Special Study

An Investigation and Evaluation of the Scientific Results from the NCSA Blue Waters Supercomputer System

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IDC OPINION

In the U.S. and other developed countries, leadership-class supercomputers have played a major role in advancing science, boosting industrial competitiveness, and improving the quality of daily life for average citizens. NCSA's Blue Waters supercomputer is well known throughout the world and, as this study shows, it has enabled many impressive innovations that would not have been possible with typical, less-capable supercomputers.

During the past five years, national political leaders in the U.S., Europe, and China have recognized the ability of leadership-class supercomputers to help transform their scientific innovativeness, economies, their societies, and their understanding of the natural world.

The intent of this study was to investigate the scientific returns from research projects conducted on the Blue Waters supercomputer system at NCSA. In this study IDC, collected quantitative and qualitative information of the value of scientific work done on the Blue Waters supercomputer. In pursuit of this goal, IDC leveraged its related research work, including but not limited to the methodology we developed and the comparative data we gathered in studies for the Department of Energy on quantifying the value/impact of HPC-enabled scientific innovations. To make the research more specific to Blue Waters, IDC surveyed a set of key Blue Waters researchers on the value of Blue Waters, using a specific survey framework. In total, IDC surveyed 31 Blue Waters-supported research projects in this study. The list of the participants and their projects can be found in the appendix.

To help show the value on the innovations, IDC used a new innovation ranking scale—a modification of the scale we have been using successfully in the DOE ROI studies—that is based on two complementary rankings of innovations, combined to form an overall ranking. We believe this new innovation index provides a useful way of looking at and ranking HPC-enabled innovations around the world.

- On both the scales, IDC has used successfully in our DOE studies—ranking the importance and the impact of HPC-enabled scientific innovations—as well as on the third scale IDC developed for the present study, Blue Waters scored very high on both of these scales.
- On the combined, innovation class scale, Blue Waters-enabled innovations as a group substantially outranked IDC's global data base of scientific innovations enabled by supercomputers.

Key Observations:

- Not once during the 31 interviews IDC conducted with Blue Waters users for this study did any of them point to shortcomings of the supercomputer. On the contrary, all of the researchers had praise for the system and enthusiastically reported on the progress it has enabled for their work.
- NCSA did an unusually thorough job of preparing for Blue Waters, first and foremost by working closely with more than 20 users group for two years to identify requirements that would help determine the most appropriate architecture and configuration for the new leadership-class supercomputer. This extreme user focus contrasts sharply with the "build-it-and-they-will-come" approach some other national HPC centers take to future supercomputers. As a result of NCSA's thoroughness, Blue Waters has been exceptionally appropriate and productive for its NSF user community.
    - IDC applauds NCSA's bold decision not to optimize Blue Waters for superior performance on the narrow benchmark test used to determine rankings on the semi-annual Top500 supercomputers list.
    - If more leadership-class HPC sites resisted this political temptation, vendors would be more motivated to design HPC systems that are applicable to a broader range of user needs.
- The innovations produced so far by Blue Waters users are crucially important as a group because they constitute substantial steps forward in major disciplines—even though it's far too soon to estimate their long-term value for scientific and industrial research. It's probably safe to say that they will contribute to a series of other notable discoveries over time.
- A substantially higher percentage of the Blue Waters-enabled innovations qualified for Class 1 & 3 innovation levels, and substantially more Blue Waters-enabled innovations ranked in the top three classes than was true of IDC's global data base of innovations.

In IDC's opinion, these findings confirm that Blue Waters has proven to be an exceptionally—and in some case uniquely—competent platform for accelerating scientific innovation. The Blue Waters-enabled innovations described and ranked in this study will produce strong benefits for the scientific disciplines they belong to. They also have great potential for benefiting U.S. industry and American society as a whole over time.

EXECUTIVE SUMMARY

In order to accelerate scientific advances and economic growth, nations around the world are increasingly investing in large, leadership-class supercomputers. These computers provide a tool that can magnify researchers' capabilities and greatly improve their efficiency in conducting science. When combined with advancements in application design, big data, and top researchers, these systems have become the backbone for new scientific discoveries.

Key Findings

- Where scientific productivity is concerned (as opposed to standard benchmark tests), Blue Waters is certainly one of the top few supercomputers in the world. Blue Water's usefulness and productivity is notable in large part because NCSA worked so closely with its user community to help determine what kind of leadership-class supercomputer would best support the demanding requirements for their scientific work.
- This study confirms that the time and money invested in Blue Waters has been paying off handsomely. Not once during the 31 interviews IDC conducted with Blue Waters users for this study did any of them point to shortcomings of the supercomputer. On the contrary, all of the researchers had praise for the system and enthusiastically reported on the progress it has enabled for their work.
- IDC has seldom encountered such a diverse group of scientific researchers who all agree on something—in this case, the value of the Blue Waters supercomputer.

Surveyed experts cited a broad range of research projects for which the Blue Waters supercomputer has been critical. A few examples will suffice here—many more appear later on in this document.

- "The computational resources at Blue Waters have been instrumental in allowing our group to perform large-scale simulations which have **allowed us to study higher dimensional effects in inertial fusion plasmas**…[Our] simulations performed on Blue Waters have been published in many high impact journals, including *Nature*."
- "Blue Waters is the only place where massively parallel sparse solver technology can be tested. This exciting technology advancement will lead to a massive leap in terms of advances in design and manufacturing, and understanding the properties of the Earth subsurface to **allow a major breakthrough in oil exploration.**"
- "Our results show the potential for **substantial reduction in Ebola spread...**"
- "Newly discovered flow features identified in our simulations indicate mechanisms that may play an important role in discerning **the most devastating, tornado-producing thunderstorms**.
- "We also implemented a **new model for black hole growth**, mergers, and feedback to realistically simulate the properties of the higher mass galaxies."
- "This will be **the first systems-level simulator that targets a specific microbe (E. coli) and will be able to simulate populations of cells with a resolution ranging from individual gene concentrations to population dynamics**.

Blue Waters is the only place where massively parallel sparse solver technology can be tested.

- "We address the problem of **decision making with uncertainty in the context of climate change** that affects the world in a non-uniform manner (more warming in the polar regions)."

Leadership-class supercomputer performance features frequently mentioned in other IDC studies include the ability to:

- Handle large three-dimensional simulations
- Analyze complex physicals systems with a high degree of precision
- Perform critical calculations in real time
- Conduct advanced multiscale and multiphysics simulations
- Reduce the need for empirical testing (including animal experimentation)
- Use data sets large enough to accurately simulate physical environments with a high degree of reliability and fidelity

Benefits of a Leadership Class Supercomputer

- **New Science.** Some stressed that a more powerful system will be needed to enable new science. Areas cited as ripe for new scientific development included personalized medicine, computational astrophysics, molecular dynamics, and social simulation.
- **Improved Simulations.** Others stated that a larger system would drive even better capabilities in existing areas of computational studies, citing the benefits of a larger, more capable system to provide more accurate simulations, enhanced simulation resolution, reduced time to solution, and greater opportunities for advanced multiscale research.
- **Less Expensive Access.** A third group indicated that a larger system would allow more users to benefit from the system, thereby increasing scientific productivity and cost-effectiveness.

Measuring the Scientific Benefits from Blue Waters

World scientific leadership and innovation leadership are becoming more dependent on the use of HPC/supercomputers every year. Economic leadership increasingly directly results from a nation's or an industry's or an enterprise's application of supercomputers in innovative and productive ways. Many countries/regions (such as the U.S., Japan, China, Russia, and Europe) are putting in place plans to gain leadership in innovation and economic progress by more broadly applying HPC/supercomputing across many different research areas.

In order to better quantify the overall impact of leadership class supercomputers for scientific innovations, IDC uses a rating system that measures both the *importance* and the *impact* of each innovation in the existing data set IDC collected for prior DOE studies, plus the new Blue Waters innovations collected in this research study. The new overall innovation ranking was created based on a combination of the two complementary rankings of the innovations, in the form of 8 class levels of innovations.

Substantially more Blue Waters-enabled innovations ranked in the top three classes than was true of IDC's global data base of innovations.

IDC Observations

- NCSA is doing an excellent job serving the needs of the researchers on Blue Waters.
- NCSA did an unusually thorough job of preparing for Blue Waters, first and foremost by working closely with more than 20 users group for two years to identify requirements that would help determine the most appropriate

architecture and configuration for the new leadership-class supercomputer. This extreme user focus contrasts sharply with the "build-it-and-they-will-come" approach some other national HPC centers take to future supercomputers. As a result of NCSA's thoroughness, Blue Waters has been exceptionally appropriate and productive for its NSF user community. IDC applauds NCSA's bold decision not to optimize Blue Waters for superior performance on the narrow benchmark test used to determine rankings on the semi-annual Top500 supercomputers list. If more leadership-class HPC sites resisted this political temptation, vendors would be more motivated to design HPC systems that are applicable to a broader range of user needs.

- The innovations produced so far by Blue Waters users are crucially important as a group because they constitute substantial steps forward in major disciplines—even though it's far too soon to estimate their long-term value for scientific and industrial research. It's probably safe to say that they will contribute to a series of other notable discoveries over time.
- A substantially higher percentage of the Blue Waters-enabled innovations qualified for Class 1 & 3 innovation levels, and substantially more Blue Waters-enabled innovations ranked in the top three classes than was true of IDC's global data base of innovations.

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Methodology

The intent of this study was to investigate the scientific returns from research projects conducted on the Blue Waters supercomputer system at NCSA.

IDC assisted NCSA by gathering quantitative and qualitative information of the value of scientific work done on the Blue Waters supercomputer. In pursuit of this goal, IDC leveraged its related research work, including but not limited to the methodology we developed and the comparative data we gathered in our studies for the Department of Energy on quantifying the value/impact of HPC-enabled scientific innovations.

