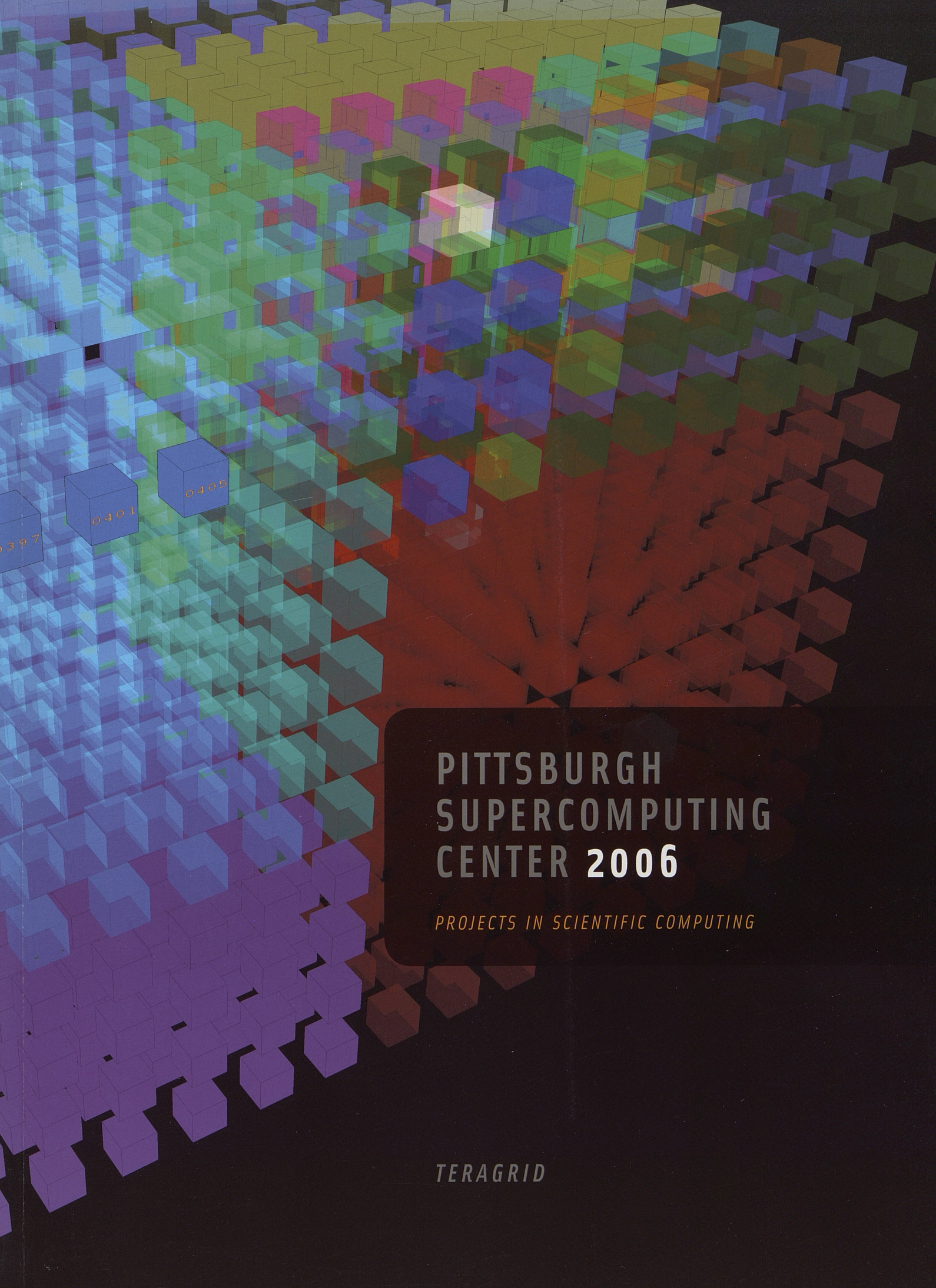

PITTSBURGH SUPERCOMPUTING CENTER 2006

PROJECTS IN SCIENTIFIC COMPUTING

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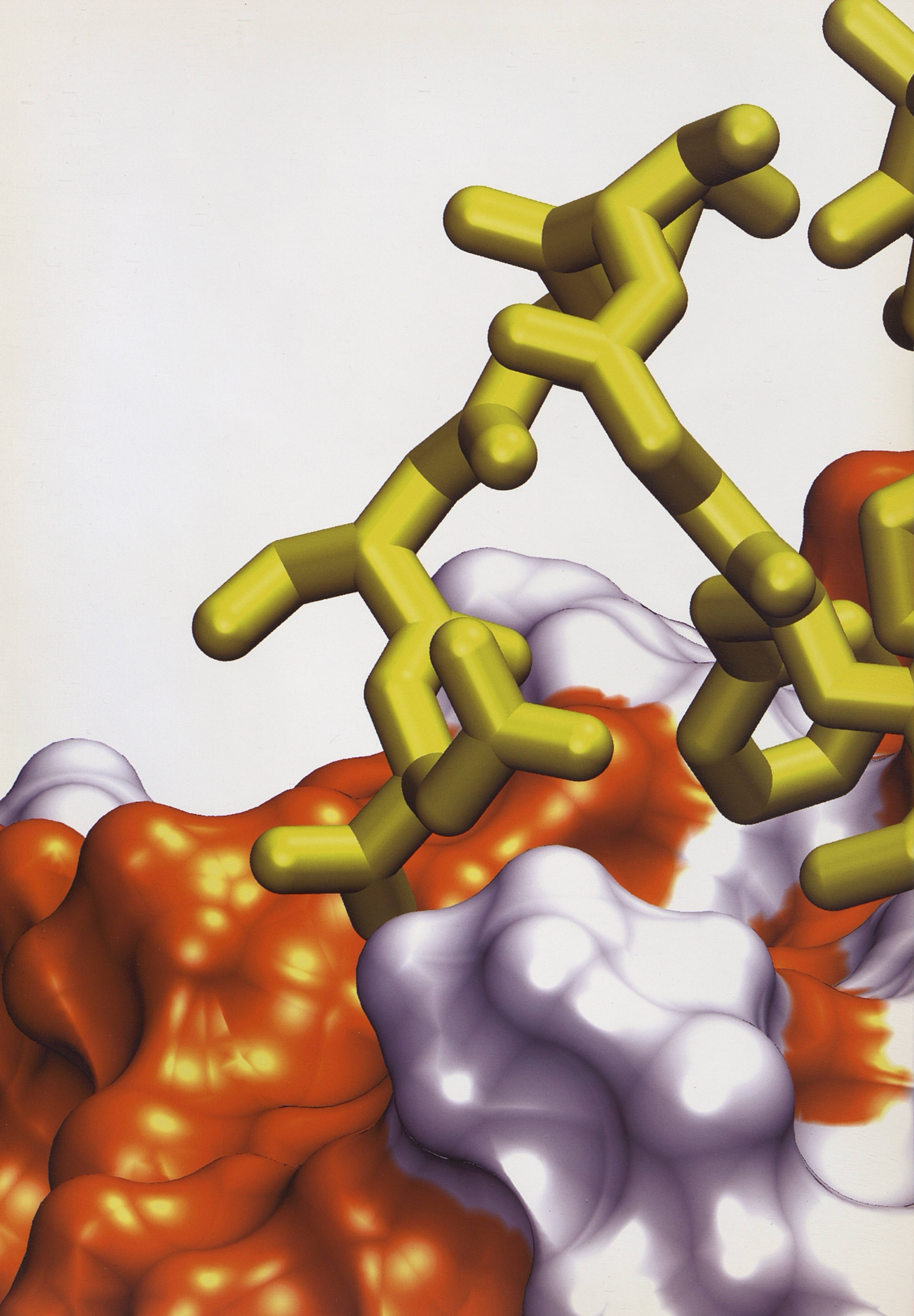


PSC.EDU/06

The Pittsburgh Supercomputing Center provides university, government and industrial researchers with access to several of the most powerful systems for high-performance computing, communications and data-handling available to scientists and engineers nationwide for unclassified research. PSC advances the state-of-the-art in high-performance computing, communications and informatics and offers a flexible environment for solving the largest and most challenging problems in computational science. As a leading partner in the TeraGrid, the National Science Foundation's program to provide a coordinated national cyberinfrastructure for education and research, PSC works with other TeraGrid partners to harness the full range of information technologies to enable discovery in U.S. science and engineering.

WWW.PSC.EDU

412-268-4960

Scientific progress at the Pittsburgh Supercomputing Center during the past year centers around our Cray XT3 system, BigBen, which has proven itself to be a massively-parallel powerhouse. As this publication demonstrates (pp. 18, 22, 26, 30, 34, 43, 45, 46), the XT3 is making possible projects and resulting new insights that would have been unthinkable before PSC brought this system into being last year as a production resource for the TeraGrid.

Our work with the TeraGrid, NSF's program to transform the nation's research capability, is advancing (p. 4), with emphasis on both scientific output and community building with PSC contributing the same staff excellence and leadership that has sustained our work for the past 20 years.

Along with celebrating our 20-year anniversary (p. 6), we moved into a new building with office space designed for PSC use. The National Resource for Biomedical Supercomputing, PSC's biomedical program, received five-year renewal funding from the NIH's National Center for Research Resources (p. 10). Our work as part of the Supercomputing Science Consortium (p. 8) and our collaboration with the U.S. Department of Energy's National Energy Technology Laboratory take on renewed importance in the context of increasing awareness of the need to develop alternative fuels.

Science is our reason for being, and we're pleased to have enabled significant new research. Some of it hints at how much more can be achieved with petascale computing, only a few years away, and for which we are preparing ourselves and the community.

Among these projects is important work from Klaus Schulten and colleagues (p. 22) in understanding a very large multi-protein complex, the nuclear pore complex, which is prelude — thanks to the XT3 — to even bigger, similar projects already underway at PSC.

Michael Klein's group has had many successes with PSC systems over the past decade. Their work on the metallo-beta-lactamase enzyme (p. 22) has crucial public health implications.

The powerful LSMS software developed at Oak Ridge has opened new insight into magnetic nanoparticles (p. 26).

New thinking about how stars form (p. 30) is the result of Mordecai-Mark Mac Low's simulations on LeMieux, and through his work PSC simulations are part of "Cosmic Collisions," a planetarium show produced by the American Museum of Natural History that will reach millions of people.

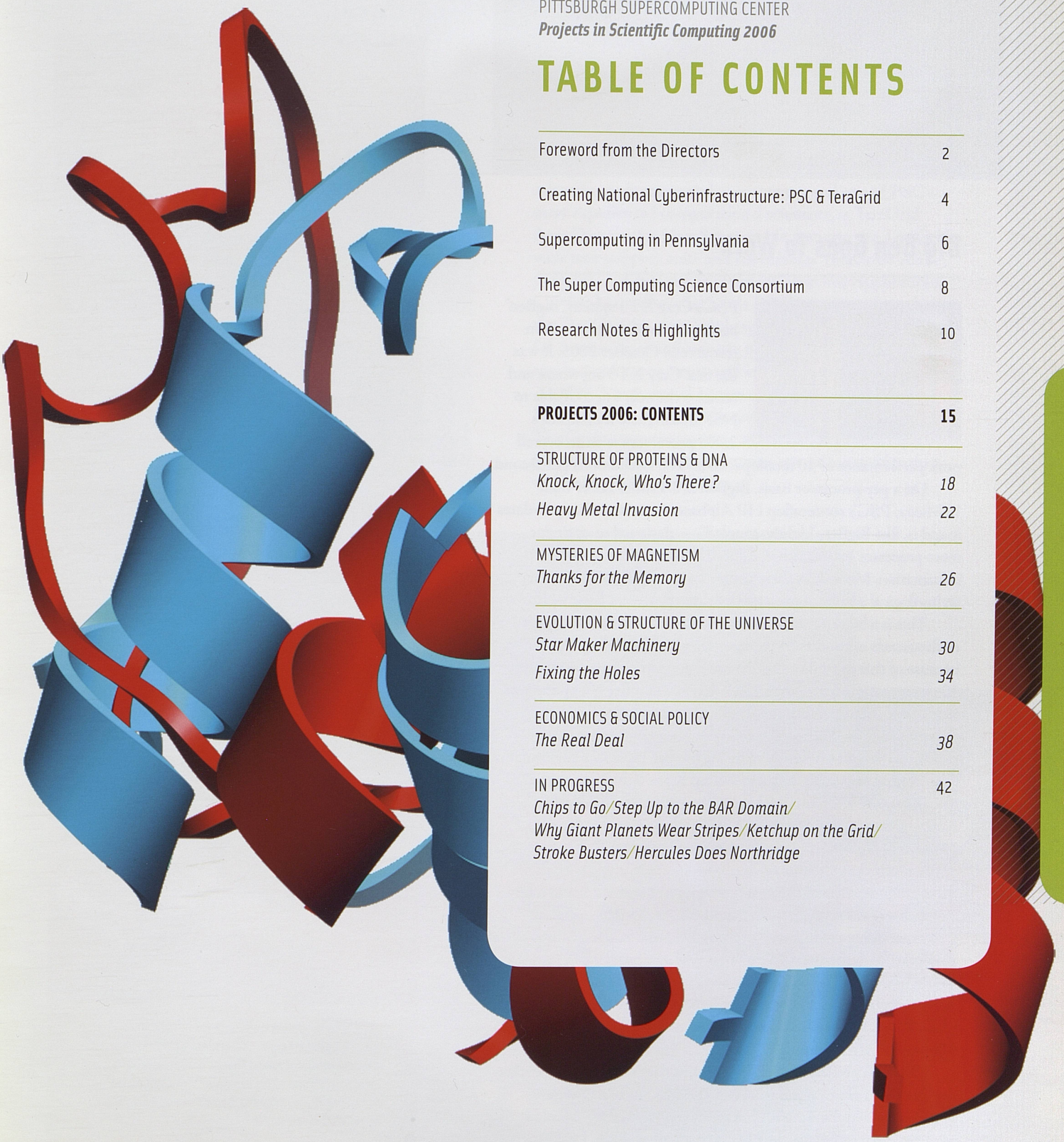
Close to home, Carnegie Mellon astrophysicist Tiziana Di Matteo made productive use of the XT3 during its "friendly-user" shakedown phase, and the result (p. 34) is major new understanding about how black holes are integral to cosmic structure.

In economics and other social sciences, supercomputing is an emerging resource. John Rust is a leader in applying these tools in this field, as evidenced by his work with the life-cycle model (p. 38).

Our success with BigBen and in other phases of our work is testimony to the knowledge, experience, creativity and energy of PSC's staff.

We are grateful for the support we receive from the National Science Foundation, the U.S. Department of Energy, the National Center for Research Resources of the National Institutes of Health, the Commonwealth of Pennsylvania and many others.

Michael Levine (right) and **Ralph Roskies**, PSC co-scientific directors, with Big Ben, Cray XT3 serial #1.



PITTSBURGH SUPERCOMPUTING CENTER
Projects in Scientific Computing 2006

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CREATING CYBERINFRASTRUCTURE

The TeraGrid is the world's most comprehensive distributed cyberinfrastructure for open scientific research. As a major partner in this National Science Foundation program, PSC plays a leadership role in shaping the vision and progress of the TeraGrid.

Big Ben Goes To Work

PSC's Cray XT3 system "BigBen" became a TeraGrid production resource in October 2005. It was the first Cray XT3 anywhere and remains the only one available to NSF researchers. It comprises 2,090 processors with an overall peak performance of 10 teraflops: 10 trillion calculations per second.

On a per-processor basis, BigBen is 2.4 times faster than LeMieux, PSC's six-teraflop HP Alphaserver system that pre-dates it and is, like BigBen, "tightly-coupled" — designed to optimize inter-processor bandwidth, the speed at which processors share information. More than sheer processor speed, BigBen's primary technological advance is its superior inter-processor bandwidth.

This is a large advantage for projects that demand hundreds or thousands of processors working together. Over the past year, because of this capability, BigBen has demonstrated performance 10 times or more better than LeMieux on a number of applications. Because of this capability also, BigBen has proven itself to be a champion at "scaling" — the ability to use a large quantity of processors without seriously reducing the per-processor performance.

Several research groups, including Klaus Schulten's group at the University of Illinois, Urbana-Champaign (p. 18) and Michael Klein's group at the University of Pennsylvania (p. 22), have found that BigBen scales to twice as many processors as the same applications on LeMieux, an improvement that, along with faster processors, represents a big gain in capability, and has led to many research successes (pp. 18, 22, 26, 30, 34, 43, 45, 46).

Researchers with large-scale parallel projects quickly caught on to BigBen's advantages. Over its first year as a production resource, nearly half of BigBen's usage has been for projects that use 1,024 processors or more, and at the last national allocation meeting, it was the TeraGrid resource most "oversubscribed" — demand in excess of available time.

BigBen's predecessor as PSC's lead system, LeMieux, remains an actively used TeraGrid resource, and PSC fulfills a unique function within the TeraGrid in providing two tightly-coupled systems. Between them, during the first half of 2006, LeMieux and BigBen provided 40 percent of overall TeraGrid usage.

TeraGrid™

TeraGrid Resource Providers
Indiana University
National Center for Supercomputing Applications
National Center for Atmospheric Research
Oak Ridge National Laboratory
Pittsburgh Supercomputing Center
Purdue University
San Diego Supercomputer Center
Texas Advanced Computing Center
The University of Chicago/Argonne National Laboratory

Jim Kasdorf, PSC director of special projects

PSC staff whose work contributes to TeraGrid include (l to r): **Laura McGinnis, Michael Schneider** (seated), **Nathan Stone, Josephine Palencia, Sergiu Sanielevici, Shandra Williams, Kathy Benninger, Rob Light, David O'Neal** (on floor), **R. Reddy, Derek Simmel, Rich Raymond, Jim Marsteller.**

TeraGrid 2006: PSC Rolls Up Its Sleeves

In several projects, PSC staff have helped to advance the technological infrastructure of the TeraGrid:

- In a major TeraGrid effort, PSC staff applied security controls for jobs run on LeMieux, PSC's terascale system, from the "portal" of the NanoHub Science Gateway. The solution involved adapting "community shell" software developed at NCSA. This PSC project is the first effort within TeraGrid to implement a security model that reconciles the community-wide reach of a Science Gateway with the secure environment of a large-scale system like LeMieux, experience we can apply to other Gateways.
- PSC network staff deployed a TeraGrid version of PSC's NPAD diagnostic service (see p. 14) on three of TeraGrid's network monitoring computers, and users have found it to be an effective tool.
- PSC staff developed software to automate the execution of "speedpage," a TeraGrid routine to measure file-transfer performance among TeraGrid sites with Globus middleware. As a result, speedpage now functions effectively to give users advance information on the file-transfer rate they can expect with these middleware routines.
- A reliable, versatile wide-area-network (WAN) file system is an important TeraGrid objective. Highly experienced in file systems across a range of architectures, PSC's systems & operations staff have implemented two separate WAN file-system projects this year. The GPFS-WAN (Global Parallel File System) developed at SDSC is now operational across TeraGrid. In a forward-looking project, PSC has led efforts to create a testbed for the flexible, open-source Lustre-WAN file system, used on PSC's TeraGrid resources. The Lustre-WAN testbed is now operational at PSC, Oak Ridge National Laboratory, Indiana University and NCSA.

Support For TeraGrid

PSC is actively involved in directing the progress of TeraGrid. Scientific director Ralph Roskies serves on the executive steering committee of the GIG, the Grid Infrastructure Group that guides TeraGrid, and scientific director Michael Levine is the principal contact for PSC as one of nine "resource provider" sites.

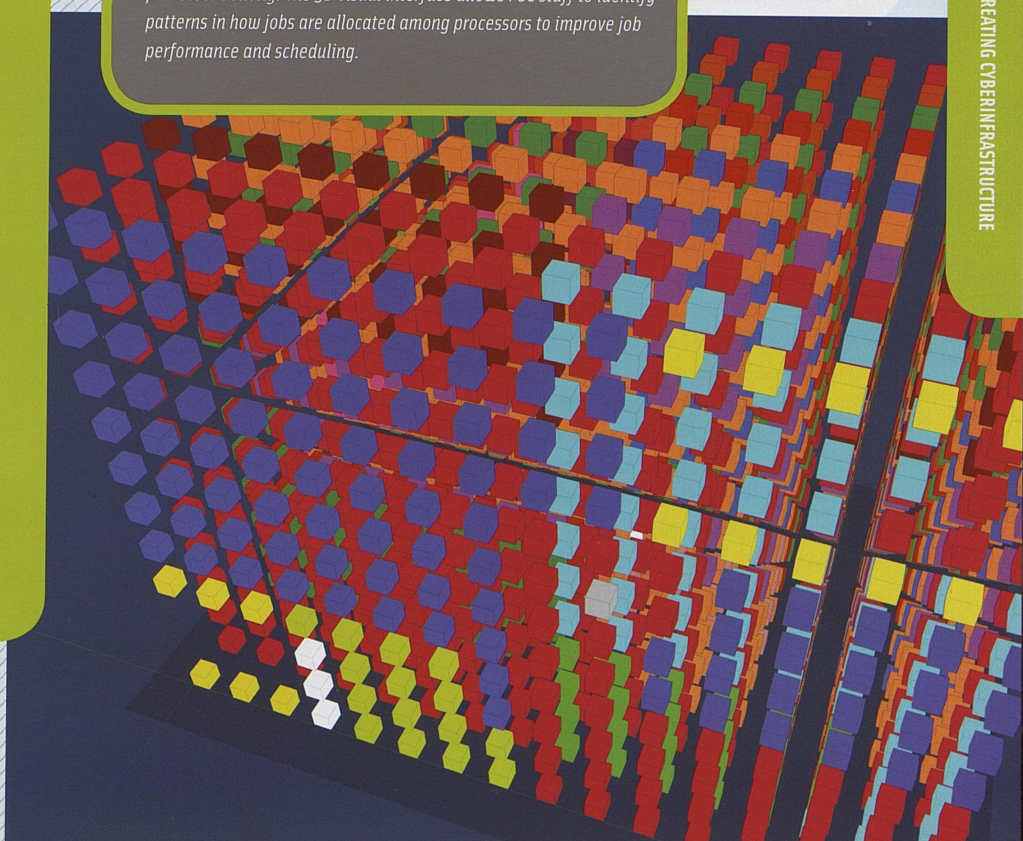
Several of PSC's key staff are committed heavily to TeraGrid work. Sergiu Sanielevici, PSC director of scientific applications and user support and one of PSC's most experienced computational scientists, is TeraGrid Area Director for User Support. He manages the TeraGrid-wide user-support team and coordinates TeraGrid's ASTA program — Advanced Support for TeraGrid Applications.

