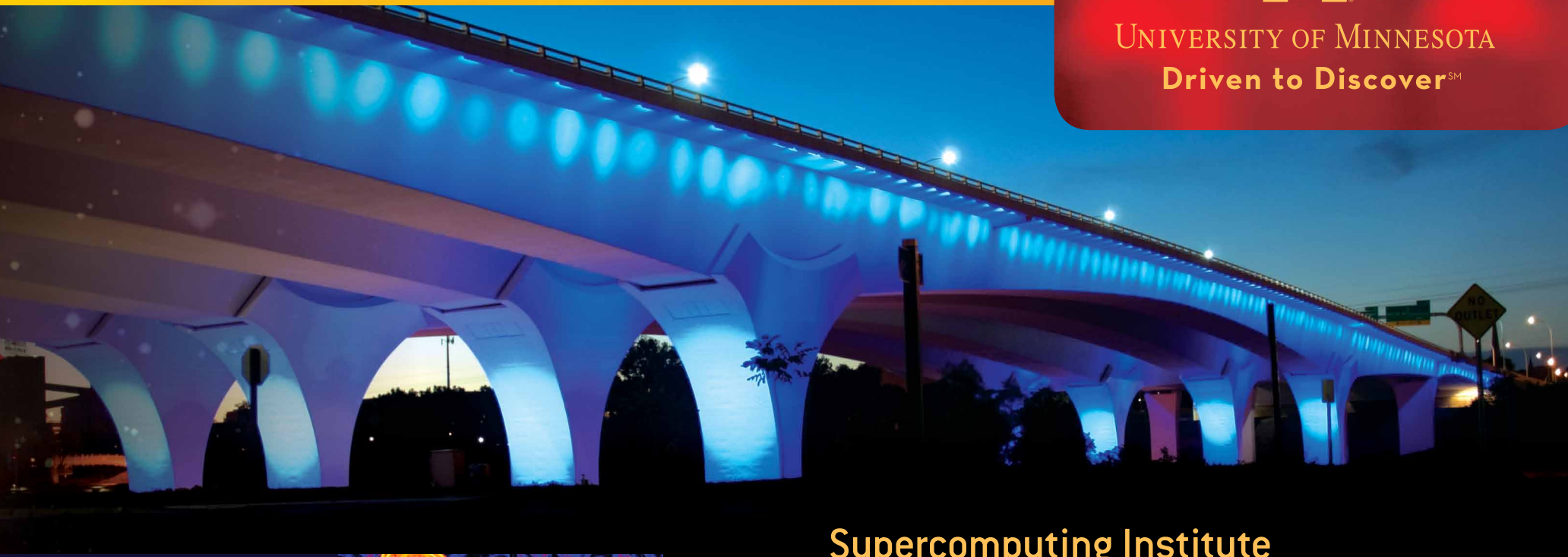
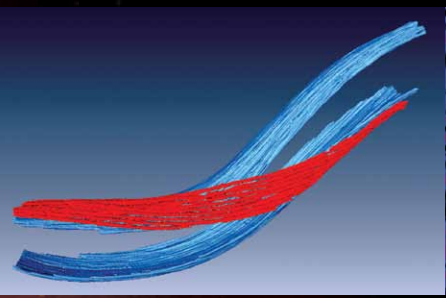


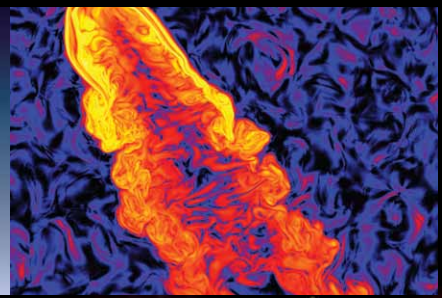
UNIVERSITY OF MINNESOTA
Driven to Discover℠

Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

a Unit of the Office of the Vice President for Research





ANNUAL *Research Highlights*

Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

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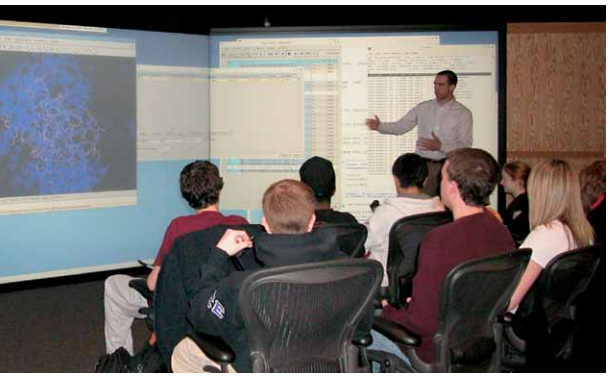

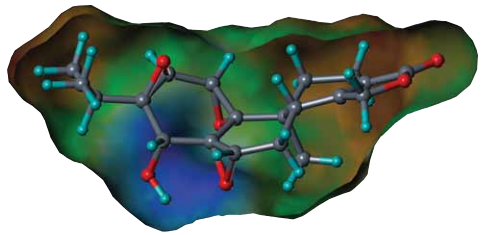

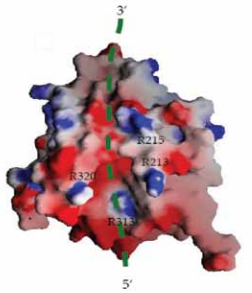

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This report was prepared by Supercomputing Institute researchers and staff.

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Editorial support and photography: Amy Danielson

Designed and printed by University Printing Services.

