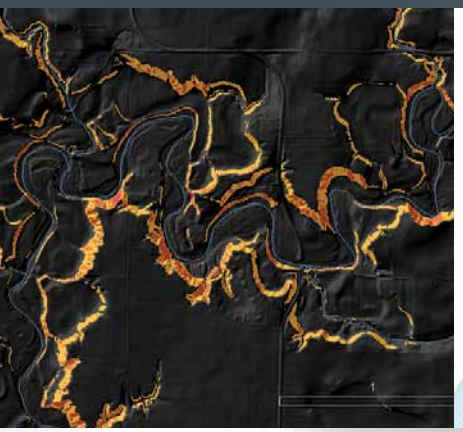
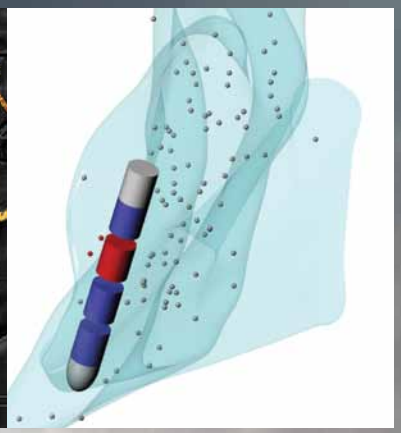
UNIVERSITY OF MINNESOTA
Driven to Discover℠





Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

a Unit of the Office of the Vice President for Research

ANNUAL Research Highlights 2011

Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

UNIVERSITY OF MINNESOTA

MSI Key Staff

Director:
Jorge Viñals
vinals@msi.umn.edu
612-624-0528

Assistant to the Director:
William Hellriegel
hellr@msi.umn.edu
612-624-1356

Assistant Director for Human Resources:
Ann Nordling
nordling@msi.umn.edu
612-624-1556

Assistant Director of HPC Operations:
Jeff McDonald
jeffrey.mcdonald@msi.umn.edu
612-625-6905

Assistant Director of Infrastructure Operations:
Bridget Kromhout
bridget@msi.umn.edu
612-624-4466

RISS Program Director:
Anne-Françoise Lamblin
lambl001@msi.umn.edu
612-625-7414

Manager of Scientific Consulting Group:
Pratik Jagtap
pratik@msi.umn.edu
612-625-6573

Manager of Application Development Services:
Benjamin Lynch
blynch@msi.umn.edu
612-624-4122

Supercomputing Institute for Advanced Computational Research
University of Minnesota
599 Walter
117 Pleasant Street SE
Minneapolis, Minnesota 55455

© 2011 by the Regents of the University of Minnesota. All rights reserved.

This report was prepared by Supercomputing Institute researchers and staff.
Editor and Photographer: Tracey A. Bartlett
Designed and printed by University Printing Services.

This publication can be made available in alternative formats for people with disabilities. Direct requests to alt-format@msi.umn.edu or call (612) 624-0528.

The University of Minnesota shall provide equal access to and opportunity in its programs, facilities, and employment without regard to race, color, creed, religion, national origin, gender, age, marital status, disability, public assistance status, veteran status, sexual orientation, gender identity, or gender expression.

Printed with vegetable ink on recycled paper, with 30% post-consumer waste.

MSI Overview

The mission of the University of Minnesota Supercomputing Institute for Advanced Computational Research is to facilitate research that involves high-performance computing at institutions of higher education throughout the State of Minnesota. This involves providing researchers in all disciplines with access to computing resources, including our supercomputers, a wide variety of software packages, and technical support and training. Research performed at MSI addresses 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.

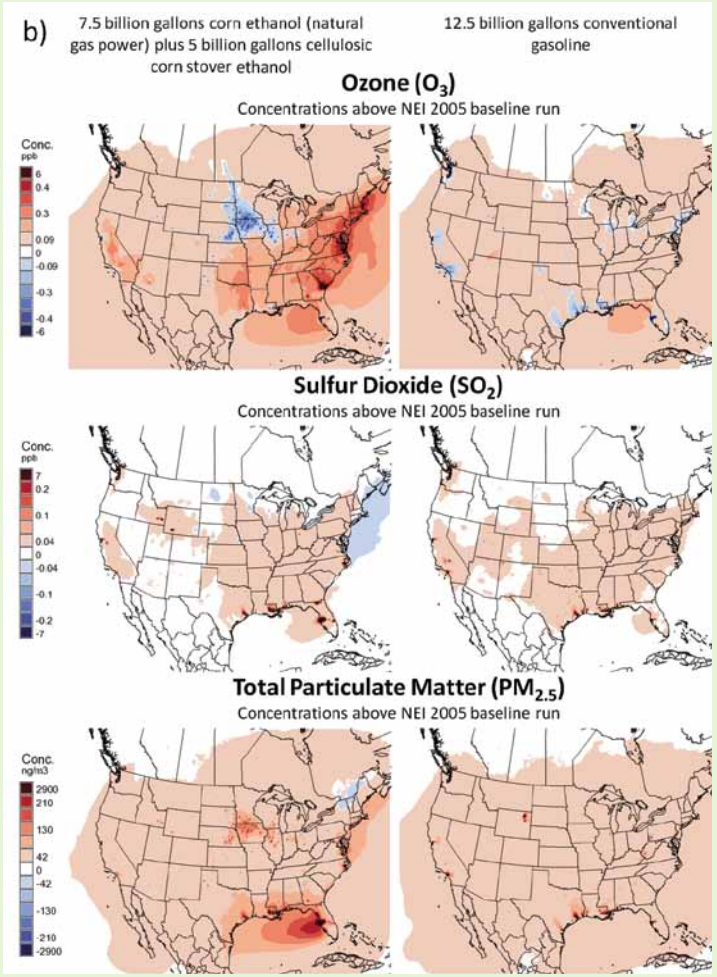
Highlights in 2010–2011:

- The SGI Altix was retired in June 2010.
- MSI hosted two classes, *Big Data for Science* and *Petascale Programming Environments and Tools*, in association with the Virtual School of Computational Science and Engineering during July 2010.
- Jorge Viñals took over as Director of the Supercomputing Institute on August 1, 2010.
- Koronis, a constellation of SGI systems, including foremost an Altix UV 1000 server, was purchased and installed in Fall 2010. Koronis was purchased with an NIH grant and is available to users with NIH funding.
- Galaxy, an integrated framework for data sharing and analysis in the life sciences, was opened for access by University of Minnesota researchers on February 16, 2011 (see story in this publication).
- Blade, the IBM BladeCenter cluster, was retired as an HPC resource in February 2011 and has been re-purposed as a batch engine for lab jobs.
- MSI underwent several organizational changes during 2010-11. Major changes include restructuring of the User Support division and acquisition of the Research Informatics Support Systems group from the Office of the Vice President for Research.

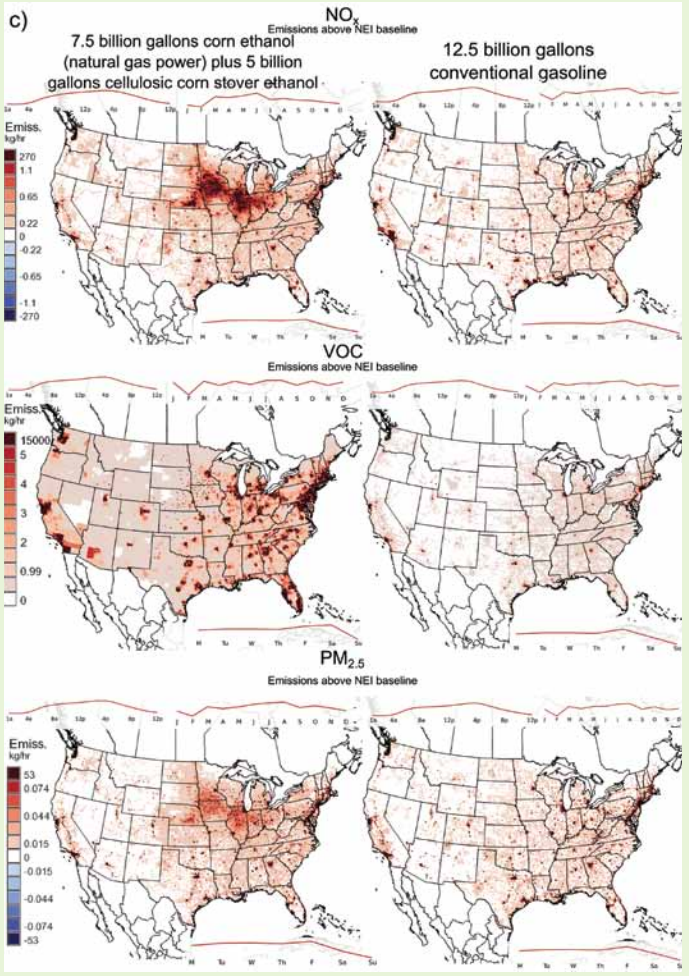
More information about MSI can be found in the Facts and Figures center section.

Modeling the Impact of *Biofuels*

MSI researcher Professor Julian D. Marshall (Civil Engineering, Institute on the Environment) is using supercomputers to study, in a comprehensive way, the emissions tradeoffs between using biofuels and fossil fuels. The production and use of biofuels and fossil fuels release differing amounts of air pollutants in different geographic locations at different times with associated ecological and human health effects that impose costs on society. This research uses advanced life-cycle assessment modeling that accounts for variations in emissions and their impacts, and also takes into account spatial and temporal variables. The researchers rely on MSI resources to run state-of-the-science meteorological, emissions, and air-quality models with very high computational requirements.

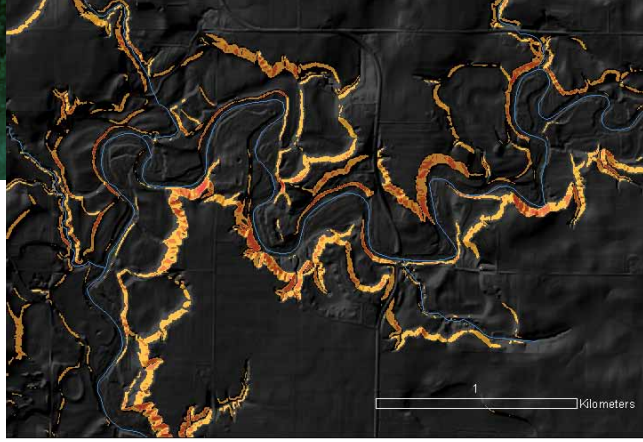


Modeled concentration changes for the pollutants ozone, sulfur dioxide, and fine particulate matter (left) ethanol and (right) gasoline production and use scenarios for the month of August. Ozone and particulate matter can cause disease and death in humans, and sulfur dioxide can cause acid rain.



