine run on Blue Waters, the BlueTide cosmological simulation. It is run with an improved version of the cosmological code P-Gadget. The simulation aims to understand the formation of the first quasars and galaxies from the smallest to the rarest and most luminous, and this process's role in the reionization of the universe. The simulation will be used to make predictions of what the upcoming WFIRST and James Webb Space Telescope (JWST; successor of Hubble, launch planned for 2018) will see.

METHODS AND RESULTS

The largest telescopes currently planned aim to study the "end of Dark Ages" epoch in the early universe, when the first galaxies and quasars form and reionization of the universe takes place.

Our main production run, BlueTides, will use the whole Blue Waters machine. It will follow the evolution of 0.6 trillion particles in a large volume of the universe (400 co-moving Mpc on a side) over the first billion years of the universe's evolution with a dynamic range of 6 (12) orders of magnitude in space (mass). This makes BlueTides by far the largest cosmological hydrodynamic simulation with the "full physics" of galaxy formation (left panel of fig. 1).

BlueTides includes a complicated blend of different physics that is nonlinearly coupled on a wide range of scales, leading to extremely complex dynamics. Significant effort was invested in code development and model validation, with several improvements to the physical models in P-Gadget:

- A relatively new pressure-entropy smoothed particle hydrodynamics (SPH) formulation [1] replaces the old density-entropy formulation, which suppresses phases mixing in a non-physical way. We also improved the effective SPH resolution with a higher-order quintic kernel that reduces the shot noise level by a factor of two without additional memory usage.
- In the regime of the simulation, the star formation is supply limited, thus it is important to consider the abundance of H_2 molecules that is the direct supply of star-forming interstellar gas. We implemented a molecular H_2 gas model based on work by Gnedin et al. [2].
- The simulation regime also overlaps the interesting Epoch of Reionization, where the entire universe turns from opaque to transparent. Traditionally a uniform UV field is introduced at the same time across space in hydrodynamical simulations. This is no longer a good approximation in a simulation of such large volume. We incorporate a patchy reionization model from Battaglia et al. [3]; the model introduces a UV field based on a predicted time-of-reionization at a different special location in the simulation.

We also improved the code infrastructure in several ways:

- *Memory efficiency:* We detached the black hole particle data from the main particle type, reducing the memory usage by one quarter for a problem of the same size. This allows us to model 600 billion particles using all of Blue Waters, while leaving some room for potential node failures.
- *Low maintainability:* The redundant code in all major physical modules is rewritten based on a new tree walk module. This inspired the base for our improvement in the threading efficiency.
- *Threading efficiency:* We replaced global critical sections with per-particle (per-node) spin locks. Because the boundaries of thread subdomains are very small, the spin locks hugely

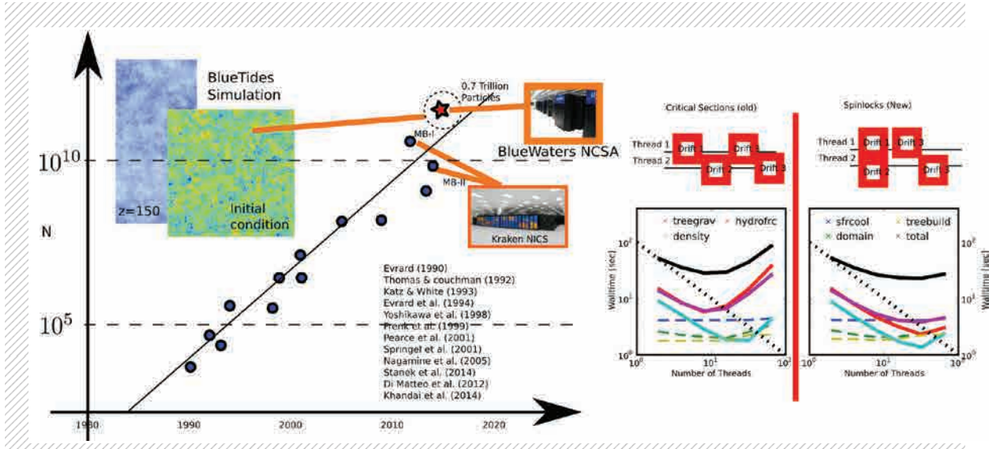


FIGURE 1: (LEFT) The number of particles in cosmological, hydrodynamical simulation of galaxy formation as a function of year. BlueTides simulation on Blue Waters is currently the largest simulation ever attempted. The green and blue colored images are the projection of the density field in the initial conditions and at the first snapshot (z=150) in the simulation. (RIGHT) Improved performance of the threading in P-Gadget. Significant improvement in wall clock time versus number of threads in our new version (bottom panels) and a schematic view of non-blocking threading synchronization scheme (top panels).

improved threading efficiency. Even though the domain decomposition and Fourier transform remains sequential, the wall time improved by about a factor of two at 32 threads. The improved threading efficiency allows us to use fewer domains, which in turn further reduces the complexity of domain decomposition and inter-domain communication, improving the overall efficiency of the code (right side of fig. 1).

- *I/O:* We enabled HDF5 compression in the snapshot files. The compression reduces the size of a snapshot by a factor of ~30%-40%.

We have generated the initial conditions for the BlueTides simulation (left side of fig. 1). This corresponds to a random realization of the density field as measured by the WMAP satellite. The full-machine simulation is underway and has produced the first snapshot (z=150 in fig. 1). Further optimization of the PM solver is currently underway. The simulation is expected to complete in early summer 2014.

WHY BLUE WATERS

Simulation predictions are of prime interest to the community as the instrumental capabilities are just reaching the point that we can explore the young universe over the next couple of decades. The challenge in understanding this epoch of the universe is that extremely large volumes need to be simulated as the first objects are rare, while at the same time extremely high resolution is required as the first galaxies and quasars are expected to be small. Blue Waters makes this possible.

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Gnedin, N. Y., K. Tassis, and A. V. Kravtsov, Modeling Molecular Hydrogen and Star Formation in Cosmological Simulations. *Astrophys. J.*, 697:1 (2009), 55.

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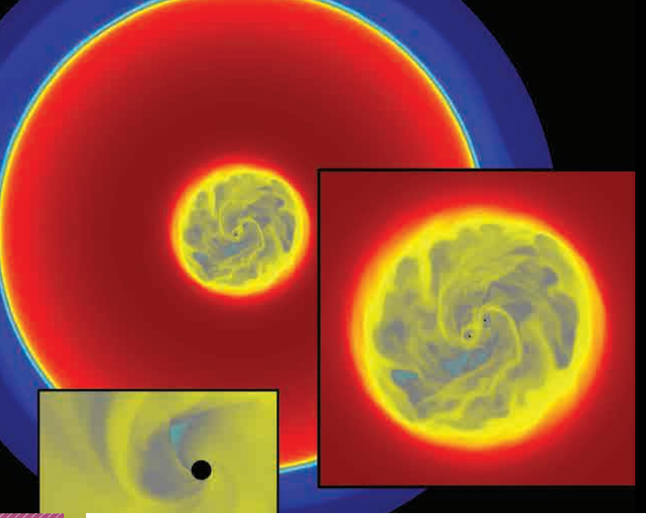

THE INFLUENCE OF STRONG FIELD SPACETIME DYNAMICS AND MHD ON CIRCUMBINARY DISK PHYSICS

FIGURE 1: Gas accreting onto two orbiting black holes from a circumbinary disk. Colors represent the gas's mass density over eleven orders of magnitude on a logarithmic color scale, from dark blue (low) to dark red (high). Each black hole is represented by a black circle. Inset images show close-ups of the background image, which spans the simulation's entire spatial extent.

Allocation: NSF/1.09 Mnh
PI: Manuela Campanelli[1]
Collaborators: Scott C. Noble[1]; Miguel Zilhão[1]; Yosef Zlochower[1]

[1]Rochester Institute of Technology

EXECUTIVE SUMMARY

The observation of supermassive black holes on the verge of merger has numerous exciting consequences for our understanding of galactic evolution, black hole demographics, plasmas in strong-field gravity, and general relativity. Our project aims to provide the astronomy community with predictions of the electromagnetic signatures of supermassive black holes using realistic initial conditions, enough model cells to resolve the essential magnetohydrodynamic turbulence that drives accretion, and sufficient duration to understand their secular trends—all of which are now possible because of Blue Waters.

Over the past year we have determined the regime where high-order post-Newtonian terms in our novel, analytic spacetime solution significantly affect the circumbinary disk's dynamics and predicted luminosity, and that nearly all the key predictions survive using a less accurate post-Newtonian model. In addition, we have begun simulations in which the black holes reside within the numerical domain to explore the development and evolution of the mini disks around each black hole.

INTRODUCTION

Supermassive black hole (SMBH) mergers are believed to happen frequently at the core of most active galaxies. Such mergers would reveal important information on the birth and growth of their host galaxies, as well as explain how highly relativistic matter behaves in the surrounding accretion disks and in the associated jets. Additionally, detection would provide a concrete example of one of general relativity's most spectacular predictions and possibly allow us to test the validity of general relativity in a truly strong-field regime. Our aim is to provide the field of astronomy with the first accurate electromagnetic (EM) predictions of these circumbinary disk environments using state-of-the-art general relativistic magnetohydrodynamics (GRMHD) simulations and general relativistic radiative transfer calculations of the simulated data.

METHODS AND RESULTS

Intensive, high-cadence astronomical surveys (e.g., Pan-STARRS, LSST) make detecting these rare mergers of SMBH binaries more likely, yet accurate theoretical predictions of the SMBH binary's EM counterpart remain to be done. The goal of this project is to develop accurate theoretical estimates of the EM signature of SMBH binaries through GRMHD simulations using the state-of-the-art HARM3d code.

High-performance computation is essential to reach our science goals because the equations are evaluated on vast domains involving tens of millions of model cells at tens of millions of time steps. Such large cell counts are required to resolve the small spatial scales of the black holes (BHs), which span tens of cells, and still cover a sufficiently large domain to include a large circumbinary disk.

It is impossible with current resources and techniques to accurately simulate the formation of SMBH binaries from the galaxy scale all the way to merger, particularly accounting for the interplay of gravitational forces between two BHs. Since our goal is to predict EM signatures when the BHs are close, we must choose initial conditions as realistic as our computational budget allows. A key goal is to understand better how the binary separation and spacetime's accuracy using the post-Newtonian (PN) approximation affect the disk's EM signatures.

In our first project [2] we exploited the ability of our new PN code [3] to exclude the highest-order terms from the metric's evaluation to see how the PN order of accuracy affected the dynamics of non-magnetized and magnetized gas. The non-magnetized runs were constrained to two spatial dimensions so that a larger parameter space could be explored. The non-magnetized runs informed the magnetized cases, which required three dimensions and the entirety of Blue Waters.

PN-order effects were obvious in the non-magnetized case starting from a separation of 20 GM/c^2. In a 3D magnetized case, many of the key qualitative conclusions were similar whether using first- or second-order PN-accurate spacetime. In both magnetized runs we discovered a unique and exciting periodic EM signature that could be used to identify SMBH binaries in the time domain and measure their mass ratio. This implies that the EM signal may be robust down to small binary separations. It remains to be seen if the quantitative differences between magnetic and non-magnetic runs are larger than systematic errors from the initial conditions. Our investigation is the first to demonstrate how the level of PN accuracy affects a circumbinary disk's evolution. It tells us the range of separation within which to trust the PN approximation and addresses the influence the initial conditions and binary separation have on simulated predictions.

Our second project focused on verifying our new code for simulations with the BHs in our domain. A non-uniform spherical-like coordinate system was constructed to focus cells near each BH and move with the BH, while asymptotically approaching a more uniform spherical grid far away from the BHs to better conserve the disk's angular momentum [1].

GM/c^2 is the gravitational radius.

WHY BLUE WATERS

Blue Waters is an essential system for our project because of its immense size. For the calculations that do not include the BHs on the domain, we often require about 10^7 cells evaluated at approximately 10^7 time steps using thousands of cores. During the past year, we finished developing and testing a novel distorted coordinate system that will allow us to resolve the BHs well and efficiently enough to include them in our simulation [1]. These simulations require about ten times more resources than their predecessors. Performing such large runs in a reasonable amount of time is only possible on the largest supercomputers like Blue Waters.

PUBLICATIONS

Zilhão, M., and S. C. Noble, Dynamic fisheye grids for binary black hole simulations. *Classical Quant. Grav.*, 31:6 (2014), 065013.

Mundim, B. C., H. Nakano, N. Yunes, M. Campanelli, S. C. Noble, and Y. Zlochower, Approximate Black Hole Binary Spacetime via Asymptotic Matching. *Phys. Rev. D*, 89 (2014), 084008.

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INFLUENCES OF ORIENTATION AVERAGING SCHEME ON THE SCATTERING PROPERTIES OF ATMOSPHERIC ICE CRYSTALS: APPLICATIONS TO ATMOSPHERIC HALO FORMATION

Allocation: Illinois/0.698 Mnh
PI: Greg M. McFarquhar[1]
Collaborators: Junshik Um[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

The Amsterdam discrete dipole approximation was used to determine the optimal orientation averaging scheme (regular lattice grid scheme or quasi Monte Carlo (QMC) method), the minimum number of orientations, and the corresponding computing time required to calculate average single-scattering properties within predefined accuracy levels for four nonspherical atmospheric ice crystal models. The QMC requires fewer orientations and less computing time than the lattice grid. The minimum number of orientations and the corresponding computing time for scattering calculations decrease with increasing wavelength, whereas they increase with particle nonsphericity.

Variations in the sizes and aspect ratios (ratio between crystal length and width) of ice crystals, which affect the size parameter at which halos first emerge, are also investigated. The threshold size at which 22° and 46° degree halos form is determined.

FIGURE 1 (TOP RIGHT): Scattering phase function P_{11} with D=16 μm: (a) L=1.6 μm, W=16.0 μm, (b) L=4.0 μm, W=16.0 μm, (c) L=8.0 μm, W=16.0 μm, (d) L=16.0 μm, W=16.0 μm. The black line in each panel indicates orientation-averaged P_{11}; color lines are P_{11} for each orientation. Scattering angles of 22° and 46° are indicated with vertical dotted lines, and a distinct peak indicates a halo.

INTRODUCTION

Cirrus clouds consist almost exclusively of nonspherical ice crystals with various shapes and sizes. The representation of cirrus in small- and large-scale models has large uncertainties mainly due to the wide variety of shapes and sizes of nonspherical ice crystals. Thus, the role of cirrus in modulating the Earth-radiation balance is poorly understood.

To determine the influence of cirrus on solar and infrared radiation for general circulation models (GCMs) and remote sensing studies, knowledge of single-scattering properties of ice crystals is required.

In this study, the single-scattering properties of realistically shaped atmospheric ice crystals were calculated using Blue Waters. The optimal orientation averaging scheme was used to calculate the single-scattering properties of ice crystals within a predefined accuracy level (i.e., 1.0%) and the impacts of size and aspect ratio (ratio between crystal length L and width W) on atmospheric halo formation were quantified.

METHODS AND RESULTS

Compute time

The optimal orientation averaging scheme (regular lattice grid scheme or quasi Monte Carlo (QMC) method), the minimum number of orientations, and the corresponding computing time required to calculate the average single-scattering properties within a predefined accuracy level were determined for four different nonspherical atmospheric ice crystal models (Gaussian random sphere, droxtal, budding Bucky ball, and column).

The QMC required fewer orientations and less computing time than the lattice grid. For example, the use of QMC saved 55.4 (60.1, 46.3), 3,065 (117, 110), 3,933 (65.8, 104), and 381 (22.8, 16.0) hours of computing time for calculating the single-scattering properties within 1.0% accuracy for 3B, droxtal, Gaussian random sphere, and column models, respectively, at λ=0.55 (3.78, 11.0) μm using 300 processors. The calculations of scattering phase function P_{11} required the most orientations and asymmetry parameter g and single-scattering albedo ω_0 the fewest. The minimum number of orientations and the computing time for single-scattering calculations decreased with increasing wavelength and increased with the surface area ratio that defines particle nonsphericity.

Atmospheric Halos

Hexagonal crystals (columns and plates) are the building blocks of the most common ice crystal habits. Previous studies have shown that atmospheric halos begin to form when the size parameter (the ratio between particle size and the wavelength of incident light) of ice crystals reaches 80 to 100. The threshold size at which atmospheric halos emerge is important because it determines the applicability of the conventional geometrical optics method (GOM) to the calculations of scattering properties of small particles.

High-resolution images of ice crystals from aircraft probes were used to define a plausible range of aspect ratios (crystal length divided by width; AR) for different sized ice crystals. Then the single-scattering properties of hexagonal crystals were calculated using the Amsterdam discrete dipole approximation (ADDA).

Hexagonal crystals with AR of 0.25, 0.50, and 1.0 (fig. 1b-d) show a distinct 22° halo, whereas only hexagonal crystals with AR of 0.50 and 1.0 produce the 46° halo. Further, both hexagonal columns and plates have more difficulty than compact crystals (AR~1.0) in generating halos. This suggests that the AR of crystals plays an important role in the formation of atmospheric halos. Hexagonal column crystals produce neither halo.

Fig. 2 shows simulated halos using different sizes and ARs of hexagonal crystals. For comparison, simulations of large crystals using a GOM are also shown in the right columns. Small crystals produce neither the 22° nor 46° halo regardless of AR (left column). Large crystals produce halos with the appearance of the 22° and/or 46° halo depending on AR (middle column). A compact hexagonal crystal produces both 22° and 46° halos.

WHY BLUE WATERS

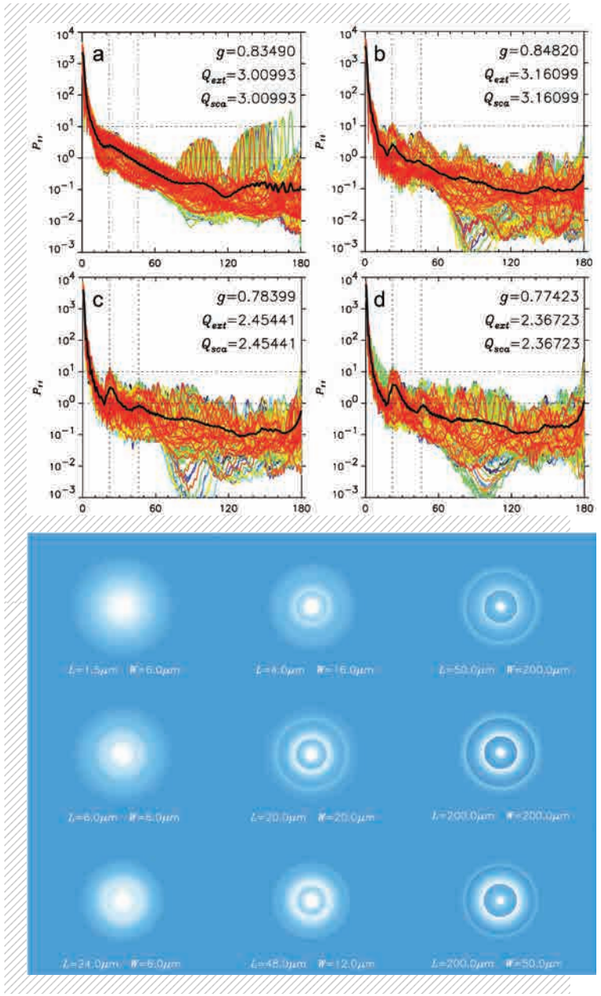
When an ice particle's size parameter was large, GOM was used to approximate the single-scattering properties. Exact methods, such as discrete dipole method, T-matrix method, and finite-difference time domain method, were used for particles with much smaller size parameters. Although the exact methods provide more accurate results, they require more computing time and memory that rapidly increases with particle size. The accuracy of radiative transfer models and satellite retrieval algorithms depends heavily on accurate calculations of single-scattering properties of ice crystals. Blue Waters is an important resource in completing these calculations.

PUBLICATIONS

Um J., and G. M. McFarquhar, Efficient numerical orientation average for calculations of single-scattering properties of small atmospheric ice crystals. *Proc. ASR Science Team Meeting*, Potomac, Md., March 18-21, 2013.

Um, J., and G. M. McFarquhar, Optimal numerical methods for determining the orientation averages of single-scattering properties of atmospheric ice crystals. *J. Quant. Spectrosc. Radiat. Transfer*, 127 (2013), pp. 207-223.

FIGURE 2 (BOTTOM): Simulated halo using different sizes and AR of hexagonal ice crystals. Left and middle columns used ADDA, right column used GOM. All panels have same scale.



EXPLORING THE PHYSICS OF GEOLOGICAL SEQUESTRATION OF CARBON DIOXIDE USING HIGH-RESOLUTION PORE-SCALE SIMULATION

Allocation: Illinois/0.05 Mnh
PI: Albert J. Valocchi[1]
Collaborators: Qinjun Kang[2]

[1]University of Illinois at Urbana-Champaign
[2]Los Alamos National Laboratory

EXECUTIVE SUMMARY:

A better understanding of the physics of geological sequestration of CO_2 is critical to engineering the injection process to maximize storage capacity and immobilization of CO_2, developing monitoring programs, and performing risk assessments. With the rapid advancement of computers and computational methods, numerical modeling has become an important tool for this problem. We developed a 3D, fully parallel code based on the color-fluid multiphase lattice Boltzmann model, which scales well on Blue Waters. We applied the code to simulate liquid CO_2 displacement of water in various homogeneous and heterogeneous pore networks and have obtained quantitative agreement with micro-model experiments fabricated and conducted using Department of Energy Environmental Molecular Science Laboratory's new micro-fabrication capability. By comparing the 2D and 3D simulations of the experiments, the 3D effect is being investigated for the first time.

INTRODUCTION

Understanding the movement of multiple fluids within pore spaces in subsurface geological formations is critical for addressing important problems such as enhanced oil recovery, groundwater pollution from leaking tanks or pipelines, geothermal energy production, and geological sequestration of CO_2. Several large-scale simulations are being used to investigate the impact of industrial-scale CO_2 injection into large geological basins. However, there is considerable scientific uncertainty about the proper way to represent pore-scale physics in these models, which leads to uncertain estimates of storage capacity and leakage probability.

Experiments at the Department of Energy's Environmental Molecular Science Laboratory (EMSL) provide validation data for high-resolution numerical simulation models. The validated models can then serve as a tool to extrapolate beyond conditions investigated in the laboratory and to develop upscaled representations of the physical processes that can be used in reservoir-scale simulations to investigate the impact of industrial-scale CO_2 injection into large geological basins.

METHODS AND RESULTS

We have developed a 3D, fully parallel code based on the color-fluid multiphase lattice Boltzmann model (CFLBM). The lattice Boltzmann method is an effective computational strategy to simulate flow of immiscible fluids in complex porous medium geometries. The CFLBM code has been shown to scale almost ideally on Blue Waters up to 32,768 cores. We have applied the code to simulate liquid CO_2 displacement of water in various homogeneous and heterogeneous pore networks, matching conditions for microfluidics experiments conducted at the state-of-the-art facilities at EMSL. We used a previous 2D version of the CFLBM code to match the experimental conditions, and found that there were some discrepancies between experimental and simulated results.

We first carried out a 3D simulation with 182 million grid points at a relatively high capillary number. The code ran 60,000 steps in one hour on 12,800 cores (400 nodes) on Blue Waters, and the simulation reached steady state after 38,400 node-hours (76.8% of our allocation). We then performed a 3D simulation with 47 million grid points at a lower capillary number, using 3,584 processor cores.

Although the 3D domain used in the simulation is considerably smaller than that used in the experiments, thus far we have found significant differences in fluid distribution between the 2D and 3D simulations and among different cross sections in the vertical (Z) direction of the 3D simulation. At Z=2, LCO_2 (liquid CO_2) didn't penetrate into the pore spaces due to the strong friction at the bottom wall. Although LCO_2 penetrates into the pore spaces at all other cross sections, it is clear that the LCO_2 fingers in the cross sections closer to the wall (e.g., Z=3) are thinner than those in the cross sections near the center (e.g., Z=12). However, this difference quickly diminishes for cross sections away from the top/bottom walls. There are no apparent differences between Z=8 and Z=12.

Comparing the 2D and 3D results at this capillary number, the LCO_2 hasn't penetrated into the pore spaces of the low-permeability domain in the 2D simulation but has started breaking through that domain in the 3D simulation. In addition, in the 3D simulation, the LCO_2 saturation is higher in cross sections away from the top/bottom walls than in the 2D simulation. More simulations with other pore networks and vertical heterogeneity are being carried out. The results and detailed analyses of fluid saturation and interfacial area will be reported in a future publication.

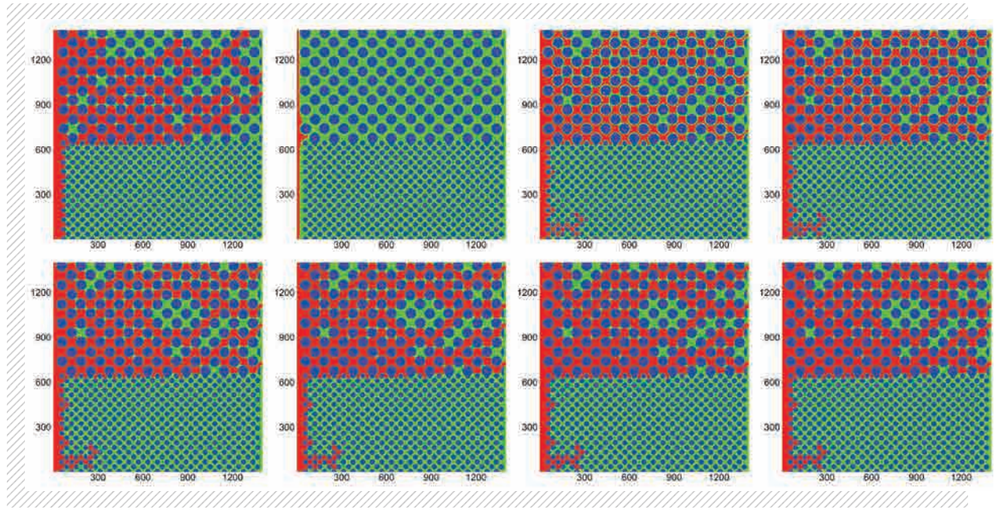


FIGURE 1: Final fluid distributions in the dual-permeability microfluidic system (1408x1400x24) at Log Ca=-4.06. Red and green denote LCO_2 and water, respectively. (Top left) 2D simulation, (Others) 3D simulations at Z=2, 3, 4, 5, 8, 10, 12 (across, then down). Total number of lattices in the Z (vertical) direction is 24.

WHY BLUE WATERS

All existing simulations of microfluidic multiphase flow experiments are based on 2D models, ignoring the effect of the top and bottom walls, as well as that of heterogeneity in the depth direction incurred during manufacturing of the micro-models. Although the 3D effects have long been speculated, a full 3D simulation has not been possible due to the formidable computational costs. Moreover, it will take a very long time for the simulations to reach steady state for analysis of fluid distribution, phase saturation, and interfacial area, etc. The computational power of Blue Waters is allowing us to conduct 3D simulations of these experiments for the first time and to rigorously study 3D effects.

PUBLICATIONS

Liu, H., A. J. Valocchi, C. Werth, Q. Kang, M. Oostrom, Pore-scale simulation of liquid CO_2 displacement of water using a two-phase lattice Boltzmann model. *Adv. Water Resour.*, (in revision).

ENABLING BREAKTHROUGH KINETIC SIMULATIONS OF THE MAGNETOSPHERE VIA PETASCALE COMPUTING

Allocation: PRAC/11.1 Mnh
PI: Homayoun Karimabadi[1,2]
Collaborators:
Vadim Roytershteyn[2]; Yuri Omelchenko[1]; William Daughton[3]; Mahidhar Tatineni[1]; Amit Majumdar[1]; Kai Germaschewski[4]

[1]University of California, San Diego
[2]SciberQuest
[3]Los Alamos National Laboratory
[4]University of New Hampshire

EXECUTIVE SUMMARY

Over 90% of the visible universe is in the plasma state. Some of the key processes in plasmas include shocks, turbulence, and magnetic reconnection. The multiscale nature of these processes and the associated vast separation of scales make their studies difficult in the laboratory. In tandem with *in situ* measurements in space, simulations have been critical to making progress. We highlight our latest progress in the areas of magnetic reconnection, plasma turbulence, and fast shocks as captured in global simulations of the magnetosphere. One of the outcomes of these studies is the dynamic interplay between these seemingly distinct processes. This synergy is demonstrated using specific examples from our work on Blue Waters.

INTRODUCTION

Fundamental plasma processes, such as magnetic reconnection, turbulence, and shocks, play a key role in the dynamics of many systems in the universe across a vast range of scales. Examples of such systems are laboratory fusion experiments, the Earth's magnetosphere, the solar wind, the solar corona and chromosphere, heliosphere, interstellar medium, and many astrophysical objects. In most of these settings, the plasma is weakly collisional, which implies that microscopic processes on the scale of the ion gyroradius and below play an important role, especially inside various boundary layers. This presents tremendous challenges for computational modeling due to the extreme separation of scales associated with the relevant systems.

The problems considered in this research are motivated by the need to better understand Earth's space environment and its interaction with the Sun, the major source of energy in the solar system. Collectively known as "space weather," this area of research is increasing in socio-economic significance due to our society's reliance on space-based communication and navigation technologies and the potential risk of catastrophic disruptions of the power grid caused by major solar events.

For example, turbulence simulations help us understand energy balance in the solar wind, the major driver of the Earth's magnetospheric activity. Similarly, global fully kinetic and hybrid simulations help us understand the response of the magnetosphere to external perturbations.

In addition to their significance for space weather, the processes and their interactions considered here are thought to play a role in many space and astrophysical settings. Consequently, the insights from this study are of great interest to a variety of fields.

METHODS AND RESULTS

Here we demonstrate in a series of examples how modern petascale simulations help address some of these challenges.

First, we discuss 3D fully kinetic simulations of decaying plasma turbulence, where the initial perturbation imposed on a system at large scales seeds a turbulent cascade. The cascade transports energy from the injection scale down to the electron kinetic scales, where it is ultimately dissipated by kinetic processes. A unique feature of these simulations is that they describe for the first time in a self-consistent manner a number of distinct dissipation mechanisms, thus helping assess their relative efficiency.

In a second example, we discuss global 2D fully kinetic simulations of interaction between solar wind and the magnetosphere. This work focuses on understanding how magnetic reconnection couples microscopic electron kinetic physics and macroscopic global dynamics driven by the solar wind.

Finally, we discuss 2D and 3D global hybrid simulations of the interaction between solar wind and the magnetosphere (3D shown in fig. 1). These simulations focus on how ion kinetic processes at the bow shock, a standing shock wave in front of the magnetosphere, drive turbulence in a narrow region behind the shock called the magnetosheath. In this hybrid simulation model, the ions are treated kinetically, while electrons are treated as a massless fluid. Consequently, the electron kinetic scales are not resolved, reducing the range of scales to be resolved by more than an order of magnitude and allowing simulation of larger scales compared to the fully kinetic case.

Our simulations are at the forefront of research in their respective communities. The simulations of decaying turbulence revealed the formation of current sheets with thicknesses from electron kinetic to ion kinetic scales. The possibility that such current sheets provide an efficient dissipation mechanism that is necessary to terminate the turbulent cascade has recently attracted considerable attention. The significance of this work is that formation of the current sheets was demonstrated in essentially first-principles simulations, which include all of the possible dissipation mechanisms.

Moreover, we demonstrated that the overall partition of the dissipated energy, the question of primary importance for solar wind studies, is not consistent with the previous assumption that resonant damping of wave-like fluctuations is the dominant dissipation mechanism.

The global hybrid and global fully kinetic simulations demonstrated the complex dynamics of the magnetosphere, where shock physics, turbulence, and reconnection interact in a complex manner not seen before in simulations. These simulations provide invaluable input into efforts dedicated to better understanding of the Earth's magnetospheric dynamics.

WHY BLUE WATERS

As we emphasized above, the topics considered in this work are characterized by extreme separation of spatial and temporal scales. Consequently, the relevant simulations require extreme computational resources and produce a large amount of data (in excess of 100 TB from a single run). Blue Waters is currently the most powerful tool available to conduct this work, enabling simulations of unprecedented scale and fidelity.

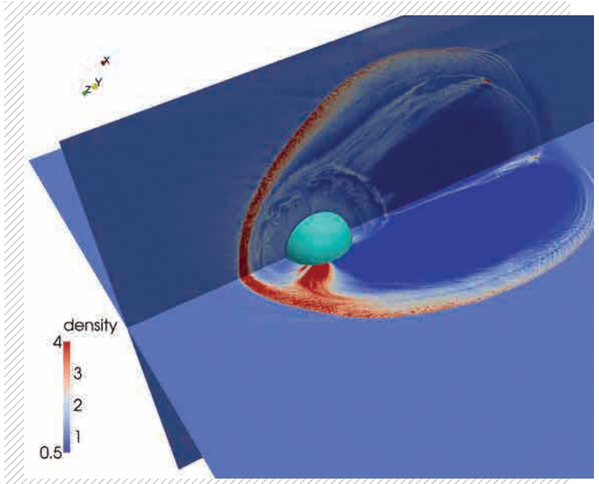


FIGURE 1: Forming magnetosphere in a global 3D hybrid simulation. (V. Roytershteyn, H. Karimabadi)

PUBLICATIONS

Karimabadi, H., et al., The link between shocks, turbulence and magnetic reconnection in collisionless plasmas, *Physics of Plasmas*, 21 (2014), 062308.

BLUE WATERS APPLICATIONS OF 3D MONTE CARLO ATMOSPHERIC RADIATIVE TRANSFER

Allocation: Illinois/0.05 Mnh, BW Prof./0.24 Mnh
PI: Larry Di Girolamo[1]
Collaborators: Alexandra L. Jones[1]; Daeven Jackson[1]; Brian Jewett[1]; Bill Chapman[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Our goal is to improve numerical weather prediction models and remote sensing algorithms for Earth's atmosphere through better treatment of radiative transfer. We produced highly accurate 3D Monte Carlo radiative transfer code that can handle the atmosphere's complexity better than prior 1D codes. The code is built to handle scattering, absorption, and emission by the Earth's atmosphere and surface, includes spectral integration, and outputs radiance, irradiance, and heating rates.

Blue Waters allowed us to reach lower noise levels (than previously achieved) by running the highly scalable code on more processing units than attempted with comparable codes. First we are applying our code to study biases in cloud products derived from NASA satellite instruments. Future directions include coupling our model with the Weather Research and Forecasting model.

INTRODUCTION

One of the least understood aspects of the weather and climate system is clouds, particularly as they interact with solar radiation. Clouds redistribute radiative energy from the sun as well as from the Earth and atmosphere. As the model representation of other physical processes has advanced with increasing spatial resolution and computing power (e.g., cloud microphysics), radiative transfer (RT) remained crude and one dimensional (up/down).

When allowed to feed back on cloud dynamics, modeled inaccuracies from this representation of RT may impact things like rainfall, surface and atmospheric heating, and photolysis rates. In remote sensing, data processing errors in satellite-derived cloud properties limit the scientific utility of the datasets, leading to a serious problem in climate research. The role of clouds is the leading source of uncertainty in predicting anthropogenic climate change. Only accurate satellite datasets can provide retrievals of global cloud properties that will improve RT in climate and weather studies. The starting point for more accurate datasets is a 3D RT model.

METHODS AND RESULTS

Thus far we have used Blue Waters to reach new benchmarking milestones with our open-source 3D Monte Carlo RT model, used the model to evaluate remote sensing algorithms, and developed new features in preparation for the model's eventual coupling to a cloud dynamics model.

We evaluated cloud retrieval algorithms used by NASA's Multi-angle Imaging SpectroRadiometer (MISR) and Moderate Resolution Imaging Spectroradiometer (MODIS). Three-dimensional RT simulations for a wide range of simulated cloud fields were generated to simulate radiance data for these instruments.

For MISR, which derives the cloud-top height via a stereoscopic technique, we demonstrated a ~30 m to ~400 m negative bias in cloud-top height, which strongly depended on the 3D distribution of the cloud liquid and ice water content, and sun and view angles. This range dwarfs the 40 m/decade trend toward lower cloud top heights in MISR that has recently grabbed the attention of climate scientists due to its implication of a negative feedback on a warming climate via greater radiative cooling to space. These results suggest that we cannot decouple actual changes in cloud-top height from changes in cloud texture. Any trend remains hypothetical.

We also have examined error in the effective radius of the cloud drop size distribution derived from MODIS, one of the most important variables in understanding the role of clouds and aerosols in our climate system. These errors are invariant to sub-pixel cloud fraction. Our simulations targeted boundary layer clouds, which are at the heart of the uncertainty in cloud feedbacks plaguing climate projections [1]. Simulated observations (example shown in fig. 1) showed that in the current algorithm used to retrieve cloud optical thickness and effective radius, spectrally varying photon leakage from cloud sides can explain the invariance. However, only the derived effective radius is affected, not optical thickness. This is an extremely useful finding as it allows us to better interpret the properties of clouds in relation to their environment.

Efforts to couple our model to the Weather Research and Forecasting (WRF) model have so far involved increasing RT model functionality by incorporating terrestrial emission (fully tested and benchmarked) and spectral integration (under development and testing) to provide radiative heating rates to WRF. Once the models are coupled, the 3D RT package will consume an estimated 99.9% of computing time because each batch of photons involves millions of scattering, emission, and absorption events. The Monte Carlo nature of our model allows work to be spread across a large numbers of processors with no communication other than the initial task assignment and summing the results.

WHY BLUE WATERS

A large increase in available processing units allowed us to extend our simulations to finer precision than ever before. Benchmark simulations ran to <0.1% Monte Carlo noise, which revealed the insufficiency of some algorithmic choices that were previously masked by the noise. Addressing those insufficiencies has led to a more robust version of our 3D Monte Carlo model. The computationally heavy nature of our simulations requires the Blue Waters infrastructure for successful and timely completion.

Our new tools on Blue Waters will also benefit the wider community by providing a solid foundation for testing future hypotheses involving the two-way interaction between cloud systems and radiation, becoming a test bed for developing practical RT parameterizations that capture the most important 3D effects at lower computational cost and addressing issues related to the interpretation of satellite observations of clouds.

PUBLICATIONS

Jones, A. L., and L. Di Girolamo, A 3D Monte Carlo Radiative Transfer Model for Future Model Parameterizations and Satellite retrieval Algorithms. *Gordon Research Conf. on Radiation and Climate*, New London, N.H., July 7-12, 2013.

Jones, A. L., and L. Di Girolamo, A New Spectrally Integrating 3D Monte Carlo Radiative Transfer Model. *14th Conf. on Atmospheric Radiation*, Boston, Mass., July 7-11, 2014.

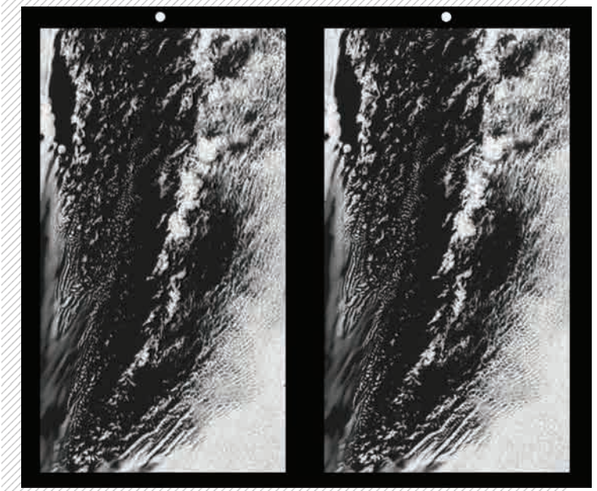


FIGURE 1: The two simulated satellite views above, with viewing angles of 0° and 5°, enable 3D viewing of the cloud scene. While staring between the side-by-side images, cross your eyes until the white dots atop each image merge in the center to form a third dot above a third, centered image. The central image will emerge as a 3D view.