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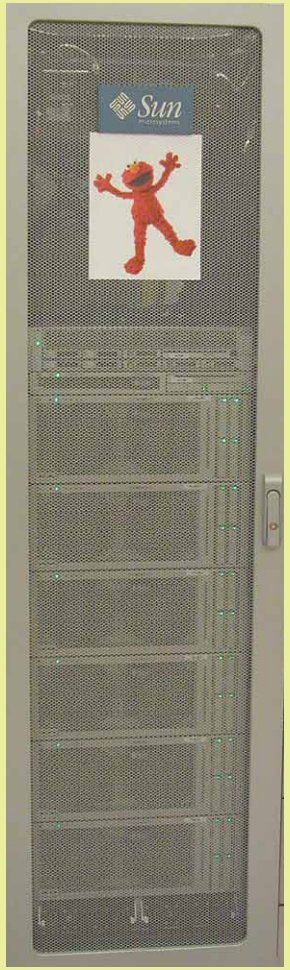
Overview

The mission of the University of Minnesota Supercomputing Institute for Advanced Computational Research (MSI) 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 2008–2009:

- 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, a Hewlett-Packard cluster with 1056 compute nodes (over 8000 cores), was purchased in June 2009. Installation began in early fall and it is expected to be available for general use by the end of 2009.
- The MSI-UMR BICB Computational Laboratory (UMBCL) became operational in June 2009. This laboratory is designed to support the University of Minnesota Rochester's Biomedical Informatics and Computational Biology Program (BICB). See page 8.

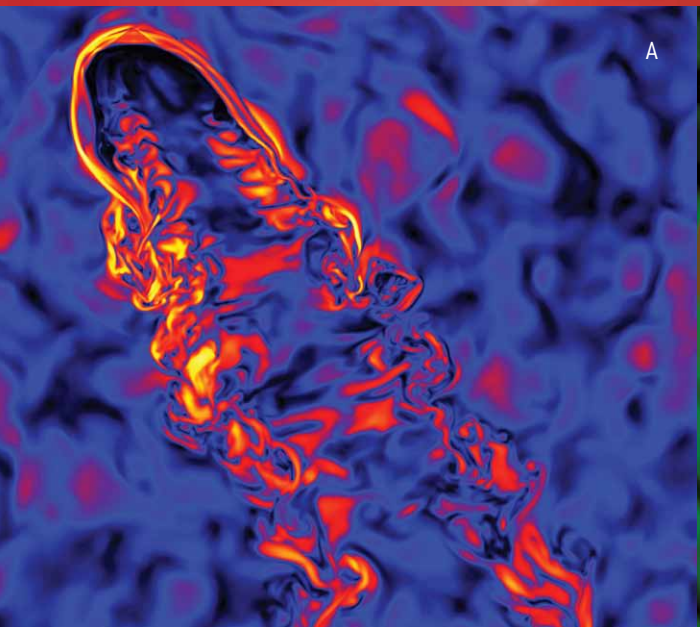
More information about MSI can be found in the Facts and Figures center section.

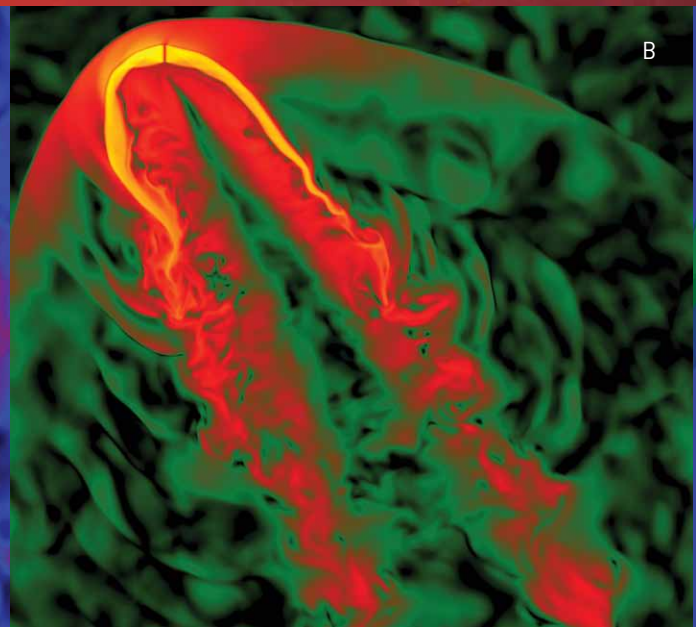
Simulating
THE COSMOS

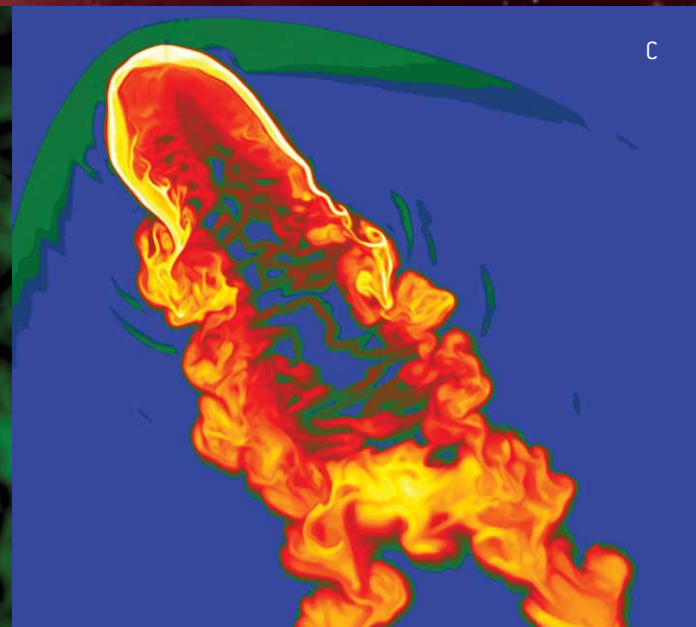
The use of massively parallel computing on powerful machines has been a great benefit to many scientific researchers. Among these are the astrophysicists, who deal with enormous datasets as they study cosmic phenomena. Professor Tom Jones, Department of Astronomy and Interim Director of the Supercomputing Institute, and his research group have successfully developed a fully parallel code that scales to several thousand cores. Using this code, the group is able to create simulations of galaxy jets.