To make the research more specific to Blue Waters, IDC surveyed a set of key Blue Waters researchers on the value of Blue Waters, using a specific survey framework.

IDC used a new innovation ranking scale -- a modification of the scale we have been using successfully in the DOE ROI studies -- that is based on two complementary rankings of innovations, combined to form an overall ranking. We believe this new innovation index provides a useful way of looking at and ranking innovations around the world.

IDC surveyed 31 Blue Waters research projects in this study. The list of the survey participants and their projects can be found in the appendix. Their inputs were reviewed by selected members of the IDC ROI review committee, which includes:

- Paul Muzio, City University of New York
- Rupak Biswas, NASA Ames
- Vijay Agarwala, Virginia Tech.
- Swamy Akasapu, General Motors
- Alex Akkerman, Ford Motor Company
- C. Scot Atkins, Industry Expert – Advanced Analytics/Dense Supercomputing
- Doug Bail, The Boeing Company
- Jeff Broughton, NERSC/Lawrence Berkeley National Lab
- Paul Buerger, Avetec
- Clayton Chandler, Credit Suisse Group AG
- Sharan Kalwani, Fermilab
- Chris Catherasoo, California Institute of Technology
- Simon Burbidge, Imperial College London
- Jack Collins, National Cancer Institute
- Steve Finn, Emagine IT
- Keith Gray, BP
- James Kasdorf, Pittsburgh Supercomputing Center
- Arno Kolster, PayPal
- Doug Kothe, Oak Ridge National Laboratory
- Jysoo Lee, KAUST

- David Martin, Argonne National Laboratory
- Michael Resch, HLRS, University of Stuttgart
- Ryan Quick, PayPal
- Stephane Requena, GENCI
- Vince Scarafino, Industry Expert
- Suzy Tichenor, Oak Ridge National Laboratory

IDC's HPC ROI and Innovation Measuring Approach

For our studies for DOE, IDC created a set of ROI macroeconomic models to quantify the impact of investments in HPC. The models include both the financial ROI (return on investment) returns and the innovation ROR (return on research) returns from projects done on supercomputers. The results of this research for DOE are published at: www.idc.com/ROI

Our 2013 pilot ROI study for DOE investigated how high-performance computing (HPC) investments can improve economic success and increase scientific innovation. This research was focused on the common good and should be useful to all HPC centers around the world. The study created two unique economic models and an innovation index:

- A *macroeconomic model* that depicts the way HPC investments result in economic advancements in the form of ROI in revenue (GDP), profits (and cost savings), and jobs.
- A *macroeconomic model* that depicts the way HPC investments result in basic and applied innovations, looking at variations by sector, industry, country, and organization size.
- A new *innovation index* that provides a means of measuring and comparing innovation levels.

For the Blue Waters study, IDC modified our DOE study methodology as described above in the Methodology section of this report.

SITUATION OVERVIEW

The world's most powerful computers, called leadership-class supercomputers, have contributed enormously to scientific advances, national security, economic progress, and the quality of life, Leadership-class supercomputers are indispensable for many applications that are important for the societies they serve, such as the following:

- Predicting severe storms that can devastate lives and property
- Providing accurate daily/weekly weather forecasts needed by the transportation, agricultural, and tourism industries
- Better understanding fundamental scientific principles
- Improving the design and safety of power plants and developing technologies to exploit alternative energy sources
- Detecting sophisticated cyber security breaches, insider threats, and electronic fraud.
- Better understanding natural processes
- Advancing fundamental science as a prerequisite for later advancements in applied research and development, including industrial R&D

International Recognition of Supercomputing's Strategic Value

Political leaders around the world have increasingly recognized the transformational power of leadership-class supercomputers and are supporting initiatives to enable their countries to compete effectively in the worldwide race to develop future supercomputers with unprecedented speed, called "exascale" computers, in the next 5-6 years. U.S. President Obama, European Commission leaders, and Chinese leaders all have endorsed initiatives to reach this goal. Japan is the only other country with the technical ability to accomplish this. In IDC's opinion, the U.S. and Japan have the greatest experience in designing leadership-class supercomputers that are capable of supporting a broad spectrum of challenging scientific and industrial research problems.

SURVEY FINDINGS

Blue Waters Scientific Innovation Success Stories (Return on Research)

IDC surveyed 31 researchers/projects that use the Blue Waters supercomputer. Descriptions of the projects are given in the tables in this section of the report. Fuller information about these researchers and their projects appears in the appendix.

Project Titles/Research Areas

- Simulation-Based Policy Analysis to Reduce Ebola Transmission Risk in Air Travel
- Hydrogen Under Extreme Conditions
- Petascale Quantum Simulations of Nano Systems and Biomolecules
- Custom Genotyping Chip for African Populations
- Dynamic Coarse-Grained Models for Simulations of Large-Scale Biophysical Phenomena
- Instrumenting Human Variant Calling Workflow on Blue Waters
- Sensing the Environment: a Glimpse into the Microscopic Mechanisms of Pain
- Simultaneous VLBA Polarimetric Observations
- VY CMa II: Component-Level Polarization Analysis
- Unlocking the Mysteries of the Most Violent Tornadoes
- Simulating the Earliest Galaxies with Enzo and Blue Waters
- ArcticDEM a White House Initiative to Produce a High-Resolution, Time-Dependent Elevation Model of the Arctic using Blue Waters
- Petascale Particle-in-Cell Simulation of Kinetic Effects in High Energy Density Plasmas
- High Resolution Earth System Modeling Using Blue Waters Capabilities
- Advancing Genome-Scale Phylogenomic Analysis
- Nuclear-Electronic Orbital Calculations on Molecular Systems
- Particle Tracking and Turbulent Dispersion at High Reynolds Number on Blue Waters
- Evolution of the Small Galaxy Population from High Redshift to the Present
- Quantum-classical Path Integral Simulations of Ferrocene-Ferrocenium Charge Transfer in Solution
- Policy Responses to Climate Change in a Dynamic Stochastic Economy
- Advanced Nanoelectronic Device Design with Atomistic Simulations
- Modeling Heliophysics and Astrophysics Phenomena with a Multi-Scale Fluid-Kinetic Simulation Suite
- Big Data on Small Organisms: Petascale Simulations of Data-driven, Whole-cell Microbial Models
- Direct Numerical Simulation of Fully Resolved Vaporizing Droplets in a Turbulent Flow
- Sparse Matrix Factorization In Solid Mechanics And Geophysics on CPUs and GPUs
- Core-Collapse Supernovae through Cosmic Time

- Location- Specific Space Weather Hazard to Electric Power Grids Calculated on a Global Scale
- Ensembles of Molecular Dynamics Engines for Assessing Force Fields, Conformational Change, and Free Energies of Proteins and Nucleic Acids
- Lattice QCD
- Predicting Protein Structures with Physical Petascale Molecular Simulations

Blue Waters Scientific Successes by Innovation Area

IDC sorted the Blue Waters scientific innovations into six high-level categories that our research experience tells us are better suited to communicating value to non-technical audiences. (Note: With fundamental science innovations such as these, it is sometimes difficult to limit their potential impact to a single category, so some of these advances might just as well have been placed in a different category.)

1. Better Products
2. Major Scientific Breakthrough
3. Cost Saving
4. Created New Approach
5. Discovered Something New
6. Helped Society

Blue Waters Successes: Supporting Better Future Products

The five project examples described in Table 1 involved innovations with strong potential to enable companies to produce better future products in a range of industries and market sectors, including:

- Electronics
- Medicine/health care
- Geospatial mapping
- Fusion energy
- Oil and gas

Key Quotes

"**The computational resources at Blue Waters have been instrumental in allowing our group to perform large-scale simulations which have allowed us to study higher dimensional effects in inertial fusion plasmas**, and to make quantitative comparisons between simulations and experiments in plasma-based accelerator. In 2015, simulations performed on Blue Waters have been published in many high impact journals, including *Nature*."

"Blue Waters is the only place where massively parallel sparse solver technology such as WSMP can be tested. This exciting technology advancement will lead to a massive leap in terms of advances in design and manufacturing, and understanding the properties of the Earth subsurface to **allow a major breakthrough in oil exploration.**"

