NICS to add more than 300 Teraflops to the NSF's computing capacity

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The Kraken supercomputer at NICS is currently ranked as the world's fourth fastest system. Credit: Oak Ridge National Laboratory and the University of Tennessee.

With twin awards from the National Science Foundation (NSF) totaling $3.4 million, the University of Tennessee-managed National Institute for Computational Sciences (NICS) will add 300 teraflops to the TeraGrid's total computational capability.

Researchers will also have access to more than 200 million additional service units, or CPU hours, per year, bringing the total available from NICS to over 800 million and benefitting the organization's entire user community.

The first part of the award will increase the size of Kraken, the first

academic petaflop computer and currently the world's fourth fastest machine, by 12 cabinets, adding 144 teraflops of computing power.

The Cray XT5 will now total 100 cabinets and provide 1.17 petaflops of computing capability and 147 terabytes of memory. While Kraken is an ideal resource for running some of the world's most computationally demanding simulations, the new cabinets will also assist the myriad of smaller jobs continually running on NICS's flagship system.

"We are extremely pleased to be able to put more continually available resources at the disposal of researchers with smaller codes, while still supporting the very largest applications," said NICS Director Phil Andrews. "The importance of a research activity cannot be defined by the size of the code involved, and we want to give all NICS users the best possible service."

Although Kraken is the only resource in the NSF's computing portfolio capable of running simulations at its full potential of 8,256 nodes, it also is a massive capacity resource.

Many of the more computationally demanding codes running on Kraken use the "sweet spot" of 8,192 nodes, the largest power of two that can be accommodated within the 8,256 node machine. While a code of this size is running, albeit for only part of each week, a maximum of 64 nodes remains for other users. The extension of Kraken to 9,408 nodes will increase this by a factor of 19, providing an additional 1,216 nodes for smaller jobs to run concurrently. This will greatly improve availability of the system for smaller, "capacity" jobs while still allowing the extremely large "capability" jobs access to the NSF's most powerful supercomputing system.

The second part of the award will fund the operation of Athena, a 166-teraflop Cray XT4 that is currently ranked as the TeraGrid's third

largest computational resource. Athena features 18,048 cores and 18 terabytes of memory and is an extremely reliable system, most recently used as a dedicated platform for climate, weather and quantum chromodynamics research. Athena will be available through the TeraGrid allocations process beginning October 1, 2010 and will be allocated in conjunction with Kraken. This will allow NICS to maximize the usefulness of both of these leading resources, each of which are running at over 90% utilization, by apportioning researchers to the most appropriate machine.

"The availability of large-scale computing resources has quickly evolved our field of biomolecular simulation and computational chemistry and has enabled a move from validation and assessment of the methods into the realm of prediction and production in applications ranging from the design of new biomaterials to computer-aided drug design," said NICS user Tom Cheatham of the University of Utah. "The addition of time comes at a critical juncture as the TeraGrid and other machines available in the US for research are over-subscribed, inhibiting science across a wide range of disciplines.

Colin Morningstar of Carnegie Mellon echoed Cheatham's enthusiasm: "The additional allocation time will definitely accelerate our lattice QCD research and allow us to study quarks and gluons in much larger volumes and using lighter quark masses. We are very excited about the new possibilities that this creates."

Provided by National Institute for Computational Sciences