HIGH-RESOLUTION CLIMATE SIMULATIONS USING BLUE WATERS

Allocation: NSF/5.11 Mnh
PI: Donald J. Wuebbles[1]
Collaborators: Arezoo Khodayari[1]; Warren Washington[2]; Thomas Bettge[2]; Julio Bacmeister[2]; Xin-Zhong Liang[3]

[1]University of Illinois at Urbana-Champaign
[2]National Center for Atmospheric Research
[3]University of Maryland, College Park

EXECUTIVE SUMMARY:

The objective of this phase has been to deliver a well-tuned global high-resolution version of the Community Atmosphere Model (CAM) version 5, the atmosphere component of the Community Earth System Model. High resolution challenges climate models since many physical processes that are clearly sub-grid at coarser resolutions become marginally resolved. High-resolution experimentation with the CAM produced a mix of changes. When the portion of convection that was parameterized increased, seasonal mean precipitation distribution generally improved, but the number of tropical cyclones per year dropped from ~100 to <10. Smoothed terrain proved problematic to precipitation in CAM's new spectral element dynamical core. Cloud-aerosol-radiation effects also diverged substantially from observations. All of these are factors in tuning the model to work well at high resolution.

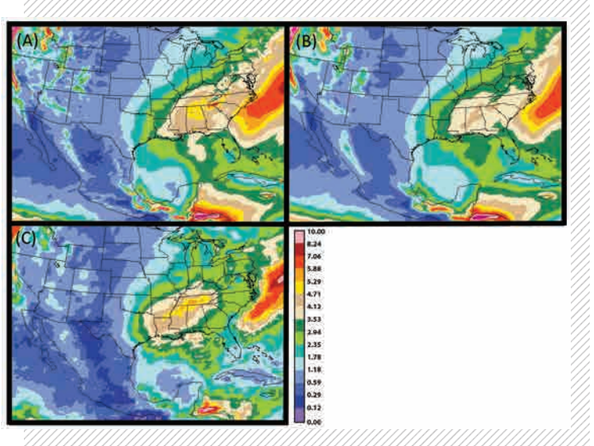


FIGURE 1: Seasonal mean precipitation for December-January-February 1980-2005 for (a) CAM5 FV at a resolution of 0.23°x0.31°; (b) CAM5 SE ne120; and (c) TRMM 1999-2005.

INTRODUCTION

This collaborative research is using Blue Waters to address key uncertainties in the numerical modeling of the Earth's climate system and the ability to accurately analyze past and (projected) future changes in climate. The objective of this phase has been to deliver a well-tuned global high-resolution version of the Community Atmosphere Model (CAM) version 5, the atmosphere component of the Community Earth System Model. In the context of global climate modeling, "high-resolution" means simulations with horizontal grid spacing near 25 km. This resolution challenges climate models since many physical processes that are clearly sub-grid at coarser resolutions become marginally resolved. In addition, a new dynamical core was introduced in CAM—the spectral element dynamical core (SE) [1]. This is a highly scalable code that allows full exploitation of massively parallel architectures such as Blue Waters. This new core revealed surprisingly large sensitivities to topographic forcing and internal dissipation.

METHODS AND RESULTS

Deep convection, seasonal precipitation, and tropical cyclones

High-resolution experimentation with the Community Atmosphere Model version 5 (CAM5) revealed a mix of changes in the simulated climate [2]. Topographically influenced circulations and the global climatology of tropical cyclones were improved. On the other hand, seasonal mean tropical ocean precipitation degraded over large areas compared to simulations with ~100 km resolution.

The time required for a convective cloud to reach maturity (τ_{cnv}), is known to be important to controlling the activity of CAM5's deep convection parameterization. As τ_{cnv} decreases, parameterized convection becomes stronger, and we suspect that problems with the heating profile associated with large-scale precipitation may contribute to biases at high resolution. To examine the effect of parameterized convection, τ_{cnv} was decreased from 3,600 seconds to 300 seconds. Seasonal mean precipitation distribution generally improved when compared to GPCP observed precipitation, but the typical number of tropical cyclones per year dropped from ~100 to <10.

Effects of Topography

When switching to CAM5's spectral element core, we found that heavily smoothing topography to reduce numerical artifacts removed many of the resolution-based improvements in topographically forced flows that were apparent in the finite volume (FV) dynamical core. Extensive development of topographic smoothing algorithms and enhanced internal divergence damping for CAM SE was conducted.

Topography is suspected to play an important role in the simulation of wintertime precipitation over the southeastern U.S. fig. 1 shows seasonal mean precipitation for December-January-February for CAM5 FV, CAM5 SE, and TRMM observational estimates. FV (fig. 1a) produces generally heavier precipitation than SE (fig. 1b) in this region. The SE simulation appears to diverge more from TRMM over much of the domain. We suspect low-level topographic effects are still underrepresented in SE, leading to weaker steering of moist Gulf of Mexico air into the southeastern U.S.

Cloud-Aerosol-Radiation Effects

Cloud-aerosol-radiation effects dominate the global climate model (GCM) climate sensitivity. The Cloud-Aerosol-Radiation (CAR) ensemble modeling system represents the comprehensive range of the mainstream parameterizations used in current GCMs [3]. Fig. 2 compares the frequency distributions for top-of-atmosphere (TOA) shortwave (SW) and longwave (LW) cloud radiative forcing averaged over 60°S-60°N in July 2004 for a fraction of CAR. The spread among the members is 30-60 Wm^{-2}, compared to 5-15 Wm^{-2} for the best observational estimates. The frequency peaks for all fluxes closely match ISCCP or SRB radiative flux estimates, suggesting that most schemes used in the leading GCMs may have been tuned to those data. Yet recent satellite retrievals from CERES instruments (except the EBAF version) fall in the tails of the model distributions.

In a subset of GCMs that produce TOA radiative balance within the observed range, the cloud radiative forcing ranges are still over three times larger than the respective observational uncertainties. Current GCMs may be tuned to reproduce the observed radiative balance by creating compensating errors among different components rather than producing the correct physics at the individual process level.

We plan to examine model uncertainties by using the regional Climate-Weather Research Forecasting model (CWRF) [4], with the built-in CAR, to estimate the range of regional climate change projections, which we anticipate will be substantial. The outcome of the CWRF will be compared with the new CESM high-resolution simulations to evaluate global versus regional model (dis)advantages in projecting future climate change.

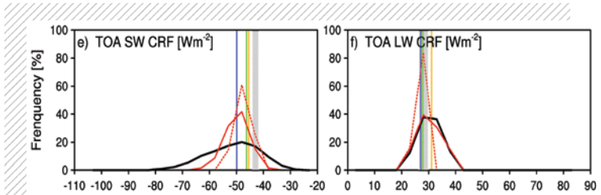


FIGURE 2: The CAR member frequency distributions (thick black curves) in predicting the top cloud radiative forcings (CRF, Wm^{-2}) averaged 60°S-60°N in July 2004 for SW (left) and LW (right) using a subset of 448 members. Red curves are results from the subset with the observational constraints on the top net SW and LW separately (dashed) and their sum (solid). The CAR ensemble mean (black) is compared with the observational data from ISCCP (red), SRB (green), various versions of CERES (purple shading), and CERES_EBAF (orange).

WHY BLUE WATERS

A new dynamical core was introduced in CAM—the spectral element dynamical core (CAM-SE) [1]. This is a highly scalable code that allows full exploitation of massively parallel architectures such as Blue Waters to run a large, high-resolution climate model.

PUBLICATIONS

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A SCALABLE PARALLEL LSQR ALGORITHM FOR SOLVING LARGE-SCALE LINEAR SYSTEM FOR TOMOGRAPHIC PROBLEMS: A CASE STUDY IN SEISMIC TOMOGRAPHY

Allocation: NSF/0.003 Mnh
PI: Liqiang Wang[1]
Collaborators: He Huang[1]; Po Chen[1]; John M. Dennis[2]

[1]University of Wyoming
[2]National Center for Atmospheric Research

EXECUTIVE SUMMARY:

Least Squares with QR factorization (LSQR) method is a widely used Krylov subspace algorithm to solve sparse rectangular linear systems for tomographic problems. Traditional parallel implementations of LSQR have the potential, depending on the non-zero structure of the matrix, for significant communication cost. The communication cost can dramatically limit the scalability of the algorithm at large core counts.

We describe a scalable parallel LSQR algorithm that utilizes the particular non-zero structure of matrices that occurs in tomographic problems. In particular, we specially treat the kernel component of the matrix, which is relatively dense with a random structure, and the damping component, which is very sparse and highly structured separately. The resulting algorithm has a scalable communication volume with a bounded number of communication neighbors regardless of core count. We present scaling studies from real seismic tomography datasets that illustrate good scalability up to O(10,000) cores on a Cray system.

INTRODUCTION

Least Squares with QR factorization (LSQR) is a member of the Conjugate Gradients family of iterative Krylov algorithms and is typically reliable when a matrix is ill conditioned. The LSQR algorithm, which uses a Lanczos iteration to construct orthonormal basis vectors in both the model and data spaces, has been shown to converge faster than other algorithms in synthetic tomographic experiments.

Unfortunately, it can be computationally very challenging to apply LSQR to a tomographic matrix with a relatively dense kernel component appended by a highly sparse damping component, because it is simultaneously compute, memory, and communication intensive. The coefficient matrix is typically very large and sparse. For example, a modest-sized dataset of the Los Angeles Basin for structural seismology has a physical domain of 496x768x50 grid points. The corresponding coefficient matrix has 261 million rows, 38 million columns, and 5 billion non-zero values. Nearly 90% of the kernel is non-zero, while damping takes approximately 10%.

METHODS AND RESULTS

To address the above challenges, we designed and implemented a parallel LSQR implementation (SPLSQR) using MPI and CUDA. Our major contributions include:

• To make our SPLQR scalable, we designed a partitioning strategy and a computational algorithm based on the special structure of the matrix. SPLSQR contains a novel data decomposition strategy that treats different components of the matrix separately. The SPLSQR algorithm provides scalable communication volume between a fixed and modest number of communication neighbors. The algorithm enables scalability to O(10,000) cores for the Los Angeles Basin dataset in seismic tomography.

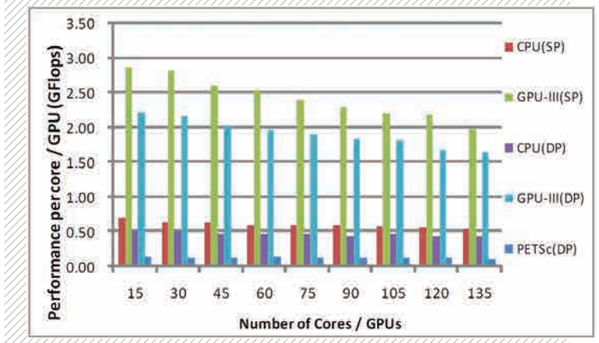
• We use CUBLAS to accelerate vector operations and CUSPARSE to accelerate sparse matrix vector multiplication (SpMV), which is the most compute-intensive part of LSQR. However, CUSPARSE is efficient in handling only regular SpMV in compressed sparse row format, but inefficient in SpMV with matrix transpose. We design two approaches to handle transpose SpMV, trading memory for better performance. The first approach utilizes a different matrix format (compressed sparse column) for transpose SpMV. Although its performance is much better than using CUSPARSE directly, it requires storing two copies of the matrix. As an alternative, we design a second approach to support both regular and transpose SpMV and avoid storing an additional matrix transpose. It has almost the same performance as the first approach on NVIDIA C2050 GPU, but is slower on NVIDIA M2070.

• To optimize memory copy between host memory and GPU device memory, we utilize a "register-copy" technique to speed up copying between by 20%. In addition, we minimize CPU operations by porting all matrix- and vector-based operations into the GPU. During computation, the intermediate results reside on device memory and only a small amount of data is copied between host and device memories for MPI communication.

• To increase parallelism, we decompose both matrix and vector. To obtain good load balance, we decompose the matrix in row-wise order and distribute rows according to the number of non-zero elements. We use MPI-IO to allow multiple MPI tasks to load data simultaneously.

We demonstrated that the SPLSQR algorithm has scalable communication and significantly reduces communication cost compared with existing algorithms. We also demonstrated that on a small seismic tomography dataset, the SPLSQR algorithm is 9.9 times faster than the PETSc algorithm on 2,400 cores of a Cray XT5. The current implementation of the SPLSQR algorithm on 19,200 cores of a Cray XT5 is 33 times faster than the fastest PETSc configuration on the modest Los Angeles Basin dataset.

In our experiment on GPUs, the single GPU code achieves up to a factor of 17.6 speedup with 15.7 GFlop/s in single precision and a factor of 15.2 speedup with 12.0 GFlop/s in double precision, compared with the original serial CPU code. The MPI-GPU code achieves up to a factor of 3.7 speedup with 268 GFlop/s in single precision and a factor of 3.8 speedup with 223 GFlop/s in double precision on 135 MPI tasks compared with the corresponding MPI-CPU code. The MPI-GPU code scales well in both strong and weak scaling tests.



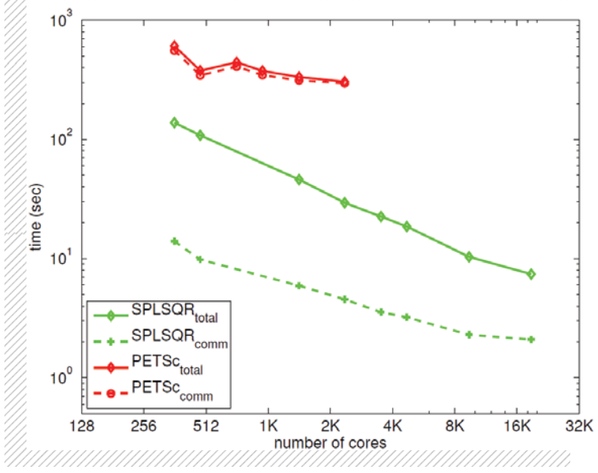


FIGURE 1 (TOP): GPU speedup and scalability on CN2008ker dataset.

FIGURE 2 (BOTTOM): Speedup and scalability of SPLSQ without GPU on Los Angeles Basin dataset from 360 to 19,200 cores.

SOLVING PREDICTION PROBLEMS IN EARTHQUAKE SYSTEM SCIENCE ON BLUE WATERS

Allocation: NSF/3.4 Mnh
PI: Thomas H. Jordan[1]
Collaborators: Scott Callaghan[1]; Robert Graves[2]; Kim Olsen[3]; Yifeng Cui[4]; Jun Zhou[4]; Efecan Poyraz[4]; Philip J. Maechling[1]; David Gill[1]; Kevin Milner[1]; Omar Padron, Jr.[5]; Gregory H. Bauer[5]; Timothy Bouvet[5]; William T. Kramer[5]; Gideon Juve[6]; Karan Vahi[6]; Ewa Deelman[6]; Feng Wang[7]

[1]Southern California Earthquake Center
[2]U. S. Geological Survey
[3]San Diego State University
[4]San Diego Supercomputer Center
[5]National Center for Supercomputing Applications
[6]Information Sciences Institute
[7]AIR Worldwide

EXECUTIVE SUMMARY:

A major goal of earthquake system science is to predict the peak shaking at surface sites on the scale of a few days to many years. The deep uncertainties in these predictions are expressed through two types of probability: an aleatory variability that describes the randomness of the earthquake system, and an epistemic uncertainty that characterizes our lack of knowledge about the system. Standard models use empirical prediction equations that have high aleatory variability, primarily because they do not model crustal heterogeneities. We show how this variance can be lowered by simulating seismic wave propagation through 3D crustal models derived from waveform tomography. SCEC has developed a software platform, CyberShake, that combines seismic reciprocity with highly optimized anelastic wave propagation codes to reduce the time of simulation-based hazard calculations to manageable levels. CyberShake hazard models for the Los Angeles region, each comprising over 240 million synthetic seismograms, have been computed on Blue Waters. A variance-decomposition analysis indicates that more accurate earthquake simulations may reduce the aleatory variance of the strong-motion predictions by at least a factor of two, which would lower exceedance probabilities at high hazard levels by an order of magnitude. The practical ramifications of this probability gain for the formulation of risk reduction strategies are substantial.

INTRODUCTION

The Southern California Earthquake Center (SCEC) coordinates basic research in earthquake science using Southern California as its principal natural laboratory. The CyberShake method produces site-specific probabilistic seismic hazard curves, comparable to Probabilistic Seismic Hazard Analysis (PSHA) hazard curves produced by the U. S. Geological Survey (USGS) that are used in national seismic hazard maps.

If the CyberShake method can be shown to improve on current PSHA methods, it may impact PSHA users including scientific, commercial, and governmental agencies like the USGS. For seismologists, CyberShake provides new information about the physics of earthquake 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 may contribute to their understanding of seismic hazards, which they may use to improve the information they report to the public. For building engineers, CyberShake represents an extension of existing seismic hazard information that may reduce some of the uncertainties in current methods, which are based on empirical ground motion attenuation models.

METHODS AND RESULTS

SCEC has used Blue Waters to perform CyberShake computational research, a physics-based, computationally intensive method for improving PSHA. We have calculated several new PSHA seismic hazard models for Southern California, exploring the variability in CyberShake seismic hazard estimates produced by alternative 3D earth structure models and earthquake source models.

SCEC's CyberShake workflow system produced a repeatable and reliable method for performing large-scale research calculations in record time. The tools used work within the shared-computer resource environment of open science HPC resources including Blue Waters. These tools have helped our team increase the scale of the calculations by two orders of magnitude over the last five years without increasing personnel .

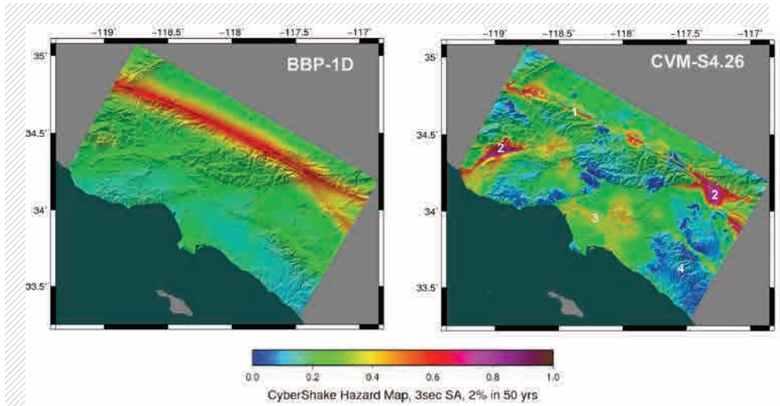


FIGURE 1: Two CyberShake hazard models for the Los Angeles region calculated on Blue Waters using a simple 1D earth model (left) and a more realistic 3D earth model (right). Seismic hazard estimates produced using the 3D earth model show lower near-fault intensities due to 3D scattering, much higher intensities in near-fault basins, higher intensities in the Los Angeles basins, and lower intensities in hard-rock areas.

Our scientific contributions to PSHA have the potential to change standard practices in the field. Models used in PSHA contain two types of uncertainty: aleatory variability that describes the intrinsic randomness of the earthquake-generating system, and epistemic uncertainty that characterizes our lack of knowledge about the system. SCEC's physics-based system science approach can improve our understanding of earthquake processes, so it can reduce epistemic uncertainties over time. As an example of the potential impact, we used the averaging-based factorization (ABF) technique to compare CyberShake models and assess their consistency with Next Generation Attenuation (NGA) models. ABF uses a hierarchical averaging scheme to separate the shaking intensities for large ensembles of earthquakes into relative (dimensionless) excitation fields representing site, path, directivity, and source-complexity effects, and it provides quantitative, map-based comparisons between models. CyberShake directivity effects are generally larger than predicted by the NGA directivity factor [1,2], and basin effects are generally larger than those from the three NGA models that provide basin effect factors. However, the basin excitation calculated from CVM-H is smaller than from CVM-S, and shows stronger frequency dependence primarily because the horizontal dimensions of the basins are much larger in CVM-H. The NGA model of Abrahamson & Silva [3] is the most consistent with the CyberShake CVM-H calculations, with a basin effect correlation factor >0.9 across the frequency band 0.1-0.3 Hz.

WHY BLUE WATERS

SCEC uses 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 jobs, and hundreds of terabytes of temporary files. These calculations are beyond the scale of available academic HPC systems, and, in the past, they required multiple months of time to complete using NSF Track-2 systems. 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. This enables SCEC scientists to improve methodology more rapidly as we work towards CyberShake calculations at the scale and resolution required by engineering users of seismic hazard information.

PUBLICATIONS

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COLLABORATIVE RESEARCH: PETASCALE DESIGN AND MANAGEMENT OF SATELLITE ASSETS TO ADVANCE SPACE-BASED EARTH SCIENCE

Allocation: NSF/4.53 Mnh
PI: Patrick Reed[1]
Collaborators: Eric F. Wood[2]; Matthew Ferringer[3]

[1]Cornell University
[2]Princeton University
[3]The Aerospace Corporation

EXECUTIVE SUMMARY:

This project is a multi-institutional collaboration between Cornell University, The Aerospace Corporation, and Princeton University advancing a petascale planning framework that is broadly applicable across space-based Earth observation systems design. We have made substantial progress towards three transformative contributions: (1) we are the first team to formally link high-resolution astrodynamics design and coordination of space assets with their Earth science impacts within a petascale "many-objective" global optimization framework; (2) we have successfully completed the largest Monte Carlo simulation experiment for evaluating the required satellite frequencies and coverage to maintain acceptable global forecasts of terrestrial hydrology (especially in poorer countries); and (3) we are initiating an evaluation of the limitations and vulnerabilities of the full suite of current satellite precipitation missions including the recently approved Global Precipitation Measurement (GPM) mission. This work will illustrate the tradeoffs and consequences of the GPM mission's current design and its recent budget reductions.

INTRODUCTION

Our satellite constellation design optimization framework is broadly applicable to the full array of National Research Council-recommended spaced-based Earth science missions. Our research proffers a critical step toward realizing the integrated global water cycle observatory long sought by the World Climate Research Programme, which has to date eluded the world's space agencies. Our research is critical for the scientific and space agency communities to overcome current computational barriers to transform the optimization of future satellite constellation architectures for delivering high fidelity data to a broad array of applications. Similarly, we envision that there is a broad array of scientists and users whose future activities will draw upon the project's scientific findings and generated data. As examples, the water-centric stakeholder community desperately requires improved monitoring and assessment of the water cycle for improved decision making related to flooding and droughts, as well as food and energy security.

METHODS AND RESULTS

Our team is exploiting access to the Blue Waters machine to radically advance our ability to discover and visualize optimal "many-objective" tradeoffs (i.e., conflicts for 4-10 objectives) encountered when designing satellites systems to observe global precipitation. Our design of satellite-based precipitation systems will explore the use of perturbing astrodynamics forces for passive control, the sensitivity of hyper-resolution global water cycle predictions on attainable satellite data frequencies, and advancing new technologies for highly scalable many-objective design optimization.

Our hypotheses related to passive control require high fidelity astrodynamics simulations that account for orbital perturbations, which dramatically increase serial design simulation times from minutes to potentially weeks. This project will be the first attempt to develop a 10,000 member Monte Carlo global hydrologic simulation at one degree resolution that characterizes the uncertain effects of changing the available frequencies of satellite precipitation on drought and flood forecasts. The simulation optimization components of the work will set a theoretical baseline for the best possible frequencies and coverages for global precipitation given unlimited investment, broad international coordination in reconfiguring existing assets, and new satellite constellation design objectives informed directly by key global hydrologic forecasting requirements.

We can categorize our project accomplishments to date within three foci: (1) scalable many-objective design optimization benchmarks, (2) advances in the use of high-fidelity astrodynamics simulation to permit passive control (i.e., minimum energy satellite constellations), and (3) benchmark the effects of reduced frequencies of satellite-based precipitation on global drought and flood forecasting.

1. With respect to many-objective design evaluation, we have completed the largest and best benchmark in terms of search quality and scalability for our team's underlying optimization algorithms. The results were made possible by the Blue Waters Friendly User period access. At 524,288 cores, our search approaches theoretically ideal performance. These results are the best benchmark ever attained for the challenge problem of focus and provide a strong foundation for our future tradeoff analyses.

2. In the context of passive control, our preliminary results focus on the patented four-satellite "Draim" constellation. Our Draim results reveal that carefully optimizing an initial orbital geometry to exploit natural perturbations (e.g., effects of sun, moon, etc.) to maintain continuous global coverage performance as a function of elevation angle. This minimizes propellant and station keeping requirements to dramatically reduce mission costs while increasing mission duration. The Draim constellation represents a stepping stone to the more complex suite of global precipitation missions that will require the analysis of more than ten satellites.

3. We are one of the first teams to show how limits in satellite-based precipitation observations propagate to uncertainties in surface runoff, evaporation, and soil moisture at distinctly different locations globally. Our results are based on the Variable Infiltration Capacity (VIC) global macroscale land surface model at 1.0° spatial resolution. For each realization of the VIC ensemble, each model grid cell's satellite precipitation is resampled at different temporal resolutions and then run through the VIC land surface model. Our results suggest differing effects of spatial and temporal precipitation sampling on each water cycle component. For example, convection plays a dominant role in the tropics and sampling will highly impact the measured precipitation. However, plant transpiration is impacted less by the intensity and frequency of storms than the sufficiency of the total precipitation. These insights have direct relevance to water security concerns in terms floods and droughts.

WHY BLUE WATERS

In simple terms, the scale and ambition of our computational experiments require that we have the ability to compress years of computational work into minutes of wall clock time to be feasible. Additionally, our applications are extremely data intensive, so Blue Waters' high core count and high memory are fundamental requirements to realizing our goals.

The global hydrologic ensemble will require approximately 30 million core hours that will yield up to 2 PB of model output. This output represents a new benchmark dataset that will be of broad interest in a variety of Earth science and engineering applications. Our satellite design trade-off analysis will expend approximately 120 million core hours to discover how quickly we deviate from the "best case" observation frequencies, with limits on spending, limits in international coordination, neglect of hydrologic objectives, and the simplified astrodynamics simulations currently employed in practice.

PUBLICATIONS

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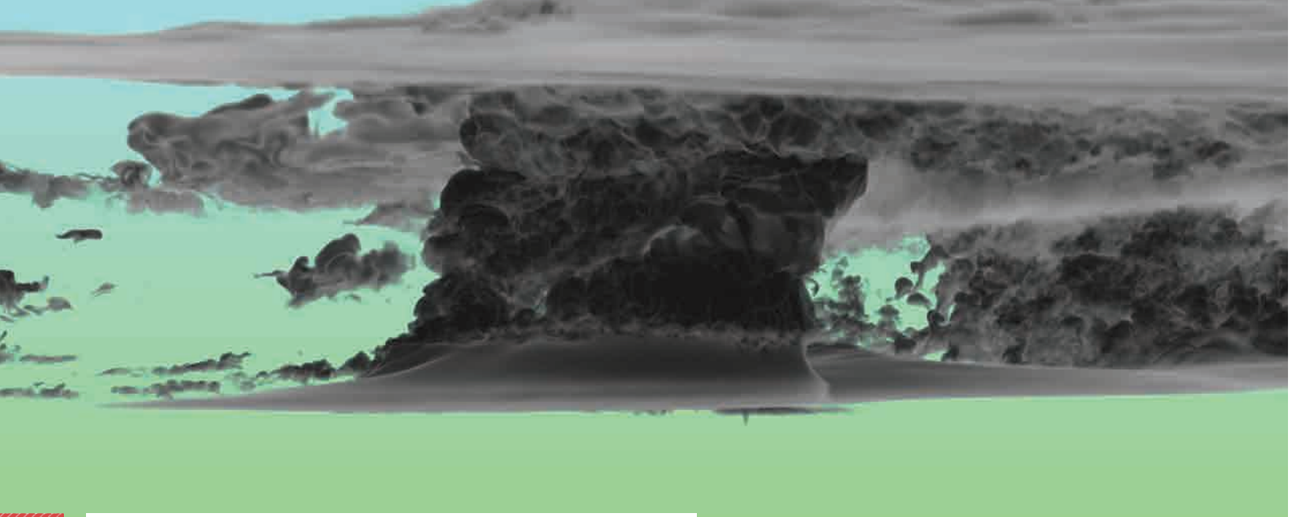

TOWARDS PETASCALE SIMULATION AND VISUALIZATION OF DEVASTATING TORNADIC SUPERCELL THUNDERSTORMS

FIGURE 1: A volume-rendered view from the south of the cloud mixing ratio field of the simulated tornadic supercell. Visible features include a tail cloud, wall cloud, and EF5 tornado beneath the mesocyclone of the simulated storm.

Allocation: Illinois/0.76 Mnh
PI: Robert Wilhelmson[1,2]
Collaborators: Leigh Orf[3]; Roberto Sisneros[2]; Louis Wicker[4]

[1]University of Illinois at Urbana-Champaign
[2]National Center for Supercomputing Applications
[3]Central Michigan University
[4]National Severe Storms Laboratory

EXECUTIVE SUMMARY:

Utilizing the CM1 model, simulations of supercell thunderstorms were conducted. Simulations varied in resolution, physics options, forcing, and the environment in which the storm formed. Concurrently, development on I/O and visualization code was completed. Two major objectives were realized:

- A VisIt plugin was developed that enables researchers to visualize both at full model scale, and also in any arbitrary subdomain. This plugin works with the new CM1 HDF5 output option that was developed and tuned on Blue Waters.
- A supercell simulation with an embedded long-track EF5 tornado was conducted and visualized with volume-rendering techniques in the VisIt plugin. To the best of our knowledge, this simulation is the first of its kind, capturing the genesis, maintenance, and decay of the strongest class of tornado. The simulated tornado traveled for 65 miles and bears a strong resemblance to an observed storm that occurred in a similar environment.

INTRODUCTION

Severe thunderstorms cause billions of dollars of damage annually to property and agriculture as well as loss of life due to flooding, lightning, and the severe winds associated with tornadoes. In the United States, prediction of severe storms continues to be a challenge, even with a large amount of dedicated and publicly supported human and technological infrastructure for protecting the public against severe weather threats.

In order to improve the accuracy of severe weather forecasts, we must improve our understanding of the severe weather phenomena being forecast. The thrust of the work conducted by our research team on Blue Waters is to understand better the inner workings of supercell thunderstorms and their most devastating product: the tornado. Specifically, we aim to capture the entire life cycle of the most devastating type of tornado: the long-track EF5, which exhibits the strongest sustained winds and the longest life cycle of all tornado types.

METHODS AND RESULTS

Long-track EF5 tornadoes are the least common of all tornadoes; in some years, none are observed in the United States even though hundreds of tornadoes occur. As expected, this infrequent observation is mirrored numerically, and it is a challenge to get a long-track EF5 to occur in a simulation. Our experience on Blue Waters indicates that, much like the real atmosphere, the likelihood that a given supercell simulation will produce a long-track EF5 is very low. In addition, very large computational resources like Blue Waters are required to simulate the entire thunderstorm, its surrounding environment, and the comparatively small-scale flow associated with tornado formation and the tornado's entire life cycle. The amount of data produced by these simulations is also very large (O(100 TB) per simulation). This amount of output presents a challenge for meaningful 3D visualization and simulation analysis.

During our time on Blue Waters we created a new output format for CM1 that dramatically reduced the wall-clock time required to do large amounts of I/O compared to existing CM1 options. HDF version 5 was chosen as the underlying data format for individual output files. In order to exploit the large amounts of memory available on Blue Waters while reducing the latency associated with frequently writing tens or hundreds of thousands of files to disk, a new approach was developed in which, for each write cycle, one rank per node collects and buffers data to memory dozens of times before flushing to disk. This approach reduced the number of files and disk operations and resulted in fewer (but larger) files being written to disk less frequently, resulting in better performance compared to other approaches.

A set of code was built around this output format (a "software plugin") that enables 3D analysis utilizing the VisIt visualization software that is supported on Blue Waters. Additional code was developed on Blue Waters that facilitates conversion from the model's raw output to other popular data formats such as netCDF and Vis5d.

We successfully simulated a long-track EF5 tornado that develops within a supercell and stays on the ground for 65 miles. To the best of our knowledge, this is the first time this has ever been accomplished. Utilizing the VisIt plugin, volume-rendered visualizations were created at very high temporal resolution, showing the development and maintenance of the EF5 tornado and the supercell that produced the tornado (example in fig. 1). In order to avoid memory exhaustion with high-quality ray casting settings, each frame was rendered on a single node and parallelization was achieved by rendering hundreds of frames concurrently. Animations produced from these frames have revealed very complex, sometimes highly turbulent, flow regimes involving dozens of constructive and destructive vortex interactions throughout the tornado's life cycle.

WHY BLUE WATERS

Blue Waters provides an infrastructure that is able to support the huge computational, communication, and storage loads inherent to our specific application. Furthermore, Blue Waters provides a robust environment that enables the rapid development of code optimizations for more efficient model performance, as well as the creation of new software in order to enable analysis and visualization of tremendous amounts of model output.

PUBLICATIONS

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73 *Direct Simulation of Dispersed Liquid Droplets in Isotropic Turbulence*

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78 *Space-Time Simulation of Jet Crackle*

80 *Petascale Quantum Simulations of Nano Systems and Biomolecules*

82 *Breakthrough Petascale Quantum Monte Carlo Calculations*

84 *Quantum Monte Carlo Calculations of Water-Graphene Interfaces*

86 *Scaling up of a Highly Parallel LBM-based Simulation Tool (PRATHAM) for Meso- and Large-Scale Laminar and Turbulent Flow and Heat Transfer*

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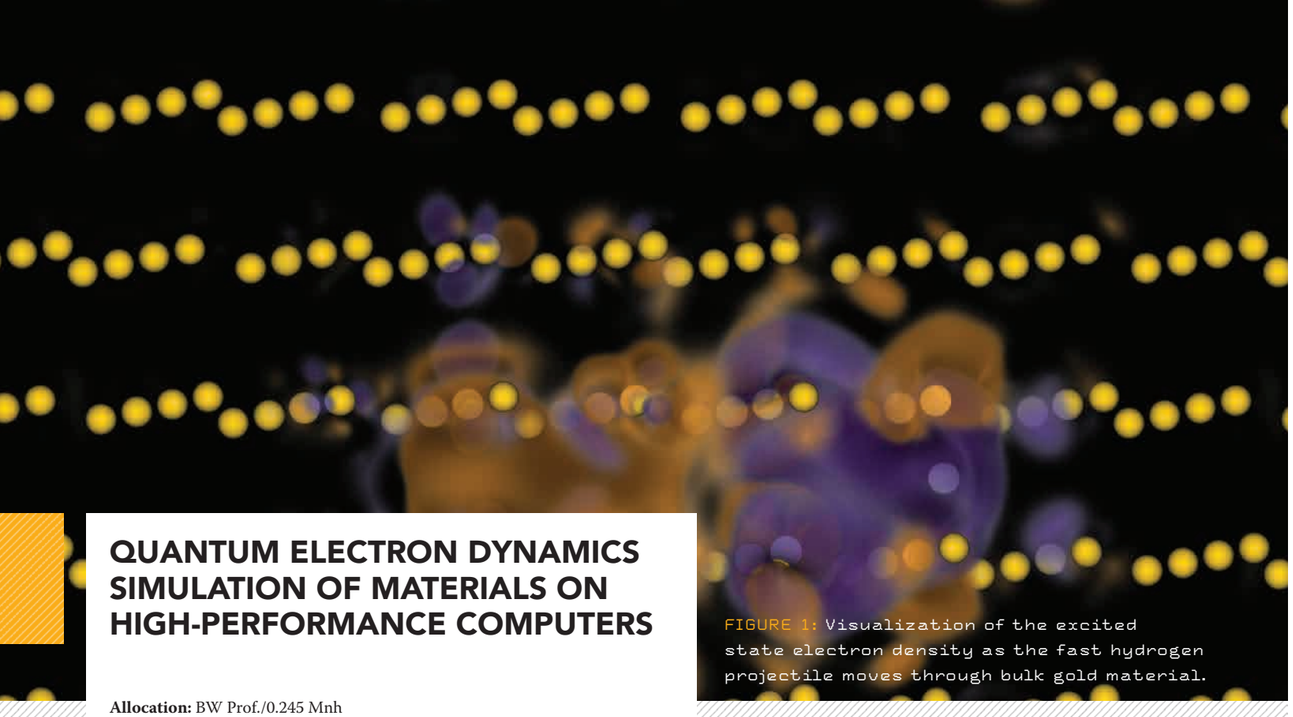

QUANTUM ELECTRON DYNAMICS SIMULATION OF MATERIALS ON HIGH-PERFORMANCE COMPUTERS

FIGURE 1: Visualization of the excited state electron density as the fast hydrogen projectile moves through bulk gold material.

Allocation: BW Prof./0.245 Mnh
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EXECUTIVE SUMMARY:

Rapidly advancing high-performance computers such as Blue Waters allow for calculating properties of increasingly complex materials with unprecedented accuracy. However, in order to take full advantage of leadership-class machines modern codes need to scale well on hundreds of thousands of processors. Here we demonstrate high scalability of our recently developed implementation of Ehrenfest non-adiabatic electron-ion dynamics that overcomes the limits of the Born–Oppenheimer approximation. We find excellent scaling of the new code up to one million compute core floating-point units. As a representative example of material properties that derive from quantum dynamics of electrons, we demonstrate the accurate calculation of electronic stopping power, which characterizes the rate of energy transfer from a high-energy particle to electrons in materials. We use the example of a highly energetic hydrogen particle moving through crystalline gold to illustrate how scientific insights can be obtained from the quantum dynamics simulation.

INTRODUCTION

In order for computational materials design to succeed, oftentimes it is crucial to develop a thorough understanding of the interaction of ions and electrons. The photon absorption of solar cells, radiation damage in materials, and defect formation are a few of many examples of properties or phenomena that have their roots in the physics of interacting electrons and ions.

The physical laws that govern this regime are well known, but directly solving the Schrödinger equation (which describes the behavior of electrons) is intractable even on modern computers. Instead scientists must rely on approximations that limit the accuracy of quantum mechanics calculations. In particular, computational cost is reduced by disregarding the quantum dynamics of electrons in many first-principles molecular dynamics approaches, which makes various interesting material properties inaccessible when using such an oversimplified method. Therefore, accurate description of electron dynamics through time-dependent quantum mechanical theory is an important challenge in computational materials physics and chemistry today.

The massively parallel and hybrid architecture of modern high-performance computers constitutes an additional challenge for numerical simulations. It is necessary to develop theoretical and algorithmic methods that are capable of fully exploiting current and future high-performance computers in electronic structure calculations while continuing to use less restrictive approximations.

METHODS AND RESULTS

We recently developed and implemented a first-principles computational methodology to simulate non-adiabatic electron-ion dynamics on massively parallel computers. The scheme is based on the time-dependent extension of density functional theory and the underlying Kohn-Sham equations. Using an explicit fourth-order Runge–Kutta integration scheme in the context of a plane-wave code, we are now able to integrate the time-dependent Kohn–Sham equations in time, which allows us to explicitly study electron dynamics. We compute Hellman–Feynman forces from the time-dependent (non-adiabatic) Kohn–Sham states and integrate ion motion using the Ehrenfest scheme. We showed that our implementation of this approach in the Qbox/qb@ll code is accurate, stable, and efficient. Using the computational power of Blue Waters as well as the BlueGene-based Sequoia high-performance computer at Lawrence Livermore National Laboratory, we showed excellent scaling of our implementation.

Owing to this new implementation, we are now able to pursue two important directions: (1) explore the scalability and applicability of the code in the context of high-performance computing, and (2) apply the code to elucidate the physics of electronic stopping in a material under particle-radiation conditions, which is a highly non-adiabatic process and, hence, crucially relies on overcoming the limitations of the Born–Oppenheimer approximation.

