ALCF Newsbytes

Argonne Leadership Computing Facility

Argonne National Laboratory

Volume 1 | April 2011

The Blue Gene/Q: Bringing Exascale to Argonne

IBM's next-generation Blue Gene supercomputer, the Blue Gene/Q, is coming to the Argonne Leadership Computing Facility (ALCF). Four times faster than today's fastest supercomputer, experts look to the unprecedented power of the ALCF's leadership-class system to propel national innovation in science and technology.

The 10-petaflops supercomputer, named "Mira," will be delivered in 2012 and made available to scientists from industry, academia, and government research facilities around the world. Scientists will use Mira to accelerate discovery in key areas, including the development of ultra-efficient electric car batteries and researching global climate change.

In addition, work done on the next-gen Blue Gene/Q will stoke economic growth and improve U.S. competitiveness for challenges like:

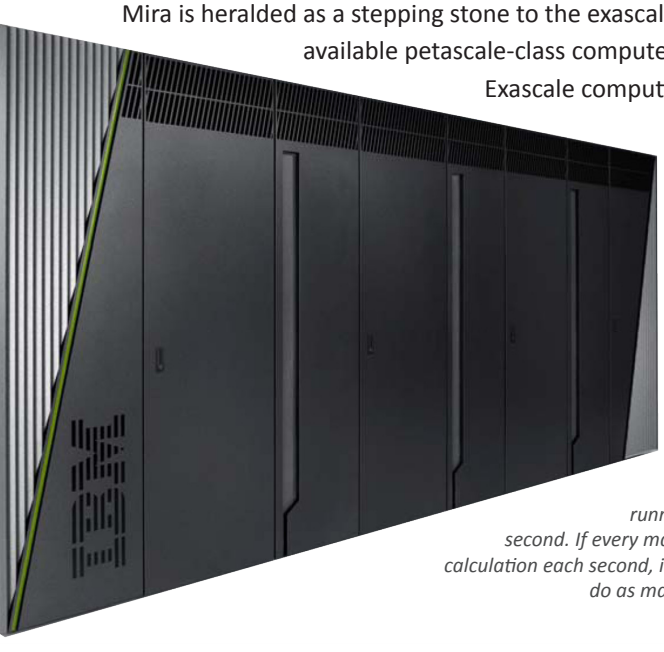
- designing safer, more efficient combustion mechanisms
- addressing human health issues through modeling cellular-scale biological processes
- studying nuclear physics reactions of critical importance to neutrino detector and accelerator experiments.

The ALCF is already working with future Q users as part of the Early Science Program—a program where researchers learn to leverage the computer's awesome power and prepare for an immediate jumpstart on discovery once the system is deployed.

Mira—the Stepping Stone to Exascale

Mira is heralded as a stepping stone to the exascale-class computers that will outpace available petascale-class computers by a factor of a thousand.

Exascale computing has the potential to address highly complex studies currently beyond our reach, not just due to their sheer size, but because of their inherent uncertainties and unpredictability. For scientists, Mira will provide an essential first glimpse into the capabilities and challenges of exascale.



Arriving in 2012, Mira will be four times faster than today's fastest supercomputer, running programs at 10 quadrillion calculations a second. If every man, woman and child in the US performed one calculation each second, it would take them almost a year combined to do as many calculations as Mira will do in one second.

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Events of Interest

2012 INCITE Call for Proposals Opens

The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program supports high-impact scientific advances through the use of the Department of Energy's Leadership Computing Facilities.
Proposals accepted through June 30, 2011.
For details, visit http://hpc.science.doe.gov/

ALCF Hosts Leap to Petascale Workshop June 7-9, 2011 Argonne National Laboratory

Take your code to the next level! Work hands-on with ALCF experts in performance and computational science to fine-tune your code. And developers of performance tools and debuggers will share ways to improve your code's performance.
Register today:
http://workshops.alcf.anl.gov/petascale2k11/

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The Blue Gene/Q: Bringing Exascale to Argonne (continued)

Design Parameters	Blue Gene/P	Blue Gene/Q	Change
Cores per Node	4	16	4×
Clock Speed (GHz)	0.85	1.6	1.9×
Flops per Clock per Core	4	8	2×
Nodes per Rack	1,024	1,024	--
RAM per Core (GB)	0.5	1	2×
Flops per Node (GF)	13.6	204.8	15×
Concurrency per Rack	4,096	65,536	16×
Network Interconnect	3D torus	5D torus	Smaller diameter
Cooling	Air	Water	~30% savings per watt