Some of the Jones group's simulations are shown on these pages; they show a 2000x2000x500 mesh simulation of a "narrow angle tail" galactic jet, which is due to a relatively weak jet in a strong wind. The jet is bent back to form a turbulent wake in a supersonic wind; the wind is due to the galaxy's motion through the inter-cluster medium. These images are at 230 million years after the galactic jet turned on. Picture A shows the magnitude of the magnetic field; picture B simulates the kinetic energy, in log scale, of the jet; picture C simulates the cosmic rays in log scale; and picture D shows the jet's vorticity in log scale.

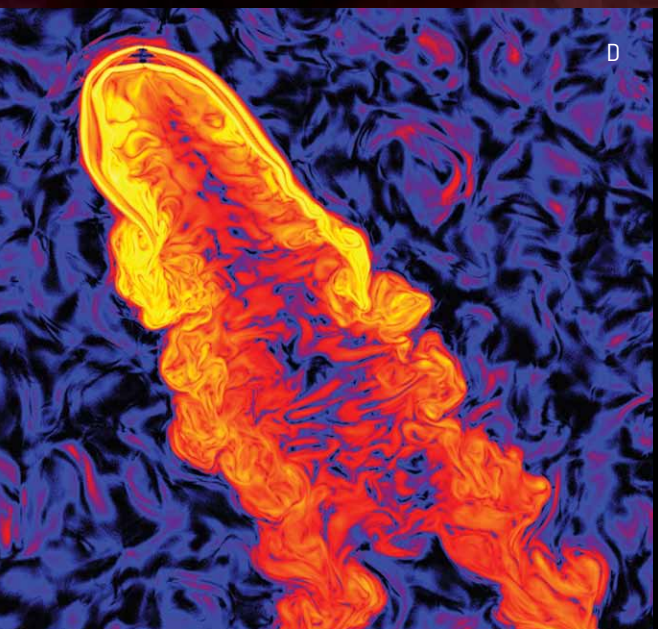
These data can be combined to compute expected emissions from the simulated jets. The dominant emissions are produced in the radio band as it turns out, so these objects are mostly studied by radio astronomers.







Picture E shows an image of what this particular object would look like to a radio astronomer. The Jones group refers to such images as “synthetic observations” of the simulated object. Fortunately, the synthetic images of the simulated object look very much like the real thing. Using methods very similar to those applied by radio astronomers on real tailed jets, the Jones group has extracted the “observed” physical properties of the simulated jets. Those properties can be compared to the actual properties of the simulated flows, in order to test the ability of radio astronomers to accurately measure the properties of real objects.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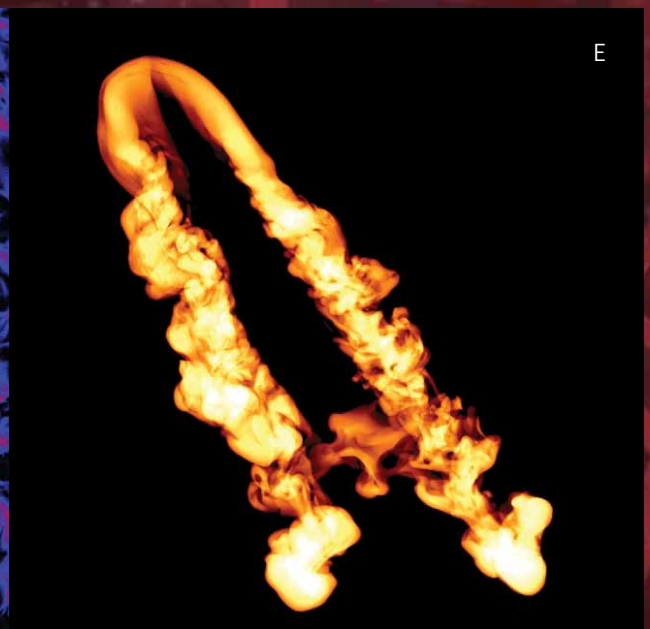
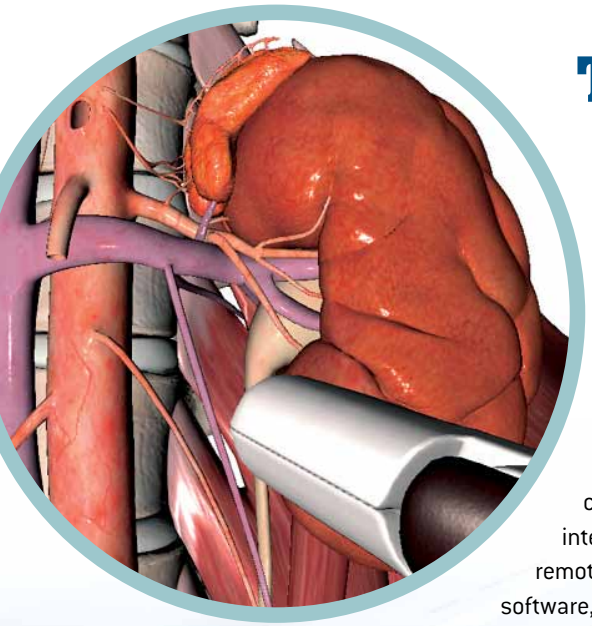

E

Modeling the New I-35W Bridge

Soon after the I-35W bridge collapsed in 2007, the design for the new bridge incorporating "smart-bridge" technology was underway. The new I-35W bridge includes sensors to investigate its structural behavior. Researchers at the University of Minnesota are involved in the interpretation and evaluation of the collected data. Professors Catherine French, Carol Shield, and Henryk Stolarski of the Department of Civil Engineering are using MSI resources for a key aspect of the data interpretation, which is the development of a detailed finite element model (FEM) to investigate the static and dynamic properties of the bridge, including time-dependent effects. Monitoring the new I-35W bridge should lead to a better understanding the behavior of post-tensioned concrete bridges in the state of Minnesota, potential improvements in the methods for analysis and design of these systems, and recommendations for instrumentation of future bridges.

