The University of Minnesota Supercomputing Institute for Advanced Computational Research, which is commonly known as MSI, celebrated its 25th anniversary this year. MSI was born and put into full operation during 1984–1986. A detailed article about those early years appeared in the Summer 2006 issue of the Research Bulletin. This article describes the Institute’s growth and the adaption of its mission to changing times.

The Early Years

In 1981, the University of Minnesota became the first U.S. university to purchase a class VI supercomputer, a 100-megaflop Cray 1. In response to the tax codes at the time, the University created a company to administer the use of the computer internally and externally, the Minnesota Supercomputing Center, Inc. (MSC). At the same time, the University was preparing for an anticipated initiative by the National Science Foundation (NSF) to create academic supercomputing centers. As part of this preparation, in 1984 the University administration created several new faculty positions to recruit leaders in supercomputer-based research, thus creating the Minnesota Supercomputer Institute. These newly recruited faculty were the first Fellows of the Institute. While Minnesota was not selected to be one of the new supercomputing centers, the University did receive some NSF funding. MSI innovations at this time included the new Cray 2 supercomputer that used the Unix operating system, and the establishment of networking connections, including the new TCP/IP protocol. None of these technologies, common today, were widely used at that time.

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After initial years in temporary, makeshift quarters, MSI moved into a remodeled former soft-drink warehouse at 1200 Washington Avenue on the University’s West Bank in September 1986. The Institute remained at this location until 2002, when it moved into Walter Library, a 1920s-era building on the East Bank Campus mall that was renovated to include state-of-the-art technology while keeping its historic architecture intact. The Washington Avenue location initially contained both the Cray 1 and Cray 2 supercomputers as well as a Cyber 205 from Control Data Corporation, making it one of the premier supercomputing centers in the world at the time.

Administration

The first MSI director was Peter Patton, who had been director of the University Academic Computing Center, and Tom Walsh, a University physics professor, was the original MSI scientific director. Both served until late 1986; after their resignations, an executive committee of MSI Fellows temporarily administered MSI. In 1987, the two director positions were merged and Donald G. Truhlar of the Department of Chemistry was appointed to the directorship. He served in that position until 2006.

In 2001, the University of Minnesota created the Digital Technology Center (DTC), an initiative that integrates research, education, and outreach in digital design, computer graphics and visualization, telecommunications, intelligent data storage and retrieval systems, multimedia, data mining, scientific computation, and other technologies. At this time, the Supercomputing Institute became part of the DTC.

In 2006, Andrew Odlyzko, the DTC Director, became Interim Director of MSI while internal and external committees of senior faculty and experts in scientific computing reviewed the Institute’s mission and activities and provided recommendations for the future. As a result, in 2008, MSI separated from the DTC and moved under the oversight of the Office of the Vice President for Research. At this time, the Institute’s official name was changed to the University of Minnesota Supercomputing Institute for Advanced Computational Research. It also absorbed the Center for Biomedical Research Informatics, which had been housed in the Academic Health Center. Tom Jones of the Department of Astronomy, a long-time MSI researcher and Institute Fellow, became Interim Director while a national search was launched for a new director. That search is expected to be completed by Summer 2010.
Growth, Development, and Impact

MSI’s resources have always been in high demand by researchers in the physical sciences and in engineering. Through the late 1990s, these research areas formed the core of MSI’s user community. With the rapid expansion of high-end computing in the biological sciences, however, MSI has become a highly sought-after resource for biologists, medical researchers, and others in fields that have not traditionally used supercomputing. MSI’s extensive collection of high-end software packages for genomics, proteomics, and related fields is available to these researchers, who without MSI might not be able to access them. As a result of the expansion in the use of high-end computing in the biological sciences, the Academic Health Center now has the highest number of MSI Principal Investigators of all University colleges.

The increase in biological research can also be seen in the research papers Institute PIs submit to the MSI Research Report series, which includes professional papers about research that used MSI resources. For the past 20 years, MSI principal investigators have submitted 200–300 reports per year to this series. In 2004, as more and more researchers in the biological sciences began to use the Institute, MSI began identifying those reports that come under the broad category of “computational biology.” Around 30% of the reports in 2004–2007 fall under this category, with the percentage increasing to 37% in 2008 and over 40% in 2009 (as of July 09).

