March 10, 2005 Supercomputer Dedicated To Bioengineering And Computational Biology Installed

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The University of California, San Diego, with support from the National Institutes of Health and the Whitaker Foundation, has installed a supercomputer dedicated to solving a wide range of challenging biological problems. The 210-node Dell PowerEdge Linux cluster capable of 2.6 trillion mathematical operations per second, the second most powerful computer cluster on campus, will be used to analyze everything from the behavior of protein molecules and subcellular structures such as nerve synapses and cardiac muscle cells, to multicellular tissue and the whole heart.

"No single computational model spans all these biological scales, but this powerful new cluster will enable us to integrate models over many of these scales, which will make it possible for us to predict, in some cases, the clinical consequences of specific genetic mutations or biochemical alterations caused by disease," said Andrew McCulloch, a professor and vice chair of the Jacobs School's Department of Bioengineering. He celebrated the installation of the cluster at a ribbon-cutting ceremony March 9 in the basement of Powell-Focht Bioengineering Hall with fellow project co-leader Peter Arzberger, principal investigator and director of the National Biomedical Computational Resource (NBCR), a program funded by the National Institutes of Health, and director of Life Sciences Initiatives at UCSD.

Arzberger said the Department of Bioengineering and NBCR Dell Rocks Cluster will be quickly integrated into a computational grid to provide the resource to as many UCSD researchers as possible. Eventually, the cluster will also be made available to computational biologists and bioengineers across the country as part of a new paradigm often referred to as grid computing.

Researchers at UCSD and collaborating institutions nearby who are planning to use the cluster, include:

Mark Ellisman, a professor of neuroscience and bioengineering at UCSD and the director of the National Center for Microscopy and Imaging Research, which is based at the university. Ellisman's group is involved in a variety of projects aimed at obtaining new insight into how the nervous system functions across multiple scales.

Jeff Hasty, a computational molecular biologist and assistant professor in the Department of Bioengineering who is focused on the development of an engineering-based methodology in the theoretical design and construction of synthetic gene regulatory networks.

Trey Ideker, an assistant professor in the Department of Bioengineering whose group has developed CYTOSCAPE, a software program being used by hundreds of labs worldwide to visualize and integrate information about genes, proteins, and their interactions into models of cellular pathways and networks.

J. Andrew McCammon, a professor of theoretical chemistry in the Department of Chemistry and Biochemistry and an investigator with the Howard Hughes Medical Institute. His research group uses molecular dynamics and other computer modeling techniques to examine how protein molecules function.

Andrew McCulloch, professor and vice chair of the Department of Bioengineering whose cardiac mechanics research group uses experimental and computational models to investigate relationships between the cellular and extracellular structure of cardiac muscle and the electrical and mechanical function of the heart during ventricular remodeling and cardiac arrhythmia.

Anouchka Mihaylova, an assistant research scientist in the Department of Bioengineering who is using experimental results and computer simulations to analyze interactions of calcium ions with macromolecular structures within cardiac cells.

Arthur J. Olson, a professor in the Department of Molecular Biology at The Scripps Research Institute in La Jolla, CA, who applies computational and computer graphic techniques to the study of protein-protein recognition, antibody-antigen complexes, and other molecular interactions.

Bernhard O. Palsson, a professor in the Department of Bioengineering and adjunct professor of medicine whose group is focused on the analysis of genome-scale biochemical reaction networks with an emphasis on cellular metabolism and transcriptional regulation, particularly in several organisms.

Michel Sanner, an associate professor of molecular biology at The Scripps Research Institute who is developing computational tools to analyze and visualize macromolecular structures and interactions.

Gabriel Silva, an assistant professor in the Department of Bioengineering who is developing treatments for degenerative retinal disorders and therapies to reverse the body's often damaging repair response to central nervous system trauma.

Shankar Subramaniam, a professor in the Department of Bioengineering and the Department of Chemistry and Biochemistry who is investigating many important aspects of computational biology, including the bioinformatics of cell signaling pathways.

The new cluster, which was purchased from Dell for less than $180,000 per Teraflops (trillion floating point operations per second), is a distributed-memory parallel computer. It is valued not only for its speed, but also because its 428 gigabytes of memory capacity and 20 terabytes of storage will enable researchers to solve ever larger and more sophisticated problems. "It's not always just a matter of computational speed with some of our models - some are memory limited," said McCulloch. "For example, our models of the propogation of an electrical impulse thorough the heart wall require us to generate matricies with millions of individual cells, and our ability to solve such problems is limited by the memory available. This new cluster will enable completely new simulations of the heart and other biological systems."

Traditional supercomputer centers have historically been the workhorses of computational biology, but McCulloch said the drive to build ever faster and more specialized supercomputers has required computational biologists to continually reinvent their modeling software. "It's not new that science has been developing large computational challenges, but what is new is the commoditization of supercomputing," said McCulloch. "These commodity clusters running with an open source operating system and management software can provide a stunning degree of performance that a few years ago simply couldn't be found in a small room in the basement of a bioengineering building."

The cluster's management tool is called Rocks, an award winning toolkit developed at UCSD by a team led by Philip Papadopoulos, director of the Advanced CyberInfrastructure Lab at the San Diego Supercomputer Center and associate research scientist in the Department of Computer Science and Engineering. The open-source Rocks toolkit has been designed for rapid and scalable deployment of clusters. It currently is used in more than 500 supercomputing clusters worldwide and supports the 64-bit processors in the new cluster. In addition to its many other features, Rocks simplifies many administration requirements.

Within a few days of unpacking more than 400 boxes containing the Dell nodes, bioengineering researchers this week had modeled how electrical impulses trigger contractions in the heart of a pig.

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