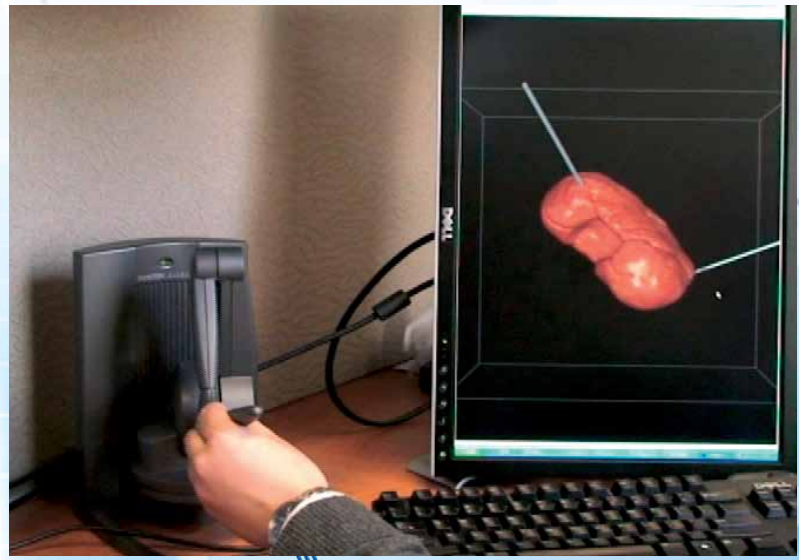


Training Surgeons With VIRTUAL REALITY

Virtual reality-based training systems are a new frontier in medical and surgical education. The Center for Research in Education and Simulation Technologies (CREST) is an exciting initiative that seeks to improve surgical training with the use of virtual reality-based trainers. In collaboration with MSI, CREST researchers are developing interactive, real-time simulation and visualization for remote surgical training; MSI is also providing hardware, software, and technical user support.

CREST is an American College of Surgeons Level 1 Center of Excellence, one of 29 in the world. It is also part of SimPORTAL (www.simportal.umn.edu), the University of Minnesota Medical School's simulation-training web portal.

Associate Professor Robert M. Sweet (CREST Director, Department of Urologic Surgery) and Professor Kumar K. Tamma (Department of Mechanical Engineering, MSI Fellow) lead a team that is developing a laparoscopic trainer as well as modules and curriculum for a transurethral procedural trainer. The team is also working on a patient-specific remote training system for delivering real-time virtual reality training to the region.

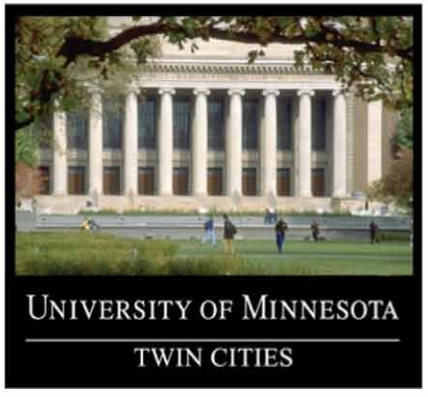


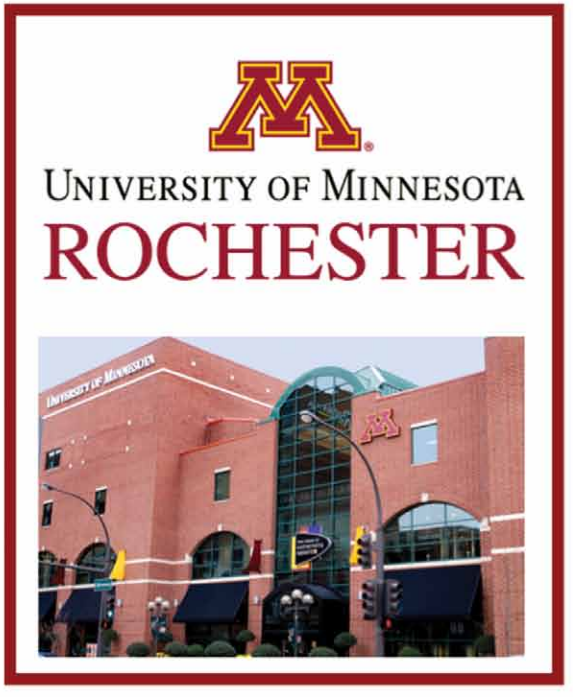
Partnership with University of Minnesota Rochester: Biomedical Informatics

The Biomedical Informatics and Computational Biology (BICB) program at the University of Minnesota Rochester (UMR) was established as part of the State of Minnesota's initiative to focus on health science, bioscience, engineering, and technology. The mission of the program is to conduct research and provide education. UMR coordinates with the University's Twin Cities campus on research and education; collaborators for the BICB program include the Mayo Clinic, IBM, and the Hormel Institute. The program is establishing an interdisciplinary, all-University graduate program in biomedical informatics and computational biology.

Besides making its high-performance computing resources and support available to BICB-affiliated researchers, MSI is partnering with the BICB program as part of a Shared University Research (SUR) Program grant from IBM. Under this grant, which was awarded in October 2008, BICB has obtained IBM Cell Blade and Power 6 computing resources. These machines are housed at MSI, and MSI staff are providing technical and user support. The machines became available in Spring 2009; information can be found at www.msi.umn.edu/labs/umbcl.

Information about the BICB program can be found at their website: www.r.umn.edu/bicb/.