Jim Marsteller, who heads PSC's security effort, chairs the TeraGrid Security Working Group. He's responsible for developing sound security practices for TeraGrid and to conduct risk assessments and incident response as necessary.

PSC's manager of systems/software projects, Laura McGinnis, has made significant contributions to the TeraGrid accounting system, which handles the complex task of tracking allocations at nine resource-provider sites with many different systems.

xt3dmon

On a 42-inch, high-definition, liquid-crystal screen, the NSF Office of Cyberinfrastructure displays a live readout from PSC-developed software called xt3dmon. This program, written by interns in PSC's training program, provides an onscreen realtime picture of BigBen's processor activity. The 3D visual interface allows PSC staff to identify patterns in how jobs are allocated among processors to improve job performance and scheduling.



SUPERCOMPUTING IN PENNSYLVANIA

With Commonwealth of Pennsylvania support, PSC provides education, consulting, advanced network access and computational resources to scientists and engineers across the state.

Twenty Years of Leadership (1986-2006)

On June 16, leaders from industry, universities and government gathered to celebrate PSC's 20th anniversary. Established in 1986, PSC has become one of the world's leading institutions in high-performance computing and communications and a catalyst for high-technology development in Pennsylvania.

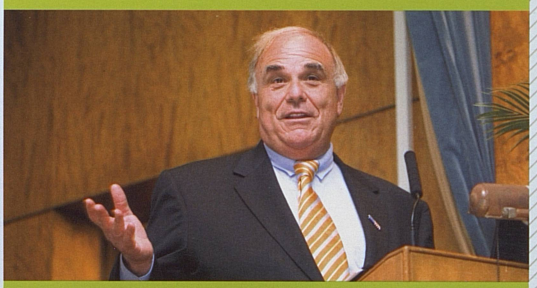
One of PSC's strengths has been its affiliation with both of western Pennsylvania's major research universities. President Jerry Cohen of Carnegie Mellon and Chancellor Mark Nordenberg of the University of Pittsburgh were on hand to help mark the occasion. Both commented on PSC's support for business and economic growth.

"This region's premiere partnership is the one we have gathered to salute today — the Pittsburgh Supercomputing Center," said Nordenberg. "It leverages the complementary strengths of three very special institutions — Carnegie Mellon University, the University of Pittsburgh, and Westinghouse."

"Alcoa, PPG, and many other private companies from this region are partners with the PSC," said Cohen. "These companies talk about how the ability to use PSC and to be supported by PSC contributes to their competitiveness in the businesses that they pursue."

Aris Candris, senior vice president, nuclear services, represented Westinghouse Electric Company, which has partnered with PSC since its beginning and provides a home for PSC's supercomputers at Westinghouse Energy Center. "Over the years," said Candris, "we have used PSC systems to supplement our Westinghouse computing capabilities. We have performed very sophisticated structural analyses and other demanding computations associated with the design of nuclear fuel systems and nuclear power plant reactor pressure vessels." While Westinghouse's business has evolved in recent years, their E-business today is based on internet connectivity provided through PSC.

PSC executive director **Beverly Clayton** coordinates PSC's program of support for research and education in Pennsylvania.



Pennsylvania Governor Edward G. Rendell, speaking at PSC's 20-year anniversary celebration, remarked on PSC's importance in helping to build Pittsburgh's reputation as a high-tech center. "Today's world runs on information," said Rendell. "For two decades, this Center has served as a resource for local businesses and academic institutions."

With nearly 7,700 technology firms in the Pittsburgh region, he added, the industry represents more than 10 percent of the area's companies. These companies employ nearly 216,000 individuals and account for 17 percent of the region's workforce, generating $10.4 billion in annual wages.

On October 3, **Beverly Clayton** accepted congratulations from **Pennsylvania Rep. Joe Markosek (D-25).** On this date, the Pennsylvania House of Representatives adopted a resolution recognizing PSC for 20 years of service to the nation and state. Rep. Markosek, who represents Monroeville and surrounding areas, including the Westinghouse Energy Center where PSC houses its supercomputing systems, introduced the resolution. Thirty other western Pennsylvania representatives joined Markosek in sponsoring the resolution

"It's fitting that we recognize the achievement of the Pittsburgh Supercomputing Center in advancing science and technology in Pennsylvania and in the country," said Markosek. "I'm proud that the Commonwealth has over the course of the past 20 years been able to sustain PSC with $30 million of support that has helped to leverage $380 million in support from federal agencies."

Support for High School Science
From June 19 to 23, PSC sponsored Computation and Science for Teachers (CAST), a workshop for science teachers in southwest Pennsylvania. Ten teachers from seven school districts completed the workshop, which is the first phase of a two-year program to incorporate computational tools into the high-school science curriculum. CAST was presented in conjunction with the Maryland Virtual High School project, with funding from the Grable Foundation, the Frick Teachers Alumnae Fund of the Buhl Foundation and NSF's Engaging People in Cyberinfrastructure) program.

RESEARCH AT PENNSYLVANIA COLLEGES & UNIVERSITIES, 2005-2006

More than 370 Pennsylvania researchers at these institutions used 4.3 million processor hours on PSC resources.

Bucknell University
Cabrini College
Carnegie Mellon University
Drexel University
Duquesne University
Edinboro University of Pennsylvania
Lehigh University
Pennsylvania State University, All Campuses
University of Pennsylvania
University of Pittsburgh, All Campuses
Ursinus College
Villanova University
Widener University

Research, Outreach & Training

Pittsburgh-based PPG Industries uses PSC systems for computational modeling in several aspects of its product lines as a global supplier of coatings, glass, fiberglass and chemicals. Medrad, Inc. in Indianola, Pennsylvania is collaborating with PSC and Carnegie Mellon to develop a novel method for safe removal of deep-vein blood clots. Through SC^2 (p. 8), Evergreene Technology Park in Greene County provides companies with access to PSC resources.

This year PSC presented the fifth in a series of annual technology-briefing days to staff from the Bechtel Bettis Atomic Power Laboratory in Pittsburgh. PSC consultants provided information on developing, managing and using a parallel distributed-computing environment.

In December 2005, PSC exhibited at the Annual Eastern Intergovernmental Technology Conference in Harrisburg, Pa. Groups who toured PSC included Science Bowl participants from Yough Area High School, students and teachers from the Elizabeth Forward School District and an Advanced Computing Machinery group from Bloomsburg College.

PSC's networking group over the past year has worked with several "K20" organizations —building collaborations among K-12 education and higher education with government and the private sector. PSC has conducted these outreach activities in collaboration with MAGPI, the Philadelphia-based network hub, leveraging their well-developed K20 program. To date, these efforts have focused on seven Intermediate Units in western Pennsylvania.

THE SUPER COMPUTING SCIENCE CONSORTIUM

Pennsylvania-West Virginia partners in development of clean power technologies.

Formed in 1999 and supported by the U.S. Department of Energy, the Super Computing Science Consortium is a regional partnership of research and educational institutions in Pennsylvania and West Virginia. $(SC)^2$ provides intellectual leadership and advanced computing and communications resources to solve problems in energy and the environment and to stimulate regional high-technology development.

Through $(SC)^2$, Evergreene Technology Park in Greene County provides a channel for companies to collaborate with local universities in southwest Pennsylvania and West Virginia and to have access to PSC computing resources.

Since the spring of 2000, a high-speed network — the first fiber-optic service to Morgantown, West Virginia — has linked the National Energy Technology Laboratory (NETL) campuses in Morgantown and Pittsburgh with PSC, facilitating NETL collaborations. Researchers at NETL and WVU have actively used this link to tap PSC computational resources. Since the founding of $(SC)^2$, 45 $(SC)^2$ researchers have used PSC systems for a range of projects, using more than three million hours of computing time, nearly 400,000 hours within the past year. This work includes:

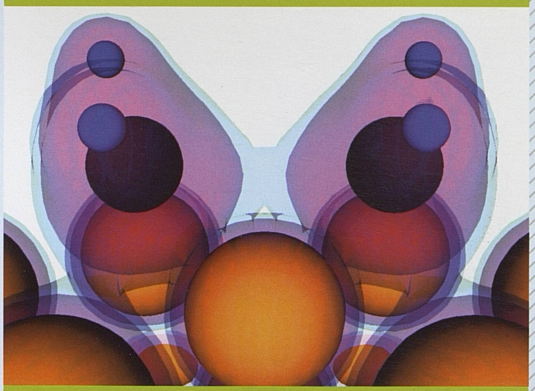
- *Gas From Black Liquor*
  http://www.psc.edu/science/2004/sc2/
- Fluidized-Bed Combustion of Silane
  http://www.psc.edu/publicinfo/netl/
- *Lean-Fuel Mixes in Next-Generation Power-Generating Turbines*
  http://www.psc.edu/science/Richards/clean_power.html
- *Industrial-Scale Technology for Coal Gasification*
  http://www.psc.edu/publicinfo/2002/sc2/
- *A New Design for a Power-Generating Turbine*
  http://www.psc.edu/science/cizmas2002.html
- *How to Produce Fuel-Quality Hydrogen*
  http://www.psc.edu/science/2005/sc2

$(SC)^2$ PARTNERS

National Energy Technology Laboratory
Pittsburgh Supercomputing Center
Carnegie Mellon University
Duquesne University
University of Pittsburgh
Waynesburg College
West Virginia University
Institute for Scientific Research
NASA Independent Verification & Validation Facility
The West Virginia Governor's Office of Technology

More Information

http://www.sc-2.psc.edu



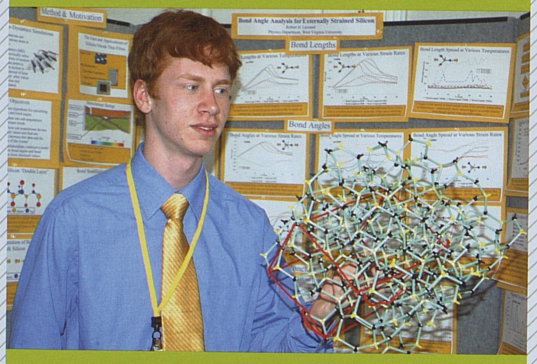
Clean Liquid Fuel

Fischer-Tropsch synthesis (FTS) is an important industrial process that offers a direct route to produce clean hydrocarbon liquid fuel from syngas (a mixture of carbon monoxide and hydrogen). Traditionally coal or natural gas have been used as feedstocks but biomass-derived hydrogen also could work, offering promise for a liquid fuel to replace fuels produced from petroleum or other fossil fuels.

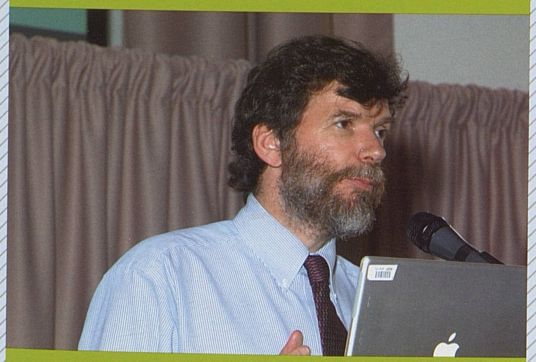
With support through NETL, Manos Mavrikakis and colleagues at the University of Wisconsin, Madison apply advanced quantum-mechanical computations at PSC to gain insight into the FTS reaction. This graphic shows the "transition state" in the formation of ethylene (C_2H_4, enclosed by two electron density surfaces) on a catalytic surface of iron (orange atoms) where the carbon-carbon bond (two dark spheres) is formed.

"Experimental techniques can't provide information about transition states," says Mavrikakis, " and computational methods are the only means to study them."

$(SC)^2$ co-chairs **Lynn Layman** of PSC (left) and **Bob Romanosky** of NETL on July 14 at Waynesburg with **Pennsylvania Governor Ed Rendell** and members of the event's planning team, (l to r) **Paul Cizmas** of Texas A&M, **Trina Wafle** of WVU, **Governor Rendell**, **Francis Van Scoy** of WVU, **Barbara Kirby** of Waynesburg College, **Robin Flaus** of PSC, **Tom Maiden** of PSC, **Laura McGinnis** of PSC, and **Don McLaughlin** of WVU.



The seminar included a poster session presenting research by students from regional colleges, including West Virginia University, Waynesburg College, the University of Puerto Rico, the University of Pittsburgh, Penn State, the University of Miami, Cornell University, Alderson Broadus College and a K-12 project from ASSET.



The keynote speech by **Stephen Meacham**, Program Director, Office of Cyberinfrastructure, National Science Foundation, highlighted high-end computing as an engine for competitiveness. "What the Supercomputing Science Consortium has done," he said, "is show how you can leverage the investment of the National Science Foundation by pulling together universities with local development opportunities. It represents a microcosm of how society can be transformed by investment."

Regional Business Opportunities in Supercomputing

Economic development was the theme of this July 14 $(SC)^2$ seminar. Sponsored by PSC, a founding partner in $(SC)^2$, and held at Waynesburg College, the event offered a learning opportunity aimed at small-to-medium-sized technology-oriented organizations.

Governor Ed Rendell spoke during an afternoon panel discussion on "Federal, State and Other Funding Opportunities for Regional Small Businesses, Colleges and Universities." He stressed the importance of a skilled workforce for economic growth. The Pennsylvania economy, he said, must compete not only against other states, but also increasingly against corporations around the world and as far away as Singapore. "The currency of where growth will occur in our new economy," said Rendell, "lies with innovation and the availability of a skilled work force."

Participants in the panel were Errol Arkilic, Program Manager, Small Business Innovation Research and Small Business Technology Transfer Programs, National Science Foundation; Chris Gabriel, Innovation Economy Program Director, Heinz Endowments; Brian Kennedy, Government Relations Director, Pittsburgh Technology Council; Paul Hill Jr., Executive Director, West Virginia EPSCoR, and Susan Zelicoff, of the Institute for Entrepreneurial Excellence at the Katz Graduate School of Business, University of Pittsburgh.

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 (NCRR), renews NRBSC for another five years.

"This grant is part of NCRR'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

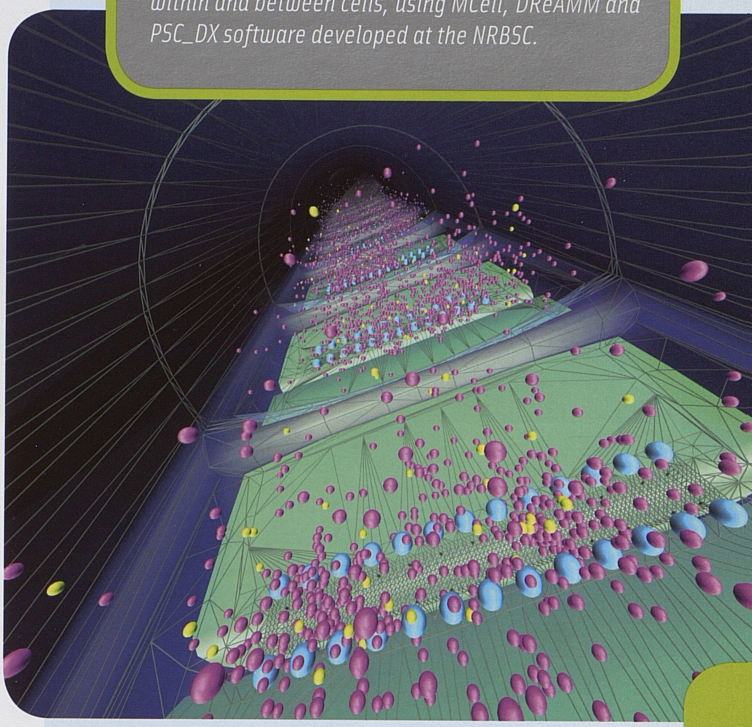
Training & Resources

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).

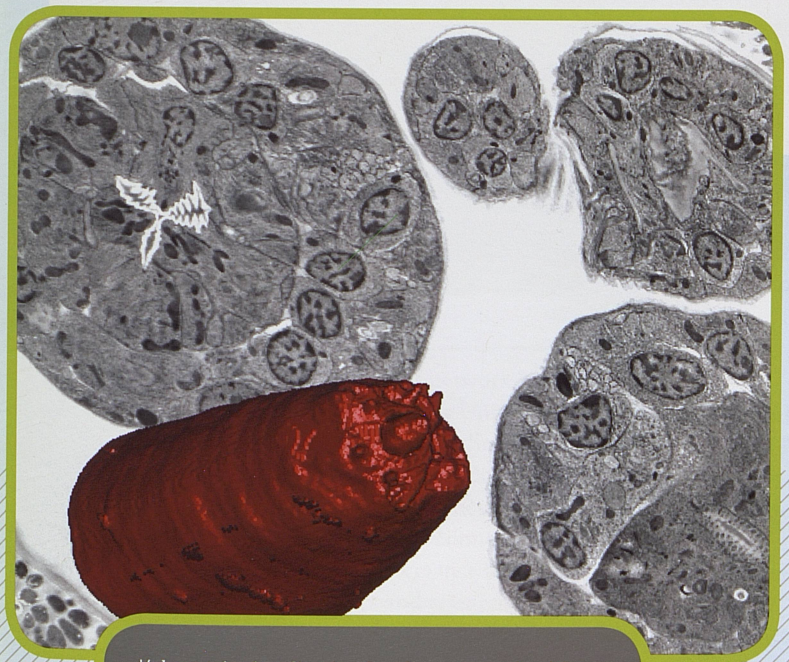
NRBSC workshops on computational biology have trained more than 3,300 researchers in the use of high-performance computing for biomedical research, in such areas as spatially-realistic cell modeling, volumetric data visualization and analysis, protein and DNA structure, genome sequence analysis and biological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



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.



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.

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.

NETWORKING THE FUTURE

One of the Leading Resources in the World for Network Know-How

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 current work with the NPAD diagnostic server — has created valuable tools for improving network performance nationally.

More information: **http://www.psc.edu/networking**

Wendy Huntoon, PSC director of networking and director of operations for National Lambda Rail (NLR), a major initiative of U.S. research universities and the private sector to provide infrastructure for research in networking technologies.

National Transit Rail

Through National Lambda Rail, PSC is participating with four other NLR members in a new project, the National TransitRail Project, to provide an intelligently managed nationwide peering and transit program. Through NLR's national network fiber infrastructure, the NTR project will work to reduce the number of "hops" required for data to get to its destination.

"NTR represents a new type of service," says PSC network director Wendy Huntoon. "It is direct peering with content providers and internet service providers. The long-term benefit is to provide a better-performing and more cost-effective link to resources than current network connections."

3R0X MEMBERS

ACADEMIC
Carnegie Mellon University, Norfolk State University, University of Pittsburgh, Pennsylvania State University, West Virginia University, Pittsburgh Public Schools, Woodland Hills School District, Intermediate Unit One

GOVERNMENT LABORATORY
The National Energy Technology Laboratory

BUSINESS
Comcast, Westinghouse Electric Co.

OTHER
Computer Emergency Response Team

NETWORK CONNECTIONS

NATIONAL RESEARCH NETWORKS
Abilene – 2.4 Gbps, TeraGrid Extensible Backplane Network – 30 Gbps.

NATIONAL COMMODITY INTERNET NETWORKS
Global Crossing – 1 Gbps; Sprint – 1 Gbps. (peering) PITX

PITTSBURGH LOCAL EXCHANGE NETWORK
Comcast, TelCove

NOTE: Gbps: a billion (Giga) bits per second.

3ROX

Through 3ROX, a high-speed network hub that serves Carnegie Mellon, Penn State, the University of Pittsburgh, West Virginia University, Norfolk State University, the Pittsburgh Public Schools and Woodland Hills School District, PSC provides advanced network resources for education and research. 3ROX connects the universities and PPS to Abilene a high-performance network linking more than 250 U.S. universities and research organizations.

3ROX News

This year Norfolk State University became the newest 3ROX member, as 3ROX expanded its network aggregation in the mid-Atlantic region to include Pennsylvania, West Virginia and Virginia. "We're pleased," says PSC network director Wendy Huntoon, "to extend services to one of the historically black colleges and universities." Norfolk State expects to work with other HBCU's in their area to share their Abilene connection through 3ROX.

3ROX this year also added Intermediate Unit One and Woodland Hills School District in the east suburbs of Pittsburgh. As a result, any university-based resources available to the school district, such as distance learning or databases, will have better performance.

Penn State expanded its network capacity by connecting to National Lambda Rail, offering up to 32 "lightpaths" — four are now active — via NLR's infrastructure, increasing its overall bandwidth from 1.2 to 40 gigabytes per second. "With the success of this completion," says Huntoon, "3ROX now maintains an advanced three-way network between Carnegie Mellon, the University of Pittsburgh and Penn State."