In addition, by studying the scientific problem of computing the electronic stopping of a hydrogen projectile in crystalline gold material, we were able to unravel the influence of the stopping geometry and to understand contributions of semi-core electrons of the gold atoms, especially for highly energetic hydrogen projectiles. Good agreement with experiments demonstrates that this approach indeed captures the key physics and even promises predictive accuracy that will be beneficial for yet unexplored systems. Using the example of hydrogen projectiles in gold we showed that we can achieve this challenging goal. In particular, the influence of the stopping geometry (i.e., the path on which the projectile atom travels through the crystal) is a crucial aspect of the problem that is often difficult to access in experiments. This application may enable first-principles design and understanding of radiation hard materials as well as the processes that underlie scintillators and radiation shielding.

WHY BLUE WATERS

In this context, it is crucial to use machines such as Blue Waters in order to validate the computational parameters such as the plane-wave basis set, check the super cell size, and study long enough trajectories in order to eliminate computational artifacts. Leadership-class machines such as Blue Waters are essential as they pave the way toward exascale computing. Using as many as 251,200 compute cores on Blue Waters is an important test that allows us to explore the limits of our parallel implementation. At the same time, since we found the scaling to be excellent, machines such as Blue Waters will allow us to tackle exciting large-scale scientific problems in the future.

PUBLICATIONS

Schleife, A., E. W. Draeger, V. Anisimov, A. A. Correa, and Y. Kanai, Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. *Comput. Sci. Eng.*, (in press).

LATTICE QCD ON BLUE WATERS

Allocation: NSF/60.1 Mnh
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EXECUTIVE SUMMARY:

• We have developed highly optimized code for the study of quantum chromodynamics (QCD) on Blue Waters and used it to carry out calculations of major importance in high energy and nuclear physics.

• We used Blue Waters to generate gauge configurations (samples of the QCD vacuum) with both the highly improved staggered quarks (HISQ) and Wilson–Clover actions. For the first time, the up and down quarks in these calculations are as light as in nature for the HISQs, leading to a major improvement in precision.

• With the HISQ configurations, we calculated a ratio of decay constants that enables determination of a key Cabibbo–Kobayashi–Maskawa matrix element to a precision of 0.2% and also obtained world-leading precision for at least half a dozen additional quantities.

• The Wilson–Clover project explored the isovector meson spectrum utilizing both the GPU and CPU nodes. On the CPU, a multi-grid solver gave an order of magnitude improvement over previous code.

INTRODUCTION

The standard model of high-energy physics encompasses our current knowledge of the fundamental interactions of subatomic physics. It has been enormously successful in explaining a wealth of data produced in accelerator and cosmic ray experiments over the past forty years. However, our knowledge is incomplete because it has been difficult to extract many of the most interesting predictions of quantum chromodynamics (QCD), those that depend on the strong coupling regime of the theory. The only means of doing so from first principles and with controlled errors is through large-scale numerical simulations. These simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, determine a number of the fundamental parameters of the standard model, and make precise tests of the standard model.

Despite the many successes of the standard model, high-energy and nuclear physicists believe that a more general theory will be required to understand physics at the shortest distances. The standard model is expected to be a limiting case of this more general theory. A central objective of the experimental program in high-energy physics, and of lattice QCD simulations, is to determine the range of validity of the standard model and search for physical phenomena that will require new theoretical ideas for their understanding. Thus, QCD simulations play an important role in efforts to obtain a deeper understanding of the fundamental laws of physics.

METHODS AND RESULTS

Our long-term scientific objective is to perform calculations of QCD, the theory of the strong interactions of subatomic physics, to the precision needed to support large experimental programs in high-energy and nuclear physics. Under our PRAC grant we are using two formulations of lattice quarks. The highly improved staggered quarks (HISQ) formulation is being used to calculate fundamental parameters of the standard model of high-energy physics and our current set of theories of subatomic physics, and to make precise tests of the standard model. In particular, the HISQ formulation is being used to calculate the masses of quarks, which are the fundamental building blocks of strongly interacting matter, and determine elements of the Cabibbo–Kobayashi–Maskawa (CKM) matrix, which are the weak interaction transition couplings between quarks. The CKM matrix elements and the quark masses are fundamental parameters of the standard model and therefore of great interest in their own right. Furthermore, in recent years a major line of research within high-energy physics has been to determine the same CKM matrix element through different processes to look for inconsistencies that would signal a breakdown in the standard model. Until now, uncertainties in the lattice calculations have limited the precision of these tests. We aim to match the precision of our calculations to that of experiments.

Our first objective with the Clover formulation of lattice quarks is to perform a calculation of the mass spectrum of strongly interacting particles (hadrons). The determination of the excited state spectrum of hadrons within QCD is a major objective for several new generations of experiments worldwide and is a major focus of the $310 million upgrade of Jefferson Laboratory. In particular, the GlueX experiment within the new Hall D at Jefferson Laboratory will search for the presence of "exotic" mesons. The existence of these particles is a signature for new states of matter, specifically the presence of gluonic degrees of freedom, predicted by QCD but thus far not clearly observed. The spectroscopy effort is intended to determine whether the equations of QCD do, in fact, realize the existence of such exotic states of matter. Because these predictions will be made before the experiments are performed, these calculations will provide crucial information about the decay signatures of such exotic states that will inform and guide the experimental searches.

Lattice QCD calculations have two steps. First, one generates and saves gauge configurations, which are representative samples of the QCD ground state. In the second step the gauge configurations are used to measure a wide range of physical quantities. The generation of gauge configurations is the rate-limiting step in the calculations and requires the most capable supercomputers available. The most computationally expensive component of the second step, the measurement routines, is to calculate the Green's functions for the propagation of quarks in the gauge configurations. For the light quarks, this calculation also requires highly capable computers.

We have made major progress in our efforts to generate gauge configurations and quark propagators using Blue Waters. These have included the most challenging ensembles undertaken to date. The new HISQ configurations have already been used to make the most precise determination to date of the decay properties

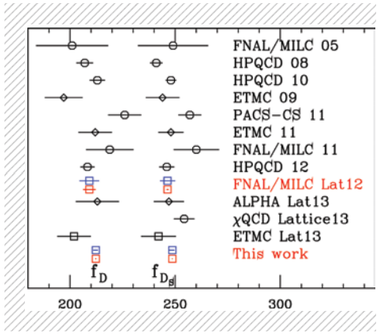

FIGURE 1: Comparison of the recent evaluation of the leptonic decay constants (x-axis) of two mesons containing a charm quark, the D and D_s mesons, by the Fermilab Lattice and MILC Collaborations (labeled "This work") with earlier work. Diamonds, octagons, and squares are calculations with two, three, and four sea quarks. [3]

of a number of mesons containing strange and charm quarks [1-3], which in turn have led to the evaluation of several CKM matrix elements that are important for tests of the standard model. They also have produced the most precise ratios among the up, down, strange, and charm quark masses [2]. Important advances have been made in the development of code for the generation of gauge configurations and quark propagators with the Clover formulation of lattice quarks [4]. The quark propagators calculated on Blue Waters with this code will play a major role in the large hadron mass spectrum calculation described above.

WHY BLUE WATERS

Lattice QCD calculations have made major progress in the last few years with a limited number of calculations reaching precision of a fraction of a percent and techniques in place to determine many more quantities to this level of accuracy. Such precision is needed to test the standard model mentioned above and for a detailed understanding of physical phenomena controlled by the strong interactions. The advent of petascale computers, such as Blue Waters, is playing a critical role in these advances because high-precision QCD calculations are enormous undertakings which require computers of the highest capability and capacity.

QCD is formulated in the four-dimensional space-time continuum. However, in order to carry out numerical calculations one must reformulate it on a four-dimensional lattice or grid. In order to obtain physical results, one must perform calculations for a range of small lattice spacings and extrapolate to the continuum (zero lattice spacing) limit while keeping the physical

size of the box within which the calculations are performed fixed. The computational cost grows roughly as the fifth power of the inverse of the lattice spacing and one must employ very fine grids to obtain high-precision results. Furthermore, the computational cost of calculations rises as the masses of the quarks decrease. Until quite recently, it has been too expensive to carry out calculations with the masses of the two lightest quarks, the up and the down, set to their physical values. Instead, one had to perform calculations for a range of up and down quark masses, and extrapolate to their physical values. Blue Waters is enabling us, for the first time, to carry out calculations with small lattice spacings and the masses of the up and down quarks at their physical values. This development has already led to a number of calculations of unprecedented precision.

PUBLICATIONS

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Winter, F. T., M. A. Clark, R. G. Edwards, and B. Joo, A Framework for Lattice QCD Calculations on GPUs. *Proc. 28th IEEE Int. Parallel Distrib. Process. Symp.*, Phoenix, Ariz., May 19-23, 2014.

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DIRECT SIMULATION OF DISPERSED LIQUID DROPLETS IN ISOTROPIC TURBULENCE

Allocation: NSF/1.24 Mnh
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EXECUTIVE SUMMARY:

The objective of our research is to enhance the understanding of the interaction between liquid droplets and a turbulent flow by performing direct numerical simulations (DNS). The freely moving deformable liquid droplets are fully resolved in three spatial dimensions and time and all the scales of the turbulent motion are simultaneously resolved down to the smallest relevant length and time scales. Our DNS solve the unsteady 3D Navier–Stokes and continuity equations throughout the whole computational domain, including the interior of the liquid droplet. The droplet surface motion and deformation are captured accurately by using the level set method. The discontinuous density and viscosity are smoothed out across the interface by means of the continuous surface force approach. A variable density projection method is used to impose the incompressibility constraint.

GOALS

This study aims to investigate the two-way coupling effects of finite-size deformable liquid droplets on decaying isotropic turbulence using direct numerical simulation (DNS). Turbulent liquid-gas flows are found in many natural phenomena and engineering devices. In particular, the study of liquid-gas interfaces is important in combustion problems with liquid and gas reagents. The main challenge in the numerical simulation of multi-phase flows is the representing the interface between the phases involved. This requires a method for the tracking the interface and a model to describe the discontinuity in density and viscosity. Furthermore, surface tension on the moving interface must be taken into account to be able to deal with capillary effects and other curvature-dependent phenomena.

We employ a level set method to capture implicitly the moving interface and a continuous surface force (CSF) approach to model density and viscosity in a continuous fashion. Finally the surface tension is included in the momentum equations as a volume force and modeled using the CSF method.

Our first simulation goal is a single water droplet falling under the effect of gravity in a fluid at rest. This features most of the physics we are interested in, namely large variations of material properties between phases, surface tension, and droplet deformation, without the added complexity of turbulence—the perfect experiment to validate our algorithm. The second objective is to repeat the experiment in a turbulent environment. Eventually we will simulate a large number of liquid droplets in decaying isotropic turbulence.

Currently we are in the final testing stage of our code. No turbulence has been considered yet since our primary focus at this time is to obtain an accurate time evolution of the droplet interface.

WHY BLUE WATERS

Performing DNS of turbulent flows is very demanding in terms of computational power and memory availability. The computational grids employed need to be fine enough to resolve the smallest flow structures accurately; this requirement becomes more and more stringent as the Reynolds number based on the Taylor micro-scale is increased. In addition, an accurate time history of the flow is sought in order to compute time-dependent statistics, thus limiting the time step interval one can use. The demand for computational power is even larger for a multi-phase flow because the standard projection method for incompressible flows must be replaced by a variable-density projection method. The latter results in a variable-coefficients Poisson's equation that is not solvable by a fast Fourier transform, thus requiring an iterative solver. We use the multi-grid preconditioned conjugate gradient solver provided by the PETSc library. Given the requirements outlined above, Blue Waters is a necessary resource for our research.

ACCELERATING NANOSCALE TRANSISTOR INNOVATION WITH NEMO5 ON BLUE WATERS

Allocation: NSF/1.24 Mnh; GLCPC/0.313 Mnh
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Collaborators: Jim Fonseca[1]; Tillmann Kubis[1]; Daniel Mejia[1]; Bozidar Novakovic[1]; Michael Povolotskyi[1]; Mehdi Salmani-Jelodar[1]; Harshad Sahasrabudhe[1]; Evan Wilson[1]; Kwok Ng[2]

Intel Corporation; PETSc Development Team, Argonne National Laboratory; NVIDIA Corporation

[1]Purdue University
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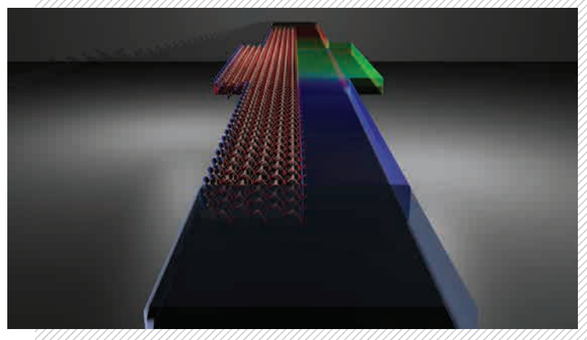
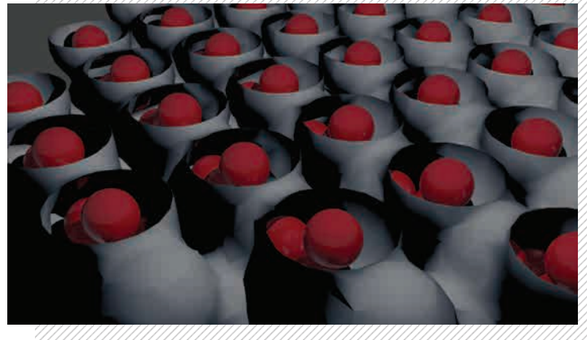
EXECUTIVE SUMMARY:

Relentless downscaling of transistor size has continued according to Moore's law for the past 40 years. According to the International Technology Roadmap for Semiconductors (ITRS), transistor size will continue to decrease in the next 10 years, but foundational issues with currently unknown technology approaches must be pursued. The number of atoms in critical dimensions is now countable. As the materials and designs become more dependent on atomic details, the overall geometry constitutes a new material that cannot be found as such in nature.

NEMO5 is a nanoelectronics modeling package designed to comprehend the critical multi-scale, multi-physics phenomena through efficient computational approaches and quantitatively model new generations of nanoelectronic devices including transistors and quantum dots, as well as predict novel device architectures and phenomena [1,2]. This technology paradigm comes full circle as the NEMO tool suite itself provides input to ITRS and is also used by leading semiconductor firms to design future devices.





INTRODUCTION

The U.S. semiconductor industry is one of the largest export industries. The global semiconductor device market is over $300 billion and the U.S. holds more than one third of this market. The U.S. is a market leader and produces a significant number of high-paying, high-technology jobs. At the same time, the end of Moore's law scaling as we know it will be reached in ten years with device dimensions expected to be about 5 nm long and 1 nm, or about 5 atoms, in its critical active region width. Further improvements in these dimensions will come only through detailed and optimized device design and better integration.

Quantum effects such as tunneling, state quantization, and atomistic disorder dominate the characteristics of these nanoscale devices. Fundamental questions need to be answered to address the downscaling of the CMOS switch and its replacement. What is the influence of atomistic local disorder from alloy, line-edge roughness, dopant placement, fringe electric fields, and lattice distortions due to strain on the carrier transport in nanometer-scale semiconductor devices such as nanowires, finFETs, quantum dots, and impurity arrays? Can power consumption be reduced by inserting new materials and device concepts?

METHODS AND RESULTS

The NEMO software suite has been used on Blue Waters to calculate design parameters for future devices, and these results have been included in the 2013 International Technology Roadmap for Semiconductors. Simulations found important deviations in the characteristics of devices as they are scaled down and raise questions about future device designs.

NEMO5 takes advantage of Blue Waters' unique heterogeneous CPU/GPU capability through the use of the MAGMA [3], cuBLAS, and cuSPARSE libraries. A specific type of non-equilibrium Green's function (NEGF), the Recursive Green's Function (RGF), which is a computational approach to handling quantum transport in nanoelectronic devices, has been implemented using the Sancho-Rubio algorithm [4]. NEGF requires storage, inversion, and multiplication of matrices on the order of the number of electronic degrees of freedom, and it is known that dense matrix multiplication and matrix inversion get respectable Flop/s on GPUs.

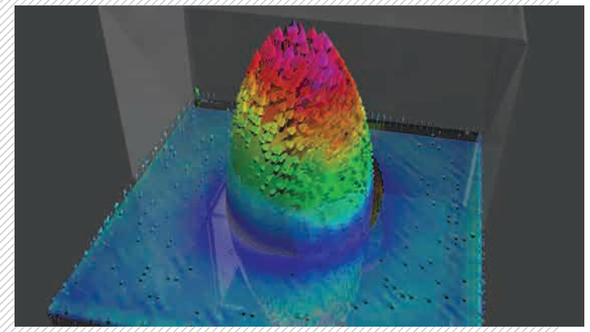
These developments have allowed NEMO5 to achieve efficient scalability past 100 nodes on Blue Waters and performance that shows a single NVIDIA Kepler K20x GPU can provide as much processing power as 40 AMD Bulldozer cores. Additionally, a PETSc–MAGMA interface has been developed in conjunction with PETSc developers for future release to the community [5].

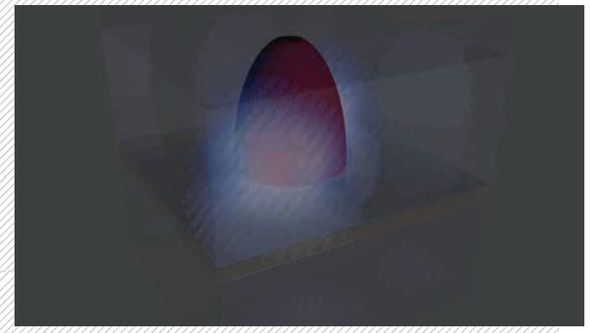
WHY BLUE WATERS

A toy calculation of a 50 nm long wire with a 3 nm diameter requires around 1 TFlop/s for a single energy point using NEGF. Resolution of a device's characteristics requires about 1,000 energy points, and this calculation must be repeated perhaps a dozen times for a full current-voltage sweep. Even with RGF, the computational time scales with the cube of cross-sectional area (relative to the direction of electron flow) and linearly with the length of the device. The treatment of a technically currently relevant finFET device would require an atomistic resolution of a device with a cross section around (20x40) nm^2, which includes the core semiconductor and the surrounding gate material.

Codes in the NEMO tool suite have been shown to scale well on leadership-class machines. A previous version of NEMO5, OMEN, demonstrated almost perfect scaling to 222,720 cores and 1.44 PFlop/s, the first engineering code to deliver a sustained 1.4 PFlop/s on over 220,000 cores on Jaguar [6].

NEMO5 is a more general code but implements the same underlying numerical approaches and framework as OMEN. Scalable algorithms that primarily use dense/sparse-dense matrix-matrix multiplication and matrix inversion have been used to take advantage of Blue Waters' GPU capabilities.





PUBLICATIONS

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Salmani-Jelodar, M., J. D. Bermeol, S. Kim, and G. Klimeck, ITRS Tool on NanoHUB. *NanoHUB User Conf.*, Phoenix, Ariz., April 9-11, 2014.

FIGURE 1 (LEFT TOP): Potential along an InAs Ultra-Thin Body (UTB) transistor.

FIGURE 2 (LEFT BOTTOM): Atomistic representation of Si, represented as diamond structure crystals.

FIGURE 3 (RIGHT TOP): InAs-GaAs quantum dot strain displacement.

FIGURE 4 (RIGHT BOTTOM): InAs-GaAs quantum dot stationary wave functions

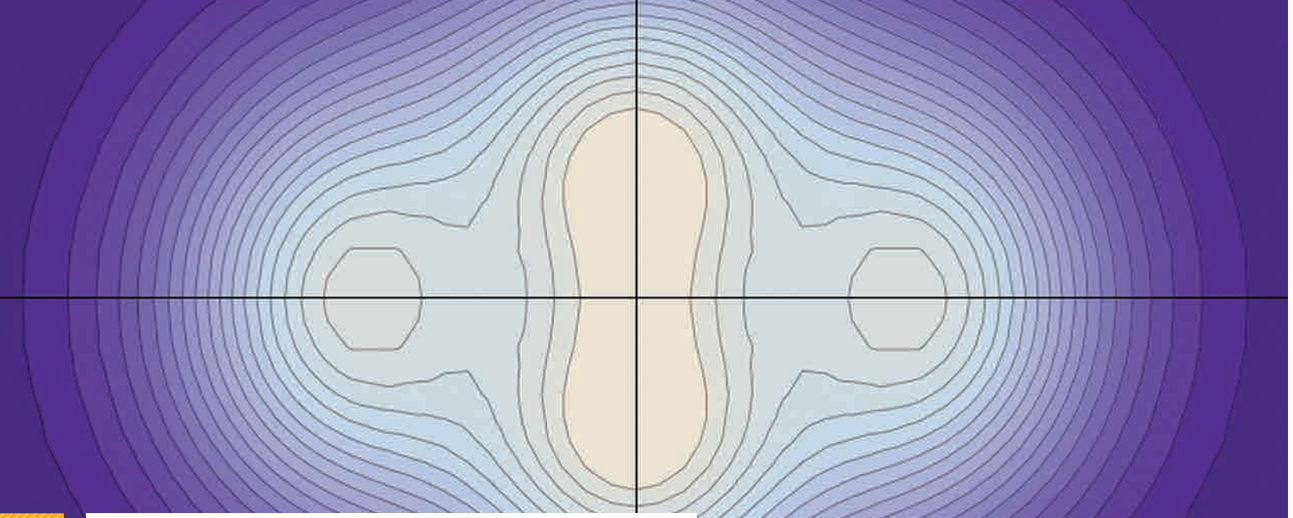

FIGURE 1: Density profile of the 20 particles in the ground state of Neon.

NEXT-GENERATION *AB INITIO* SYMMETRY-ADAPTED NO-CORE SHELL MODEL AND ITS IMPACT ON NUCLEOSYNTHESIS

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[2]Czech Technical University in Prague
[3]Iowa State University
[4]The Ohio State University
[5]Old Dominion University

EXECUTIVE SUMMARY:

We have developed a next-generation first-principle (*ab initio*) symmetry-adapted no-core shell model (SA-NCSM). The SA-NCSM capitalizes on exact as well as important approximate symmetries of nuclei; it also holds predictive capability by building upon first principles, or fundamentals of the nuclear particles. These theoretical advances coupled with the cutting-edge computational power of the Blue Waters system have opened up a new region for first investigations with *ab initio* methods, the intermediate-mass nuclei from Fluorine to Argon isotopes. For example, reliable descriptions of Neon isotopes are already available. Such solutions are feasible due to significant reductions in the symmetry-adapted model space sizes compared to those of equivalent ultra-large spaces of standard no-core shell models. This is essential for further understanding nucleosynthesis, as nuclear energy spectra and reaction rates for many short-lived nuclei involved in nucleosynthesis are not yet accessible by experiment or reliably measured for the astrophysically relevant energy regime.

INTRODUCTION

Theoretical advances of the *ab initio* symmetry-adapted no-core shell model (SA-NCSM) [1] coupled with the cutting-edge computational power of the Blue Waters system open up a new region of the periodic table, the "*sd* shell" (or intermediate-mass region), including O, F, Ne, Na, Mg, Al, Si, P, S, and Ar isotopes, for first investigations with *ab initio* methods that hold predictive capabilities. This is essential for further understanding nucleosynthesis, as nuclear masses, energy spectra, and reaction rates for many short-lived nuclei involved in nucleosynthesis are not yet available by experiment or reliably measured for the astrophysically relevant energy regime.

In addition, one of the most challenging problems in nuclear physics today is to achieve an *ab initio* nuclear modeling of the Hoyle state in ^{12}C, which affects, for example, results of core-collapse supernovae simulations and stellar evolution models, predictions regarding X-ray bursts, as well as estimates of carbon production in asymptotic giant branch stars.

METHODS AND RESULTS

We advance an *ab initio* (i.e., from first principles) large-scale nuclear modeling initiative that proffers forefront predictive capabilities for determining the structure of nuclear systems, including rare isotopes up through medium-mass nuclei that are inaccessible experimentally and fall far beyond the reach of other *ab initio* methods. We aim to provide nuclear structure information of unprecedented quality and scope that can be used to gain further understanding of fundamental symmetries in nature that are lost in massive datasets or require petascale (or even exascale) architectures, and to extract essential information for astrophysics (e.g., nucleosynthesis and stellar explosions), neutrino physics, and energy-related applied physics problems.

Our NSF-sponsored OCI-PetaApps award resulted in a practical and publicly available, platform-independent and highly scalable computational realization of SA-NCSM [2-5]. The success of this first demonstration means new regions of the chart of nuclides are open for investigation within the framework of *ab initio* methods.

Targeted nuclei represent a considerable challenge requiring more than 100,000 cores. The following list describes the results and projected studies:

- We have provided the first *ab initio* description of ^{20}Ne. This is an example for an open-shell nucleus in the intermediate-mass region, with complexity far beyond the reach of complementary *ab initio* methods. Following this success, we target *ab initio* modeling of Ne, Mg, and Si isotopes, especially those close to the limits of stability (at proton and neutron drip lines), providing important input to nuclear reaction studies. Such reactions in the intermediate-mass region are key to further understanding phenomena like X-ray burst nucleosynthesis or the Ne-Na and Mg-Al cycles.
- We have studied electron scattering off ^{6}Li with wave functions calculated in the *ab initio* SA-NCSM. Results show the efficacy of the SA-NCSM model space selection, for the first time, toward reproducing the low- and high-momentum components of the ^{6}Li wave function. This finding is crucial for planned studies of neutrino scattering off of ^{12}C and ^{16}O nuclei, the ingredient nuclei in the neutrino experiment detectors.
- A work-in-progress focuses on one of the most challenging problems in nuclear physics today: achieving an *ab initio* nuclear modeling of the first excited 0^+ state (the so-called Hoyle state) in ^{12}C, the resulting state of the essential stellar triple-alpha process. Knowing the structure of low-lying states of ^{12}C is key to modeling nucleosynthesis and stellar explosions.

WHY BLUE WATERS

The SA-NCSM was specifically designed to efficiently handle complex data in large-scale applications, and its efficacy has been demonstrated already, with the largest production run successfully utilizing 363,616 processors on Blue Waters for a 100-terabyte nuclear Hamiltonian matrix. This was facilitated by our new hybrid MPI+OpenMP implementation of the SA-NCSM, developed and optimized with assistance from the Blue Waters technical team.

The unique features of the SA-NCSM and the Blue Waters system are crucial to advancing *ab initio* methods for nuclei in the lower *sd* shell and beyond, as well as highly deformed states exemplified by the Hoyle state in ^{12}C. And in return, targeted scientific achievements of the types performed as well as proposed here could help prove the value of current HPC resources, and maybe even serve to help shape future HPC facilities.

PUBLICATIONS

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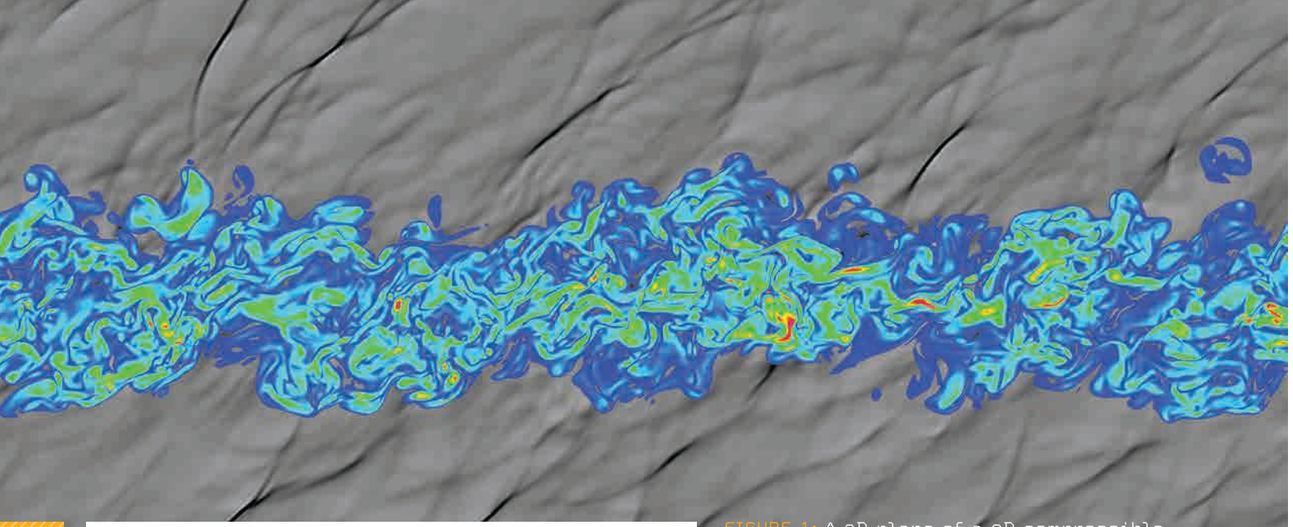

FIGURE 1: A 2D plane of a 3D compressible turbulent temporal shear layer showing magnitude of vorticity (color) and dilatation (grayscale). Dark gray inclined waves are weak shocks with sharp peaked pressure compressions that lead to the 'crackling' character of sound.

SPACE-TIME SIMULATION OF JET CRACKLE

Allocation: Illinois/0.075 Mnh
PI: David Buchta[1]; Jonathan B. Freund[1]

[1]University Of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

Exploratory simulations are proposed as part of our research studying the noise from high-specific thrust jet exhausts, such as on military jets. This noise, known as crackle, exhibits a distinctive rasping fricative sound that is harsher than a typical civilian transport. The sound is generated by the complex flow turbulence interactions in the jet. Blue Waters provides simulation capabilities that allow us to examine the complex root mechanisms with unprecedented detail.

We employ large-scale simulations to study the nonlinear turbulence interactions that generate crackle. Three simulations at increasing flow speeds of technological importance—Mach numbers 1.5, 2.5, and 3.5—have been executed with excellent parallel scaling on Blue Waters. They show a fundamental change of character in the generation of the noise. Taking advantage of Blue Waters' I/O capabilities, we ran small-scale tests, loading in large portions of solution fields to evaluate higher resolution space-time correlations of turbulence and sound. Results of this work will advance scientific understanding of root causes and guide engineering mitigation of crackle.

INTRODUCTION

Many of us have heard a jet aircraft and thought it sounded different than usual. Looking up, we discover it is a military jet. Though their noise can be more intense, what often attracts notice is its distinct character—a rasping fricative sound, harsher than a typical civilian transport. People near airbases experience it a lot, often unhappily, and those who work closely around such aircraft can even sustain aural injury.

Since the identification of this peculiar, intense sound from high-speed jet exhausts, the source mechanisms of crackle have been debated. It is thought that supersonically advecting turbulent eddies surrounding the jet can radiate Mach-wave-like sound, which leads to its peculiar and intense character, now called "crackle." The question remains: what gives these waves the steepened, skewed signature that correlates with crackle?

The extreme flow conditions and the space-time character of the turbulence and its sound challenge experimental diagnostics. Advanced large-scale simulations such as ours are offering a microscope for studying its root mechanisms. We are focusing on the nonlinear turbulence interactions that generate the sound and the nonlinear acoustics that seem to give crackle some of its features, which may reveal a new set of "knobs" to control it. Such a control space may be applied to aircraft and ship detection, environmental noise reduction, and perhaps fine-tuning bio-medical acoustic procedures.

METHODS AND RESULTS

We have designed the present simulations to provide a detailed description of the turbulence that generates acoustic fields associated with crackle. While jet noise is the target application, we chose to study a compressible temporally developing turbulent planar shear layer because it provides a clearer perspective of the root mechanisms of this sound generation. It can be considered as a model for the near-nozzle region of a high-Reynolds number jet, where the turbulence is concentrated in a weakly curved shear layer between the high-speed potential core flow and the surrounding flow. Because the model is focused on this small region, we can explicitly resolve a larger range of turbulence scales than could be represented in a full jet simulation.

We have executed three simulations at increasing flow speeds of technological importance—Mach numbers 1.5, 2.5, and 3.5—with excellent parallel scaling on the Blue Waters system. These show a fundamental change of character in the generation of the noise, and their noise exhibits crackle levels comparable to full-jet simulations and experiments. Taking advantage of Blue Waters' I/O capabilities, we have run small-scale tests that load in larger portions of solution fields than we have previously employed to evaluate higher resolution space-time correlations of the turbulence and sound.

To provide a realistic and detailed description the flow, we solve the three-dimensional compressible Navier–Stokes equations without modeling approximations. The computational domain for ongoing simulations is discretized in Cartesian coordinates by ~1.6 billion points. High-order finite differences and fourth-order Runge–Kutta time advancement provide the high resolution needed for both the turbulence and its acoustic radiation.

WHY BLUE WATERS

With Blue Waters we increased the Reynolds number by an order of magnitude beyond prior runs, allowing us to address important questions regarding scale similarity of the crackle phenomenon. This has foundational implications for crackle asymptotics in the high-Reynolds number limit that is representative of the full-scale engineering applications.

The other, more substantial and Blue Waters-specific goal is to examine the possibility of rapid space-time analysis of the full three-dimensions-plus-time databases we generate. Sound generation is fundamentally unsteady and turbulence is fundamentally three-dimensional. Typical post-processing of massive DNS databases requires compromises in resolution. However, Blue Waters can hold the entire database in memory. It has the potential to calculate key quantities for the whole database, such as space-time correlations of theoretical noise sources, without the usual I/O limitations of most modern systems. This could introduce a new paradigm for the analysis of such databases.

PUBLICATIONS

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Buchta, D., A. Anderson, J. Freund, Near-Field Shocks Radiated by High-Speed Free-Shear-Flow Turbulence. *35th AIAA Aeroacoustics Conference,* Atlanta, Ga., June 16-20, 2014.

PETASCALE QUANTUM SIMULATIONS OF NANO SYSTEMS AND BIOMOLECULES

Allocation: NSF/3.2 Mnh
PI: Jerzy Bernholc[1]
Co-PIs: Shirley Moore[2]; Stanimire Tomov[3]; Wenchang Lu[1]; Miroslav Hodak[1]

[1]North Carolina State University
[2]University of Texas at El Paso
[3]University of Tennessee, Knoxville

EXECUTIVE SUMMARY:

This project focuses on high-performance electronic structure calculations and development of petascale methods for such simulations. We describe two applications: (1) Mechanistic investigation of the action of copper-containing nitrite reductases, which catalyze the reduction of nitrite to nitric oxide, a key step in the denitrification process. We identify its mechanism of action and determine the activation energies, transition states, and minimum energy pathways. (2) We use first-principles techniques combined with molecular dynamics simulations to calculate transport properties of B-DNA connected to carbon nanotubes. We find that the DNA conformation and especially the overlaps between sequential guanine bases play a critical role in electron transport, which is governed by charge delocalization. We also describe recent optimizations and enhancements to the Real Space Multigrid (RMG) code suite developed at North Carolina State University. RMG reached 1.144 Pflop/s on Blue Waters while using 3,872 XK (GPU-based) nodes. A portable library of routines suitable for inclusion in other HPC codes has also been developed.

INTRODUCTION

Denitrification has become a critical part of remediating human impact on our planet, as human activity has dramatically increased the amount of bio-available nitrogen. The considered enzyme, copper-containing nitrite reductase (CuNiR), is a key enzyme catalyzing the committing step of this process. This class of enzymes has been extensively investigated already, but many mechanistic aspects remain controversial.

The electrical conductivity of DNA is of fundamental interest in the life sciences. However, experimental measurements of conductivity differ dramatically for this system, depending on the method of sample preparation and the experiment being performed. We are thus investigating several factors affecting conduction, including DNA sequence, the presence of water, counterions, and linkers.

The current work addresses two issues: (1) the conversion of biologically active nitrogen back into atmospheric nitrogen, and (2) the mechanism of charge flow in DNA, understanding of which could lead to new DNA-based sensors and devices. Another goal of this project is to adapt our main quantum simulation code, Real Space Multigrid (RMG), to petascale supercomputers and release it to the scientific community, enabling many more petascale simulations of nano systems and biomolecules.

METHODS AND RESULTS

We have investigated theory of the enzymatic function of CuNiR and found that only a single mechanism is consistent with the structural data available for key intermediates. We found that the key part of the catalytic cycle involves changes of Asp^{98} configuration from "proximal" to "gatekeeper" to "proximal", and we identified the origins of the two protons needed for the reaction as coming from Asp^{98} and His^{255}, respectively. We have also found that the previously observed side-on coordination of the NO intermediate does not occur during the normal function of CuNiR.

CuNiR has the potential for use in environmental remediation and removal of excess nitrogen from aquatic environments. We find that nitrite reduction and attachment are the main rate limiting steps with energy barriers of 20.05 and 15.44 kcal/mol, respectively. The former barrier may be reduced by optimizing the T2 Cu binding site, while the latter can be decreased by improving the substrate channel leading to the catalytic site.

We have also investigated charge transport in DNA. While a lot of experimental studies have been performed, the results are contradictory and the process is poorly understood. Our calculations consider 4 and a 10 base-pair (bp) poly (G) poly (C) DNA fragments connected to (5,5) carbon nanotube leads via alkane linkers. To capture the thermal fluctuations, the systems are first investigated using molecular mechanics (MM) with full solvation.

We found that conductivity changes of 6 to 12 orders of magnitude for 4 bp and 12 bp DNA, respectively. The main factor causing these changes is the structure of DNA. Further analysis shows that the most relevant parameter is the area of overlap between successive guanines: the most conductive configurations have high values of this parameter between all neighboring base pairs. For these configurations, highly delocalized conductive states spanning the entire molecule exist (fig. 1), while a break in overlap between neighboring guanines causes the conductive states to be more localized, decreasing conductivity.

Additionally, we have investigated the effect of different sequences by replacing one of the GC pairs with AT, GT, and AC pairs. The first one is a well-matched case, whereas the other two pairs are mismatched. Our investigation finds that in an ideal DNA structure, these substitutions decrease conduction through the DNA by a factor of 5 for the well-matched case and a factor of 50 when a mismatch is present. However, when considering dynamical effects by averaging over multiple snapshots from MM simulations, we find that all cases have very similar conductances.

Ab initio electronic structure calculations have been very successful in studies of a wide range of scientific problems ranging from semiconductors to biological systems. Such calculations are rather computationally expensive and adapting the codes and algorithms to maximize performance on new computer architectures is an ongoing effort. The RMG code, which uses a sequence of grids of varying resolutions to perform quantum mechanical calculations, is very well suited to highly parallel architectures. It avoids fast Fourier transforms, which require global communications, and parallelizes easily via domain decomposition. It has been adapted to petascale architectures and GPUs during this proposal period and run at 1.14 Pflop/s on Blue Waters using 3,872 of the XK nodes.

WHY BLUE WATERS

Both applications described above require a very large parallel supercomputer with a high-speed interconnect between the nodes (due to frequent exchanges of substantial amounts of data between nodes). Each project required many runs to explore its various scientific issues, with a substantial amount of analysis between the runs. High availability and quick turn around on Blue Waters are very important for timely progress in our research.

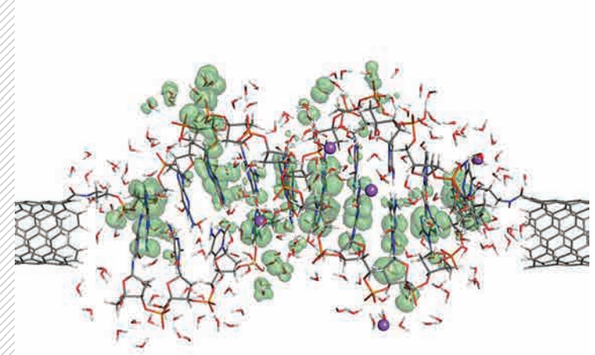

FIGURE 1: Isosurface of charge density of the most conducting HOMO state from a high-conductivity DNA configuration. The HOMO state is extended over most of the guanine bases.