Getting Time on Mira

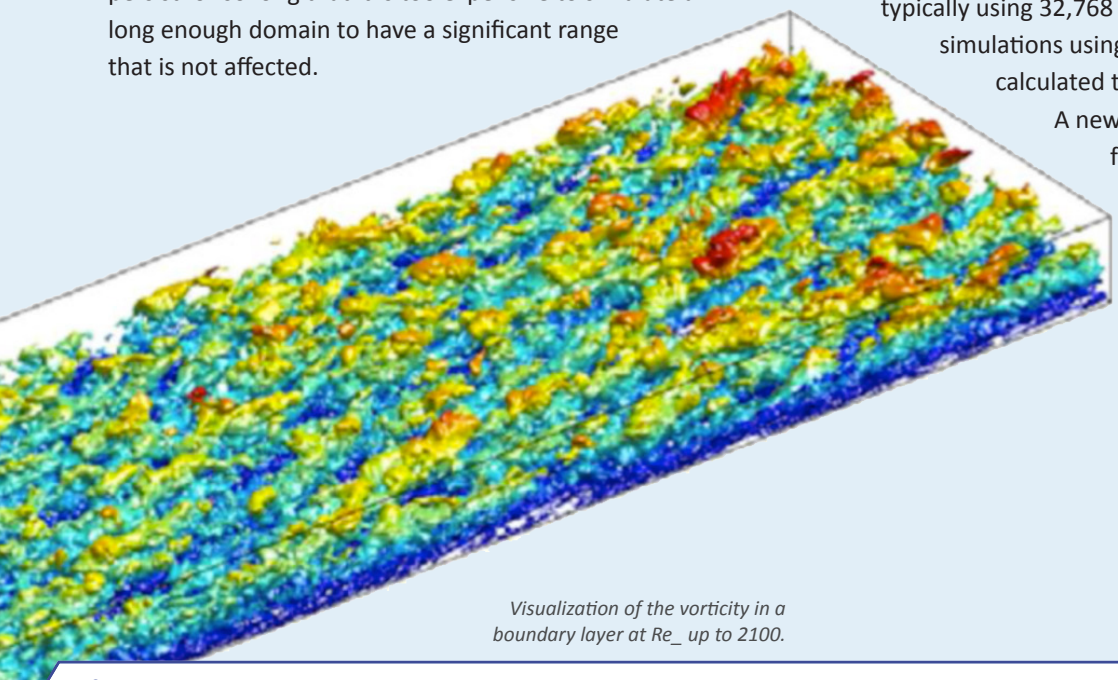
Once Mira is in production, the DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) and the ASCR Leadership Computing Challenge (ALCC) programs will award blocks of computing time via a peer-reviewed, competitive process to researchers working on scientific challenges that are best addressed by the capabilities of leadership-class supercomputers.

A New Approach to Understanding Boundary Layers Using High Reynolds Numbers

Boundary layers are the primary interface between vehicles (e.g., airplanes, boats) and the medium in which they move. Their physical understanding is not only an intellectual challenge but also a prerequisite for better vehicle design.

INCITE researchers from the University of Texas at Austin discovered that at large Reynolds numbers the boundary layer relaxes slowly from the artifacts of the inlet conditions. This appears to be physical and implies that boundary layers have longer memory than had previously been thought. However, particularly for the recycling inflow used, the inlet artifacts persist for so long that it is too expensive to simulate a long enough domain to have a significant range that is not affected.

Using the IBM Blue Gene/P system at the Argonne Leadership Computing Facility, the researchers developed a new approach in which an effectively longer spatial domain is simulated by breaking the domain into two shorter pieces, with a plane at the end of the useful range of the first simulation used as an inlet condition for the second. This has a significant advantage, since the first domain can be simulated with much coarser resolution, making it about 10 times less expensive to simulate this portion than it would be as part of a unified single simulation. This approach has been implemented and tested during the course of 34M hours (29M capability hours), typically using 32,768 cores for each job. Coarse resolution simulations using this approach are now being calculated to eliminate statistical transients. A new set of production simulations will follow.