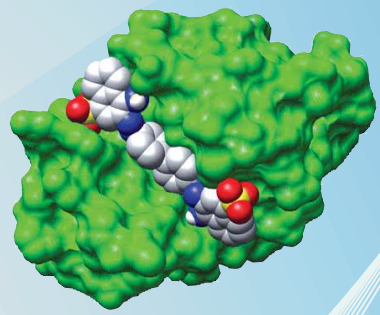


Facts and Figures

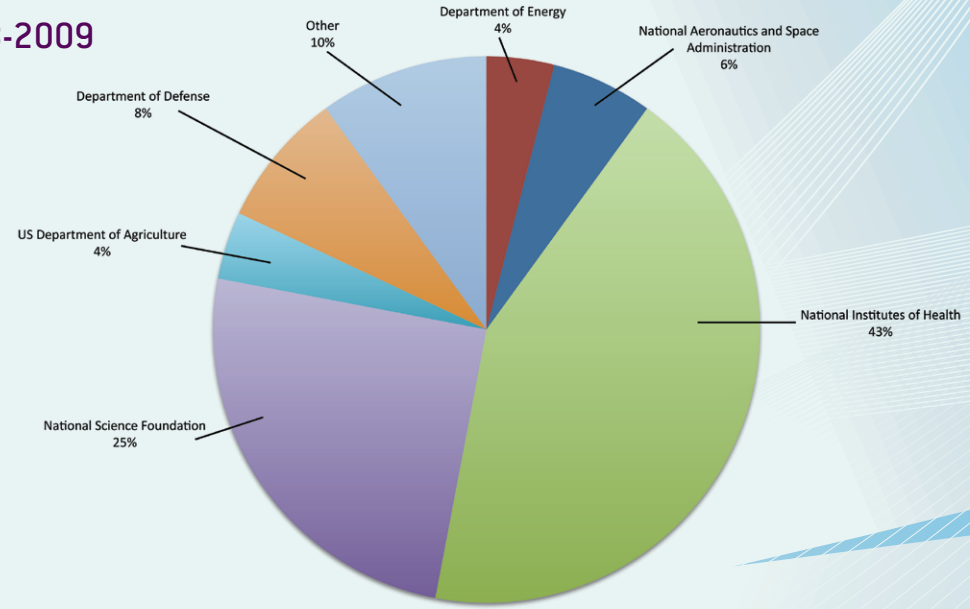
2008-09

External Funding

Funding Source	Amount, 2007–08	Amount, 2008–09
Department of Energy	$4,289,614	$4,062,068
National Aeronautics and Space Administration	$3,038,433	$6,640,465
National Institutes of Health	$50,772,711	$44,879,416
National Science Foundation	$20,652,936	$26,042,899
US Department of Agriculture	$4,582,522	$4,296,155
Department of Defense	$11,235,527	$6,968,986
Other	$9,174,502	$10,977,567
Total External Funding	**$103,746,245**	**$103,867,556**



Breakout for 2008-2009



Facts and Figures

2008-09

People

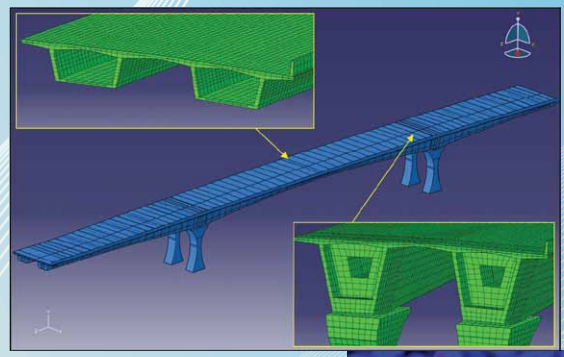
MSI Principal Investigators Active During January 2008 Through June 2009

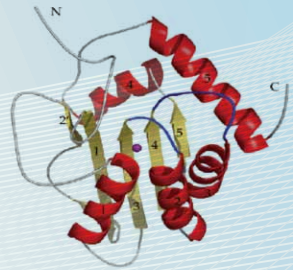
Number of PIs at University of Minnesota Twin Cities

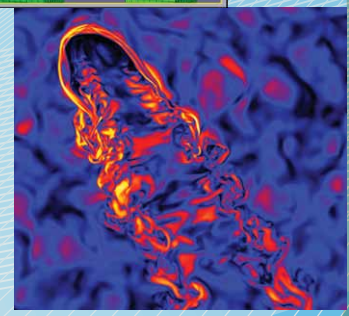
School/College	#PIs
Academic Health Center	*251*
AHC Centers	12
College of Pharmacy	35
College of Veterinary Medicine	13
Medical School	121
School of Dentistry	7
School of Nursing	1
School of Public Health	11
Joint CBS/Medical School	51
College of Biological Sciences	*89*
CBS departments	24
Joint CBS/Medical School	51
Joint CBS/CFANS	14
College of Food, Agricultural, and Natural Resource Sciences	*67*
CFANS departments	49
Joint CBS/CFANS	14
Joint CFANS/IT	4
College of Education and Human Development	*1*
College of Liberal Arts	*7*
Curtis L. Carlson School of Management	*3*
Institute of Technology	*175*
Institute of Technology departments	171
Joint CFANS/IT	4

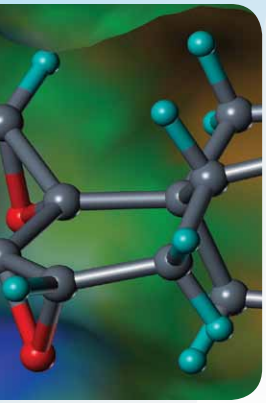
School/College	#PIs
Office of the Vice President for Research	*3*
Hormel Institute	2
Minnesota Population Center	1
Total Number of UMTC PIs January 2008–June 2009	*527**

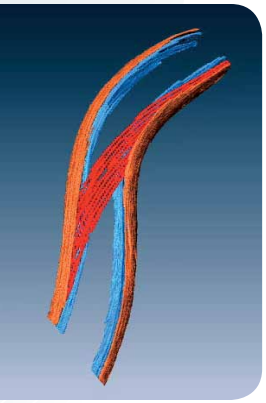
**note: numbers do not add up to total because PIs in jointly-administered departments are counted in both colleges*











Number of PIs at Non-UMTC Institutions

Institution	#PIs
Bethel University	1
Gustavus Adolphus College	2
Hamline University	1
Mayo Clinic College of Medicine	4
Metropolitan State University	1
Minnesota State University, Mankato	3
St. Cloud State University	1
St. Olaf College	2
University of St. Thomas	2
University of Minnesota Duluth	
College of Pharmacy Duluth	1
Medical School Duluth	4
Swenson College of Science and Engineering	13
University of Minnesota Morris	
Division of Science and Mathematics	3
University of Minnesota Rochester	
BICB Program	1

