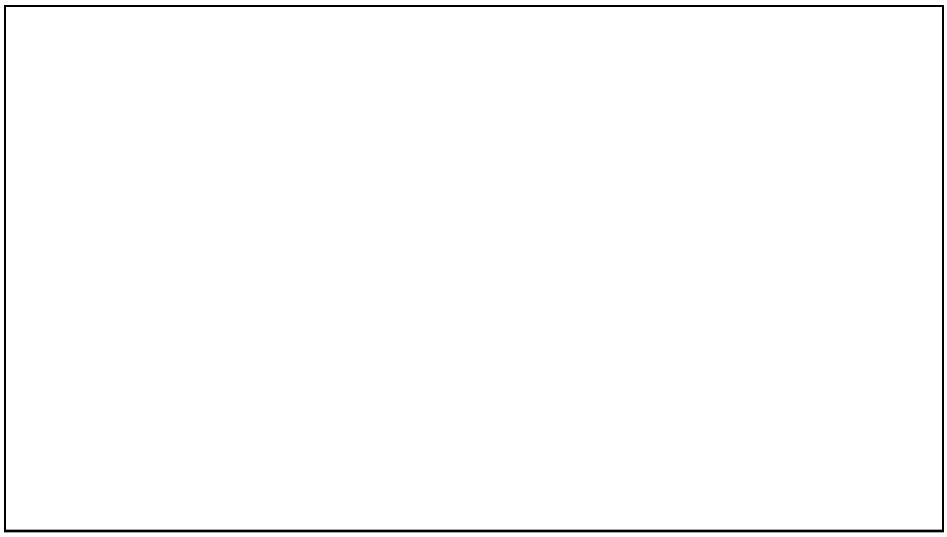
Celebrating Two Years of Blue Waters Supercomputing at NCSA

April 8, 2015 by staff

This week NCSA celebrated two years of Blue Waters supercomputing in an event convened by U.S. Senator Mark Kirk. The powerful Cray supercomputer is used by scientists and engineers across the country to tackle challenging research for the benefit of science and society.

The event featured a panel of Blue Waters users—four from among the 200

teams across the country that have used the system—then briefly described how the supercomputer accelerates their research:



Leigh Orf, professor of Atmospheric Science at Central Michigan University, is part of a research team using Blue Waters to better understand the inner workings of supercell thunderstorms and their most devastating product: the tornado. Orf said that while our ability to predict tornadoes has improved, we still need to understand more about how the storms form so warnings can be more accurate.

"We want to have fewer false alarms, more targeted alarms, and ultimately saved lives," Orf said.

Using Blue Waters, his research team has simulated powerful EF5 tornadoes, identifying new flow structures that have not been seen previously. This new information could help explain what makes these devastating storms unique.

> *"You can't do this kind of thing without supercomputers," Orf said. And the 20,000-core simulation that produced 100 terabytes of data "couldn't have happened on other [supercomputers]."*

Randy Huber, Advanced Virtual Product Development Manager at Caterpillar, explained why Cat has been a long-time member of NCSA's Private Sector Program.

> *We came to NCSA (in the 1980s) for high-performance computing. The high-performance computer of today is the industrial work station of tomorrow," he said. By working with cutting-edge resources and expert staff at NCSA, Cat stays ahead of the curve. Huber added that collaborating with NCSA opens up new opportunities for Cat, helping the company's employees realize that "maybe that problem CAN be solved, maybe I CAN do something I haven't been able to do before."*

Huber said that in order for Cat to design and build products that will help its customers work more effectively and efficiently, the company needs more knowledge and more realism. "We have to get realism in simulation, and high-performance computing is an ingredient in helping us get there," he said.

The research of Rohit Bhargava, professor of Bioengineering at the University of Illinois at Urbana-Champaign, focuses on developing novel chemical imaging technology and structures that can be employed to detect, diagnose and understand tissue structure and cancer pathology. He believes that new technology—essentially a computational microscope that combines spectroscopy and chemistry—can lead to more effective and less expensive cancer diagnosis and care.

Rohit Bhargava

> *What we're really after is an image that tells the clinician what is shown in the image—including what might be cancerous. And it's done in our laboratory entirely without human intervention, entirely with computation," Bhargava said. But this technique produces huge datasets and requires computational power to be clinically feasible. "Just running the first step on a desktop 10 years ago took 23 days. Just running the iteration once for one set of samples takes several days now. That's not fast enough," he said.*

That's where a powerhouse like Blue Waters comes into play. Bhargava's most

recent results with the new technique have beat the current medical paradigm in predicting which samples show dangerous prostate cancer (as opposed to a slow-growing, much less threatening form of prostate cancer), with an accuracy rate of 85 percent.

> *Perhaps with more computing power, we can tell people reliably whether their prostate cancer is dangerous or can remain untreated" and patients can avoid unnecessary complications and side effects, he said.*


Klaus Schulten

Klaus Schulten, a professor of Physics and Blue Waters Professor at the University of Illinois at Urbana-Champaign and leader of the Theoretical and Computational Biophysics Group at the Beckman Institute, calls Blue Waters "the ultimate microscope." Schulten's research team uses Blue Waters to study a variety of biological systems, including the amyloid fibers that are thought to cause Alzheimer's disease, the mechanism by which the antibiotic erythromycin fights bacteria, and fundamental aspects of photosynthesis. He recently was awarded an additional Blue Waters allocation to study the Ebola virus.

Using Blue Waters, Schulten's team was able for the first time to determine the chemical structure of the HIV capsid, a protein shell that protects the virus's genetic material. "The capsid is far from just being a boring container," he said. "It needs to communicate with the cell in order to have successful infection. Thanks to Blue Waters, we learned about previously unknown infection chemistry."

> *Blue Waters is really getting us close to understanding living systems at a completely new level."*

The discussion concluded with remarks from Jim Kurose, assistant director of the Directorate for Computer and Information Science and Engineering at the National Science Foundation (NSF).

> *The breakthrough research achievements we've heard today*

> *demonstrate why Blue Waters is such a compelling investment," he said. "Taken all together—the hardware, the software, the data and the networks, and, probably most importantly, the people—make Blue Waters an incredibly versatile scientific instrument. We can think of it as a microscope and a telescope. It can allow us to look inside tornadoes. It can help us eradicate epidemics. It can be a job creator as well."*

He pointed out that Blue Waters is part of a nationwide "ecosystem" supported by the National Science Foundation—a smorgasbord of computing, data, software, and support resources that also includes the Extreme Science and Engineering Discovery Environment (XSEDE) project led by NCSA.

> *We at NSF are committed to continuing to support his ecosystem into the future," Kurose said. "As a national resource, Blue Waters helps ensure that the United States remains a global leader."*

Source: NCSA

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