Annual average gridded emissions of three pollutant species: oxides of nitrogen (NO_x), volatile organic chemicals (VOCs), and fine particulate matter ($PM_{2.5}$). Temporal profiles are included to show variation by month of year, day of week, and hour of day. Two scenarios are compared: the production and use of (left) ethanol from a mix of corn and corn stover and (right) an equivalent amount of gasoline.

Research IN MINNESOTA



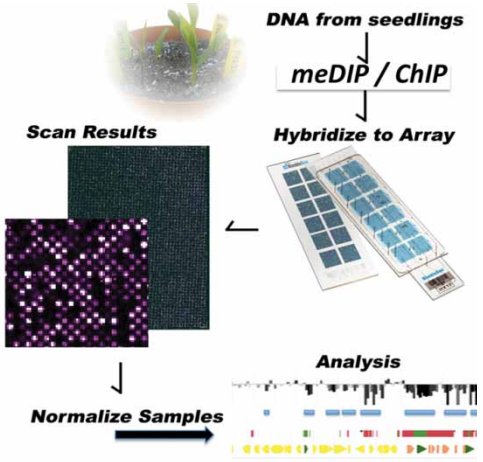
Many MSI researchers are investigating problems that have a direct effect on the State of Minnesota. These include ecological questions, the condition of waterways in the state, and ways to improve agriculture. The Principal Investigators on these pages are studying areas of great interest to the people who live and work here.

Sediment in the Le Sueur River Basin

The Le Sueur River Basin in southern Minnesota is a major source of sediment in the Minnesota River and in Lake Pepin. Excess sediment can adversely affect the ecosystems of rivers and lakes. Assistant Professor Karen B. Gran (Geological Sciences, University of Minnesota Duluth) is studying sediment in the Le Sueur River Basin in support of work by the Minnesota Pollution Control Agency, which seeks to evaluate and control the condition of the river. The Gran group is using two approaches for the project. In the first, they use radionuclide tracers to provide an estimate of the proportional contribution from different sources, integrated over a large area, which is crucial for examining non-point source pollutants. The second approach uses in-field measurements, sediment gauging stations, and air photo analyses to provide information on location and rates of sediment erosion and supply, allowing targeting of the most impaired areas. The two approaches apply different principles and methods and provide independent corroboration. MSI is used to store large spatial datasets used in the development and execution of the sediment routing model and to facilitate data sharing between researchers.

Ecological Research at Cedar Creek

Cedar Creek Ecosystem Science Reserve (CCESR) is a University of Minnesota-owned ecology research site, designated by the NSF as a Long-Term Ecological Research site (photo at right). Since 1964, data have been collected at CCESR and archived in various electronic formats. To better serve the research community, Professor G. David Tilman, (Ecology, Evolution, and Behavior) and his group are establishing an SQL database that houses all data and metadata collected at CCESR. These data and metadata are made available dynamically through web applications on the Cedar Creek website (www.cedarcreek.umn.edu), which the researchers are migrating to the Supercomputing Institute. The CCESR website also serves as an education and outreach tool for scientists to communicate with the public, both on a local and a national level.