PUBLICATIONS

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BREAKTHROUGH PETASCALE QUANTUM MONTE CARLO CALCULATIONS

Allocation: NSF/2.66 Mnh
PI: Shiwei Zhang[1]
Co-PIs: David Ceperley[2]; Lucas Wagner[2]; Elif Ertekin[2]
Collaborators: J. Grossman[3]; R. Hennig[4]; P. Kent[5]; H. Krakauer[1]; L. Mitas[6]; A. Srinivasan[7]; C. Umrigar[4]

[1]College of William & Mary
[2]University of Illinois at Urbana-Champaign
[3]Massachusetts Institute of Technology
[4]Cornell University
[5]Oak Ridge National Laboratory
[6]North Carolina State University
[7]Florida State University

EXECUTIVE SUMMARY:

The central challenge that our PRAC team aims to address is accurate, *ab initio* computations of interacting many-body quantum mechanical systems. The Blue Waters petascale computing framework has enabled highly ambitious calculations of a diverse set of many-body physics and engineering problems, spanning from studies of model systems in condensed matter (3D Hubbard model) to superconductivity in high-pressure hydrogen to the simulation of real materials of current research interest for energy applications. Over the past year, we have carried out simulations aiming to address these three general target areas. In our symposium presentation, we gave an overview of the team's activities and highlighted the latest science results. We focused on several of our explorations, including near-exact Hubbard model calculations, the dissociation of the chromium dimer, the adsorption of cobalt atoms on graphene, the metal-insulator transition in vanadium dioxide, and calculations of defects in semiconductors for photovoltaic and other applications.

INTRODUCTION

Many-body interactions are at the heart of both fundamental and applied physics problems. For decades, direct numerical solution of interacting systems has been computationally intractable, necessitating the use of approximate or effective models. Direct approaches accounting for many-body effects are critical to overcoming key barriers to predictive, accurate simulation.

Two key challenges addressed by our team are: (1) the development of high-accuracy computational methods for predictive, quantitative analysis of interacting physics; and (2) the application of these methods across a spectrum of problems, ranging from fundamental physics to real engineering materials design.

METHODS AND RESULTS

Chromium dimer

The chromium dimer has become a landmark test for electronic structure computation (fig. 1a). The quest for a scalable method capable of its accurate treatment is ongoing. We carried out phaseless auxiliary-field quantum Monte Carlo (ph-AFQMC) calculations using large, realistic basis sets. In parallel, we performed exact AFQMC calculations for smaller basis sets to systematically improve the ph-AFQMC accuracy. The calculated spectroscopic properties are in good agreement with experimental results.

Adsorption of cobalt atoms on graphene

Cobalt atoms adsorbed on graphene is of intense research interest because of their possible use in spintronics applications. We use auxiliary-field quantum Monte Carlo (QMC) and a size-correction embedding scheme to accurately calculate the binding energy of Co/graphene for several high-symmetry adsorption sites and benchmark a variety of different theoretical methods. A theory to explain recent experimental observations based on the calculations was provided in our talk at the 2014 symposium.

Metal-insulator transition in VO_2

We have been able to describe the metal insulator transition in the material VO_2 using QMC calculations. To our knowledge, this is the first time this material has been accurately simulated without using adjustable parameters.

Nitrogen doping in zinc oxide

Can nitrogen doping make zinc oxide a p-type semiconductor? This question has long been debated, with several experimental results indicating no, while several (less accurate) computational methods suggest yes. Our results, the first ever QMC assessment, are summarized in fig. 1b; they are in very good agreement with recent experimental results and are a very promising illustration of the capacity of QMC in historically very challenging systems.

Defect chemistry of the earth–abundant photovoltaic material CZTS

Two relatively new semiconducting materials, CuZnSnS and CuZnSnSe, have received substantial attention as potential earth-abundant alternatives to conventional silicon photovoltaics, but the influence of defects on properties is unknown. We are studying the formation of defect clustering reactions that can be detrimental to charge carrier transport.

WHY BLUE WATERS

The Blue Waters computing framework provides the exciting opportunity to apply direct stochastic solution methods—namely, QMC methods—to highly ambitious problems. The numerical methods are highly parallelizable, demonstrating nearly linear scaling up to several tens of thousands of cores.

PUBLICATIONS

Ma, F., S. Zhang, and H. Krakauer, Excited state calculations in solids by auxiliary-field quantum Monte Carlo. *New J. Phys.*, 15 (2013) 093017.

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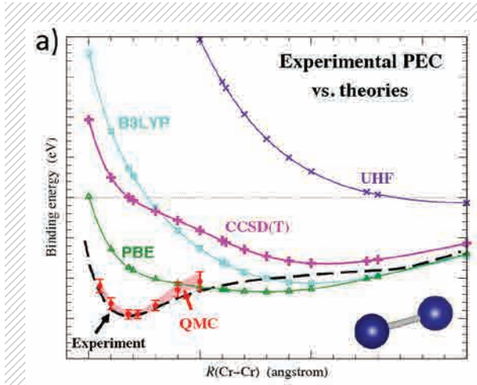


FIGURE 1 (A): The quantum Monte Carlo method enables unprecedented accuracy in capturing the dissociation physics of the chromium molecule, a long-standing physics challenge.

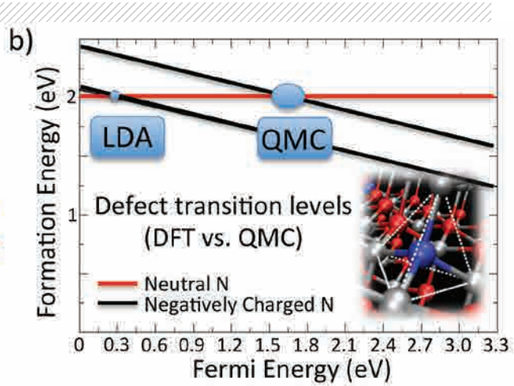


FIGURE 1 (B): Using quantum Monte Carlo methods, we can answer fundamental questions about semiconductor defect physics such as the nature of nitrogen impurities in zinc oxide, a question that has historically posed challenges to the defect community.

QUANTUM MONTE CARLO CALCULATIONS OF WATER-GRAPHENE INTERFACES

Allocation: Illinois/0.45 Mnh
PI: Narayana R. Aluru[1]
Co-PI: Lucas Wagner[1]
Collaborators: Yanbin Wu[1]; Huihuo Zheng[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

We are using the power of Blue Waters to perform highly accurate calculations of the electronic structure of water adsorbed on graphene surfaces. An accurate theoretical picture of the graphene-water potential energy surface will not only establish the basics of graphene-water interactions, but will also pave the way for revolutionary carbon-based applications related to energy, medicine, and water purification. Our diffusion Monte Carlo (DMC) calculations show strong graphene-water interaction, indicating the graphene surface is more hydrophilic than previously believed. The unusually strong interaction can be attributed to weak bonds between graphene and water. Our DMC calculations are of unprecedented accuracy, based on the first-principles Hamiltonian, and can provide insight for experimentalists seeking to understand water-graphene interfaces and for theorists seeking to improve density functional theory for weakly bound systems.

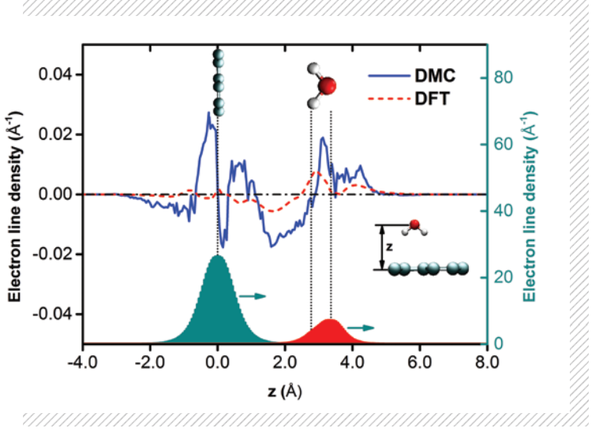


FIGURE 1: Electron redistribution when graphene and water approach each other. A positive value means accumulation of electron density and a negative value means depletion of electron density.

INTRODUCTION

An accurate theoretical picture of the graphene-water potential energy surface will not only establish the basics of graphene-water interactions, but will also pave the way for revolutionary carbon-based applications related to energy, medicine, and water purification. The outcome of our calculations will have several important scientific benefits:

1. A physical picture of the interaction of water with graphene. The interaction of water with surfaces is still very much an open problem, with ramifications in biology, atmospheric science, and global warming research, in addition to technological applications like water purification. Being able to examine the water-surface interaction with first-principle calculations has the potential to be a game changer in the study of these systems.

2. The development and testing of an accurate water-graphene surface potential based on the highly accurate energies given by the *ab initio* calculations. The water-graphene surface potential will be utilized in molecular dynamics simulations.

3. Reference data for the development of density functional theory (DFT) in the weak interaction limit.

METHODS AND RESULTS

We are using the power of Blue Waters to perform highly accurate calculations of the electronic structure of water adsorbed on graphene surfaces. Estimating graphene-water interaction energies based on *ab initio* calculations is challenging because graphene-water interaction is a weakly bounded system. As such, the electron correlation has to be properly described with adequate precision. Conventional DFT fails to do this.

For this reason, a correction to DFT focused on improving the description of the dispersion term. Recent reports of graphene-water binding energies using various electronic structure methods vary widely. The scatter of this data is mainly due to approximations in the electron structure methods that are necessary to be able to capture big graphene systems. A method that describes electron correlation accurately and scales well with system size is needed to study graphene-water interaction.

To achieve these goals, we perform a set of highly accurate quantum Monte Carlo calculations (QMC) on multiple water molecules interacting with a graphene surface. QMC is a class of methods that directly approach the many-body quantum problem. In this work, we plan to use two of the most prevalent flavors of QMC: variational Monte Carlo (VMC) and fixed node diffusion Monte Carlo (FN-DMC or DMC), both of which solve for the many-body ground state of a system of particles.

Our DMC calculations show strong graphene-water interaction, indicating the graphene surface is more hydrophilic than previously believed. The graphene-water binding energy computed in our DMC calculations is in good agreement with the heat of the adsorption energy measured using the gas chromatogram technique [1]. The unusually strong interaction can be attributed to weak bonds between graphene and water. Charge transfer may also contribute to the interaction. An isolated water molecule has one unoccupied band lying below the Fermi level of the graphene. When graphene and water approach each other, charge transfers from graphene to water, which can be shown from electron density analysis using DMC calculations as shown in fig. 1.

WHY BLUE WATERS

The DMC calculations are quite computationally expensive. To compute one interaction energy point between water and graphene, 200,000 core-hours are needed. It is ideal to run these DMC calculations on the large-scale resources of Blue Waters since QWalk, the QMC package we use, scales very well up to 64,000 cores (as tested on Blue Waters). Simulations that used to take weeks on other systems can now be done within days or even hours on Blue Waters so that multiple configurations can be explored to obtain unprecedented accuracy in interaction energy profiles.

SCALING UP OF A HIGHLY PARALLEL LBM-BASED SIMULATION TOOL (PRATHAM) FOR MESO- AND LARGE-SCALE LAMINAR AND TURBULENT FLOW AND HEAT TRANSFER

Allocation: Illinois/0.05 Mnh
PI: Rizwan Uddin[1]
Collaborators: Sudhakar V Pamidighantam[2]; Prashant Jain[3]
Associated Researchers: Kameswararao Anupindi[4]; Emilian Popov[3]

[1]University of Illinois at Urbana-Champaign
[2]National Center for Supercomputing Applications
[3]Oak Ridge National Laboratory
[4]University of Southampton

EXECUTIVE SUMMARY:

In the present work, we enhance, validate, and test the scalability of PRATHAM (PaRAllel Thermal Hydraulics Solver using Advanced Mesoscopic applications), a lattice Boltzmann method-based code for solving incompressible, time-dependent laminar and turbulent fluid flow in 3D domains. PRATHAM code is enhanced with a new lattice type (D3Q27), an immersed boundary method to handle complex geometry, and the capability to collect and report turbulent statistics. Using some of these new enhancements, the code is first tested for turbulent flow in a lid-driven cavity (LDC), turbulent flow in a circular pipe. The results obtained for flow in a LDC at a Reynolds number of 22,000 are compared with the available DNS data in the literature and this step acts as a validation of the PRATHAM solver. PRATHAM is found to scale well as the processor count is increased on Blue Waters.

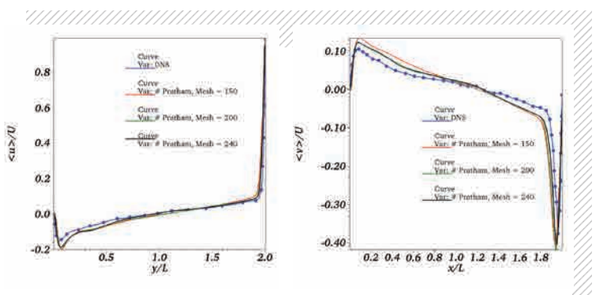


FIGURE 1: (left) Comparison of u component of velocity in the y direction on the central z plane. (right) Comparison of v component of velocity in the x direction on the central z plane.

METHODS AND RESULTS

PRATHAM is being developed at Oak Ridge National Laboratory to demonstrate the accuracy and scalability of a lattice Boltzmann method for turbulent flow simulations that arise in nuclear applications. The code is written in FORTRAN90 and made parallel using a message-passing interface. Silo library is used to write the data files in a compact form, and VisIt visualization software is used to post-process the simulation data in parallel.

PRATHAM has a variety of models implemented in it. For example, the collision between lattice points can be modelled using either a single or multiple relaxation time approximation. Lattice models such as D3Q19 and D3Q27 are implemented in a generic manner so that new types can be incorporated easily into the code. Large eddy simulation (LES) is used to simulate turbulent flows. In LES the larger turbulent structures are directly resolved, whereas turbulent structures smaller than the grid are modelled using a sub-grid scale (SGS) model. The present work uses the simple and widely used Smagorinsky SGS. This model modifies the fluid viscosity by an additional eddy viscosity that mimics energy dissipation in the sub-grid eddies, which is proportional to the resolved strain rate tensor. An immersed boundary method is also implemented so the code can simulate turbulent flow in complex geometries that are typical in nuclear applications. A ghost-point immersed boundary method is implemented which works starting from a geometry file in stereo lithography format.

In order to validate the solver we used flow in a lid-driven cavity (LDC) as a test case. A LDC is a simple geometry that shows several interesting flow features such as bifurcation and corner eddies. Direct numerical simulation data are available in the literature for comparison.

Flow in a LDC at a Reynolds number of 22,000 is simulated and mean and fluctuating turbulent quantities are computed. Fig. 1 shows a comparison of mean velocities with the DNS data as the mesh is refined from 150 mesh points to 240 mesh points in each direction. As the mesh is refined the results approach that of the DNS. A mesh size of 200 points in each direction seems to be an optimum size for this problem. We found that PRATHAM scales well up to a processor count of $O(10^4)$.

PETASCALE PARTICLE-IN-CELL SIMULATIONS OF KINETIC EFFECTS IN PLASMAS

Allocation: NSF/4.69 Mnh
PI: Warren Mori[1]
Collaborators: Frank S. Tsung[1]

[1]University of California, Los Angeles

EXECUTIVE SUMMARY:

In the past two years, the Blue Waters supercomputer has allowed us to perform very large-scale simulations which have provided qualitative and quantitative understanding in many different topics in plasma physics, including plasma-based accelerators and laser fusion. The simulation results (described below) have significantly impacted our understanding in these areas. Furthermore, we will discuss the need to move toward exascale computing and our development plans for future architectures, including Intel Phis and GPUs.

METHODS AND RESULTS

We study the electron beam evolution in an electron beam-driven plasma wakefield accelerator when the accelerated beam has a very small transverse emittance and a very small matched spot size that can cause the plasma ions to collapse toward the beam. The improved quasi-static particle-in-cell code QuickPIC allows us to use very high resolution and to model asymmetric spot sizes. Simulation results show that the accelerated beam will reach a steady state after propagating several centimeters in the plasma. We find that for round beams the (Li^+) ion density is enhanced by a factor of 100, but the emittance only grows by around 20%. For asymmetric spot sizes, the ion collapse is less, and emittance growth is zero in the plane with the largest emittance and about 20% in the other plane.

Recent experiments with the Callisto laser in the Jupiter laser facility have demonstrated the formation of a mono-energetic ring with an average energy of 150-250 MeV. OSIRIS 3D simulations have shown that injected electrons from a first bucket create a defocusing area in the front of a second bucket. As the electrons from the second bucket de-phase and move toward the front, they feel this defocusing force and begin to spread out. A small focusing region between the first and second buckets captures some of these electrons in the second bucket, causing the mono-energetic ring to form.

Laser-driven inertial fusion energy (IFE) can be detrimentally affected by the coupling of laser light waves to the plasma through which it propagates. In stimulated Raman scattering (SRS), the incident laser wave decays into an electron plasma wave (EPW) and a scattered light wave, potentially resulting in a direct loss of drive energy, inefficiency in drive symmetry, and pre-heating of the fusion fuel due to hot electrons generated by the daughter EPW.

We have performed 2D PIC simulations of SRS in inhomogeneous plasmas and with speckled laser beams. The laser beams in inertial confinement fusion experiments consist of a distribution of high-intensity hot spots, or speckles. While only a small percentage of these may be above the instability threshold for SRS, waves and particles generated by SRS in one speckle can stream into a neighboring speckle and cause it to undergo SRS even if it's below the threshold. Simulations of two-speckle scenarios have allowed us to study the conditions for which scattered light waves, EPWs, and hot electrons generated by SRS in above-threshold speckles can trigger SRS in neighboring, below-threshold speckles. Larger-scale simulations of multi-speckle ensembles show that SRS cascades triggered by scattered light can lead to pump depletion, dominating the recurrence of SRS.

These complex interactions could not be understood without simulations performed on Blue Waters.

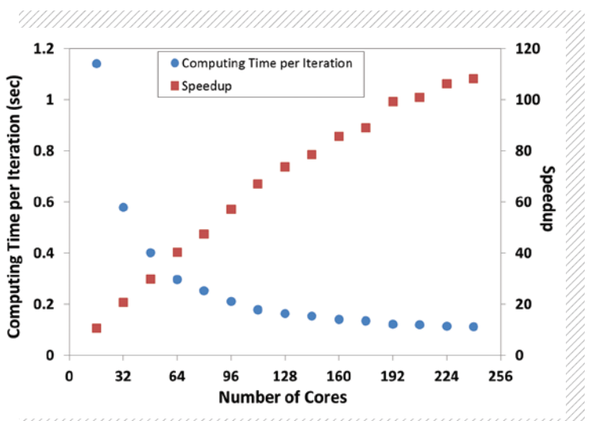
PRELIMINARY EVALUATION OF ABAQUS, FLUENT, AND CUFLOW PERFORMANCE ON BLUE WATERS

Allocation: Illinois/0.1 Mnh
PI: Brian G. Thomas[1]
Co-PIs: Lance Hibbeler[1]; Kai Jin[1]; Rui Liu[1]; Seid Koric[1]; Ahmed Taha[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

This project advances the state of the art in computationally intensive models of turbulent flow, mechanical behavior, heat transfer, and solidification in the continuous casting of steel. These models provide practical insight into how to improve this important manufacturing process. The performance of and preliminary results from the commercial codes FLUENT and ABAQUS and an in-house code are presented. FLUENT has been tested with a 3D, two-phase turbulent flow simulation and demonstrates a speed-up factor of about 100 with 256 cores. ABAQUS/Standard has limited speed-up capabilities because of its direct solver and works best with about 64 cores; the vast amount of memory on Blue Waters has improved the simulation time of a thermo-mechanical model of the mold and waterbox by a factor of about 40. A maximum speed-up factor of 25 has been observed on a single Blue Water XK7 node for the in-house GPU code for flow simulations.



INTRODUCTION

Continuous casting is used to produce 95% of steel in the world in the form of semi-finished shapes such as slabs, blooms, billets, beam blanks, and sheets. Even small improvements to this process can have a wide impact. Most defects arise in the mold region of the casting process due to the entrapment of inclusion particles into the solidifying shell and crack formation in the newly solidified steel shell. These defects persist into the final products and cannot be removed. Thus, the best method to improve steel products is to fully understand the mechanisms of defect formation and find operation conditions that avoid these problems.

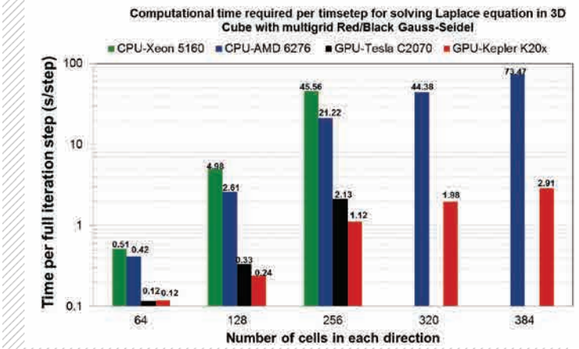
Owing to the high temperatures and harsh commercial environment, it is difficult to conduct comprehensive measurements in the manufacturing process. Accurate and efficient computational models are needed to optimize various process variables (nozzle geometry, steel and gas flow rates, electromagnetics, taper of the mold walls, etc.). In addition to improving the manufacturing process, development and validation of better computational methodologies is useful in the modeling of many other processes.

METHODS AND RESULTS

For the stress analysis, several runs with a mesh of 375,200 elements, 754,554 nodes, and 2,263,662 degrees of freedom (DOFs) were completed on Blue Waters with implicit ABAQUS, which allows input and use of the phase field. The CPU time for one Newton iteration, consisting of 0.57 Tflop/s, is presented in table 1 for different numbers of threads. The optimum number of threads is ~64. Efficiency appears to be limited by the FEM assembly process, coupling between DOFs during solving, or communication across processors. Results from this model match with plant inclinometer measurements on the cold-face exterior [11].

To evaluate performance of the commercial package, FLUENT, for fluid flow modeling on Blue Waters, argon-steel two-phase turbulent flows in a continuous casting mold was modeled on several computers. The test consisted of 0.66 million hexahedral mapped computational cells and ~8.4 million DOFs. One hundred iterations of FLUENT ran about 108 times faster on 240 nodes on Blue Waters than on a single-core Dell Precision T7600 workstation. Further simulations on Blue Waters with a different number of computer nodes showed almost linear speed-up with more nodes (fig. 1). Results from this model show that dithering (oscillation) of the slide gate to lessen clogging also causes mold flow oscillations, which may become unstable at certain frequencies [12].

For the in-house GPU code, CUFLOW, the pressure Poisson equation (PPE) solver was tested on a single Blue Waters XK7 node by solving a heat conduction problem in a 3D cube. The solver uses V-cycle multi-grid technique and a red/black successive over-relaxation (SOR) method. Both CPU and GPU versions were developed and tested. Increasing grid size from 0.26 million to 0.56 billion cells increased speedup to a maximum of 25 (fig. 2). The model is being applied to predict the entrapment locations of inclusion particles in the solidified strand for conditions where measurements were obtained at an operating commercial caster [13].



# THREADS	DAYS REQUIRED
32	6.80
64	5.25
128	5.50
256	5.50

WHY BLUE WATERS

All of the models used in this work are very computationally demanding. For the stress analysis part, multi-scale thermal-mechanical simulations of mechanical behavior the solidifying steel shell are being conducted using ABAQUS/Explicit. By aiming to capture physical phenomena involving detailed behavior on the small scale of the microstructure, this model requires advanced computational resources like Blue Waters.

For the fluid flow simulation, the Navier–Stokes equations are solved using the finite volume method for large eddy simulations (LES) incorporating the multi-phase flow via Eulerian–Lagrangian coupling [7-8]. Our previous LES simulations with about 1.5 million cells requires about four months to simulate only 30 seconds of model time on high-end workstations [9-10]. Proper mesh resolution requires over 10 million cells, and resolving the main periodic frequencies identified in plant experiments require over 60 seconds of model time. Thus, we explore the feasibility of using FLUENT on Blue Waters, with the help of ANSYS, Inc.

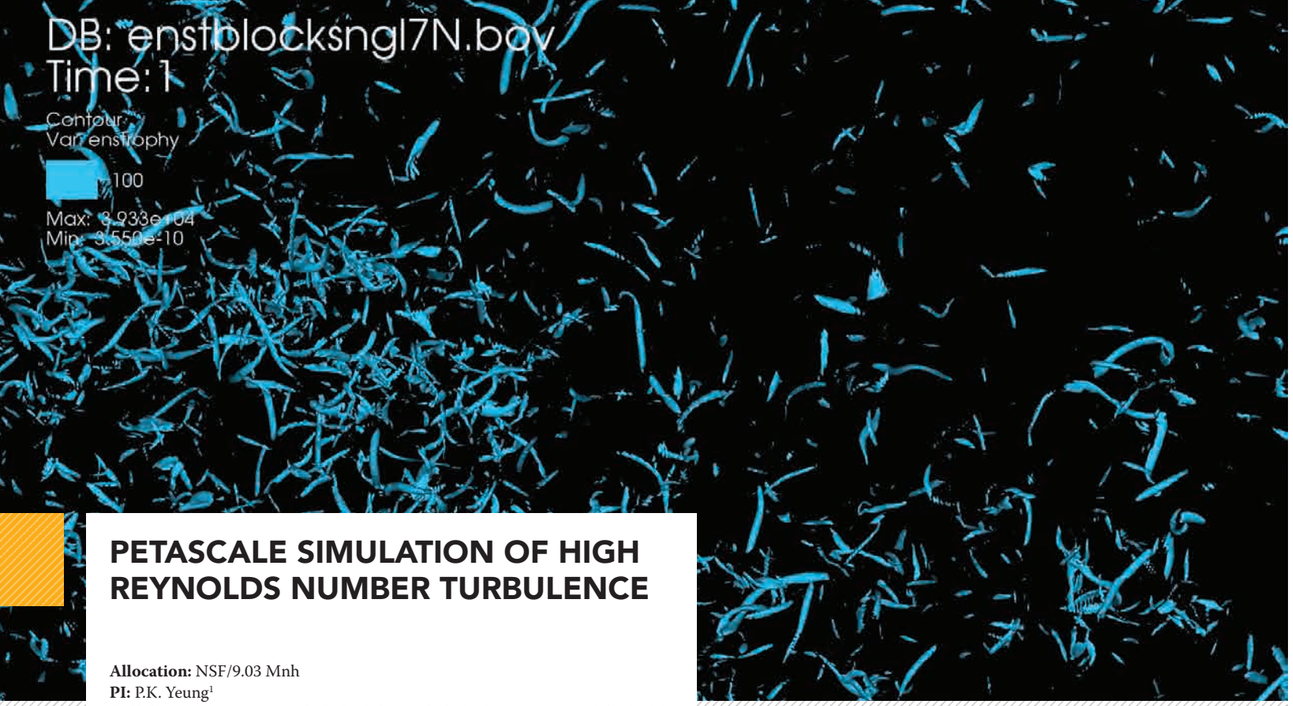
PUBLICATIONS

Hibbeler, L. C., B. G. Thomas, R. C. Schimmel, and H. H. Visser, Simulation and Online Measurement of Narrow Face Mold Distortion in Thin-Slab Casting. *Proc. 8th European Continuous Casting Conf.* , Graz, Austria, June 23-26, 2014.

FIGURE 1 (LEFT): FLUENT computational cost on Blue Waters (per iteration) with speed-up relative to a lab workstation.

FIGURE 2 (ABOVE): PPE solver performance on Blue Waters CPU and GPU.

TABLE 1: ABAQUS runs on Blue Waters. CPU time required for 1 second simulation for different numbers of threads



PETASCALE SIMULATION OF HIGH REYNOLDS NUMBER TURBULENCE

Allocation: NSF/9.03 Mnh
PI: P.K. Yeung[1]
Collaborators: A. Majumdar[2]; D. Pekurovsky[2]; R. D. Moser[3]; J.J. Riley[4]; K.R. Sreenivasan[5]; B.L. Sawford[6]

[1]Georgia Institute of Technology
[2]San Diego Supercomputer Center
[3]University of Texas at Austin
[4]University of Washington
[5]New York University
[6]Monash University, Australia

EXECUTIVE SUMMARY:

We study the complexities of turbulent fluid flow at high Reynolds number, where resolution of fluctuations over a wide range of scales requires massively parallel petascale computation even in simplified geometries. The power of Blue Waters, combined with the use of remote memory addressing and reserved partitions to minimize communication costs, has made feasible a simulation at record resolution exceeding half a trillion grid points.

Early science results include new insights on fine-scale intermittency, spectral transfer, and the connection between extreme events observed in fixed and moving reference frames. Phase 1 of this project has focused on algorithm enhancement and the study of velocity field structure. Phases 2 and 3 will focus on mixing passive substances and slow-diffusing chemical species, and dispersion of contaminant clouds at high Reynolds number. Collaborative work based on the new data is expected to lead to significant advancements in theory and modeling.

FIGURE 1 (BACKGROUND): Slender vortex filaments showing the complexity of fine-scale structure in high Reynolds number turbulence at $8{,}192^3$ resolution.

INTRODUCTION

Turbulence at high Reynolds number arises in numerous types of natural phenomena and engineering devices where disturbances in one form or another are generated by some physical mechanism, transported over some distance in space, or dissipated through molecular viscosity or diffusivity. The prediction of wind gusts in a storm, the life of marine organisms in the ocean, the propulsive thrust provided by jet aircraft engines, and the dispersion of pollutants in an urban environment—all depend on the study of turbulence and are of concern to our society.

Our project will help provide a much better understanding of the underlying flow physics that also apply to turbulent flows in more realistic geometries. Improved resolution and higher Reynolds number will also help settle long-standing questions about local isotropy and sub-grid scale modeling in turbulent mixing. We will also be able to address a pressing concern in turbulence simulations, namely how to parameterize Reynolds number dependence well enough so that important conclusions about the flow physics can be extrapolated safely toward Reynolds numbers that remain out of reach.

METHODS AND RESULTS

Our computational challenge is to simulate incompressible turbulence in a periodic domain at a resolution of $8{,}192^3$, with more than half a trillion grid points, at a Reynolds number that exceeds previous known work, while also resolving the small scales better than standard practice in the literature. The presence of a wide range of scales is crucial to many key properties such as the intermittency of extreme events, the spectral transfer from the large scales to the small scales, the effective mixing of transported substances compared to molecular diffusion, and the relative dispersion of contaminants carried along highly convoluted fluid element trajectories. Although several well-known hypotheses of scale similarity provide an approximate description of the flow physics, well-resolved numerical simulation data at a Reynolds number higher than achieved in the recent past are still necessary for theory and model development at the next level of physical realism.

As of April 2014 we obtained a $8{,}192^3$ velocity field which is statistically stationary and isotropic, at a Taylor-scale Reynolds number close to 1,300, with a grid spacing which resolves scale sizes down to about 1.5 times the Kolmogorov scale. Many instantaneous snapshots of velocity fields spanning about 2.5 large-eddy turnover times have been saved. When running under a reserved partition of appropriate network topology the wall time on 262,144 MPI tasks is consistently under 10 seconds per time step, which gives essentially perfect strong scaling if compared with the same problem size using 65,536 cores without a reserved partition.

Substantial effort is directed at studying the intensity of the local straining and rotation of fluid elements subjected to the distorting effects of velocity fluctuations. Results on the probability distributions of these variables provide strong validation of conclusions from recent work on the likelihood of extreme events approaching 10,000 times the mean value. Comparisons of the statistics of acceleration (which is also highly intermittent) in fixed and moving reference frames show a strong degree of mutual cancellation between the effects of unsteadiness at a fixed location and of turbulent transport in space. Conditional statistics also verify quantitatively the connection between intermittency in the energy dissipation rate and in the acceleration, which is very important in the modeling of turbulent dispersion.

WHY BLUE WATERS

The rapid increase in the range of scales in length and time with Reynolds number is such that, in general, a $8{,}192^3$ simulation is almost 16 times as expensive as one at $4{,}096^3$ resolution (which was first reached in 2002, on the Earth Simulator in Japan). The cost also increases considerably (by at least a factor of two) when we include mixing and dispersion in addition to the basic flow field. Consequently, our intended science target can only be reached using a large allocation of time on a multi-petaflop computer such as Blue Waters. At the same time, our code performance benefitted greatly from Cray personnel helping us with remote memory addressing, and from the Blue Waters project staff in arranging reserved partitions of up to 8,192 32-core Blue Waters nodes, which largely overcomes the issue of network contention with other jobs running on the system.

PUBLICATIONS

Yeung, P. K., Early Results from High Reynolds Number DNS at $8{,}192^3$ resolution. *Second International Conference on Mathematical Theory of Turbulence via Harmonic Analysis and Computational Fluid Dynamics*, Nara, Japan, March 3-5, 2014.

Iyer, K. P., Studies of turbulence structure and turbulent mixing using Petascale computing. (PhD thesis, Georgia Institute of Technology, 2014).

Iyer, K. P., and P. K. Yeung, Structure functions and applicability of Yaglom's relation in passive-scalar turbulent mixing at low Schmidt numbers with uniform mean gradient. *Phys. Fluids*, **26** (2014), 085107.

COMPUTATIONAL EXPLORATION OF UNCONVENTIONAL SUPERCONDUCTORS USING QUANTUM MONTE CARLO

Allocation: Illinois/0.508 Mnh
PI: Lucas K. Wagner[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

The interactions between electrons create many unique quantum states and electronic devices, such as superconductors. To date, efforts to simulate these quantum states have had great difficulty achieving enough fidelity to describe these states. Using Blue Waters and modern algorithms, we performed state-of-the-art many-body simulations of strongly interacting quantum systems VO_2 and several superconductor parent materials to unprecedented detail. These simulations have given insight into how these materials perform their function and offer hope that simulations of this type will be able to achieve the dream of computationally guided correlated material design.

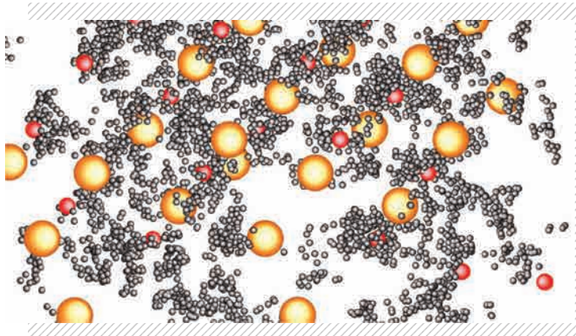


FIGURE 1: A sample of electronic positions pulled from a calculation on the MgO solid. Each sample corresponds to the positions of all electrons. Density of samples represents the amplitude of the wave function.

INTRODUCTION

One of the grand challenges in condensed matter physics is to describe the behavior of strongly correlated electronic systems—materials in which the interactions between electrons are critical to their behavior. Electron interactions are responsible for a number of unique properties of these materials including high-temperature superconductivity, giant magnetoresistance, high-efficiency catalysis, and many others. The strong correlation challenge is particularly interesting in that the fundamental equation to be solved, the time-independent electronic Schrödinger equation, is well known. There is no known general, efficient, and exact solution to this problem.

METHODS AND RESULTS

We are using Blue Waters to simulate correlated electrons directly using the diffusion Monte Carlo algorithm. This method is based on a mapping from the Schrödinger equation to the dynamics of stochastic particles. These particles diffuse, drift, and branch, and in their equilibrium configuration their density represents the amplitude of the lowest energy state, the most important state for condensed matter physics.

There is one major approximation in diffusion Monte Carlo. Since the stochastic particles are all positive, they cannot easily represent a function with positive and negative regions. Further, the ground state of electrons is required to have both positive and negative regions by fundamental physics. We thus must approximate the zeroes of the wave function to fix the positive/negative regions. This is called fixed-node diffusion Monte Carlo (FN-DMC). In practice, the fixed node approximation has been shown to be very accurate on realistic simulations of quantum systems. This method has been implemented and scaled up by the authors to run on a large fraction of Blue Waters [1].

We have completed two pilot studies on correlated electronic systems. Both of these studies are on materials that have been known for several decades, but to date have resisted description by either first-principles calculations (Schrödinger equation) or assumed models. The lack of a reliable first-principles description is particularly limiting for design of materials with strongly correlated effects. At the 2014 Blue Waters Symposium, we present our results on the metal-insulator transition in VO_2 and the spin-lattice interaction in the high Tc superconducting cuprate parent materials using Blue Waters and the FN-DMC method to describe their electronic structure accurately.

The successful description of these correlated materials opens the door to many further calculations that may help uncover the mechanism for high-temperature superconductivity and potentially allow for design of these unique materials. Since the FN-DMC method is generally applicable to the many-body Schrödinger equation, developments in this arena carry over to other important issues in materials physics, such as the prediction of doping behavior, magneto-electric coupling, and catalysis.

PUBLICATIONS

Zheng, H., and L. K. Wagner, The mechanism of metal-insulator transition in vanadium dioxide from a first-principles quantum Monte Carlo perspective. (submitted). arxiv:1310.1066

Wagner, L. K., and P. Abbamonte, The effect of electron correlation on the electronic structure and spin-lattice coupling of the high-T_c cuprates: quantum Monte Carlo calculations. (submitted). arXiv:1402.4680

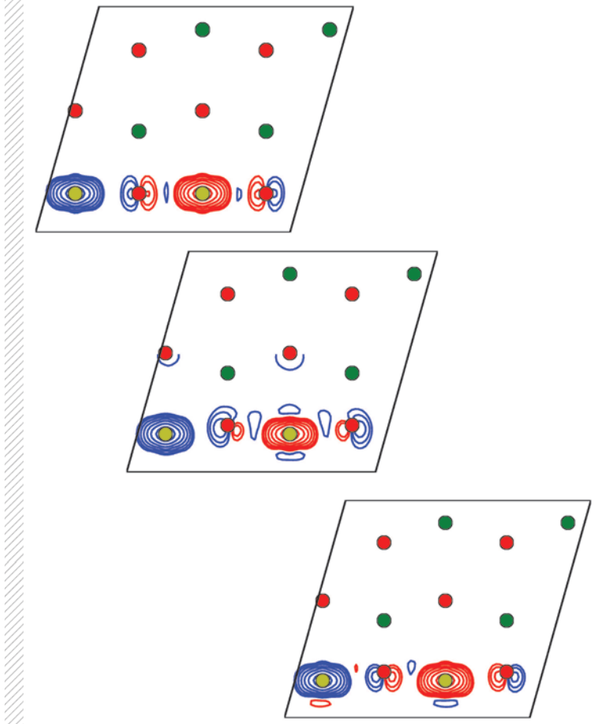


FIGURE 2: 2D projection of the resultant spin densities for the high temperature superconducting material La_2CuO_4. Copper atoms are gold, oxygen atoms are red, and lanthanum atoms are green. Shown is the response of the spin density to different phonon modes.

COMPUTER SCIENCE & ENGINEERING

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100 *System Software for Scalable Computing*

102 *Scalability Analysis of Massively Parallel Linear Solvers on the Sustained Petascale Blue Waters Computing System*

HYBRID DATAFLOW PROGRAMMING ON BLUE WATERS

Allocation: GLCPC/0.375 Mnh
PI: Michael Wilde[1,3]
Collaborators: Scott J. Krieder[2]; Justin M. Wozniak[1]; Timothy Armstrong[3]; Daniel S. Katz[1,3]; Ian T. Foster[1,3]; Ioan Raicu[2,3]

[1]Argonne National Laboratory
[2]Illinois Institute of Technology
[3]University of Chicago

EXECUTIVE SUMMARY:

This work presents the analysis of hybrid dataflow programming over XK7 nodes of Blue Waters using a novel CUDA framework called GeMTC. GeMTC is an execution model and runtime system that enables accelerators to be programmed with many concurrent and independent tasks of potentially short or variable duration. With GeMTC, a broad class of such "many-task" applications can leverage the increasing number of accelerated and hybrid high-end computing systems. GeMTC overcomes the obstacles to using GPUs in a many-task manner by scheduling and launching independent tasks on hardware designed for SIMD-style vector processing. We demonstrate the use of a high-level many-task computing programming model (the Swift parallel dataflow language) to run tasks on many accelerators and thus provide a high-productivity programming model for the growing number of supercomputers that are accelerator enabled. While still in an experimental stage, GeMTC can already support tasks of fine (sub-second) granularity and execute concurrent heterogeneous tasks on 86,000 independent GPU warps spanning 2.7 million GPU threads on Blue Waters.