Graduate Students

MSI has always been a valuable resource for graduate students. Besides the large number of graduate students who work in MSI research groups, the Institute has supported the Graduate Program in Scientific Computation since its inception. This interdisciplinary graduate program provides a combination of studies for solving scientific computational problems, building on the strength of existing programs at the University in formulating real problems based on the physical system or the traditional discipline. It augments field-specific work relating to mathematical and numerical modeling.

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### MSI Laboratories

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<thead>
<tr>
<th>Laboratory</th>
<th>Opened</th>
<th>Description</th>
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| **Scientific Development and Visualization Laboratory (SDVL)**             | 1984    | • Main workstation laboratory; provides equipment that allows researchers to develop new applications and to create high-quality visualizations  
• Contains various kinds of workstations, a broad mix of application software, and equipment for making short videos |
| **Biomedical Modeling, Simulation, and Design Laboratory (BMSDL)**         | 1994    | • Originally created as the Medicinal Chemistry-Supercomputing Institute Visualization/Workstation Laboratory (VWL) and co-managed by the Department of Medicinal Chemistry; mainly used for medicinal-chemistry applications and scientific visualization  
• Renamed in 2008 to reflect broader scope of available software and hardware |
| **Basic Sciences Computing Laboratory (BSCL)**                           | 1995    | • Provides a unique mixture of computational servers, workstations, and visualization tools, including a stereo projection system with a 64” by 80” screen                                                                 |
| **Computational Genetics Laboratory (CGL)**                              | 2003    | • Designed for the computational biology community, especially in the areas of genomics, bioinformatics, proteomics, and system biology                                                                                                                                 |
| **Scientific Data Management Laboratory (SDML)**                         | 2005    | • Virtual laboratory designed to meet the evolving data-management needs of MSI researchers                                                                                                                                                                         |
| **LCSE-MSI Visualization Laboratory (LMVL)**                             | 2008    | • Managed in coordination with the Laboratory for Computational Science and Engineering  
• Provides researchers with access to a state-of-the-art large-screen visualization system that can be used in high-resolution mode to display detailed visualizations or as an immersive visualization system using active three-dimensional stereo and motion tracking |
| **MSI-UMR BICB Computational Laboratory (UMBCL)**                         | 2009    | • Supports the University of Minnesota Rochester’s Biomedical Informatics and Computational Biology Program (BICB)  
• Available for interdisciplinary and collaborative BICB projects between IBM, Mayo Clinic, the Rochester and Twin Cities campuses of the University of Minnesota, and the University’s Hormel Institute |
| **Digital Technology Center Computational Biology Laboratory (CBL)**      | 2001; closed 2007 | • Allowed special and focused stimulation of interdisciplinary and interdepartmental digital technology collaboration among research groups involved in computational biology  
• Mission was absorbed into other labs in early 2007 |
| **Laboratory for Large-Scale Data Analysis (LLSDA)**                     | 2002; closed 2005 | • Partnership with Unisys; designed to promote the use of the Orion computer for large problems and large datasets that demonstrated the capabilities of the hardware, operating system, and software  
• Orion converted to core resource in 2005 |

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**Supercomputing Institute History**

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with state-of-the-art techniques for scientific computation in an integrated manner. Most of the faculty in this program are Principal Investigators of the Institute, and many are Fellows or Associate Fellows.

MSI also supported the Neuro-Physical Computational Sciences Program, an interdisciplinary pre-doctoral fellowship program that integrated training in neuroscience with physical-computational studies. Predoctoral fellows pursued degrees in biomedical engineering, chemistry, computer science, mathematics, neuroscience, physics, and scientific computation. Fellows majoring in neuroscience pursued a minor or supporting program in computation or physical science, and those majoring in any other discipline minored in neuroscience. The program began in 1998 and continued through 2008.