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

Seed Grant Program Awards for 2009–2010

PI: Gary W. Meyer, Department of Computer Science and Engineering
Color Appearance Modeling for Physics-based Coatings

PI: Chad L. Myers, Department of Computer Science and Engineering
Machine Learning Approaches for Inference of Genetic Interaction Networks in Yeast

PI: Fernando Porté-Agel, Department of Civil Engineering, St. Anthony Falls Laboratory, and MSI Fellow
A High-Performance Large-eddy Simulation Technique to Study Land-Atmosphere Fluxes Over Multiscale Topography

PI: Thomas E. Schwartzentruber, Department of Aerospace Engineering and Mechanics
Highly Scalable Particle Simulation for Multiscale Gas Flows

Undergraduate Internship Program, Summer 2010

Bradley C. Abell
Platinum Clusters: A Computational Study in the Search for Better Catalysts

Scott M. Adams
Feedback of Narrow-angle Tail Galaxies in Galaxy Clusters

Gregory A. Barnett
High Rayleigh Number, 3-D Mantle Convection With Standard and Compact Finite Difference Methods Implemented on the GPU

Adam W. Birdsall
Comparative Docking Studies of Gleevec

Erik M. Fritz
Determining Relative Acidities in Carboxylic Acids

Erik R. Gustafson
Structure-based Design and Optimization of Anthrax Lethal Factor Inhibitors

Sarah E. Kragt
Solvation Energies of Biomedical Molecules

Abhrajeet V. Roy
Applying Pharmacophore Mapping and Genetic Algorithms Towards the Development of Novel Anthrax Lethal Factor Inhibitors

Jacob L. Stricherz
A Study of Beta Lactamase Inhibitors

Aurora J. Turgeon
^{15}N and ^{13}C Isotope Effects of Substituted Anilines

Yi Z. Wang
Molecular Dynamic Simulation of TOAC Amino Acid Spin Label

Robin M. Weiss
A System for Web-based, Interactive Visualization of Large Datasets in Real Time

Facts and Figures

2008-09

Resources

MSI Supercomputers

Altix (SGI Altix Cluster)
Blade (IBM BladeCenter Linux Cluster)
Calhoun (SGI Altix SE 1300 Linux Cluster)
Elmo (Sun Fire X4600 Linux Cluster)
Itasca (Hewlett-Packard c-Class BL280 Linux Cluster)

MSI Computing Laboratories

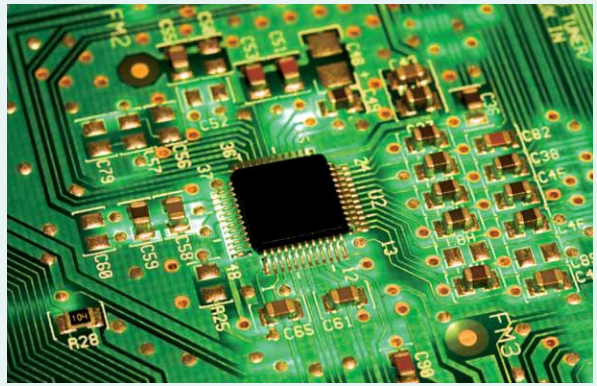
Basic Sciences Computing Lab
Biomedical Modeling, Simulation, and Design Lab
Computational Genetics Lab
LCSE-MSI Visualization Lab
MSI-UMR BICB Computational Lab
Scientific Data Management Lab
Scientific Development and Visualization Lab

Software

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

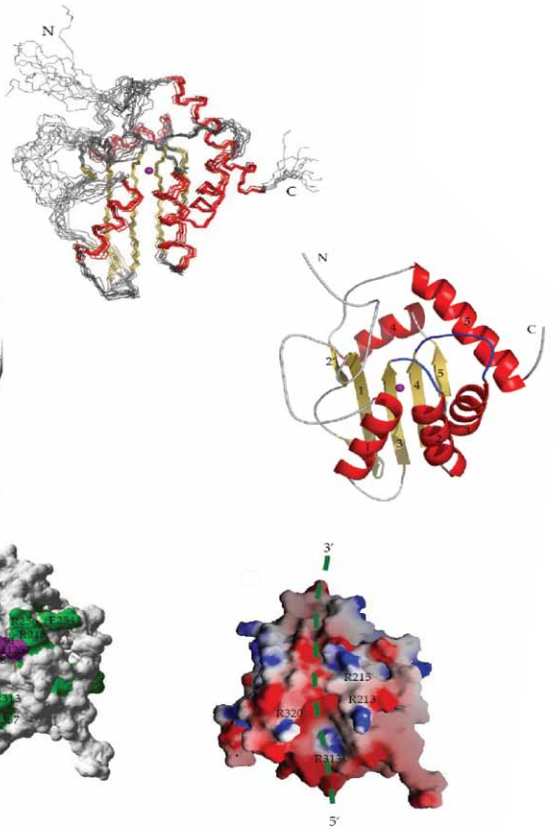
User Support

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.