Narrowing the Wizard Gap

The Internet is extremely robust because Internet protocols include recovery procedures that silently self-correct network failures. These procedures hide network problems at the cost of reducing performance. Within a local network, this slowdown is likely to be trivial, but can lead to unacceptably slow wide-area traffic — because the increased network round-trip time multiplies the delay. The self-correction also masks the flaws, making it very difficult to pinpoint the ultimate causes of the reduced performance. With the NPAD (Network Path and Application Diagnostics) Project, PSC network engineers and the National Center for Atmospheric Research have developed diagnostic tools — based on tools PSC developed in a project called Web100 — that analyze and determine the nature of any observed path failures.

The primary audience for NPAD is data-intensive scientific users. "The goal," says PSC engineer Matt Mathis, "is to easily — and in many cases automatically — diagnose problems that impede performance at this scale." The diagnostics (called pathdiag) are run through a web interface. With NPAD deployed on a local network, a user can with a couple clicks test the path to a client for flaws, determine whether it will support a long fast flow, and make suggestions how to fix any observed problems.

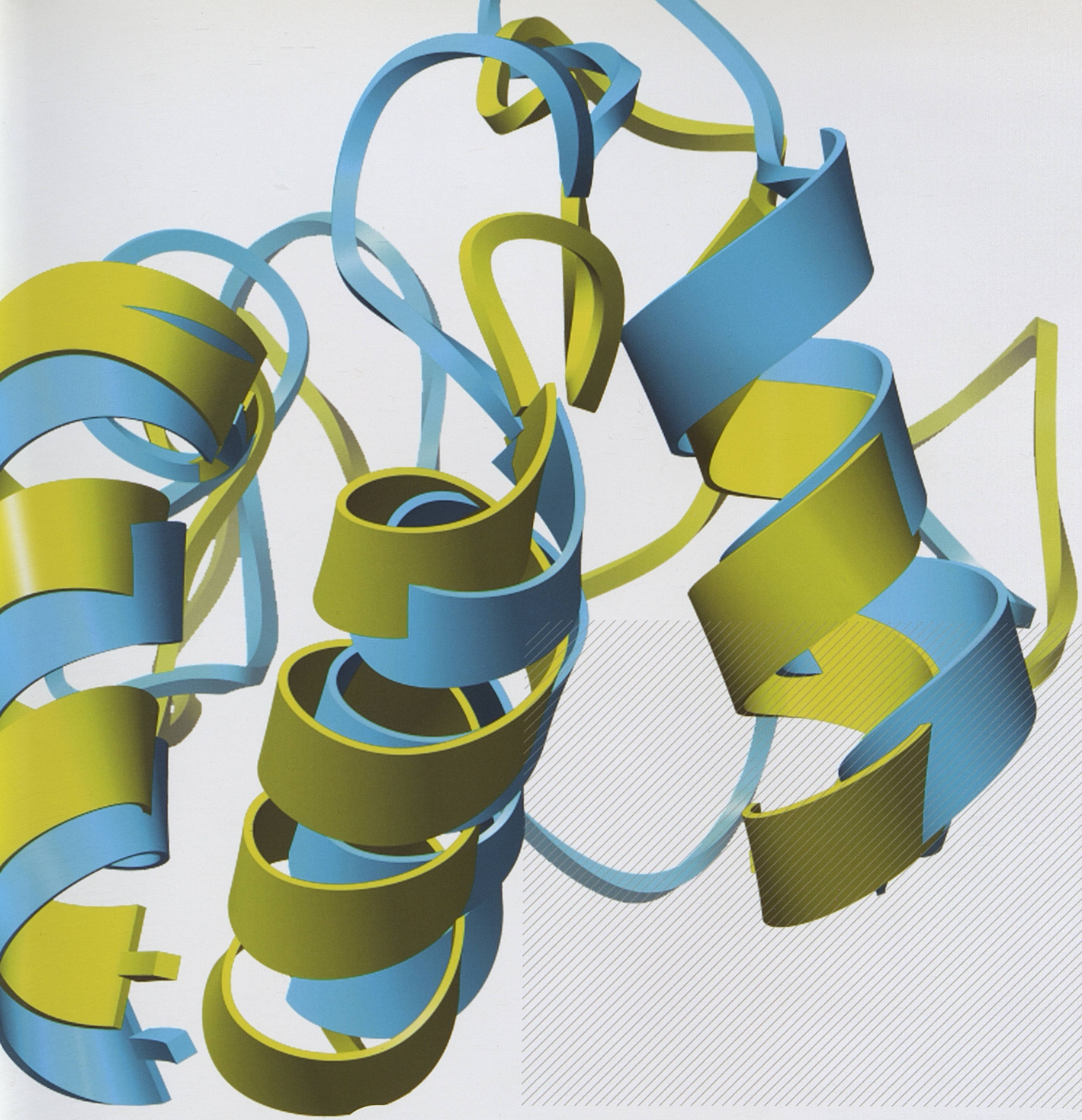
NPAD, says Mathis, can substantially narrow the "wizard gap" — the gap in available network performance between network wizards and typical users. "Several network researchers have demonstrated 40 gigabits per second under a variety of environments, but this does little to help typical domain scientists with observed median performances of only three megabits per second. The difference is a factor of 10,000, and most of the problems that cause half this gap — the first factor of 100 — can be completely and automatically diagnosed by pathdiag."

Pittsburgh Supercomputing Center Workshops (2005-2006)

Introduction to the Cray XT3
Bioinformatics (for minority-serving institutions)
Developing Bioinformatics Programs
Computational Methods for Spatially-Realistic Microphysiological Simulations
Nucleic Acid and Protein Sequence Analysis
Computational Biophysics

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

The PSC operational management team playing "railroad tycoon," a board game of technological infrastructure: (l to r) **Katie Vargo**, manager, scientific computing systems; **John Kochmar**, HPC facilities manager, systems and operations; **J. Ray Scott**, director, systems and operations; **Bob Stock**, associate director; **Gwendolyn Huntoon**, director, networking; **David Kapcin**, manager, financial affairs; **Nick Nystrom**, director, strategic applications; **Rich Raymond**, manager, user support; **Sergiu Sanielevici**, director, scientific applications and user support. Not in photo: **Janet Brown**, manager, networking.



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IN SCIENTIFIC COMPUTING
2006

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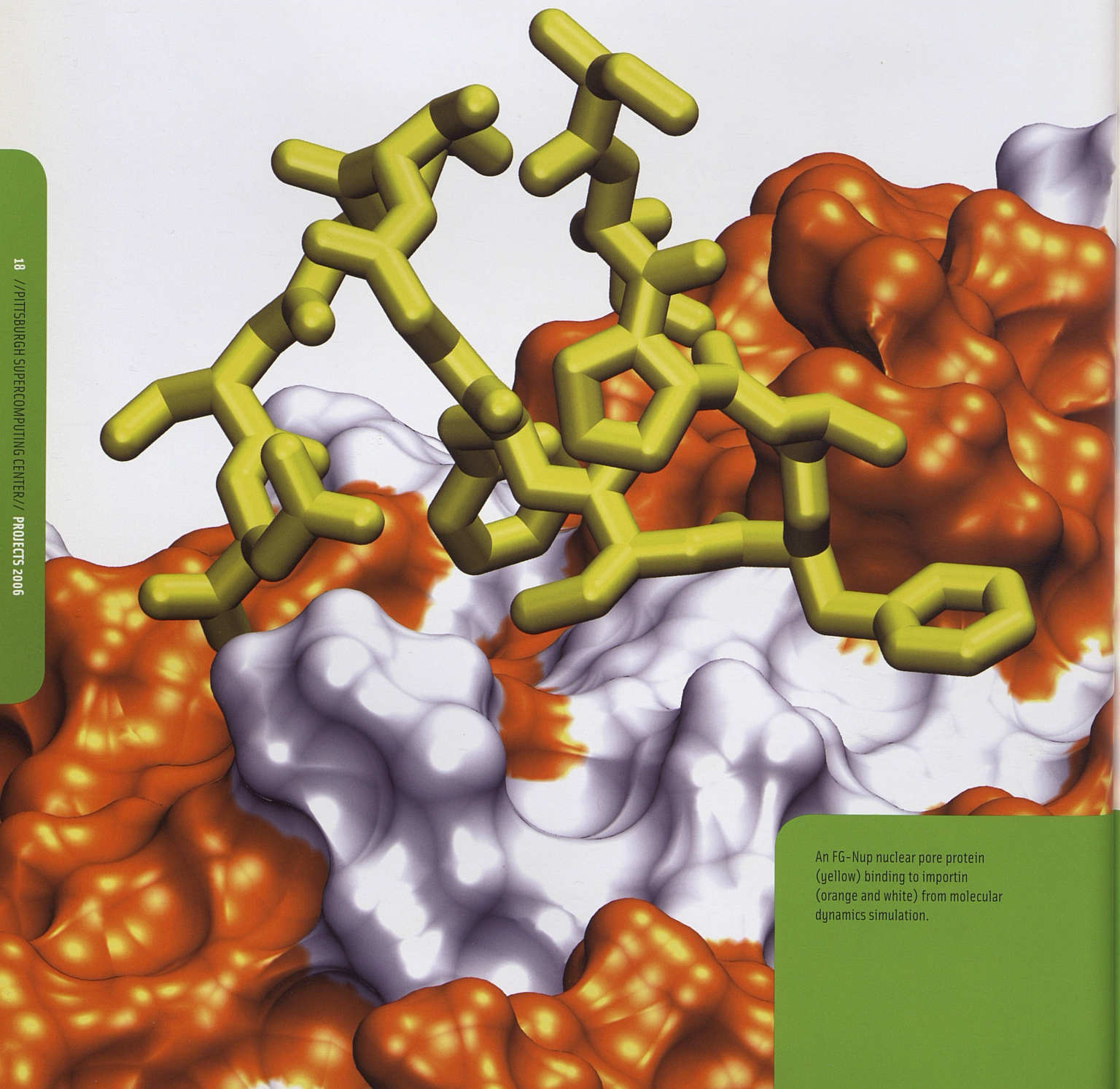
KNOCK, KNOCK, WHO'S THERE?



An FG-Nup nuclear pore protein (yellow) binding to importin (orange and white) from molecular dynamics simulation.

SIMULATIONS REVEAL NEW INFORMATION ABOUT THE GATEWAY TO THE CELL NUCLEUS

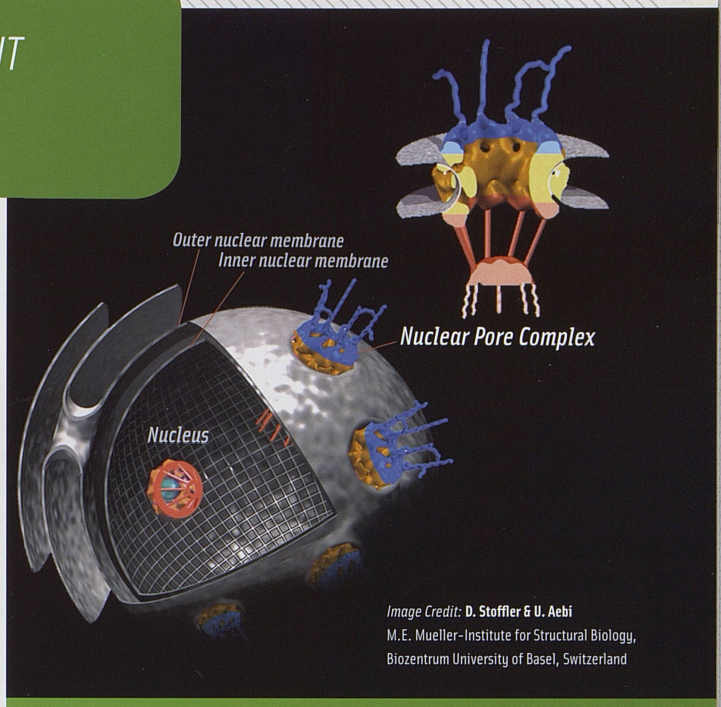


Image Credit: **D. Stoffler & U. Aebi**
M.E. Mueller-Institute for Structural Biology,
Biozentrum University of Basel, Switzerland

NUCLEAR PORE COMPLEX

Think of yourself as a big protein. You're inside a cell, milling around in the aqueous molecular crowd called the cytoplasm, and you'd like to get into the nucleus. If you've ever attended a black-tie event with someone at the door to check your engraved invitation and escort you arm-in-arm through the doorway, where you can pass only if the escort displays correct credentials to a very serious bouncer — that's a rough idea of what it's like to pass into or out of the cell nucleus.

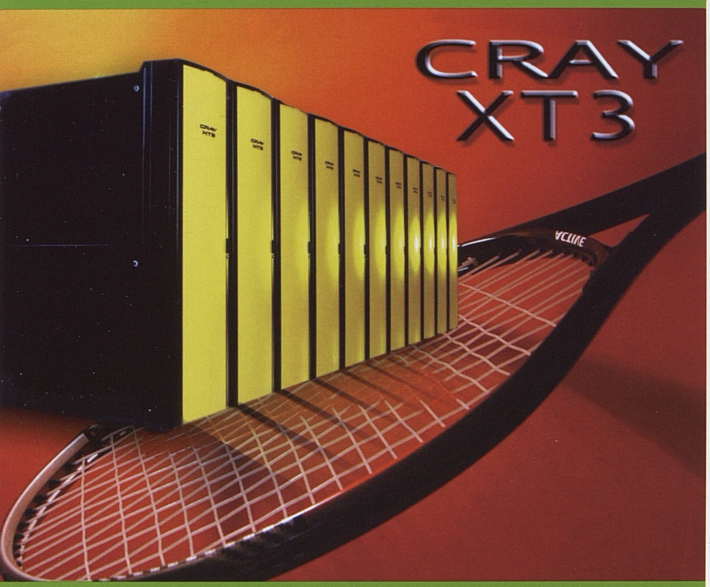
The doorway with built-in security apparatus you'd have to go through is called the nuclear pore complex. Hundreds to thousands of NPCs are embedded in the nuclear envelope of each cell, a double membrane that houses and protects the organism's genetic information. The NPC's ability to pick and choose which large proteins pass is crucial, protecting the nuclear DNA and, at the same time, allowing transit of proteins and strands of RNA involved in the manufacture of new proteins, the cell's bottom-line business.

Small proteins pass freely, but for a large protein to pass through the NPC may be only slightly less complicated than the proverbial rich man getting to heaven. "The mechanism by which the NPC selectively allows the transit of certain large proteins while restricting the passage of others is poorly understood," says biophysicist Klaus Schulten, who directs the Theoretical Computational Biophysics Group at the University of Illinois Beckman Institute.

The NPC's selection process involves signal proteins, energy-transfer reactions and it relies strongly on a group of proteins — called transport receptors — whose job is to escort large proteins through the NPC. In a late 2005 study, Schulten and graduate student Timothy Isgro looked at a transport receptor called importin-ß and how it interacts with other proteins in the NPC interior. Their molecular dynamics (MD) simulations — using TeraGrid resources at PSC, SDSC and NCSA — provide the first atomic-level view of NPC selectivity, and they show that these interactions are more numerous than had been thought.

Their work confirms experimental findings about importin and goes beyond experiments to predict new "binding spots," one of which has been subsequently verified. Schulten and Isgro's ability to reveal previously unknown details of the NPC process with simulations attracted attention, including commentary in *Science* (January 6, 2006) and *Structure* (December 2005), which stated "the predictive power of their MD work is convincingly displayed...."

Klaus Schulten (left) and **Tim Isgro,**
University of Illinois, Urbana-Champaign



ONWARD TO THE RIBOSOME

The life sciences, says Klaus Schulten, are moving on to bigger things. When it comes to understanding processes in living systems at the molecular level, it's become possible—thanks to technology such as the Cray XT3—to look at very large systems, of which the nuclear pore is one example. "The XT3," says Schulten, "is a terrific computer platform for this new generation of work."

Encouraged by success with the NPC, Schulten has (as of late August 2006) begun to use his powerful software NAMD on PSC's XT3 to simulate the ribosome. This huge aggregate protein-RNA assembly is a cellular factory that reads the genetic blueprint from messenger RNA and uses it to manufacture proteins. "It's possible to do this now with the XT3." Schulten's MD simulations of the ribosome (2.7 million atoms) are using NAMD with 1,000 XT3 processors—unprecedented large-scale parallelism for molecular dynamics.

Because of the XT3's fast inter-processor communication, NAMD can use the entire system efficiently, 2,000 processors, for a single simulation. "This is just the right system for this kind of project," says Schulten. "If you have a tennis racquet, it has a sweet spot where you can hit best, and for this project the sweet spot is the entire XT3 at Pittsburgh."

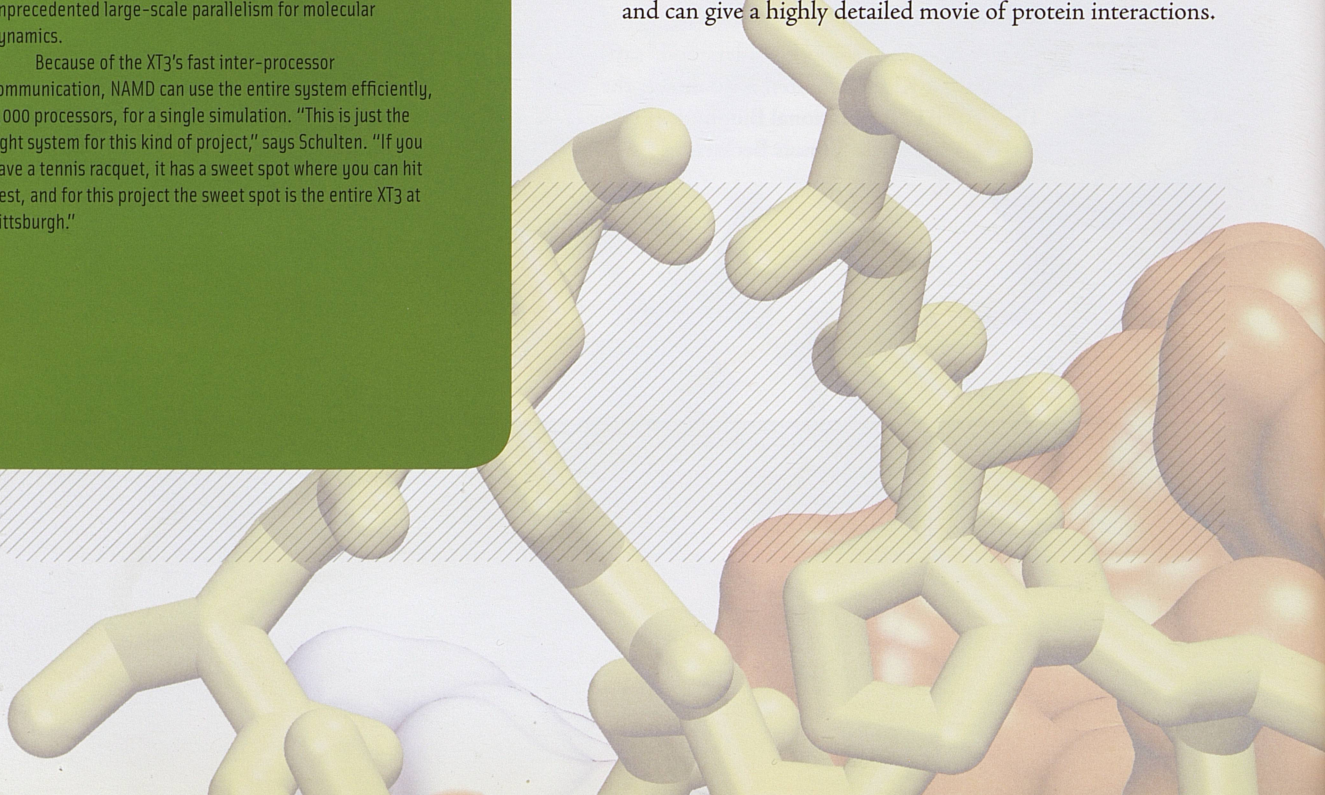
GATEWAY TO THE NUCLEUS

In the world of proteins, the NPC is a behemoth. Its mass in vertebrates is 125 megaDaltons, probably the largest protein complex in the cell. Not a single protein, the NPC is comprised of many distinct proteins, called nucleoporins — "Nups" for short. "There are whole machines in living cells that are made of hundreds or thousands of proteins," says Schulten, "and the nuclear pore is one of those systems. It's actually one of the most magnificent systems in the cell."

The immense size of the NPC makes it difficult to study in detail. Over the past decade, electron microscopy has provided much information about its large-scale structure, and other laboratory studies have looked at the transport process. Recent work resolved the structure of importin, laying a foundation for Schulten and Isgro's MD simulations. "The mystery," says Isgro, "is how exactly does the nuclear pore complex transport things into and out of the cell nucleus."

Experiments have shown that a specific subset of Nups — called "FG-Nups," because of a repeating sequence of the amino acids phenylalanine and glycine — is involved in NPC selectivity. "Presumably the NPC recognizes importin as a protein that's allowed to pass and shuttle its cargo through the pore," says Isgro. "The question is what is the recognition process? Experiments have implicated the FG-Nups."

FG-Nups have been shown to occupy the central pore region of the NPC, through which a transport receptor and its cargo must pass, and they have been shown to interact with importin at binding sites on the importin surface. To get a detailed picture, Schulten and Isgro turned to MD simulations, which track how the atoms move with time, and can give a highly detailed movie of protein interactions.



THEY IDENTIFIED SIX PREVIOUSLY UNKNOWN BINDING SPOTS.

PREVIOUSLY UNKNOWN SITES

As a first step, Isgro used PSC's LeMieux to simulate FG-Nups alone, without importin. The question was whether it would be feasible to see results from a simulation of importin with FG-Nups in the amount of biological time it would be possible to simulate — tens of nanoseconds (one nanosecond is a billionth of a second) being the limit with a practical amount of computing.

"I didn't know," says Isgro, "if tens of nanoseconds would be enough time for the FG-Nups to diffuse through solution and bind to the surface of importin." Using MD software called NAMD, developed in Schulten's research group, with 128 processors of LeMieux for a series of sixteen 24-hour simulations, Isgro found that the FG-Nups associated with one another in a few nanoseconds, which suggested that a simulation with importin would be fruitful.