Table 1

Blue Waters Scientific Successes: Supporting Better Future Products

Project Title	Project Description
Petascale Quantum Simulations of Nano Systems and Biomolecules	This project builds on a set of open-source petascale quantum simulation tools being developed via the PetaApps program; these tools enable quantum simulations of unprecedented size in the broad area of nanoscience and nanotechnology. The goals of this project are to radically advance the fundamental understanding of key nanoscale phenomena and processes in the following areas: (i) graphene-based electronics, which will likely form the basis for new generations of ultrafast, ultradense electronic circuitry, (ii) catalytic growth of carbon nanotubes, aiming at discovering the catalysts and conditions that would lead to controlled growth of carbon nanotubes with desired electronic properties, (iii) DNA-based sensor structures for detection of DNA damage, and (iv) metal-induced accelerated onset of Alzheimer's disease.
ArcticDEM a White House initiative to produce a high-resolution, time-dependent elevation model of the Arctic using Blue Waters	Last summer, President Obama announced that a complete DEM of the Arctic will be completed by next year. The ArcticDEM will be a continous, 8m and then 2m DEM mosaic of all land masses above 60 degrees North (above the latitude of SRTM), constructed from DigitalGlobe Inc. satellite imagery. SETSM is the primary software for DEM extraction for ArcticDEM and we have been working feverishly to ramp up data processing on the Blue Waters Supercomputer while simultaneously continuing SETSM development and post-processing, mosaicking and registration methods. Nearly all of Alaska, Greenland, Scandanavia and large parts of Russia and Canada have already been processed to 8m. This enables data filtering and algorithm development. Once complete, the resolution will be increased to 2m for the final product.
Petascale Particle-in-Cell Simulation of Kinetic Effects in High Energy Density Plasmas	The UCLA Simulation Group has been on the frontier of high performance kinetic simulation of plasmas since its early days with its founder John Dawson. Over the subsequent 40+ years, the group has developed a full suite of codes (with various models for fields and particles) to study kinetic effects in plasmas for a variety of applications, including plasma-based accelerators, laser fusion, and basic plasma physics. The computational resources at Blue Waters have been instrumental in allowing our group to perform large-scale simulations which have allowed us to study higher dimensional effects in inertial fusion plasmas, and to make quantitative comparisons between simulations and experiments in plasma-based accelerator. In 2015, simulations performed on Blue Waters have been published in many high impact journals, including Nature. These simulation results and our code development efforts, including the latest timing results on GPU's and the Intel Xeon Phi processors, will be presented.
Advanced Nanoelectronic Device Design with Atomistic Simulations	Advanced Nanoelectronic Device Design with Atomistic Simulations
Sparse Matrix Factorization in Solid Mechanics And Geophysics on CPUs and GPUs	Sparse matrix factorization is a critical algorithm in many science, engineering, and optimization applications. The performance of the massively parallel direct multi-frontal solver Watson Sparse Matrix Package (WSMP) for solving large sparse systems of linear equations arising in an implicit finite element method in solid mechanics and an inversion problem in geophysics was evaluated on Blue Waters and achieved new records in sparse matrix factorizations. We performed fullscale benchmarking tests up to 65,536 cores (100 Tflop/s) on XE6 nodes using assembled global stiffness matrices and load vectors with 5 million to 40 million unknowns. Blue Waters is the only place where

Table 1

Blue Waters Scientific Successes: Supporting Better Future Products

Project Title	Project Description
	massively parallel sparse solver technology such as WSMP can be tested. This exciting technology advancement will lead to a massive leap in terms of advances in design and manufacturing, and understanding the properties of the Earth subsurface to allow a major breakthrough in oil exploration.

Source: IDC 2016

Blue Waters Successes: Major Scientific Breakthroughs

The project examples described in Table 2 involved scientific innovations with strong potential to benefit society at large and deepen human understanding of the natural world in the following areas and others:

- Epidemic diseases
- Bacteriology
- Severe weather prediction
- Cosmology
- Space exploration
- Air travel (wind shear)

Key Quotes

"Our results show the potential for **substantial reduction in Ebola spread** by changing current [aircraft] boarding and disembarkation procedures. This approach leads to high computational cost, which is handled through massive parallelization on Blue Waters."

Our results show the potential for substantial reduction in Ebola spread

"[The project involves] the application of CG models and software to the study of model systems such as **the nucleation and growth of the HIV-1 capsid protein lattice**…with specific emphasis placed on the use of the Blue Waters platform."

"Newly discovered flow features identified in our simulations indicate mechanisms that may play an important role in discerning **the most devastating, tornado-producing thunderstorms** from those that are much more common and less destructive.

"Further progress was made concerning **tropical cyclone behavior**."

"A substantial algorithmic change in the interpolation of fluid particle velocities on a distributed domain has led to a **dramatic improvement in the scalability of the particle tracking algorithm at 262,144 cores**. We present a number of important results, such as the Lagrangian acceleration autocorrelation, and the scaling of velocity increment statistics conditioned upon the dissipation rate."

"We also implemented a **new model for black hole growth**, mergers, and feedback to realistically simulate the properties of the higher mass galaxies."

"This will be **the first systems-level simulator that targets a specific microbe (E. coli) and will be able to simulate populations of cells with a resolution ranging from individual gene concentrations to population dynamic**s. The Blue Waters Supercomputer with its unique architecture, large-scale simulation capabilities and professional support staff provides the ideal platform to achieve this ambitious goal."

Table 2

Blue Waters Scientific Success: Major Scientific Breakthroughs

Project Title	Project Description
Simulation-Based Policy Analysis to Reduce Ebola Transmission Risk in Air Travel	Air travel is a major cause of the spread of infections. This led to calls for ban on air travel during the recent Ebola outbreak. However, such bans have serious human and economic consequences. Our project is identifying policies and procedures that can provide the same benefit without the negative consequences. This is accomplished using a fine-scale model that tracks individual passenger movement in airplanes. Inherent uncertainties in human behavior make it difficult to accurately predict the consequences of any particular policy choice. Instead, it is more fruitful to determine vulnerabilities under a variety of possible scenarios. We parameterize the sources of uncertainty and perform simulations to cover the range of uncertainties. This approach leads to high computational cost, which is handled through massive parallelization on Blue Waters. Our results show potential for substantial reduction in Ebola spread by changing current boarding and disembarkation procedures.
Dynamic Coarse-Grained Models for Simulations of Large-Scale Biophysical Phenomena	Atomic-resolution computer simulations can provide highly detailed information about biomolecular systems, but are restricted to time- and length-scales that may be insufficient for the study of certain biological phenomena. One alternative technique is the use of “coarse-grained” (CG) models, where degrees of freedom are removed to generate simpler molecular representations while retaining the essential characteristics of the detailed system. Due to their computational efficiency, coarse-grained models provide an appealing tool for the study of relatively large-scale biomolecular phenomena. The application of CG models and software to the study of model systems such as the nucleation and growth of HIV-1 capsid protein lattice will be discussed, with specific emphasis placed on the use of the Blue Waters platform.
Unlocking the Mysteries of the Most Violent Tornadoes	Devastating, long-lived tornadoes are rare, but the death and destruction they cause is significant. We reviewed nearly four years of our work on Blue Waters, focusing on recent supercell thunderstorm simulations in which long-lived, violent tornadoes occur. Newly discovered flow features identified in our simulations indicate mechanisms that may play an important role in discerning the most devastating, tornado-producing thunderstorms from those that are much more common and less destructive. Recent simulations run with 20-meter isotropic grid spacing reveal the internal structure of a long-lived, devastating tornado, which undergoes morphological transitions from a narrow, single-celled tornado to a wide, multiple-vortex tornado.
High Resolution Earth System Modeling Using Blue Waters Capabilities	This project addresses uncertainties associated with numerical modeling of Earth’s climate system and with modeled present and future climate change by conducting high-resolution simulations with the Community Earth System Model (CESM). Pushing model resolution, our group is conducting the first-of-its-kind simulations including the fully-coupled ¼° atm/lnd coupled to the 1° ocn/ice configuration and the fully-coupled ¼° atm/lnd coupled to a 1/10° ocn/ice RCP8.5 scenarios. The former set is used to assess climate sensitivity, 20th Century climate changes, and future climate changes while the latter simulation allows exploration of very high resolution impacts on regional features and climate change processes.

Table 2

Blue Waters Scientific Success: Major Scientific Breakthroughs

Project Title	Project Description
Nuclear-Electronic Orbital Calculations on Molecular Systems	The nuclear-electronic orbital (NEO) method treats electrons and select nuclei quantum mechanically on the same level using an orbital-based formalism with the goal of obtaining a computationally tractable method that includes non-Born-Oppenheimer effects as well as nuclear quantum effects. The NEO method is ideal for studying chemical phenomena such as proton-coupled electron transfer (PCET) because the timescale for proton tunneling is often faster than the timescale for electronic transitions, thereby leading to a breakdown of the Born-Oppenheimer approximation. In applications of the NEO method to PCET, all electrons and one or a few protons are treated quantum mechanically, and a mixed nuclear-electronic time-independent Schrödinger equation is solved using explicitly correlated wavefunctions. Recent advances to the NEO method involving wavefunction and density functional theory will be discussed and benchmarking calculations on small molecules for basis sets will be presented.
Particle tracking and turbulent dispersion at high Reynolds number on Blue Waters	As reported last year, a half-trillion-grid points simulation of turbulence performed on Blue Waters has provided clear evidence of extreme events where local measures of the deformation and rotation of local fluid elements are much stronger than and have topological properties different from previously thought. In this talk we focus on turbulent dispersion at high Reynolds number in the Lagrangian reference frame of an observer moving with the flow. A substantial algorithmic change in the interpolation of fluid particle velocities on a distributed domain has led to a dramatic improvement in the scalability of the particle tracking algorithm at 262,144 cores. We present a number of important results, such as the Lagrangian acceleration autocorrelation, and the scaling of velocity increment statistics conditioned upon the dissipation rate. Particle pair trajectories are also followed both forward and backward in time, which provide unique insights for the physics of enhanced mixing in turbulence.
Evolution of the small galaxy population from high redshift to the present	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 is undertaking this modelling with the specific goal of interpreting Hubble Space Telescope observations of high redshift galaxies. To do this modelling, we are using the highly scalable N-body/Smooth Particle Hydrodynamics code, ChaNGa, based on the Charm++ runtime system on Blue Waters to perform a simulation of a 25 Mpc cubed volume of the Universe with a physically motivated star formation/supernovae feedback model. We also implemented a new model for black hole growth, mergers, and feedback to realistically simulate the properties of the higher mass galaxies.
Modeling Heliophysics Phenomena With A Multi-Scale Fluid-Kinetic Simulations Suite	The investigated physical phenomena occurring when the solar winds (SW) interacts with the local interstellar medium (LISM). These problems include (1) issues related to the mixing of the SW and LISM plasma at the heliopause (the boundary of the heliosphere, the spherical region around the Sun that is filled with solar magnetic fields and the outward-moving solar wind consisting of protons and electrons) in particular due to the heliosphere instability and magnetic reconnection at its surface; (2) the influence of the heliosphere on the observed anisotropy of teraelectronvolt (TeV) galactic cosmic rays; (3) the dynamic effect of non-thermal ions, and (4) the influence of time-dependent phenomena on the energetic neutral atom flux observed by the Interstellar Boundary Explorer (IBEX) space mission.
Big Data on Small Organisms: Petascale Simulations of Data-driven,	This project aims to develop the next-generation of genome-scale, data-driven models for microbial organisms. The project first focuses on the most-studied microbe, the gram-negative bacterium Escherichia coli. Accurate prediction of microbial fitness and cellular state can have profound implications to the way we test hypotheses that are directly related to health, social or economic benefits. This will be a boon for the development and training of the next generation of data-driven predictive methods in molecular and cellular biology. This will be the first systems-level simulator that