Visualization of the vorticity in a boundary layer at Re_ up to 2100.

Contact: Robert Moser, rmoser@ices.utexas.edu

2011 ALCF Winter Workshop Series Offers Hands-on Experience to Users

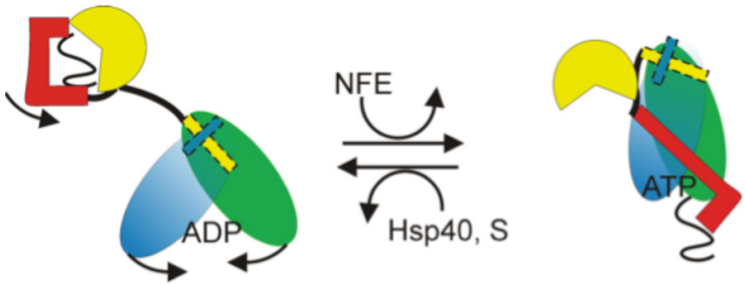
The January 2011 Winter Workshop Series, sponsored by the Argonne Leadership Computing Facility, drew 68 attendees. The *Getting Started* workshop, held January 18, provided users with key information on ALCF services and resources, technical details on the IBM Blue Gene/P architecture, as well as hands-on assistance in porting and tuning of applications on the Blue Gene/P. In the *Productivity Tools for Leadership Science* workshop, held January 19-20, ALCF experts helped boost users' productivity using TAU, Allinea, and other HPC tools. The workshop covered parallel I/O, visualization and data analysis, and libraries on the IBM Blue Gene/P system at the ALCF. Hands-on assistance was provided. Attendees remarked on the helpfulness of the hands-on demos and the one-on-one interaction with ALCF staff.

In addition, 54 registered for the ALCF-sponsored webinar, *INCITE Proposal Writing*, held January 24. Scientists from the ALCF and Oak Ridge Leadership Computing Facility provided tips and suggestions to improve the quality of proposal submissions. This workshop was presented concurrently as a live event and a webinar.

To download workshop and webinar presentations, visit the ALCF websites
http://workshops.alcf.anl.gov/wss11/agenda/
and
http://workshops.alcf.anl.gov/pww11/

Simulation of Molecular Chaperones Offers Insight into Protein Folding, Unfolding

A study conducted at the Argonne Leadership Computing Facility by INCITE researchers at Cornell University is the first to successfully simulate functionally important motions of special proteins that play a fundamental role in biological processes. The simulations were run using more than 6.2 million core-hours on the IBM Blue Gene/P at the ALCF. The insight gained from these simulations led to the formulation of a mechanism that provides a unifying explanation of known experimental facts.



A plausible mechanism of Hsp70 chaperone opening deduced from coarse-grained simulations of 2KHO.

The dynamics of proteins and mechanisms of protein folding and unfolding are key in enzymatic reactions, signal transduction, immunological response, cell motility, and in diseases such as cancer and amyloid formation. The native three-dimensional structure of a protein is entirely encoded in its amino-acid sequence and corresponds to the global minimum of the free energy of the protein, plus the surrounding solvent. However, *in vivo* folding is assisted by special proteins called molecular chaperones. Heat shock proteins (Hsps) are essential molecular chaperones present both in prokaryotic and eukaryotic cells of all organisms.

The functionally important motions lead to the transition between the SBD-closed and SBD-open conformation of Hsp70 chaperones (an essential step in chaperone-assisted protein folding, refolding, or repair), using the coarse-grained molecular dynamics approach and a nucleotide-free closed form of the DnaK chaperone from E. coli as a model. Based on the results of the simulations, a plausible mechanism of interdomain communication has been proposed, which agrees with the information from chaperone opening/closing experiments.

Contact: Harold Scheraga, has5@cornell.edu

Spotlight on ALCF Staff: Ray Loy

ALCF Newsbytes recently commandeered a few moments with Ray Loy, part of the Performance Engineering team here at the Argonne Leadership Computing Facility, and one of the facility's first employees.

NEWSBYTES What is the role of the Performance Engineering group at the ALCF?

RAY LOY We're here to help users achieve the best performance from their applications. We work hands-on with them to port, tune and parallelize their applications on ALCF computers, and to resolve I/O issues inhibiting performance.

NEWSBYTES What's your educational background?

