THE BLUE WATERS project team had several challenging months last year, but what a comeback. Blue Waters is now firmly back on track.

The Blue Waters system that our new partner, Cray Inc., will install in the National Petascale Computing Facility will be a CPU-GPU hybrid computing system. With its massive computing capability; large, fast memory subsystem; improved interconnect; and large, fast I/O subsystem, it will bring sustained-petaflop performance to a broad range of science and engineering applications in fields like climate change, the spread of epidemics, earthquakes, fundamental chemistry and physics, and materials science. And, with its equally impressive GPU capability, it will serve as a bridge to the technologies on which future supercomputers will be based.

Cray has already delivered the first forty-eight (48) computational racks of Blue Waters. This initial system, a Cray XE6 system, is the Phase 1 Early Science System and will be made available to a select number of the NSF-approved Science Teams next month. By mid 2012, the entire set of Cray XE6 nodes and the racks for the XK nodes will be in place. The Kepler GPU units will be installed in the XK racks in the fall of 2012.

It has taken several months of intense effort to bring this new plan into full focus. But a few things stood out while the plan was still emerging. They were absolutely essential to our success then and will continue to be essential as we move forward.

First among those is the NCSA staff—knowledgeable, experienced, and dedicated. All organizations do well when times are good. What distinguishes an outstanding organization is how well it does when times are uncertain. I am extremely proud of the way that the NCSA staff handled themselves during these trying times—they kept their focus on the goal and brought years of experience and expertise to bear to ensure the right outcome for the science and engineering community.

The staff had the know-how to right the project, and they have the know-how to see that the project lives up to its fullest potential. We have everything we need to ensure that the researchers who use Blue Waters will have an outstanding computing system and technical support. With this, they will be able to take full advantage of the extraordinary capabilities that Blue Waters provides.

Cray and its impressive staff were also crucial. They entered a tricky situation with great resolve, and they have been a trustworthy and able partner from the outset. To say Cray had to hit the ground running is an understatement. Their commitment is obvious and greatly valued.

The entire team—at NCSA, Illinois, Cray, Cray’s suppliers and our academic partners throughout the country who are part of the Great Lakes Consortium for Petascale Computation—understands the core principle behind Blue Waters. That is: It’s more than just a hardware acquisition, more than just a chase for a high peak performance number or a ranking on the Top 500 list—it is about making a super ecosystem that is absolutely the best at real work.

Blue Waters is a project that was focused from the beginning on transforming the role of computing in science and engineering while providing a world class platform to continue science discovery during this transformation. The National Petascale Computing Facility was built with flexibility in mind. The external networking for the system is up and running, and the archive system will follow soon. The science teams who will use Blue Waters were already working with NCSA staff to prepare their codes to run at the scale required. That work is continuing unabated and has been expanded to embrace GPU accelerators. Similarly, the Blue Waters education programs have been training hundreds of students in the skills they need to exploit extreme-scale computing systems—including GPUs.

This mindset allowed us all to evaluate our options and move quickly to select a new hardware solution with Cray. The Cray heterogeneous system will allow NCSA to serve the national science and engineering community as it has for the last 25 years—driving new discoveries, advancing engineering practice, and improving our world. These are lofty goals, and we are keenly aware that they come with a certain amount of risk. But they are also timeless and vital and exciting. These are the kinds of risks we will continue to take and the kind of goals we will continue to pursue.

Thom Dunning
Blue Waters Project Director

Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign, its National Center for Supercomputing Applications, Cray, and the Great Lakes Consortium for Petascale Computation. It is supported by the National Science Foundation, the University of Illinois at Urbana-Champaign, and the state of Illinois.
The Cray Blue Waters system

This new Cray supercomputer will support significant research advances in a broad range of science and engineering domains, meeting the needs of the most compute-intensive, memory-intensive, and data-intensive applications. Blue Waters is expected to deliver sustained performance, on average, of more than one petaflop on a set of benchmark codes that represent those applications and domains.

The Blue Waters system is intentionally designed to be the most balanced and most effective system of its generation. Instead of chasing a theoretical peak performance operation rate, or a Linpack measure, the system design follows the consistent project philosophy. Hence, the vast majority of the computation resources, 90%, are general purpose CPUs usable immediately by science teams. To support the transformation of science applications, 10% of the physical resources (but about 1/3 of the peak FLOPs), are the hybrid GPU nodes, making Blue Waters one of the largest GPU clusters in the world. Blue Waters also invested in more aggregate memory and what could be described as the most intense storage sub-systems than any other HPC system known.

Blue Waters will be composed of 244 Cray XE6 cabinets based on the recently announced AMD Opteron™ 6200 Series processor (formerly code-named “Interlagos”) and 32 cabinets of a future version of the recently announced Cray XK6 supercomputer with NVIDIA®’s Kepler™ GPU computing capability incorporated into a single, powerful hybrid supercomputer, making this by far the largest system Cray has delivered to date. These Cray XK nodes will further increase the measured sustained performance on real science problems.