Table 2

Blue Waters Scientific Success: Major Scientific Breakthroughs

Project Title	Project Description
Whole-cell Microbial Models	targets a specific microbe (E. coli) and will be able to simulate populations of cells with a resolution ranging from individual gene concentrations to population dynamics. The Blue Waters Supercomputer with its unique architecture, large-scale simulation capabilities and professional support staff provides the ideal platform to achieve this ambitious goal.
Direct Numerical Simulation of Fully Resolved Vaporizing Droplets in a Turbulent Flow	This numerical study employs direct numerical simulations (DNS) to examine the two-way interactions between freely moving vaporizing droplets and isotropic turbulence. The droplets are fully resolved in 3-D space and time, i.e., not treated as point particles, and all the scales of the turbulent motion are resolved down to the smallest relevant length- and time-scales (the Kolmogorov scales). The emphasis is on the two-way exchange of mass, momentum, and energy between the vaporizing droplets and surrounding turbulent gas. The turbulence is assumed to be isotropic as a first step before considering turbulent shear flows in future studies.
Core-Collapse Supernovae Through Cosmic Time	We study the explosive deaths of massive stars, supernovae, and their contribution to the evolution of the elemental content of the universe. Core-collapse supernovae (CCSNe) are tightly coupled multi-physics events without natural symmetry and require physically and spatially detailed 3D simulations to resolve. The progenitor stars of CCSNe vary in mass, heavy element composition, rotation, and other parameters that affect how the explosion develops, or if it develops at all, and the elemental abundances of the ejecta. Over the course of our project we will compute CCSN models that broadly cover the range of masses and compositions representative of massive stars throughout the history of the universe. In prelude to that survey, we are conducting studies with Blue Waters that will assess the impact of spatial resolution on our simulations.

Source: IDC 2016

Blue Waters Successes: Cost Savings

The project examples described in Table 3 involved scientific innovations with strong potential to benefit broad areas of science and later on to reduce R&D costs for industry in areas including (but not limited to) the following:

- Pharmaceuticals
- Applied biology
- Electronics

Key Quotes

"Harnessing the computation capabilities of Blue Waters, **we explored several pathways of activation [for novel analgesics]** and characterized ion channel conductance and selectivity. Our calculations reveal a novel mechanism for sensing temperature and osmolarity."

"[Our] **new method (HIP-HOP) for classifying sequences into gene families**…substantially improves the accuracy compared to all current alternative methods (including BLAST). [Our version of BAli-Phy] shows scalability to 10,000 sequences, whereas the original implementation could only analyze about 100 sequences.

Table 3

Blue Waters Scientific Successes: Cost Savings

Cost Savings	
Project Title	Project Description
Sensing the environment: a glimpse into the microscopic mechanisms of pain	TRP channels are central to environmental sensation in animals, fungi, and unicellular eukaryotes. Clarifying how TRP channels convert physical and chemical stimuli from the environment into the allosteric signals underlying channel activation is key to understanding how they control cell excitability in both physiological and pathological conditions. Their relevance in the molecular pathways mediating pain makes them promising targets of novel classes of analgesics. Building on the structural information made recently available for TRPV1 thanks to a series of cryo-microsopy experiments, we performed free energy (metadynamics) simulations on models of TRPV1 embedded in a lipid bilayer. Harnessing the computation capabilities of Blue Waters, we explored several pathways of activation and characterized ion channel conductance and selectivity. Our calculations reveal a novel mechanism for sensing temperature and osmolarity.
Advancing Genome-Scale Phylogenomic Analysis	Research Highlights: 1. Scalable versions of BAli-Phy (3), a Bayesian method for statistical co-estimation of multiple sequence alignments and trees so that they can analyze large datasets (our current implementations show scalability to 10,000 sequences, whereas the original implementation could only analyze about 100 sequences). 2. A new method (HIP-HOP) for classifying sequences into gene families, that substantially improves the accuracy compared to all current alternative methods (including BLAST (1)). 3. New supertree methods with improved accuracy and scalability that will enable the development of divide- and-conquer methods for estimating large phylogenetic trees.
Quantum-classical path integral simulations of ferrocene-ferrocenium charge transfer in solution	Condensed phase electron transfer reactions play a vital role in most biological and synthetic energy transfer pathways. The costs of quantum mechanical calculations scale exponentially with system size; thus, performing highly accurate simulations of realistic condensed phase reactions is notoriously demanding. Quantum-classical path integral (QCPI) is a recently developed highly parallelizable methodology designed to efficiently and accurately simulate the dynamics of a quantum system immersed in a condensed phase environment. It combines a classical treatment of the environment with a path integral representation of the system. The local nature of the quantum paths allows for the system-solvent interaction to be treated exactly, free of approximation. Using Blue Waters' resources, we utilized QCPI to simulate the charge transfer process of the ferrocene-ferrocenium pair in solution with unprecedented accuracy.

Source: IDC 2016

Blue Waters Successes: Creating New Approaches

The project examples described in Table 4 involved innovations that created new and better approaches to scientific investigation in the following domains:

- Astronomy/astrophysics
- Cosmology

- Economic impacts of climate change policy

Key Quotes

"We developed new Quantum Monte Carlo simulation methods to [support] understanding [of] the giant planets, Jupiter and Saturn. However, the observations [from our two experiments] do not agree with each other, **This motivated us to repeat our earlier calculations on Blue Waters**."

"Accurately modeling the **formation and evolution of galaxies over the lifetime of the universe** presents tremendous technical challenges. [We] present simulations (and accompanying published results) that the Enzo collaboration has recently done on the Blue Waters supercomputer."

"We address the problem of **decision making with uncertainty in the context of climate change** that affects the world in a non-uniform manner (more warming in the polar regions)."

Table 4

Blue Waters Scientific Successes: Creating New Approaches

Project Title	Project Description
Hydrogen Under Extreme Conditions	The properties of hydrogen and helium are important for understanding the giant planets, Jupiter and Saturn, but experiments under the relevant conditions are challenging. We have developed new Quantum Monte Carlo simulation methods to treat such systems and using them, have studied molecular dissociation in liquid hydrogen and have observed clear evidence of an extra liquid-liquid phase transition. During the past year, two experiments have reported observations of the transition we predicted, however, the observations do not agree with each other, differing in pressure by a factor of two. This motivated us to repeat our earlier calculations on Blue Waters. It is essential for progress in the high pressure community to resolve the difference between the experiments and computation. After validation, the method can be used with more confidence in modeling the wide variety of astrophysical objects being observed, composed largely of hydrogen and helium under extreme conditions.
Simulating the Earliest Galaxies with Enzo and Blue Waters	Galaxies are complex - many physical processes operate simultaneously, and over a huge range of scales in space and time. As a result, accurately modeling the formation and evolution of galaxies over the lifetime of the universe presents tremendous technical challenges. In this talk I will describe some of the important unanswered questions regarding galaxy formation, discuss in general terms how we simulate the formation of galaxies on a computer, and present simulations (and accompanying published results) that the Enzo collaboration has recently done on the Blue Waters supercomputer. In particular, I will focus on the transition from metal-free to metal-enriched star formation in the universe, as well as the luminosity function of the earliest generations of galaxies and how we might observe it with the upcoming James Webb Space Telescope.
Policy Responses to Climate Change in a Dynamic Stochastic Economy	We extend our Integrated Assessment Model framework, called DSICE (Dynamic Stochastic Integration of Climate and the Economy), for evaluating alternative policy responses to future climate change under both economic and climate uncertainty. We incorporate five interacting climate tipping points into DSICE, and find that the present social cost of carbon (SCC) increases nearly eightfold. Moreover, passing some tipping points increases the likelihood of other tipping points occurring, so that the SCC increases abruptly. The optimal mitigation policy requires zero industrial emission after this midcentury and leads to a path of global average temperature less than 1.5 degree Celsius. We also examine the impact of Bayesian learning of uncertain critical parameters (e.g., climate sensitivity) to decision rules. Furthermore, we address the problem of decision making with uncertainty in the context of climate change that affects the world in a non-uniform manner (more warming in the polar

Table 4

Blue Waters Scientific Successes: Creating New Approaches

Project Title	Project Description
	regions).

Source: IDC 2016

Blue Waters Successes: Discovered Something New

The project examples described in Table 5 involved innovations centered on new discoveries in the following domains:

- Biology

Key Quotes

"No MD [molecular dynamics] simulation can yet fold a protein larger than around 120 amino acids. But most biologically important proteins are bigger. With this Blue Water allocation, we hope to **achieve the computational folding of larger proteins…that can tell some of biology's most interesting stories**."

