

NOTES & HIGHLIGHTS

NETWORKING

One of the leading resources in the world for network know-how

THE FUTURE

PSC's Advanced Networking group is one of the leading resources in the world for knowledge about networking. Through 3ROX (Three Rivers Optical Exchange), a high-speed network hub, they provide high-performance networking for research and education. Their research on network performance and analysis — in previous projects such as Web100 and the NPAD diagnostic server — has created valuable tools for improving network performance nationally.

MORE INFORMATION: <http://www.psc.edu/networking/>

PSC ADVANCED NETWORKING GROUP
(seated, l to r):

Stephen Petko, Wendy Huntoon, and Michael Lambert, (standing) Chris Rapier, Kathy Benninger, Joe Lappa, Andrew Adams, Steve Cunningham, Ken Goodwin, Shane Filus, John Heffner, Matt Mathis and Jim Miller.

Not in photo, **Janet Brown.**

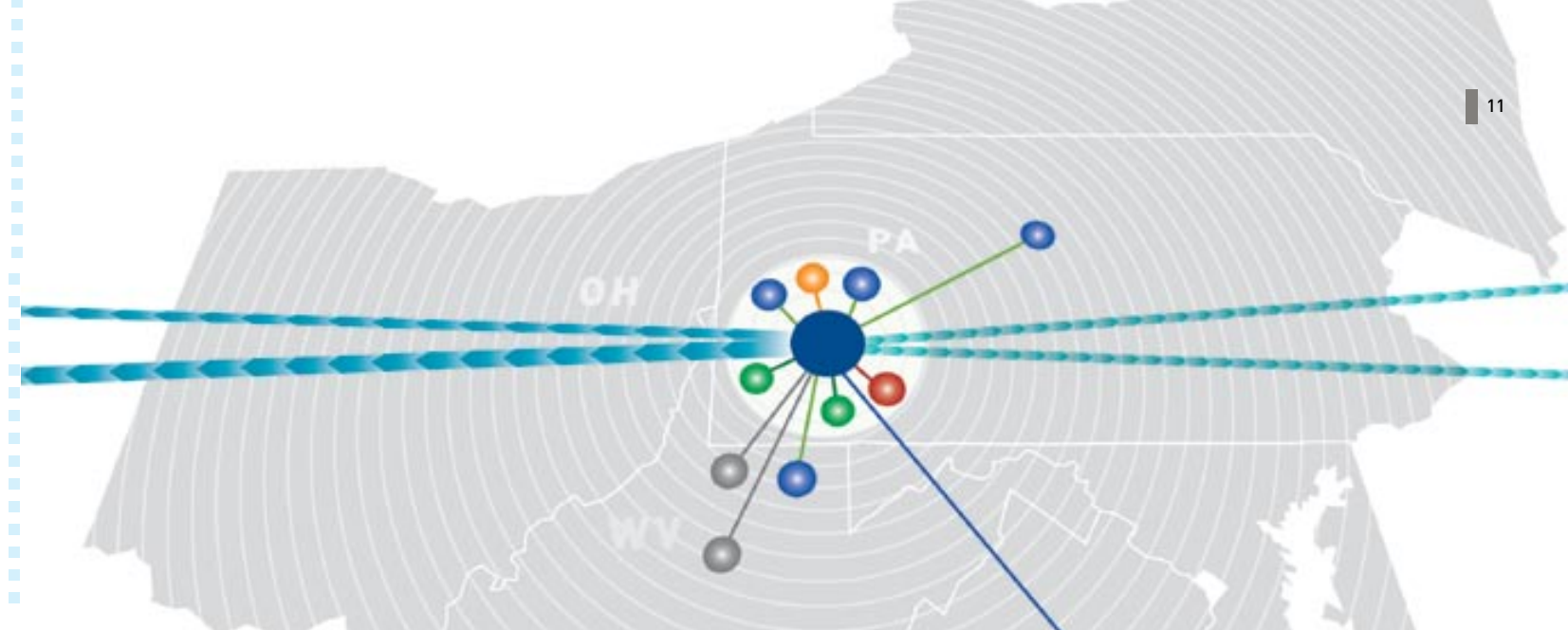


HUNTOON ELECTED

TO INTERNET2 RESEARCH ADVISORY COUNCIL

PSC director of networking Wendy Huntoon, who also directs operations for National LambdaRail (NLR), a major initiative of U.S. research universities and the private sector to provide infrastructure for research in networking technologies, this year was elected to a regional network seat on Internet2's Research Advisory Council.

