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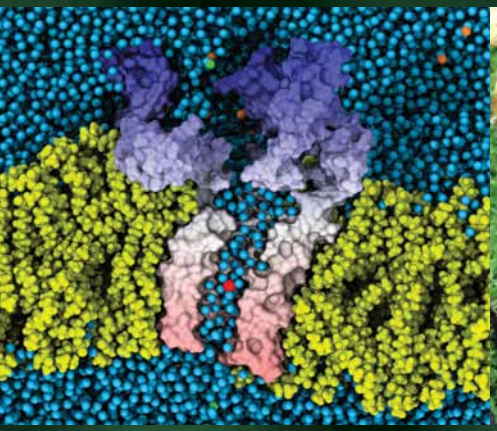
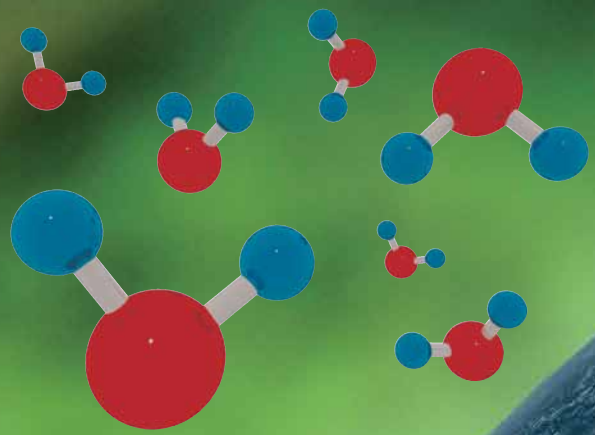


Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

a Unit of the Office of the Vice President for Research

ANNUAL Research Highlights 2010



Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

UNIVERSITY OF MINNESOTA

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Overview

The mission of the University of Minnesota Supercomputing Institute for Advanced Computational Research is supercomputing research, which is defined broadly to include a variety of research activities from many disciplines. This research involves the use of high-performance computing environments to address problems in the physical, biological, medical, mathematical, and computing sciences and engineering as well as other fields that use computers in their research. The goal is to promote successful attacks on problems that could not otherwise be attempted.

The Institute is an interdisciplinary research program spanning all colleges of the University of Minnesota. The Institute provides supercomputing resources and user support to faculty and their research groups. It is a linchpin program in the University's broad-based digital technology effort, provides a focal point for collaborative research on supercomputing within the University and the State, and provides an interdisciplinary focus for undergraduate and graduate education related to supercomputing and scientific computing. The Institute's hardware and software resources and technical support are available to researchers at the University of Minnesota and other post-secondary educational institutions in the State of Minnesota.

Changes in 2009–2010:

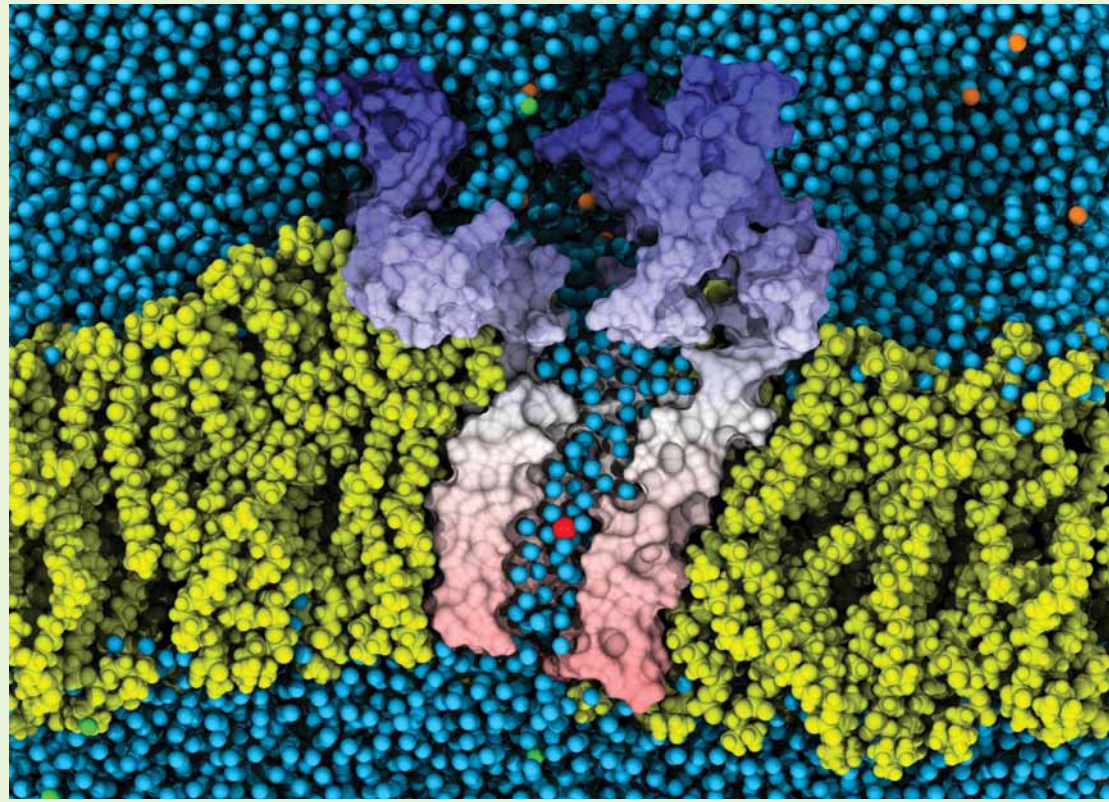
- Jorge Viñals became the Director of the Supercomputing Institute on August 1, 2010, succeeding Tom Jones, who had served as Interim Director since July 2008.
- Elmo, a set of six Ethernet-connected Sun Fire X4600 Linux systems, became available to users in January 2009.
- Regatta, the IBM Power4, was retired on April 1, 2009.
- Itasca, an HP Linux cluster with HP ProLiant BL280c G6 blade servers, was purchased and installed in 2009. Itasca was made available to users in July 2010.
- The SGI Altix was retired in June 2010.