Table 5

Blue Waters Scientific Successes: Discovered Something New

Project Title	Project Description
Simulating the Earliest Galaxies with Enzo and Blue Waters	Galaxies are complex - many physical processes operate simultaneously, and over a huge range of scales in space and time. As a result, accurately modeling the formation and evolution of galaxies over the lifetime of the universe presents tremendous technical challenges. In this talk I will describe some of the important unanswered questions regarding galaxy formation, discuss in general terms how we simulate the formation of galaxies on a computer, and present simulations (and accompanying published results) that the Enzo collaboration has recently done on the Blue Waters supercomputer. In particular, I will focus on the transition from metal-free to metal-enriched star formation in the universe, as well as the luminosity function of the earliest generations of galaxies and how we might observe it with the upcoming James Webb Space Telescope.
Policy Responses to Climate Change in a Dynamic Stochastic Economy	We extend our Integrated Assessment Model framework, called DSICE (Dynamic Stochastic Integration of Climate and the Economy), for evaluating alternative policy responses to future climate change under both economic and climate uncertainty. We incorporate five interacting climate tipping points into DSICE, and find that the present social cost of carbon (SCC) increases nearly eightfold. Moreover, passing some tipping points increases the likelihood of other tipping points occurring, so that the SCC increases abruptly. The optimal mitigation policy requires zero industrial emission after this midcentury and leads to a path of global average temperature less than 1.5 degree Celsius. We also examine the impact of Bayesian learning of uncertain critical parameters (e.g., climate sensitivity) to decision rules. Furthermore, we address the problem of decision making with uncertainty in the context of climate change that affects the world in a non-uniform manner (more warming in the polar regions).

Table 5

Blue Waters Scientific Successes: Discovered Something New

Project Title	Project Description
Direct Simulation Of Dispersed Liquid Droplets In Isotropic Turbulence	The objective of our research is to enhance understanding of the two-way interactions 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. A DNS of single phase isotropic turbulence at Reynolds number 300 requires a grid of 2,0483 mesh points, and about 12 hours on 65,536 processors to cover seven large eddy turnover times. Given the requirements outlined above, Blue Waters is a necessary tool for our research.
Ensembles of Molecular Dynamics Engines for Assessing Force Fields, Conformational Change, and Free Energies of Proteins and Nucleic Acids	This project uses computer simulation methods within the AMBER to simulate the atomic motions of proteins and nucleic acids in their native environment to better understand the structure, dynamics and interactions among various bio-molecules. Preliminary work on the Blue Waters Supercomputer has demonstrated reproducible and complete sampling of the conformational distributions of RNA tetranucleotides, tetraloop RNA structures, and also the internal portion of a B-DNA helix. With complete sampling, it is now possible to reliably assess, validate, and improve the applied force fields. Preliminary simulations on Blue Waters, reducing times to solution from months-years to days-weeks, show that although it is possible to converge the conformational distributions of nucleic acids like RNA tetranucleotides and tetraloops, one does not find conformational distributions that completely agree with experiments.
Lattice QCD	Calculations of QCD must support large experimental programs in high energy and nuclear physics. QCD is a strongly coupled, nonlinear quantum field theory; lattice QCD is a first principles calculation tool that requires large scale computer power. A central goal of nuclear physics is to predict new bound states of quarks, properties of glue balls and exotic states that are not predicted by quark models.
Predicting Protein Structures with Physical Petascale Molecular Simulations	We have a new computational method (MELD) for predicting protein structures. Unlike others, it is based on physics of atomic interactions. The power of physical methods is that they help us understand how proteins perform their biological actions as catalysts, motors, pumps, transporters and transducers of energy and light. In the past, physics-based structure prediction was much too computationally costly. Our work with MELD so far has shown that we can use atomistic molecular dynamics to fold 15 out of 20 small proteins to their correct native structures, and to fold 3 small proteins with very high accuracy. No MD simulation can yet fold a protein larger than around 120 amino acids. But, most biologically important proteins are bigger. With this Blue Water allocation, we hope to achieve the computational folding of larger proteins. With Blue Waters' GPU resources, we hope to bring the power of atomistic MD to folding and mechanisms that can tell some of biology's most interesting stories.

Source: IDC 2016

Blue Waters Successes: Helped Society

The project examples described in Table 6 involved innovations centered on new discoveries in the following domains:

- Ethnology
- Biology/Medicine
- Weather

Key Quotes

"This computational project aimed to produce genomic variant calls for the design of a cost-effective genotyping chip that would **capture the genetic diversity in populations of African origin**, including African-Americans… We also demonstrated, in a production-grade project, the capability of Blue Waters to **conduct high-throughput analysis of human genomes**."

"If **whole genome sequencing and analysis** become part of the standard of care in many hospitals within the next few years, then human genetic variant calling will need to be performed on hundreds of incoming patients on any given day… We [are investigating] the kinds of computational bottlenecks that can be expected, as well as the tools and methods to overcome them."

"The historical record suggest that extreme space weather is likely to impact the Earth again in the future…We are…[calculating] location specific **space weather hazards to electric power grids**. Blue Waters permits us to account for the Earth's topography, oceans, variable composition of the lithosphere as well as variable ionospheric composition and source conditions according to time, altitude, and position around the globe."

Table 6

Blue Waters Scientific Success

Project Title	Project Description
Custom Genotyping Chip for African Populations	This computational project aimed to produce genomic variant calls for the design of a cost-effective genotyping chip that would capture the genetic diversity in populations of African origin, including African-Americans. This work will enable the identification of genetic variation specific to African populations, which will help better understand the links between genotype and disease in people of African origin, and thus extend the principles of personalized medicine to these underserved populations. It will also permit deeper study of African genetic diversity, which will bring important insights into the history and evolution of humans in general. We also demonstrated, in a production-grade project, the capability of Blue Waters to conduct high-throughput analysis of human genomes. Lots of benchmarking data were collected, and the computational workflow was hardened with many quality control steps to ensure delivery of correct results. The code is posted on GitHub, to be shared with the community.
Instrumenting Human Variant Calling Workflow on Blue Waters	High throughput Human Variant Calling Workflow on BlueWaters. If whole genome sequencing and analysis become part of the standard of care in many hospitals within the next few years, then human genetic variant calling will need to be performed on hundreds of incoming patients on any given day. At this scale, the standard workflow widely accepted in the research and medical community, will use thousands of nodes at a time and have I/O bottlenecks that could affect performance even on a major cluster like BlueWaters.
Location- Specific Space Weather Hazard to Electric Power Grids Calculated on a	The historical record suggest that extreme space weather is likely to impact the Earth again in the future. However, modern electrotechnologies will be affected by space weather to a much larger degree than in the past. We are using a global Maxwell's equation model of the Earthionoshere waveguide to calculate location specific space weather hazards to electric power grids. Specifically, we are calculating and analyzing electromagnetic field behavior during recent geomagnetic storm in

Table 6

Blue Waters Scientific Success

Project Title	Project Description
Global Scale	March 2015. Blue Waters permits us to account for the Earth's topography, oceans, variable composition of the lithosphere as well as variable ionospheric composition and source conditions according to time, altitude, and position around the globe. Blue Waters also allows us to calculate and analyze ground-level electromagnetic fields spans over time-spans of hours over microsecond time resolution (as required by algorithm).

Source: IDC 2016

The Innovation Metrics Used In the Study

In order to better quantify the overall impact of leadership class supercomputers for scientific innovations, IDC uses a rating system that measured both the *importance* and the *impact* of each innovation in the existing data set, plus the new Blue Waters innovations collected in this research study. The new overall innovation ranking was created based on a combination of the two complementary rankings of the innovations:

1) The IMPORTANCE this innovation compared to all other innovations in this field over the last ten years:

5. One of the top 2 to 3 innovations in the last decade

4. One of the top 5 innovations in the last decade

3. One of the top 10 innovations in the last decade

2. One of the top 25 innovations in the last decade

1. One of the top 50 innovations in the last decade

2) The IMPACT of this innovation to multiple organizations:

5. An innovation that is useful to over 10 organizations

4. An innovation that is useful to 6 to 10 organizations

3. An innovation useful to 2 to 5 organizations

2. An innovation only useful to 1 organization

1. An innovation that is recognized ONLY by experts in the field

3) Combing these measures, IDC's used these overall innovation ratings for this project:

- Class 1 innovations – One of the top 2-3 innovations in a field over the last ten years PLUS useful to over 10 organizations
- Class 2 innovations -- One of the top 5 innovations in a field over the last ten years PLUS useful to over 10 organizations
- Class 3 innovations – One of the top 5 innovations in a field over the last ten years PLUS useful to at least 5 organizations
- Class 4 innovations – One of the top 10 innovations in a field over the last ten years PLUS useful to at least 5 organizations
- Class 5 innovations – One of the top 25 innovations in a field over the last ten years PLUS useful to at over 10 organizations
- Class 6 innovations – One of the top 25 innovations in a field over the last ten years PLUS useful to at least 2 organizations

- Class 7 innovations – One of the top 50 innovations in a field over the last ten years PLUS useful to at least 2 organizations
- Class 8 innovations – innovations that are typically only useful to one organization and/or are minor innovations in a given research field