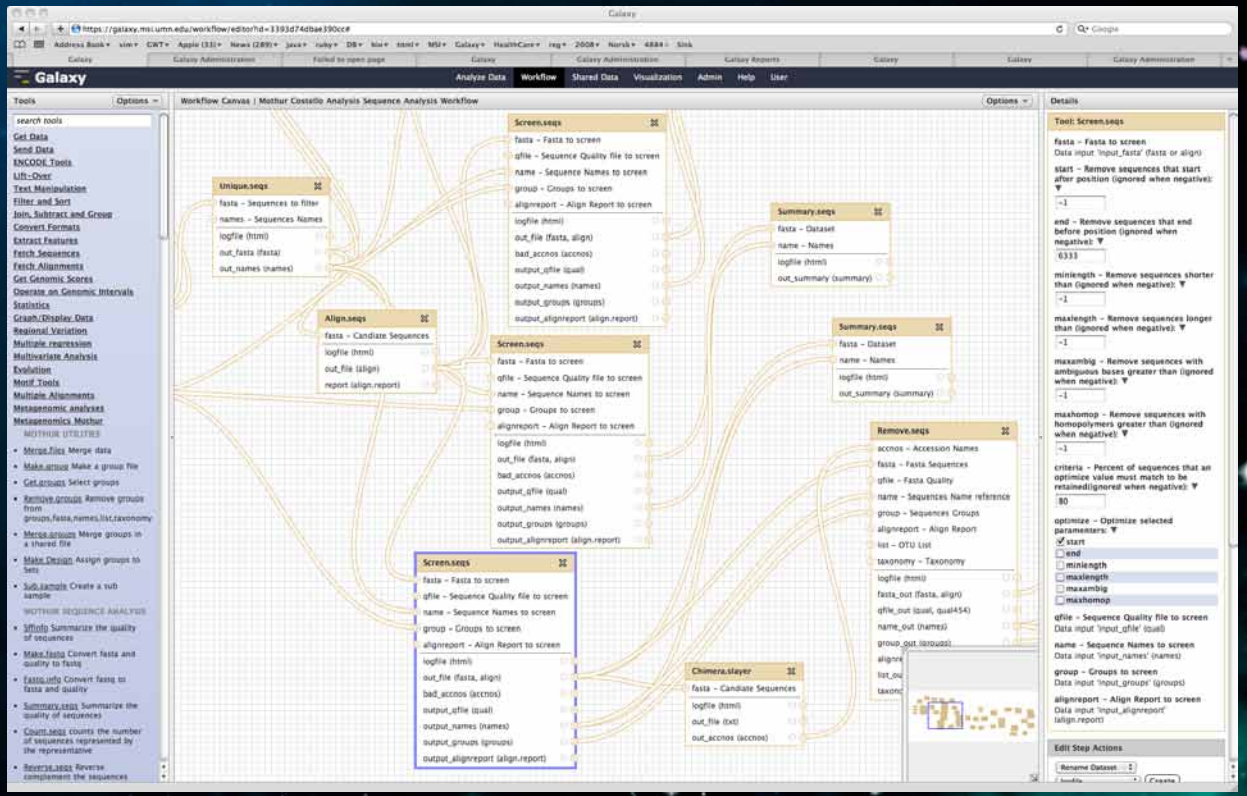


Improving Crops

Many researchers at the University of Minnesota are concerned with improving the food crops grown in the Midwest. MSI researchers are studying these crops in order to develop strains that are hardier, more disease-resistant, and have better yields. Associate Professor Nathan M. Springer (Plant Biology; MSI Associate Fellow) studies variations among different lines of maize (corn). His group has profiled structural variation in the genome of different maize lines and expression differences among genotypes. They are now profiling the distribution of epigenetic markers (chemical additions to the genetic sequence) throughout the genomes of different individuals. A long-term goal of this research is to understand the contributions of epigenetic changes and structural changes to variations in characteristics within a species. The datasets used for the research are quite large, which necessitates the use of MSI laboratories for analysis and visualization of the data.

Galaxy Software

Galaxy is a framework developed at Penn State and adopted for use at the University of Minnesota as part of its core life sciences cyberinfrastructure. The Galaxy informatics tool provides the University's researchers with the necessary integrated environment to access data, run analytical workflows or pipelines, and share information. The initial focus of the installation is urgent needs in genomics research, and more specifically Next Generation Sequencing data analysis and data management. On February 16, 2011, the Galaxy informatics tool was opened for general access by University researchers. Dr. James Taylor from Emory University, a member of the original Galaxy team, gave two workshop presentations on Galaxy and its applications in genomics research. Dr. Anne-Françoise Lamblin, MSI's Research Informatics Support Systems Program Director, is also the program director for Galaxy at the University of Minnesota. More information can be found at the Galaxy website, *www.msi.umn.edu/events/galaxyrelease.html.*



Facts and Figures

2010-11

MSI by the Numbers

Over **3,000** unique users

Two data centers with over **1 MW** of IT capacity

MSI provides:

- four supercomputers providing **128,000,000** core hours every year
- parallel high-performance and enterprise storage totaling **2.3 petabytes**
- over **5 petabytes** of archival storage
- dual **10-Gbps** connections, one to the University backbone, the other to BOREAS-Net

71 onsite workshops during September 2010–August 2011

45 staff members and student employees

2010-11

RESEARCHER BASE

Principal Investigators Active During January 2010 Through May 2011

Number of PIs at UMTC Schools and Colleges

School/College	#PIs
Academic Health Center (AHC)	**229**
AHC Centers	13
College of Pharmacy	18
College of Veterinary Medicine	23
Medical School	116
School of Dentistry	8
School of Nursing	3
School of Public Health	9
Joint CBS/Medical School	39
College of Biological Sciences (CBS)	**70**
CBS departments	11
Joint CBS/CFANS	15
Joint CBS/CSE	5
Joint CBS/Medical School	39
College of Education and Human Development	**3**
College of Food, Agricultural, and Natural Resource Sciences (CFANS)	**61**
CFANS departments	43
Joint CFANS/CBS	15
Joint CFANS/CSE	3

Number of PIs at UMTC Schools and Colleges

School/College	#PIs
College of Liberal Arts	**13**
Curtis L. Carlson School of Management	**6**
College of Science and Engineering (CSE)	**181**
(before July 1, 2010, Institute of Technology)	
College of Science and Engineering departments	173
Joint CSE/CBS	5
Joint CSE/CFANS	3
Hubert H. Humphrey Institute of Public Affairs	**1**
Office of the Vice President for Research	**3**
Hormel Institute	2
Minnesota Population Center	1
Total Number of UMTC PIs, January 2010–June 2011	**504**

** 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

2010-11

Number of PIs at Non-UMTC Institutions

Institution	#PIs
Augsburg College	2
Bethel University	1
College of St. Benedict	1
Gustavus Adolphus College	1
Mayo Clinic College of Medicine	7
Metropolitan State University	1
Minnesota State University, Mankato	2
St. Olaf College	1
University of Minnesota Duluth	
College of Pharmacy Duluth	1
Medical School Duluth	3
Swenson College of Science and Engineering	15
University of Minnesota Morris	
Division of Science and Mathematics	2
University of Minnesota Rochester	
BICB Program	2
Center for Learning Innovation	2
University of St. Thomas	4
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*

Facts and Figures

2010-11

RESOURCES AND SERVICES

MSI Supercomputers
Calhoun (SGI Altix SE 1300 Linux Cluster)
Elmo (Sun Fire X4600 Linux Cluster)
Itasca (Hewlett-Packard ProLiant Linux Cluster)
Koronis (SGI Altix UV 1000 server and constellation)

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

Data Centers
MSI's data centers provide over 1 megawatt of IT capacity.