"LeMieux," says Isgro, "provided a fast and efficient computing platform that enabled us to see the full atomic structures and dynamics of nuclear pore proteins interacting with one another for the first time."

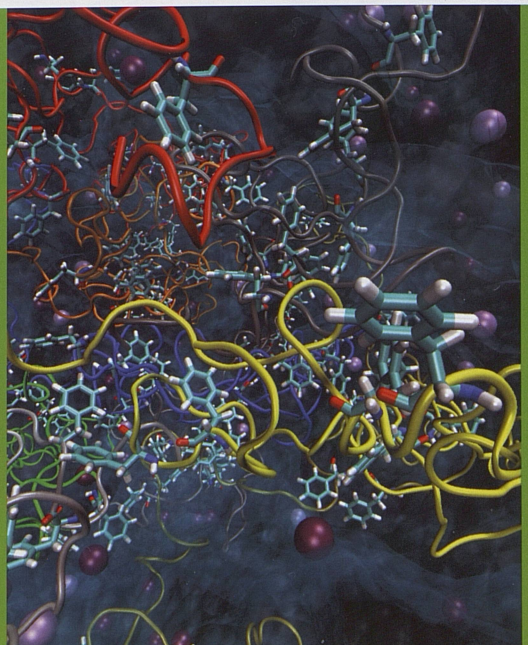
To simulate the interaction of importin with FG-Nups, Schulten and Isgro also used NAMD and a system at NCSA. They did five different simulations, using different FG-Nup sequences in solution with importin. They simulated a total of over 200 nanoseconds, each simulation lasting several tens of nanoseconds, enough time to see FG-Nups bind to the surface of importin.

As a further step, the researchers aligned the amino-acid sequences of eight different forms of importin to identify likely "hot spots" for FG-Nup binding. With this combination of MD simulations and sequence alignment, their computations confirmed three out of four FG-Nup binding sites on importin that had been previously identified in experiments. Their study also identified six previously unknown binding spots.

An experimental study subsequently verified one of these newly predicted binding spots. These additional binding spots, says Schulten, suggest that importin has more extensive ability to interact with the NPC than had been expected before this work. The observed interactions between FG-Nups and importin are consistent with several prevalent models of how the NPC recognizes transport receptors and allows them to pass. "These results," says Schulten, "are the first atomic-scale look at these novel binding spots for FG-Nups, and they suggest that the extent of binding on the surface of importin is much larger than previously realized."

With this success under their belt, Schulten and Isgro in 2006 turned to another transport receptor, NTF2 (nuclear transport factor2). As they did with importin, they looked at the interactions between NTF2 and FG-Nups. For this project, PSC's Cray XT3 was available to speed up completion of the work. Once again, the researchers found previously unknown FG-Nup binding spots on the transport receptor, and the simulations provide previously unavailable structural detail of the binding interactions. (MS)

MORE INFORMATION:
http://www.psc.edu/science/2006/schulten.html



FG-Nups in Solution
A snapshot from simulation on PSC's LeMieux shows FG-Nups (various color strands) interacting with one another. This is a hypothesized view of the center of the nuclear pore complex, in which the disordered FG-Nups would block large proteins, yet allow passage of transport receptors, such as importin, with their large protein cargo. Phenylalanine residues (the "F" of "FG") are displayed in blue (hexagons). Ions are shown as spheres.

HEAVY METAL INVASION

Matteo Dal Peraro (left) and **Michael Klein,** University of Pennsylvania

So much for miracles. Penicillin and its derivatives have saved uncountable lives, but evolution, in its robustly creative way, has improvised potent countermeasures to Alexander Fleming's miracle drug. Infectious bacteria have shown protean ability to adapt, survive and reassert themselves as a threat to human health.

Over the last two decades, bacterial resistance to antibiotics has become widely recognized as a serious problem. The National Health Council estimates that 14,000 Americans die annually in U.S. hospitals because available antibiotics don't work. Like Nosferatu the undead, tuberculosis has resurrected itself as a worldwide killer because of the TB bacterium's antibiotic resistance. Many other bacteria have also developed resistance. In response, molecular biologists, as if in a weapons race, have devised ever-newer drugs to overcome bacterial defenses. Various multi-drug regimens have proven to be effective, but current research, nevertheless, finds more and more bacteria capable of resisting even these drugs.

The most widely used antibiotics are penicillin and its derivatives, a family called "beta-lactam" antibiotics — so-named for their chemical structure. As you might expect, because of wide use over more than half a century, bacteria have evolved a defense to these drugs — an enzyme that attacks and inactivates the beta-lactam structure. "The clinical use of beta-lactams, the most widespread antibiotics on the market today," says University of Pennsylvania biophysicist Matteo Dal Peraro, "has exerted a large evolutionary pressure on bacteria, triggering several resistance mechanisms. The most effective of these mechanisms is biosynthesis of beta-lactamases, a group of enzymes that inactivate the drugs."

Dal Peraro, a post-doctoral researcher, collaborates with Michael Klein, who directs the University of Pennsylvania's Center for Molecular Modeling and who leads a range of studies on enzymes and how they catalyze reactions. For a number of years, Klein's research group has used PSC systems to good effect, and they were among the first research groups to have success with BigBen, PSC's Cray XT3. "For the kind of calculations we do," says Klein, "the XT3 is the most productive resource available to our group. It is allowing us to undertake projects we couldn't do before in a reasonable time."

Klein's focus on enzymes and his development of powerful computational methods to study them, led him and Dal Peraro along with Alejandro Vila and Paolo Carloni to look at a particularly nefarious class of beta-lactamases, a group that includes zinc, a heavy metal, in its structure. Known as metallo-beta-lactamase (MßL), this class of enzymes is newer than other beta-lactamases and so far not as widespread. Existing multi-drug regimens, however, are ineffective against MßLs, and they pose a potentially serious threat.

In a series of simulations starting with LeMieux, PSC's first terascale system, and finishing this year with BigBen, the Klein team uncovered previously unknown atomic-level information about how MßL works and the reactions that occur as it attacks beta-lactam antibiotics — vital information for pharmaceutical researchers as they work to develop drugs that can inhibit MßLs before the bacteria that produce them become more dangerous.

QUANTUM SIMULATIONS WITH THE XT3 TAKE A STEP TOWARD DEFEATING A DANGEROUS STRAIN OF ANTIBIOTIC-RESISTANT BACTERIA

BREAKING THE RING

Although beta-lactams have been used since the 1940s, scientists still lack a complete, exact picture of how they work. What's clear is they disrupt bacterial ability to synthesize cell walls, and the disruption is lethal.

The distinctive feature of beta-lactams is the beta-lactam ring — a four-sided structure, three carbon and one nitrogen atoms. The antibiotic effect depends on the integrity of this ring. Beta-lactamase enzymes attack the ring and "hydrolyze" it, cutting it and rendering the drug harmless as an antibiotic.

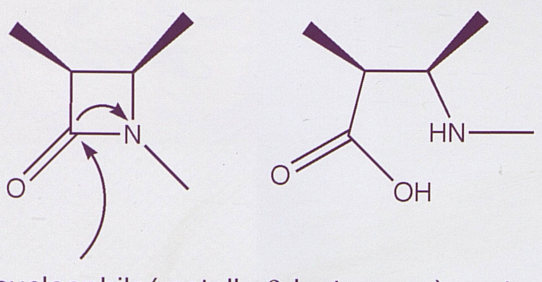
The ability of beta-lactamase enzymes to break the beta-lactam ring depends on the presence of a "nucleophile" — a chemical group that can donate electrons — in the active site of the enzyme. In the older, better known beta-lactamases the nucleophile is attached to the amino-acid serine.

"These normal beta-lactamases," says Dal Peraro, "which are sometimes called serine beta-lactamases, have been around since the 1970s, and inhibitors have been designed to limit their effectiveness." A widely used multi-drug formulation is augmentin, which teams the antibiotic amoxicillin in a one-two punch with clavulanic acid, an inhibitor that binds with and occupies the beta-lactamases, allowing amoxicillin to have its lethal effect.

In alarming ways, however, MßLs differ from their serine beta-lactamase cousins. They wield the same chemical tactic, a nucleophile in the active site, but they rely on zinc ions, either one or two — mono or bizinc MßLs — rather than serine, and because of this difference, they are immune to existing inhibitors.

"This is a new class of beta-lactamases," says Dal Peraro, "first discovered more than 10 years ago. There are no useful inhibitors in the market to inactivate these enzymes, so all beta-lactam antibiotics are ineffective against MßL bacteria. Fortunately, MßLs aren't as widespread as the older beta-lactamases, but microbiologists who study this problem find they are continuously spreading in the clinical setting. They are already dangerous and have led to deaths from post-operative infection, but they will be more dangerous in the future if they continue to spread."

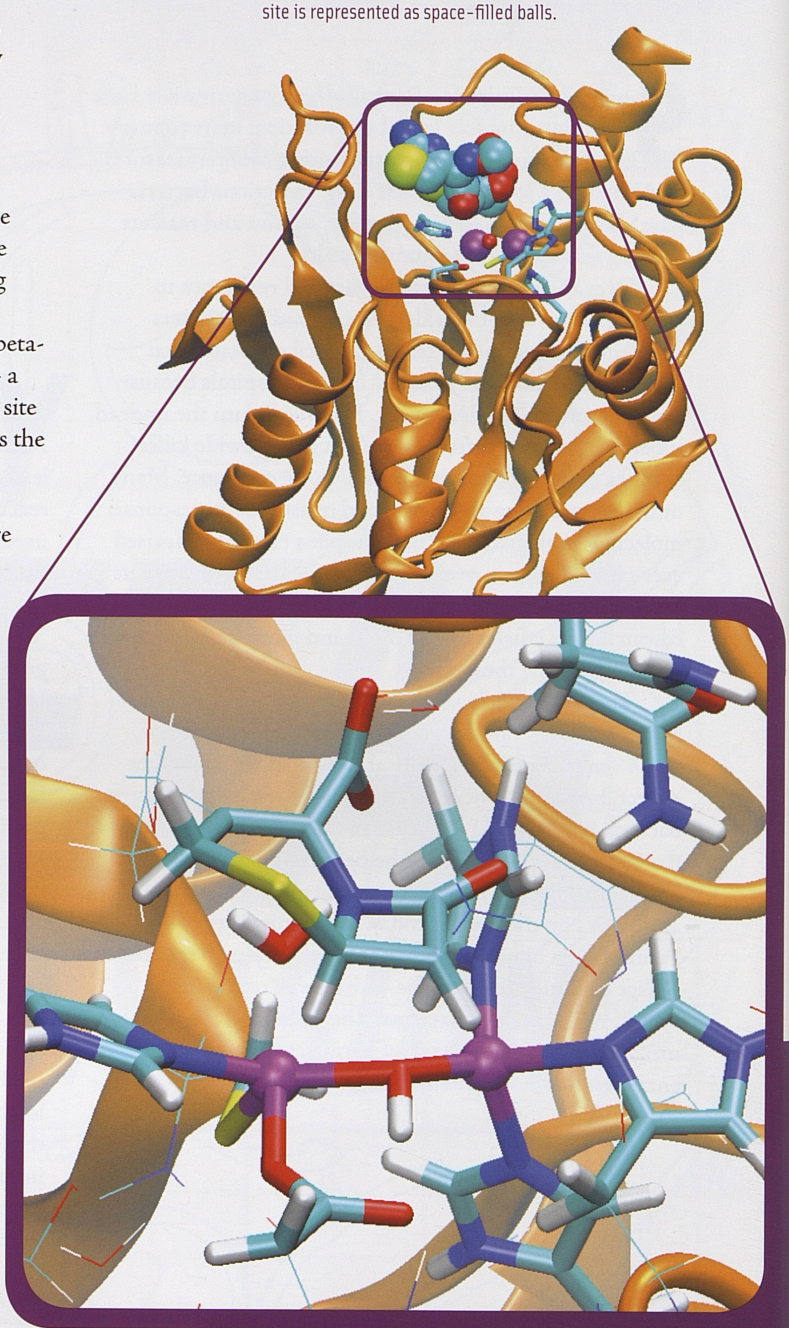
"There is an urgent need," says Klein, "to understand the function of these enzymes at the molecular level."



nucleophile(metallo β-lactamase)+water

Metallo beta-lactamase enzymes wield a nucleophile to break the beta-lactam ring.

This ribbon structure depicts the metallo-beta-lactamase enzyme simulated by the researchers. Two zinc ions (purple spheres) are in the enzyme's active site with amino acids coordinating the metals (represented as sticks). A beta-lactam antibiotic bound at the active site is represented as space-filled balls.



Closeup on the Action

This closeup on the bizinc MßL active site shows the conformation of the reactants (in stick representation) from the QM/MM simulation. The beta-lactam ring of the antibiotic is in the center of the picture. Other parts of the enzyme, not included in the quantum-mechanical part of the simulation, are shown as thin lines. The QM treatment of the active site reveals that a hydroxide group (red & white, OH-) bridging the two zinc ions (purple spheres) interacts with a water molecule (red with two white wings, above the left zinc atom) between one of the metals and the antibiotic. This water shuttles a proton (H+) to break the beta-lactam ring.

"FOR THE KIND OF CALCULATIONS WE DO THE XT3 IS THE MOST PRODUCTIVE RESOURCE AVAILABLE TO OUR GROUP."

GETTING A FIX ON ZINC

For the pharmaceutical industry to identify and gain approval of a new antibiotic is a major undertaking, requiring as much as eight years and $500 million. As a big step in the direction of an MßL inhibitor, the Klein team set out to precisely characterize the reactions that occur when an MßL enzyme interacts with a beta-lactam antibiotic.

"Computational studies of enzyme catalysis," says Klein, "go back a long way — to the pioneering work of Arieh Warshel and Michael Levitt, now at USC and Stanford respectively, who introduced the notion of QM/MM [quantum mechanics/molecular mechanics], which treat the active site with quantum mechanics and the rest by classical molecular dynamics. More rigorous treatments are possible now in both regions. Our modest contribution is to employ Car-Parinello density-functional based methodology for the QM region. To implement this, our group uses code developed by one of our former post-doctoral researchers, Ursula Roethlisberger of EPFL (Ecole Polytechnique Fédérale de Lausanne) Switzerland and her group."

Traditional classical "molecular dynamics" tracks the movement of atoms and, therefore, changes in molecular structure with time, but doesn't track the making and breaking of bonds that occur during reactions. The powerful Car-Parinello approach makes it feasible to obtain this quantum-level information with a practical amount of computing.

Reactions involve transition states that occur almost instantaneously as a reaction moves from reactant to product states. "With this kind of study," says Dal Peraro, "we want to characterize the transition state of the reaction, because what we know from experiment is only the resting state of the enzyme, not the pathway that leads to the products. With this information you have a better chance to design an efficient inhibitor."

The role of zinc in the MßL enzyme reaction hasn't been well defined, despite a large amount of experimental study. Klein and Dal Peraro designed a simulation that tracked a particular bizinc MßL with their QM/MM approach as it reacts with three different beta-lactam antibiotics.

For initial phases of the project, the researchers relied on LeMieux, PSC's terascale system, but when BigBen became available in late 2005, they turned to the new system and it became a major advantage to their work. With the QM/MM code, Dal Peraro was able to use up to 128 BigBen processors at a time, twice as many as he could efficiently use on LeMieux. He submitted ensemble jobs using up to 1,280 BigBen processors for up to 10 different parallel, simultaneous 128-processor simulations that scanned the reaction pathway in several windows over a total reaction time of more than 50 picoseconds (trillionths of a second).

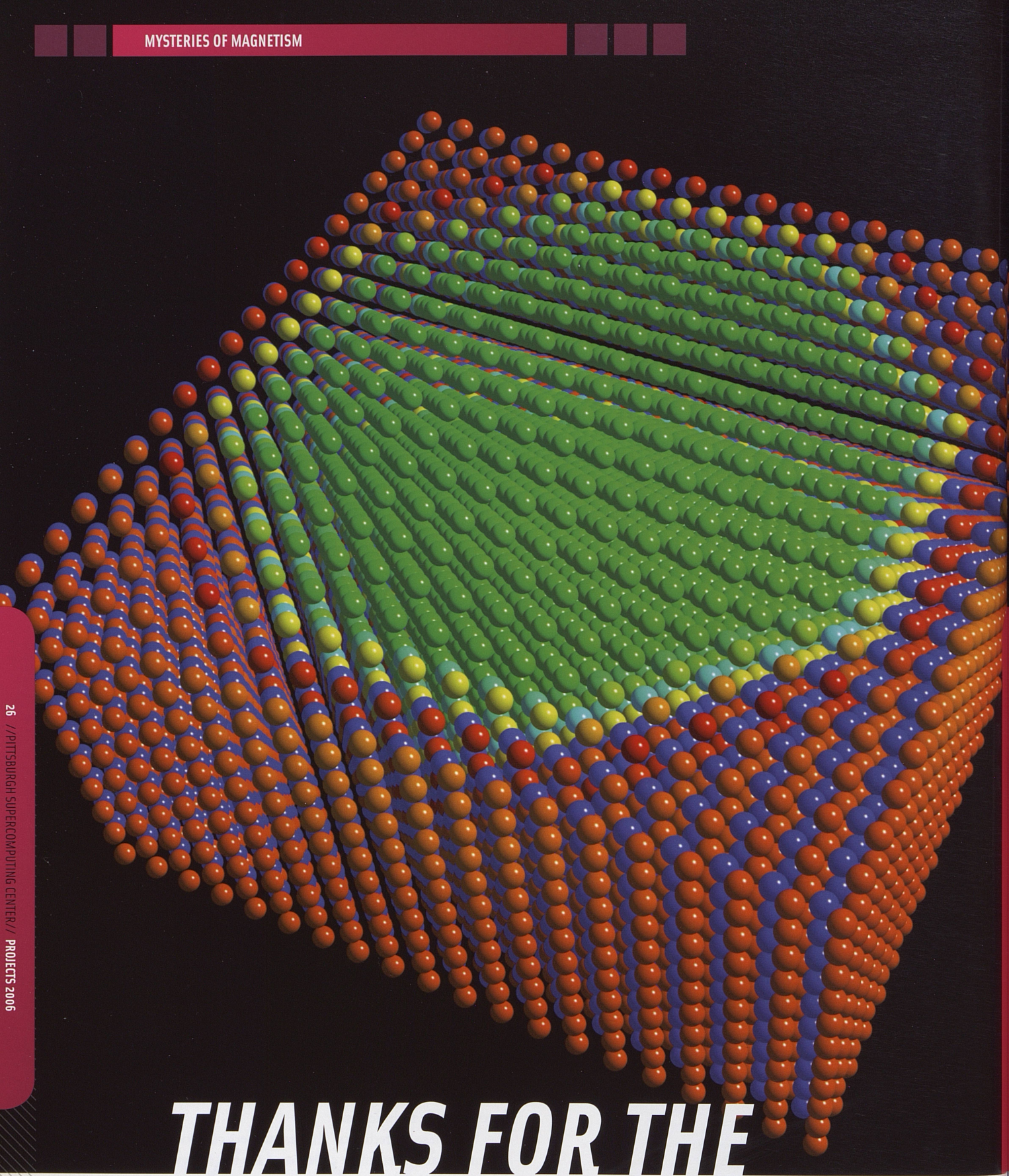
After a series of these simulations, they arrived at several new findings. They found that a water molecule forms a bridge between the MßL active site and the antibiotic, and this water shuttles a proton (H+) that is instrumental in cleaving the carbon and nitrogen of the beta-lactam ring. "This is important," says Dal Peraro, "because you can model inhibitors based on the position of that water molecule and its importance in the enzyme reaction."

What also emerged from the simulations is that the bizinc form is more efficient. "The second zinc," says Dal Peraro, "helps to make the reaction faster." With bizinc MßL, the reaction happens in one step, as opposed to two steps with the monozinc form. This suggests that the bizinc form is more of a threat, a finding that aligns with experimental evidence that bizinc MßL "is the most evolutionarily advanced form of the enzyme and ultimately more dangerous."

Another surprising finding has to do with the "coordination sphere" of the zinc ions, which refers to the number and geometry of bonds associated with the ions. The zincs shift their coordination during the reaction, between being bound to either four or five other molecular groups. This shift and the flexibility it shows, say the researchers, is of paramount importance in appreciating how the enzyme works, and it is revealed only by computation. "Experimentally you can't see these movements," says Dal Peraro, "because it's really fast and also because zinc and other metals are silent, not visible to spectroscopic techniques."

"All these ingredients," the researchers conclude, "are important and need to be considered for the design of new inhibitors." (MS)

MORE INFORMATION:
http://www.psc.edu/science/2006/enzyme.html



THANKS FOR THE MEMORY

POWERFUL QUANTUM METHODS AND THE CRAY XT3 OPEN A DOOR TO NEXT-GENERATION MAGNETIC STORAGE

A slice from the 2005 simulation, an iron nanoparticle embedded in an iron-aluminide matrix, shows charge distribution on the atoms (blue to red, positive to negative). In the nanoparticle itself, neutral iron (green) is bounded by iron atoms (yellow & light blue) that lose electrons. Other boundary iron atoms gain electrons to become more negative (red). In the matrix, aluminum atoms (blue) lose electrons to iron atoms (orange).

Computational scientists and other computer users in the future may hum this tune of gratitude, though perhaps few will appreciate how today's supercomputing helped to realize those even more capable hard drives of the future, as well as better iPods, DVDs, and who knows what?