**Undergraduate Students**

Undergraduates have also found valuable educational experiences through MSI. One of its most successful programs has been the Undergraduate Internship Program, in which undergraduates from the University of Minnesota and other colleges and universities spend a period working with Principal Investigators and their research groups on projects using MSI resources. These projects usually involve visualization and graphics. The goal of the program is to introduce undergraduates to the kind of research they would do as graduate students at the University of Minnesota. The program was established in 1991 and continues to this day; 566 undergraduates have participated through Summer 2009. Many of these students continue to work with their faculty mentors during the following school year, and some eventually return to the University of Minnesota as graduate students.

**Post-doctoral Researchers**

For many years, MSI enhanced the supercomputing research programs of faculty investigators through the Research Scholarship Program, which was in existence through 2008. This program provided grants to post-doctoral researchers. The grants provided important opportunities for the creation and pursuit of research projects that might not otherwise have been attempted. Numerous publications arose out of this research. MSI awarded 229 research scholarships over the course of the program.

**External Funding**

MSI research attracts a considerable amount of external funding to the University. The first year
MSI tracked external funding, the 1989–90 academic year, the amount of external funding received by MSI researchers was over $11,500,000. This amount increased to over $106,000,000 for the 2008–09 academic year.

**Equipment and Resources**

MSI’s core mission, to provide supercomputing resources to academic researchers and to encourage frontier computational research, has grown and developed over the years. The Institute has continued to purchase new and faster computers with more state-of-the-art processing power. These machines have included computers from Cray, Control Data Corporation, ETA Systems, HP, IBM, SGI, Unisys, and Sun. Machines in use as of September 2009 include an IBM BladeCenter Linux cluster, an SGI Altix XE1300 cluster, an SGI Altix shared-memory system, and a Sun Fire x4600 Linux cluster. A newly purchased Hewlett-Packard Intel-CPU-based cluster with over 8,000 compute cores is being tested at MSI as of this writing.

But MSI does not only provide supercomputers. Several MSI computer laboratories provide workstations, software, and technical support to researchers who need high-end computing support but not the very large, high-performance machines. In addition, MSI hosts an increasing assortment of sophisticated databases and research websites. A list of MSI laboratories is shown on page 4.

**The Future**

In its first quarter century MSI has established itself as a vital resource to the University of Minnesota in facilitating ground-breaking research, while attracting top faculty and students as well as enhancing its competitive advantage in the search for external funding. Going forward, MSI is expected to play an even more central role at the University, since high-end computation and data-intensive analysis and visualization are increasingly critical to a broad and growing range of disciplines well beyond the fields that traditionally have utilized MSI. As its scope broadens and as computational tools continue to improve, MSI will surely evolve. On the other hand, MSI’s core mission will remain to support and stimulate research and education at the cutting edge through computational tools that are at the cutting edge.
Itasca, MSI’s Newest Supercomputer

MSI’s newest machine, a cluster of HP ProLiant blade servers, was installed in September 2009 and is now being tested. The new system has 1,083 HP ProLiant BL280 G6 servers with 8,664 computing cores. In an overwhelming vote, the MSI staff chose the name “Itasca” for the new system.

Itasca delivers a theoretical 97 teraFLOPS of computing performance, which is three times the aggregate theoretical peak of all MSI’s other core resources combined. The system is also number 67 on the November 17, 2009 TOP500 list of the world’s most powerful supercomputers.

Itasca completed Phase I Acceptance Testing in October 2009. It ran a Top500 High-Performance LINPACK (HPL), achieving 74.39 TF of 94.6 TF theoretical (78.6% efficiency) on 1,056 of the 1,083 nodes. It also successfully completed a series of HPL runs over a 108-hour “stability testing” phase.

In Phase II Acceptance Tests, underway as of this writing, HP will replicate their projected timings on MSI’s suite of benchmark codes and then a selected number of MSI PIs (six to eight) will each do real science runs using their own codes at full scale across the entire machine.