Software
MSI provides access to hundreds of commercial and academic software packages.

User Consultants
MSI's team of experts provides assistance to researchers in all fields with high-level computation, modeling, simulation, database development, and web-based services.

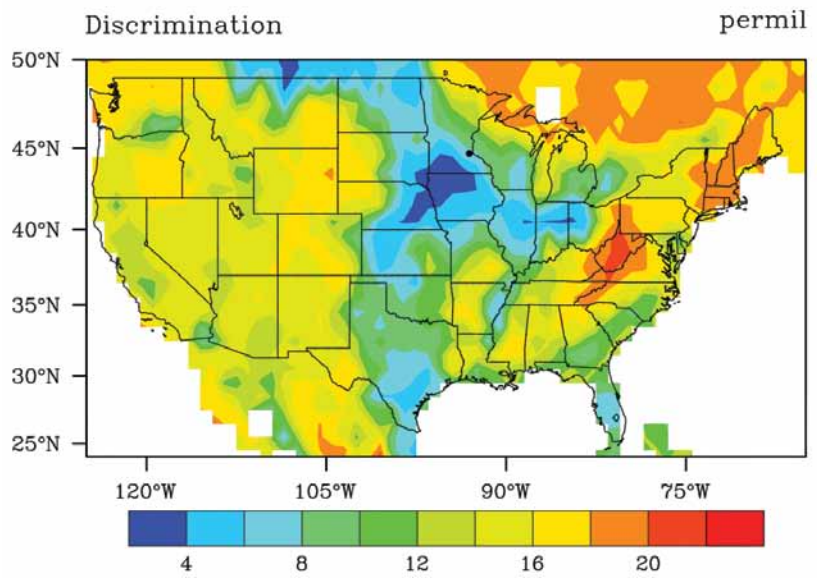
Paid Services
While most resources at MSI are provided free of charge to University researchers, longer-term, dedicated services tailored to specific research initiatives or development programs are also available for at-cost fees.

MSI is also a certified External Sales Organization of the University. Companies and other organizations in Minnesota can buy time on the supercomputers and technical consulting and training.

Carbon Modeling

IN THE UPPER MIDWEST

Associate Professor Timothy J. Griffis, (Soil, Water, and Climate), is working to improve the scientific understanding of the biophysical processes and discrimination mechanisms controlling the exchange of carbon dioxide between the land and atmosphere at the ecosystem, landscape, and regional scales. This research uses a model called Community Earth System Model 1.0 (CESM1.0) to study how climate variations versus land cover change impact regional carbon cycling, carbon isotope discrimination, and the carbon isotope budget of the Upper Midwest. The latest version of the model was released by the National Center for Atmospheric Research in June 2010. It has the capacity to simulate energy, water, and carbon fluxes at high spatial and temporal resolution (globally). Ph.D. student Ming Chen is adding carbon and water isotope algorithms to the model to help improve our ability to trace the flow of carbon and water between the land and atmosphere. This model is computationally very demanding and therefore requires the use of a supercomputer.



The growing season ^{13}C-CO_2 photosynthetic discrimination as simulated using the Community Earth System Model. The dark blue shading reveals the influence of corn and other C_4 species on carbon cycling. These discrimination values can be used to help trace the flow of carbon between the land and atmosphere and are used in inverse modeling studies to help constrain regional carbon budgets.

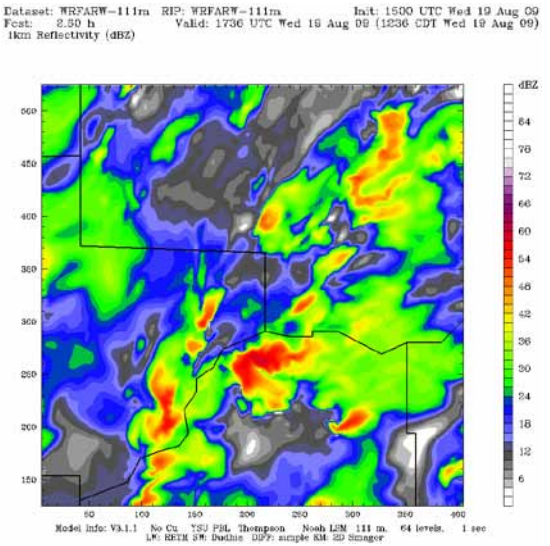
Forecasting Tornadoes

Residents of the Midwest know very well the dangers of thunderstorms and tornadoes. In the Twin Cities metropolitan area, tornado sirens are a common sound during the worst parts of thunderstorm season, and, in 2010, Minnesota led the nation in the number of tornadoes that developed. Obviously, it's important to have timely and accurate systems in place to warn the public so that they are able to seek shelter when a tornado is approaching.