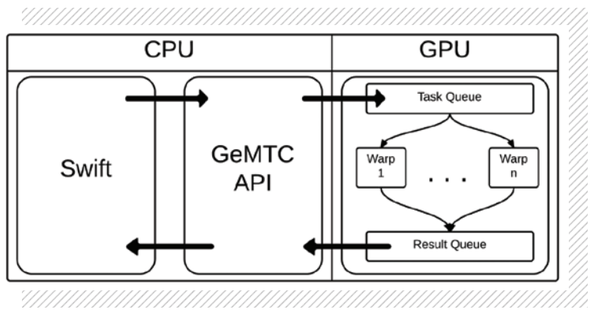


FIGURE 1: Flow of a task in GeMTC driven by Swift.

INTRODUCTION

This work explores methods for, and potential benefits of, applying the increasingly abundant and economical general purpose graphics processing units (GPGPU) to a broader class of applications. It extends the utility of GPGPU from the class of heavily vectorizable applications to irregularly structured many-task applications. Such applications are increasingly common, stemming from both problem-solving approaches (i.e., parameter sweeps, simulated annealing or branch-and-bound optimizations, uncertainty quantification) and application domains (climate modeling, rational materials design, molecular dynamics, bioinformatics).

In many-task computing (MTC) [1], tasks may be of short (even sub-second) duration or highly variable (ranging from milliseconds to minutes). Their dependency and data-passing characteristics may range from many similar tasks to complex, and possibly dynamically determined, dependency patterns. Tasks typically run to completion; they follow the simple input-process-output model of procedures, rather than retaining state as in web services or MPI processes.

METHODS AND RESULTS

Fig. 1 shows a high-level diagram of GeMTC [2] driven by tasks generated by the Swift [3] parallel functional dataflow language. GeMTC launches a daemon on the GPU that enables independent tasks to be multiplexed onto warp-level GPU workers. A work queue in GPU memory is populated from calls to a C-based API, and GPU workers pick up and execute these tasks. After a worker has completed a computation, the results are placed on an outgoing result queue and returned to the caller.

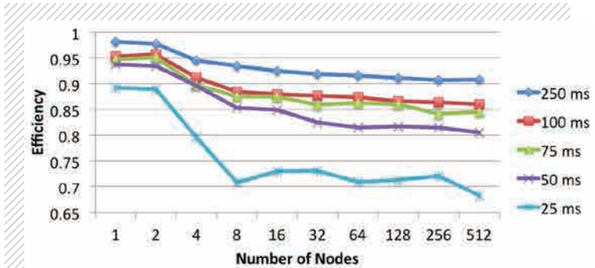
We first ran a multi-node scaling experiment where the number of simulations is set equal to the number of workers. At each data point there are two times as many workers as at the previous data point, so we run twice as much work. In an ideal system without any overhead we would expect a flat line demonstrating the ability to conduct the same amount of work at each step. Even after eight nodes we achieve 96% utilization. Future work aims to evaluate our system at even larger scales on Blue Waters. We also obtain 70% of ideal throughput with 10,000-way concurrency using Swift+GeMTC.

Fig. 2 demonstrates an upper bound of GeMTC by launching efficiency workloads on multiple GPU nodes with only a single active GeMTC worker per GPU. We next enable 168 GeMTC warp workers per GPU (the maximum) and evaluate the efficiency of workflows with varied task granularities up to 86,000 individually operating GPU workers on Blue Waters. After adding 167 additional workers per GPU we require longer-lasting tasks to achieve high efficiency. We attribute this drop in performance to greater worker contention on the device queues and the fact that Swift must now drive 168 times the amount of work per node.

In fig. 3 we observe that tasks exceeding one second achieve high efficiency up to scales of 40,000 workers. Although we have not yet identified the cause for this drop in performance, we expect that the performance degradation at extreme levels of concurrency comes from the loading of shared libraries from the remote parallel file system. In future work we will continue to improve system-wide performance by reducing the reliance on dynamic loadable shared libraries and using larger scale evaluation on all ~4,000 XK7 nodes.

While we observe a drop in performance moving from a single worker to 168 workers, we achieve 168 times the amount of work with only a five-fold increase in time. These numbers improve even more when the time for computing versus data transfer increases. In future work we will continue to improve system-wide performance and evaluation at even larger scale.

Future work includes performance evaluation of diverse application kernels (e.g., data pipelining, detecting cancer-related genes, glass modeling, and protein structure simulation); analysis of the ability of such kernels to effectively utilize concurrent warps; enabling of virtual warps which can both subdivide and span physical warps; support for other accelerators such as the Xeon Phi; and continued performance refinement.



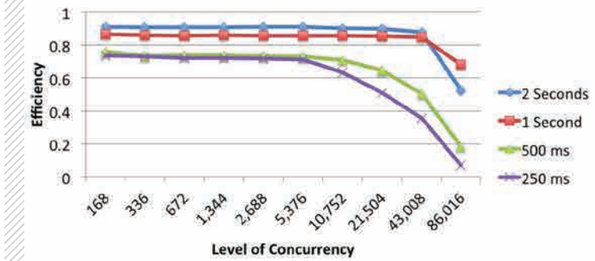


FIGURE 2 (TOP): GeMTC + Swift efficiency up to 512 nodes, 1 GeMTC worker.

FIGURE 3 (BOTTOM): Efficiency for workloads with varied task granularities up to 86,000 independent warps of Blue Waters. 168 active workers/GPU.

REDESIGNING COMMUNICATION AND WORK DISTRIBUTION IN SCIENTIFIC APPLICATIONS FOR EXTREME-SCALE HETEROGENEOUS SYSTEMS

Allocation: GLCPC/0.319 Mnh
PI: Karen Tomko[1]
Co-PI: Dhabeleswar K. Panda[2]
Collaborators: Khaled Hamidouche[2]; Hari Subramoni[2]; Jithin Jose[2]; Raghunathan Raja Chandrasekar[2]; Rong Shi[2]; Akshay Venkatesh[2]; Jie Zhang[2]

[1]Ohio Supercomputer Center
[2]The Ohio State University

EXECUTIVE SUMMARY:

In this project we explore communication performance for modern programming models at large scale. Specifically, we evaluate the performance of point-to-point and collective communications for CraySHMEM and UPC PGAS models. We tune a hybrid high-performance LINPACK implementation to leverage both CPU and GPU resources for systems with mixed node types. We evaluate collective algorithm performance at very large scale, starting with Broadcast and extending to more complicated operations such as Reduce, All-Reduce, and All-to-All. Additionally, we evaluate the cost of I/O for checkpoint operations to understand the impact of system-level checkpointing on applications.

INTRODUCTION

The field of computer architecture, interconnection networks, and system design is undergoing rapid change that enables very large supercomputers such as Blue Waters to be built. System advances have come in the form of increased parallelism from many-core accelerators and improved communication interfaces. To leverage these advances, applications must be revamped to use new capabilities of the interconnection networks and more sophisticated programming models. Without these corresponding software advances the vision of science breakthroughs cannot be achieved.

METHODS AND RESULTS

We have evaluated the performance and scalability of point-to-point and collective operations of Cray-SHMEM and Cray-UPC using the Ohio State University Micro-benchmark suite. For point-to-point experiments, we evaluate both intra- and inter-node cases for put, get, and atomic operations. UPC collectives are evaluated for Broadcast, Scatter, Gather, Allgather, Alltoall, and Barrier operations. Similarly, OpenSHMEM collective operations such as Broadcast, Barrier, Collect, and Reduce are evaluated. Our evaluations indicate good point-to-point performance results for both OpenSHMEM and UPC. Further, many of the collective operations (UPC-Scatter, OpenSHMEM-Broadcast) show good scalability characteristics. However, for some of the collectives the performance is lower than the corresponding MPI collective operations.

We have tuned a mixed-node version of high-performance LINPACK (HPL) to utilize both XE6 and XK7 Blue Waters nodes in a single run. Our HPL tests with different versions of the benchmark: standard HPL from Netlib, NVIDIA's HPL running on pure CPU nodes, NVIDIA's HPL running on pure GPU nodes, and our hybrid HPL running across both CPU and GPU nodes. For the underlying math libraries, we measure the performance among ACML, OpenBLAS, and LibSci.

OpenBLAS and ACML achieve better performance than LibSci for standard HPL with the peak performance of a single CPU node around 202 GFlop/s. When measuring NVIDIA's HPL on pure CPU nodes (modified version), we measure the multi-thread computation capacities among different math libraries, and OpenBLAS performs better than ACML in this case, with peak performance of a single CPU node around 190 GFlop/s. We also measure the peak performance efficiency achieved by our hybrid HPL compared to the sum of pure CPU and GPU nodes. We get above 70% efficiency with 16 GPU nodes and 64 CPU nodes.

The performance of collectives on Blue Waters has been evaluated with OSU's Micro-benchmark suite. The experiments focus on the aspects of scalability of the collectives with increasing message size as well as with increasing process count in the MPI job. All the collectives have been run on the MPI_COMM_WORLD global communicator of the MPI job. Results indicate that the performance of both Broadcast and Reduction operations are quite scalable with fairly short latencies considering the scale of the job. Reduction operations are especially scalable owing to the use of dedicated hardware support in the Gemini interconnect. Other dense collective operations, such as MPI_Allgather and MPI_Alltoall, are quite time consuming at a process scale of 128,000 and indicate an area that needs attention at scale.

MPI implementations typically provide system-level fault-tolerance support by means of transparent checkpoint restart. We are developing an I/O kernel that mimics the I/O pattern of coordinated checkpointing protocols and are using this benchmark to study the performance impact of system-level checkpointing on MPI applications. We do not have results to report on this activity at this time.

WHY BLUE WATERS

There are very few systems nationally that provide a test bed for scaling communications to tens or hundreds of thousands of cores, yet communication runtimes and the applications built upon them are expected to run effectively at these scales and beyond. Blue Waters provides this test bed. The system's unique mix of XE6 and XK7 nodes enable investigation of application-level designs for mixed CPU and GPU node systems. Additionally, the system's high-bandwidth Lustre file system supports evaluation of large-scale checkpoint/restart costs.

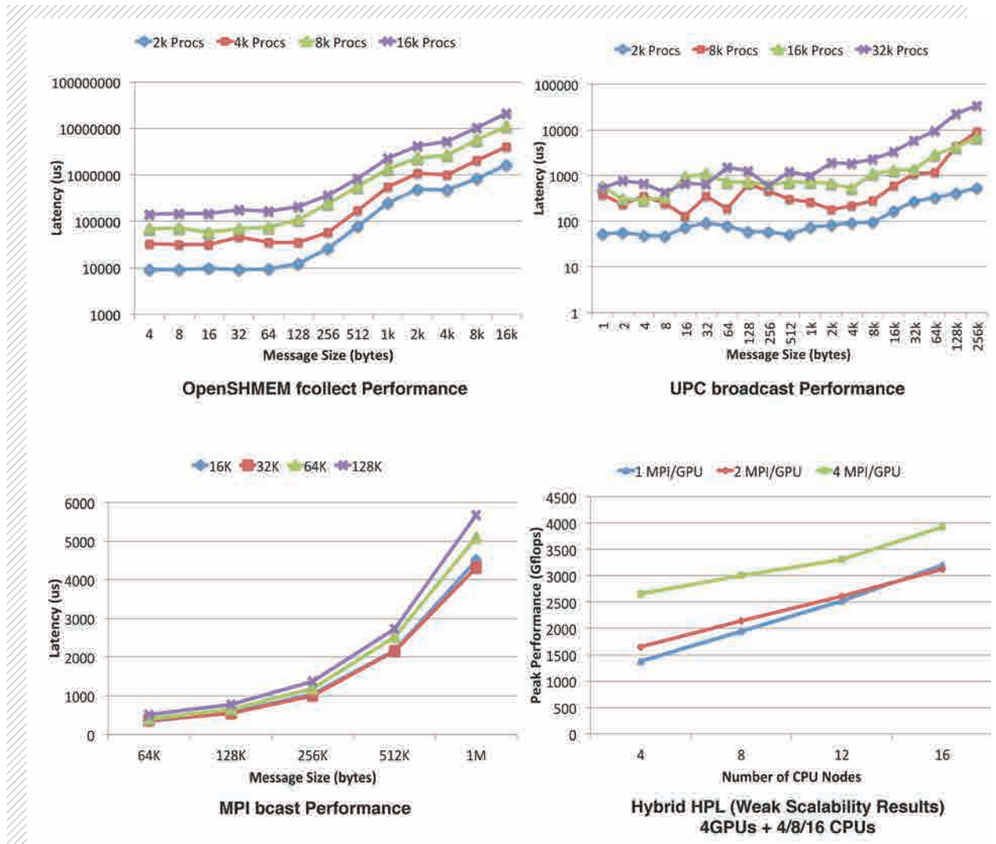


FIGURE 1 (RIGHT): Communication performance and scalability of modern programming models on Blue Waters. Clockwise from upper left:

(A): Latency of the OpenSHMEM fcollect collective communication operation by message size for 2,000 to 16,000 processes.

(B): Latency of the UPC all_broadcast collective communication operation by message size for 2,000 to 32,000 UPC threads.

FIGURE 1 (C): Performance of the hybrid HPL implementation for different CPU-to-GPU node ratios and with differing MPI processes per GPU node.

(D): Latency of the MPI_Bcast collective operation by message size for 16,000 to 128,000 processes.

SYSTEM SOFTWARE FOR SCALABLE COMPUTING

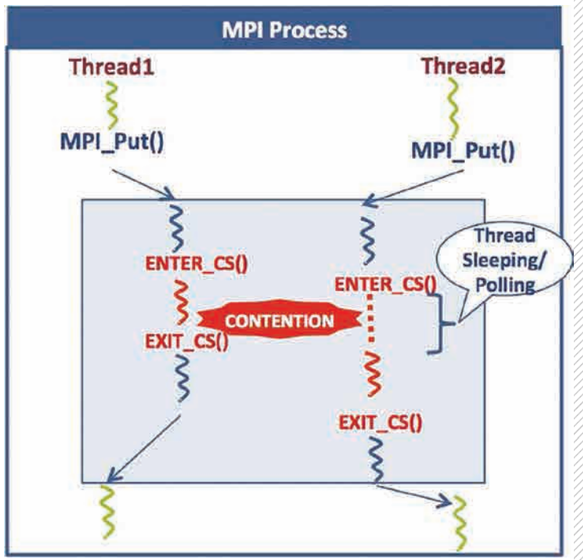
Allocation: BW Prof./0.245 Mnh; NSF/0.613 Mnh
PI: William Gropp[1]
Collaborators: Pavan Balaji[2]

[1]University of Illinois at Urbana-Champaign
[2]Argonne National Laboratory

EXECUTIVE SUMMARY:

The goal of the System Software for Scalable Computing project was to study the performance of low-level communication systems such as MPI in various environments on the Blue Waters system and propose optimization techniques to address performance shortcomings. Over the past year, we focused on two such areas: (1) MPI communication in multi-threaded environments, and (2) MPI communication in irregular communication environments such as graph algorithms.

FIGURE 1: Lock contention in an MPI+threads application



INTRODUCTION

Because of power constraints and limitations in instruction-level parallelism, computer architects are unable to build faster processors by increasing the clock frequency or by architectural enhancements. Instead, they are building more and more processing cores on a single chip and leaving it up to the application programmer to exploit the parallelism provided by the increasing number of cores. MPI is the most widely used programming model on HPC systems and many production scientific applications use an MPI-only model. Such a model, however, does not make the most efficient use of the shared resources within the node of an HPC system. For example, having several MPI processes on a multicore node forces node resources (such as memory, network FIFOs) to be partitioned among the processes. To overcome this limitation, application programmers are increasingly looking at using hybrid programming models comprising a mixture of processes and threads, which allow resources on a node to be shared among the different threads of a process.

With hybrid programming models, several threads may concurrently call MPI functions, requiring the MPI implementation to be thread safe. In order to achieve thread safety, the implementation must serialize access to some parts of the code by using either locks or advanced lock-free methods. Using such techniques and at the same time achieving high concurrent multithreaded performance is a challenging task [2-4].

METHODS AND RESULTS

Our first focus area is MPI communication in multi-threaded environments. The Blue Waters system, while rich in the number of cores per node, is unfortunately not as well optimized for communication when multiple threads issue MPI operations simultaneously. In this work, we analyzed sources of thread contention in representative MPI+thread applications using several benchmarks, ranging from micro-benchmarks and stencil computation to graph traversal applications [1]. In our study, we found that one of the primary sources of lock contention is lock monopolization stemming from unfair mutex-based critical sections (fig. 1). When a thread spends a short period between two lock acquisition attempts and an arbitration is not performed, the thread holder may reacquire the lock before other threads notice the lock was relinquished. If this happens repeatedly, it will lead to lock monopolization.

Based on this analysis, we designed a way to mitigate this issue with a FIFO (first-in, first-out) arbitration (ticket-based locking) as well as a prioritized locking scheme that favors threads doing useful work. Experimental results show that our new locking scheme significantly increases the throughput of MPI+thread applications.

Our second focus area involving Blue Waters is a large-scale graph application. While a number of users have demonstrated scaling regular applications on Cray XE platforms, it is more challenging to scale distributed graph algorithms to a large scale because of the load balance problem caused by their irregular communication. To solve the load balance problem, we are designing a parallel asynchronous breadth-first search (BFS) algorithm on distributed memory systems [5]. This work is in its early stages, but we showcased some initial performance numbers at the symposium.

Different from level-synchronous BFS, asynchronous BFS will not wait until all vertices in the same level have been visited to start traversing a new level. Instead, it will start visiting its neighbors as soon as it receives a message from its parent, so it removes the waiting time. However, because vertices do not synchronize at each level, some vertices may receive a delayed message with a smaller distance to the root. So the algorithm has to send messages to all its children again to correct the distance, thus bringing redundant communication to the algorithm. In order to minimize the redundant communication, we plan to use priority queues to give a partial order to different messages handled by each processor. We will also evaluate the tradeoff of computation and communication in graph algorithms in different problem scales.

WHY BLUE WATERS

Some problems are not observed when we run them at a small scale, but Blue Waters gives us a unique opportunity to evaluate and design our algorithm at a large scale with state-of-the-art network and computer systems.

SCALABILITY ANALYSIS OF MASSIVELY PARALLEL LINEAR SOLVERS ON THE SUSTAINED PETASCALE BLUE WATERS COMPUTING SYSTEM

Allocation: Private sector/0.002 Mnh
PI: Seid Koric[1]
Collaborators: Anshul Gupta[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Solving linear systems of equations lies at the heart of many problems in computational science and engineering and is responsible for 70-80% of total computational time consumed by the most sophisticated multi-physics applications.

Recent solver comparisons [1,2] have shown that the Watson sparse matrix package (WSMP) solver from IBM's "Watson" initiative [3] is unique, however, as it is the only solver that has shown sufficient scalability and robustness to tackle problem sizes of many millions of equations on many thousands of processor cores. This project involves porting WSMP to Blue Waters and performing full-scale benchmarking tests using assembled global stiffness matrices and load vectors ranging from 1 million to 40 million unknowns extracted from commercial and academic implicit finite element analysis applications.

We have ported WSMP to the Blue Waters Cray Linux Environment (CLE) and adapted it to use PGI's compiler and AMD's math library ACML. We could not build the library with Cray's own compiler, since Cray's libsci math library had issues with p-threads in WSMP. The issue with thread safety of p-threads under libsci was reported in the JIRA ticket system and forwarded to Cray for review.

So far we have managed to solve and benchmark a couple of large test systems ("M20" with 20 million degrees of freedom (DOFs) and "M40" with 40 million DOFs) using WSMP on Cray XE6 nodes. The M40 system, with over 40 million DOFs and 3.3 billion non-zeros, is the largest ever to be benchmarked with direct solvers, as best as we can discern from our review of existing literature.

FIGURE 1: WSMP Factorization wall clock time M40

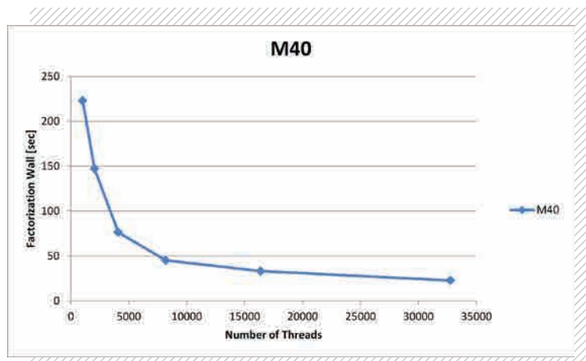
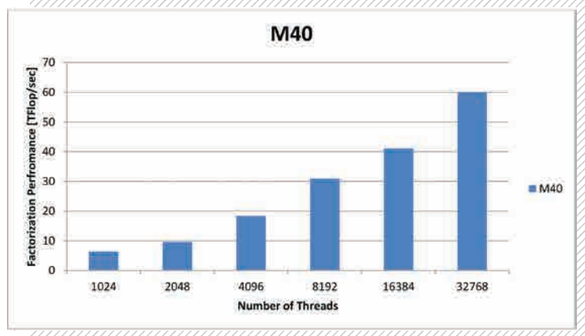


FIGURE 2: WSMP Factorization Performance M40



WHY BLUE WATERS

We have scaled this problem size to over 32,000 cores on Blue Waters while achieving 60 Tflop/s, which are unprecedented numbers for sparse linear solvers (figs. 1-2).We are most eager to test WSMP at an even wider scale on Blue Waters, as well as to build and test WSMP with Intel's compiler and MKL when they become available to users.

PUBLICATIONS

Vazquez, M., et al., Alya: Towards Exascale for Engineering Simulation Codes. *SC 2014*, New Orleans, La., November 16-21, 2014 (in review).

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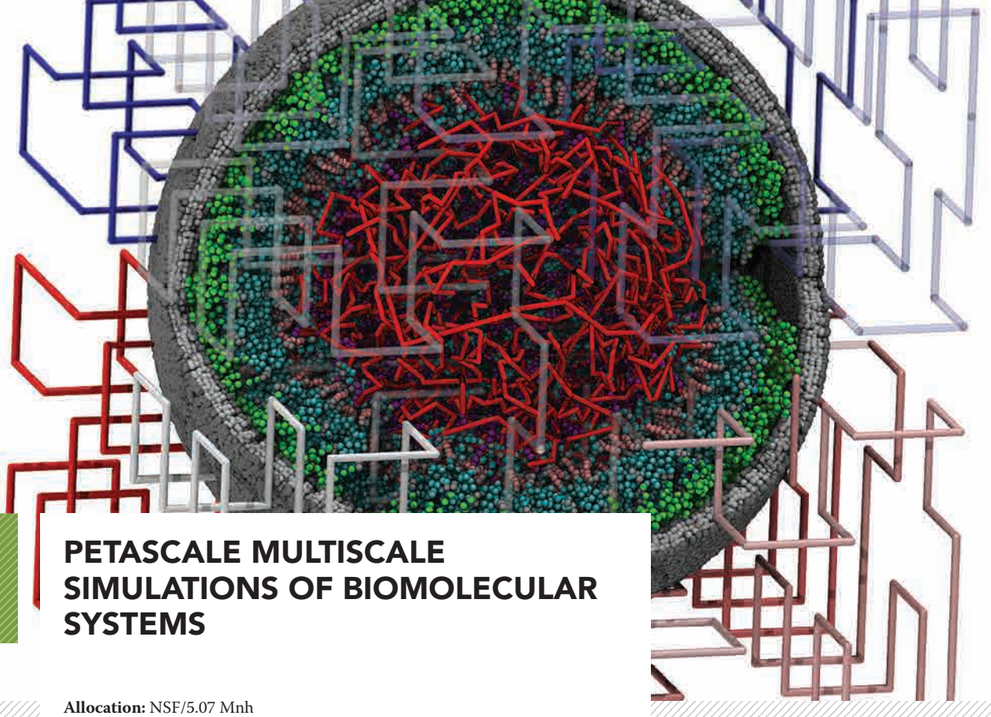

PETASCALE MULTISCALE SIMULATIONS OF BIOMOLECULAR SYSTEMS

Allocation: NSF/5.07 Mnh
PI: Gregory A. Voth[1]
Collaborators: John Grime[1]

[1]University of Chicago

FIGURE 1 (BACKGROUND): Example coarse-grained model of an immature HIV-1 viral particle enclosed by a Hilbert space-filling curve (as used in load balancing by the UCG-MD software).

EXECUTIVE SUMMARY:

Computer simulations offer a powerful tool for high-resolution studies of molecular systems. Increases in the potential scope of computer simulations are driven not only by theoretical developments but also by the impressive (and growing) power of modern supercomputers. Very large-scale molecular systems can nonetheless present a serious challenge for simulations at atomic resolutions. In such cases, "coarse-grained" (CG) molecular models can significantly extend the accessible length and time scales via the careful generation of simpler representations.

Although CG models are computationally efficient in principle, this advantage may be difficult to realize in practice. Conventional molecular dynamics (MD) software makes certain assumptions about the target system for computational efficiency, and these assumptions may be invalid for dynamic CG models. To address these issues, we developed the UCG-MD software. Our presentation at the 2014 symposium outlined key algorithms of the UCG-MD code and demonstrated their utility for representative CG models of biological systems.

INTRODUCTION

The application of "coarse-grained" (CG) molecular models can significantly extend the scope of computer simulations, particularly where the effects of any explicit solvent molecules are instead represented implicitly in the CG solute interaction potentials. Recent advances in the theory of CG model generation offer the concept of "ultra-coarse-grained" (UCG) molecular models [1], further increasing the accessible time and length scales for computer simulations. Although CG and UCG models are computationally efficient, parallel simulations of very large-scale CG and UCG systems typically do not realize the full potential of these models. The use of molecular models with atomic resolution has driven the design of traditional molecular dynamics (MD) software. Where molecular topologies and interaction potentials are fixed at runtime, the properties of atomic-resolution systems heavily influence the nature of the numerical algorithms used.

METHODS AND RESULTS

Three key challenges hinder the efficient use of advanced CG/UCG models on modern supercomputers: (1) the load balancing of extremely heterogeneous systems, (2) the memory requirements of very large simulations, and (3) the inability to easily represent systems with highly dynamic contents. Some (or all) of these problems can restrict the straightforward application of CG/UCG models to truly dynamic cell-scale biological processes using conventional MD software.

We developed an unorthodox MD code designed to alleviate these issues, with the hope of enabling entirely new classes of molecular simulation [2]. Major aspects of this software include the use of Hilbert space-filling curves for dynamic load balancing, the use of on-demand sparse data structures to reduce memory requirements, and the implementation of dynamic molecular descriptions to enable highly variable molecular topologies and interactions at runtime. These aspects of the software were described and motivated by "real-world" examples in our 2014 symposium presentation to illustrate where and how such functionality would prove useful in the context of large-scale biological systems.

The UCG-MD code was tested for example systems of relevance to CG/UCG biological models, and the resultant fundamental performance measurements were described in our presentation. In particular, superior performance was highlighted with reference to a conventional MD archetype for both load balancing and memory use, with the dynamic topological capabilities of the UCG-MD code introducing minimal runtime overhead. The UCG-MD code thus presents a versatile platform for efficient CG/UCG simulations of very large-scale molecular systems, even in cases where more traditional MD approaches can face significant difficulties.

WHY BLUE WATERS

Even with the efficient application of CG/UCG models, the ability to access molecular phenomena featuring very large numbers of molecules interacting in spatial volumes on the order or microns or larger still requires significant parallel computational power. The Blue Waters supercomputing resource thus proved to be critical for the implementation and deployment of the UCG-MD software, offering not only an extremely large number of parallel compute nodes but also an environment for close collaboration between external researchers and expert NCSA technical support staff. This latter aspect was particularly crucial in the design and implementation of advanced software functionality using the Blue Waters network hardware. The Blue Waters "point-of-contact" model is therefore considered to be an impressive model for any future supercomputing facilities.

PUBLICATIONS

Dama, J. F., A. V. Sinitskiy, M. McCullagh, J. Weare, B. Roux, A. R. Dinner, and G. A. Voth, The Theory of Ultra-Coarse-Graining. 1. General Principles. *J. Chem. Theory Comput.*, 9:5 (2013), pp. 2466-2480.

Grime, J. M. A., and G. A. Voth, Highly Scalable and Memory Efficient Ultra-Coarse-Grained Molecular Dynamics Simulations. *J. Chem. Theory Comput.*, 10:1 (2014), pp. 423-431.

MECHANISMS OF ANTIBIOTIC ACTION ON THE RIBOSOME

Allocation: GLCPC/0.33 Mnh
PI: Alexander Mankin[1]
Collaborators: Nora Vasquez-Laslop[1]; Klaus Schulten[2,3]

[1]University of Illinois at Chicago
[2]University of Illinois at Urbana-Champaign
[3]Beckman Institute for Advanced Science and Technology

EXECUTIVE SUMMARY:

The ribosome, one of the ubiquitous molecular machines in living cells, is responsible for the critical task of translating the genetic code into functional proteins. The antibiotic drug erythromycin (ERY) acts as a protein synthesis inhibitor. The molecular mechanisms underlying the effects of such drugs are unknown, and bacterial resistance to antibiotics is a growing problem. To promote novel designs of the next generation of antibiotics that are more effective, we investigated the molecular mechanisms underlying the antibiotic action of ERY on bacterial ribosomes. Our results showed that the ERY drug takes antibiotic effect by altering the structure of the bacterial ribosome.

FIGURE 1(A): The ribosome contains a large and a small subunit. The nascent protein elongates from the core of the ribosome and egresses through the ribosomal exit tunnel to the outside of the ribosome. ERY binds to the exit tunnel.

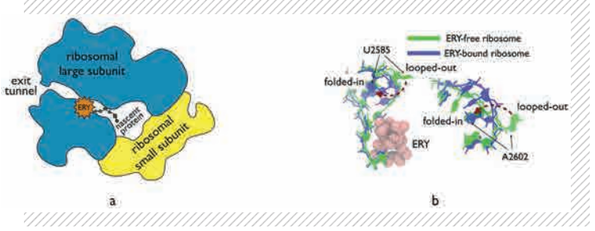

FIGURE 1(B): Molecular dynamics simulations show drug-induced nucleotide-flipping in the ribosome.

INTRODUCTION

The ribosome, one of the ubiquitous molecular machines in living cells, is responsible for the critical task of translating the genetic code into functional proteins. The bacterial ribosome is the target of over 50% of antibiotic drugs [1,2], including the widely-prescribed erythromycin (ERY; a macrolide drug) which is on the WHO essential medicines list [3,4]. The antibiotic action of such drugs has been known for over 50 years; however, the molecular mechanisms underlying the effects of these drugs are unknown [5].

Bacterial resistance against antibiotics is developing into a major global concern because no new antibiotic drugs have been developed for nearly 30 years while new strains of bacteria have evolved to be resistant to existing drugs [6]. To promote novel designs of the next generation of antibiotics that are more effective and less resistance inductive, we investigated the molecular mechanisms underlying the antibiotic action of ERY on bacterial ribosomes.

METHODS AND RESULTS

ERY acts as a protein synthesis inhibitor [7] and binds to the ribosomal exit tunnel of bacterial ribosomes (fig. 1a) [8,9]. Contrary to prior beliefs [10-14], we found that the macrolide drugs may act on the ribosome directly without the presence of the nascent protein. We modeled an ERY-bound empty ribosome (without nascient protein) and a drug-free empty ribosome based on the complete crystal structures of ribosomal complexes [8,15], respectively).

We found that ERY reproducibly induced conformational changes of the universally conserved ribosomal nucleotides U2585 and A2602 (fig. 1b), in agreement with experiments. Flipping of U2585 and A2602 from a looped-out orientation, required for aligning tRNA substrates to prepare the peptide-bond transfer [16,17], to a folded-in orientation was observed in the ERY-bound ribosome simulations. We note that A2602 in the looped-out orientation is also required to prevent premature nascent protein release [18]. By contrast, the two nucleotides predominantly assumed looped-out orientation in drug-free ribosome simulations [19]. This finding unveils a new view of the antibiotic action of macrolides on bacterial ribosomes.

WHY BLUE WATERS

The Blue Waters supercomputer provided us computational efficiency to perform sub-microsecond time scale all-atom simulations with our complete ribosome systems.

PUBLICATIONS

Sothiselvam, S., et al., Macrolide antibiotics allosterically predispose the ribosome for translation arrest. *Proc. Natl. Acad. Sci. USA*, (2014), doi: 10.1073/pnas.1403586111.

POLYAMINE MEDIATES SEQUENCE- AND METHYLATION-DEPENDENT COMPACTION OF CHROMATIN

Allocation: Illinois/0.922 Mnh; BW Prof./0.24 Mnh
PI: Aleksei Aksimentiev[1]
Collaborators: Jejoong Yoo[1]; Haijin Kim[1]; Taekjip Ha[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

Most biological problems can be reduced to questions about gene regulation mechanisms. Experimental advances in the last decade have shown that spatial location and eukaryotic chromatin conformations are highly correlated to gene activities. Although it is clearly shown that DNA sequence and methylation patterns determine the chromatin conformations, the underlying driving force that dominates this phenomenon is unclear. Our research aims to investigate how polybasic histone tails or biogenic polyamine molecules control the sequence/methylation-dependent inter-DNA and internucleosomal interactions.

BACKGROUND

Most biological problems can be reduced to questions about gene regulation mechanisms. For example, development and differentiation of the cells are controlled by turning on and off specific sets of genes. Several factors can affect gene regulation: DNA wrapping around nucleosomes, histone tails and their chemical modifications, DNA modifications such as methylations of CpG dinucleotides, and transcription factors.

Programmed gene regulation by chemical modifications of DNA and histone tails—epigenetics—is fundamentally important because it is the central mechanism of human development. All the cells of a human body share exactly the same genome sequence, but cells can play different roles depending on tissue type. Epigenetic markers, not DNA sequence, determine the tissue type. Many diseases, such as cancer, are caused by defective genes or failure in gene regulation. Cancer cells are a specialized cell type showing specific epigenetic marker patterns [1,2] and, presumably due to the epigenetic markers, show peculiar chromatin architecture [3]. Understanding how epigenetic markers control the chromatin architecture can lead us to understand how differentiation and cancer occur.

The conventional view of gene regulation says that controlling the binding of transcription factors to a specific gene, such as modifying histone tails and DNA, achieves finely tuned gene regulation. However, experimental advances in the last decade have radically changed our view on eukaryotic chromatin structure so that, unlike prokaryotes, spatial location and chromatin conformations are highly correlated to gene activities. In this new framework, gene locations are not random but highly controlled as programmed.

For example, recent experiments [4-6] revealed chromosomal territories on an even larger scale than before. Fragments containing 0.1-1 million DNA bases co-localize according to their AT content into topologically associated domains (TADs). The inner surface of a nucleus attracts AT-rich TADs [7,8]. Moreover, highly methylated TADs are known to form compact clusters [9], which presumably enables reversible chromatin reorganization.

Although the correlation between chromatin conformations and gene activities is well founded and it is clearly shown that DNA sequence and methylation patterns determine the chromatin conformations [9], the underlying driving force that dominates this phenomenon is unclear.

GOALS

Our research aims to investigate how polybasic histone tails or biogenic polyamine molecules control the sequence/methylation-dependent inter-DNA and internucleosomal interactions. This task requires that we consider various methylation/sequence patterns to extract their effects on DNA compactions. We will run multiple free-energy simulations in parallel using advanced sampling techniques of all-atom molecular dynamics simulations, which can be done efficiently only by using a powerful computer like Blue Waters.

SIMULATION OF THE MOLECULAR MACHINERY FOR SECOND-GENERATION BIOFUEL PRODUCTION

Allocation: Illinois/0.25 Mnh
PI: Isaac Cann[1]
Collaborators: Rafael C. Bernardi[1,2]; Michael A. Nash[3]; Hermann E. Gaub[3]; Klaus Schulten[1,2]

[1]University of Illinois at Urbana-Champaign
[2]Beckman Institute for Advanced Science and Technology
[3]Ludwig-Maximilians-Universität München, Germany

EXECUTIVE SUMMARY:

Biofuels are a well-known alternative to fossil fuels. However, competition with food production raises ethical concerns. The production of so-called second-generation biofuels, made from agricultural waste, is more favorable but is not yet cost competitive. Our project wants to find a more cost-competitive strategy using bacteria.

Some bacteria, especially from the genus *Clostridium*, employ several synergistic enzymes docked extra-cellularly on a highly modular and remarkably flexible molecular framework, the cellulosome. Our project employed molecular dynamics simulations that complement single-molecule experiments from our collaborators to characterize the protein modules docked together to form cellulosomes. Our experiments measured that the docking complexes are extremely strong. Simulations revealed that pulling the complexes apart actually strengthens the complexes before they rupture. The resulting strength is the largest ever seen in macromolecular complexes. Presently, we are running 13-million-atom simulations of cellulosomes on Blue Waters to further explore the properties and technical potential of cellulosomes.

INTRODUCTION

Deconstruction of plant cell walls to fermentable sugar using enzymatic hydrolysis is being pursued for the production of so-called second-generation biofuels. Driven by significant research efforts worldwide, a large number of enzymes and enzymatic complexes that may be used for biofuel production have been identified and biochemically characterized. Among the most intricate enzymatic complexes are the cellulosomes, found especially in anaerobic environments.

While keeping a commonplace biochemical affinity, cellulosomes' building blocks can maintain their mechanical integrity under strong shear forces. The assembly and disassembly of these protein networks is mediated by highly specific cohesin/dockerin interactions, the main building blocks of the cellulosomes. It is believed that the cellullosomes' high activity is related to its extremely flexible scaffoldin, constituted of cohesin domains connected by a very flexible linker. In this work we aim to identify cellulosomal network components with maximal mechanical stability and characterize the extreme flexibility of the cellulosomal complex.

METHODS AND RESULTS

With the intention of further studying this synergism, we employed Blue Waters to model the entire cellulosome complex (fig. 1). Presently, we carry out 13-million-atom simulations of cellulosomes on Blue Waters to further explore properties and technical potential of cellulosomes.

To perform the calculations we utilized the molecular dynamics program NAMD, which employs the prioritized message-driven execution capabilities of the Charm++ parallel runtime system, allowing excellent parallel scaling. The CHARMM36 force field along with the TIP3 water model were used to describe all systems. To characterize the coupling between dockerin and cohesin, we performed steered molecule dynamics simulations of constant velocity stretching (SMD-CV protocol) employing three different pulling speeds: 1.25 Å/ns, 0.625 Å/ns, and 0.25 Å/ns. The stochastic generalized simulated annealing (GSA) method, implemented in the GSAFold plugin for NAMD, was employed to generate millions of different conformations for the cellulosome complex.

Cellulosome assemblages consist of a scaffoldin backbone onto which dockerin-containing catalytic modules and carbohydrate binding modules are appended. Analogous to a "Swiss Army knife," these cellulosomes contain a plethora of different catalytic and substrate binding activities that facilitate the degradation of plant cell wall material. The dockerin/cohesin interactions are the main building blocks of the cellulosomes and their interaction is known to be stronger than common protein-protein interactions. The exceptionally high rupture forces we measured (600-800 pN) are hugely disproportionate to the dockerin/cohesin biochemical affinity, which at KD≈20 nM is comparable to typical antibody-antigen interactions. Antibody-antigen interactions, however, will rupture at only ~60 pN at similar loading rates. To the best of our knowledge, the dockerin/cohesin complex is the highest protein ligand-receptor rupture force ever reported at more than half the rupture force of a covalent bond.

The simulation results reproduced the experimental force profile and were able to identify key hydrogen bonding contacts previously identified as important for dockerin cohesin. Analysis of the binding interface and associated contact surface area of the molecules in the mechanically loaded and unloaded state suggests a catch bond mechanism may be responsible for the remarkable stability. Dockerin modules in the simulated binding interface seem to clamp down on the cohesin upon mechanical loading, resulting in increased stability and decreased accessibility of water into the hydrophobic core of the bound complex.

The scaffoldin and its cohesins and the enzymatic domains with dockerins are the main building blocks that characterize the macrostructure of the cellulosomes. It was reported that *Clostridium thermocellum*, the most studied cellulosomal organism, exhibits one of the highest rates of cellulose utilization known in nature, and the cellulosomal system of this bacterium is reported to display a specific activity against crystalline cellulose that is fifty-fold higher than the corresponding non-cellusomal fungal system in *Trichoderma reesei*.