Updated information about Itasca will be posted on the MSI website, www.msi.umn.edu/hardware/, as it becomes available.
Open House 2009

The Supercomputing Institute held an Open House on the afternoon of November 4, 2009. Events included a presentation about high-performance computing by Mr. Richard Kaufmann of Hewlett-Packard, an address by University of Minnesota Vice President for Research Tim Mulcahy, and a panel discussion concerning “Research Computing in the Life Sciences as It Impacts the State of Minnesota.” The panel was moderated by Dean John Finnegan of the School of Public Health. Panel members included: State Senator Kathy Saltzman (DFL-District 56); Mr. Drew Flaada of IBM; Professor Bin He, Department of Biomedical Engineering; and Professor Julie Jacko, Director, Institute for Health Informatics.

Other activities during the Open House included tours of the machine room, visualization demonstrations in the LMVL, research and software demonstrations in the SDVL, and presentations and posters by MSI researchers (see page 11). Over 200 people attended.

Three attendees won door prizes. The prizes included an iPod Touch, donated by Sun Microsystems; a printer, donated by Dell; and “A Night on the Town,” which included gift cards for dinner at a Minneapolis restaurant and for the Minnesota Orchestra, donated by Intel.

MSI is extremely grateful for the support of sponsors who provided donations for the refreshments and for the goody bag gifts. Sun Microsystems, Schrödinger, SGI, and Microsoft all gave donations to the refreshments. Goody bag gifts were donated by Hewlett-Packard, IBM, Intel, Schrödinger, and Sun Microsystems.

Top left: Vice President for Research Tim Mulcahy addressed the audience about MSI and its mission. (Photo by Amy Danielson)
Top right: Mr. Richard Kaufmann, Distinguished Technologist at Hewlett-Packard, gave a presentation about high-performance computing. (Photo by Amy Danielson)
Bottom: Dean John Finnegan, School of Public Health, moderated the panel discussion. Panel members, left to right, are: Minnesota State Senator Kathy Saltzman (DFL-District 56); Mr. Drew Flaada, IBM; Professor Bin He, Department of Biomedical Engineering; and Professor Julie Jacko, Director, Institute for Health Informatics.
Events and Symposia

Top, left to right: Dr. H. Birali Runesha, MSI Director of Scientific Computing and Applications; Professor Bin He, Department of Biomedical Engineering; Professor Julie Jacko, Director, Institute for Health Informatics; Minnesota State Senator Kathy Saltzman (DFL-District 56); Mr. Drew Flaada, IBM. Professor He, Professor Jacko, Senator Saltzman, and Mr. Flaada participated in a panel discussion on “Research Computing in the Life Sciences as It Impacts the State of Minnesota.”

Bottom: Gabe Turner, HPC Systems Administrator, gives a tour of the machine room.
Top: An Open House attendee learns about MSI’s support of the Jane Goodall Institute Center for Primate Studies’ database of digital images and videos from Assistant Professor Michael Wilson.
Bottom: Guests at the Open House enjoy lunch prior to the presentations.
Events and Symposia

Posters From the MSI 2008–2009 Seed Grant Program

Efficient Coupling of Ab-Initio and Bifurcation Techniques for Structural Transformations in Materials
Principal Investigator: Matteo Cococcioni, Department of Chemical Engineering and Materials Science

Accounting for Sib Correlation for Testing SNP Single-locus and Epistasis Effects in Genome-wide Association Analysis
Principal Investigator: Yang Da, Department of Animal Science

Multi-scale Modeling and Simulation of Turbulent Reacting Multiphase Flows
Principal Investigator: Sean C. Garrick, Department of Mechanical Engineering, MSI Associate Fellow

Plasmotic Nanohole Arrays for Label-free Kinetic Biosensing in a Lipid Membrane Environment
Principal Investigator: Sang-Hyun Oh, Department of Electrical and Computer Engineering

An Integrated Computational and Experimental Approach to a Molecular-level Understanding of Complex Atmospheric Nucleation Processes
Principal Investigator: J. Ilja Siepmann, Department of Chemistry, MSI Fellow

Displays of Research Using MSI Resources

The Biomedical Genomics Center
The Center for Mass Spectrometry and Proteomics
The Jane Goodall Institute’s Center for Primate Studies
The National Center for Earth-surface Dynamics
St. Anthony Falls Laboratory
The University of Minnesota Biocatalysis/Biodegradation Database
The Virtual Laboratory for Earth and Planetary Materials
The Supercomputing Institute is pleased to announce its Undergraduate Internship Program for Summer 2010. Appointments are for full-time, 10-week internships, and will run from June 7 through August 13, 2010. A student interested in becoming an intern must still be an undergraduate in August 2010 and must be a citizen or permanent resident of the United States or its possessions. Interns will be paid a stipend of $5,000 and are responsible for their own travel and housing costs.