Huntoon also serves on the steering committee for NSF's community-based planning activity, which gathers input on the infrastructure required by the science and engineering research and education community after the current TeraGrid project awards expire in early 2010.



3ROX MEMBERS

- **Universities**
Carnegie Mellon University, Norfolk State University, Pennsylvania State University, University of Pittsburgh, Waynesburg University, West Virginia University
- **K-12 Institutions**
Pittsburgh Public Schools, Woodland Hills School District, Intermediate Units 1, 2 (Pittsburgh), 3 (Allegheny), 5 (Northwest Tri-County), 6 (Riverview), 27 (Beaver Valley) and 28 (ARIN)
- **Government Laboratory**
The National Energy Technology Laboratory
- **Business**
Comcast, Westinghouse Electric Co.
- **Other**
Computer Emergency Response Team

NETWORK CONNECTIONS

- ← **National Research Networks**
Internet2 — 1 Gbps, National LambdaRail PacketNet — 10 Gbps, TeraGrid Extensible Backplane Network — 30 Gbps
- Other Network Connections**
Southern Crossroads (SOX) — 1Gbps, TransitRail — 1Gbps
- ← **National Commodity Internet Networks**
Global Crossing — 1 Gbps; Sprint — 1 Gbps. (Pittsburgh Local Exchange Networks) Comcast

Note: Gbps: a billion (Giga) bits per second

3ROX

Through 3ROX, a high-speed network hub, PSC provides advanced network resources for education and research. 3ROX connects universities and public schools to high-performance networks, such as Internet2, which links leading U.S. universities, corporations, government research agencies, and not-for-profit networking organizations.

3ROX NEWS

3ROX contracted this year with FiberTech for a "co-location space" at Allegheny Center Mall (ACM) on Pittsburgh's near North Side. This network co-location space will provide a redundant location for 3ROX members to connect, initially only for commodity network connectivity, and eventually to include all services supported by 3ROX. ACM also provides an additional primary connection point for 3ROX members and collaborators.

Waynesburg University became a 3ROX member this year, and the University of Pittsburgh upgraded their connection to 3ROX from one to 10 Gbps. This new connection allows them to take better advantage of the NLR related services associated with 3ROX, including connectivity to PacketNet and the TransitRail peering service.

3ROX this year added several school district intermediate units, including Beaver Valley, Allegheny and a shared connection for Riverview, Northwest Tri-County and ARIN. These schools now have connectivity to Internet and NLR research and education networks as well as regional networks.

ADVANCED NETWORK RESEARCH

Through projects such as Web100 (www.web100.org), PSC's networking group has played a major role nationally in engineering the Internet. During this past year, they have authored and published several RFCs, official standards of the Internet Engineering Task Force, an open international community of network designers, operators, vendors, and researchers concerned with evolution and operation of the Internet.

In May, PSC researchers Matt Mathis and John Heffner authored "Packetization Layer Path MTU Discovery," a new standard for improved Internet performance. This work describes a method to automatically assess the best Maximum Transfer Unit (MTU) — the biggest data packet a connection can efficiently use — for a given network connection.

In June, Mathis, Heffner and Rajiv Raghunathan of Cisco published "TCP Extended Statistics MIB." This important standard, essentially the main deliverable from the Web100 project, describes extended performance statistics for TCP (transmission control protocol), a core software protocol that underlies the majority of Internet applications. With the performance statistics defined by this document, diagnostic tools can — in situations of poor network performance — directly ask TCP why it is slow and gather information on the nature of the problem.

"It takes the guesswork out of network debugging," says Mathis. "If a network-based application is performing poorly, TCP can determine if the bottleneck is in the sender, the receiver, or the network itself. If the bottleneck is in the network, TCP can provide specific information about its nature." Prototypes implemented to this RFC were incorporated into a number of operating systems, including Linux and Microsoft Vista.