The Cray Blue Waters system will employ:

- Cray’s scalable Gemini high-performance interconnect, providing a major improvement in message throughput and latency.
- AMD’s 8-core Opteron™ 6200 Series processors, selected by the editors of HPCwire as one of the top five new technologies to watch in 2011.
- Cray’s XK6 blades with NVIDIA® Tesla™ GPUs, based on NVIDIA’s next-generation ‘Kepler’ architecture, which is expected to more than double the performance of the Fermi GPU on double-precision arithmetic.
Blue Waters Stats

- Cray X60 cabinets: 244
- Cray XK6 cabinets: 32
- Total cabinets, including storage & server cabinets: >300
- Compute nodes: >25,000
- Usable Storage Bandwidth: >1 TB/s
- Aggregate System Memory: >1.5 Petabytes
- Memory per core: 4 GB
- Interconnect Topology: 3D Torus
- Number of disks: >17,000
- Number of memory DIMMS: >190,000
- Usable storage: >25 Petabytes
- Peak performance: >11.5 Petaflops
- Number of AMD processors: >49,000
- Number of AMD x86 cores: >380,000
- Number of NVIDIA GPUs: >3,000
- External network bandwidth: 100 Gb/s scaling to 300
- Integrated near line environment: scaling to 500 PBs
- Bandwidth to near-line storage: 100 GB/s

The multi-year and multi-phase contract with Cray, consisting of products and services, is valued at more than $188 million. Blue Waters is expected to be fully deployed by the end of 2012.

As supercomputers continue to grow in scale and complexity, it becomes more challenging to effectively harness their power. Since the Blue Waters project was launched in 2008, NCSA has helped researchers prepare their codes for the massive scale of this and other extreme-scale systems. NCSA also initiated a broad range of research and development projects designed to improve the performance of the existing HPC software stack and facilitate the development and use of applications on Blue Waters and other petascale computers. The Blue Waters project is now prepared to mount a major, community-based effort to move the state of computational science into the petascale era. The center will work with the computational and computer science and engineering communities to help them take full advantage of Blue Waters as well as future supercomputers. The effort will focus on scalability and resilience of algorithms and applications, use of accelerators to improve time to solution for science and engineering problems, and simultaneous use of computational components with different characteristics.

GLCPC aids education, other efforts

The Great Lakes Consortium for Petascale Computation (GLCPC) is a collaboration of colleges, universities, national research laboratories, and other educational institutions. The consortium is a key element of the Blue Waters project and facilitates the widespread and effective use of petascale computing, through the development of new computing software, applications, and technologies. A comprehensive educational and workforce development program ensures that advances made by consortium members are passed on to the next generation of researchers and applied to frontier research questions in science, technology, engineering, and the social sciences. Current GLCPC officers are:

- President: Stan Ahalt, RENCI
- President Elect: Steve Gordon, OSC/OSU
- Past President: Maxine Brown, University of Illinois at Chicago
- Secretary/Treasurer: Patricia Jacobs, Shodor
- Executive Committee / Member At Large: Srinivas Aluru, Iowa State University, Tom Jones, University of Minnesota, Greg Moses, University of Wisconsin-Madison, Joe Paris, Northwestern, Padma Raghavan, Penn State

Watch Blue Waters’ installation!

View a live video feed of the floor at the National Petascale Computing Facility: http://timelapse.ncsa.illinois.edu/pcf/inside2/index.php
New PRAC teams cover many disciplines

With the Blue Waters sustained-petascale computer, researchers believe they’ll be able to gain important insights into problems some have been exploring for years. To take full advantage of the new technologies of Blue Waters, however, codes must be rewritten. Petascale Computing Resource Allocations (PRAC awards) from the National Science Foundation allow research teams to work closely with the Blue Waters project team in preparing their codes. The codes and projects address key challenges faced by our society and explore fundamental scientific and engineering problems.

These collaborations include help porting and re-engineering existing applications. In some cases, the teams will build entirely new applications based on new programming models. Current projects represent a wide range of disciplines. They will drive scientific discovery for years to come. Projects announced in the last half of 2011 are:

- **Accelerating nano-scale transistor innovation**
  Principal Investigators: Gerhard Klimeck, Purdue, Thomas Hacker, Purdue, Mathieu Luisier, Purdue

- **Simulating vesicle fusion on Blue Waters**
  Principal Investigator: Vijay Pande, Stanford

- **Using petascale computing capabilities to address climate change uncertainties**
  Principal Investigators: Donald Wuebbles and Xin-Zhong Liang, University of Illinois at Urbana-Champaign

See the complete list of PRAC teams at: http://www.ncsa.illinois.edu/BlueWaters/sci-eng.html

**Events of interest**

- **Improving the Eclipse Parallel Tools Platform**, monthly user conference call held the fourth Wednesday of every month
  http://wiki.eclipse.org/PTP/PTP_User_Meetings

- **2012 Symposium on Application Accelerators in High-Performance Computing**, (SAAHPC), July 10-12, Argonne National Laboratory
  http://saahpc.ncsa.illinois.edu/

- **2012 XSEDE Conference**, July 16-19, Chicago, IL
  www.xsede.org

**About the Blue Waters Project**

Blue Waters is expected to be one of the most powerful supercomputers in the world for open scientific research when it comes online. Scientists will create breakthroughs in nearly all fields of science using Blue Waters.

For more information visit: www.ncsa.illinois.edu/BlueWaters

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