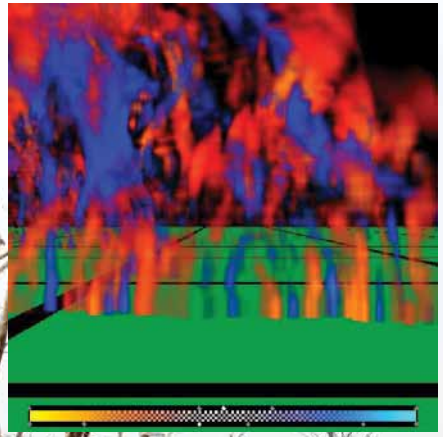
The current method of determining when to activate the warning systems can be thought of as "warn on detect." Professor Doug Dokken (Mathematics, University of St. Thomas) and his colleagues Professor Kurt Scholz (Mathematics, University of St. Thomas) and Thomas Hultquist (National Oceanic and Atmospheric Administration) are among many researchers across the country working towards a "warn on forecast" method. This method would allow authorities to figure out when a tornado is more likely to form in a particular storm or within given atmospheric conditions, and so be able to warn those in the storm area to seek shelter. Using weather-modeling tools, the researchers are analyzing past tornadoes to better understand the processes that cause them. This research is highly computationally intensive.

EF-4 tornado in Bowdle, SD on May 22, 2010. Credit: John Wetter, Skywarn Coordinator.

EF-4 tornado near Campbell, MN on August 7, 2010. Credit: John Wetter, Skywarn Coordinator.



Simulated radar imagery for a model run using MSI resources at a 111-meter grid spacing that re-creates the August 19, 2009 Minneapolis tornadic storm (this storm produced a weak tornado in South Minneapolis). The simulation has also done a very good job depicting similar storms with tornadic characteristics.



Simulation showing counter-rotating loops of vorticity (hairpins) being lifted up along a gust front of a simulated supercell storm. Adjacent loops will merge and cancel, forming longer loops (arching vortex loops). The Dokken group is applying the vortex-gas theory of A. Chorin to understand tornado genesis. The vortices near the ground form a vortex gas, which is treated analogously to a molecular gas.

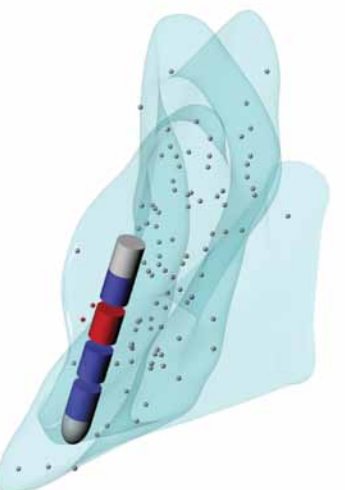
Computational Modeling of Deep Brain Stimulation

Simulation showing a DBS lead in the pedunculopontine nucleus for treatment of Parkinson's disease.

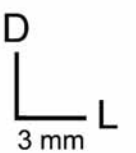
Deep brain stimulation (DBS) is a surgical therapy for several neurological disorders that are often refractory to medication. Some examples include Parkinson's disease, dystonia (in which muscle contractions cause twisting and repetitive movements or abnormal postures), and essential tremor (a disorder that causes involuntary shaking). DBS therapy involves placing small electrodes in regions of the brain that exhibit pathological activity, which contributes to the neurological disorder, and then stimulating those regions with continuous pulses of electricity.

Assistant Professor Matthew D. Johnson (Biomedical Engineering) and his research team use supercomputing resources to simulate the activity patterns of thousands of computational neuron models during DBS. The neuron models consist of sets of mathematical equations that replicate the biophysical properties of membrane and synapse dynamics of neurons located within or near the stimulated nucleus. These neuronal dynamics are coupled with finite element analysis of the voltage distribution generated in the brain during stimulation. The Johnson lab uses MSI visualization resources to create patient-specific models using both anatomical brain imaging and clinical programming notes from each patient. The models are providing a basis for the design of new stimulation strategies and new electrode arrays that enable improved therapeutic outcome in DBS patients with neurological disorders.

Simulation showing activation of axonal fibers of passage during therapeutic DMS in the pedunculopontine nucleus.

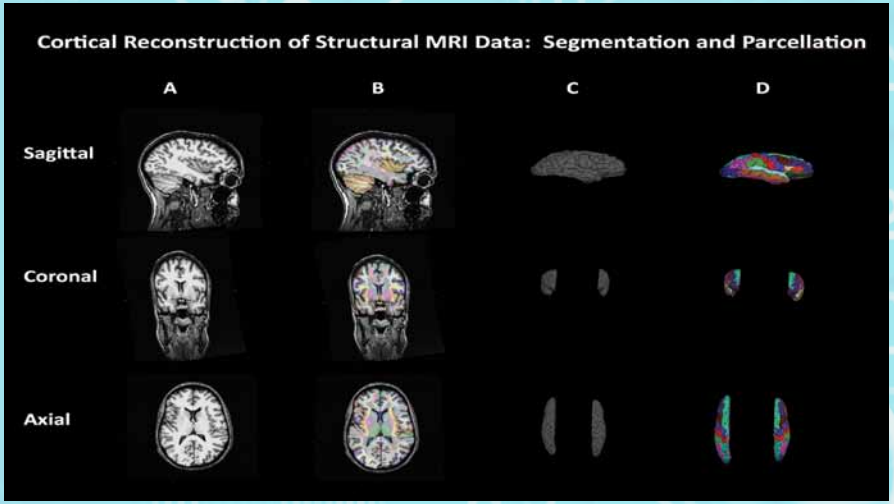


Simulation of the reconstructed location of a DBS lead implanted in the ventral intermediate nucleus of the thalamus of a patient for treatment of Essential Tremor.