THE NRBSC TEAM (l to r): →

Pallavi Ishwad, Art Wetzel, Jacob Czech, Alex Ropelewski, Jenda Domaracki, Boris Kaminsky, Demian Nave, Jack Chang, Hugh Nicholas, Joel Stiles, Troy Wymore, Greg Hood, Stu Pomerantz, Markus Dittrich, Adam Marko and Christal Banks



NOTES & HIGHLIGHTS CONTINUED

THE NATIONAL RESOURCE FOR BIOMEDICAL SUPERCOMPUTING

National Leadership in High-Performance Computing for Biomedical Research

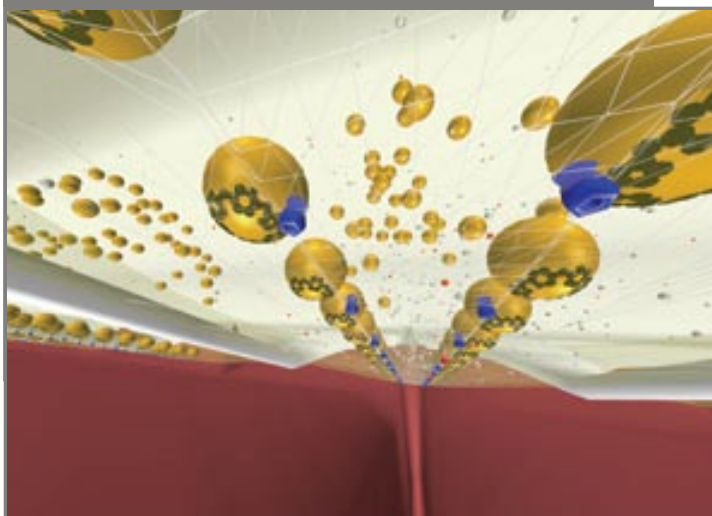
Established in 1987, PSC's National Resource for Biomedical Supercomputing (NRBSC) was the first external biomedical supercomputing program funded by the National Institutes of Health (NIH). Along with core research at the interface of supercomputing and the life sciences, NRBSC scientists develop collaborations with biomedical researchers around the country, fostering exchange among experts in computational science and biomedicine and providing computational resources, outreach and training. In October 2006, NRBSC received \$8.5 million from NIH's National Center for Research Resources (NCRR) to renew its work for five years.

"Over the past decade, computing has become essential to almost all aspects of biomedicine," says PSC's Joel Stiles, director of NRBSC, a medical doctor who also holds a doctorate in physiology. "Here at the NRBSC, we're developing and distributing computational tools in simulation, visualization, and education that are helping to transform our understanding of life and disease."

MORE INFORMATION: <http://www.nrbsc.org>

RESEARCH

NRBSC research focuses on three areas of biomedicine that span many scales of space and time: spatially realistic cell modeling, large-scale volumetric visualization and analysis, and computational structural biology.



Spatially realistic cell modeling centers on realistic 3-D simulations of movements and reactions of molecules within and between cells, to better understand physiological function and disease. As illustrated in this image, MCell, DReAMM and PSC_DX software is developed at the NRBSC and is used to model events like neurotransmission between a nerve and muscle cell.

NRBSC Biomedical Collaborations

Albert Einstein College of Medicine

Carnegie Mellon University

Cornell University

Duke University

Howard University

Janelia Farm, Howard Hughes Medical Institute

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 Kansas

University of North Carolina, Chapel Hill

University of Pittsburgh

University of Pittsburgh School of Medicine

University of Puerto Rico, Medical Sciences Campus

COMPUTATIONAL SERVICE & TRAINING

Since its inception, NRBSC has provided access to computing resources for more than 1,200 biomedical research projects involving more than 3,800 researchers at 255 research institutions in 45 states and two territories. Among these are several projects featured in this booklet (pp. 26 & 30).