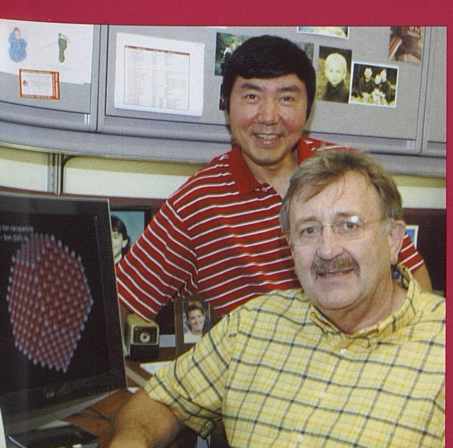
Technology has made steady advances in the ability to write and store vast quantities of information in smaller, more manageable forms, but current technologies are approaching their limit. How much smaller can you make grains of magnetized material before they start to act like the mind of an overstressed, aging human who steps out of the shower and can't remember if he's washed his hair?

Not much, which is why researchers are seeking a way to magnetize a single nanoparticle reliably, so that such a particle — rather than "grains" used in current magnetic-storage media — can record one bit of digital data. The door to this breakthrough is understanding what happens at the quantum level for each atom in a nanoparticle. Laboratory methods, for all their usefulness, can't provide this information. Over the past year, however, Malcolm Stocks, Yang Wang and their colleagues — using PSC's Cray XT3 — have shown that computational simulations can do the job.

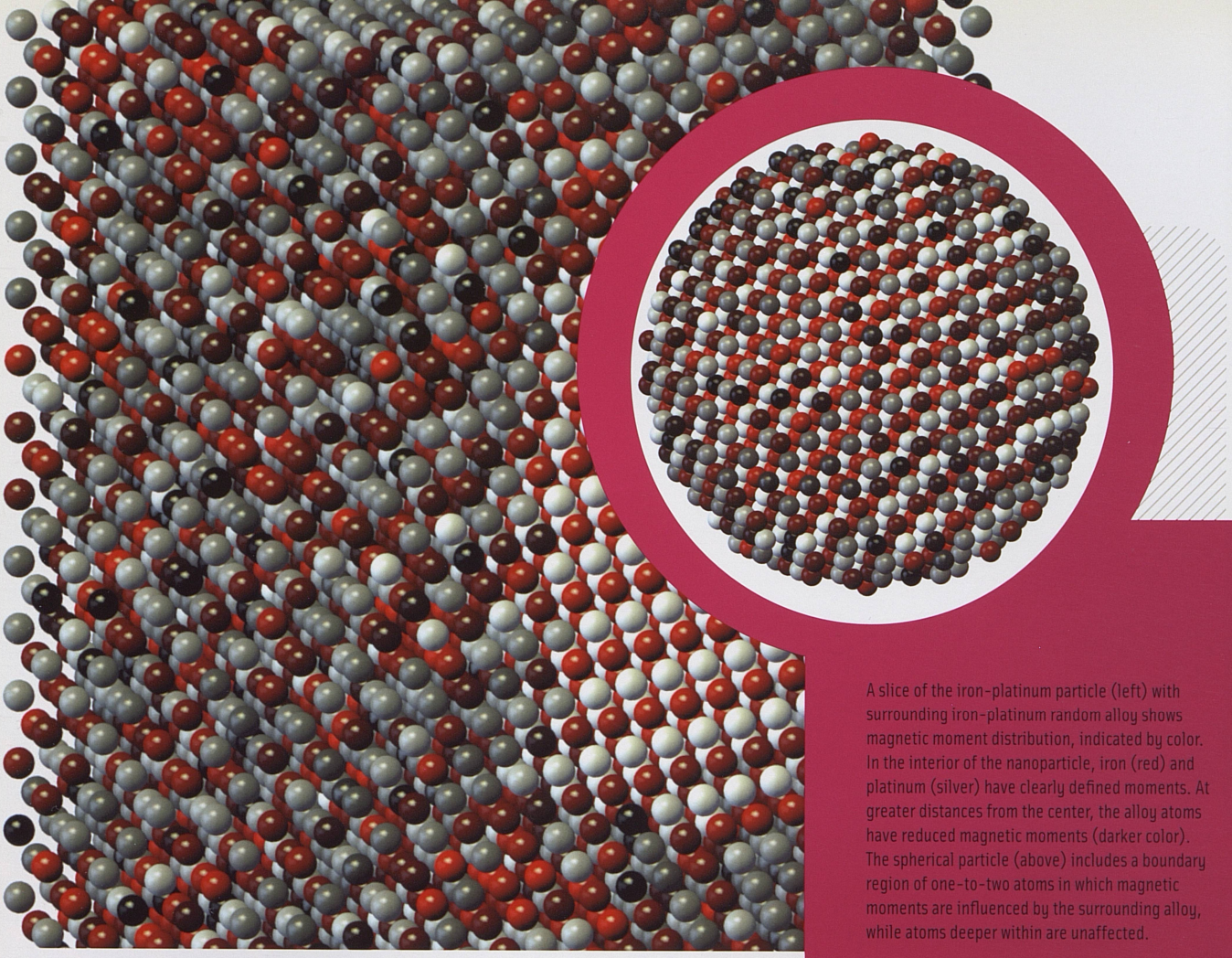
"Experimenters can tell us a lot about the magnetic and electrical properties of a nanoparticle as a whole," says PSC physicist Wang, "but simulations are the only way we have to determine the magnetic moments and electrical charges of individual atoms and therefore to understand the underlying mechanisms that drive the particle's electro-magnetic behavior."

Quantum-level simulations of even the smallest nanoparticles present huge challenges. "Consider that even a five nanometer-sized cube of iron contains on the order of 12,000 atoms," says Oak Ridge National Labs physicist Stocks, who leads a team — including Wang, Aurelian Rusanu, Don Nicholson and Markus Eisenbach of Oak Ridge — who have carried out large-scale nanoparticle simulations with powerful software they developed and the XT3.

Along with proving the feasibility of their approach, they have with their most recent simulation — a 14,400 atom iron-platinum nanoparticle — revealed unexpected electro-magnetic features. They found that a boundary region of nanoparticle atoms isolates the particle interior from quantum disturbances — a finding that opens a new window for design and development of nanostructured magnetic materials.



Malcolm Stocks (right), Oak Ridge National Laboratory, and **Yang Wang**, Pittsburgh Supercomputing Center



A slice of the iron-platinum particle (left) with surrounding iron-platinum random alloy shows magnetic moment distribution, indicated by color. In the interior of the nanoparticle, iron (red) and platinum (silver) have clearly defined moments. At greater distances from the center, the alloy atoms have reduced magnetic moments (darker color). The spherical particle (above) includes a boundary region of one-to-two atoms in which magnetic moments are influenced by the surrounding alloy, while atoms deeper within are unaffected.

THE SUPERPARAMAGNETIC LIMIT

Steady increases in data-storage density — which have doubled annually for decades — and the similar trend in faster processors have driven us into the information age. Today's magnetic storage can record data at 100 gigabits per square inch, and the next milestone is a terabit, a trillion bits per square inch. Roughly, that's all the x-ray data in a large hospital, or about 5,000 trees worth of printed paper, on one square-inch of magnetic material.

The dominant storage media are films of magnetic particles, composed of complex alloys of various metals, on fast-spinning hard disks. Whether the information is a rap tune on an iPod or a cryptogram on a CIA server, it's written to the disk by magnetizing minute patches of these particles, one patch for each bit of information. The smaller and fewer the particles that can be given a uniform magnetic field to represent binary "1" or "0," the greater the density.

The roadblock that looms — called the superparamagnetic limit — is that as the grains become smaller, heat effects (called thermal fluctuations) disturb the magnetic moments, resulting in noise, false sensor response, and long-term data loss. Storing information reliably — 10 years is a typical industry standard — requires stable magnetization at room temperature, but at grain sizes much smaller than current technologies, thermal fluctuations, even at room temperature, tend to scramble the data.

Proposed new designs, such as a patterned magnetic nanoparticle media in which each bit is stored in a single nanoparticle, require better understanding of quantum-mechanical behaviors. "There are big pieces of the underlying physics," says Stocks, "that we don't understand."

"We want to be able to predict for each nanoparticle," says Wang, "how much energy it takes to flip the magnetic moment from up to down. And because thermal fluctuations can flip the moment, we need to know the smallest size a particle can be and resist the fluctuation, and we want to understand the interactions between nanoparticles — how close they can be one to another — because we don't want to flip one particle and affect another one."

RESULT: A DETAILED PICTURE OF A REALISTIC NANOPARTICLE'S ELECTRONIC AND MAGNETIC STRUCTURE

AN ELECTROMAGNETIC SCREENING REGION

To get some of these answers, the Oak Ridge-PSC team turned to LSMS (the locally self-consistent multiple scattering method), powerful software they developed to simulate the quantum properties of solid-state materials. When implemented at PSC in 1998 (on the Cray T3E), LSMS broke the teraflop barrier. It was the first research software (as opposed to benchmark codes) to sustain performance over a teraflop (a trillion computations a second), an achievement that won the 1998 Gordon Bell Prize for high-performance computing.

On the XT3, running on 2,048 processors, LSMS zooms at over eight teraflops, more than 80 percent of the XT3's theoretical peak. "A powerful innovation of LSMS is its linear scaling," says Stocks. "As the number of atoms increases, computing time increases by only the same multiple." Without the innovations of LSMS, a realistically sized particle of tens-of-thousands of atoms would be too large to simulate. With a conventional approach, the amount of computing increases by the number of atoms cubed N^3 — so that as the particle size changes, for instance, from 1,000 to 10,000 atoms, the computing would take 1,000 times as long, rather than, as with LSMS, only ten times.

"Quantum-mechanical calculations are very time-consuming," says Stocks, "even on big computers. What we've done with LSMS is develop methods that allow you to do calculations for a sufficient number of atoms so the nanoparticle that the theory people talk about gets very close to the size that the experimentalists can make and measure."

In 2005, Stocks, Wang and colleagues used LSMS to carry out one of the first projects on PSC's then newly installed XT3. They calculated the electronic and magnetic structure of an iron nanoparticle embedded in an iron-aluminide matrix, a total of 16,000 atoms. This was the first quantum-based calculation of a physical system several nanometers in scale, and it successfully laid the groundwork for their next simulation.

The 2005 calculations were limited by an assumption that the magnetic moments for each atom of the nanoparticle were aligned in the same direction. "In reality," says Yang, "because of surrounding materials, that won't be the case." This year, taking the next step, they simulated an iron-platinum nanoparticle — at three different sizes, 2.5, 3.86 and 5.0 nanometers — in a matrix of surrounding alloy, totaling in each case 14,400 atoms, without any a priori assumptions about alignment of the magnetic moments. They focused on iron-platinum, says Wang, because industry leaders are interested in its potential as a storage medium. The computations occupied 1,200 XT3 processors — 12 atoms assigned to each processor — running for more than 50 hours.

"Iron-platinum," says Stocks, "is an important material because of its high magnetic anisotropy compared to most metals. This means it takes more energy for the magnetic moment to flip. As particle size gets smaller, this is more and more important."

The result of the LSMS simulations is a detailed picture of a realistic nanoparticle's electronic and magnetic structure. Atoms in the particle interior settle into an organized pattern of essentially the same amount of net charge and magnetic moment as bulk crystalline iron-platinum. Iron atoms gain electrons from the platinum atoms to become negatively charged, and conversely the platinum atoms become positively charged.

The most interesting finding is a boundary region, just a few atoms in thickness, that isolates the nanoparticle from disruptive quantum effects from the surrounding alloy. In this region, about four angstroms, net charge and magnetic moment fluctuate from influence of the alloy. The four-angstrom width of this region was constant for all three simulations, suggesting that it is independent of particle size. "The perturbed surface of the particle," says Stocks, "is like a fishbowl, separating the interior from outside effects. This is a piece of knowledge we didn't have before, and it will prove useful."

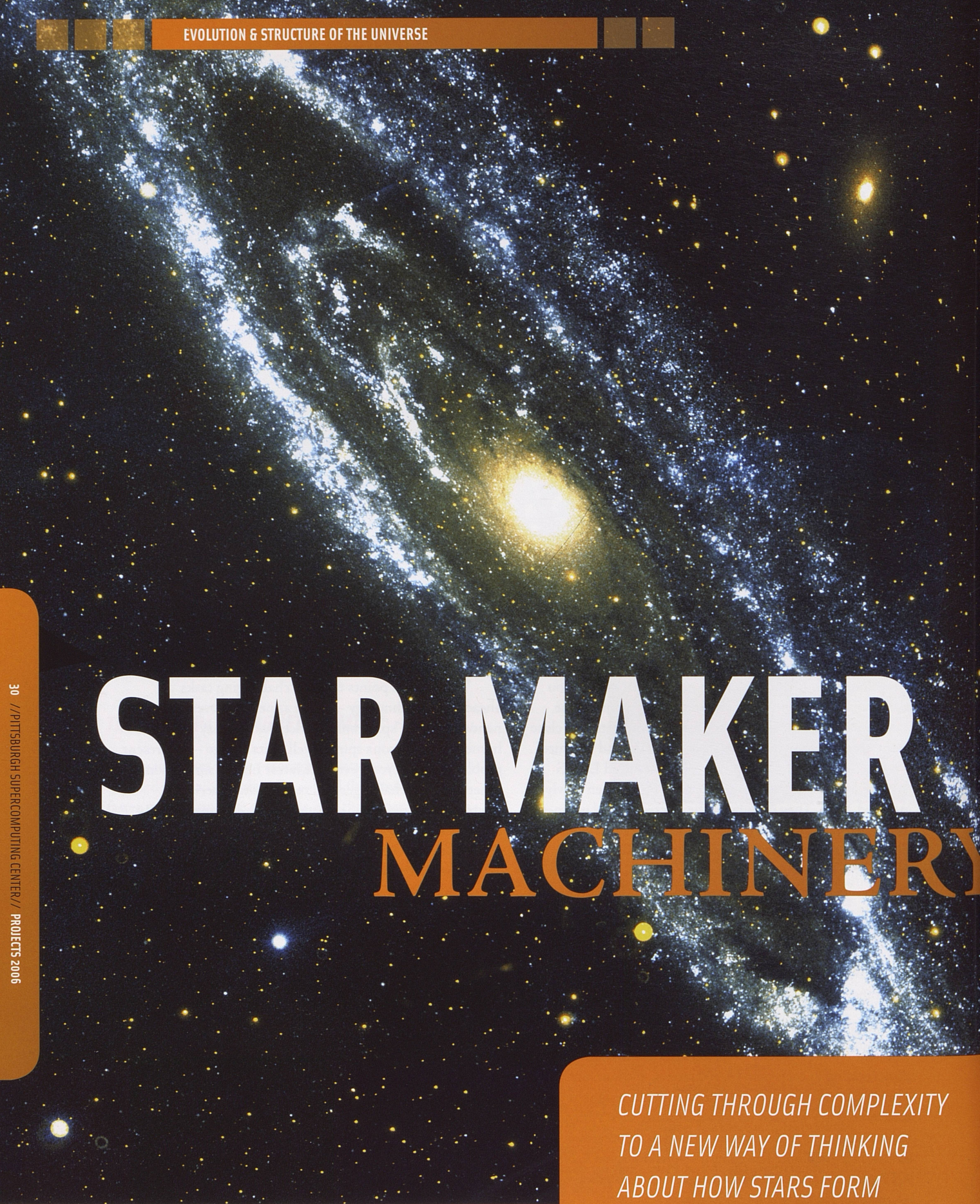
This success points to more challenging tasks ahead. Nanotechnology — such as new discoveries in nanostructured "spintronic" devices, which may be able to harness the electron's spin as well as its charge — represent problems well beyond even the latest LSMS simulation. Meeting those challenges will require characterizing electronic and magnetic structures on scales approaching millions of atoms, rather tens-of-thousands, and the computational cost will rise by a factor of hundreds.

Eventually, simulations such as these will aid in developing the more powerful computers needed for the next round of simulations. "Without the magnetic storage advances to date," says Stocks, "we wouldn't be able to do these calculations, which will help develop the next level of materials for the disk drives we'll need for the next level of calculations."

"Ultimately," says Wang, "the success of direct quantum mechanical simulation of nanostructured electronic devices relies on the advent of petaflop computing technology." (GH)

MORE INFORMATION:

http://www.psc.edu/science/2006/nano.html



STAR MAKER MACHINERY

CUTTING THROUGH COMPLEXITY TO A NEW WAY OF THINKING ABOUT HOW STARS FORM

How are stars made? — no, not pop stars and movie stars, the other kind, the ones that bring light to cosmic darkness. Like people, the brilliant light points in space have a birth-to-death cycle, and their birth is a tempestuous, uncertain process.

A star comes into being when a region of cold gas in a galaxy collapses —like a basketball contracting to the size of a dot — until the core gets so dense that the atoms begin to fuse. Astrophysicists mark the onset of nuclear fusion — when the thermonuclear furnace at a star's core begins to heat up — as the moment of star birth.

Not all galactic regions of collapsing gas, however, result in newborn stars. One scenario sees the birth process as a kind of competition between energies. Swirling, turbulent gas as it collapses builds up tremendous pressure, which — as it becomes dense enough — sends a sound wave outward. If this outward pressure wave travels fast enough, it can stop the collapse. On the other hand, if the collapse happens faster than the pressure wave's ability to slow it, known as Jeans instability, nuclear fusion starts and voilá — a new star.

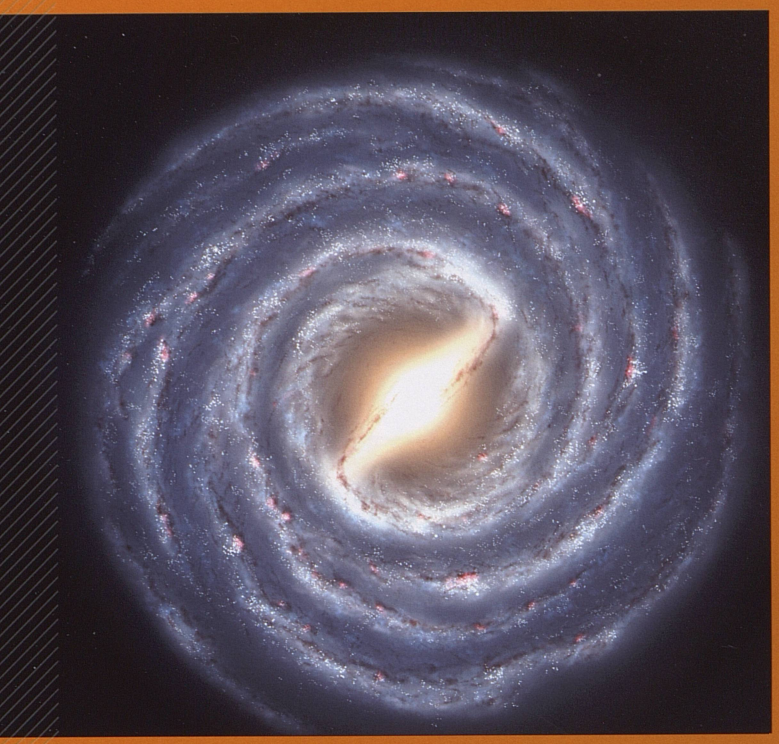
Underlying this simplified scenario, however, is a complex stew of physical processes, with many factors involved, including temperature of the gas, its chemical composition, its magnetization, and the rate at which the collapsing gas cools. Depending on how galaxy behavior is understood, scientists have proposed numerous theories of star birth and have long sought a clear explanation.

Why do we care how stars form? Simple, says Mordecai-Mark Mac Low, an astrophysicist at the American Museum of Natural History in New York. Without star birth, there wouldn't be life. "Ultimately our research tells us why we are here," he says. "In our models of star formation, we're basically trying to figure out how the galaxy we live in and all the galaxies we see around us behave. And how does that behavior contribute to our own presence?"

In recent work, Mac Low and colleagues Yuexing Li of Columbia University — now at the Harvard-Smithsonian Center for Astrophysics, and Ralf S. Klessen of the Astrophysical Institute of Potsdam — now at the University of Heidelberg, used LeMieux, PSC's terascale system, to simulate billions of years of galactic evolution. Their results cut through the galactic fog and reduce a complex story to one key element.

"Gravitational instability," says Mac Low, "appears to be the dominant mechanism controlling the formation of stars."

Mordecai-Mark Mac Low, the American Museum of Natural History



COSMIC COLLISIONS

Simulations Featured in Planetarium Show

"Two spiral galaxies, spinning like jeweled spiders, approach, flow through each other, separate as arms of stars flow gracefully akimbo and then draw together again in a double-yoked embrace..."

This poetic prose in the *New York Times* (by science writer Dennis Overbye) describes the grand finale of "Cosmic Collisions," a space show at the Hayden Planetarium of the American Museum of Natural History (AMNH), New York City. The scene, a simulation that depicts the Milky Way and Andromeda galaxies colliding and eventually merging five billion years from now, owes its existence to the computational horsepower of LeMieux, PSC's terascale system.

A high level of scientific accuracy in the show results from a decision to use supercomputer simulations instead of artists' renderings of cosmic phenomena. In the case of the Milky Way–Andromeda merger, that meant a simulation by Mac Low and colleagues Li and Klessen and John Dubinski of the University of Toronto using 64 LeMieux processors for 40,000 processor hours. It was the first galaxy-merger simulation to track individual star clusters and follow them on their orbits, and its results support hypotheses that merger processes partially explain the origin of the dense globular clusters of stars that orbit galaxies, whose birth has been observed by the Hubble Space Telescope in the past decade.

AMNH distributes "Cosmic Collisions" nationally and internationally and expects that it will be seen by millions of people.

SINK PARTICLES

To get to this conclusion, Mac Low's team modeled the matter within galaxies as particles, using a method called "smoothed particle hydrodynamics." They implemented this approach with simulation software, called GADGET, developed by Volker Springel at the Max Planck Institute for Astrophysics in Garching, Germany. Instead of overlaying a fixed grid and monitoring changes within each cube of the grid — a common approach to modeling movement of objects in space, GADGET scatters particles across the galaxy, with each particle assigned an initial density, pressure, and velocity. The simulations track these particles — their changes in position, density, pressure and velocity — through billions of simulation years.