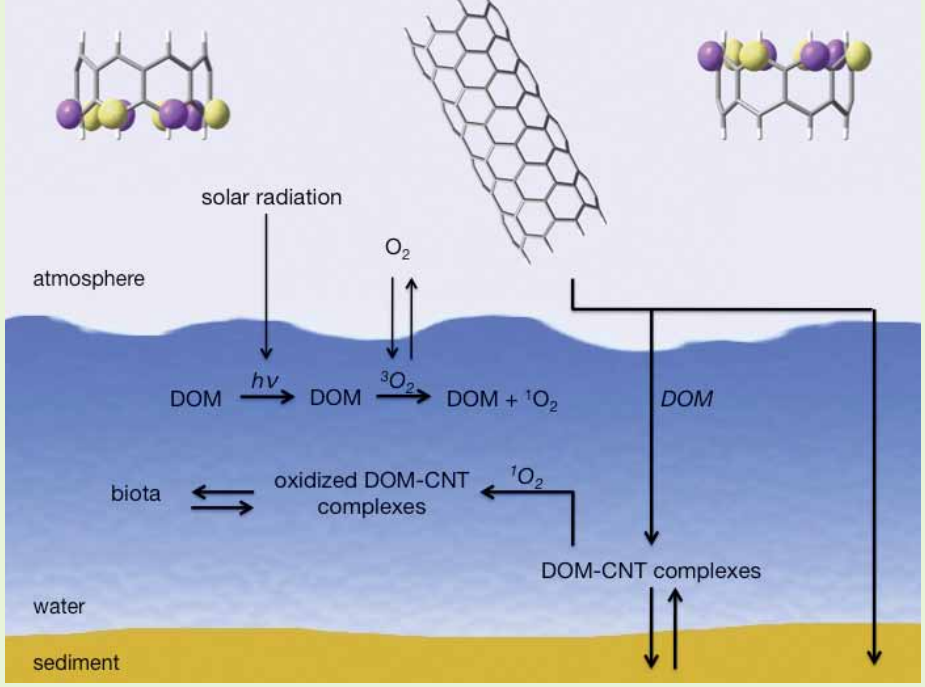
More information about MSI can be found in the Facts and Figures center section.

Computational Chemistry

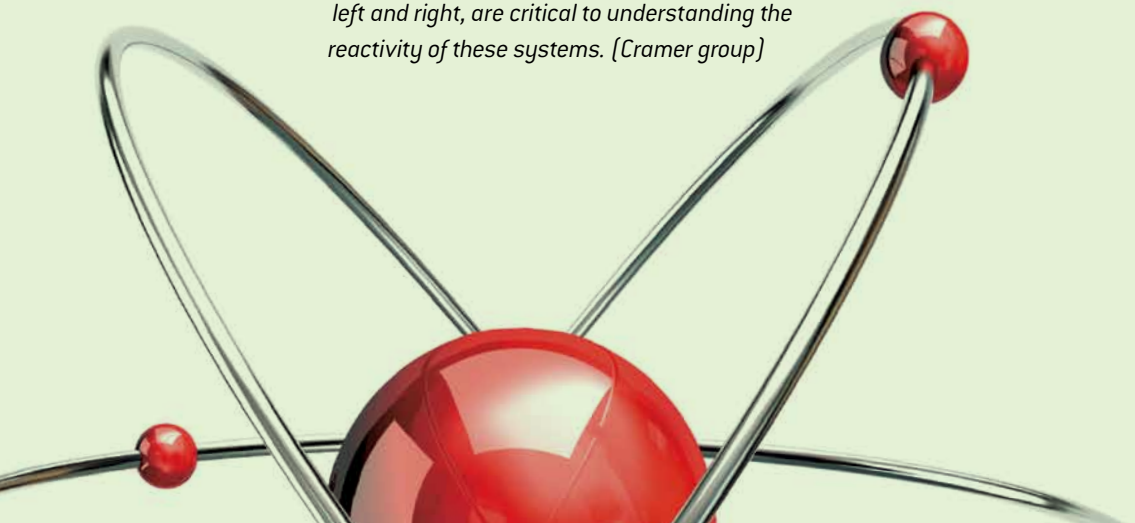
Mention chemistry, and many people think of labs with test tubes and white-coated scientists creating mysterious substances. But the computational chemists work with computers and codes. Computational chemists apply chemistry, mathematics, and computing to interesting chemical problems. Using efficient computer codes and fast, powerful machines, computational chemists can generate the properties of molecules and simulate experimental results. Because the amount of computing time increases as the problems become more complex, supercomputers are important to this branch of chemistry. The images on these pages are from the research of three MSI Fellows who have used MSI resources for many years: Professor Christopher J. Cramer, Professor Jiali Gao, and Regents Professor Donald G. Truhlar.

Below: Phospholamban is a transmembrane protein responsible for the regulation of muscle contraction, including heartbeat. Its pentameric complex has a channel-like structure that researchers believe may funnel calcium and chloride ions through the membrane. Molecular dynamics simulations in explicit membranes have shown that, while ion and water passage through the channel is possible, it cannot happen under actual physiological conditions due to the energetic penalty caused by the hydrophobic core of the pentamer. (Gao group)

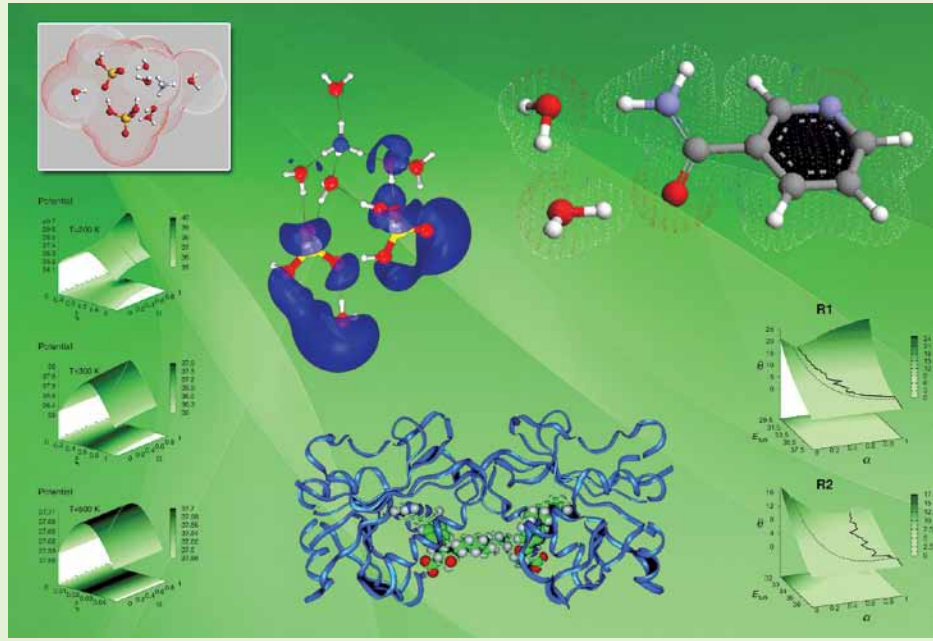




Above: The environmental fate of carbon-based nanomaterials such as carbon nanotubes (CNTs) in aquatic systems is dependent on complexation with dissolved organic matter (DOM) and surface oxidation by photochemically produced reactive oxygen species, such as singlet oxygen. Using cyclacenes as model CNTs, quantum mechanical electronic structure calculations are used to predict the thermodynamics and kinetics of such oxidation pathways. The frontier molecular orbitals, like those shown at upper left and right, are critical to understanding the reactivity of these systems. (Cramer group)