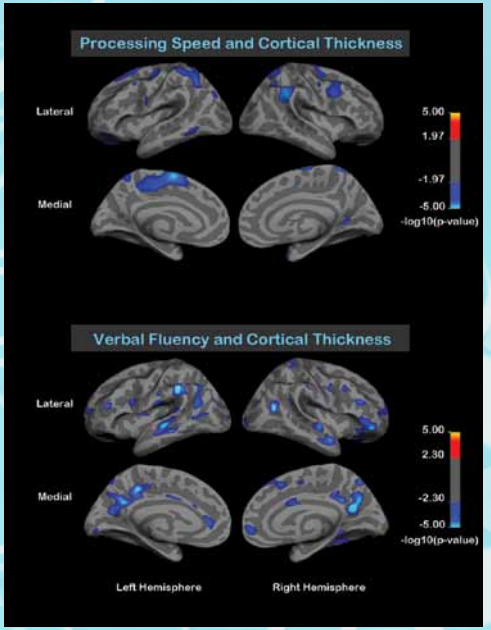


Adolescent Brain Development and Drug Abuse

One of the main functions of the brain's prefrontal cortex (PFC) is to exert control over a person's behavior so that the person can act with purpose, instead of thoughtlessly and emotionally. Professor Monica Luciana (Psychology) hypothesizes that the PFC's ability to control behavior under challenging situations is still developing in late adolescence, rendering teens vulnerable to their emotional impulses. She, along with her collaborator Professor Kelvin O. Lim (Psychiatry) and other members of her research group, are using structural neuroimaging, neurocognitive assessments, and genetic data to research the neurodevelopment of the PFC in adolescents. Tools now exist that allow researchers to quantify aspects of gray and white matter maturation that represent connectivity across brain structures. Since these tools are computationally intensive, this group must use MSI resources.



Structural MRI scan. Column A shows "volume-based" raw data that have not been processed; column B illustrates the same data after intense computational processing that classifies different brain tissue and identifies different brain regions with color; column C shows the same brain using a 3D surface representation; and column D shows this surface representation with the anatomical labels represented by different colors. These metrics allow Professor Luciana to examine multiple aspects of various brain regions with high specificity.



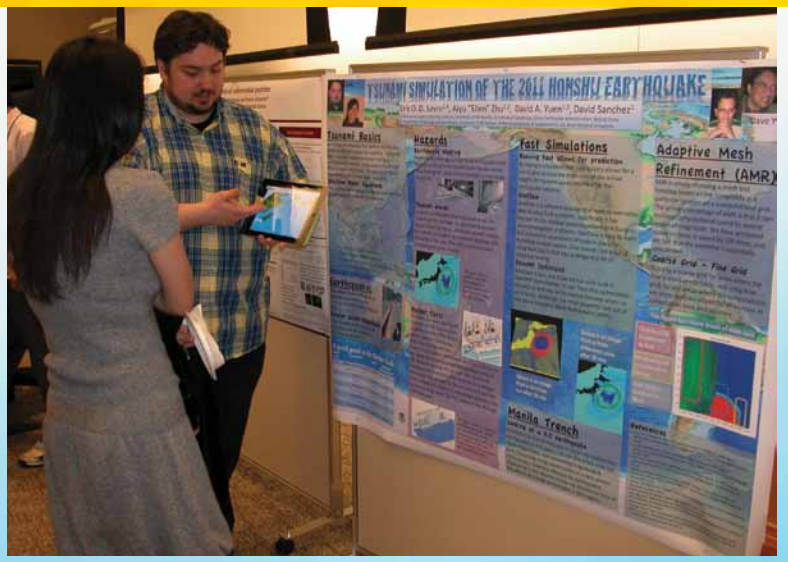
Results of analyses using subjects' behavioral performance data to predict their local cortical thicknesses. These analyses illustrate that, in specific, localized regions, having a thinner cortex (blue areas) is related to improved performance across adolescent development (age range 9-24 years old). During adolescent development, the cortex as a whole becomes thinner, compared to childhood levels. These analyses show that the extent to which maturational processes have remodeled the cortex in specific locations has an impact upon an individual's behavioral performance.

MSI Events and Outreach | *June 2010–June 2011*

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; each works with a faculty member and his or her research group on a project using MSI. For many of these students, the program is the first opportunity they have to participate in this kind of world-class research. Eleven undergraduates participated in the 2010 program, and there were nine interns in the 2011 program.