"Instead of a regular grid where the resolution is fixed everywhere," says Mac Low, "you have an unstructured grid, where the resolution follows the gas flow. This is good if you're looking at problems of collapse, because you put the most resolution in the densest regions."

Along with this advantage, however, the particle method imposes a challenging computational problem. When collapse starts, the particles crowd closer and closer, in tighter and tighter orbits about each other. Maintaining high resolution in such a region requires more and more computation to advance the same amount of physical time, which eventually leads to an impasse — to advance a year of galactic time can require a year of computation.

The solution is to let collapse proceed until it's certain the collapsing region will achieve critical stellar density, then replace the thousands of gas particles in this region with a single absorbing particle of the same mass and velocity — called a "sink" particle because it acts as a sink, as opposed to a source, of mass. In that region, LeMieux now has to track only one particle, instead of thousands. By measuring the mass of a sink particle, scientists can quantify how much gas has collapsed to form a star cluster. "Effectively it becomes," says Mac Low, "a star particle."

Mac Low first worked with sink particles on a cluster computer at the American Museum of Natural History before he approached PSC for time on LeMieux. "You don't want to get on a high-performance machine," he says, "until you know where you're going and what you want to accomplish. Once we started our million particle runs, to do it right we needed something like LeMieux."

Their model galaxies comprise a disk of stars and uniform temperature (isothermal) gas surrounded by a spherical "halo" of dark matter; picture a globe filled with dark matter and a swirling disk of gas and stars at the equator. Through a series of about 20 simulations of single galaxies, over nearly two years starting with the AMNH cluster and then with LeMieux, they varied the number of gas particles from one to six million, and they varied other parameters — the fraction of gas, the size and rotation rate of the galaxies, effectively varying the strength of gravitational instability — and observed the effect on star birth.

THE SIMULATIONS IDENTIFY A RELATIONSHIP BETWEEN THE RATE OF STAR BIRTH AND THE TOOMRE INSTABILITY PARAMETER.

GRAVITY RULES

The results show that star particles form more readily in regions that are more gravitationally unstable. In disk galaxies, gravitational instability is known as Toomre (pronounced Toom-ray) instability, for Alar Toomre, who first described it in 1964.

The Toomre gravitational instability parameter quantifies how sensitive a region of gas is to changes in local conditions. If additional gas is added to the region, or the strength of rotational shear changes, how likely is it that this will initiate collapse? Regions with an instability parameter above 1.0 are relatively stable and vice-versa.

Two factors bear on Toomre instability: pressure support and shear support. Pressure support involves a sound wave traveling outward through a collapsing region, as described earlier. If the gas collapses faster than the sound wave can stabilize it, the region becomes pressure unstable, meeting the Jeans instability criterion.

The other factor is shear support, which takes into account the "differential rotation" of material orbiting in a disk. Particles close to the center of the disk revolve faster than particles at the outer edges, just as in our Solar System where planets distant from the Sun travel more slowly along their orbit than planets close to the Sun. Because of differential rotation, gas on one side of a collapsing region can shear away from gas on the other side before collapse occurs, preventing star formation. For Toomre instability, the gas region must collapse fast enough so that (1) sound waves can't provide pressure support, and (2) shear doesn't tear the region apart before it collapses.

Mac Low's simulations with LeMieux show that sink particles form more readily in regions where the Toomre gravitational instability parameter is smaller. This is true regardless of changes in other variables — galaxy size, quantity of gas particles, rotation rate and gas fraction of the galactic disk. The simulations identify an exponential relationship between the rate of star birth and the Toomre instability parameter. Therefore, Mac Low concludes, Toomre instability alone is sufficient to explain star formation.

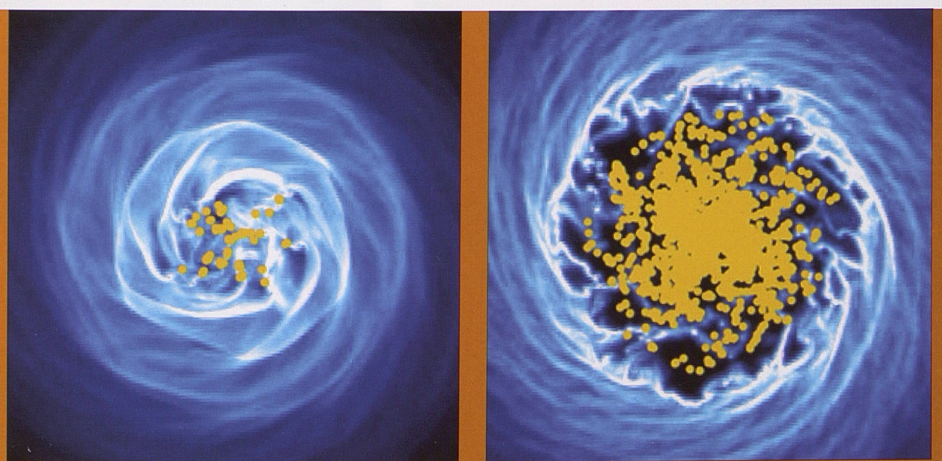
This conclusion departs from a number of previous theories. Some theorists believe that cooling is key — if you cool the gas in a galactic disk to a low enough temperature, star formation will inevitably occur. Others argue that magnetic support is crucial, with star formation occurring only in regions sufficiently neutral to decouple from the magnetic field.

Mac Low's results, however, strongly suggest that these ideas are due for rethinking. "I'm arguing," he says, "that cooling is incidental. The first thing you do is start the collapse, and if you raise the densities high enough, the cooling will happen very quickly, more or less regardless of details. Similarly, if a massive enough region collapses, magnetic support can simply be overwhelmed."

To follow-up on these findings, Mac Low and his colleagues plan to simulate galaxies at finer and finer resolution until they reach the resolution of an individual star. Currently, he and M. K. Ryan Joung of Columbia University are using 1,000 LeMieux processors to simulate a small fraction of a galaxy — to test whether supernovas act as galactic "stirrers" that stir and heat gas, impeding collapse.

Better knowledge of how a star is born, he says, helps us to comprehend "the grand history that ends up producing a kind of average star two-thirds of the way out in a larger-than-ordinary galaxy, a star that happens to have planets around it — one of which we live on." (TP)

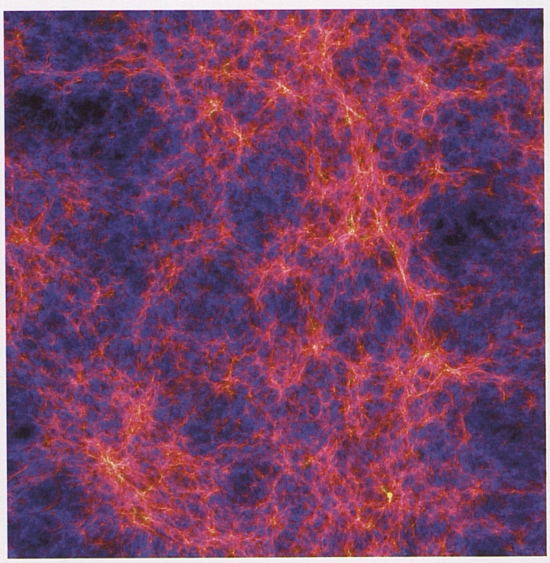
MORE INFORMATION:
http://www.psc.edu/science/2006/starmaker/starmaker.php

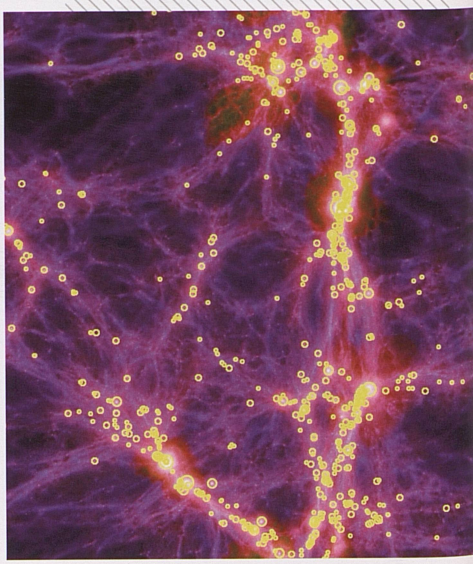


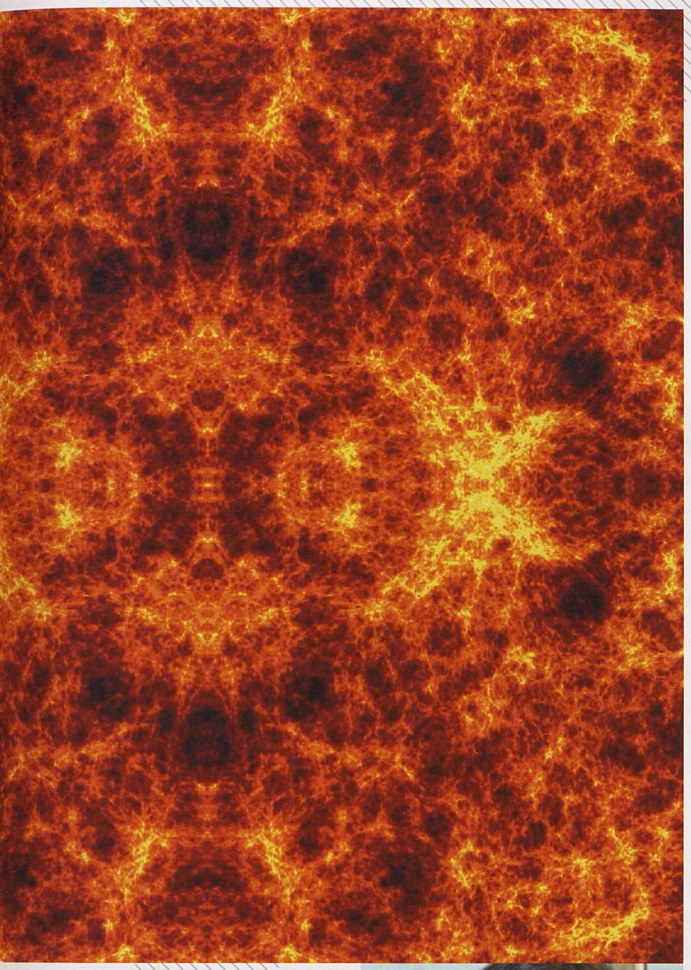
Simulations of star formation in two galaxies with different masses after a billion years. A galaxy 10 times more massive (right) than the other is much more unstable gravitationally, which leads to the formation of a greater number of star clusters, as represented by the yellow sink particles. The surface density of atomic gas in these galaxies is represented by the white and blue regions, with white indicating the highest density and dark blue the lowest.

FIXING THE HOLES

Evolution of Structure in the Cosmos
Snapshots from the simulation show evolution of structure in a large volume of the universe. Gas density is shown (increasing with brightness) with temperature (increasing from blue to red color). Yellow circles indicate black holes (diameter increasing with mass). At about 450 million years after the big bang (left), as the early universe still shows a relatively uniform structure, the first black hole appears. At about 6 billion years (right), the universe has many black holes and a pronounced filamentary structure.







Tiziana Di Matteo,
Carnegie Mellon University

Once thought to be rare, exotic bodies, black holes have turned out to be fundamental focal points in the architecture of the cosmos. Among the sprawling, intricate arrangement of matter in every galaxy, they are the invisible centerpiece. Their tremendous mass, which can be many billion times the mass of the Sun, gives them gravitational pull to swallow huge quantities of interstellar gas. As this gas swirls outside the lip of the drain, just before falling in, it heats to extreme temperatures and radiates energy as light waves, producing one of the brightest bulbs in the universe — a quasar. Once over the edge of this lip, however, nothing escapes, not even light.

Despite their ubiquitous presence, black holes and the quasars they spawn have been until now absent from large-scale simulations of the universe — too small to be resolved within the big picture of cosmic structure. With PSC's Cray XT3, however, Carnegie Mellon University astrophysicist Tiziana Di Matteo and her colleagues included black holes in what is perhaps the most computationally demanding cosmological simulation ever, encompassing a sizeable fraction of the universe. Their intentions were bold. "We wanted to simulate the universe," says Di Matteo, "and go from the Big Bang until today."

The result can be viewed as a movie that shows evolution of structure over the 14 billion years of the universe's existence, with black holes in a lead role. Far from being only destroyers, gobbling up any matter within reach, black holes in this new picture are also regulators: Their mass is related to the size of the galaxy they reside in as well as to its total star mass.

The goal is a more fundamental understanding of the evolution of the universe. "What kind of quasars formed in what kind of galaxies at what time?" asks Di Matteo. "What is the progenitor of the most massive black hole today?" There is also a more immediate benefit — directing astronomers where to aim the Next Generation Space Telescope — the successor to the Hubble Space Telescope — to observe the formation of the first galaxies and black holes.

BY INCLUDING BLACK HOLES FOR THE FIRST TIME IN A LARGE-SCALE COSMOLOGICAL SIMULATION, PHYSICISTS UNCOVER THEIR FUNCTION IN REGULATING THE GROWTH OF GALAXIES

A NEW COSMIC RECIPE

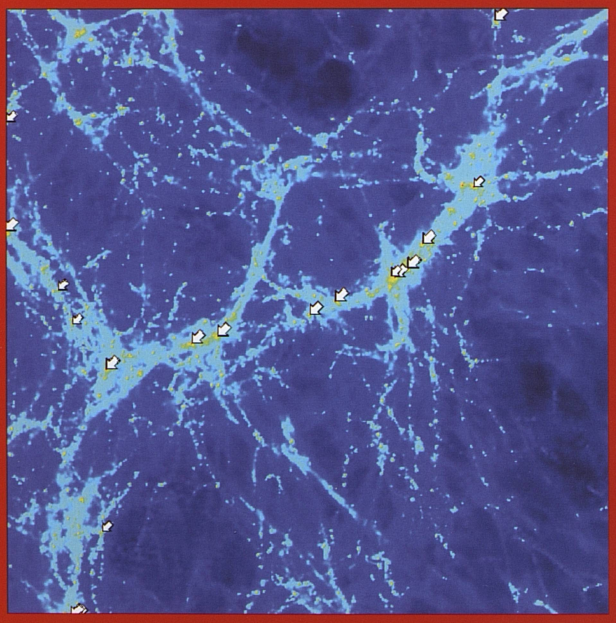
For this huge simulation, Di Matteo started with the software called GADGET-2 developed by Volker Springel of the Max Planck Institute for Astrophysics. To account for black holes, Di Matteo added code to "seed" black holes at the centers of forming galaxies. Next, she added an equation to describe how black holes "accrete" or swallow gas, adding to their mass and gravitational pull. Finally, she included calculations for "feedback" — heating of surrounding gas in the galaxy by quasar radiation produced at the lip of the black hole.

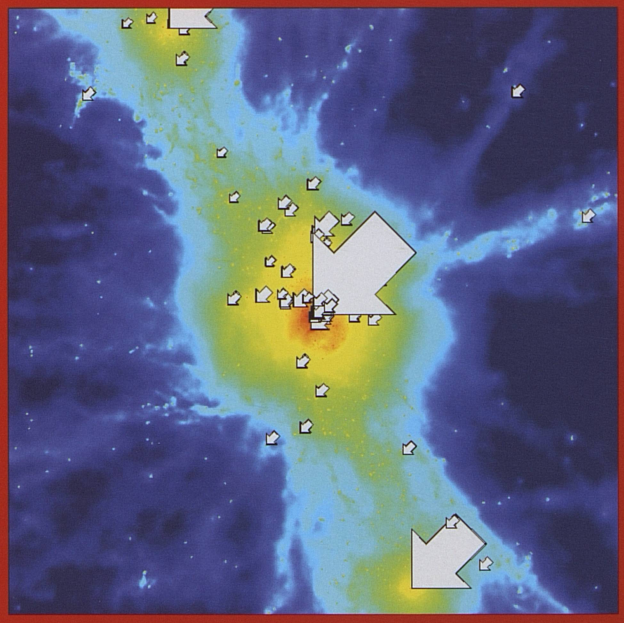
The researchers first applied this approach on a small system of two colliding galaxies with black holes at their centers. The success of this simulation, which revealed new behavior when black holes were included, led to a 2005 paper in *Nature*. It also prompted Di Matteo to move to a much bigger scale. The idea, says Di Matteo, was to simulate a large portion of the universe "at the same resolution and with the same spatial scale as those idealized calculations."

To obtain this high resolution, the researchers scattered 230 million hydrodynamic particles over a 33 megaparsec cube, a huge volume encompassing a million galaxies, a representative chunk of the universe. To track these particles, the simulation used 2,000 XT3 processors — the whole system — over four weeks of run time. They followed the evolution of superclusters of galaxies — the largest structures in the universe — while simultaneously resolving the growth of black holes at the centers of galaxies. The XT3 was key.

"The XT3 is ideal for this simulation because it has incredibly fast built-in communication," says Di Matteo. "If we didn't have the bandwidth to communicate large chunks of data among 2,000 processors, it would have been really tough. I don't think we could run this simulation anywhere else right now."

Galaxy Closeup
These simulation snapshots zoom-in on the galaxy that hosts the most massive black hole in the universe today. This galaxy resides in one of the most massive elliptical galaxies, at the center of a large galaxy cluster. At about 600 million years after the big bang (left), matter is more diffuse than it is about 4.5 billion years later. Gas density increases from blue to red, and arrows indicate black holes (arrow-size relative to mass).





"THE XT3 IS IDEAL FOR THIS SIMULATION BECAUSE IT HAS INCREDIBLY FAST BUILT-IN COMMUNICATION."

REPENTANT OVEREATERS

While the researchers are still analyzing the huge quantity of data from this simulation, about ten trillion bytes, initial results are exciting. The major finding is the regulatory role black holes play in galaxies. It turns out that after gobbling gas for millennia, a black hole eventually begins pushing gas away, like a repentant overeater. "The black hole tries to swallow a lot of gas," says Di Matteo, "but this growth is kind of suicidal. As it tries to swallow more and more it will radiate so much energy that it will affect its surroundings and stop more gas from flowing in."

This first effect of this purging "feedback" process is that it shuts off the quasar associated with the black hole. Because gas is no longer falling in, gas at the lip of the black hole is no longer heated and eventually radiation stops. In effect, feedback blows out the candle of the quasar, which explains why — though virtually every galaxy had a quasar when the universe was young — now there are quasars in only about one in 10,000 galaxies.

While blowing out the quasar, the black hole also expels most of the galaxy's interstellar gas into inter-galactic space. As a result, since interstellar gas is the stuff that stars are made of, stars stop forming. This helps to explain the "red and dead" phenomenon with which astronomers have long struggled: the preponderance of old galaxies in which no new stars are forming. Old galaxies tend to appear red due to the overwhelming dominance of old stars. Stars should form readily if there is interstellar gas to feed the process, yielding young blue stars. Di Matteo's simulation shows that there is very little interstellar gas left, leaving old galaxies "red and dead."

Another conundrum was the common ratio found between the mass of the central black hole and the mass of its host galaxy. Precise measurement using the Hubble Space Telescope and other instruments has shown that the black hole has a mass approximately 1/1000th the mass of the stars in its galaxy. This same ratio emerged from Di Matteo's simulation, which helps to validate the model, but the reason for the ratio is not yet evident. Some mechanism related to a galaxy's critical mass might cause the black hole to stop swallowing when it does, but that mechanism remains a mystery. "Black holes clearly regulate how the galaxy forms in some way that is still debated," says Di Matteo, "and that is what we are still trying to understand."

Perhaps one of the most exciting end products of this huge calculation is a movie showing how the universe evolved over 14 billion years. The simulation begins before galaxies have formed, and the first frames (each frame is about half a million years) show a virtually uniform universe, with matter dispersed rather evenly, and just small perturbations in this background — corresponding well with the picture provided by cosmic microwave background studies. The first black holes appear when the universe is 300 million years old — just a child.