Below: Images clockwise from top right: solvent accessible surface for nicotinamide complex with two water molecules; variation of the imaginary-action integral with the parameter at each of the tunneling energies (in kcal/mol); $DHFR_2MTX_2$ chemically induced dimer; effective potentials (in kcal/mol) at the representative tunneling energy of a reaction at different temperatures; solvent accessible surface for $(H_2SO_4)(HSO_4)(NH_4^+)(H_2O)$ cluster; negative valued molecular electrostatic potential isosurface for $(H_2SO_4)(HSO_4^-)(NH_4^+)(H_2O)$ cluster. (Truhlar group)

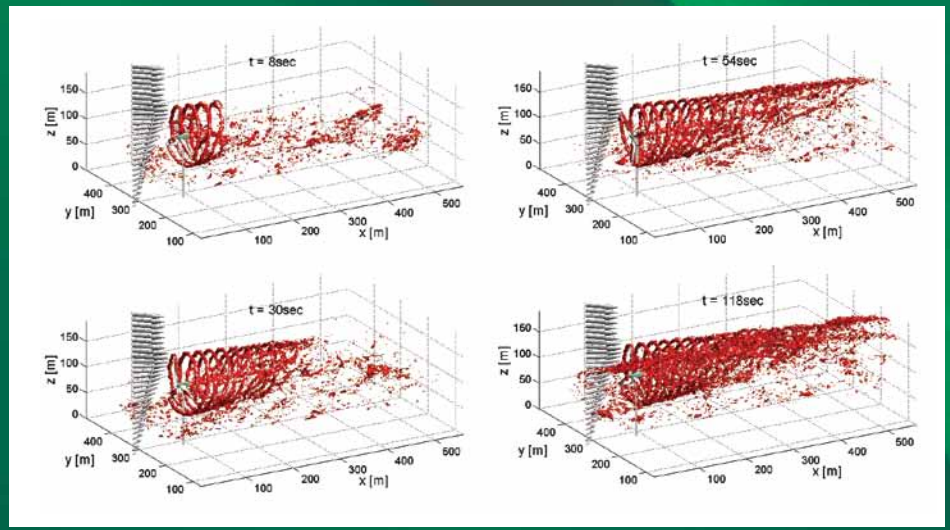


Modeling THE WIND

Alternative energy sources are a hot topic in the early 21st century. Wind power has many advocates, and researchers are investigating ways to harness wind to power our lives. MSI researchers at St. Anthony Falls Laboratory (SAFL) are using the supercomputers to model wind turbines and airflow. The kinds of computations used in this research require huge amounts of computing power.

Professor Fotis Sotiropoulos (SAFL Director and MSI Fellow) uses MSI's supercomputers to perform numerical simulations of wind and hydrokinetic turbine flows. These models can show how wind interacts between turbines and the ground and also between two or more turbines. A result from one of the models can be seen in the figure on the opposite page (top left), which shows simulations of air currents in the wake of a two-blade wind turbine rotor. This research will directly affect the way that wind farms are designed. Professor Sotiropoulos is also the Principal Investigator for a multi-million-dollar Department of Energy grant to a consortium led by the University of Minnesota. The goal of this project is to develop improved methods of wind-energy generation. This includes building more efficient and durable wind turbines, creating optimum designs for wind farms, and developing novel energy transmission systems and electric generators. Industrial partners in this consortium include Siemens Energy, Barr Engineering, Eaton Corporation, Honeywell, Lockheed Martin, Luna Innovations, 3M, and WindLogics.

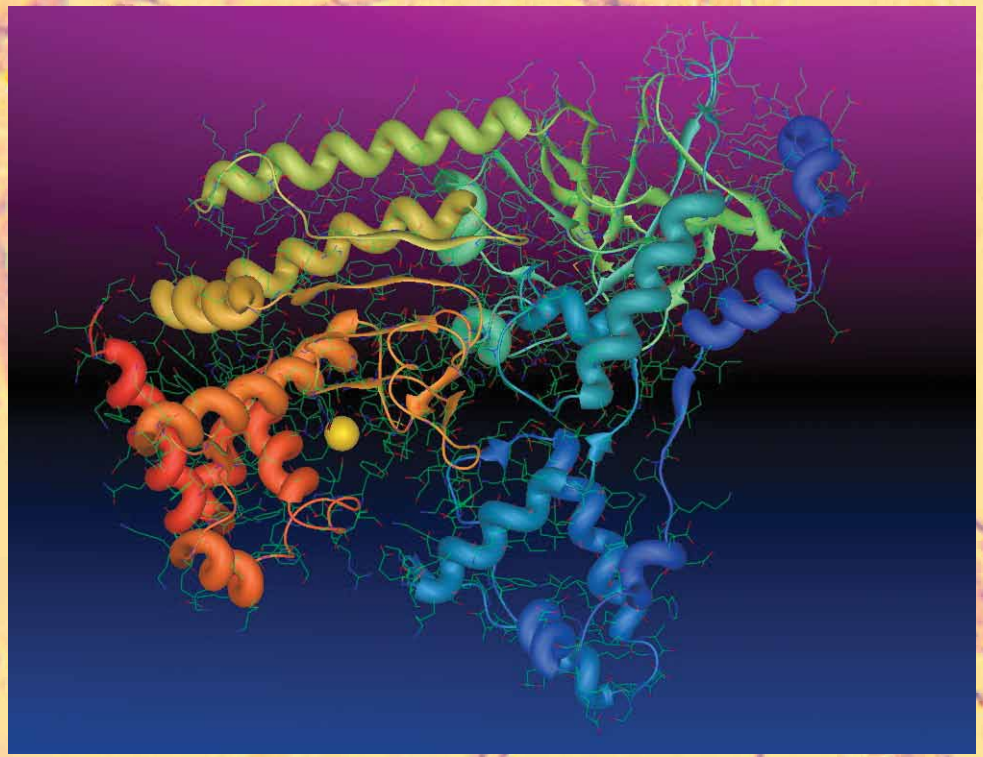
Another researcher at SAFL, Professor Fernando Porté-Agel (MSI Fellow), uses MSI's supercomputers for large-eddy simulation (LES) modeling of the atmosphere. LES is a state-of-the-art numerical modeling technique that is used to calculate unsteady three-dimensional transport in turbulent flows. Professor Porté-Agel's research group has recently begun a project to develop high-resolution simulations of atmospheric boundary layer turbulence and its interaction with wind turbines and interference effects among wind turbines. The images at right are simulations of blade-induced three-dimensional helicoidal tip vortices. The four images are taken at different times of the simulation along the axial domain.



Investigating Anthrax

Anthrax is an acute infectious disease caused by the spore-forming, rod-shaped bacterium *Bacillus anthracis*. It occurs most commonly in livestock and wild animals. Naturally occurring anthrax infections are rare in humans, and have usually resulted from exposure to infected animal carcasses and/or wool. In recent years, however, *B. anthracis* has been used as a biological warfare and terrorism agent. The inhaled form of the anthrax infection is usually lethal, and the cutaneous and gastrointestinal forms can also be deadly. Anthrax spores sent through the mail to several media offices and to two U.S. Senators in September 2001 killed five people and infected many more.