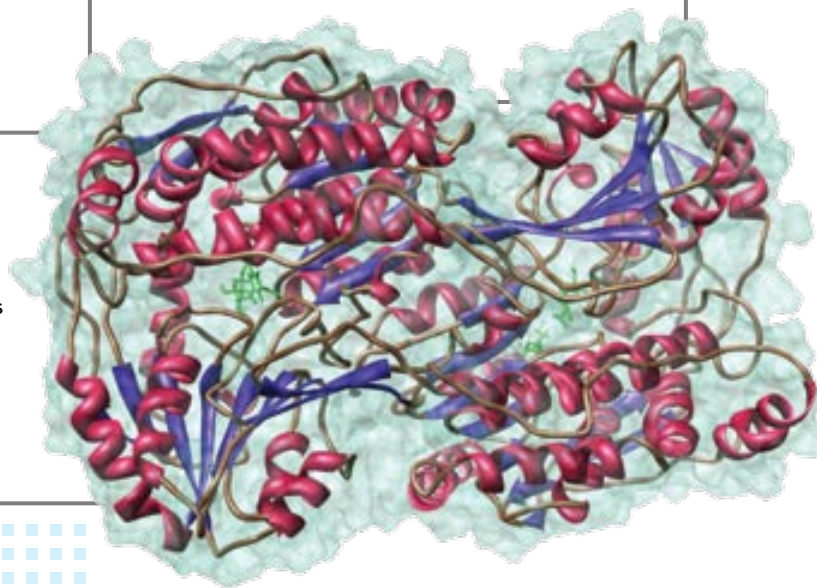
NRBSC training activities reach hundreds of scientists each year. More than 3,400 researchers have participated in NRBSC workshops in such areas as spatially realistic cell modeling, volumetric data visualization and analysis, protein and DNA structure, genome sequence analysis and biological fluid dynamics.

NRBSC participates in a range of undergraduate and graduate training programs. These include:

- A joint Carnegie Mellon and University of Pittsburgh Ph.D. program in computational biology (www.compbio.cmu.edu).
- The Ray and Stephanie Lane Center for Computational Biology at Carnegie Mellon (lane.compbio.cmu.edu).
- The University of Pittsburgh Department of Computational Biology (www.ccbb.pitt.edu).
- The undergraduate Bioengineering & Bioinformatics Summer Institute (www.ccbb.pitt.edu/bbsi), sponsored by NRBSC, Carnegie Mellon, the University of Pittsburgh, and Duquesne University, and funded jointly by NSF and NIH.



Volumetric visualization is based on the NRBSC's PSC_VB software, enabling multiple users to share, view and analyze extremely large datasets and time series obtained from light and electron microscopes, CAT and MRI scanners, etc. This image illustrates Visible Human data from the National Library of Medicine, analyzed with PSC_VB and rendered with DReAMM.



NRBSC structural biology focuses on computational tools used to determine the structure of proteins from their amino acid sequence and development of quantum-mechanical simulation methods for biomolecules such as enzymes. This image shows the 3-D structure of human p5cdh, an enzyme involved in metabolism of sugars.

NOTES & HIGHLIGHTS CONTINUED

K-12 SCIENCE OUTREACH

The NRBSC and PSC are developing innovative Computational Modules In Science Teaching (CMIST) for high-school biology, chemistry, physics, computer science and math. CMIST modules bring critical concepts to life in novel ways, using realistic models and simulations with visually appealing, scientifically accurate animations. NRBSC distributes the modules online and on DVDs. They include lecture slides, animations, lesson plans aligned to national and state standards, worksheets and answer keys. NRBSC developed the pilot module, "Molecular Transport in Cells," through a summer 2007 series of workshops with 37 western Pennsylvania high-school science teachers from 17 school districts, who gave enthusiastically positive feedback.

Pittsburgh Supercomputing Center Workshops (2006-2007)

Petascale Applications Symposium

Computational Methods for Spatially-Realistic Microphysiological Simulations

Summer Institute in Bioinformatics (for minority-serving institutions)

Parallel Programming

Toward Multicore Petascale Applications

Introduction to the Cray XT3

Methods and Applications of Hybrid QM/MM Simulations to Biomolecular Systems

Bioinformatics

A workshop underway in the PSC Computer Training Center, the David W. Deerfield II Training Center, equipped with 30 "dual-boot" workstations and a projector for overhead display of the instructor's desktop.



↑
PSC'S DIRECTORS AND MANAGERS (front, l to r):

Cheryl Begandy, outreach manager; **Elvira Prologo**, manager of administration; **Bob Stock**, PSC associate director; **Rich Raymond**, manager of user support; **Wendy Huntoon**, director of networking; **Sergiu Sanielevici**, director of scientific applications and user support; (back): **David Kapcin**, director of financial affairs; **Joel Stiles**, director of NRBSC; **John Kochmar**, manager of high-performance computing facilities; **J.Ray Scott**, director of systems & operations; **Katherine Vargo**, manager of scientific computing systems.

Not in photo: **Nick Nystrom**, director of strategic applications; **Laura McGinnis**, manager of data & information resource services; **Janet Brown**, manager of networking; **Clint Perrone**, manager of systems and operations.

PROJECTS

IN SCIENTIFIC COMPUTING

2007