Established in 1987, PSC’s National Resource for Biomedical Supercomputing (NRBSC) was the first external biomedical supercomputing program funded by the National Institutes of Health (NIH) and has continued uninterrupted since then. Along with core research at the interface of supercomputing and the life sciences, NRBSC scientists develop collaborations with biomedical researchers around the country, fostering exchange among experts in computational science and biomedicine and providing computational resources, outreach and training.

In September 2012, NRBSC gained renewed NIH support as a participant in a newly funded Biomedical Technology Research Center (BTRC) on High-Performance Computing for Multiscale-Modeling of Biological Systems. This $8 million grant, from NIH’s National Institute of General Medical Sciences, establishes a collaboration between the University of Pittsburgh, Carnegie Mellon University and PSC. The principal investigator of the BTRC, Ivet Bahar, chairs the Department of Computational & Systems Biology at the University of Pittsburgh School of Medicine. Markus Dittrich of NRBSC leads the PSC component, and Robert F. Murphy, director of the Lane Center for Computational Biology, leads Carnegie Mellon’s participation.

“This collaboration opens many opportunities as NRBSC goes forward,” says Dittrich. “Through the new BTRC, we continue our work in cellular modeling, structural biology, and large-scale volumetric image analysis, and we gain through synergy with the outstanding computational biology programs at the University of Pittsburgh and Carnegie Mellon.”

Anton Program Extended

A supplementary award to the newly established BTRC also provides $1.1 million to extend the Anton program (see pp. 26-31) for another two years. In partnership with D. E. Shaw Research (DESRES), this program makes an innovative computing system available to U.S. biomedical scientists. Having served 91 research projects by more than 70 individual research groups in two years, the Anton program commenced a new round of allocations in November 2012.

“We are thrilled about the impact that Anton has had over the last two years,” says Markus Dittrich of NRBSC, “and we are excited to be able to offer continued access to this great resource for the biomedical community.”

More info: http://www.nhsc.org

Biomedical image processing using NRBSC-developed software enables accurate three-dimensional reconstruction of brain circuits from massive serial-section electron microscopy image sets. The example shown here spans a cortical region of mouse brain and is built from 3000 individual camera images at four nanometer resolution. After registration at the NRBSC, the large sectional reconstruction occupies 12 gigabytes. Thousands of these sections are then combined and aligned into 3D volumes for visualization and analysis of neural pathways.

Research

NRBSC research focuses on three areas of biomedicine that span many scales of space and time:

Spatially realistic cell modeling centers on stochastic computer simulations of movements and reactions of molecules within and between cells, to better understand physiological function and disease. MCell and CellBlender software is developed at the NRBSC and used to model and visualize events such as shown in this image) neurotransmission between nerve and muscle cells.

NRBSC structural biology focuses on computational tools to determine the structure of proteins from their amino-acid sequence and quantum-mechanical simulation methods for biomolecules such as enzymes. This image shows structure for the oxacillinase class D beta-lactamase enzyme, with the “active site” in blue. Beta-lactamase is a bacterial enzyme that is a major mechanism of antibiotic resistance. PSC-developed software enables researchers to simulate enzyme reactions and gain new insight into enzyme function, which facilitates design of new therapeutic drugs.

NRBSC and PSC have also developed educational programs, CRFT and BEST (see pp. 8-9), that have provided training to high-school and undergrad students and educators in the Pittsburgh region and nationally.