Defeating HIV

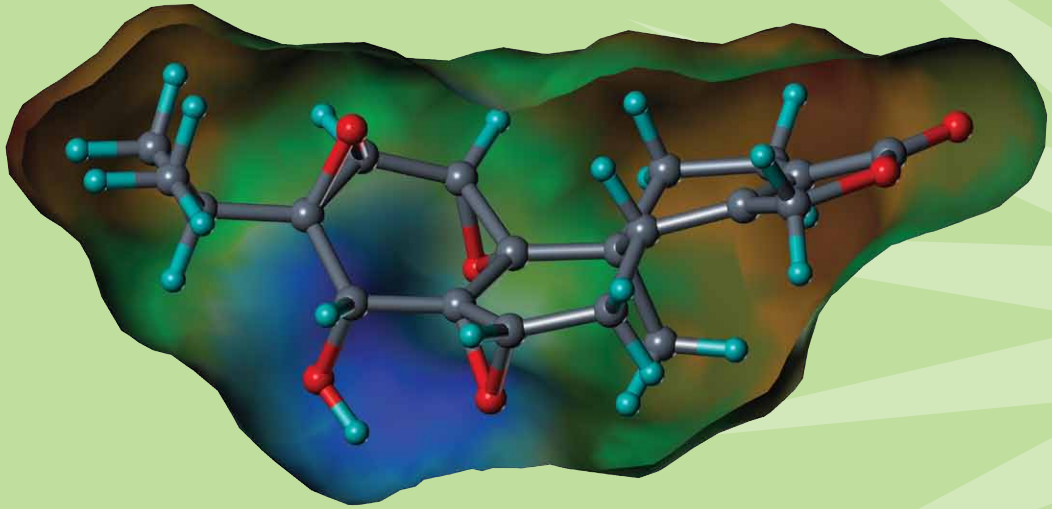
Associate Professors Hiroshi Matsuo (MSI Associate Fellow) and Reuben Harris of the Department of Biochemistry, Molecular Biology, and Biophysics lead a team of researchers studying ways of fighting HIV. Specifically, they are studying a protein called APOBEC3G, or A3G, which can alter the HIV genome by deaminating cytosines to uracils. (Cytosine is one of the bases in DNA; uracil is a base in RNA.) DNA deamination can genetically inactivate HIV and it has the potential to prevent the development of AIDS. A3G interacts with the HIV virion infectivity factor (Vif) protein. While HIV/AIDS researchers have assembled a wealth of genetic and biochemical details about this conflict, Professors Matsuo and Harris and their team are working to get a clear picture of the interaction at the atomic level. The group's work was featured in the prestigious journal *Nature* in 2008, and Professor Harris was recently awarded a $100,000 Grand Challenges Explorations grant from the Bill and Melinda Gates foundation to continue this important research. The pictures on this page are examples of computer-generated images of molecular models used by the team to graphically depict structures determined by magnetic resonance scanning and other means. This graphic includes modifications of Figures 2 and 4 in Chen et al., *Nature*, **452**, 116-119 (2008).



The Institute for Therapeutics Discovery and Development

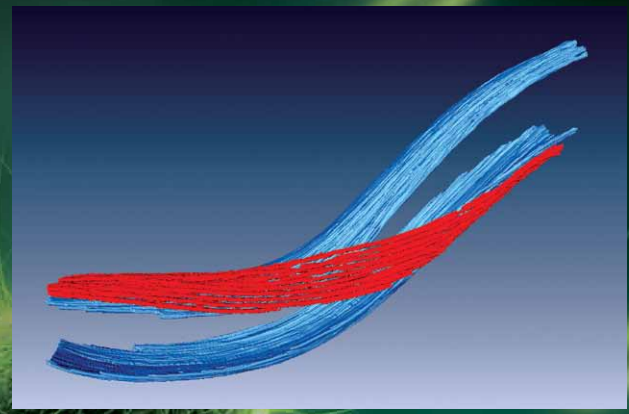
The quest for potential new drugs and molecules that can serve as probes of biochemical processes is a major effort at the University of Minnesota. At the Institute for Therapeutics Discovery and Development (ITDD), researchers conduct interdisciplinary research in drug discovery and development and provide scientific services to research and business communities. Professor Gunda I. Georg, an internationally known medicinal chemist, directs the institute. Researchers at the Institute focus on medicinal chemistry, high-throughput screening, lead discovery, combinatorial chemistry, and chemical process development. As part of the Department of Medicinal Chemistry in the College of Pharmacy, the ITDD also serves as a training ground for the drug discoverers of the future.

The discovery and development of new therapeutics requires specialized software not normally found in an academic setting. Researchers at the ITDD employ MSI hosted resources to (1) design and model new compounds to help medicinal chemists select compounds to prepare and test, (2) track information on the over 200,000 compounds currently in the GPHR compound screening collection, and (3) safely and securely record and manage the enormous amount of biological data that is generated during the drug discovery process.



Visualizing TINY ORGANISMS

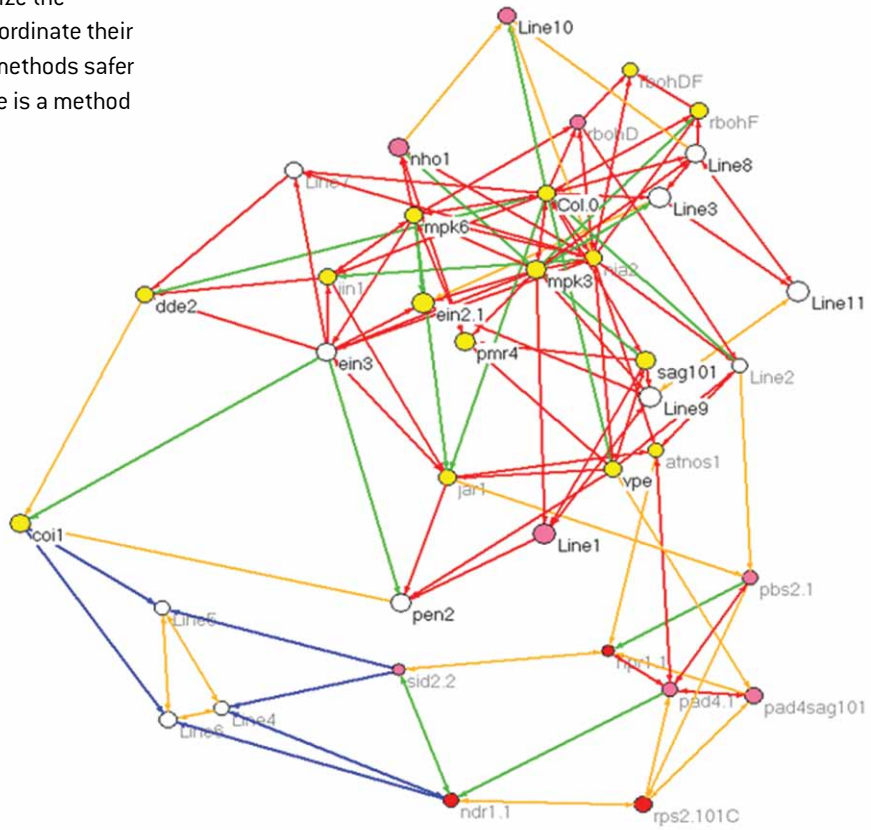
One of the obvious problems with studying the organisms that cause disease is that they tend to be very, very small. Modern researchers are able to use high-powered electron microscopes to study these tiny organisms, and they can then use computers to create graphical representations of them.