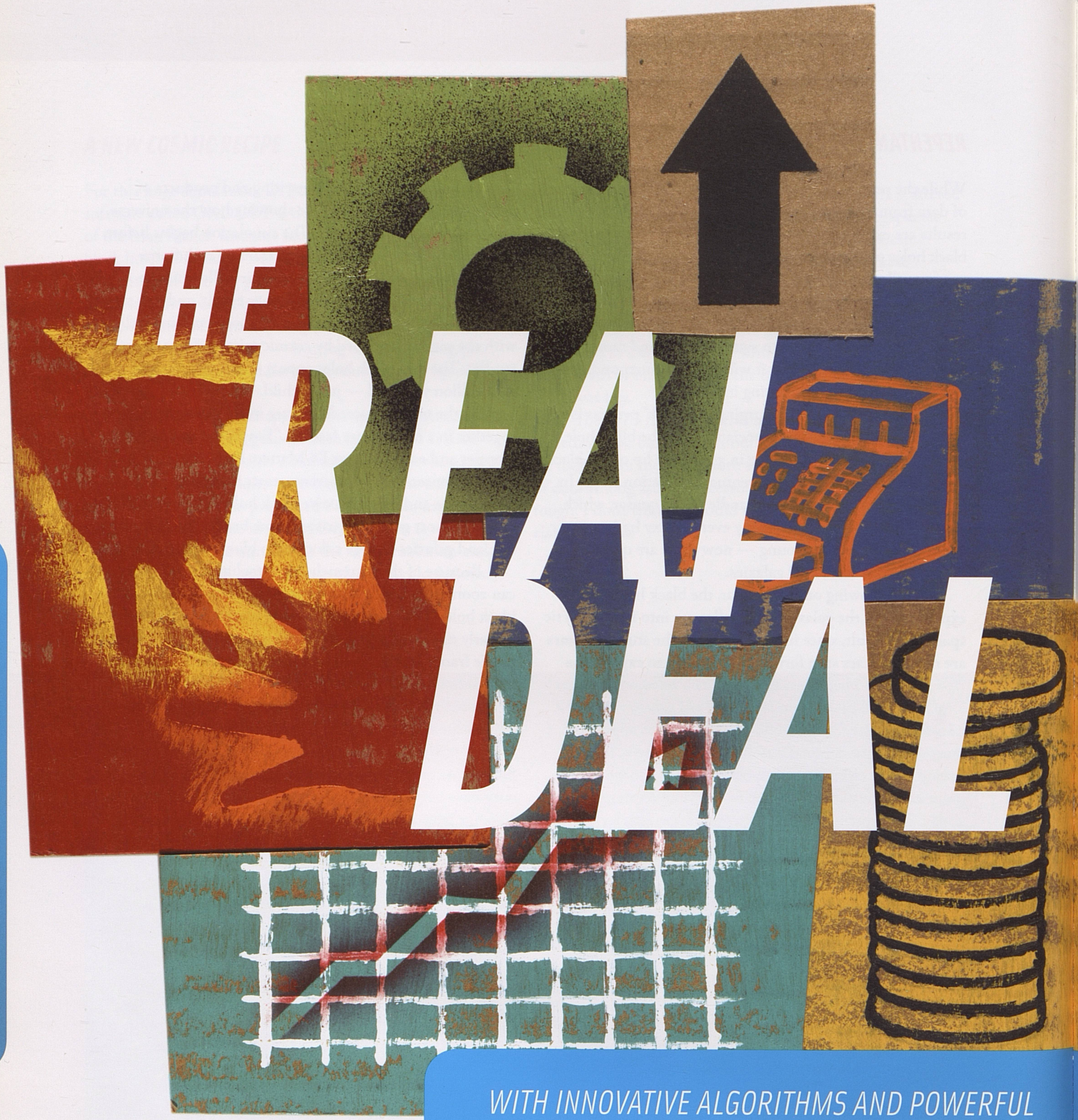
As the movie proceeds, matter in the universe clumps together in a filamentary fashion. "Empty regions become emptier and emptier," says Di Matteo. Dense regions become denser, and the universe starts to look like a spider web. By the end, supermassive black holes are lurking in the center of most galaxies, quasars shine bright and then blow out, and galaxies change colors from blue to red as they age.

Because of the extremely high resolution, Di Matteo can zoom in at any time and watch the growth of a particular black hole. "This is the most massive black hole that forms at an early time," she says, pointing to a specific black hole on a movie frame, "but it does not end up being the largest black hole today. It grows really fast then it stops. Other black holes start to grow later on and they grow at a faster rate at a much later stage, and so that's very exciting too."

Di Matteo and her colleagues don't know what other fascinating results await them in the huge mass of data they have begun to analyze. Perhaps they will learn where to point telescopes to see the remnants of the first quasars, or maybe they will see astronomical phenomena never dreamed of before. "The hugest challenge was to do this very large simulation," says Di Matteo. Analyzing the data will be a pleasure. "Both in terms of the resolution and the physics," she says, smiling, "nobody else has a simulation like this right now." (TP)

MORE INFORMATION:

http://www.psc.edu/science/2006/blackhole.html



THE REAL DEAL

WITH INNOVATIVE ALGORITHMS AND POWERFUL COMPUTERS, ECONOMISTS ARE GETTING REAL WITH THE LIFE-CYCLE MODEL

Who among us hasn't pondered strange human behaviors? Some people invest in beanie babies. Some wear bell-bottom hip huggers. Some of us live in populous cities located in earthquake or flood zones.

Despite many irrational human behaviors, economists have the professional task of making reliable predictions about the economy, a task that involves trying to find underlying logic in the processes by which people make decisions in consumer spending, housing, employment, savings, healthcare and many other economic-related realms of activity. One of the best tools economists have to help forecast economic weather, despite the inherent vagaries of human decision-making, is the *life-cycle model*.

"The life-cycle model is one of the central paradigms in economics," says John Rust, professor of economics at the University of Maryland at College Park. "With this approach, observed behavior can be explained as rational 'best responses' based on the structure of economic institutions, such as the social security system, and the real uncertainties individuals face regarding health, earnings, prices and many other uncertainties."

The life-cycle model mathematically formulates decision-making as a series of sequential decisions influenced by variables over the course of a lifetime. It has been applied usefully in many areas of policy making. Nevertheless, the model's predictive ability has been limited because it hasn't been possible to solve complex formulations that account for a realistically broad range of variables. "The theoretical predictions of the model," says Rust, "haven't been well understood since, except for trivially simple special cases, the model doesn't have a closed-form solution."

Beginning several years ago, Rust used PSC's Cray T3E to develop novel algorithms that, for the first time, make it possible to apply the computational muscle of massively parallel systems to the life-cycle model. With this powerful approach, he and graduate students Joseph Nichols and Gaobo Pang have used LeMieux, PSC's terascale system, to solve the largest, most realistically specified versions of the life-cycle model ever attempted.

Their approach has yielded insights in a number of areas. Nichols, now at the Federal Reserve, used LeMieux to develop the first realistic life-cycle model treatment of housing and mortgages, resolving a previously puzzling question about why people hold a large fraction of investment in housing assets. A study by Pang used LeMieux and a detailed life-cycle model to find that, contrary to expectation, tax-deferred savings accounts would lead to substantial new savings and could induce earlier retirement.

With his innovative algorithms and LeMieux, Rust — an advisor to the Social Security Administration during the Clinton presidency — has applied the life-cycle model in many areas. Among several government-policy related studies, he developed and tested a proposal by which the Social Security Administration can improve its disability benefit process, targeting those who are truly disabled at less cost than current procedures.

"When the life-cycle model is fully estimated and tested," says Rust, "it has a number of practical uses for predicting the impacts of proposed changes to the Social Security program, including raising the early retirement age, introducing individual accounts, and changing Medicare coverage." Modeling these proposed changes instead of passing them with no prior study can protect the American public, says Rust, from becoming "inadvertent crash-test dummies."

Most interesting, perhaps, in Rust's work with LeMieux are the surprises that emerge from the ability to solve more realistic formulations of the model — such as his recent work on a long-puzzling question about decline in consumption after retirement. Contrary to prior studies, Rust's computations — taking into account variables not before considered — show that this decline is a rational response consistent with the life-cycle model. The result has stirred controversy.

"This is the power of computational economics," says Rust, "to arrive at results we're not able to anticipate by our economic intuitions from simpler versions of the model. It takes supercomputing to show how basically simple, elegant equations can yield answers we would never guess at or otherwise be able to see."

John Rust,
University of Maryland

"IT'S ONLY THROUGH WHAT THE SUPERCOMPUTER SHOWS US THAT WE CAN OPEN OUR EYES AND THINK IN NEW WAYS."

BREAKING THE CURSE

How do you quantify the complexities of human behavior? Economists have wrestled with this problem since at least the 1940s, when researchers in a number of fields — notably John von Neumann and Oskar Morgenstern — arrived at an approach called "backward induction." In the simplest terms, backward induction means starting at the end and working backward to see what decisions led to the final outcome.

The life-cycle model uses backward induction and assumes that people try to make the best decisions possible, based on the information available to them. The beauty of the model is that it can accommodate uncertainty — saving for retirement being a classic example. No one knows, in a precise way, how much to save since no one knows how long they'll live or what kinds of health problems they might experience, not to mention future rates of inflation or other economic factors.

The life-cycle model, furthermore, is predicated on preferences and beliefs — such as individual priorities about leisure versus work or perceptions about future health and longevity. Rust's algorithms implementing the model are best described as "polyalgorithms" — an inner algorithm does the backward induction (often called "dynamic programming") within an outer algorithm that searches for values of the preferences and beliefs parameters. The inner algorithm solves the model hundreds or thousands of times to find optimal decisions and iterates back and forth with the outer algorithm until the predicted behavior matches well with observed behavior over the life cycle.

Although variables will change and details of the model specification differ, life-cycle models can be applied to a huge variety of problems. "The life-cycle model has the ability to provide an explanation for almost everything we do in our lives," says Rust, "starting with child rearing, learning and schooling, dating and sex, going to college, searching for the first job, getting married, buying a first home, choosing whether to have children and how many, saving for their college and your retirement, or deciding when to retire."

A serious limitation of the life-cycle model has been the so-called "curse of dimensionality." For each decision cycle, the program must find optimal values for the variables, and a single solution requires many billions of algebraic operations. For every variable added, increasing its realism, the computing time increased exponentially. Rust's novel algorithms introduce a randomizing routine that, in effect, breaks the curse of dimensionality. He achieves linear scaling on parallel architectures for as many as 800 processors, making it possible to solve problems that would take many hours on a single processor in a matter of minutes on a parallel system such as LeMieux.

Bellman equation for rental problem

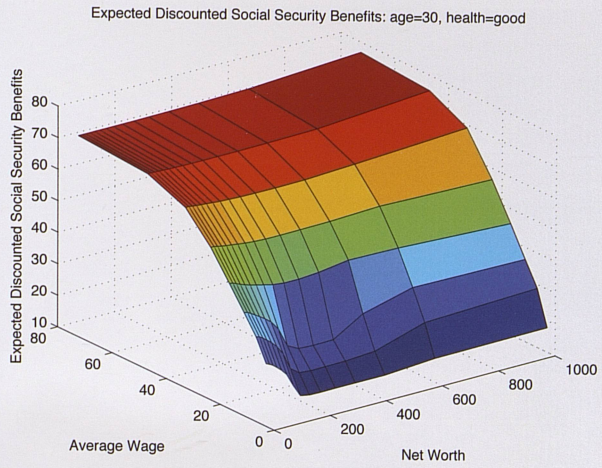
$$V(r,d,0) = \max\left[E\Pi(0) - \bar{P} + \beta EV(r_0,0,0),\ ER(r,d,0) - EM + \beta EV(r,d,0) \right]$$

HOW TO MAKE (MORE) MONEY RENTING CARS

In a much different application of his methods, Rust looked at a car-rental business and the question of what is the best timing to replace older cars with new models. Even in the case of a company making good profit, the modeling shows they could substantially increase profit by using cars longer with a "discount menu" rental rate.

"We found that the company is getting burned," says Rust, "by the rapid initial price depreciation in cars. By holding cars longer, they amortize the initial depreciation over a longer horizon, earning more rental revenue, which helps to defray the cost of replacing older with newer models."

The modeling also accounts for the economic reality that customers will be less inclined to rent older vehicles – showing that with age or odometer-based discounts on rental, the company can earn significantly higher profit, and customers have greater choice. "With PSC resources," says Rust, "we found a win-win situation that this company is seriously considering adopting."



Expected present value of social security benefits for a 30-year-old person in good health, as a function of average wage and net worth. (Units are in thousands of dollars.) Benefits are a concave function of average wage, showing that high-wage individuals have lower proportionate return than low-wage individuals, an indication of the "progressivity" of the system.

THE PROBLEM WITH TOYS

Rust's recent modeling of retirement consumption goes beyond prior life-cycle modeling of this problem and suggests — contrary to prevailing wisdom — that, with a sufficiently realistic statement of the life-cycle model, retirement data that's been seen as "irrational" can be explained as a rational response. By taking into account the "labor-effect factor" — the possibility that people choose to retire earlier with less income than they otherwise might, because they value leisure — his modeling arrived at a new way of fitting the model with observed behavior.

Earlier this year in an invited talk at the Federal Reserve Board in Chicago, Rust stirred controversy when he presented these findings. Previous work on this problem has relied on a concept called "consumption smoothing" — which assumes people adjust consumption gradually in response to anticipated events. Skepticism about his finding, Rust believes, comes in part from reliance on life-cycle models — "toy models" — that don't account realistically for the choices people face as retirement nears. Consumption smoothing is a strong intuition that economists arrived at from toy models, and "it doesn't really generalize."

The inadequately specified "toy models" can lead to bad or unnecessary policy changes. "Some economists point to the drop in consumption after retirement as 'proof' that individuals are myopic," says Rust, "and experts therefore think that having a large, mandatory Social Security program is the way to protect these poor decision makers in old age and keep them out of poverty. My work indicates that the drop in consumption need not be a sign of myopia and can indeed be an optimal response by a rational, forward-looking consumer. In general, if people are rational, it only hurts them when the government forces them to save in a certain way, especially if it makes them save too much in the early part of their life when they are liquidity constrained."

Beyond the challenging theoretical insights from Rust's work, there are significant practical applications. From a public policy perspective, says Rust, being able to model human behavior at this level of detail is far more cost effective than attempting to measure behaviors in a population.

"These models can get so complex," he says, "that it's only through what the supercomputer shows us that we can open our eyes and think in new ways. This represents an important contribution to the science of economics that, I believe, will become more and more important over time — as the tools become more powerful and more economists learn to use them." (DA)

MORE INFORMATION:
http://www.psc.edu/science/2006/realdeal.html

Chips To Go

U.S.-JAPAN GRID TESTBED LINKS SIX SUPERCOMPUTERS FOR QUANTUM SIMULATIONS OF CHIP FABRICATION

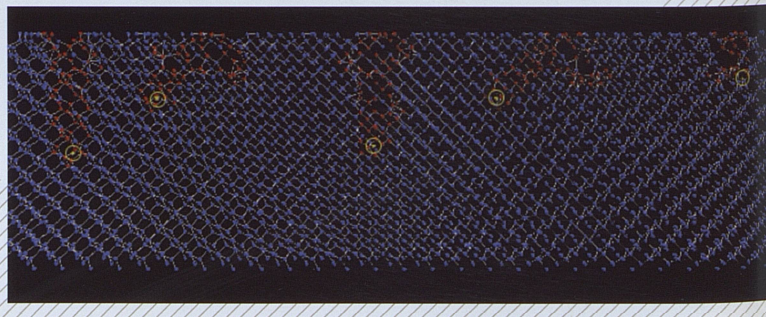
From cell phones to laptops, integrated circuits — "chips" — that run fast on low power are the brains of our mobile electronic culture. SIMOX (separation by implantation of oxygen) is the favored method for sculpting circuits in SOI (silicon over insulator) chips — the usual choice for portable, battery-powered devices.

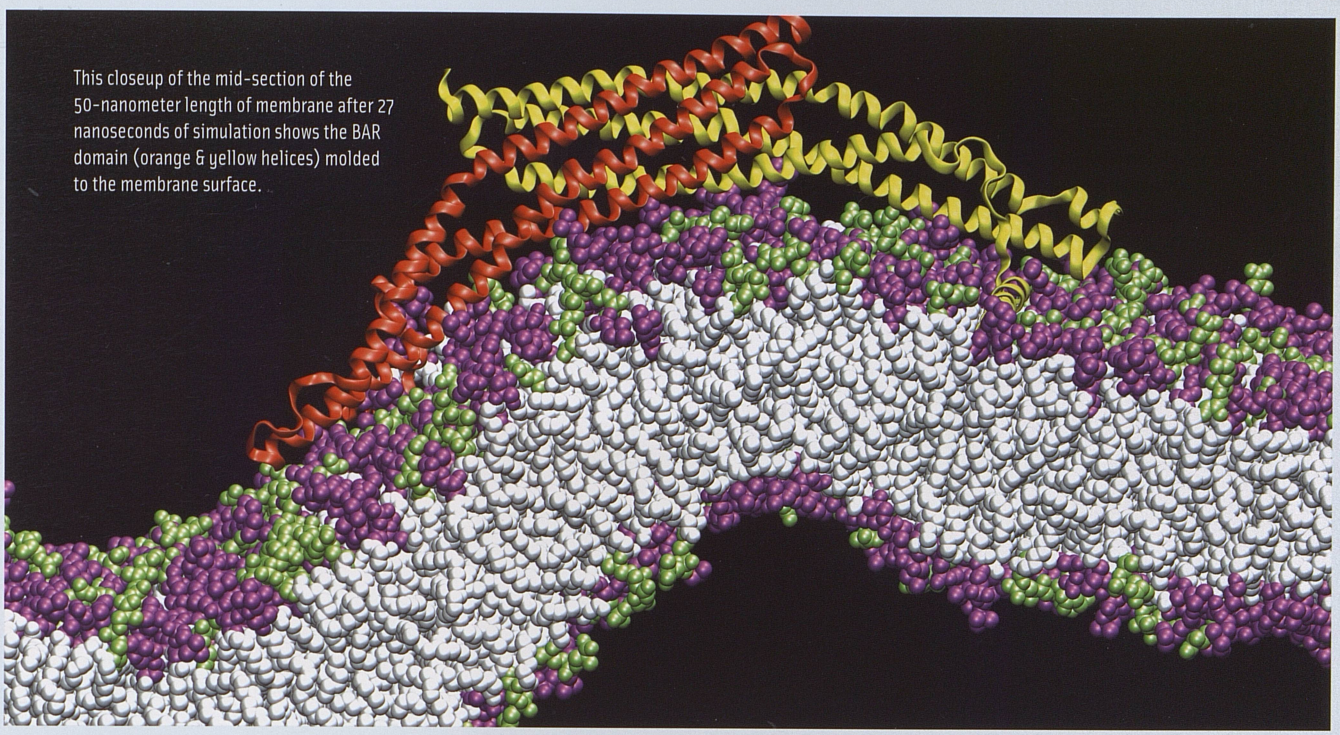
With energized beams of oxygen, SIMOX oxidizes a thin layer of silicon deep inside a chip. For further advances in chip design, the oxygen beams need to be able to sculpt thinner layers, from 10 microns currently to 10 nanometers, 1,000 times thinner, which means using 1,000 times lower energy. This requires atomic-level understanding of how oxygen atoms migrate through silicon at these low energies.

Quantum-level simulations can provide this knowledge, but they demand extraordinary amounts of computation. To harness the necessary resources, researchers from Advanced Industrial Science and Technology (AIST) and the Nagoya Institute of Technology in Japan teamed with materials scientists at the University of Southern California (USC) to create a U.S.-Japan grid testbed. Led by Yoshio Tanaka of AIST and Aiichiro Nakano of USC, they created a grid-enabled framework that allowed them to do quantum-mechanical (QM) simulation of oxygen atoms moving through silicon. The QM models were embedded in classical molecular dynamics (MD) simulations for the surrounding silicon.

They used TeraGrid systems at NCSA and SDSC along with clusters at AIST and relied heavily on PSC's LeMieux. The simulation ran in total for 150,000 processor hours. Results reveal that the depth of oxygen penetration depends strongly and critically on the incident position of the oxygen beam.

A snapshot from the MD/QM simulations of SIMOX shows oxygen atoms (yellow circles) injected perpendicular to a silicon surface of 110,000 atoms. Each of five QM regions of silicon (red) penetrated by oxygen expands and changes shape tracking the migration of the oxygen and the breaking and reforming of silicon-silicon bonds.





This closeup of the mid-section of the 50-nanometer length of membrane after 27 nanoseconds of simulation shows the BAR domain (orange & yellow helices) molded to the membrane surface.

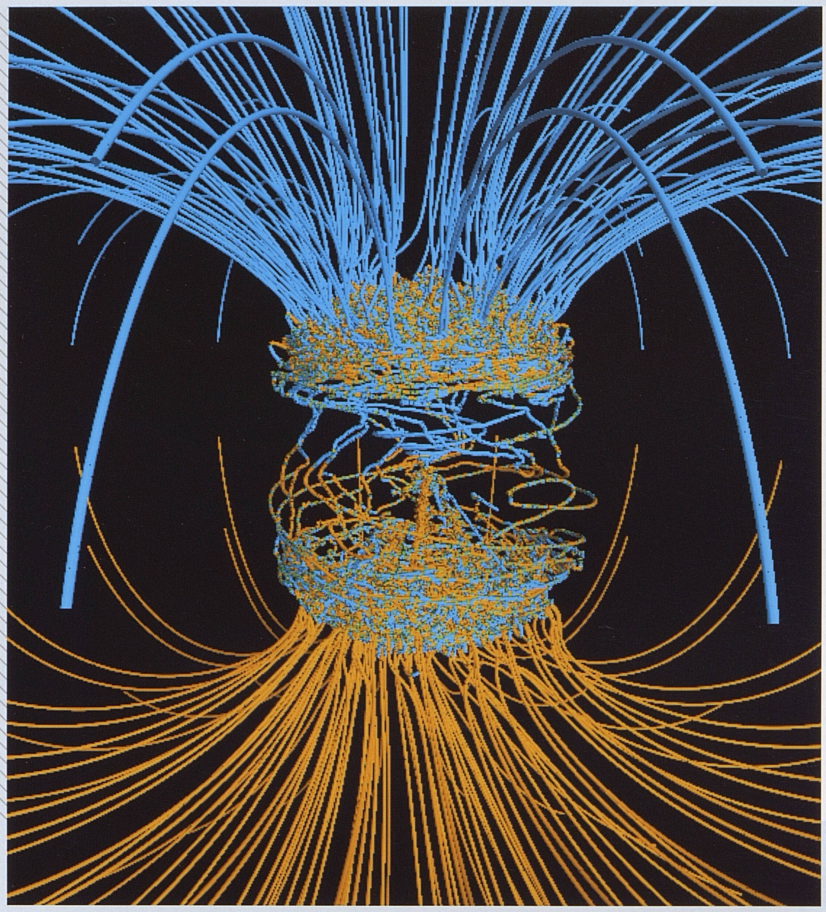
Step Up To The Bar Domain

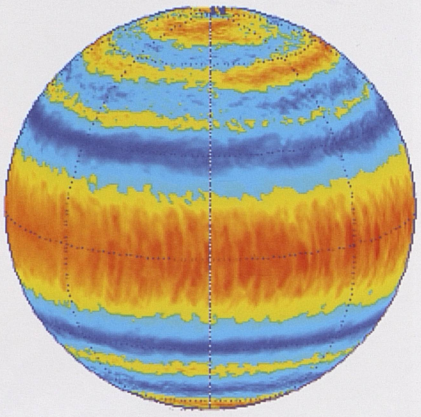
ONE OF THE LARGEST BIOLOGICAL SIMULATIONS EVER SHOWS HOW BANANA-SHAPED PROTEINS INDUCE MEMBRANES TO CURVE

University of Utah chemist Gregory Voth and grad student Phil Blood are using PSC's Cray XT3 to tackle a basic question of endocytosis — the life-sustaining process by which cells absorb material from outside the cell by bending their membrane to form a "vesicle" and engulf it. All animal cells depend on endocytosis, which involves various steps, but begins with curvature of the membrane.