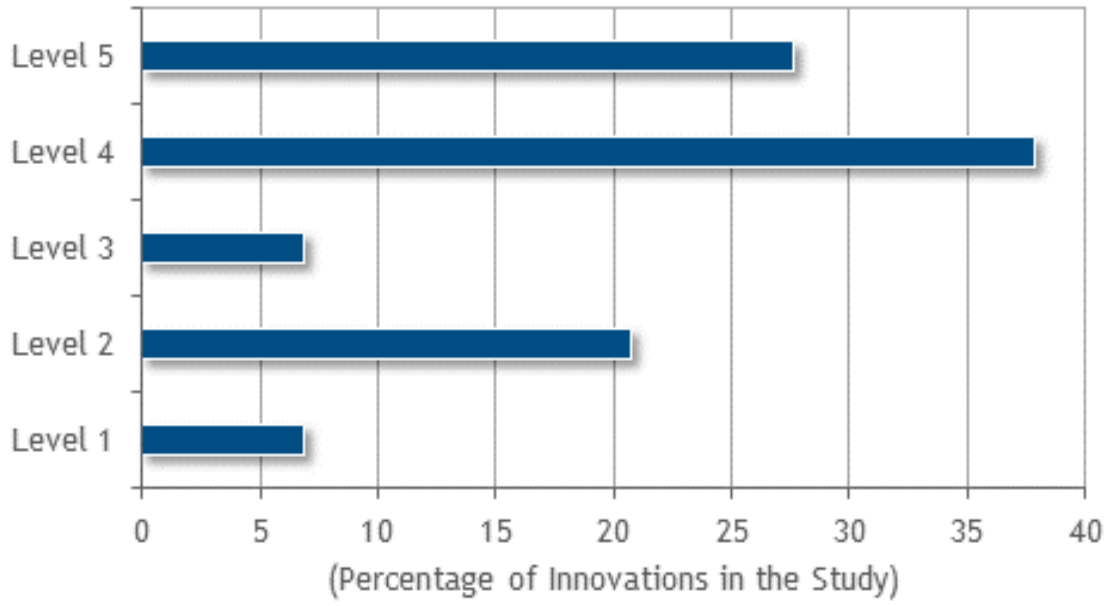
Blue Waters Innovation Rankings

Innovation Importance Levels

Figure 1 shows the scale of innovation importance (explained above), where level 5 is most important and level 1 least important. As the figure indicates, many of the innovations enabled by Blue Waters were in the high-importance levels 4 and 5 categories.

FIGURE 1

Blue Water Innovations: Innovation Importance Levels



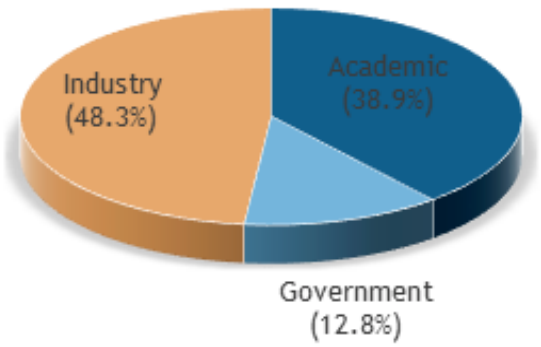
Source: IDC 2016

Innovation Importance Levels: Compared to Worldwide Averages

The profile of the worldwide sites in this study shown in Figures 2 and 3, and in Table 7.

FIGURE 2

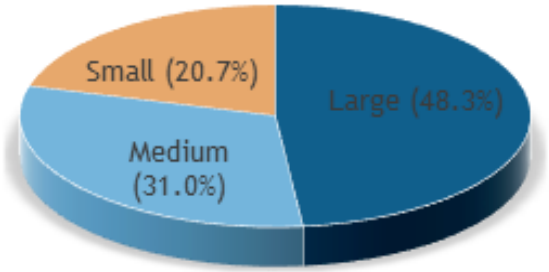
Profile of Worldwide Participants in the Study: By Sector



Source: IDC 2016

FIGURE 3

Profile of Worldwide Participants in the Study: By Size



Source: IDC 2016

Table 7

Mix Profiles of Worldwide participants in the Study

Sector	Organization Size	Count of Applied Innovations	Count of Basic Innovations	Total Number of Innovations
Academic	Large	20	10	30
	Medium	4	31	35
	Small	8	6	14
Academic Total		32	47	79
Government	Large	5	5	10
	Medium	2	3	5
	Small	5	6	11
Government Total		12	14	26
Industry	Large	48	10	58
	Medium	17	6	23
	Small	15	2	17
Industry Total		80	18	98
Grand Total		124	79	203

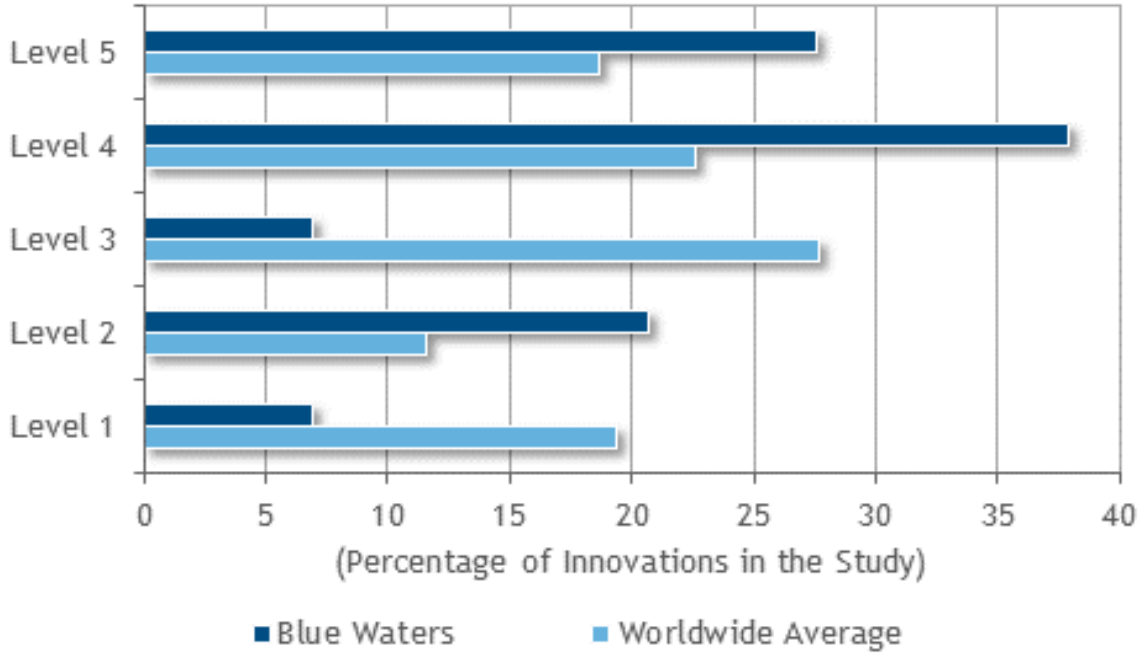
Source: IDC 2016

Figure 4 compares the importance of the scientific innovations enabled by Blue Waters with a global collection of examples IDC assembled for our DOE research studies. Compared to all worldwide sites, a significantly higher percentage of the Blue Waters-enabled innovations fell into the top two levels of importance, and far fewer Blue Waters innovations fell into the level 1 category of least importance.

Comparisons are also shown for all US innovations, and for US academic only innovations. Looking at the top two rating categories, Blue Waters is similar to other US academic sites. And way fewer Blue waters innovations are in the level 1 category.

FIGURE 4

Blue Water Innovations: Innovation Importance Levels



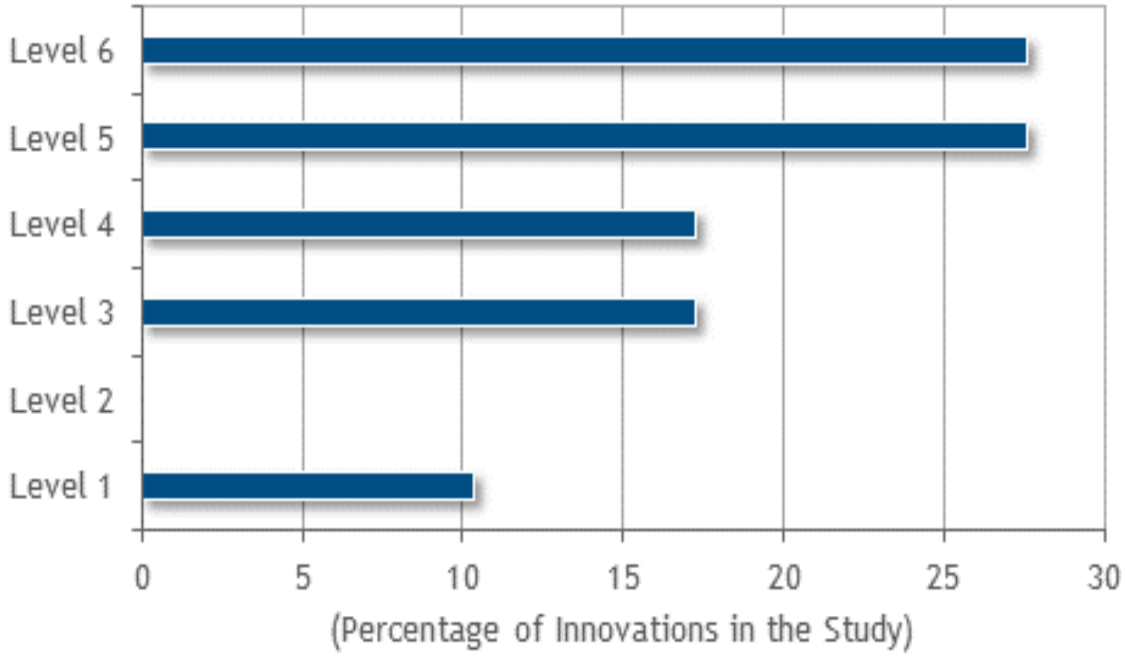
Source: IDC 2016

Innovation Impact Levels

Figure 5 displays the impact levels of the Blue Waters-enabled scientific innovations. The figure shows that more than half of the Blue Waters innovations qualified for levels 5 or 6, representing innovations having the largest impacts to multiple organizations.

