For more than 25 years, the National Center for Supercomputing Applications (NCSA), located at the University of Illinois at Urbana-Champaign, has provided scientists and engineers from across the United States with access to some of the world’s most powerful high-performance computing (HPC) resources. Researchers use those resources to untangle the mysteries of protein folding, analyze the potential effects of earthquakes on buildings, understand the formation of galaxies and more.

In 2007, the National Science Foundation (NSF) funded the acquisition and deployment of a petascale system at NCSA to help researchers solve more complex problems, increase the resolution of simulations and improve the fidelity of physical models. Named “Blue Waters,” the new supercomputer is a collaborative effort by the University of Illinois, NCSA, the Great Lakes Consortium for Petascale Computation and IBM. From its inception, Blue Waters was expected to be one of the most powerful supercomputers in the world, with sustained performance of more than 1 petaFLOP (1 quadrillion calculations per second) on a wide range of science and engineering codes.

IBM TECHNOLOGIES PROVIDE THE FOUNDATION FOR BLUE WATERS

The NCSA team selected IBM® Power Systems™ based on IBM POWER7® technology to provide the robust foundation required for Blue Waters. NCSA will use the IBM Power Systems IH supercomputing node, which includes four 8-core POWER7 chips in a single multichip module (MCM). When Blue Waters is fully deployed, it will include more than 300,000 POWER7 cores.

The supercomputing node features a new IBM interconnect technology that draws from IBM Federation supercomputing switches and InfiniBand. With the ability to scale to hundreds of thousands of cores, the interconnect technology can help create a high-bandwidth, low-latency network. The NCSA team also decided to adopt the IBM General Parallel File System (GPFS™) to manage large-scale storage requirements for the supercomputer.

“With IBM Power Systems, we can create balanced nodes for Blue Waters with exceptional usable compute power—as well as sufficient memory, communication and I/O bandwidth—to deliver exceptional science and engineering results,” says Cristina Beldica, senior project manager at NCSA.

“We wanted to achieve the petaFLOP performance with the fewest possible number of cores, not only to reduce the system’s footprint but also to help ensure that applications could scale sufficiently,” says Bob Fiedler, technical program manager for science and engineering applications at NCSA. “By using IBM Power Systems with POWER7 processors in the IH configuration, we can create a dense infrastructure that has the memory bandwidth per core to handle scientific workloads and the high-speed connections between processors to remove scalability bottlenecks.”
IBM Power Systems will also help NCSA control energy costs and adhere to the organization’s commitment to minimizing the environmental impact of supercomputing. “Many of the components in IBM Power Systems are integrated onto a small number of circuit boards, so we can avoid using the additional power supplies and cooling fans required for other systems,” says Fiedler. “We also plan to use IBM water-cooling technology to reduce the energy required to remove the heat generated by the nodes.”

EARLY TESTING REVEALS SIGNIFICANT PERFORMANCE GAINS
To gauge the performance POWER7 technology might deliver for Blue Waters, the NCSA team ran performance tests for key HPC applications using first a POWER7 simulator and then an IBM Power 780 server with POWER7 processors. IBM provided access to additional systems in IBM labs so the NCSA team could see how performance would scale. “Even with these early tests, we saw significant gains in performance for several HPC applications,” says Fiedler. “For example, the standard MILC NSF ‘XL’ benchmark runs three times faster on the POWER7 than on our POWER5+ and POWER6 interim systems.” When the final system is deployed with enhanced processors, chipsets and finely tuned system software, the NCSA team could see even higher performance than in the test and development environments.

BLUE WATERS PREPARES FOR NEW SCIENCE AND ENGINEERING BREAKTHROUGHS
By offering considerably greater computing performance than existing clusters, Blue Waters could facilitate important new breakthroughs in a number of fields. For example, molecular biologists will be able to study longer cellular processes and entire subsystems within cells to advance scientific knowledge and contribute to drug development. Engineers will work at an atomic level to design new manufacturing materials to meet precise engineering needs. Weather researchers will use full-fidelity models to trace the genesis and evolution of tornadoes. Epidemiologists will predict the spread of communicable diseases with greater accuracy. And seismologists will study the effects of earthquakes on smaller structures than before, including hospitals and apartment complexes, to help improve building design.

NCSA LOOKS AHEAD TO EXASCALE COMPUTING
By the time the Blue Waters deployment is complete, the NCSA team will be deep into the planning of future projects. “We are already working closely with IBM to investigate emerging technologies and determine how they might contribute to the next generation of supercomputers,” says Beldica. “Exascale systems—which deliver a thousand times the performance of petascale systems—are on the horizon.”

To learn more about Blue Waters, visit: www.ncsa.illinois.edu/BlueWaters

To read additional IBM HPC customer success stories, visit: ibm.com/systems/deepcomputing/success/index.html