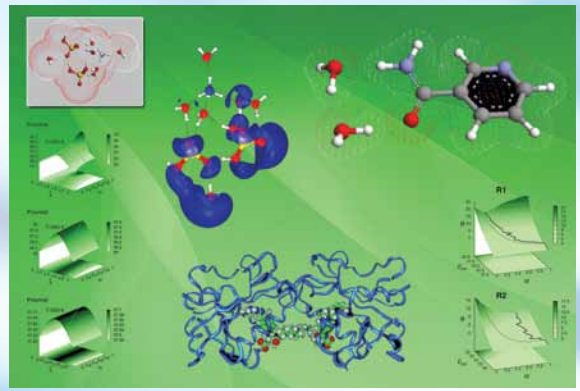
Assistant Professor Elizabeth A. Amin (Medicinal Chemistry, MSI Associate Fellow) and her research team are using molecular modeling techniques as part of their research into ways of counteracting the anthrax toxin lethal factor (LF) enzyme, which is the chief agent in anthrax that is toxic to cells. LF from weaponized anthrax can remain in the human system for days after the anthrax bacterium has been killed with antibiotics. This residual LF can cause fatal toxemia, and there is currently no clinical therapy against it. The Amin group is investigating compounds that may be used for future drug designs targeting LF. The image on this page shows LF domains II-IV (residues 297-809) with catalytic Zn^{2+}.



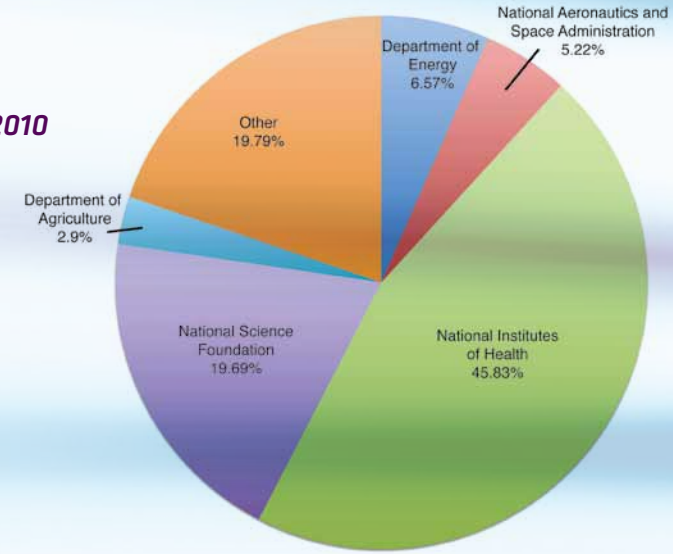
Facts and Figures

EXTERNAL FUNDING

Funding Source	*Amount, 2008–09*	*Amount, 2009–2010* (as of July 31, 2010)
Department of Energy	$4,062,068	$9,795,784
National Aeronautics and Space Administration	$6,640,465	$7,785,242
National Institutes of Health	$44,879,416	$68,314,350
National Science Foundation	$26,042,899	$29,350,774
US Department of Agriculture	$4,296,155	$4,326,446
Other	$17,946,553	$29,496,484
Total External Funding	**$103,867,556**	**$149,069,080**



External Funding Breakout for 2009–2010



2009-10

People

MSI Principal Investigators Active During January 2009 Through May 2010

Number of PIs at UMTC Schools and Colleges School/College	#PIs
Academic Health Center (AHC)	**238**
AHC Centers	19
College of Pharmacy	20
College of Veterinary Medicine	17
Medical School	120
School of Dentistry	8
School of Nursing	3
School of Public Health	13
Joint CBS/Medical School	38
College of Biological Sciences (CBS)	**65**
CBS departments	14
Joint CBS/Medical School	38
Joint CBS/CFANS	13
College of Education and Human Development	**2**
College of Food, Agricultural, and Natural Resource Sciences (CFANS)	**55**
CFANS departments	39
Joint CBS/CFANS	13
Joint CFANS/CSE	3
College of Liberal Arts	**9**
Curtis L. Carlson School of Management	**3**

Number of PIs at UMTC Schools and Colleges School/College	#PIs
College of Science and Engineering (CSE)	**175**
(before July 1, 2010, Institute of Technology)	
College of Science and Engineering departments	172
Joint CFANS/CSE	3
Office of the Vice President for Research	**4**
Hormel Institute	3
Minnesota Population Center	1
Total Number of PIs, January 2009–June 2010	**497**

** note: numbers in right-hand column do not add up to the total because PIs in jointly-administered departments are counted in both colleges*

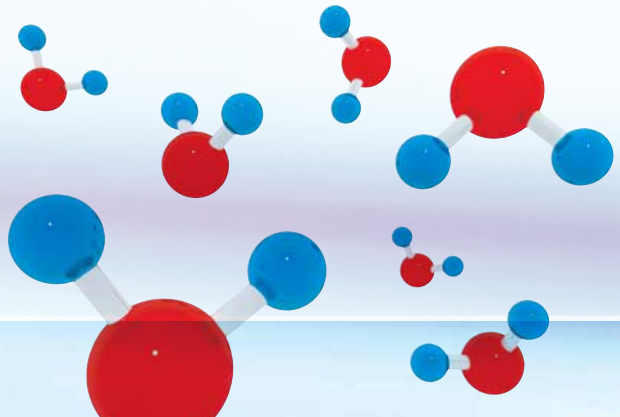
Facts and Figures

2009-10

Number of PIs at Non-UMTC Institutions

Institution	#PIs
Augsburg College	1
Bethel University	1
Gustavus Adolphus College	2
Hamline University	1
Mayo Clinic College of Medicine	4
Metropolitan State University	1
Minnesota State University, Mankato	2
St. Cloud State University	1
St. Olaf College	2
University of St. Thomas	4
University of Minnesota Duluth	
College of Pharmacy Duluth	1
Medical School Duluth	4
Swenson College of Science and Engineering	14
University of Minnesota Morris	
Division of Science and Mathematics	2
University of Minnesota Rochester	
BICB Program	2
Winona State University	1

Project abstracts for PIs can be found in MSI Research Abstracts Online, www.msi.umn.edu/about/publications/res_abstracts.html



Undergraduate Internship Program, Summer 2010

Bjorn K. Berntson, University of Minnesota
Advisor: Professor Christopher J. Cramer, Department of Chemistry

Erik M. Fritz, University of Minnesota
Advisor: Professor Steven Kass, Department of Chemistry

Timothy M. Hecht, Brigham Young University
Advisor: Professor J. Woods Halley, Department of Physics

Michelle S. Lenz, Bethel University
Advisor: Regents Professor Donald G. Truhlar, Department of Chemistry

Aatif Mansoor, University of Minnesota
Advisor: Assistant Professor Elizabeth A. Amin, Department of Medicinal Chemistry