All applications are evaluated competitively based on the qualifications of the applicant and the availability of a suitable project. Prospective applicants should review the research projects list and indicate projects in which they are interested, although they may be offered other projects due to availability.

Projects are available in the disciplines shown below. Students may qualify for projects outside their majors, and are encouraged to apply for these if they are interested in them.

Complete application information, application forms, and project lists are available on the Supercomputing Institute website (see contact information below). Applications, transcripts, and letters of recommendation must be received by March 1, 2010.

### Project Areas

- Aerospace Engineering and Mechanics
- Astronomy
- Biochemistry
- Biology
- Biomedical Engineering
- Biophysics
- Bioproducts and Biosystems Engineering
- Chemical Engineering
- Chemistry
- Civil Engineering
- Computer Science
- Computer Engineering
- Geology and Geophysics
- Materials Science
- Mechanical Engineering
- Medicinal Chemistry
- Molecular Biology
- Pharmaceutics
- Physical Chemistry
- Physics
- Structural Biology

### Contact Information

Website: www.msi.umn.edu/programs/undergraduateinternship.html
Email: uip@msi.umn.edu
Phone: 612-624-2330
Fax: 612-624-8861
Postal address: Undergraduate Internship Coordinator, University of Minnesota Supercomputing Institute, 599 Walter Library, 117 Pleasant Street SE, Minneapolis, MN 55455
Biochemistry, Molecular Biology, and Biophysics

2009/79 and CB 2009-33
Systematic Comparison of the Human Saliva and Plasma Proteomes

Chemical Engineering and Materials Science

2009/78 and CB 2009-32
Multi-scale Crystal Growth Computations via an Approximate Block Newton Method
A. Yeckel, L. Lun, and J. J. Derby

2009/81
Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals

2009/82
Parameters Influencing Diffusion Dynamics of an Adsorbed Polymer Chain
N. Hoda and S. Kumar

Computer Science and Engineering

2009/86
Curvature Effects on Optical Response of Si Nanocrystals in SiO2 Having Interface Silicon Suboxides
P. Carrier

Mechanical Engineering

2009/80
Dislocation Onset and Nearly Axial Glide in Carbon Nanotubes Under Torsion
D.-B. Zhang, R. D. James, and T. Dumitrica

Microbiology

2009/83 and CB 2009-34
Evidence of a Role for Monocytes in Dissemination and Brain Invasion by Cryptococcus neoformans
C. Charlier, K. Nielsen, S. Daou, M. Brigitte, F. Chretien, and F. Dromer

Physics

2009/84
Emergence of Triplet Correlations in Superconductor/Half Metallic Nanojunctions With Spin Active Interfaces
K. Halterman and O. T. Valls

2009/85
The Phase Diagram of Vortex Matter in Layered Superconductors With Tilted Columnnar Pinning Centers
C. Dasgupta and O. T. Valls

Surgery

2009/77 and CB 2009-31
Creating a Technology Hybrid for Efficient Data Management and Analysis In Pre-Clinical and Clinical Research
P. Tokachichu, G. J. Beilman, J. G. Chipman, and S. T. Parente

Names of Supercomputing Institute principal investigators appear in bold type. This list contains reports entered into the reports database during August–November 2009.
For more information on the University of Minnesota Supercomputing Institute, please visit the Supercomputing Institute’s website:

www.msi.umn.edu

This information is available in alternative formats upon request by individuals with disabilities. Please send email to alt-format@msi.umn.edu or call 612-624-0528.

Editor/photographer: Tracey A. Bartlett

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