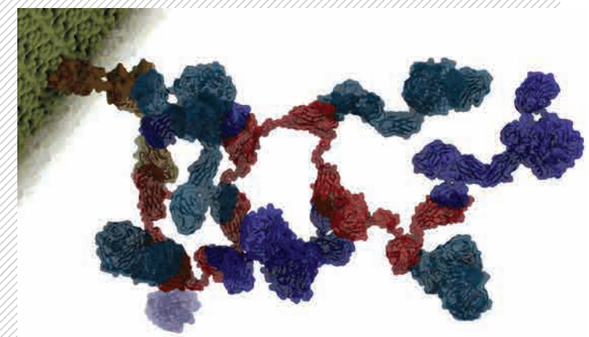

FIGURE 1: Cellulosome model built using partially available crystallographic structures combined with similarity-based molecular modeling and generalized simulated annealing.

WHY BLUE WATERS

The size of the cellulosome had been out of reach of molecular dynamics simulations before the advent of Blue Waters, and even studying fragments of the cellulosome would be a challenge for any supercomputer except Blue Waters.

PETASCALE SIMULATIONS OF COMPLEX BIOLOGICAL BEHAVIOR IN FLUCTUATING ENVIRONMENTS

Allocation: NSF/0.003 Mnh
PI: Ilias Tagkopoulos[1]

[1]University of California, Davis

EXECUTIVE SUMMARY:

One of the central challenges in computational biology is the development of predictive multi-scale models that can capture the diverse layers of cellular organization. Even scarcer are models that encode biophysical phenomena together with evolutionary forces in order to provide insight into the effect of adaptation at a systems level.

The goal of this project is to create a scalable model and simulation framework to (a) investigate the dynamics of microbial evolution in complex environments, and (b) assess its effect on microbial organization across the various biological layers. The simulation framework should be focused on the general principles governing evolution and microbial organization so it can be generalized.

Over the last five years, our lab has created a multi-scale abstract microbial evolution model that unifies various layers, from diverse molecular species and networks to organism and population-level properties. With the help of Blue Waters and the NCSA team, we are able to scale up to hundreds of thousands of cells, an unprecedented scale of simulation. (It is, however, only a fraction of the billions of cells that are present in a bacterial colony.) Here, we present our scalability results, the methods that we employed to achieve them, and our current work on a data-driven, genome-scale, population-level model for *Escherichia coli*.

INTRODUCTION

Microbes are the most abundant and diverse forms of life on Earth. Their impact on the human race and our ecosystem as a whole is difficult to exaggerate. They have been used extensively in industrial applications, ranging from bioremediation to production of organic compounds, and they are relevant to human health as both probiotics and pathogens.

Over the past decades, we have studied microbial organisms extensively and gained valuable insights into their system-level properties, as well as the mechanistic underpinnings of their complex behavior. Less is known about their potential to acquire new traits and become resilient to adverse environmental conditions through evolutionary forces such as random mutations, horizontal gene transfer, and genetic drift. Elucidating the effect of such environments on their gene regulatory and biochemical networks is particularly interesting. In turn, it can lead to a better understanding of what is possible, likely, and potentially transformative to the environment they occupy. From antibiotic resistance to stress-resistant biotechnological strains for recombinant protein production, such knowledge will have a tremendous impact on various industrial, agricultural, and medical fields. While there have been many studies of adaptive laboratory evolution in the past couple of years, these are limited to a few thousand generations that can hardly capture the vast phenotypic space that microbes can explore. Hence, the development of computational modeling and simulation tools that can capture these phenomena across multiple scales can lead to transformative advances in this field.

METHODS AND RESULTS

There are a number of challenges we need to address to achieve our goals. First, a model of biological organization that is both biologically realistic and computationally feasible is paramount, incorporating the right level of biological abstraction. Second, the spatial and temporal scales of a model that encompasses genes, proteins, networks, cells, and populations are very diverse, which creates additional hurdles when applying numerical methods to solve them. Third, since evolution is based on random mutations and natural selection, it is inherently hard to predict and can lead to imbalances in the distribution of active cells, and by extension, computational tasks. Fourth, a typical microbial colony has billions of cells, while current simulations are at most in the thousands. This leads to size-specific artifacts (size does matter). Finally, storing and visualizing the fossil record of an evolutionary trajectory, especially since dozens of them are needed for assessing statistical significance for any hypothesis-testing experiment, is not an easy task since a simulation can easily lead to terabytes of complex data that require analysis.

We have created the Evolution in Variable Environments (EVE) v3.0 synthetic ecology framework, which is currently the most sophisticated, abstract simulator for microbial evolution, with the capacity to scale up to 8,000 MPI processes and 128,000 organisms. To compare, our previous work (before the PRAC award) scaled up to 200 organisms with a less complex underlying model [1].

To cope with unforeseen computational load due to the emergence of complex phenotypes, we have developed both static and adaptive load balancers that can account for both fixed and non-fixed population sizes [2,3]. We developed intuitive visualization tools [4], HDF5 storage solutions, and novel analysis algorithms based on network flows [5] to efficiently project data to accelerate biological discovery. The EVE simulator has since been used to investigate the effect of horizontal gene transfer [6], distribution of fitness effects, and the hypothesis of accelerated evolution through guided, step-wise adaptation [7] with interesting results that drive biological experimentation [8,9].

Future work includes pushing the limits of microbial simulations to break the one-million-cell barrier, parallelization of organism-specific, data-driven models that integrate omics layers, starting from our recent work in the model bacterium *Escherichia coli* [10], and integration with synthetic biology computer-aided design tools for targeted, chassis-aware genome engineering [11-14].

WHY BLUE WATERS

Over the last five years, our lab has created a multi-scale abstract microbial evolution model that unifies various layers, from diverse molecular species and networks to organism and population-level properties. With the help of Blue Waters and the NCSA team, we are able to scale up to hundreds of thousands of cells, an unprecedented scale of simulation.

PUBLICATIONS

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EPISTATIC INTERACTIONS FOR BRAIN EXPRESSION GWAS IN ALZHEIMER'S DISEASE

Allocation: Private sector/0.031 Mnh
PI: Nilufer Ertekin-Taner[1]
Collaborators: Mariet Allen[1]; Liudmila Mainzer[2,3]; Curtis Younkin[1]; Victor Jongeneel[2]; Thierry Schüpbach[4]; Gloria Rendon[2]; Julia Crook[1]; Julie Cunningham[5]; Summit Middha[5]; Chris Kolbert[5]; Dennis Dickson[1]; Steven Younkin[1]

[1]Mayo Clinic in Jacksonville
[2]University of Illinois at Urbana-Champaign
[3]National Center for Supercomputing Applications
[4]Swiss Institute of Bioinformatics
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EXECUTIVE SUMMARY:

Alzheimer's disease (AD) is likely influenced by the interaction of many genetic and environmental factors, some of which may act by influencing brain gene expression. The aim of this study is to test for pairwise genetic variant interactions (epistasis) that influence brain gene expression levels using existing data from our expression GWAS study of 359 temporal cortex samples (181 AD, 178 non-AD), 223,632 SNP genotypes and ~24,000 transcripts that were measured using an expression array. The analysis of epistatic effects in large studies, such as ours, requires powerful computational resources and would not be possible without the unique computing capabilities of Blue Waters. The first of three planned analyses has been completed for 17,284 array probes detected in >75% of AD samples. Analyses of the non-AD and combined (AD + non-AD) groups will follow shortly.

INTRODUCTION

The primary goal of this study is to identify novel genetic loci that influence gene expression in the brain in order to identify Alzheimer's disease (AD) candidate genes, although it is both feasible and likely that our findings will have broader implications. It is well established that AD has a significant genetic component. Therefore, identifying the genetic factors that influence AD risk can have a significant impact on the development of novel therapeutic targets, identification of potential, premorbid biomarkers, and generation of *in vivo* disease models, much needed for pre-clinical development and testing of novel therapies.

METHODS AND RESULTS

We have previously conducted an expression genome-wide association study (eGWAS) for ~200 AD subjects and ~200 subjects with other non-AD pathologies using samples from the temporal cortex and cerebellum of post-mortem brain tissue to identify genetic variants that influence brain gene expression [1]. Using this single SNP/single phenotype approach we identified 2,089 significant SNP/probe associations that replicated across the two tissues we investigated and identified an enrichment of human disease-associated variants. Our findings demonstrate the utility of this study design and confirm that genetic variants that influence risk for human disease can also influence brain expression of genes in cis.

However, the single SNP/single phenotype approach employed in GWAS studies is simplistic and likely not an accurate reflection of the complex biological interactions that take place in an organism. Gene (or SNP) interactions, known as epistasis, allow for the study of interaction effects of pairs of SNPs on a given phenotype and can uncover additional genetic factors that influence gene expression and disease. In this study we leverage our existing brain eGWAS data to identify pairs of SNPs that associate with brain gene expression measures with the goal of identifying additional genetic factors that might influence Alzheimer's disease risk.

Through our work with our collaborators at the University of Illinois and NCSA we were able to address many of the challenges that a project of this scope presented. Considering the thousands of phenotypes we proposed to analyze, it was imperative that we identify an efficient software package that could facilitate analysis of multiple phenotypes at one time. We had initially targeted the epistasis tools available through the genetic analysis software PLINK [1]; however, this did not allow for parallelization of multiple phenotypes and would have been time limiting, even with the capabilities of Blue Waters.

We subsequently utilized the application FastEpistasis [2], which builds on the analysis paradigm used by PLINK, but is a multi-threaded software and runs up to 75 times faster by splitting the analysis into three phases. Using FastEpistasis we are able to analyze multiple phenotypes simultaneously. After conducting some optimization tests we found that running 32 phenotypes at one time was the most efficient way to run the analysis on Blue Waters. Due to the large computation requirements for epistasis analysis, incorporation of covariates in regression models is limiting and is not routinely executed. We were able to account for important covariates in our analysis, such as RNA Integrity Number (RIN), age, and gender, by first regressing our gene expression phenotypes with key covariates (in R) to generate residuals. We then used the residuals as our phenotypes for epistasis analysis. We have extensively tested smaller datasets and determined that epistasis analysis executed in FastEpistasis and PLINK generate identical results and have also demonstrated that single variant analysis using residuals as the phenotype gives identical results to multivariable linear regression analysis using the full model.

Finally, in order to reduce the size of the output data and make it more manageable for transfer and entry into a database, we changed the p-value threshold for results that are output in the final phase of FastEpistasis from $p<10^{-4}$ to $p<10^{-7}$, which decreased the output for many phenotypes by more than 75% while retaining results that are well above the p-value threshold following correction for multiple testing. As of this writing, we have completed analysis of the initial dataset of AD subjects sampled from the temporal cortex: 181 AD subjects, 223,632 SNPs and 24,526 probes of which 17,284 are reliably measured in >75% of the subjects. Analysis of 178 non-AD subjects for the same set of SNPs and the same number of phenotypes is under way and will be followed by analysis of the complete dataset of 359 (AD + non-AD) subjects with RNA sampled from the temporal cortex.

WHY BLUE WATERS

The computation of epistatic interactions for hundreds of samples, hundreds of thousands of SNPs and a single phenotype is computationally intensive; for thousands of phenotypes it is virtually impossible without the use of specialized applications and petascale computation. Furthermore, the storage architecture of Blue Waters is highly compatible with the data generated from the epistasis analysis software package implemented for this analysis, FastEpistasis. We have been able to address many of these challenges through our interactions with our collaborators at NCSA and the University of Illinois.

PUBLICATIONS

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CHARACTERIZING STRUCTURAL TRANSITIONS OF MEMBRANE TRANSPORT PROTEINS AT ATOMIC DETAILS

Allocation: Illinois/0.686 Mnh
PI: Emad Tajkhorshid[1,2]
Co-PIs: Mahmoud Moradi[1,2]; Giray Enkavi[1,2]; Po-Chao Wen[1,2]; Jing Li[1,2]

[1]Beckman Institute for Advanced Science and Technology
[2]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Membrane transporters are specialized molecular devices that couple active transport of materials across the membrane to various forms of cellular energy. Their fundamental role in diverse biological processes makes them key drug targets, furthering widespread interest in their mechanistic studies. Large-scale conformational changes (on the order of milliseconds to many seconds) are central to the mechanism of membrane transporters. Studying such conformational transitions requires sampling complex, high-dimensional free energy landscapes that are inaccessible to conventional sampling techniques such as regular molecular dynamics simulations. We have developed a novel approach combining several extensive search and state-of-the-art sampling techniques and used it to study a number of membrane transporters. The method, which Blue Waters has made feasible only recently for large macromolecular systems, has greatly impacted the scope of our computational studies of this important family of membrane proteins.

INTRODUCTION

All living organisms rely on continuous exchange of diverse molecular species (e.g., nutrients, precursors, and reaction products) across cellular membranes for their normal function and survival. Membrane transporters are specialized molecular devices that provide the machinery for selective and efficient transport of materials across the membrane. They actively pump their substrates across the membrane by taking advantage of different forms of cellular energy. The biological and biomedical relevance of mechanistic studies of membrane transporter proteins cannot be overstated, given their central role in a myriad of key cellular processes and their involvement in a vast number of pharmaceuticals. Their importance is also evident in the major shift in the focus of experimental structural biological studies in recent years towards characterizing representative structural states formed during the function of these proteins.

Large-scale conformational changes are central to the mechanism of membrane transporters. A major goal in computational studies of membrane transporters, therefore, is to describe, at an atomic level, the pathways and energetics associated with structural transitions involved in their function. Given the technical challenges involved in experimental characterization of these structural phenomena, simulation studies currently provide the only method to achieve the spatial and temporal resolutions required for complete description of the transport cycle in membrane transporters.

METHODS AND RESULTS

We have recently developed a knowledge-based computational approach to describing large-scale conformational transitions using a combination of several distinct enhanced sampling techniques. In the proposed approach we use non-equilibrium, driven simulations by designing mechanistically relevant, system-specific reaction coordinates whose usefulness and applicability to the transition of interest are examined using knowledge-based, qualitative assessments along with non-equilibrium work measurements which provide an empirical framework for optimizing the biasing protocol in a series of short simulations.

In the second stage, we use the string method with swarms-of-trajectories in a high-dimensional collective variable space to further relax the most optimized non-equilibrium trajectory from the first stage. We use the relaxed trajectory to initiate bias-exchange umbrella sampling (BEUS) free energy calculations and characterize the transition quantitatively. Using a biasing protocol fine tuned to a particular transition not only improves the accuracy of the resulting free energies but also speeds up the convergence. By assessing the efficiency of the sampling we are able to detect possible flaws and provide potential improvements in the design of the biasing protocol.

We studied the structural transition between the outward-facing and inward-facing states in several transporter systems from different classes including the bacterial ABC transporter MsbA, and two secondary transporters, GlpT and Mhp1, using NAMD, a highly scalable molecular dynamics code. These simulations resulted in the most detailed description to date of the transition process, and at atomic resolution for the first time. The simulations provided novel insight into the details of the energy coupling mechanisms in these proteins; they also have hinted at the presence of previously uncharacterized intermediate states. We are in the process of experimentally verifying these intermediates through our collaborations with leading experimental groups. These intermediates largely expand our repertoire of structures that can be used for docking and drug design studies. As novel structural entities, they can provide new targets for better and more selective drugs.

WHY BLUE WATERS

Our research approach relies on multiple-copy algorithms (MCAs) that couple the dynamical evolution of a large set of replicas/copies of a system (e.g., to enhance sampling or refine transition pathways). In our simulations, we employ BEUS scheme as well as a parallel variation of string method, both of which are MCAs and are well suited to Blue Waters due to their use of distributed replicas that communicate with a low overhead cost. Given that every copy of the simulation would require thousands of cores for its simulation, simulating a large number of interacting replicas simultaneously can only be accomplished on massive computing resources such as Blue Waters. NAMD also has been extensively tested and optimized for Blue Waters, showing sustained petascale performance.

PUBLICATIONS

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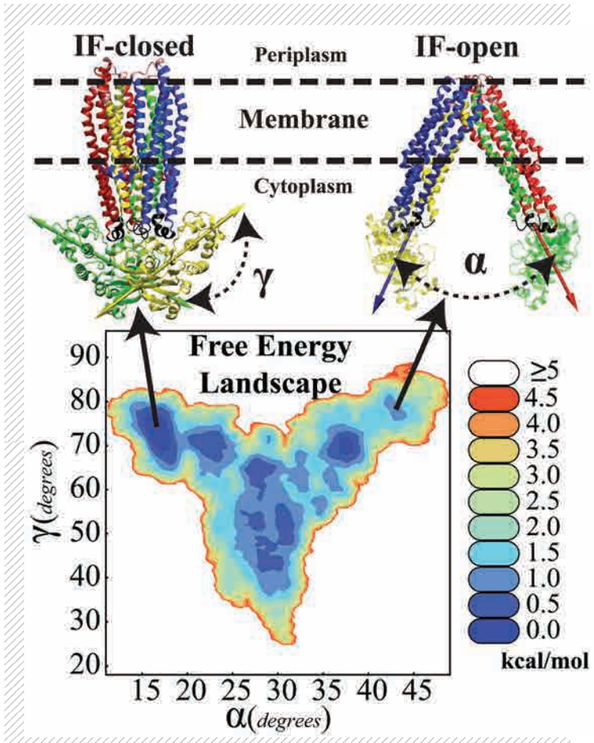
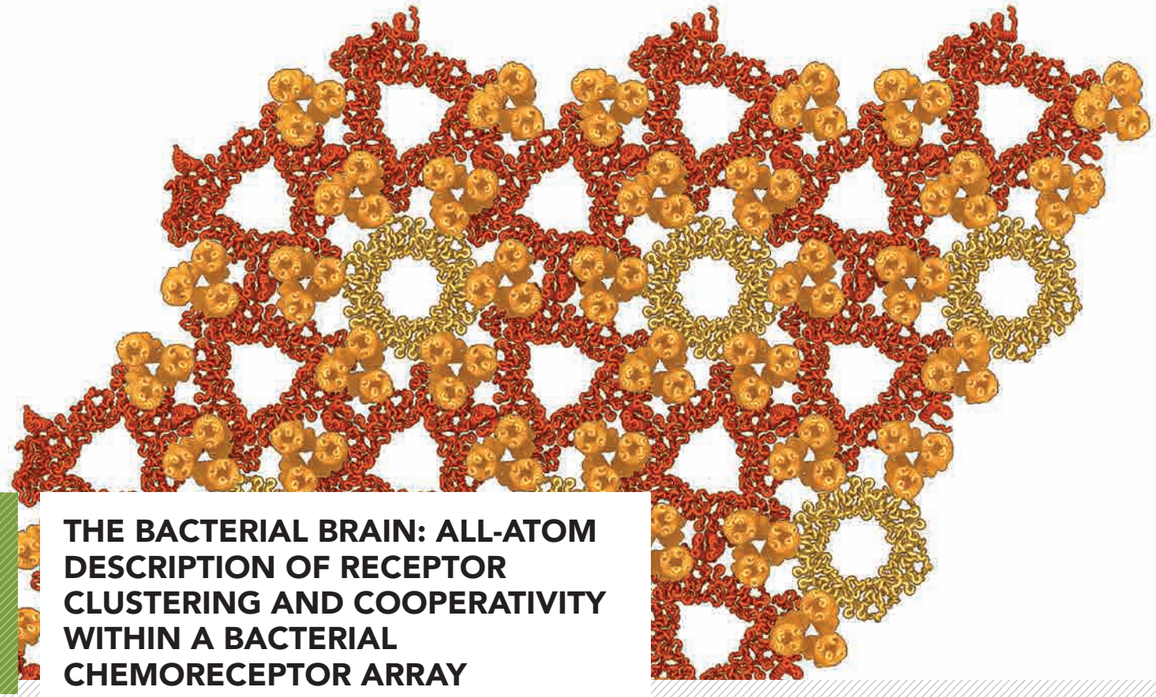


FIGURE 1: Conformational Free energy landscape of opening and closing of the cytoplasmic end of ABC transporter MsbA. Free energies were calculated using a bias-exchange umbrella sampling (BEUS) scheme and plotted in the (α,γ) space, which describe the relative orientations of different molecular domains as shown in the figure. Inward-facing-closed and inward-facing-open conformations shown in the figure are low-resolution (4.5 Å) crystal structures used to design the sampling protocol.



THE BACTERIAL BRAIN: ALL-ATOM DESCRIPTION OF RECEPTOR CLUSTERING AND COOPERATIVITY WITHIN A BACTERIAL CHEMORECEPTOR ARRAY

Allocation: Illinois/0.15 Mnh
PI: Yann Chemla[1]
Collaborators: Klaus Schulten[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

The ability of an organism to sense, interpret, and respond to environmental signals is central to its survival. Chemotaxis is a ubiquitous signaling system by which cells translate environmental chemical information into a motile response. Bacteria in particular have evolved sophisticated protein networks that survey chemicals in the environment and position cells optimally within their habitat. These networks are functionally analogous to the brains of higher organisms: an array of chemoreceptors senses chemical stimuli and transmits adaptive signals through an extended, multi-million-atom protein lattice, which evaluates these signals to appropriately affect the cell's swimming behavior. Here, we present an all-atom structure of the intact bacterial chemoreceptor array, based primarily on crystallographic and electron microscopy data. Molecular dynamics simulations on Blue Waters are being used to investigate the dynamical properties of the array and provide insight into its amazing information processing and control capabilities.

INTRODUCTION

A central problem in the chemotaxis field concerns the intermolecular cooperativity, which emerges from the organized clustering of proteins within the chemoreceptor array. Indeed, experimental and quantitative modeling studies have shown receptor clustering to be an essential functional feature of bacterial chemotaxis, giving rise to many of the network's enhanced signaling properties. However, due to the sheer size (tens of thousands of individual proteins in an average-sized array) and irreducible nature of the array's multi-component machinery, the detailed molecular mechanisms by which these proteins cooperate to robustly transduce signals have remained elusive.

Similarly, another important signaling feature emerges from the collective nature of the chemoreceptor array, namely the ability to variably regulate responses to environmental signals. Through the reversible methylation of chemoreceptors at several key sites along their cytoplasmic domains, bacteria are able to adapt to background chemical concentrations over several orders of magnitude in order to efficiently forage their habitat. How exactly this remarkable adaptation affects the regulatory properties of the array at the molecular level, however, is still quite mysterious.

As the centerpiece of perhaps the most thoroughly studied sensory signal transduction system in all of biology, namely the chemotactic network of *E. coli*, the chemoreceptor array represents the next frontier towards a complete understanding of a basic, naturally evolved biological computer. The bacterial chemoreceptor array possesses the essential functional features of higher-level signaling assemblies arising in more complex eukaryotic cells such as neurons and lymphocytes. Hence, new insights into the collective function of the chemoreceptor array will help elucidate the fundamental mechanisms by which biological systems process information in general.

METHODS AND RESULTS

We constructed an all-atom model of the unit cell from the bacterial chemoreceptor array based on crystallographic structures of component proteins and a 16 Å resolution cryo-electron microscopy density of the chemoreceptor array from *E. coli*. The model involves over one million atoms per unit cell. This unit cell model was equilibrated and subsequently simulated for 250 ns on Blue Waters using NAMD, a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Superior to previous studies, the experimentally guided unit cell model explicitly couples each protein component to its proper native array neighbor so that the structure evolves under its native contacts. The resulting stable model and simulations mark the first all-atom description of the structure and dynamics of an intact chemoreceptor array.

In order to further characterize the collective dynamics of the chemoreceptor array, equilibrium molecular dynamics (MD) simulations on Blue Waters were used to extend the total sampling time of the unit cell system up to 3 μs. Principal component analysis was used to extract, from the thermal fluctuations present in these MD simulations, important structural information regarding the natural modes of motion of the individual array oligomers as well as the global motions arising within the array itself. The preliminary results reveal coupled excitations of the individual oligomer modes within the modes of the complete unit cell, potentially establishing routes of communication between individual proteins and hinting at a signaling mechanism. More refined collective dynamics analysis will hopefully provide further insights into the functional relationships between these proteins and the deep cooperativity underlying the chemoreceptor array's computing ability.

WHY BLUE WATERS

Until recently, the relatively immense spatial and temporal scales needed to describe collective phenomena in large, multi-protein complexes such as the chemoreceptor array rendered it impractical to address these problems with available computational techniques and facilities. With the intense parallel computing power of Blue Waters, it is now feasible to explore such necessarily large systems computationally. The unique atomistic perspective afforded by Blue Waters will provide a framework to explicitly test theoretical hypotheses and help elucidate the connections between diverse experimental results as well as inform future experiments.

FIGURE 1 (BACKGROUND): Central to their chemotactic ability, bacteria possess a universally conserved, multi-million-atom protein lattice known as the chemoreceptor array. Scientists in Klaus Schulten's group at the University of Illinois at Urbana-Champaign have recently constructed the first all-atom model of the chemoreceptor array and are using Blue Waters to investigate its amazing information processing and control capabilities.

THE DYNAMICS OF PROTEIN DISORDER AND ITS EVOLUTION: UNDERSTANDING SINGLE MOLECULE FRET EXPERIMENTS OF DISORDERED PROTEINS

Allocation: Illinois/0.05 Mnh
PI: Gustavo Caetano-Anollés[1]
Co-PI: Frauke Gräter[2]
Collaborators: Cédric Debès[2]; Davide Mercadante[2]; Fizza Mughal[1]

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[2]Heidelberg Institute for Theoretical Studies, Germany

EXECUTIVE SUMMARY:

Intrinsically disordered proteins (IDPs) play crucial roles in cells. They also introduce a source of conformational heterogeneity in 3D protein structure that can be experimentally explored using Förster Resonance Energy Transfer (FRET) methods. Here we study this heterogeneity with molecular dynamics simulations of nucleoporin Nup153 peptides using the GROMACS 4.6 platform, benchmarked against FRET experiments. Nup153 is a crucial nuclear pore IDP involved in membrane trafficking. Our analyses show that the non-structured molecules collapse quickly, reaching consistent values of gyration radius. As expected from FRET experiments, the ends of the protein chain exhibited higher dynamics. Remarkably, we found an unanticipated increase in the dynamics of intra-chain segments for short fragments compared to medium fragments. This difference is due to the reduced influences of chain termini when fragments are below a certain size.

INTRODUCTION

Intrinsically disordered proteins (IDPs), which comprise ~10% of all proteins and are especially common in eukaryotes [1], pose an enormous experimental challenge due to the heterogeneous conformational ensemble they sample. In this regard, Förster Resonance Energy Transfer (FRET) experiments have provided unprecedented insight into the dynamics of disordered proteins less than 100 amino acid residues long [2]. They have shown molecular fluctuations with reconfiguration time scales of ~100 ns for free termini of the semi-flexible chains [3,4]. In this study we use FRET experiments as benchmarks for molecular dynamics (MD) simulations of nucleoporin proteins (Nups) of three different lengths to assess the dependency of chain dynamics on chain length. Nups control transport of molecules across the nuclear membrane by inducing changes in their structure. The mechanisms responsible for these changes are yet to be established.

Here we focus on MD simulations of Nup153, a membrane pore crucial to membrane trafficking. Our long-term goal is to extend these kinds of analyses to non-structured loop and disordered regions of proteins that have been associated with the rise of molecular flexibility and genetics in molecular evolution [5,6].

METHODS AND RESULTS

We simulated trajectories of one microsecond and beyond on Nup153 fragments of three different lengths. Since the resulting conformational ensemble likely depends on the starting conformation, which is randomly chosen, we ran three simulations for each fragment. Trajectories were examined to compute reconfiguration time scales as a function of polymer length, yielding correlations of distance fluctuations between fixed points on the chain.

Single molecule FRET results on Nup153 show unexpectedly reduced dynamics in the 10-100 ns range compared to other unfolded or disordered proteins investigated previously [4]. While the Nup153 from this experiment were obtained from the full-length 900 amino acid residue IDP, previous analogous experiments have all been performed on shorter peptides (<100 residues) that were labeled at the termini. An obvious assumption is that embedding a fragment under consideration with labels at its termini into a much larger disordered protein significantly reduces the inter-label dynamics.

We also monitor correlations of distance fluctuations between fixed points on the chain to calculate reconfiguration time scales as a function of chain length, fulfilling our expectation that the increase in chain length causes the characteristic ~100 ns dynamics [3,4]. Specifically, we find that the non-structured Nup153 chains, which lack secondary structure, collapse quickly in the trajectories, reaching consistent values of gyration radius (fig. 1). Calculation of reconfiguration time scales as a function of chain length revealed that the ends of the molecules (the termini of the coils) exhibited higher dynamics than the rest of the molecules. In contrast, we found that there was an unanticipated increase in the dynamics of intra-chain segments for short fragments compared to medium fragments due to the reduction of the influence of chain termini when fragments are below a certain size. The increased dynamics of short intra-chain segments may enhance the sampling of the molecular conformational spectrum and facilitate the molecular function of the nucleoproteins.

Increased dynamics of small coils in non-structured loops and short intrinsically disordered segments that are abundant in proteins could facilitate a wide range of molecular functions by enhancing the molecular flexibility of these regions. In fact, a structural phylogenomic analysis of millions of proteins in hundreds of proteomes revealed that the rise of genetics was associated with these flexible regions [5].

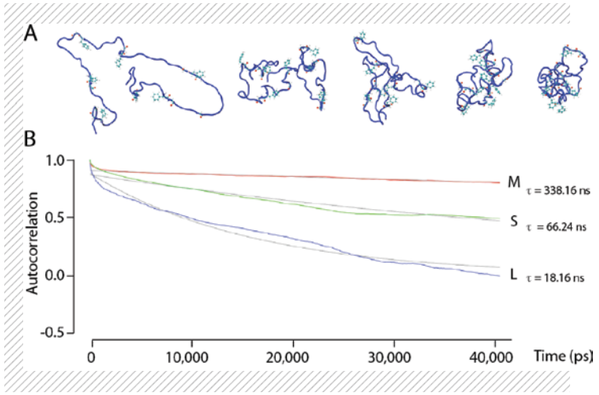

FIGURE 1: Equilibrium MD simulations of Nup153 fragments of different lengths show the intra-chain dynamics of the protein coils. (A) A series of representative images, ranging from extended (left) to more collapsed states (right), depict the simulated trajectories of the long Nup153 fragment. The protein backbone is shown as a random coil while the FG-repeats along the sequence are represented by balls and sticks. (B) Autocorrelation values plotted against simulation time. The fluctuations of short (S) 29-residue, medium (M) 49-residue, and long (L) 79-residue fragments of Nup153 are in line with simpler polymer models.

WHY BLUE WATERS

The results of our proof-of-concept study now provide a foundation for a Blue Waters-enabled high-throughput MD simulation study of the dynamics of a massive number of intra-chain protein regions. Such a study could yield unprecedented atomistic details of non-bonded interactions, secondary structure propensities, and other properties of the random coils of proteins, which are linked to constraints imposed by billions of years of molecular evolution that are responsible for structuring both proteins and the genetic code.

THE COMPUTATIONAL MICROSCOPE

Allocation: NSF/30 Mnh, BW Prof./0.24Mnh
PI: Klaus Schulten[1]
Collaborators (HIV Project): Peijun Zhang[2]; Christopher Aiken[3]
Collaborators (Chromatophore Project): Neil Hunter[4]; Simon Scheuring[5]

[1]University of Illinois at Urbana-Champaign
[2]University of Pittsburgh
[3]Vanderbilt University
[4]University of Sheffield
[5]INSERM/Université Aix-Marseille

EXECUTIVE SUMMARY:

Cells are the building blocks of life, yet they are themselves constructed of proteins, nucleic acids, and other molecules, none of which are, in and of themselves, alive. How living things can arise from the "behavior" of molecules, which are simply obeying the laws of physics, is the essential question of modern biology. Molecular dynamics simulations can be used as a "computational microscope," offering the ability to explore living systems at the atomic level and providing a necessary complement to experimental techniques such as crystallography, nuclear magnetic resonance (NMR), and cryo-electron microscopy.

With the rise of petascale computing, we take a critical step from inanimate toward animate matter by computationally resolving whole cellular organelles in atomic detail. Herein we discuss recent enhancements to the enabling programs NAnoscale Molecular Dynamics (NAMD) and Visual Molecular Dynamics (VMD) and successful research on several large-scale biomolecular systems being studied on Blue Waters, including the HIV capsid and a photosynthetic organelle.

INTRODUCTION

Bridging the gap between single protein simulations and organelle or cell-scale simulations is challenging on many levels. Because molecular dynamics simulations on the order of hundreds of millions of atoms require substantial computational power, efficient codes, as well as appropriate analysis and visualization techniques, must be developed. Such simulations open up new possibilities to understand biological systems on a new level, such as evaluating the effects of pharmaceuticals on the stability of a virus capsid, or unraveling the complex interplay between the many processes that enable photosynthesis.

Simulations interpret data, suggest new experiments, and do what experiments cannot, which is to give an atomic-level picture of what is going on inside living systems. The ability to explore living systems via the "computational microscope" of molecular dynamics simulations has a profound impact not only on the progress of basic science, but also in the treatment of disease, development of drugs, and development of new energy technologies.

METHODS AND RESULTS

The HIV capsid project produced the first ever atomic-level structure of a native, mature HIV capsid [1]. Since then, the capsid model has continued to be used to analyze the dynamics of motion of the HIV capsid subunits and has been used to explore the interactions of the capsid with drugs and host cell factors. We have explored the interactions of the full HIV capsid with small molecules, including the controversial Pfizer PF74 drug (which interferes with host cell binding to the capsid), the PF1385801 drug (which results in ultra-stable capsids), and compounds BI01/02 (which trigger premature disassembly). In the early stages of the replication cycle, the HIV capsid interacts with various host cell factors, such as cyclophilin A (which stabilizes and assists capsid assembly), and TRIM family factors, which disrupt the capsid and assist in nuclear import. Together with experimental collaborators, computational scientists were able to describe the action of cyclophilin A on the capsid and are presently working on the mechanism of restriction by TRIM-family proteins. Such studies may help scientists understand better how the HIV capsid infects the host cells and could lead to new HIV therapies.

The photosynthetic chromatophore project is creating the first all-atom model of a cellular organelle. Chromatophores are spherical organelles in photosynthetic bacteria which allow the bacteria to absorb sunlight and turn it into chemical fuel that drives many processes in the cell. The chromatophore is composed of about 200 proteins and carries out about 20 processes. By modeling the full organelle, it is possible to see how these processes interlock, much like the gears in a fine Swiss watch, and see how they allow the bacteria to make ATP fuel out of sunlight [2].

The chromatophore project is still underway, but a smaller chromatophore-membrane system has been simulated and recently published [3]. This smaller, 20-million-atom simulation of a flat membrane filled with photosynthetic light harvesting complexes (based on AFM images from a bacterium with flat chromatophore membranes), served as proof of concept for the chromatophore organelle simulation and explored the relationship between the organization of the light-harvesting proteins and the efficiency with which those proteins can transfer energy between them. A newly published model of the spherical chromatophore organelle recently revealed, for the first time, the locations not only of the light-harvesting complexes, but of the bc1 complex and ATP synthase, two other critical proteins whose locations were previously unknown. Deciphering the inner workings of this model photosynthetic system can guide the development of bio-hybrid green energy devices to help address mankind's energy needs. The chromatophore model is currently being prepared for simulation.

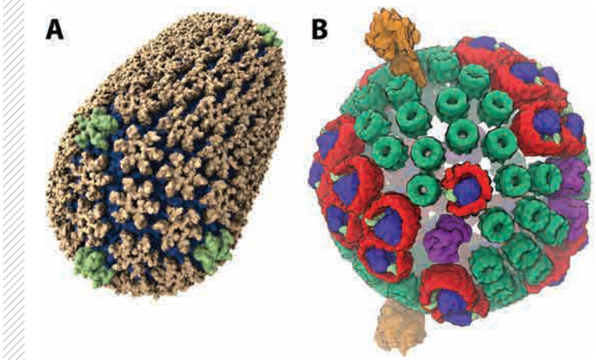

FIGURE A: Klaus Schulten's group at the University of Illinois at Urbana-Champaign was able to construct and simulate the first atomic-resolution model of a mature HIV capsid. This capsid model is now being simulated on Blue Waters to test the interactions of HIV drugs and host cell factors with the capsid, which could help lead to the design of new HIV therapies.

FIGURE B: Scientists in Schulten's group have also constructed an atomic-resolution model of a whole photosynthetic organelle, called a chromatophore. With Blue Waters and other petascale computers, scientists are no longer limited to looking at one or two proteins at a time. It is becoming possible to look at all of the interlocking processes inside an organelle made of many proteins.

WHY BLUE WATERS

Without Blue Waters and other petascale computing resources, neither the HIV nor the chromatophore project would be possible. The HIV project involves simulations of about 65 million atoms, and the chromatophore project requires simulations of up to 100 million atoms; both simulations require thousands of nodes on Blue Waters to run effectively. These projects are examples of how Blue Waters enables bold, new projects that push the limits of what can be done with scientific computing. In our case, that means expanding molecular dynamics simulation capabilities from simulating just a few proteins to simulating full organelles.

PUBLICATIONS

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Cartron, M. L., et al., Integration of energy and electron transfer processes in the photosynthentic membrane of Rhodobacter sphaeroides. *BBA-Bioenergetics*, (2014), in press.

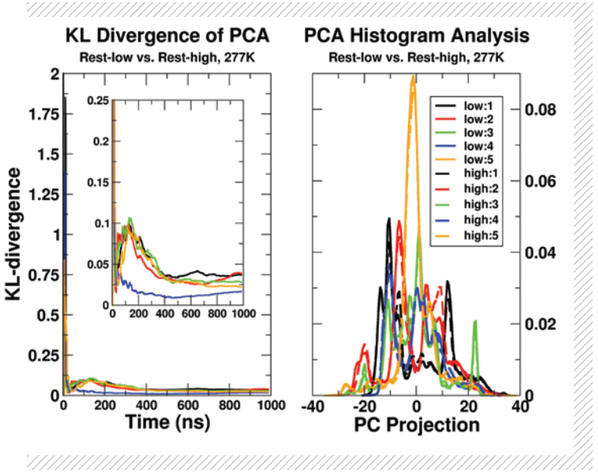
HIERARCHICAL MOLECULAR DYNAMICS SAMPLING FOR ASSESSING PATHWAYS AND FREE ENERGIES OF RNA CATALYSIS, LIGAND BINDING, AND CONFORMATIONAL CHANGE

Allocation: NSF/14 Mnh
PI: Thomas Cheatham, III[1]
Co-PIs: Adrian Roitberg[2]; Carlos Simmerling[3]; Darrin York[4]

[1]University of Utah
[2]University of Florida
[3]Stony Brook University
[4]Rutgers University

EXECUTIVE SUMMARY:

A collaborative team of AMBER developers has been focusing on the development and application of methods that couple together ensembles of highly GPU-optimized molecular dynamics engines to fully map out the conformational, energetic, and chemical landscape of biomolecules. Through applications of the recently released AMBER 14 codes on Blue Waters, the team has shown the ability to not only efficiently converge conformational distributions of RNA tetranucleotides, RNA tetraloops, and DNA helical structure, but also shown reproducibility in the results under different initial conditions.



INTRODUCTION

A continually growing community of researchers is using atomistic biomolecular simulation methods in a variety of applications aimed at, for example, aiding in the refinement of experimental structures, probing ligand-receptor interactions, investigating protein and RNA folding, and generally to understand biomolecular structure and dynamics better. Yet, very few of the force fields are well validated and few studies show complete converge and reproducibility. It is estimated that more than 40% of compute cycles on resources allocated through the NSF's Extreme Science and Engineering Discovery Environments (and a large fraction of Blue Waters cycles) are for the application of these types of simulation methods. If these force fields have limitations, this impacts the reliability of the simulation results and could alter interpretations of the data. Although it is very likely there are still issues with the force fields and sampling, as we show, the situation is not entirely dire since many groups have shown that with reliable starting structures (i.e., high-resolution structures from experiment) and good sampling near these experimental structures, excellent reproduction of experimental observables can be seen and new insight inferred.