Brendan A. Murphy, University of Minnesota
Advisor: Assistant Professor Tay Netoff, Department of Biomedical Engineering

Ashwin P. Srikrishna, North Carolina State University
Advisor: Assistant Professor Kevin Dorfman, Department of Chemical Engineering and Materials Science

Adam M. Novak, Harvey Mudd College
Advisor: Professor Victor H. Barocas, Department of Biomedical Engineering

David A. Sanchez, University of Minnesota
Advisor: Professor David A. Yuen, Department of Geology and Geophysics

Andrew J. Wesson, Carnegie Mellon University
Advisor: Professor Thomas W. Jones, Department of Astronomy

Alexandra M. Zudova, University of Minnesota
Advisor: Professor David D. Thomas, Department of Biochemistry, Molecular Biology, and Biophysics

RESOURCES

MSI Supercomputers
Altix (SGI Altix Cluster) (retired 6/30/10)
Blade (IBM BladeCenter Linux Cluster)
Calhoun (SGI Altix SE 1300 Linux Cluster)
Elmo (Sun Fire X4600 Linux Cluster)
Itasca (Hewlett-Packard ProLiant Linux Cluster)

MSI Computing Laboratories
Basic Sciences Computing Lab
Biomedical Modeling, Simulation, and Design Lab
Computational Genetics Lab
LCSE-MSI Visualization Lab
Scientific Data Management Lab
Scientific Development and Visualization Lab
MSI-UMR BICB Computational Lab

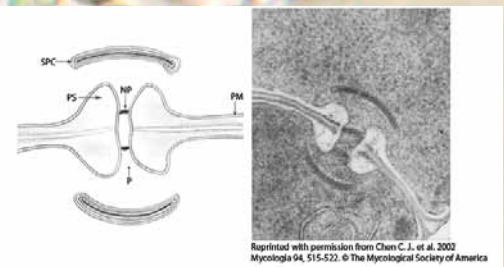
Software
MSI provides access to over 400 commercial and academic software packages.

User Support
MSI's team of experts provides assistance with high-level computation, modeling, simulation, and database development. User support staff members have expertise in various fields, including computational chemistry, computational fluid dynamics, structural mechanics, design optimization, data mining, structural and molecular biology, bioinformatics, computational biology, computational genomics, proteomics, scientific visualization, and geophysics.

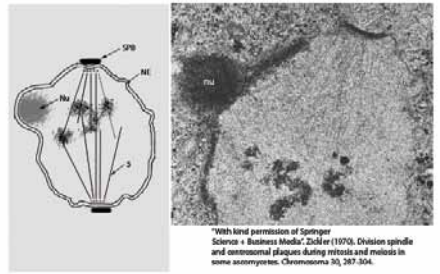
THE LINEAGE *of Fungi*

Fungi are one of the largest branches of the tree of life, with an estimated 1.5 million species. Because they are decomposers, pathogens, and mutualistic symbionts, they are of profound ecological and economic importance. Professor David J. McLaughlin (Plant Biology) and his research group participated in a collaborative project called *Assembling the Fungal Tree of Life* (*AFTOL*) and are now involved in its successor project, *AFTOL: Resolving the Evolutionary History of the Fungi.* This project, which involves researchers at ten universities and many collaborators in the mycological community, will contribute to understanding the lineage of fungi—fungi phylogeny—at multiple levels and will promote training and education in fungal biology.

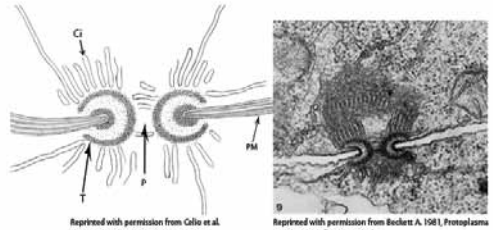
In support of this project, the McLaughlin group at the University of Minnesota is coordinating analysis of subcellular characters as well as studying molecular phylogenetics of selected species. They are using the Computational Genetics Laboratory for phylogenetic analyses of molecular and subcellular data and are creating a Structural and Biochemical Database. This database will become a major resource for the scientific community, managing and providing morphological and biochemical information on fungi and serving as a phyloinformatics tool. The illustrations shown at right are images from the database.



Reprinted with permission from Chen C. J. et al. 2002 Mycologia 94, 515-522. © The Mycological Society of America



"With kind permission of Springer Science + Business Media". Zickler (1970). Division spindle and centrosomal plaques during mitosis and meiosis in some ascomycetes. Chromosoma 30, 287-304.