BAR domains are a family of banana-shaped proteins shown to bind to cellular membrane as it curves. Experiments suggest that BAR domains mold their concave surface to a section of membrane and induce a corresponding curvature. Voth and Blood undertook molecular dynamics simulations to look more closely. With the XT3 they've been able to run efficiently, using software called NAMD, with as many as 1,024 processors. "The XT3 has been amazing," says Blood. "We haven't found a hard limit on scaling up the number of processors."

They used TeraGrid systems at SDSC, NCSA and University of Chicago/Argonne to construct a model and to explore how long a stretch of membrane they needed for curvature to occur. Their final simulations used the XT3 to include the protein with a 50-nanometer length of membrane — probably the longest patch of membrane ever simulated — for a total of 738,000 atoms. Their results, reported in *Proceedings of the National Academy of Sciences* (2006), show that the orientation of the BAR domain as it attaches to the membrane determines the degree of curvature.





Top: Results from Glatzmaier's 3D simulation represent banded zonal flow on a giant planet's surface, with eastward flow (red and yellow) contrasted with westward (blue). **Left:** A snapshot of the generated magnetic field shows lines of force outward (orange) and inward (blue).

Why Giant Planets Wear Stripes

SIMULATIONS SUGGEST A BETTER EXPLANATION FOR DIFFERENTIAL ROTATION

Wind in the upper atmosphere of giant planets like Jupiter and Saturn blows both ways, west and east — shifting with latitude in banded zones. Known as differential rotation, this phenomenon has stirred much interest and several theories, but scientists have yet to settle on a conclusive explanation for how these banded wind patterns are maintained or how deep below the surface they extend.

Like the Sun, a giant gaseous planet has a fluid interior that transports heat outward by turbulent convective motions. Because of this thermal convection and effects of the planet's 10-hour rotation period, the fluid interior, instead of rotating as a solid body, rotates at different rates at different latitudes and depths. The resulting shear flow of the electrically conducting fluid generates a magnetic field. In 1995, running at PSC, Gary Glatzmaier of the University of California, Santa Cruz, used a computational model he developed to produce the first self-consistent simulation of convection and magnetic-field generation in Earth's fluid core. With a modified version of that code, he is now simulating convection, differential rotation and magnetic-field generation in giant planets.

In recent work, Glatzmaier and graduate students Martha Evonuk and Tamara Rogers propose a mechanism more robust than previous theories for differential rotation in the interiors and atmospheres of giant planets. Previous models have neglected the effects of the large variation of density with depth and how this generates vorticity as rising fluid expands and sinking fluid contracts. Simulations of the newly proposed mechanism, using LeMieux, PSC's terascale system, demonstrate how it can maintain differential rotation and a global magnetic field similar to those observed on the surfaces of Jupiter and Saturn.

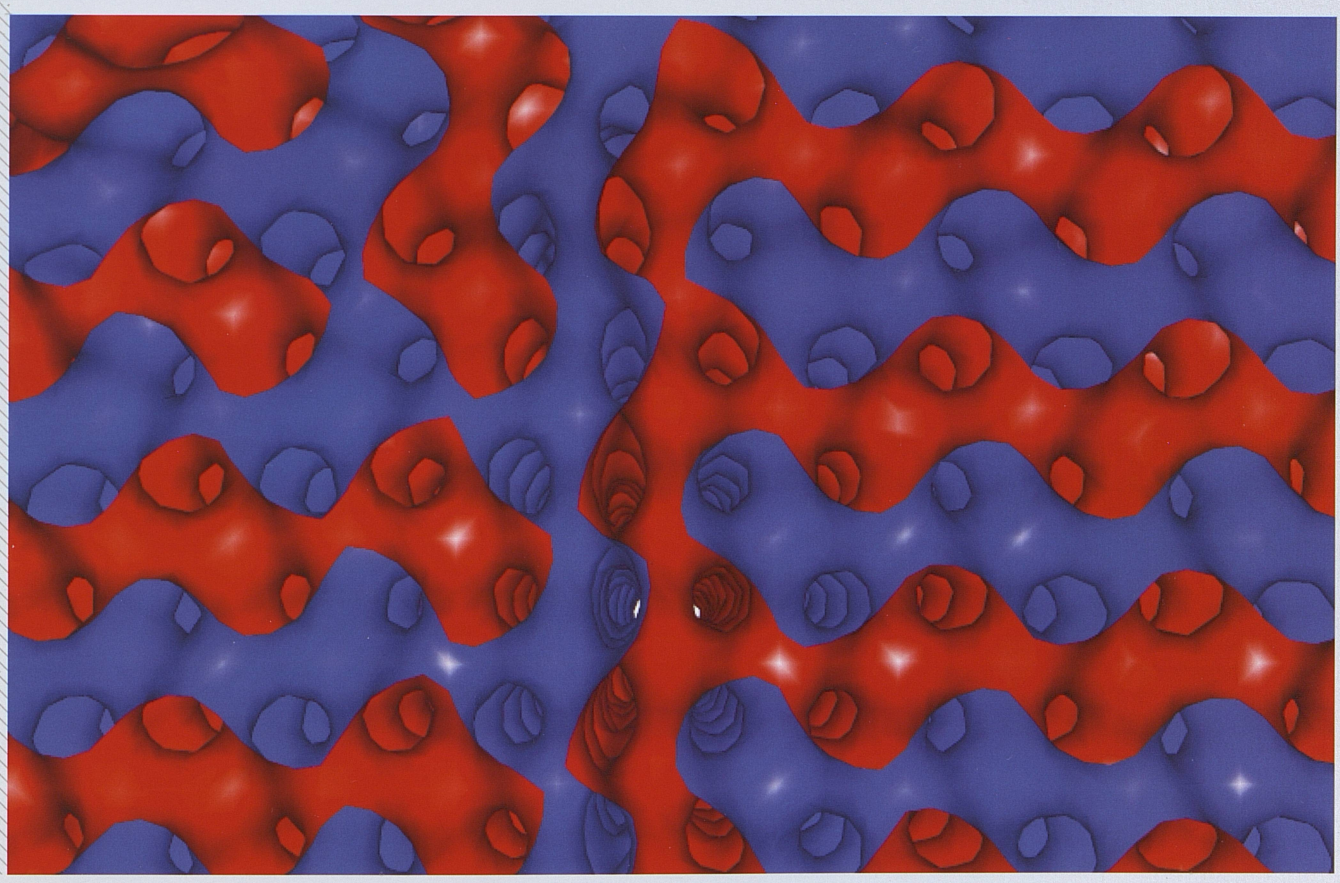
Ketchup On The Grid

TRANSATLANTIC GRID PRODUCES NEW UNDERSTANDING OF LIQUID CRYSTALS

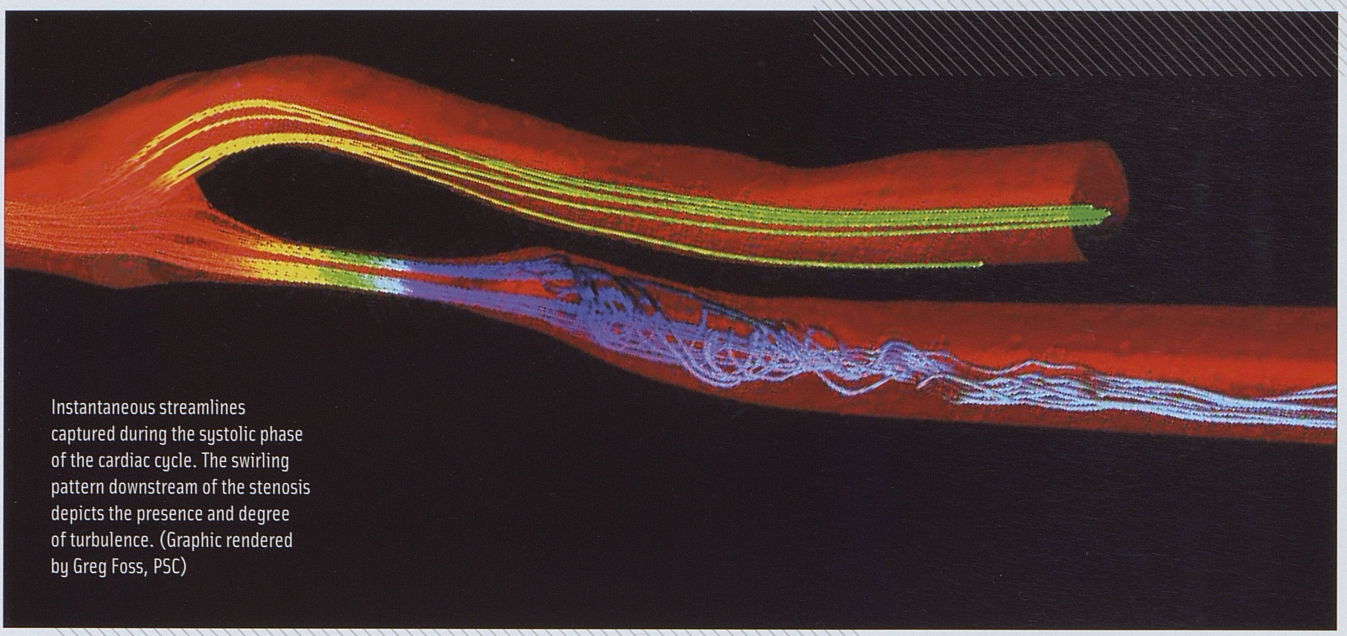
Turn a bottle of ketchup upside down. It's a liquid and therefore should pour, right? New scientific findings from a large-scale transatlantic project may not make ketchup flow smoothly, but they describe never-before-known details of liquid mixtures, such as ketchup, that act like solids.

Led by theoretical chemist Peter Coveney of University College London and Bruce Boghosian of Tufts University, and jointly funded by the National Science Foundation and the UK's Engineering and Physical Sciences Research Council, the project used resources at four TeraGrid sites — PSC, NCSA, SDSC and UC/Argonne — along with U.K. resources at Daresbury Lab and Manchester. The researchers steered multi-site simulations to zero-in on a defect phase of the gyroid, and then used LeMieux, PSC's terascale system, for a very large-scale simulation of this defect phase. The results show formation and evolution of realistic "gyroid" systems, structures that are a fascinating hybrid of liquid and solid physical features. Such systems are widespread both in living organisms — where they are thought to feature in certain lipid structures — and in the electronics display industry, where there's much interest in understanding how they operate.

Published in June 2006 by the Royal Society, the U.K.'s national academy of science, the findings present the first analysis of gyroid self-assembly and defect dynamics. "Liquid-crystal systems are scientifically important, and this study was possible only because multisite grid resources were available," says Coveney, who with his colleague Jonathan Chin, authored the Royal Society paper. "We're in a region where nobody has studied these properties until now and we've been able with computation to make predictions and invite experimentalists to take a look."



Two gyroid domains with a domain wall running vertically between them. The gyroid phase forms in a mixture of oil (red), water (blue) & surfactant. The image shows opposite handedness of the two domains.



Instantaneous streamlines captured during the systolic phase of the cardiac cycle. The swirling pattern downstream of the stenosis depicts the presence and degree of turbulence. (Graphic rendered by Greg Foss, PSC)

Stroke Busters

SIMULATING TURBULENCE IN A STENOSED CAROTID ARTERY

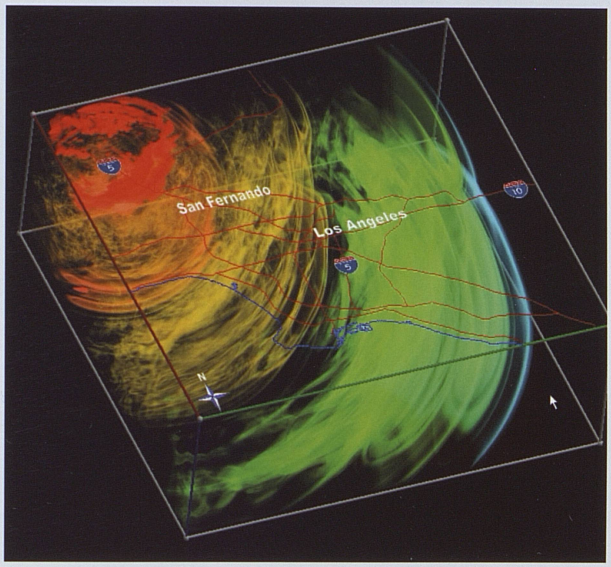
Probably the main cause of strokes is arterial narrowing — stenosis — due to atherosclerosis in the carotid artery, the main thoroughfare for blood to the brain. Plaque that builds up in a stenosed region can break loose and block an artery downstream, a problem that's most dangerous in the internal carotid artery, just past where the carotid splits into two branches.

A predictor of the possible risk of plaque breakup is shear stress produced by blood flow in the stenosed region. Experiments show that such flows can become turbulent downstream of severely narrowed regions. To gather insight into this phenomenon and obtain more accurate data than is possible from experiment, a team led by George Karniadakis of Brown University has undertaken direct numerical simulation of realistic 3D flow through a stenosed artery. For these demanding computations, they applied Nektar, a high-order spectral element code developed at Brown, with a realistic 3D geometry of a stenosed carotid artery reconstructed from MRI. They ran simulations on TeraGrid resources at NCSA and on PSC's Cray XT3, using up to 196 processors.

"We discovered a transition to turbulence during the systole phase," says Karniadakis. This transition occurs downstream from the throat where the internal carotid artery narrows. This turbulence decays downstream, and also decays during the diastolic phase. The simulations show that shear stress on the artery wall increases during this turbulent phase. With the availability of more powerful computation, such as anticipated petascale systems, this information could become useful to help predict patients at high risk for stroke.

Hercules Does Northridge

END-TO-END EARTHQUAKE MODELING WITH REAL-TIME VISUALIZATION



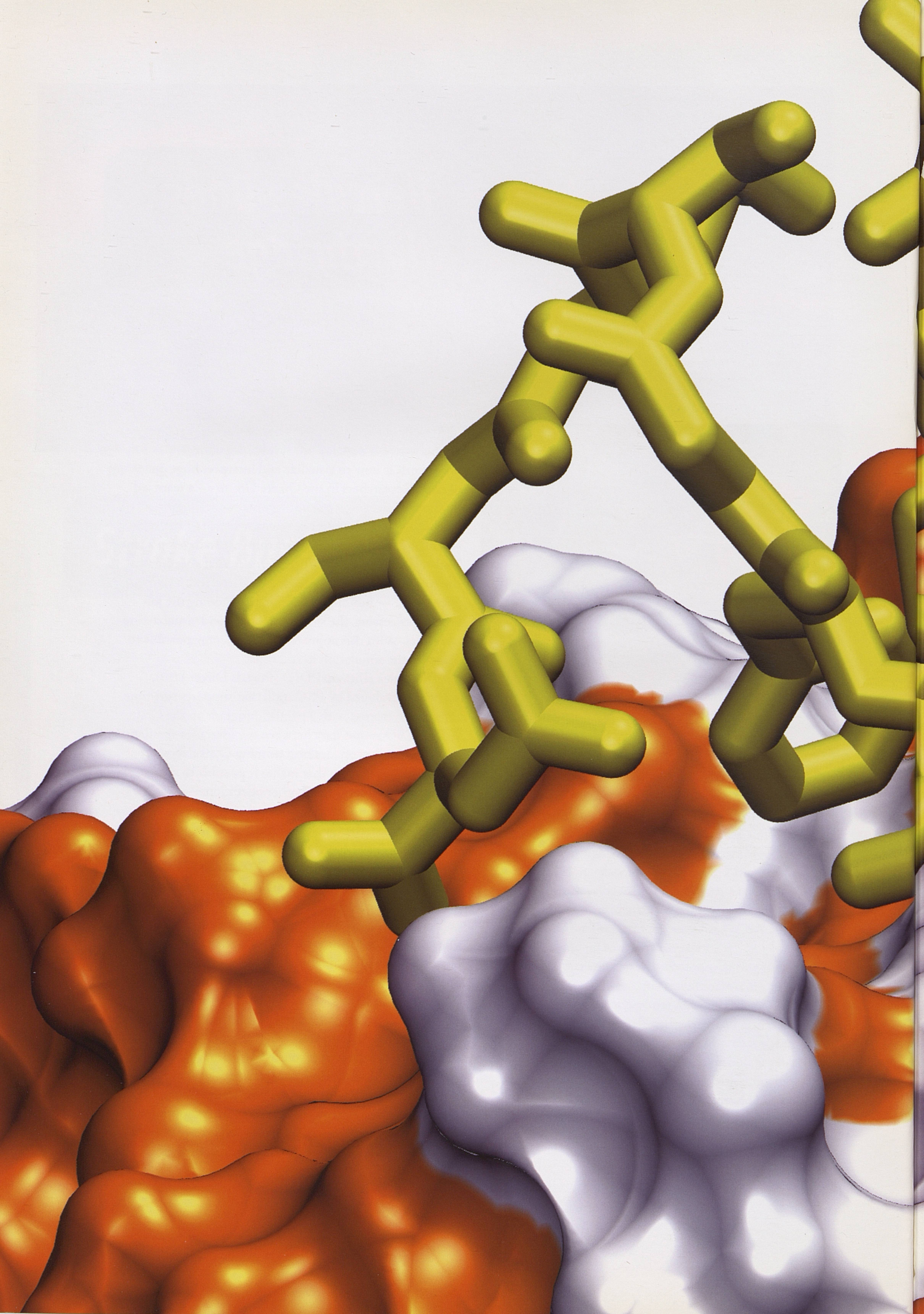
This snapshot from QuakeShow during an earthquake simulation shows amplified seismic waves in the San Fernando Valley.

A major challenge with large-scale parallel simulations, as with PSC's Cray XT3, involving thousands of processors, is how to visualize and interpret huge quantities of data. Researchers in the Quake Group — a team led by Carnegie Mellon civil and computational engineer Jacobo Bielak and computer scientist David O'Hallaron — collaborated with PSC staff this year to develop a new "end-to-end" approach, called *Hercules*, that coordinates the components of earthquake simulation into a unified framework — building the mesh, partitioning the job among processors, the simulation itself, and visualization of results. With this approach, it has become possible to visualize the simulation in real time.

Hercules relies on PDIO (Portals Direct I/O), software developed by PSC staff, that supports run-time remote interaction with a parallel program on the Cray XT3. PDIO routes data between the Hercules simulation and a remote laptop/desktop running QuakeShow, a visualization program that makes it possible to change view angles, zoom in or out and other operations — while the simulation is running.

In August, the Quake team applied Hercules to simulate the 1994 Northridge earthquake. Using 1,024 XT3 processors, they simulated 80 seconds of earthquake with an adaptive mesh of 9.9 million elements. Real-time visualization every 10 time steps allowed the researchers to view difficult-to-observe physical phenomena. "We were able to see strong concentrations of seismic energy in both the San Fernando Valley and the Los Angeles Basin," says Bielak, "while seismic waves in the nearby Santa Monica Mountains and San Gabriel Mountains had dissipated — a validation that sedimentary basins trap seismic energy during strong earthquakes."

The researchers plan to use Hercules with the XT3 to simulate a magnitude 7.7 scenario quake along the San Andreas fault in a large region of Southern California at higher frequencies, requiring much more computation. Higher vibration frequencies are important because they present the greatest danger to most city structures.



PITTSBURGH SUPERCOMPUTING CENTER

The Pittsburgh Supercomputing Center is a joint effort of Carnegie Mellon University and the University of Pittsburgh together with Westinghouse Electric Company. It was established in 1986 and is supported by several federal agencies, the Commonwealth of Pennsylvania and private industry.

PSC GRATEFULLY ACKNOWLEDGES SIGNIFICANT SUPPORT FROM THE FOLLOWING

The Commonwealth of Pennsylvania
The National Science Foundation
The National Institutes of Health
The National Energy Technology Laboratory
The National Archives and Records Administration
The U. S. Department of Defense
The U. S. Department of Energy
Cisco Systems, Inc.
Cray Inc.
DataDirect Networks
Hewlett-Packard Company
The Buhl Foundation
The Grable Foundation

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GRAPHICS RESEARCH, PHOTOGRAPHY DIRECTION, COPY EDITING
Shandra Williams, PSC
(Thanks also to PSC alumnus Sean Fulton)

TRANSCRIBING
Ryan Omecene, Jessica Dailey and Megan Hackworth, PSC.

PHOTOGRAPHY
Photography & Graphic Services at Mellon Institute.

GRAPHICS
Thanks to Greg Foss, PSC, for nanoparticle and carotid artery graphics; and Derek Simmel, Jared Yanovich and Bob Budden, PSC, for xt3dmon images.

We dedicate this year's edition of Projects in Scientific Computing to the memory of PSC scientist David W. Deerfield II.

DESIGN
Wall-to-Wall Studios, Inc.

PRINTING
Broudy Printing

Printed on Sappi McCoy Gloss Paper, a premium sheet with 10 percent post-consumer waste fiber, with vegetable-based inks.

PITTSBURGH SUPERCOMPUTING CENTER
300 SOUTH CRAIG STREET
PITTSBURGH, PENNSYLVANIA 15213