

# THE NATIONAL RESOURCE FOR BIOMEDICAL SUPERCOMPUTING

Twenty Years of Leadership  
Renewed for Five More Years

In October, PSC received \$8.5 million from the National Institutes of Health to renew its program in biomedical supercomputing, renamed last year as the National Resource for Biomedical Supercomputing. Through NRBSC, PSC scientists pursue research in the life sciences and foster exchange nationwide among experts in computational science and biomedicine.

Established in 1987, PSC's biomedical supercomputing program was the first such program in the country external to NIH. Along with core research, NRBSC develops collaborations with biomedical researchers at many centers around the country and provides computational resources, outreach and training. The current award, from NIH's National Center for Research Resources (NCR), renews NRBSC for another five years.

"This grant is part of NCR's ongoing commitment to bring together leading-edge computational resources and experts in computing with experts in biology and medicine," said Ralph Roskies, PSC co-scientific director.

"A great deal of important biomedical work over the last decade owes thanks to NIH support for this program," said PSC senior scientist Joel Stiles, scientific director of NRBSC. "We've developed computational tools in simulation and visualization that are helping scientists nationwide."

More information: <http://www.nrbsc.org>

## Core Research

The renewal award supports NRBSC's research in three core areas: spatially realistic cellular modeling, large-scale volumetric visualization and analysis, and computational structural biology.

"Our long-term vision," said Stiles, "includes integration of these areas to enable multiscale modeling of molecules, cells and tissues, with a substantial future impact on human health care."



The NRBSC team (l to r): Joel Stiles, Stuart Pomerantz, Jack Chang, Alex Ropelewski, Boris Kaminsky, Greg Hood, Jenda Domaracki, Demian Nave, Hugh Nicholas, Markus Dittrich, Bob Bourne, Christal Banks, Adam C. Marko, Art Wetzel, Troy Wymore.

### NRBSC BIOMEDICAL COLLABORATIONS

Albert Einstein College of Medicine  
Carnegie Mellon University  
Duke University  
Hospital for Sick Children, Toronto  
Howard University  
Marine Biological Laboratory, Woods Hole  
Morgan State University  
North Carolina Central University  
Rockefeller University  
The Salk Institute  
The Scripps Research Institute  
University of California at Davis  
University of California at San Diego  
University of North Carolina, Chapel Hill  
University of Pittsburgh  
University of Pittsburgh School of Medicine  
University of Puerto Rico, Medical Sciences Campus

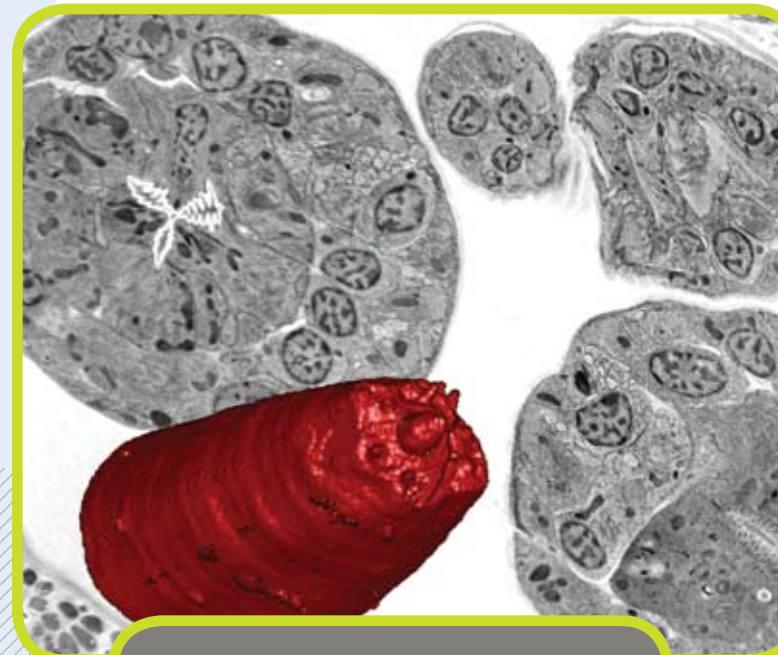
## Training & Resources

NRBSC training activities reach hundreds of scientists each year. Since its inception, NRBSC has provided access to computing resources for more than 1,200 biomedical research projects involving more than 3,500 researchers at 245 research institutions in 46 states and two territories. Among these are several projects featured in this booklet (p. 18 & 22).

NRBSC workshops on computational biology have trained more than 3,300 researchers in the use of high-performance computing for biomedical research, in such areas as spatially-realistic cell modeling, volumetric data visualization and analysis, protein and DNA structure, genome sequence analysis and biological fluid dynamics.

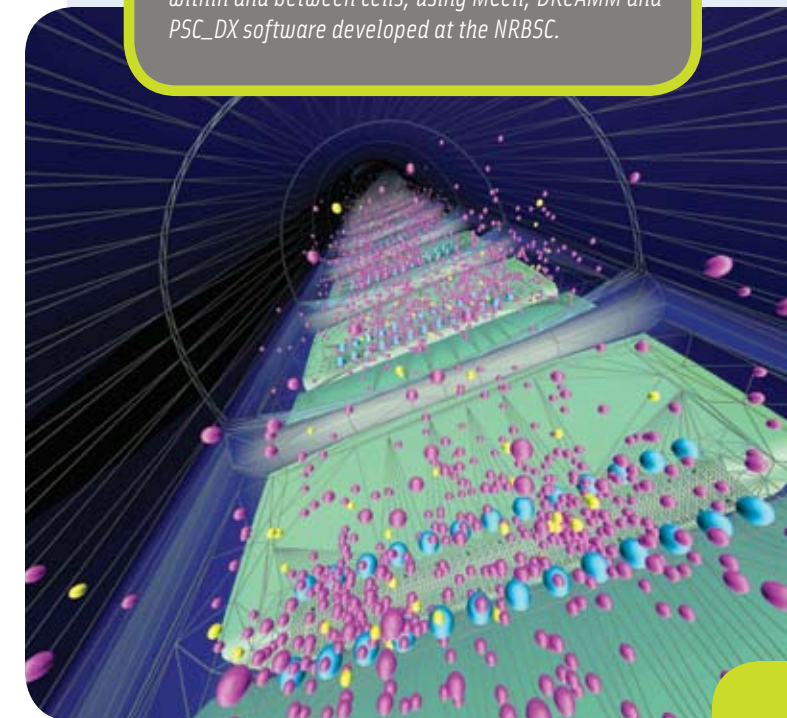
This year a Bioengineering & Bioinformatics Summer Institute program funded jointly by NSF and NIH was renewed for three more years. NRBSC participates with the University of Pittsburgh, Carnegie Mellon and Duquesne University in this 10-week summer intensive that trains promising college students for research in computational biology-related fields. NRBSC director Joel Stiles serves on the core faculty and other NRBSC scientists act as research mentors.

More information on BBSI: <http://www.ccbb.pitt.edu/bbsi>



Volumetric visualization involves research with software called PSC\_VB, also developed at NRBSC, that enables multiple users to share, view and analyze very large-scale three-dimensional and four-dimensional datasets, such as time series of mouse cardiac function obtained from high resolution CAT scan imaging.

Spatially realistic cellular modeling centers on realistic three-dimensional cellular models to simulate the movements and reactions of molecules within and between cells, using MCell, DReAMM and PSC\_DX software developed at the NRBSC.



Structural biology focuses on the development of computational tools used to determine the structure of proteins from their amino-acid sequence and also the development of quantum-mechanical simulation methods for biomolecules such as enzymes.