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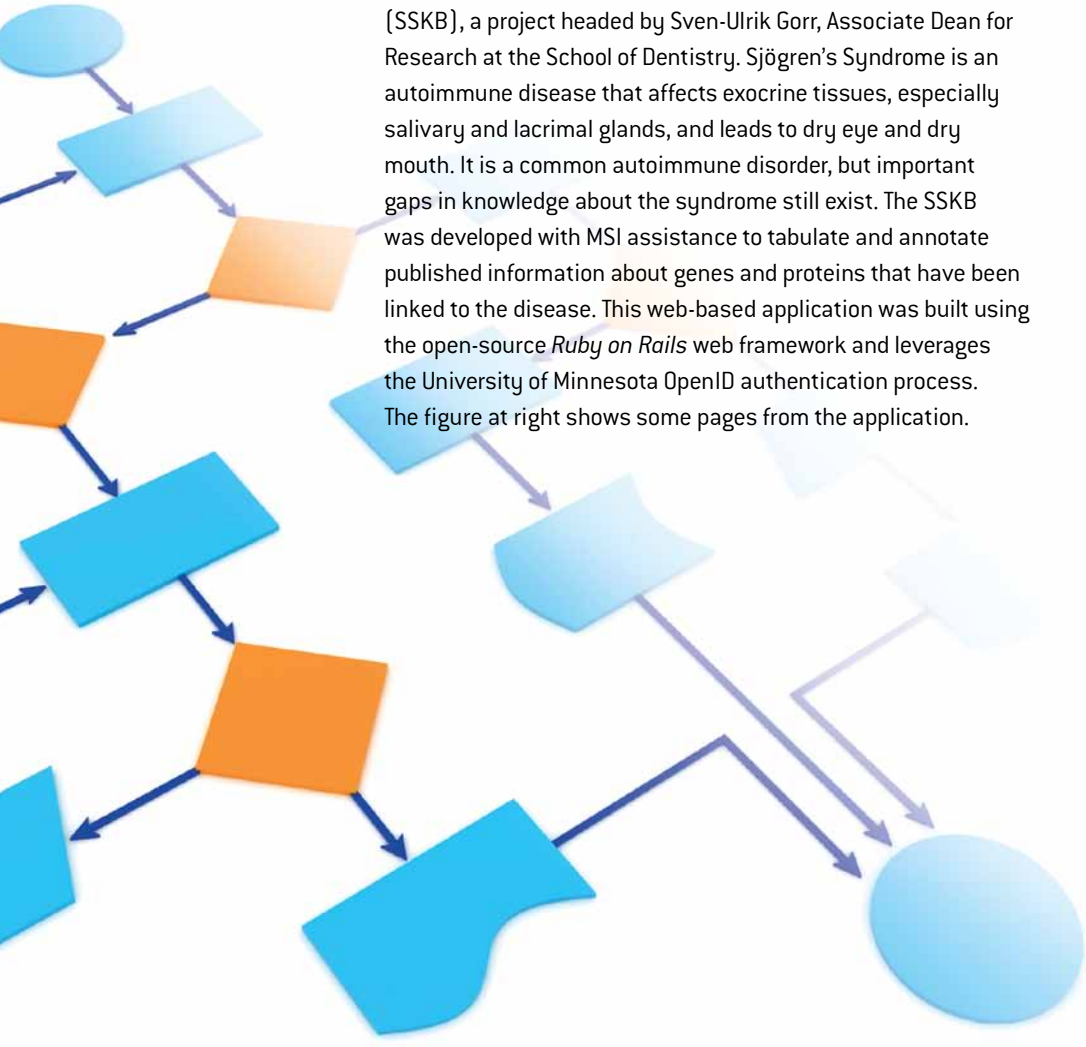
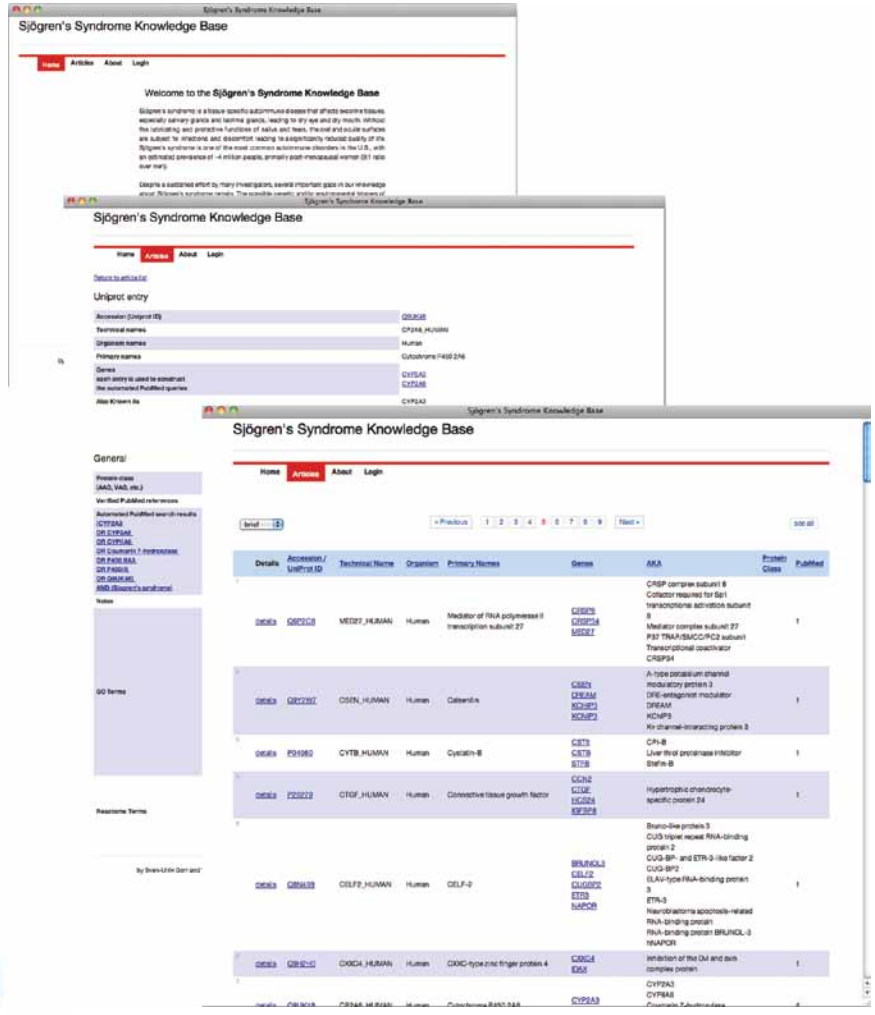
Databases

MSI hosts and develops many databases for its user community. These include public, project-specific, and commercial databases that serve a wide number of fields. Many of them are integrated into specific software for researchers. MSI provides hardware, software, and advanced user support for maintaining and using the databases.



One such database is the Sjögren's Syndrome Knowledge Base (SSKB), a project headed by Sven-Ulrik Gorr, Associate Dean for Research at the School of Dentistry. Sjögren's Syndrome is an autoimmune disease that affects exocrine tissues, especially salivary and lacrimal glands, and leads to dry eye and dry mouth. It is a common autoimmune disorder, but important gaps in knowledge about the syndrome still exist. The SSKB was developed with MSI assistance to tabulate and annotate published information about genes and proteins that have been linked to the disease. This web-based application was built using the open-source *Ruby on Rails* web framework and leverages the University of Minnesota OpenID authentication process. The figure at right shows some pages from the application.



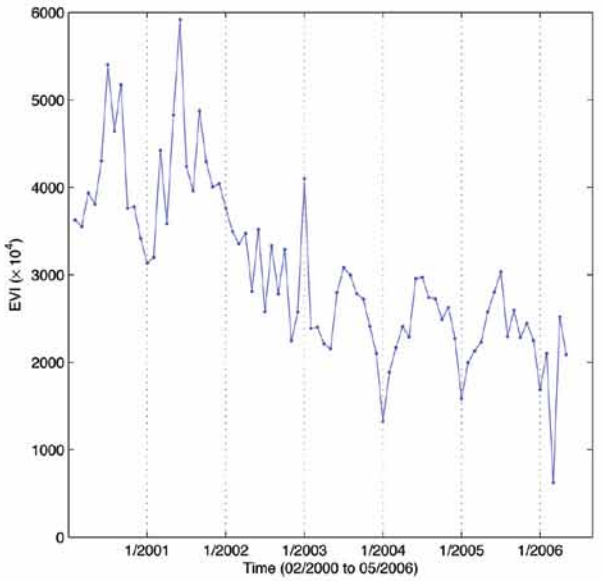
Another database under development will contain digitized photographs and videos of the chimpanzees in Gombe National Park, Tanzania. This project is for the Jane Goodall Institute's Center for Primate Studies at the University of Minnesota, which houses records from the decades of work by Dr. Goodall. The long-term aim of the project is to allow researchers and educators to search the database on the web. In the photograph below, Professor Michael Wilson, the Center's associate director, explains the database to a visitor at the MSI Open House.