FIGURE 5

Blue Water Innovations: Innovation Number of Organizations Impacted



Source: IDC 2016

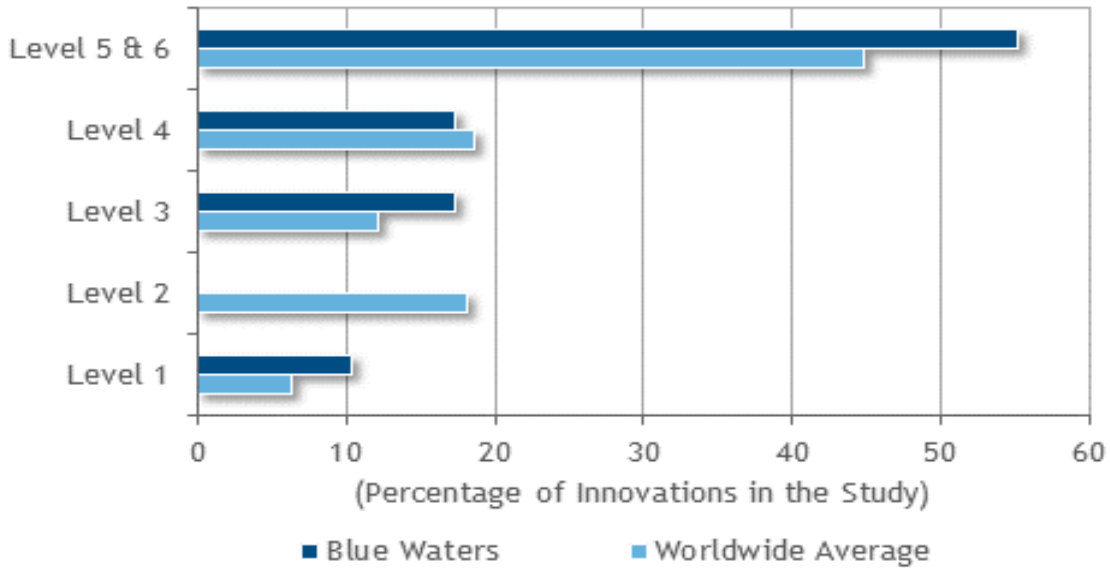
Innovation Impact Levels: Compared to Worldwide Averages

A notably higher percentage of scientific innovations conducted using Blue Waters qualified for impact levels 5 and 6 than was true for IDC's global data base of supercomputer-enabled scientific innovations (see Figure 6).

Comparisons are also shown for all US innovations, and for US academic only innovations. Looking at the top rating category, Blue Waters is similar to other US academic sites.

FIGURE 6

Blue Water Innovations: Innovation Number of Organizations Impacted



Source: IDC 2016

Innovation Overall "Class" Levels:

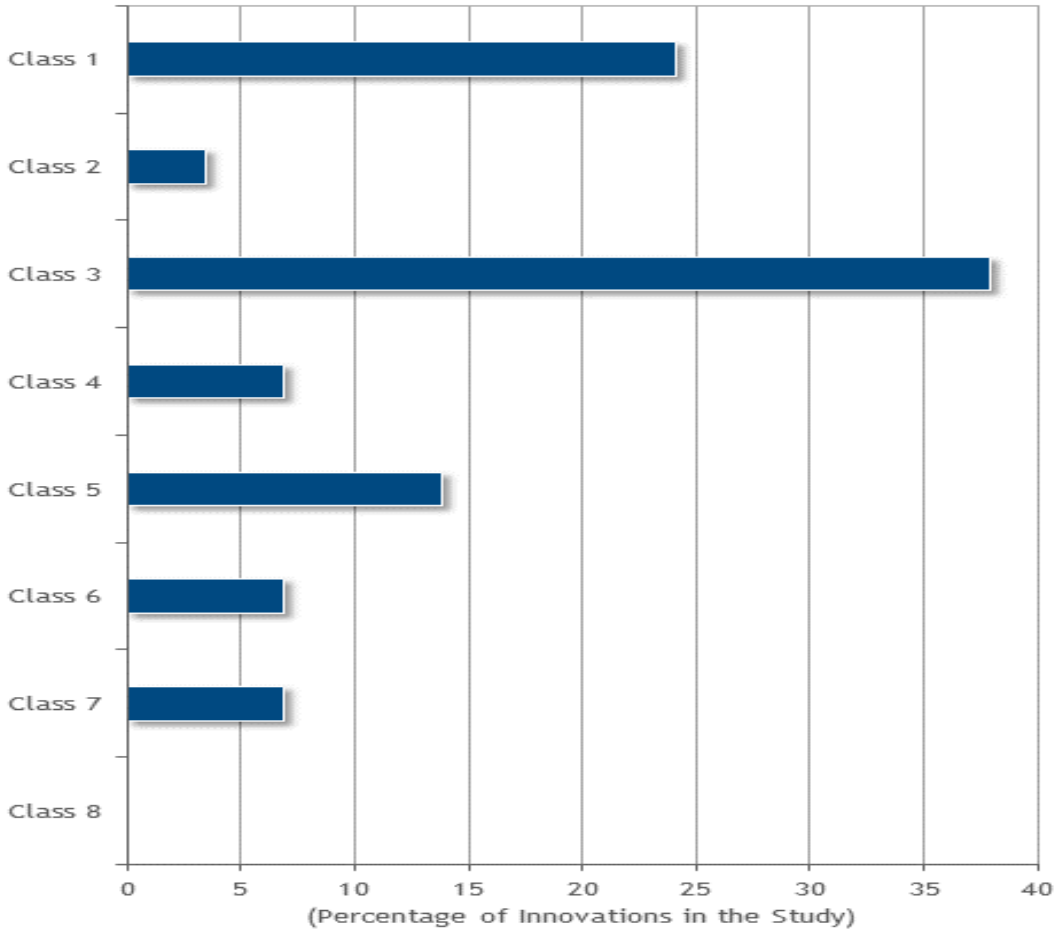
Figure 7 shows the rankings of Blue Waters-enabled innovations when both importance and impact are considered, using the following definitions:

- Class 1 innovations – One of the top 2-3 innovations in a field over the last ten years PLUS useful to over 10 organizations
- Class 2 innovations -- One of the top 5 innovations in a field over the last ten years PLUS useful to over 10 organizations
- Class 3 innovations – One of the top 5 innovations in a field over the last ten years PLUS useful to at least 5 organizations
- Class 4 innovations – One of the top 10 innovations in a field over the last ten years PLUS useful to at least 5 organizations
- Class 5 innovations – One of the top 25 innovations in a field over the last ten years PLUS useful to at over 10 organizations
- Class 6 innovations – One of the top 25 innovations in a field over the last ten years PLUS useful to at least 2 organizations
- Class 7 innovations – One of the top 50 innovations in a field over the last ten years PLUS useful to at least 2 organizations
- Class 8 innovations – innovations that are typically only useful to one organization and/or are minor innovations in a given research field

In this hybrid classification method IDC created for the present study, 62% of the Blue Waters-enabled innovations ranked in the top three classes.

FIGURE 7

Blue Water Innovations: Innovation Class Level



Source: IDC 2016

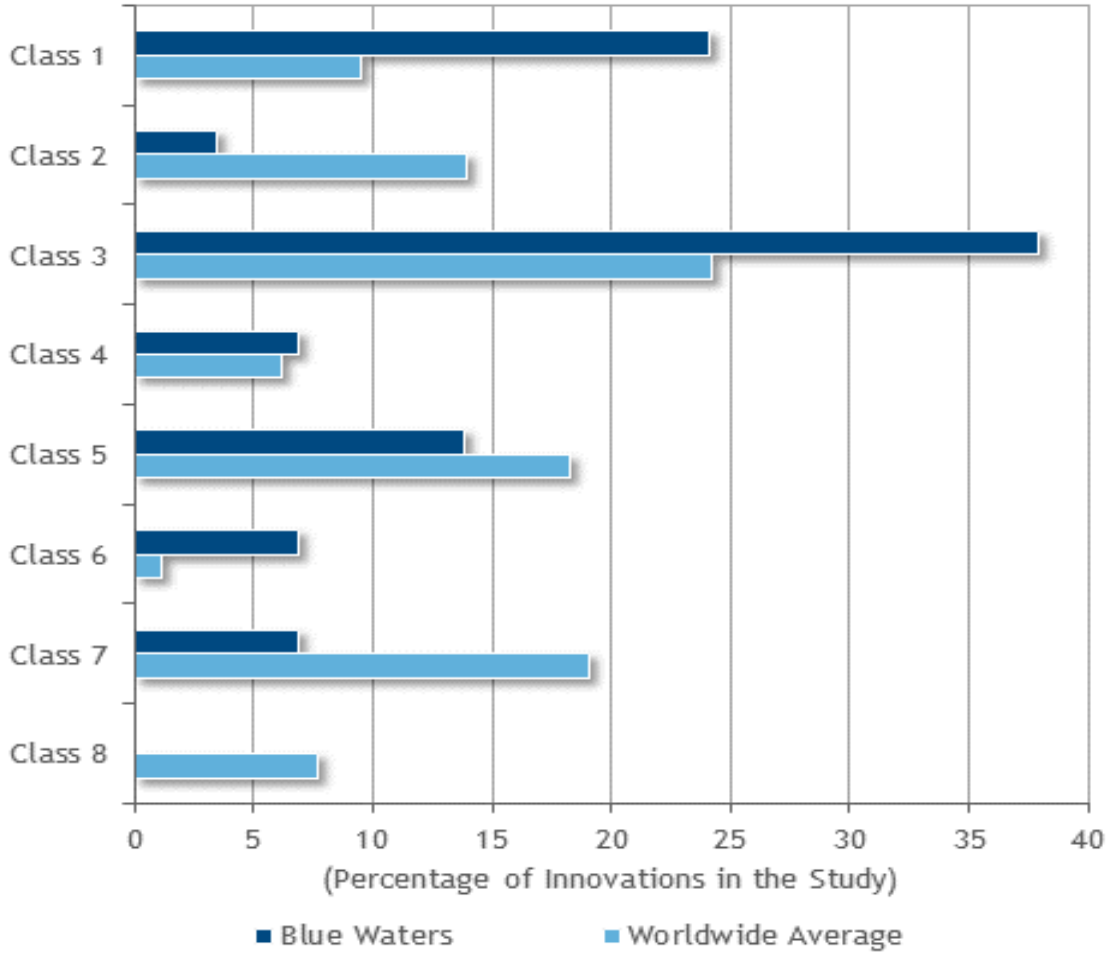
Innovation Overall "Class" Levels: Compared to Worldwide Averages

Figure 8 shows that a substantially higher percentage of the Blue Waters-enabled innovations qualified for Class 1 & 3 innovation levels, and substantially more Blue Waters-enabled innovations ranked in the top three classes than was true of IDC's global worldwide data base of innovations.