LOY I have a bachelor's in Engineering with a major in Computer Science from the School of Engineering at Columbia University. I did my graduate work at Rensselaer Polytechnic Institute where my thesis involved parallel adaptive unstructured mesh computation.

NEWSBYTES There's a lot of breakthrough research underway at the ALCF. Where do your interests gravitate?

LOY Climate modeling and molecular dynamics. In performance engineering, I'm most interested in parallel I/O and parallel debuggers.

NEWSBYTES We've heard you're now "President" Loy.

LOY Yes, I recently accepted the presidency of ScicomP, the IBM HPC Systems Scientific Computing User Group. ScicomP is a forum for computational scientists and engineers who want to maximize performance and scalability on the big IBM HPC platforms, including the Blue Gene. Our annual meeting is in May in Paris. Organizing it has been a lot of work, but I'm very excited to be involved.

NEWSBYTES What did you want to be when you grew up?

LOY The Monty Python fan in me wants to reflexively say a Chartered Accountant or a lumberjack. But really, I was always interested in how things worked, so it was inevitable I would become an engineer or scientist of some sort.

NEWSBYTES How did you come to join the ALCF?

LOY In 2005, I was with the closely linked Mathematics and Computer Science division at Argonne, using the ALCF's Blue Gene/L to work on the Model Coupling Toolkit and the scalability of the Community Climate System Model (CCSM). As an early Blue Gene user, I was often called on to help other users—first in workshops, later by providing application support. It was a logical transition for me to join the ALCF when it became its own division in 2006. I've seen it grow from a staff of four to over 60.

NEWSBYTES What aspects of work at the ALCF would likely surprise our readers?

LOY I think people would be surprised by how much work goes into the procurement of a leadership-class machine. Pretty much the day after we finished acceptance testing of our current Blue Gene/P, we started working on the next system, the Blue Gene/Q—defining requirements, projecting the new types of scientific simulations that will be possible, collaborating on the design, and passing round after round of reviews. The process literally takes years, and only at the completion of acceptance testing and transition to operations do the users see a result.

NEWSBYTES What do you like most about working for the ALCF?

LOY We not only get to work with the newest, most powerful machines, but also, through our collaboration with IBM, we get to be part of their design.

NEWSBYTES Is there a particularly fascinating project you worked on here that stands out in your mind?

LOY Benoit Roux's INCITE project performed a molecular simulation of potassium ions filing through a voltage-gated membrane channel. Given the incredibly small timescale of the molecular interactions, and the amount of computation involved, the resulting animation was truly amazing.

View Benoit Roux's animation here:
http://www.ks.uiuc.edu/Research/kvchannel/Movie_Sim1.mpg
http://www.ks.uiuc.edu/Research/kvchannel/kv1.2-2048-large.mpg

For more information about the Performance Engineering Team, contact Ray Loy: rloy@alcf.anl.gov

ALCF Staff Mentor Middle-School Girls at 10th Annual IGED

Argonne hosted 76 6th-, 7th- and 8th-grade girls from Illinois, Indiana, and Wisconsin during its 10th Annual Introduce a Girl to Engineering Day (IGED) on February 24. Held in celebration of National Engineering Week, the event focused on introducing girls to engineering careers through hands-on activities and direct interaction with engineers and scientists.

The girls spent the day with Argonne mentors to explore their interests in math, science, and engineering. A number of middle-school girls who previously attended IGED also shared their experiences with this year's participants. The day opened with a career presentation—"Engineering is Fun!" An Engineering Expo featured chemistry and transportation technologies, magnets, geographical information systems, and the conversion of plants into biodiesel fuel, among other exhibits. The girls participted in hands-on activities and experiments, such as designing a model car and creating materials. In addition, each girl took a tour relating to her particular area of interest in biology, engineering, applied energy systems, or the Advanced Photon Source.

Sreeranjani Ramprakash, Technical Support Specialist, and Marta Garcia, Assistant Computational Scientist, at the Argonne Leadership Computing Facility served as mentors during the event.

"We exposed the girls to a wide variety of science, engineering, and technology fields," noted Sreeranjani. "The event gave us the opportunity to explain the different types of technical careers that are available to them."

Read more (http://students.ne.anl.gov/schools/iged11.php)

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ALCF Newsbytes is a publication of the Argonne Leadership Computing Facility.
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