MSI staff have helped to develop several databases for various core research facilities around the University, and MSI provides computer hosting for these large databases. In general, these large databases allow researchers to share and distribute data. They use the University's authorization system to maintain the security of the data. In some cases, MSI's code is integrated with commercially available software to provide the most streamlined and efficient way of dealing with large amounts of data. Some of the core research facilities using MSI for their databases include the Biomedical Genomics Center, the Center for Mass Spectrometry and Proteomics, the College of Biological Sciences Imaging Center, the Academic Health Center Biomedical Image Processing Lab, and the Institute for Therapeutics Discovery and Development.

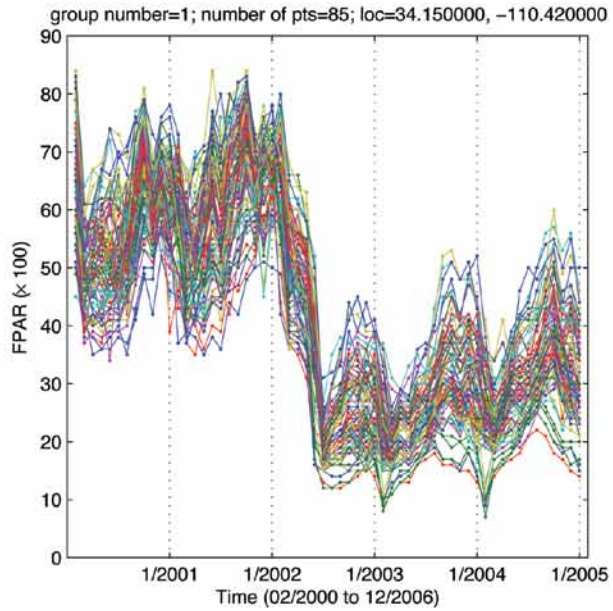
Using Data Mining to *Monitor the Planet*

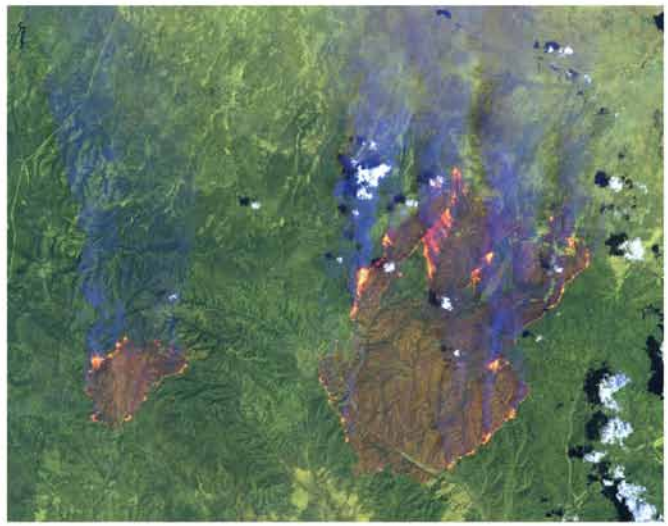
Data mining is a computational technique that uses sophisticated search capabilities and statistical algorithms to find patterns in data. Professor Vipin Kumar (Computer Science and Engineering, MSI Fellow) and his research team have developed scalable algorithms to detect changes in land cover using data from NASA's Earth Observing System (EOS) satellites, and have shown their effectiveness in detecting changes in forest cover due to fires, logging, and other events. Deforestation is an area of concern to scientists studying climate change. Changes in forests account for as much as 20% of the greenhouse gas emissions into the atmosphere, second only to fossil fuel emissions.

In 2009, the University of Minnesota entered a partnership with the Planetary Skin Institute (www.planetaryskin.org), an organization that is developing a global "nervous system" known as Planetary Skin. This system will integrate data from sensors monitoring the earth's surface into a form that policymakers can use. Professor Kumar's software is being integrated into the first prototype of Planetary Skin.



A vegetation time series (left) identified by the change detection algorithm shows a sustained decrease in vegetation. The corresponding satellite image from Google Earth (right) shows that logging has indeed occurred in this forested area located in Northern California.





The collection of time series (left) identified by the change detection algorithm shows a dramatic drop in vegetation index around the summer of 2002. Satellite imagery (right) for this location (a forested area near Phoenix) from June 2002 shows a large-scale forest fire in progress—the well-documented Rodeo Fire.

MSI Events and Outreach | *June 2009–June 2010*

As part of our mission to support research, the Supercomputing Institute is involved in events and outreach activities to publicize the work being done with our equipment and facilities and to provide learning experiences for students.

Undergraduate Internship Program

Each summer, undergraduate students from across the U.S. come to Minnesota for ten weeks to work with a faculty member and his or her research group on a project using MSI. For many of these students, this is the first opportunity they have to participate in this kind of world-class research. Eleven undergraduates from six colleges and universities around the country participated in the Summer 2010 program. In the picture below, interns participate in a lunchtime seminar.

Annual Supercomputing Conference

MSI participated in the annual Supercomputing Conference in November 2009. The conference (SC09) was held in Portland, Oregon on November 16–20, 2009. MSI researchers gave several presentations about the work being done using our facilities and equipment. In the picture above, Dr. Ben Lynch of the MSI User Support staff gives a presentation.

Open House 2009

MSI held an Open House on November 4, 2009 to showcase its resources and highlight some of the groundbreaking research being done using them. Activities included talks, a panel discussion, tours of the labs and machine room, and poster displays by several MSI research groups. Above: Moderator John Finnegan (Dean, School of Public Health) introduces the panel discussion at the Open House. Panel members, left to right: State Senator Kathy Saltzman (DFL-District 56), Mr. Drew Flaada (IBM), Professor Bin He (Department of Biomedical Engineering), and Professor Julie Jacko (Director, Institute on Health Informatics).

25 Anniversary Research Exhibition

To celebrate MSI's 25th anniversary, we held a Research Exhibition poster competition on April 30, 2010. Forty-four posters were displayed by MSI researchers in a number of fields. The Grand Prize winner was Pierre Carrier of the Department of Computer Science and Engineering. The other prize winners were Ke-Jung Chen (Physics), shown below left explaining his poster to Professor Tom Jones, Astronomy and MSI Interim Director; Dane Coffey (Computer Science and Engineering); Raamesh Deshpande (Computer Science and Engineering); and Binh K. Lieu (Electrical and Computer Engineering).

Youth Outreach–BioSMART

MSI hosted students and faculty from the BioSMART program at Arlington High School in St. Paul, Minnesota on March 17, 2010. The students toured the MSI facilities, learned about the "innards" of computers (below right), and programmed a short movie, which they got to see displayed on the LMVL.