MSI Research Exhibition

MSI held a Research Exhibition, including a poster competition, on April 25, 2011. Over 40 posters were displayed by MSI researchers in a number of fields. The Grand Prize winner was Ken Chen, who is a graduate student of Professor Alexander Heger (MSI Fellow) in the School of Physics and Astronomy. All the finalists can be seen on the event webpage, *www.msi.umn.edu/events/researchexhibition2011.html.*

Minnesota State Fair

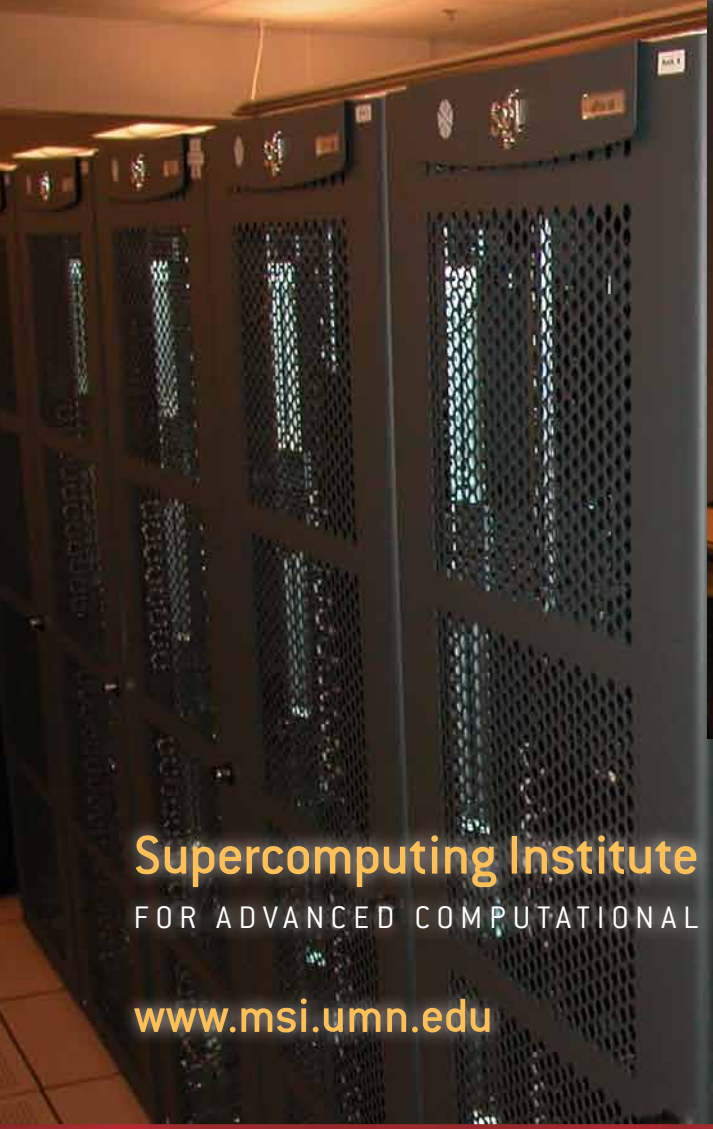
For the third year, MSI joined with the Medical Devices Center (MDC) to demonstrate to attendees at the Minnesota State Fair how supercomputers are used in medicine. Visitors were able to see three-dimensional simulations of a fly-through through a human heart as well as other simulations created by researchers at the MDC.

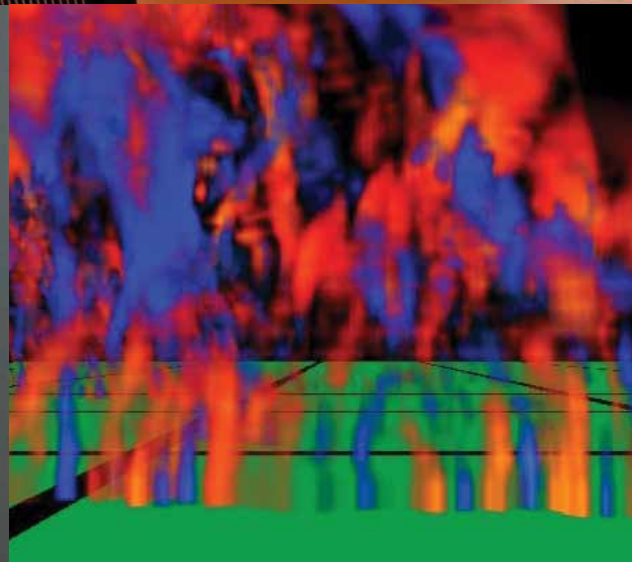
Outreach to Elementary and High Schools

MSI participates in several events each year that are aimed at younger students. MSI's displays and hands-on exhibits allow the visitors to handle the "innards" of computers, build model molecules, and see how scientists use computers to make molecule simulations. We also host visits from school and camp groups who learn about high-performance computing and visualization.

School Outreach Events

- College of Science and Engineering Math and Science Fun Fair, November 2010.
- ¡Amantes de la Cienca! at the Science Museum of Minnesota (St. Paul, Minnesota), January 11, 2011.
- Visit from middle-school students from the Washington Technology Magnet Middle School in St. Paul, Minnesota on October 14, 2010. The students were part of the BioSMART (Biologically focused Science, Math, Academic Rigor, and Technology) Program.
- "Body Forward," the 2010 Minnesota FIRST LEGO League (www.firstlegoleague.org) robotics competition. The program used the LMVL as part of the University of Minnesota Research Workshop hosted by the College of Science and Engineering.
- Visits from students interested in applying to the College of Science and Engineering. The Department of Computer Science and Engineering hosted these students and visited the LMVL for several sessions during March 2011
- The College of Science and Engineering's Exploring Careers in Engineering and Physical Science summer camp for high-school students. MSI participated in these camps during the summers of 2010 and 2011.





Supercomputing Institute

FOR ADVANCED COMPUTATIONAL RESEARCH

www.msi.umn.edu

UNIVERSITY OF MINNESOTA