The research group of Professor Stuart Goldstein of the Department of Genetics, Cell Biology, and Development studies the structure of the Lyme disease spirochete, *Borrelia burgdorferi*. The group has been using electron cryotomography, an electron-microscope technique that reveals three-dimensional structures, to discover the motility mechanisms of *B. burgdorferi*. MSI resources are used to create three-dimensional color graphics of the structures that show their forms and relationships within the cell. The image on this page was created using this technique. A similar computer image appeared on the cover of the January 2009 *Journal of Bacteriology*, which featured an article about this research.

Self-defense for Plants

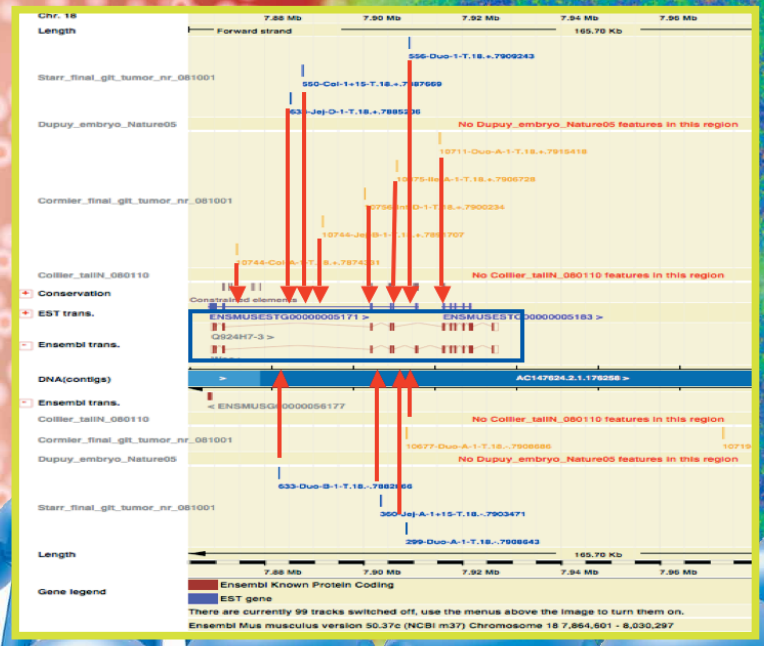
It's not easy being a plant. There are any number of pathogens just waiting to attack you, and, being a plant, you can't run away. Fortunately, plants can defend themselves, and the research group of Associate Professor Fumiaki Katagiri, Department of Plant Biology and MSI Associate Fellow, is studying how. Their cross-disciplinary research, which involves molecular biology, biochemistry, genetics, reverse genetics, genomics, expression profiling, proteomics, structural biology, and computational biology, investigates how plants recognize the molecular signals of pathogen attack and how they then coordinate their defense responses. This work may lead to disease-control methods safer for humans and for the environment. The image on this page is a method of visualizing relationships among mutant plants.



Finding Cancer Genes

The source of cancer truly lies in our genes, and researchers are working hard to discover the genes that, when mutated, could make you more likely to get a specific form of cancer. Some researchers are using transposons, or "jumping" genes, to help with this research. One transposon, dubbed "*Sleeping Beauty*" by its discoverers, is used by the research team of Professor David Largaespada, Department of Genetics, Cell Biology, and Development and the Masonic Cancer Center. The Largaespada group has made great contributions towards improving *Sleeping Beauty*'s jumping efficiency and making it useful for cancer gene discovery. The team uses the transposon to activate or inactivate a gene's normal function, which allows them to identify genes associated with certain cancers.

The researchers make the *Sleeping Beauty* transposons jump within a cell nucleus in specific tissues of mice. Sometimes the transposon lands within the gene that normally blocks tumor formation, effectively lifting the brakes on the process of cell proliferation. The Largaespada group has identified genes that are associated with both colorectal cancer and liver cancer. These cancers are the second and third leading causes of cancer death in the world. MSI provides equipment and technical support that helps the team perform sequence analysis of their gene data. This work has been published in the prestigious scientific journals *Science* and *Nature Biotechnology*.



MSI Outreach

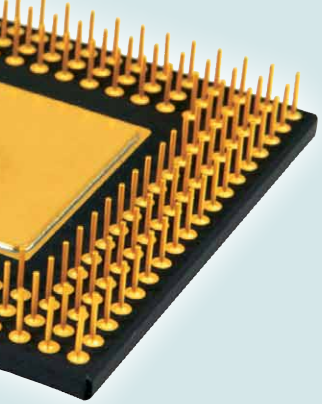
As part of our mission to support research, the Supercomputing Institute is involved in various outreach activities to publicize the work being done with our equipment and facilities. We also provide intern opportunities for undergraduate students that allow them to get involved in research using the supercomputers and to find out what it's like to be a graduate student.

Annual Supercomputing Conference

For the first time, MSI participated in the annual Supercomputing Conference in November 2008. Supercomputing 2008 (SC08) was held in Austin, Texas on November 17–21. MSI researchers gave several presentations about the work being done using our facilities and equipment.

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.



Youth Outreach

MSI has expanded its efforts to work with younger children to get them interested in science.

- Faculty members from the Arlington BioSMART High School in St. Paul, Minnesota have visited the Institute to learn about the kinds of research performed here. BioSMART's program introduces students to careers in biotech industries.
- Attendees at Amantes de la Ciencia on April 25, 2009 at the Minnesota Science Museum got to see how researchers use Institute computers to create pictures of molecules. Amantes de la Ciencia is an annual event that introduces the public to scientists and educators in the Twin Cities' Latino and Hispanic communities.

Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

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