Comparisons are also shown for all US innovations, and for US academic only innovations. Looking at the top three innovation class rating categories, Blue Waters well ahead of other US organizations and other US academic sites. And way fewer Blue waters innovations are in the class levels 1 and 2 categories.

FIGURE 8

Blue Water Innovations: Innovation Class Level



Source: IDC 2016

IDC OBSERVATIONS

The Blue Waters supercomputer at NCSA is a pioneering achievement in HPC design. And where scientific productivity is concerned (as opposed to standard benchmark tests), Blue Waters is certainly one of the top few supercomputers in the world. As noted earlier, Blue Water's usefulness and productivity is notable in large part because NCSA worked so closely with its user community to help determine what kind of leadership-class supercomputer would best support the demanding requirements for their scientific work.

This study confirms that the time and money invested in Blue Waters has been paying off handsomely. Not once during the 31 interviews IDC conducted with Blue Waters users for this study did any of them point to shortcomings of the supercomputer. On the contrary, all of the researchers had praise for the system and enthusiastically reported on the progress it has enabled for their work. IDC has seldom encountered such a diverse group of scientific researchers who all agree on something—in this case, the value of the Blue Waters supercomputer.

LEARN MORE

Related IDC Research

- Worldwide HPC Server Forecast, 2016-2020 Jun 2016 Doc #US41318216 Earl C. Joseph, Ph.D., Steve Conway, Robert Sorensen, Kevin Monroe
- NSCI Update: Rolling Up Its Sleeves and Getting to Work Mar 2016 Doc #IcUS41072416 Robert Sorensen
- EU Consortium Gathers Core Capabilities to Build Exascale HPC Prototype Feb 2016 Doc #IcUS41048816 Robert Sorensen
- Next Steps for the NSCI: Looking to Ensure a Long and Lively Life Span Jan 2016 Doc#IcUS40980816 Robert Sorensen
- IDC Study: U.S. Private Sector Cybersecurity Best Practices Jan 2016 Doc#US40688815 Steve Conway, Sean Pike
- Baidu's Deep Learning Efforts: Notable Progress on Many Fronts Dec 2015 Doc#IcUS40704215 Robert Sorensen
- Worldwide HPC Server Forecast Update, 2015-2019 Nov 2015 Doc #259950 Earl C. Joseph, Ph.D., Steve Conway, Robert Sorensen
- The U.S. National Strategic Computing Initiative as a "Moonshot": Taking Its First Small Steps Sep 2015 Doc #259288 Flash Earl C. Joseph, Ph.D., Steve Conway, Robert Sorensen
- White House Announces Strategic HPC Plan: A Good Start on a Long Road Aug 2015 Doc #258194 Flash Robert Sorensen, Earl C. Joseph, Ph.D., Steve Conway
- Global HPC Market Dynamics in 2013 Apr 2014 Doc #248137 Chirag Dekate, Ph.D., Earl C. Joseph, Ph.D., Steve Conway
- Industrial Partnership Programs and High-Performance Computing: HPC User Forum, April 7-9, 2014, Santa Fe, New Mexico Apr 2014 Doc #248113 Earl C. Joseph, Ph.D., Steve Conway, Chirag Dekate, Ph.D.
- International Perspectives on Industrial High-Performance Computing Partnerships: HPC User Forum, April 7-9, 2014, Santa Fe, New Mexico Apr 2014 Doc #248122 Steve Conway, Earl C. Joseph, Ph.D., Chirag Dekate, Ph.D.
- Catalyst Supercomputer Heralds Shift to More Balanced Architectures Nov 2013 Doc #IcUS24437513 Steve Conway, Earl C. Joseph, Ph.D.
- National and International Initiatives: HPC User Forum, September 2013, Boston, Massachusetts Oct 2013 Doc # 243776 Steve Conway, Chirag Dekate, Ph.D., Earl C. Joseph, Ph.D.
- High-Performance Data Analysis in the Life Sciences: HPC User Forum, September 2013, Boston, Massachusetts Oct 2013 Doc # 243774 Steve Conway, Chirag Dekate, Ph.D., Earl C. Joseph, Ph.D.
- World's Fastest Supercomputer Set to Reach Customer in Oct 2013 Sep 2013 Doc #IcUS24300913 Steve Conway, Earl C. Joseph, Ph.D.
- Worldwide High-Performance Data Analysis 2013-2017 Forecast Jun 2013 Doc #241315 Steve Conway, Chirag Dekate, Ph.D., Earl C. Joseph, Ph.D.

- Top Issues for HPC Sites: HPC User Forum, April 29-May 1, 2013, Tucson, Arizona Jun 2013 Doc #241463 Chirag Dekate, Ph.D., Steve Conway, Earl C. Joseph, Ph.D.
- Livermore Lab Expands Industry Partnerships: Economic Security Is Vital for National Security Mar 2013 Doc #240232 Steve Conway, Earl C. Joseph, Ph.D., Chirag Dekate, Ph.D.
- Advanced Research at the South Ural State University Supercomputing Center Dec 2012 Doc #238225 Chirag Dekate, Ph.D., Steve Conway, Earl C. Joseph, Ph.D.
- IDC Special Study for NCSA/NSF on Industrial Use of HPC, Presented at Supercomputing 2012 Nov 2012 Doc #237984 Steve Conway
- HPC End User Site Update: RIKEN Advanced Institute for Computational Science Earl C. Joseph, Ph.D., Steve Conway, Chirag Dekate, Ph.D. Mar 2012 Doc # 233690

APPENDIX

Participants In The Survey

Table 8

Survey Participants

Investigator	Project Name
Ashok Srinvassan	Simulation-Based Policy Analysis to Reduce Ebola Transmission Risk in Air Travel
David Ceperley	Hydrogen Under Extreme Conditions
Jerry Bernholc	Petascale Quantum Simulations of Nano Systems and Biomolecules
Gerrit Botha	Custom Genotyping Chip for African Populations
John Grime	Dynamic Coarse-Grained Models for Simulations of Large-Scale Biophysical Phenomena
Liudmila Mainzer	Instrumenting Human Variant Calling Workflow on Blue Waters
Vincenzo Carnevale	Sensing the environment: a glimpse into the microscopic mechanisms of pain
Athol Kemball	Simultaneous VLBA polarimetric observations of the v={1,2} J=1-0 and v=1, J=2-1 SiO maser emission toward VY CMa II: component-level polarization analysis
Leigh Orf	Unlocking the Mysteries of the Most Violent Tornadoes
Brian O'Shea	Simulating the Earliest Galaxies with Enzo and Blue Waters
Paul Morin	ArcticDEM a White House initiative to produce a high-resolution, time-dependent elevation model of the Arctic using Blue Waters
Frank Tsung	Petascale Particle-in-Cell Simulation of Kinetic Effects in High Energy Density Plasmas
Susan Bates	High Resolution Earth System Modeling Using Blue Waters Capabilities
Tandy Warnow	Advancing Genome-Scale Phylogenomic Analysis
Kurt Brorsen	Nuclear-Electronic Orbital Calculations on Molecular Systems
PK Yeung	Particle tracking and turbulent dispersion at high Reynolds number on Blue Waters
Tom Quinn	Evolution of the small galaxy population from high redshift to the present
Nancy Makri	Quantum-classical path integral simulations of ferrocene-ferrocenium charge transfer in solution
Yongyang Cai	Policy Responses to Climate Change in a Dynamic Stochastic Economy

Table 8

Survey Participants

Investigator	Project Name
Gerhard Klimeck & Jim Fonseca	Advanced Nanoelectronic Device Design with Atomistic Simulations
Nikolai Pogorelov	Modeling Heliophysics and Astrophysics Phenomena with a Multi-Scale Fluid-Kinetic Simulation Suite
Ilias Tagkopoulos	Big Data on Small Organisms: Petascale Simulations of Data-driven, Whole-cell Microbial Models
Said Elghobashi	DIRECT SIMULATION OF DISPERSED LIQUID DROPLETS IN ISOTROPIC TURBULENCE
Seid Koric	SPARSE MATRIX FACTORIZATION IN SOLID MECHANICS AND GEOPHYSICS ON CPUS AND GPUS
Eric Lentz	Core-Collapse Supernovae Through Cosmic Time
Jamesina Simpson	Location- Specific Space Weather Hazard to Electric Power Grids Calculated on a Global Scale
Thomas Cheatham	Ensembles of Molecular Dynamics Engines for Assessing Force Fields, Conformational Change, and Free Energies of Proteins and Nucleic Acids
Robert Sugar	Lattice QCD
Ken Dill	Predicting Protein Structures with Physical Petascale Molecular Simulations

Source: IDC 2016

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