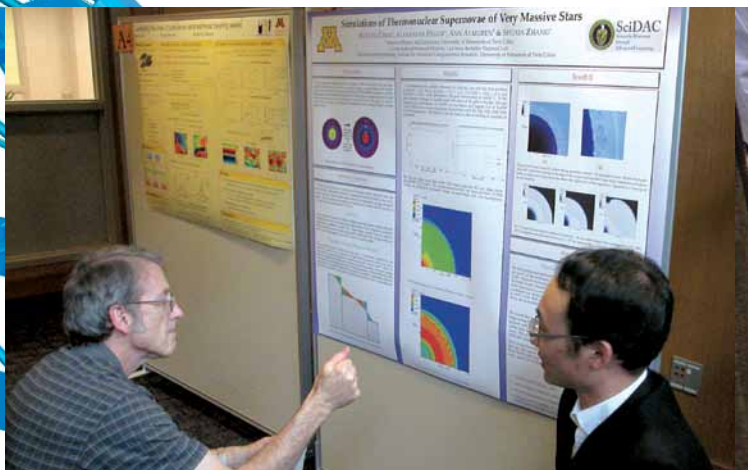
Other Conferences

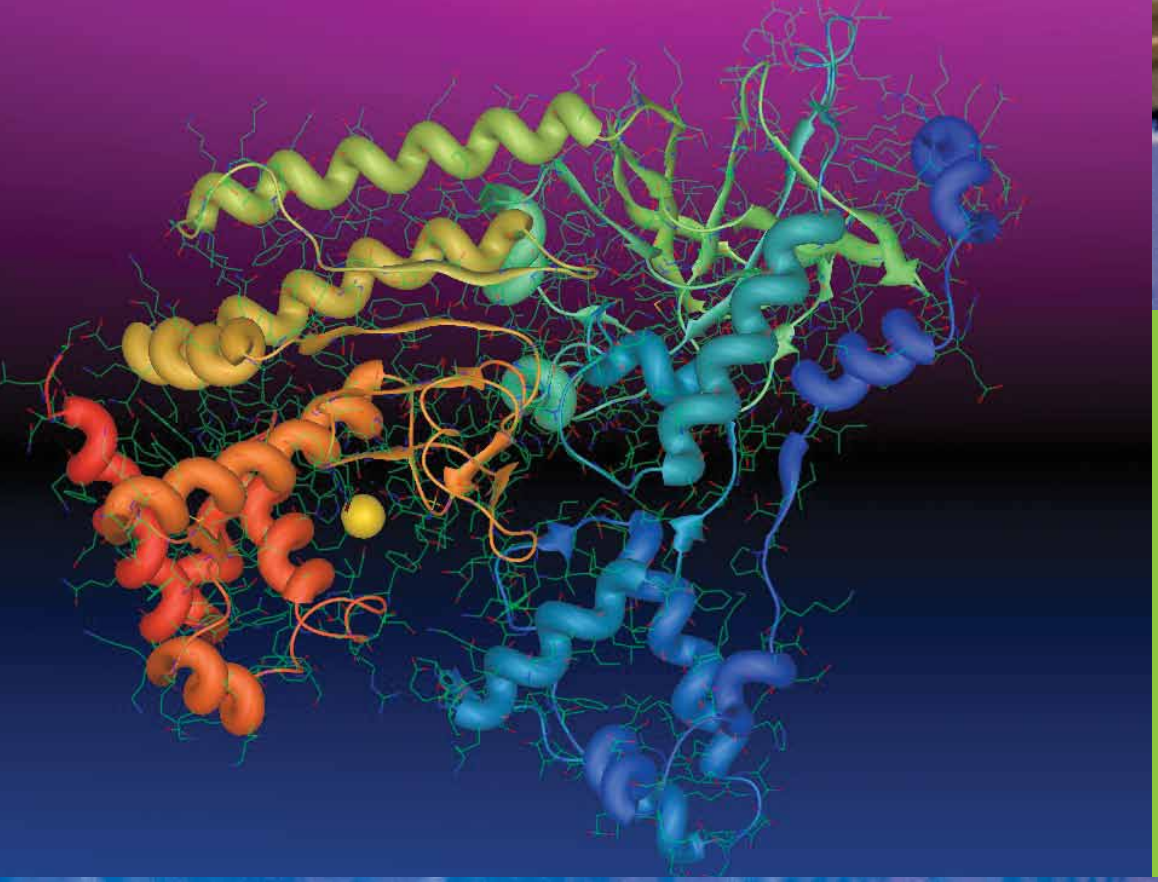
BICB Symposia, *July 2009 and January 2010*

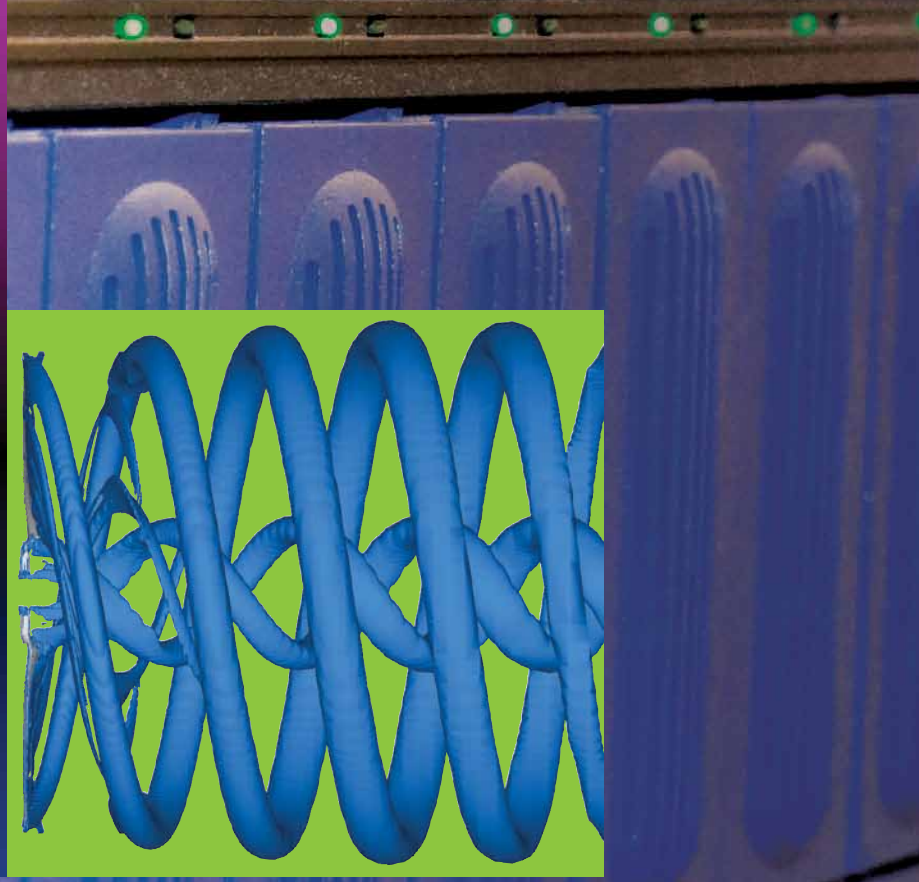
American Physical Society/Division of Fluid Dynamics conference, *November 22–24, 2009*

LifeScienceAlley, *December 9, 2009*

Designing Medical Devices Conference, *April 13–15, 2010*







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