METHODS AND RESULTS

Applying these simulation methods we can understand better the properties of biomolecules such as proteins and nucleic acids with such fine-grained detail that the methods accurately account for their native environments of solvent, salts, and other molecules, and complement experimental results. Two key challenges exist. The first centers on the means to effectively and completely sample the complex conformational landscape or, at the least, sufficiently sample the time scales of the processes of interest. This is challenging since biomolecular processes occur over a wide range of time scales, coupling fast and localized dynamics on the femtosecond to nanosecond timescales to larger collective motions over microseconds to milliseconds and beyond. The other key challenge centers on force field accuracy and the ability of the models to properly describe the energetic and dynamic landscape.

The initial focus was on simulations of the RNA tetranucleotide r(GACC) in explicit solvent for which good NMR is available to assess. A number of papers demonstrate that not only can we converge the conformational ensemble of this tetranucleotide, but we can do it reproducibly under different initial conditions.

Unpublished recent work is on the UUCG tetraloop structure that has been a challenge for many current and available force fields, despite the fact that this is the most stable tetraloop structure observed in nature. Given the reliability of the experimental data, this makes UUCG a good test system for improvements to the force fields. Our primary challenge was to converge the distribution of loop structures for UUCG.

In fig. 1 we demonstrate qualitative convergence between two restrained-stem simulations. To demonstrate convergence, the principal components of the combined ensembles were calculated. The Kullback–Leibler divergence of the first five principal components decreases quickly, but still shows significant non-zero values (left panel). The histogram projection of the principal components shows us areas where the primary motions of the loop differ, specifically in the first two modes (right panel).

WHY BLUE WATERS

A key enabler of our work is the extensive work in optimizing the AMBER molecular dynamics (MD) simulations on GPUs by the AMBER development team. AMBER is arguably one of the fastest, if not the fastest, MD engines on NVIDIA GPUs, and this high-performing code was released to the larger community in April 2014. To take advantage of this speed, we have developed and optimized methods that couple together ensembles of independent simulations that exchange information periodically to enhance sampling. We have developed a multi-dimensional replica exchange (M-REMD) framework and set of analysis tools that enable independent simulations to exchange information (temperature, pH, Hamiltonian or "force field") to enhance sampling. Applying these, we have learned which methods help with speed to solution and which do not.

PUBLICATIONS

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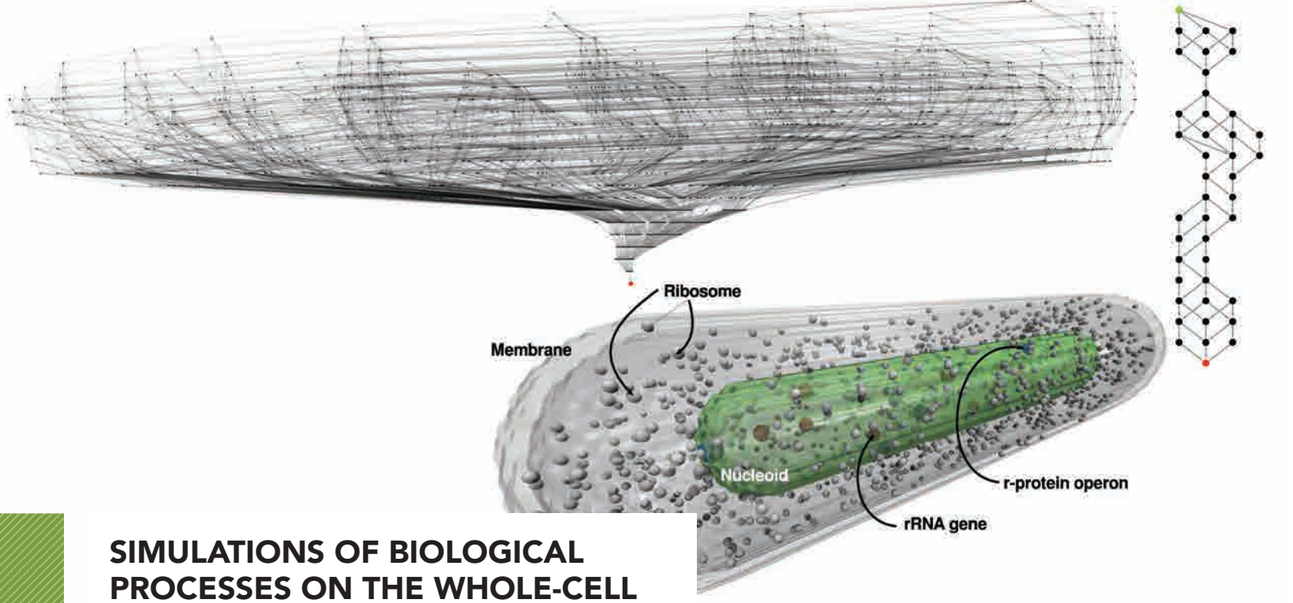
Thibault, J. C., D. R. Roe, J. C. Facelli, and T. E. Cheatham, III, Data model, dictionaries, and desiderata for biomolecular simulation data indexing and sharing. *J. Cheminform.*, 6:1 (2014), doi:10.1186/1758-2946-6-4.

Roe, D. R., C. Bergonzo, and T. E. Cheatham, III, Evaluation of enhanced sampling provided by accelerated molecular dynamics with Hamiltonian replica exchange methods. *J. Phys. Chem. B*, 118:13 (2014), pp. 3543-3552.

Swails, J. M., D. M. York, and A. E. Roitberg, Constant pH replica exchange molecular dynamics in explicit solvent using discrete protonation states: Implementation, testing, and validation. *J. Chem. Theory Comput.*, 10:3 (2014), pp. 1341-1352.

FIGURE 1 (BOTTOM LEFT): Convergence of principal components and overlap of projections between two independent simulations of the UUCG tetraloop with weak or tighter stem loop base pair restraints. (Left) Kullback-Leibler divergence between projections of individual simulation principal components calculated over the combined trajectories from both simulations as a function of time, sampled over 350 replicas in multidimensional replica exchange. (Right) Overlap of principal component projections from the two independent simulations for the first five principal components.



SIMULATIONS OF BIOLOGICAL PROCESSES ON THE WHOLE-CELL LEVEL

Allocation: Illinois/0.592 Mnh
PI: Zaida Luthey-Schulten[1,2]
Collaborators: Michael J. Hallock[1]; Ke Chen[1]; Tyler M. Earnest[1]; Joseph R. Peterson[1]; John A. Cole[1]; Jonathan Lai[1]; John E. Stone[2]

[1]University of Illinois at Urbana-Champaign
[2]Beckman Institute for Advanced Science and Technology

EXECUTIVE SUMMARY:

Recent experiments are revealing details of fundamental cellular processes involved in protein synthesis and metabolism. However, a dynamical description of these processes at the whole-cell level is still missing. With Blue Waters we have been able to develop a kinetic model of ribosome biogenesis that reproduces *in vivo* experimental observations. Stochastic simulations with our GPU-accelerated Lattice Microbe software have extended the model to the entire bacterial cell by computationally linking the transcription and translation events with ribosome assembly on biologically relevant time scales.

INTRODUCTION

Translation is the universal process that synthesizes proteins in all living cells. The ribosome constitutes approximately one fourth of a bacterial cell's dry mass and is central to translation. Biogenesis of the ribosome, together with all cellular activities involved in translation, consume a significant portion of the cell's total energy. However, the cell's effort to enforce such balance between metabolism and macromolecular synthesis is yet to be recognized. We envision that a whole-cell model of ribosome biogenesis is crucial to understanding cell growth and how it is regulated in response to environmental perturbations.

In bacterial cells, ribosomal assembly requires the cooperation of many molecular components: approximately 55 r-proteins, translated in different regions of the cell, to find and bind with the rRNA in the correct order of assembly, and approximately 20 assembly cofactors are engaged to facilitate the process at various assembly stages.

Nomura et al. [1] originally mapped out the hierarchical dependency of the r-proteins binding to the *E. coli* 16S rRNA using equilibrium reconstitution experiments. Progress in biophysical approaches boosted our understanding of *in vitro* ribosomal self-assembly mainly for the protein-assisted dynamics of RNA folding [2-4] and the kinetic cooperation of protein binding [5-7]. However, protein binding orders derived from thermodynamic and kinetic experiments do not always agree, which hampers our investigation of the assembly under an *in vivo* environment. A comprehensive model that captures the topology of the protein-RNA interaction network is needed to decipher the underlying rules governing the assembly of the ribosome.

METHODS AND RESULTS

To address the global complexity in *in vivo* ribosome biogenesis, we simulated a kinetic model of the 30S ribosome assembly using the Lattice Microbe software (LM) on Blue Waters. LM [8-10] is a package of stochastic solvers for simulating the kinetics of biological systems. The reaction diffusion master equation (RDME) solver incorporates spatial information and only allows molecules to interact with others that are nearby. The RDME allows for a more realistic description of biological systems *in vivo* than the alternative, the chemical master equation (CME) solver. Molecular crowding and initial distributions of ribosomes within the cells are obtained from proteomics and cryo-electron tomography reconstructions, and this data can be used by the RDME to describe the cellular environment [11].

We construct a model that explicitly uses the dependencies of the Nomura map [1] to decreases the size of the network to a manageable level, taking effective r-protein binding rates published by the Williamson lab [7]. To further reduce the network size, we use well-stirred stochastic simulations to identify the intermediates in which the majority of the reaction flux flows through. Intermediates which are underutilized by the reaction network are removed from the network along with their associated reactions. This analysis allowed us to reduce the assembly network from 1,633 to 62 species (42 assembly intermediates) and 7,000 to 69 reactions.

To test the validity of this severely pruned network, we compared the protein binding curves, which show the fraction of r-protein bound to intermediates as a function of time, from the well-stirred simulations using the full network and simulations of the reduced network. We saw no greater than 0.1 % root-mean-square error. After subsequent tuning with the competing folding conformations identified in our previous studies [4, 12-14], the model successfully reproduced the structural intermediates reported in the single particle electron microscopy experiments [15]. Furthermore, the model predicted new assembly intermediates that will guide further experimental discoveries.

WHY BLUE WATERS

Even the reduced network is considerably larger than any cellular network we have simulated to date. It is absolutely crucial to have high-performance GPUs to finish the simulation in a timely manner. Many simulations were run to test the sensitivity of the runs to changing parameters and produce an adequate pool of results to make statistical inferences. We could not have done this without Blue Waters. Our long-range goal is to unite the kinetic model of translation with other cellular networks extending over several cycles of cell division so that whole-cell simulations of bacteria responding to various stimuli and environmental factors can be achieved.

As development of LM progresses, Blue Waters will continue to be a prime resource for our simulations. Support for distributed simulations that span multiple nodes over MPI is in development, and features such as Blue Waters' high-speed interconnect, GPU-to-fabric DMA, and a highly parallel file system will be key components for a successful and scalable application.

FIGURE 1 (BACKGROUND): (Upper left) The full reaction network of ribosomal intermediates during the binding of ribosomal proteins to the 16S rRNA (green node) to form the 30S subunit (red node). (Upper right) The full network can be reduced significantly by the analysis of flux through each intermediate. By eliminating intermediates whose flux is less than 0.7% of the most active species, we can prune the network to 62 species and 69 reactions. (Lower right) The reduced small subunit assembly network is simulated within the environment of a living cell. Using our Lattice Microbes whole-cell simulation software [8-10], we are investigating the spatial-temporal effects of a complicated cellular environment on ribosomal biogenesis. The genes encoding the ribosomal proteins and rRNA are placed according to their location in the genome and allowed to diffuse throughout the nucleoid region. Ribosomes are placed within the cytoplasm according to their experimental distribution. In addition to the ribosomal protein binding network, transcription of r-proteins and rRNA and translation of r-protein mRNA are simulated. With the effect of transcription and translation, a realistic simulation of *in vivo* ribosome biogenesis can be performed.

PREDICTIVE COMPUTING OF ADVANCED MATERIALS AND ICES

Allocation: BW Prof/0.12 Mnh
PI: So Hirata[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Two breakthroughs in the algorithms of *ab initio* electronic structure theory developed recently by the Hirata group will be deployed on Blue Waters to perform predictively accurate calculations for the optoelectronic properties of large conjugated molecules used in advanced materials and for the structures, spectra, and phase diagram of nature's most important crystals, such as ice and dry ice, or even molecular liquids such as water, all from first principles. These *ab initio* methods go beyond the usual workhorse of solid-state calculations (density-functional approximations) in the fidelity of simulations that can be achieved and also use a novel stochastic algorithm, an embedded-fragment algorithm, or both to realize unprecedented scalability with respect to both molecular system and computer sizes.

INTRODUCTION

Computational chemists are facing an exciting prospect of being able to apply systematically accurate, and thus predictive, computational methods, the so-called *ab initio* methods, to large molecules, solids, and even liquids, which include nature's most important solids and liquids such as ice and liquid water as well as advanced materials used in optoelectronic devices. This is thanks to the combination of half a century of effort that numerous computational chemists put into refining theories and algorithms of molecular electronic structures and our recent breakthroughs (to be described below) allowing them to be applied to solids, as well as the supercomputers reaching speeds that can make such calculations routine. Chemists, physicists, and materials scientists now anticipate a major transformation in computational or quantitative aspects of solid-state physics and materials science via high-performance computing—that is, the same kind of transformation that occurred in molecular sciences but potentially with even greater impact on society. The theories and their accuracy go beyond the usual workhorse (density-functional approximations) of solid-state computation.

METHODS AND RESULTS

Our group has recently made two breakthroughs in computational chemistry for large molecules and solids (and liquids). One weds second-order and higher many-body perturbation theories (MP2, MP3, etc.) with quantum Monte Carlo (QMC) methods, enabling massively parallel, systematically accurate electronic structure calculations for larger molecules and solids [2,3]. It changes the usual matrix-algebra formulation of electronic structure theories, which is fundamentally non-scalable with respect to system or computer size, into the more scalable stochastic formulation.

The other breakthrough is the method that allows such high-level calculations to be applied to an infinitely extended molecular solid (either periodic or non-periodic) or molecular liquids by dividing them into fragments embedded in the electrostatic field of the solid. The fragments are then treated by well-developed molecular theories and software in a highly parallel algorithm. Our group used this method to study the structures, spectra, equation of state, thermodynamics (heat capacity, enthalpy, Gibbs free energy), Fermi resonance, phase transition, etc. of various phases of ice and dry ice, but at such high theoretical levels as MP2 and coupled-cluster theory [4-6].

With either or both of these, our group plans to predict a variety of properties of all known molecular phases of ice and dry ice to construct *ab initio* phase diagrams of these important solids. A successful outcome will greatly impact geochemistry, astrophysics, and planetary science where probing high-pressure phases of the ices of atmospheric species on Earth or other planets are important but experimentally difficult and expensive.

We also plan to extend this to liquid water using *ab initio* Born-Oppenheimer molecular dynamics. We will also apply Monte Carlo MP2, MP3, and MP4 to predict the stacking interaction energies (important for morphology and thus functions) and optoelectronic parameters (ionization and electron attachment energies, band gaps) of conjugated organic molecular solids and supramolecular assemblies. They include solids that serve as bases of advanced materials such as bulk heterojunction organic solar cells, batteries, sensors, smart windows, field-effect transistors, and light-emitting diodes. The optoelectronic parameters are the quantities of prime importance in determining the solids' performance and functions, but the usual density-functional approximations are known to be poor for these properties. Here, our new method is uniquely useful and accurate. This portion of our research will broadly impact energy science and technology.

In only two months on Blue Waters, the Monte Carlo MP2 code has already been ported and tested using the small allocation provided to a graduate student (Matthew R. Hermes) as a prize of the student's ACS Graduate Student Award. Using this, we have run electron-correlated electron affinity calculations of C_{60}, whose derivatives are used as an electron acceptor in many bulk heterojunction solar cells [1]. A postdoctoral researcher (Dr. Soohaeng Y. Willow) implemented the aforementioned embedded-fragment method at the MP2 level for direct *ab initio* molecular dynamics simulations of liquid water and a large water droplet with a halogen anion. This is being tested on Blue Waters and, if successful, will be a major breakthrough in computational chemistry. Dr. Willow has also implemented a massively parallel embedded-fragment program for solids on Blue Waters and our group will commence ice phase diagram calculations at MP2 or higher levels.

WHY BLUE WATERS

Today's workhorse computational methods for solids (density-functional methods) are routine on a small computer cluster, but with limited accuracy. Therefore, the most meaningful use of Blue Waters in this area (high-pressure chemistry, materials science, geochemistry, etc.) is to fundamentally improve the accuracy rather than system size (which is already formally infinite). In electronic structure theory, this means switching from density-functional methods to *ab initio* theories, which solve the fundamental equation of motion of chemistry rigorously and using systematic approximations with controlled errors. As mentioned, conventional matrix algebra algorithms of *ab initio* theories are fundamentally non-scalable. The aforementioned Monte Carlo MP methods and embedded-fragment methods are among the few that may be realistically and usefully deployed on the large number of processors available on Blue Waters. Such calculations, in turn, may directly address or answer some outstanding scientific questions of solids or large optoelectronic materials, purely computationally and with sufficient accuracy.

PUBLICATIONS

Willow, S. Y., M. R. Hermes, K. S. Kim, and S. Hirata, Convergence acceleration of parallel Monte Carlo second-order many-body perturbation calculations using redundant walkers. *J. Chem. Theory Comput.*, 9:10 (2013), pp. 4396-4402.

NON-BORN–OPPENHEIMER EFFECTS BETWEEN ELECTRONS AND PROTONS

Allocation: BW Prof/0.24 Mnh
PI: Sharon Hammes-Schiffer[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

The quantum mechanical behavior of nuclei plays an important role in a wide range of chemical and biological processes. The inclusion of nuclear quantum effects and non-Born–Oppenheimer effects between nuclei and electrons in computer simulations is challenging. Our group has developed the nuclear-electronic orbital (NEO) method for treating electrons and select nuclei in a quantum mechanical manner on the same level using an orbital-based formalism. The NEO code uses a hybrid MPI/OpenMP protocol, but the calculations require a large number of processors and a substantial amount of memory. We have used Blue Waters to perform NEO calculations on systems in which all electrons and one proton are treated quantum mechanically and have tested approximate methods that enable the study of larger systems.

INTRODUCTION

The inclusion of nuclear quantum effects such as zero-point energy and tunneling in electronic structure calculations is important for the study of a variety of chemical systems, particularly those involving hydrogen transfer or hydrogen-bonding interactions. Moreover, non-adiabatic effects, also called non-Born–Oppenheimer effects, between electrons and certain nuclei are significant for many of these systems. In this case, the electrons cannot be assumed to respond instantaneously to the nuclear motions, and the concept of the nuclei moving on a single electronic potential energy surface is no longer valid. This type of non-adiabaticity has been shown to play a critical role in proton-coupled electron transfer (PCET) reactions, which are essential for a wide range of chemical and biological processes, including photosynthesis, respiration, enzyme reactions, and energy devices such as solar cells. The development of non-Born–Oppenheimer methods to enable accurate and efficient calculations of PCET reactions will impact many scientific endeavors, from drug design to the design of more effective catalysts for solar energy devices.

METHODS AND RESULTS

In the NEO approach, typically all electrons and one or a few protons are treated quantum mechanically, and a mixed nuclear-electronic time-independent Schrödinger equation is solved. To include the essential electron-proton correlation, we developed an explicitly correlated method, denoted NEO-XCHF. Although explicitly correlated methods have been shown to be highly accurate for model systems, they are computationally expensive and are currently intractable for larger systems of chemical interest.

Recently, we proposed an alternative ansatz with the primary goal of improving computational tractability to enable the study of larger systems of chemical interest. In this approach, denoted NEO-RXCHF, only select electronic orbitals are explicitly correlated to the nuclear orbital(s) and certain exchange terms are approximated, thereby substantially decreasing the number of multi-particle integrals that must be calculated.

The computational bottleneck is the calculation of two-, three-, and four-particle integrals that arise from computing matrix elements of the explicitly correlated wave function over the mixed nuclear-electronic Hamiltonian. Since these integrals can be calculated completely independently from one another we applied the OpenMP protocol, providing almost perfect scaling with respect to the number of threads.

When considering calculations on larger proton-containing systems, two drawbacks with the shared-memory-based OpenMP model are of immediate concern: (1) the parallelization is restricted to the number of cores on a single machine, which is usually 32 at most, and (2) the calculations must be performed using the memory of a single machine. A hybrid MPI/OpenMP protocol obviates the need for all integrals to be stored simultaneously and allows the division of the calculation over different machines. This version of the code scales very well with respect to the number of MPI processes.

We performed initial NEO-RXCHF calculations on proton-containing systems on Blue Waters. We analyzed the nuclear densities of the protons and compared them to highly accurate grid-based densities. Our calculations illustrate that this approach can provide accurate descriptions of the protons that are treated quantum mechanically. We also have tested new approximate methods that will enable the study of larger proton-containing systems. Current work focuses on refining these approximate methods and investigating larger systems of chemical and biological interest. Our long-term objective is to use these non-Born–Oppenheimer methods to study PCET in molecular catalysts that are directly relevant to solar energy conversion.

WHY BLUE WATERS

Our in-house NEO code has been adapted to incorporate a hybrid MPI/OpenMP protocol, but the calculations require a large number of processors and a substantial amount of memory. The highly parallel computing system on Blue Waters is essential for the application of this approach to systems of interest, where the computational bottleneck is the embarrassingly parallelizable calculation of many integrals. Most importantly, the large memory requirements of storing these integrals render this problem impossible when a large number of nodes cannot be used simultaneously, as on other computer systems. As our code has demonstrated excellent scaling, we are able to directly benefit from using a large number of nodes simultaneously on Blue Waters with very little overhead.

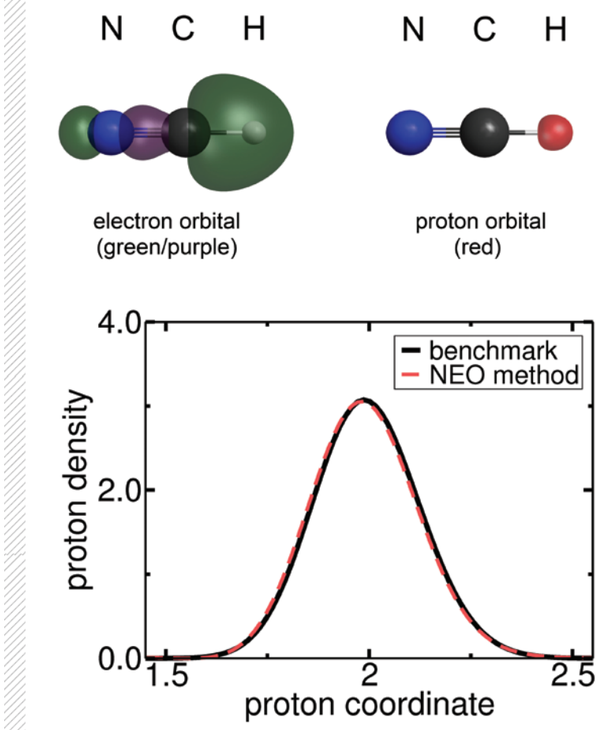


FIGURE 1: The results of a NEO-RXCHF calculation performed on the hydrogen cyanide molecule. (Top) Correlated electron and proton molecular orbitals obtained from the NEO calculation. The electron orbital is shown in green and purple, indicating its two phases, and the proton orbital is shown in red. (Bottom) The proton density along the N-C-H axis, comparing the results of the NEO calculation (red dashed) to a numerically exact benchmark grid-based calculation (black solid).

THE MECHANISM OF THE SARCO/ENDOPLASMIC RETICULUM ATP-DRIVEN CALCIUM PUMP

Allocation: GLCPC/0.6 Mnh
PI: Benoît Roux[1]
Co-PI: Avisek Das[1]

[1]University of Chicago

EXECUTIVE SUMMARY:

Sarco/endoplasmic reticulum Ca^{2+}-ATPase is an integral membrane protein that uses ATP hydrolysis as a source of free energy to pump two calcium ions per ATP molecule from calcium-poor cytoplasm of the muscle cell to the calcium-rich lumen of the sarcoplasmic reticulum, thereby maintaining a ten-thousand-fold concentration gradient. Two major outstanding issues are the pathways of the ions to and from the transmembrane binding sites and a detailed understanding of the large-scale conformational changes among various functionally relevant states. We hope to shed some light on these important issues by simulating conformational transition pathways between experimentally known stable states. The optimal path is determined by string method with swarms-of-trajectory, which involves running thousands of all-atom molecular dynamics trajectories that communicate at a regular interval. Our recent simulations on Blue Waters have revealed unprecedented molecular details of several key steps of the pumping cycle.

INTRODUCTION

Membrane proteins form an important class of biomolecules that are associated with the membrane dividing the inside of a cell (or a cellular compartment) and its environment. These proteins play essential roles in controlling the bi-directional flow of material and information. Our project aims to understand the function of an integral membrane protein called sarco/endoplasmic reticulum Ca^{2+}-ATPase (SERCA) [1-3] that uses ATP hydrolysis as a source of free energy to pump two calcium ions per ATP molecule from calcium-poor cytoplasm of the muscle cell to the calcium-rich lumen of the sarcoplasmic reticulum. This process is important for relaxation of skeletal muscle that is regulated by calcium ions, and a close analogue in the cardiac muscle is a therapeutic target.

Over the past few years a number of structural studies [1-6] have provided atomic resolution models for several important states along the pumping cycle. Two major outstanding issues are the pathways of ions from either side of the membrane to the transmembrane binding sites and a detailed description of the conformational changes that will elucidate how various parts of the protein communicate over fairly large distances in order to achieve coupled ATP hydrolysis and calcium transport. We intend to simulate the transition pathways between experimentally known end points to shed some light on these important issues.

METHODS AND RESULTS

The most important computational tool for studying the dynamics of large systems at biologically relevant temperatures is classical molecular dynamics (MD) simulation [7] with all-atom resolution. Conformational changes in large biomolecules are complex and slow, taking place on timescales that are far beyond the reach of brute-force MD simulations. For example, even a microsecond-long all-atom MD trajectory is not enough to connect two end points of a conformational transition. To overcome these problems we have employed a robust computational algorithm called the "String method with swarms of trajectories" [8,9]. For meaningful results, more than a thousand copies of the system and hundreds of iterations are required. Simulations were carried out using a modified version of NAMD 2.9 [10].

We have determined a transition pathway between the calcium bound non-occluded (PDB ID: 1SU4) [1] and occluded (PDB ID: 1VFP) [4] states of SERCA. This transition is responsible for the occlusion process which prevents the escape of bound calcium ions in the transmembrane binding sites to the cytoplasmic side. The string was represented by 35 images, and for each image we used 32 trajectories to estimate the drifts (a total of 1,120 copies of the system). Each iteration involved 20 picoseconds of simulation; about 100 iterations were performed for production calculation.

Before embarking on a full-scale production run, several scaling studies and trial runs were performed. The convergence of the string is determined by monitoring the image-wise distances from the initial string as well as all possible Frechet distances between strings corresponding to two different iterations. The Frechet distance between two strings is a global measure of similarity of two strings which takes into account the proper order of the images. The final converged string revealed the mechanism of occlusion process in unprecedented molecular details. The large-scale motions of the cytoplasmic domains induce small-scale motions of key hydrophobic side chains in the transmembrane helices. These side chain movements block the cytoplasmic ion pathway and lock the bound calcium ions inside the membrane.

WHY BLUE WATERS

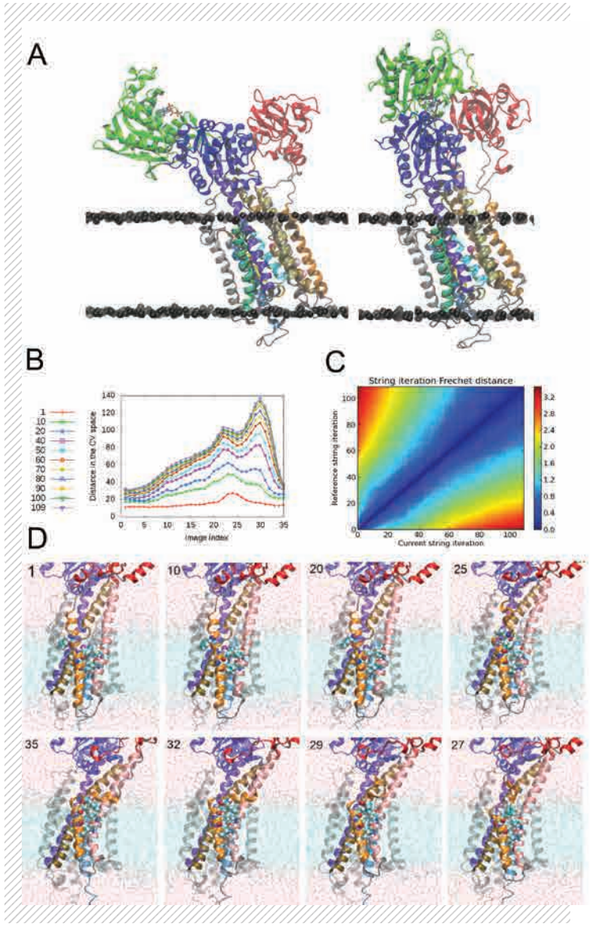
To perform this calculation on SERCA (~290,000 atoms), a single job requires more than 6,000 nodes, which is more than the node count of an entire machine for many small- to medium-sized supercomputers. Therefore, the massively parallel architecture of Blue Waters played a crucial role in the successful implementation of our project.

FIGURE A: Crystal structures of non-occluded (left, PDB ID: 1SU4) and occlude (right, PDB ID: 1VFP) states of sarco/endoplasmic reticulum Ca^{2+}-ATPase. The protein has three large cytoplasmic domains: nucleotide binding domain N (green), phosphorylation domain P (blue) and actuator domain A (green). The ten transmembrane helices are color coded as follows: M1 (orange), M2 (pink), M3 (tan), M4 (ochre), M5 (violet), M6 (cyan), M7 (dark green), M8 (sky blue), M9 (yellow), M10 (silver).

FIGURE B: Convergence of string iterations monitored by image-wise distances. The image-wise distances from the initial string in the space of the collective variables (CV) are plotted for several iterations.

FIGURE C: Convergence of string iterations monitored by pairwise Frechet distances between strings at different iterations. The blue patch at the upper right corner indicates a converging string.

FIGURE D: Snapshots of selected images of the final string showing the occlusion of ions in the transmembrane binding sites by upward motions of M1 and M2 and bending of M1. Purple spheres are calcium ions and space fills show several key residues. Due to the motions of the above-mentioned side chains, the cytoplasmic ion pathway is blocked by hydrophobic side chains during the transition from the non-occluded state (image 1) to the occluded state (image 35).



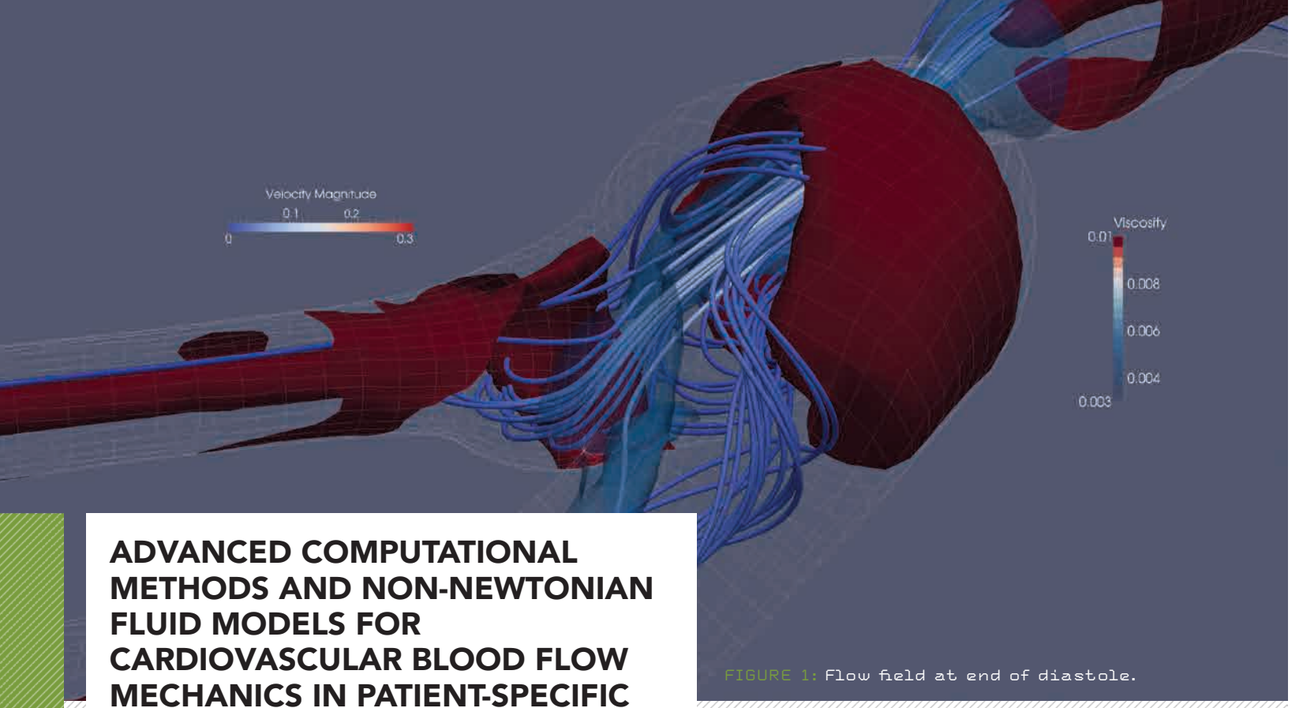


FIGURE 1: Flow field at end of diastole.

ADVANCED COMPUTATIONAL METHODS AND NON-NEWTONIAN FLUID MODELS FOR CARDIOVASCULAR BLOOD FLOW MECHANICS IN PATIENT-SPECIFIC GEOMETRIES

Allocation: Illinois/0.042 Mnh
PI: Arif Masud[1]
Collaborators: JaeHyuk Kwack[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

We have developed novel numerical methods that are integrated with non-Newtonian constitutive models to simulate and analyze blood flow through patient-specific geometries in the cardiovascular system. The current Blue Waters project helped us to achieve two objectives: (1) Further explore the mathematical constructs of our hierarchical multiscale methods on Blue Waters hardware architecture. Our new methods exploit the local resident memory on the processing nodes to make the macro elements "smart," thereby reducing the size of the global problem and minimizing data communication. (2) Extract flow physics in patient-specific models of carotid artery via high-fidelity blood flow simulations.

METHODS AND RESULTS

Blood shows significant viscoelastic- and shear-rate-dependent response, and under arterial disease conditions such as stenosis and/or aneurysms of the artery, this viscoelastic feature becomes dominant. We have developed non-Newtonian models for blood that account for its viscoelastic response [1,2]. We have also developed hierarchical multiscale finite element methods with local and global (coarse and fine) description of the variational formulations that results in telescopic depth in scales [3,4]. This scale split leads to two coupled nonlinear systems: the coarse-scale and the fine-scale subsystems. The fine-scale solution is nonlinear and time dependent, and it is extracted from the fine-scale sub-problem via a direct application of residual-free bubbles approach over element subdomains. The fine-scale solution is then variationally projected onto the coarse-scale space, and it leads to the hierarchical multiscale method with enhanced stabilization properties. The telescopic depth in scales helps reduce the size of the global problem, while increasing "local-solves" that are cost effective on Blue Waters-type architectures. From computational and algorithmic perspectives, the hierarchical multiscale framework leads to substantially reduced global communication in favor of increased local computing. This feature is of tremendous benefit in massively parallel computing as it reduces communication costs across the partitioned subdomains.

We have verified the robustness of our method under diverse flow conditions that are found in the human vasculature, and have applied it to a patient-specific model of a carotid artery that suffers from stenosis and aneurysm. The geometric model of the carotid artery was constructed from MRI images. Figs. 1 and 2 show snapshots of velocity streamlines and time-varying viscosity of blood during a typical heart beat at the end of diastole and middle of systole, respectively. At the end of diastole (fig. 1) where the shear rate is at its minimum, substantial viscosity buildup can be seen. This effect is more pronounced in the aneurysm where, due to the ballooning effect, local velocity is lower than the mean flow velocity.

Through this study we found that in the middle of the diastole the Newtonian and the shear-rate dependent non-Newtonian models yield significantly different results, where the non-Newtonian model predicts higher shear stresses as compared to the Newtonian model. Consequently, using the Newtonian model in clinical applications can provide a non-conservative estimate that is not appropriate for patient care. This work was highlighted in the spring/summer 2014 issue of NCSA's Access magazine.

One of the intended applications of our effort is to employ these models for optimizing Ventricular Assistive Devices (VADs) for patient-specific requirements, as well as possibly help in the design of these devices. We believe that new methods and the associated computer programs that we have developed will help optimize the performance of VADs for patient-specific needs, and thus help in personalized medicine.

WHY BLUE WATERS

Blue Waters has a unique hardware architecture that provides substantial local memory at the level of the processing nodes. Our new computational methods take advantage of this resident memory and carry out high-intensity local calculations that make the elements "scale aware" or "smart." Accuracy on coarse meshes is the same as that from highly refined meshes if standard finite element techniques are used. These new methods are mathematically robust and computationally economical, and these attributes have been verified on highly nonlinear and transient test problems.

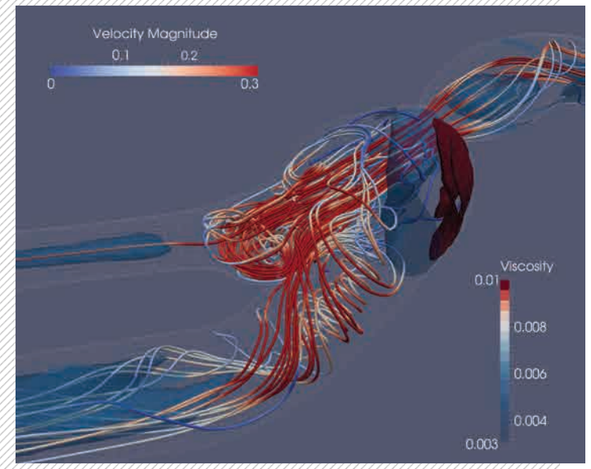
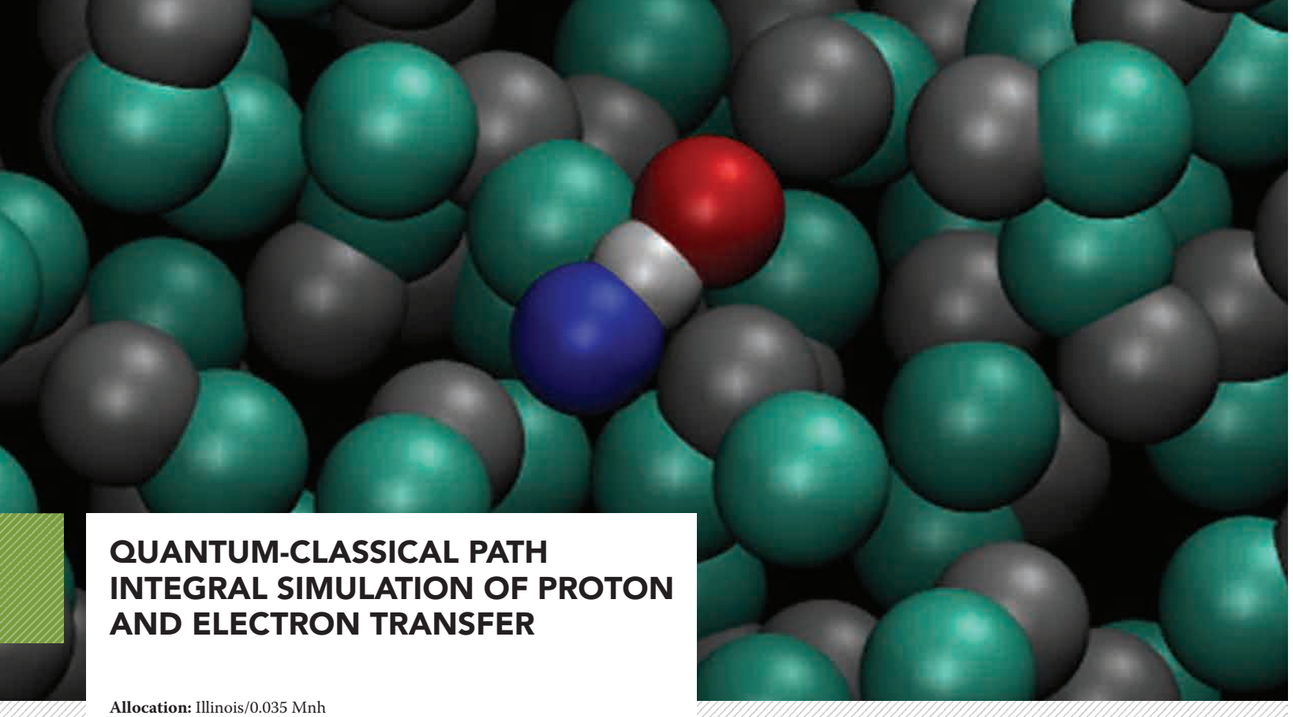


FIGURE 2: Flow field at middle of systole.

PUBLICATIONS

Kwack, J., and A. Masud, A stabilized mixed finite-element method for shear-rate dependent non-Newtonian fluids: 3D benchmark problems and application to blood flow in bifurcating arteries. *Comput. Mech.*, 53:4 (2014), pp. 751-776.



QUANTUM-CLASSICAL PATH INTEGRAL SIMULATION OF PROTON AND ELECTRON TRANSFER

Allocation: Illinois/0.035 Mnh
PI: Nancy Makri[1]
Co-PI: Thomas Allen[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Quantum mechanical effects play an essential role in chemical and biological processes and are important for understanding energy storage and designing novel materials. The simulation of quantum dynamical phenomena in condensed-phase and biological systems continues to present major challenges. We have been pursuing rigorous quantum-classical formulations based on Feynman's path integral formulation of quantum mechanics. Current work involves the first implementation of quantum-classical path integral (QCPI) to the simulation of two paradigm chemical processes. Upon completion of this phase of the work, the QCPI calculations will offer quantitative results for the kinetics of the chosen proton and electron transfer processes, along with a detailed picture of the underlying mechanism, including the time scale of correlations and decoherence, the distinct roles of fast and sluggish solvent motions and associated quantum effects, as well as the importance of nonlinear solvent effects on the dynamics.

INTRODUCTION

Quantum mechanical effects play an essential role in chemical and biological processes and are important for understanding energy storage and designing novel materials. The major challenge in the development of quantum mechanical simulation algorithms stems from the non-local nature of quantum mechanics, which leads to exponential scaling of computational effort with the number of interacting particles.

For many processes of interest, quantum mechanical effects are vital in the treatment of a small number of degrees of freedom (e.g., those corresponding to a transferring electron or proton), while the remaining particles (solvent molecules or biological medium) could be adequately described via Newtonian dynamics. However, the traditional Schrödinger formulation of quantum mechanics (which is based on delocalized wave functions) does not lend itself to a combination with Newtonian trajectories (which are local in phase space) unless severe approximations are introduced. Thus, the simulation of quantum dynamical phenomena in condensed-phase and biological systems continues to present major challenges.

METHODS AND RESULTS

We have been pursuing rigorous quantum-classical formulations based on Feynman's path integral formulation of quantum mechanics. The major appeal of this approach stems from the local, trajectory-like nature of the Feynman paths, which leads naturally to combined quantum-classical treatments that are free of approximations. Recent work has described a quantum-classical path integral (QCPI) methodology, which incorporates these ideas as well as several advances in the understanding of decoherence processes. QCPI treats a small subsystem using full quantum mechanics, while the effects of the environment are captured via standard molecular dynamics (MD) procedures. Since all quantum interference effects and their quenching by the solvent are accounted for at the most detailed (non-averaged) level, QCPI leads to correct branching ratios and product distributions, allowing simulation of important chemical and biological processes with unprecedented accuracy.

Current work involves the first implementation of QCPI to the simulation of two paradigm chemical processes. The first calculation (by Thomas Allen) is on the proton transfer reaction of the phenol-amine complex in methyl chloride. This system has been employed in many computational investigations using a variety of approximations. The accurate QCPI results will lead to an unambiguous picture of the proton transfer mechanism in this system and will serve as much-needed benchmarks. The second process (by Peter Walters and Tuseeta Banerjee) involves the ferrocene-ferrocenium charge transfer pair in benzene and hexane solvents. This system was chosen for its significance in electrochemistry.

Two widely used MD packages, NAMD and LAMMPS, have been combined with the QCPI software and adapted to yield trajectories subject to forces obtained using the proton or electron coordinates specified by the given quantum path. We have simulated the early dynamics of the transferring particles and obtained the time evolution of the state populations. A set of convergence tests is performed to determine the optimal parameters for longer time calculations. These processes are dominated by solvent effects, and some high-frequency vibrations of the solvent molecules are strongly coupled to the transferring particle. Thus, in addition to the quantum tunneling effects associated with the proton or electron, the QCPI calculations reveal substantial solvent-induced quantum mechanical effects on the dynamics of these reactions.

Upon completion of the present phase of the work, the QCPI calculations will offer quantitative results for the kinetics of the chosen proton and electron transfer processes, along with a detailed picture of the underlying mechanism, including the time scale of correlations and decoherence, the distinct roles of fast and sluggish solvent motions and associated quantum effects, as well as the importance of nonlinear solvent effects on the dynamics.

FIGURE 1 (BACKGROUND): Phenol-amine proton transfer in methyl chloride.

WHY BLUE WATERS

Implementation of the QCPI methodology requires integration of a large number of classical trajectories, and accompanying Feynman paths of the quantum subsystem, from each initial condition sampled from the solvent density. Because the trajectories are independent and generally relatively short, it is possible to assign a single trajectory to each core within a given processor while maintaining computational efficiency. This multi-level approach has the benefit of minimizing communication time while maximizing concurrent processing, since related classical and quantum mechanical calculations are performed within the same node, where communication between processors should be much faster than if the information were more widely distributed. By exploiting the very mechanism of decoherence, we are able to circumvent the exponential proliferation of the number of trajectories with propagation time. The QCPI formulation is well suited to decomposition based on multi-level parallelism, and Blue Waters provides the ideal platform for its implementation.

INVESTIGATING LIGAND MODULATION OF GPCR CONFORMATIONAL LANDSCAPES

Allocation: NSF/3.13 Mnh
PI: Vijay S. Pande[1]
Collaborators: Morgan Lawrenz[1]; Diwakar Shukla[1]; Kai Kohloff[1,2]; Russ Altman[1]; Gregory Bowman[1]; Dan Belov[2]; David E. Konerding[2]

[1]Stanford University
[2]Google

EXECUTIVE SUMMARY:

We have completed and ongoing research projects that utilize the extensive computing infrastructure of Blue Waters to study G-protein coupled receptors (GPCRs), key signaling proteins that are the targets of ~40% of commercially available drugs. Our workflow involves massively parallel biomolecular simulations that are aggregated by a statistical model that maps the connectivity and stability of receptor states. We have completed work on the β2 adrenergic receptor and used our approach to provide the first atomistic description of this receptor's ligand-modulated activation pathways [1]. We targeted intermediate states along these pathways with extensive small molecule virtual screens and demonstrated that these intermediates select unique ligand types that would be undiscovered without knowledge of the full activation pathway. These results show that our model of biomolecular simulations significantly contributes to understanding of both biological mechanisms and drug efficacy for GPCRs.

INTRODUCTION

G-protein coupled receptors (GPCRs) regulate a large variety of physiological processes by transmitting signals from extracellular binding of diverse ligands to intracellular signaling molecules, a property called functional selectivity. Central to this phenomenon is the well-accepted biophysical paradigm of conformational selection, in which a ligand selectively stabilizes a state from an ensemble. GPCRs provide rich examples of conformational selection. We hypothesize that there are general principles describing the dynamics of ligand-modulated GPCR activation. Detailed structural understanding of this mechanism for β2AR can inform studies of over 19 known subfamilies of class-A GPCRs which share sequence and structural features. Because of their central role in cellular signaling, these proteins are also prominent drug targets. β2AR is implicated in type-2 diabetes, obesity, and asthma. Knowledge of ligand-modulated GPCR conformational dynamics can improve our understanding of drug efficacy at these receptors and allow development of more effective structure-based drug design approaches.

METHODS AND RESULTS

We generated an extensive dataset from molecular dynamics simulations of β2AR and identified kinetically stable states along ligand-modulated activation pathways. We used massively parallel small molecule docking to target these Markov state model (MSM) states and demonstrate that our approach incorporates our rich structural data into a drug discovery workflow that could lead to drugs that interact more closely with diverse receptor states, leading to overall increased efficacy and specificity.

MSM states from high flux activation pathways identified in this study were targeted with small molecule docking of a database of β2AR agonists, antagonists, and decoys with the program Surflex. For both agonists and antagonists, docking to the MSM states along activation pathways gives high values for area under the receiver operating characteristic (ROC) curve, which evaluates selection of true ligands from decoys. These results are a statistically significant improvement over results from docking to the active and inactive crystal structures and to randomly selected snapshots from long-time-scale, agonist-bound β2AR deactivation simulations.

Next, we show that docking to MSM states expands the chemical space of our docking results, an essential advantage in docking approaches. Top-scoring ligands for each MSM state were selected for 3D shape- and chemistry-overlap calculations using the program ROCS. These calculations give Tanimoto scores for overlap of ligands, which were used to cluster the results and revealed a diversity of chemotypes that are highly ranked, or enriched, differentially by MSM states along the activation pathways. We can show examples of chemotypes that would have been undiscovered by virtual screen docking to the crystal structures alone or without knowledge of the full activation pathway. These results highlight MSMs as a tool for picking functional intermediate GPCR states that have different estimated affinities for known ligand chemotypes. Information on this correspondence between ligand type and receptor conformation may be beneficial for future drug design efforts and can predict ligands that may preferentially bind and isolate rare intermediate conformations of receptors.

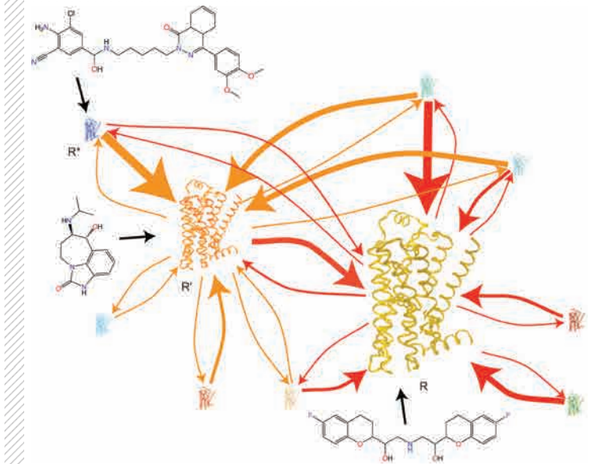


FIGURE 1: Markov state models (MSMs) of receptor dynamics allow discovery of intermediate receptor states that aid discovery of new drug classes. A network representation of a ten-state MSM from GPCR molecular dynamics simulations shows examples of inactive (R), active (R*), and kinetically stable intermediate states (R') connected by arrows that are weighted by transition probability. We show that these intermediate states preferentially bind to different ligand types, which may be fruitful for future drug design efforts and can give testable predictions for ligands that may isolate rare intermediate conformations of receptors.

WHY BLUE WATERS

The extensive architecture of Blue Waters gives us two unique advantages: (1) the resource allows generation of many long timescale, equilibrated molecular dynamics simulations which can give useful information on receptor dynamics and also be used synchronously with distributed computing resources to generate exceptionally sampled conformational data for our biological targets; and (2) the resource allows us to rigorously test a new computational protocol for identifying new small molecules that requires massively parallel calculations. For β2AR, we have 140 unique, kinetically stable receptor states that we wanted to target with a rigorous small docking algorithm, which takes approximately two minutes per molecule. This would take ~80,000 hours to run all molecules on a single CPU core for a full initial screen of our data, but takes only a week using available Blue Waters cores. A similar savings in time applied to all the molecule overlap calculations for the clustering approach. This quick evaluation of our computational protocol was integral to the demonstration of a new computational approach.

PUBLICATIONS

Kohloff, K. J., D. Shukla, M. Lawrenz, G. R. Bowman, D. E. Konerding, D. Belov, R. B. Altman, and V. S. Pande, *Nature Chemistry*, 6:1 (2014), pp. 15-21.

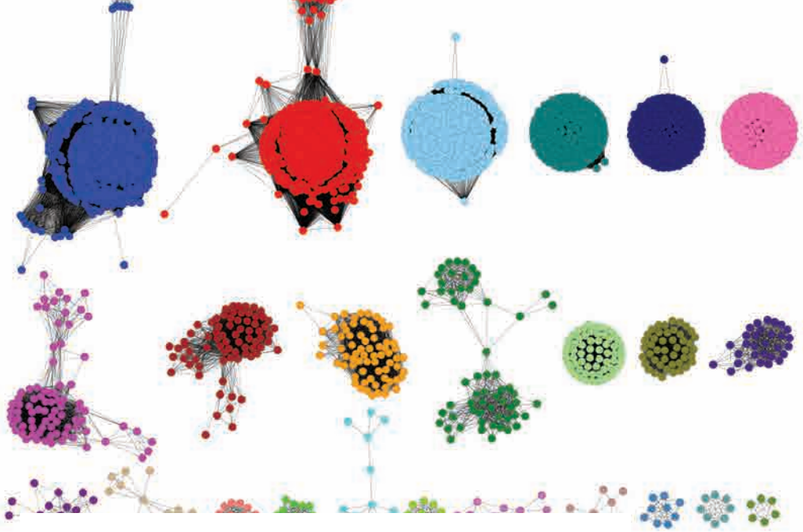


FIGURE 1: Sequence similarity network (SSN) for PF08794, the proline racemase family, displayed with a BLAST e-value threshold of 10-110 (50% sequence identity). The colors are used to distinguish predicted isofunctional clusters.

SEQUENCE SIMILARITY NETWORKS FOR THE PROTEIN "UNIVERSE"

Allocation: Illinois/0.625 Mnh
PI: John A. Gerlt[1]
Collaborators: Daniel Davidson[1]; Boris Sadkhin[1]; David Slater[1]; Alex Bateman[2]; Matthew P. Jacobson[3]

[1]University of Illinois at Urbana-Champaign
[2]European Bioinformatics Institute
[3]University of California, San Francisco

EXECUTIVE SUMMARY:

The Enzyme Function Initiative (EFI) is a large-scale collaborative project supported by the National Institutes of General Medical Sciences (U54GM093342-04) [1]. The EFI is devising strategies and tools to facilitate prediction of the *in vitro* activities and *in vivo* metabolic functions of uncharacterized enzymes discovered in genome projects. The Blue Waters allocation enables generation of a library of pre-computed sequence similarity networks for all Pfam families and clans of proteins in the UniProtKB database that will be provided to the scientific community. We are using Blue Waters to calculate all-by-all BLAST sequence relationships as well as statistical analyses of the BLAST results.

INTRODUCTION

The UniProtKB database contains 56,555,610 sequences (release 2014_5; 14-May-2104). The majority of the entries are obtained from genome sequencing projects, with the rationale that knowledge of the complete set of proteins/enzymes encoded by an organism will allow its biological/physiological capabilities to be understood. However, if many of the proteins/enzymes have uncertain or unknown functions, researchers cannot capitalize on the investments in genome projects.

Bioinformatics tools are integral to the EFI's strategies. The EFI's goal is to provide to the biological community an "on-demand" library of sequence similarity networks [2] for the 14,831 families and 515 clans in the Pfam database (Release 27.0; March 2013) and to update this library on a minimum three-month refresh cycle. Sequence similarities are quantitated by the BLAST e-values between pairs of sequences.

METHODS AND RESULTS

The EFI and University of Illinois at Urbana-Champaign's Institute for Genomic Biology (IGB) collaborated on development of scripts that allow facile generation of sequence similarity networks (SSNs) for protein families using sequences from the Pfam sequence database. However, the BLAST calculations are computationally intensive, so the user must wait hours to days for these to complete.

Also, instead of requiring users to initiate SSN generation, the EFI and IGB are using the petascale capabilities of Blue Waters to calculate the BLASTs as well as statistical analyses for all Pfam families and clans so that a complete library of pre-computed SSNs can be provided using an EFI-supported webserver.

The Blue Waters allocation was awarded in mid-October 2013. Since that time, we have been evaluating how to run and optimize two pieces of code, as well as the Perl scripts that control the flow of data and collect the results:

BLAST v2.x (blastall) is a widely used program developed by the National Center for Biotechnology Information (NCBI). Blastall is not efficiently multi-threaded, so we are running as many single-threaded processes per node as there are integer cores available.

CD-Hit is a sequence clustering algorithm [3] that we use to both generate merged datasets of input sequences and/or post-process sequences flagged as being similar to each other by blastall.

The majority of the Pfam families and clans contain <200,000 sequences, so the BLAST and downstream statistics calculations are straightforward and efficient. However, for the largest families and clans (the largest contains ~3 million sequences) the computation time increases exponentially with the number of sequences and the RAM requirements become more demanding because of the number of sequences and BLAST results becomes large.

BLAST results totaling 33 TB of data have been obtained for virtually all of the 515 Pfam clans and 14,831 Pfam families. We now are addressing the problem of filtering the BLAST data to remove redundant pairs. With the BLAST results, we will perform statistical analyses that are required for the user to choose parameters for generating the SSNs.

Our recent activities address the necessary experimentation to determine the most efficient pipeline for performing the BLASTs and the downstream statistical analyses so that the process can be automated and performed with a minimum three-month refresh cycle so that the library of SSNs will remain current as the sequence databases are updated.

WHY BLUE WATERS

The project uses an embarrassingly parallel computing model to perform the BLAST analyses. Because of (1) the scales of the computations used (number and sizes of Pfam families and clans and the number of sequences in each family and clan) and (2) the time sensitivity of the production of the output relative to database updates, only a resource the scale of Blue Waters can perform the job in a reasonable time frame.

BENCHMARKING THE HUMAN VARIATION CALLING PIPELINE

Allocation: Illinois/0.05 Mnh
PI: Christopher J. Fields[1]
Collaborators: Liudmila S. Yafremava[1]; Gloria Rendon[1]; C. Victor Jongeneel[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

Researchers increasingly use genome sequencing for medical purposes. The standard pipeline used for this purpose presently carries a high computational cost, and if hospitals begin to sequence every arriving patient, the total ongoing storage requirement would reach the petabytes scale. This is a major hurdle for the routine implementation of genome-based individualized medicine.

We scaled the pipeline to hundreds of genomes and documented the disk space and compute requirements for performing daily production runs as expected in a personalized medicine clinic. Our results are comparable to those published by other groups, but Blue Waters has enough nodes and disk space to actually demonstrate the scalability, as opposed to estimating it from smaller number of genomes.

INTRODUCTION

Researchers increasingly use genome sequencing for medical purposes. A key application is to generate a genomic variation profile—the set of differences between a patient's genome and that of a population average, as well as between a tumor and normal tissue from a single person. This profile is then used to predict the patient's susceptibility to disease, their response to various therapies, or the underlying causes of extant pathologies.

The standard pipeline used for this purpose presently carries a high computational cost. This is a major hurdle for the routine implementation of genome-based individualized medicine. Still, it is believed that whole-genome sequencing and analysis will become the standard of care in medicine within the next few years, requiring that this pipeline be run for every patient who comes through a hospital's doors on any given day. Our project seeks to explore the computational bottlenecks, performance limitations, and tradeoffs between speed and accuracy that arise at scale.

METHODS AND RESULTS

Accuracy vs. speed

In collaboration with members of the University of Illinois CompGen initiative, we created a comprehensive suite of synthetic sequence data, which sweeps across a number of parameters that can affect the accuracy and robustness of the pipeline. Specifically, we generated over 200 datasets, including synthetic whole exomes and genomes, by simulating a range of sequencing error rates, base substitution transition probabilities, and read lengths. Known synthetic variants were introduced into each dataset, which we compared with the workflow output. We used these synthetic data to probe the limits of accuracy of the workflow and determine the conditions under which the variants could no longer be reliably detected. The accuracy can sometimes be rescued by using alternative software tools, which are more comprehensive at the expense of longer compute time. We documented this continuum of tradeoffs between accuracy and speed and determined the extent to which specificity and sensitivity are affected by noise in the input data. As a reality check, we compared the results with pipeline runs on the freely available human exomes from the 1000 Genomes Project.

We took advantage of the opportunity to perform comprehensive profiling of those tools while running the above accuracy benchmarking on the synthetic data files. When using the pipeline at the expected production rate, we believe that the bandwidth of the file system will be a big contributor to performance degradation when scaling up.

Using an embedded launcher

The standard bioinformatics software is not parallelized across cluster nodes, is sometimes single threaded, and is intended to run on embarrassingly parallel data. At the same time, the procedure itself is fairly complex, with multiple split/merge points, numerous conditional forks, and several data entry points into the workflow. When running on sets of several hundred genomes at once, the pipeline can generate over 1,000 separate jobs, which can result in low job priority and break the per-user limit on the number of jobs in the queue. We collaborated with the Blue Waters support team to use an embedded job launcher, which submits a single PBS job for each of the three major embarrassingly parallel blocks of the workflow, reserving the required number of nodes, and launches the pipeline jobs within it.

Blue Waters enables production-grade scaling

Using the embedded job launcher described above, we scaled the pipeline to hundreds of genomes and documented the disk space and compute requirements for performing daily production runs as expected in a personalized medicine clinic. Running the variant calling on one whole human genome uses up to 20 nodes concurrently for 2-4 days, depending on depth of sequencing. If hospitals begin to sequence every arriving patient, a compute facility can expect to deal with hundreds of datasets daily. Because each run takes several days, the runs on data from different days will overlap, tying up several thousand nodes every day. During the course of this production, ~250 TB of storage has to be dedicated to the input data alone. The output data, including intermediary files, uses 10 times as much disk space, provided that the data are deleted immediately upon production and delivery.

Emerging collaborations

In the effort to gain as much speed as possible, we collaborated with Novocraft, the Malaysian company that developed Novoalign, the widely used and currently most accurate short read aligner. An MPI version of Novoalign was developed on Blue Waters and yields a four-fold speedup in the first phase of the pipeline.

We collaborated with scientists from the Department of Electrical and Computer Engineering, NCSA, and the CompGen initiative at the University of Illinois at Urbana-Champaign to perform an in-depth study of performance, robustness, and scalability of the pipeline. With their involvement, we have identified the following exciting new directions that should help harden and speed up the pipeline even further:

- Investigate the possibilities of running the entire pipeline in RAM
- Investigate the benefits of converting the data streaming parts of the pipeline into a map/reduce framework
- Eliminate the bottleneck resulting from merge steps along the workflow by rewriting that step with a better, multi-threaded code

WHY BLUE WATERS

Our results are comparable to those published by other groups [1], but Blue Waters has enough nodes and disk space to actually demonstrate the scalability, as opposed to estimating it from smaller number of genomes. If hospitals begin to sequence every arriving patient, the total ongoing storage requirement would reach the petabytes scale, provided that the data are deleted immediately upon production and delivery. No other supercomputing center thus far has directly documented its ability to sustain such work.

SOCIAL SCIENCE, ECONOMICS, & HUMANITIES

146 *Benchmarking Computational Strategies for Applying Quality Scoring and Error Modeling Strategies to Extreme-Scale Text Archives*

148 *An Extreme-Scale Computational Approach to Redistricting Optimization*

150 *Policy Responses to Climate Change in a Dynamic Stochastic Economy*

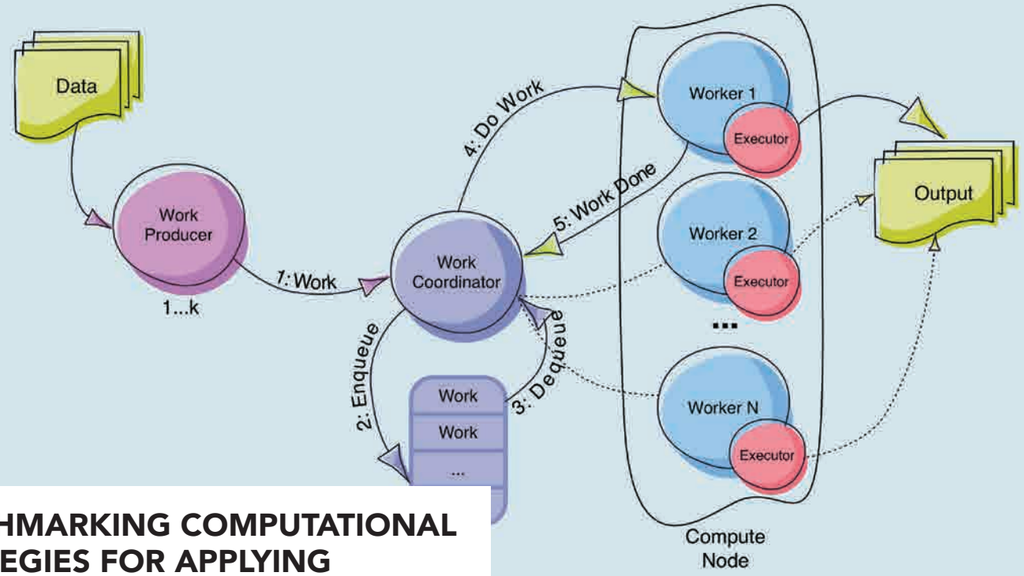


FIGURE 1: Akka framework for running share-nothing, highly parallel, distributed processing on Blue Waters.

BENCHMARKING COMPUTATIONAL STRATEGIES FOR APPLYING QUALITY SCORING AND ERROR MODELING STRATEGIES TO EXTREME-SCALE TEXT ARCHIVES

Allocation: Illinois/0.05 Mnh
PI: Scott Althaus[1]
Collaborators: Loretta Auvil[1]; Boris Capitanu[1]; David Tcheng[1]; Ted Underwood[1]

[1]University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY:

At present, the most important barrier to extreme-scale analysis of unstructured data within digitized text archives is the uncertain Optical Character Recognition (OCR) accuracy of scanned page images. We used Blue Waters to evaluate OCR errors on the HathiTrust Public Use Dataset, which is the world's largest corpus of digitized library volumes in the public domain, consisting of 3.2 million zipped files totaling nearly 3 TB. The primary aim is to develop error quality scoring strategies that can enhance the volume-level metadata managed by the HathiTrust Research Center with probabilistic quality metrics. A secondary aim is to develop a JVM distributed computing solution based on Scala and Akka for Blue Waters. Our task was to calculate a metric to indicate quality of text on each page of a given volume. An initial run took about 8 hours to score the entire dataset at a processing rate of approximately 110 volumes per second.

INTRODUCTION

Researchers in the humanities and social sciences often analyze unstructured data in the form of images and text that have been scanned and digitized from non-digital sources. For this type of research, the most important barrier to conducting extreme-scale analysis of unstructured data is the uncertain quality of the textual representations of scanned images derived from Optical Character Recognition (OCR) techniques. Only when OCR quality is high can automated analysis safely rely on natural language processing and machine learning methods to correctly extract information from unstructured data. Assessing the quality of unstructured data and developing strategies for correcting errors in such data are therefore among the most important research tasks for unlocking the potential for extreme-scale analysis of unstructured data in historical archives. Our project is using Blue Waters to detect, score, and correct OCR errors in the HathiTrust Public Use Dataset, which is the world's largest corpus of digitized library volumes in the public domain, consisting of over 1.2 billion scanned pages of OCR text.

METHODS AND RESULTS

The scale of our research problem and its embarrassingly parallel nature demanded a distributed solution. We chose to leverage Akka since it claimed to provide a high-performance JVM-based framework featuring simple concurrency and distribution.

When engineering an Akka-based solution for running in a distributed environment, the Akka cluster extension is often used because it "provides a fault-tolerant decentralized peer-to-peer based cluster membership service with no single point of failure or single point of bottleneck… using gossip protocols and an automatic failure detector" [1]. The cluster extension provides simpler coordination between distributed actors and makes it easier to adopt a "let it crash" [2] philosophy for enhancing system robustness.

Our first research prototype using this framework evaluated the OCR quality of documents from the HathiTrust corpus by tokenizing the text and examining the tokens against a set of rules defining characteristics expected of regular words (e.g., whether the tokens consist of exclusively alphabetic characters, or exhibit a "normal" character frequency distribution). Each page of the ~3.2 million volumes was scored based on two quality metrics.

Fig. 1 shows the architecture of this initial prototype framework. In this prototype we used a single Work Producer whose job was to traverse the directory structure where the documents were stored and send each document path as a work item to the Work Coordinator. The worker Executor was programmed to accept as input the document path and run the necessary analysis summarized above to produce the OCR quality score measures. Given the size of our documents and the complexity of the analysis, an initial performance evaluation of the prototype on a subset of the data showed that optimal performance was reached when using 192 to 224 workers. Beyond performance plateaued, likely due to an I/O bottleneck. We are planning several optimizations to alleviate this bottleneck.

The final run on the entire dataset was completed in 8 hours and 5 minutes and used a total of eight compute nodes. The average processing speed was about 110 documents per second.

WHY BLUE WATERS

With a corpus of this size, the computational demands of using natural language processing, machine learning, or rule-based scoring strategies would severely tax the capabilities of other HPC platforms. Only Blue Waters offers the computational scale required to carry out the necessary quality scoring and error correction strategies in a timely fashion.

FIGURE 1 (CONTINUED): Each circle represents an actor. Actors exchange messages to collaborate on a task, which in our case represents some work that needs to be performed. In general, the Work Producers take input data and package it into independent units of work to be sent to the Work Coordinator, which in turn stores those in a queue. The Work Coordinator assigns one work unit at a time to a Worker. Executing the work inside the Worker actors is done via an internal asynchronous Executor actor that allows the worker itself to remain responsive to external queries (e.g., status updates). This allows the Worker to detect and handle Executor failures that may arise from the execution of the work while remaining available to execute future work (spawning a new Executor, if necessary).

AN EXTREME-SCALE COMPUTATIONAL APPROACH TO REDISTRICTING OPTIMIZATION

Allocation: Illinois/0.6 Mnh
PI: Shaowen Wang[1,2]
Collaborators: Wendy K. Tam Cho[1,2]; Yan Liu[1,2]

[1]University of Illinois at Urbana-Champaign
[2]National Center for Supercomputing Applications

EXECUTIVE SUMMARY:

The redistricting problem, or drawing electoral maps, amounts to arranging a finite number of indivisible geographic units into a smaller number of larger areas (i.e., districts). The primary goal of our work is to develop and implement computational capabilities that can generate and objectively evaluate alternative redistricting schemes and compare them to one another based on compliance with voting laws as well as with various notions of "fairness" and adherence to democratic principles. Our approach is implemented by enhancing a scalable parallel genetic algorithm (PGA) library. The improved library has scaled well in tests on Blue Waters with minimal impact on the numerical performance of our PGA. Using massive computing power on Blue Waters, deeper understanding of the problem space and solution search strategies applied to large redistricting problems will lead to a series of innovations in the development of scalable heuristic strategies and algorithmic operations.

INTRODUCTION

The redistricting problem [1], or drawing electoral maps, amounts to arranging a finite number of indivisible geographic units into a smaller number of larger areas (i.e., districts). Redistricting [2] has attracted significant interest in political science, geographic information science, and operations research. Due to the limited computational capability of existing solutions, the study of redistricting problems at fine spatial scales (e.g., census block) has been difficult, if not impossible.

Our research proposes a scalable computational approach to address this fundamental challenge and provides an open research tool for solving fine-scale redistricting problems. The primary goal is to develop and implement computational capabilities that can generate and objectively evaluate alternative redistricting schemes and compare them to one another based on compliance with voting laws as well as with various notions of "fairness" and adherence to democratic principles. Political and geographical constraints include:

- *Competitiveness*: districts with similar proportions of different partisans, resulting in competitive elections;
- *Contiguity*: all parts of every district must be physically connected;
- *Compactness*: no overly irregular shaped districts;
- *Equi-population*: to make sure votes are as equally weighted as possible;
- *Preservation of communities of interest and local political subdivisions*: keep identifiable communities together;
- *Incumbent protection*: ensure that incumbents are not pitted against one another, which, if excessive, may disrupt the political process; and
- *Minority districts*: comply with the Voting Rights Act.

METHODS AND RESULTS

Finding an exact optimal solution to redistricting is computationally intractable. In our research, we develop a heuristic algorithm by combining attention to the idiosyncrasies of the specific redistricting problem with a genetic algorithm (GA) [3] to produce nearly optimal redistricting maps. Our computational approach considers the development of both redistricting-specific strategies to reduce the number of iterations needed to identify an optimal solution and scalable algorithms for exploiting the massive computational power provided by high-performance computing resources such as Blue Waters.

Our approach is implemented by enhancing a scalable parallel genetic algorithm (PGA) library [4] developed by the authors. The PGA library runs a large number of independent PGA processes simultaneously with a migration strategy that exchanges solutions between any two directly connected PGA processes. This library eliminates the global synchronization cost at the migration step which would increase dramatically when using a large number of processors. The library scaled up to 16,384 processors on the retired Ranger supercomputer at the Texas Advanced Computing Center.

On Blue Waters, we further improved scalability by resolving a major bottleneck in our PGA library. The original asynchronous migration strategy developed for this library scaled well on 16,000 processor cores with fine-tuned PGA parameters, but scaled poorly on a larger number of faster processors and caused MPI communication layer failure. The outgoing message buffer controlled by MPI experienced buffer overflow. We extended our library to manage the sending buffer better at the application level and explicitly specified the degree of overlap between GA iterations and message sending. The improved library has scaled well in tests on Blue Waters with minimal impact on the numerical performance of our PGA. The communication cost stayed consistently around 0.17% when the number of cores increased from 8,192 to 65,536.

Solving the redistricting problem using GA requires a series of spatial GA operators to consider the spatial distribution of political units and districts in order to satisfy explicit or implicit spatial constraints. These spatial operations are much more computationally intensive than the conventional GA operators. As a result, a new set of spatial GA operators, including initial solution generation, crossover, and mutation, is developed for redistricting. The slow-down from higher computational intensity increases as the number of processor cores involved increases. More efficient heuristic strategies for solution space searching, such as path relinking, are being considered to allow more intensified local search and diversified global search.

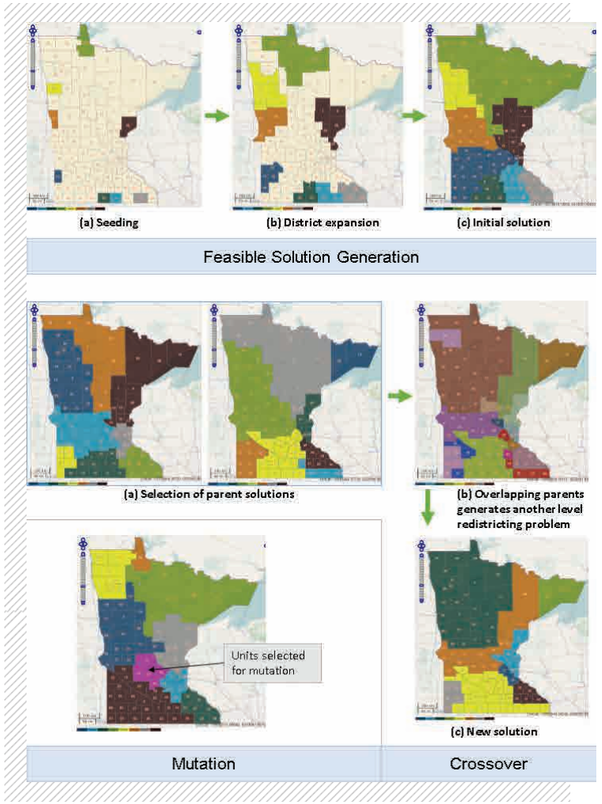


FIGURE 1: Spatial genetic algorithm (GA) operators for redistricting problem solving.

WHY BLUE WATERS

Exploiting high-performance computing resources such as Blue Waters is crucial for achieving our goal of gaining a better understanding of the redistricting process and its impact on democratic rule. For instance, dividing 55 blocks into six districts, the number of possibilities is 8.7×10^{39}, a formidable number, and the magnitude of the problem rises exponentially with the number of geographic units. Given the large number of census blocks in each state (e.g., 259,777 in Minnesota; 710,145 in California), our goal would be inconceivable given the prohibitively large sizes of these problem instances. Using massive computing power on Blue Waters, deeper understanding of the problem space and solution search strategies applied to large redistricting problems will lead to a series of innovations on the development of scalable heuristic strategies and algorithmic operations.

PUBLICATIONS

Liu, Y. Y., and S. Wang, A Scalable Parallel Genetic Algorithm for the Generalized Assignment Problem. *Parallel Comput.*, (in press).

POLICY RESPONSES TO CLIMATE CHANGE IN A DYNAMIC STOCHASTIC ECONOMY

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EXECUTIVE SUMMARY:

We developed tools for evaluating alternative policy responses to challenges posed by future climate change in models that merge uncertainties related to both economic factors and their interaction with the climate. We extended past work on computational methods for solving dynamic programming problems, dynamic games, and empirical estimation of economic models.

We have combined numerical methods for quadrature, approximation, and optimization problems to develop efficient approximations of the Bellman operator for up to 20 dimensional discrete-time dynamic programming. We have also developed methods for computing all Nash equilibria of dynamic games. Our code scales nicely up to 160,000 processes for realistic problems.

One initial substantive result is that the optimal carbon tax is three to four times larger than usually estimated when we incorporate empirically justified specifications for the social desire to reduce risk [1].

METHODS AND RESULTS

This project aims to develop tools that determine optimal policies and outcomes of competitive processes for use in economics research.

Dynamic optimization problems reduce to solving Bellman equations arising from dynamic programming problems. In general, solving Bellman equations grows rapidly in complexity as the dimension rises. However, we identified mathematical properties of a wide range of economics problems (i.e., portfolio allocation and optimal greenhouse gas mitigation) which allow us to solve high-dimensional problems. These properties concern the shape and smoothness of the solution to the Bellman equation. Smoothness allows for efficient approximation of multi-dimensional functions and efficient quadrature methods for evaluating integrals contained in the Bellman operator; concavity is a strong qualitative property that we use to stabilize the numerical procedures [2,3]. Many problems we solved have nine continuous dimensions. Only a machine with the scale of Blue Waters can solve such complex problems in reasonable time.

Solving for all Nash equilibria of dynamic games requires solving a fixed-point mapping on finite lists of convex polytopes in n-dimensional Euclidean space, where n is the number of players. Again, such problems can only be solved on Blue Waters-like machines.

These tools open up the possibility to explore dynamic optimization and dynamic strategic problems in a quantitative manner never before feasible. (Economists generally confine their games to have few moves and a small number of players, or focus on finding only one equilibrium even though they know there are many equilibria.) Our dynamic programming tools have shown that the social costs of greenhouse gases is a stochastic process with great variation, and that the appropriate policy needs to be flexible to deal with unexpected events. We have shown that the chance of needing aggressive policies is much larger than usually thought.

This is the first time that economics problems of this nature and scale have been solved. It is clear that economics problems need and can efficiently use high-power computing.

WHY BLUE WATERS

Modeling realistic dynamic stochastic economics problems requires massive computational power. Each value function iteration (or more generally, the application of a contraction mapping in a Banach space) consists of millions of nonlinear programming problems that can be solved in parallel. Our code allocates the tasks so that all cores are busy at almost all times. The Blue Waters architecture is an excellent fit for this problem.

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Blue Waters is supported by the National Science Foundation

ISBN 978-0-9908385-1-7