

UNIVERSITY OF MINNESOTA

Institute of Technology

Supercomputing Institute

for Digital Simulation and Advanced Computation

Programs, resources, and user support
2006–07

For more information, see:

www.msi.umn.edu

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Table of contents

Supercomputing Resource Allocations on Core Computing Machines	1
Basic Sciences Computing Laboratory.....	4
Computational Genetics Laboratory.....	6
Digital Technology Computational Biology Laboratory	8
Medicinal Chemistry-Supercomputing Institute Visualization/Workstation Laboratory.....	10
Scientific Data Management Laboratory.....	11
Scientific Development and Visualization Laboratory.....	13
Supercomputing Institute User Support.....	15
Research Scholarship Program.....	16
Travel Awards Program.....	17
Undergraduate Internship Program	18

Supercomputing Resource Allocations on Core Computing Machines

Overview

The Supercomputing Institute offers computer time, software, and technical support on core machines. Each core machine has a large number of fast processors, considerable disk space, and fast input/output. All Institute core machines can be used for serial and parallel codes written in C, C++, FORTRAN 77, and FORTRAN 90. For parallel codes, MPI and the easier-to-use OPENMP are available on all Institute core machines. However, OPENMP is limited to the number of processors on an individual node. The Institute provides numerous commercial and public domain software packages.

To determine the system that is best for your use, please contact the Institute's user support staff by sending email to help@msi.umn.edu or calling (612) 626-0802. You may also contact Dr. H. Birali Runesha, the Institute's User Support Manager, at (612) 624-8857 or runesha@msi.umn.edu.

Description

The Supercomputing Institute currently provides supercomputing resource allocations and technical support for the IBM BladeCenter H LINUX Cluster, IBM Power4, IBM Netfinity LINUX Cluster, SGI Altix, and Unisys ES7000.

The IBM BladeCenter H LINUX Cluster is a new resource available starting in September 2006. It has AMD Opteron processors and is used primarily for parallel jobs. Complete information about the BladeCenter can be found at:

www.msi.umn.edu/bladecenter/index.html

The IBM Power4 system is a constellation of several shared-memory nodes. Users submit to a single queue on an interactive node, and a fair-share scheduling system schedules each job on an appropriate available node; users may also request a particular node or nodes. The operating system is AIX, IBM's brand of UNIX. The nodes are either pSeries 690+ nodes (called Regatta nodes) or pSeries 655+ nodes. All nodes are connected to an IBM High Performance Switch (HPS) network. Complete information can be found at:

www.msi.umn.edu/power4/index.html

The Netfinity LINUX Cluster consists of compute nodes, an interactive node, and file server nodes. The compute nodes have Intel Pentium 4 or Pentium III processors. The nodes are connected together using Gigabit Ethernet, Fast Ethernet, and Myrinet. Complete information can be found at:

www.msi.umn.edu/netfinity/index.html

The SGI Altix Cluster consists of 11 shared-memory machines running the LINUX operating system. Complete information can be found at:

www.msi.umn.edu/altix/

The Unisys ES7000 has Intel Itanium processors and runs the Red Hat Enterprise LINUX operating system. The machine provides both interactive and batch resources. Complete information can be found at:

www.msi.umn.edu/es7000/index.html

Currently, one service unit (SU) will provide a fixed number of hours of CPU time on each platform as follows:

IBM BladeCenter H* LINUX Cluster	3.5
IBM Power4	3.5
Netfinity LINUX Cluster	12
SGI Altix	3.5
Unisys ES7000	40

A disk service unit (DSU) will be charged when a group's usage has exceeded 500 GB of disk usage on a system for more than an hour. There will not be a charge for disk usage on scratch spaces. DSUs will be charged per the rates on our Web site:

www.msi.umn.edu/general/Programs/Descriptions/resources.html

There is no service unit charge for software usage, technical support, or for other laboratory resources.

Eligibility

Allocations are available to faculty members at the University of Minnesota and other faculty researchers at accredited institutions of higher education in the state of Minnesota for their work and that of their students and research groups. All proposals requesting an allocation must be sponsored and signed by a faculty member of the University of Minnesota or other accredited institution of post-secondary education in the state of Minnesota. Information on requesting Supercomputing Institute resources can be found at:

www.msi.umn.edu/general/Programs/obtain/resources.html

Review procedures

Supercomputing resource allocations are awarded based upon a competitive review by the Supercomputing Resources Peer Review Panel. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu. In addition, the criteria are stated on the allocation request form.

Deadlines

Deadlines for submitting a proposal requesting an allocation are October 15, 2006 for the January 1 to June 30, 2007 period and April 15, 2007 for the July 1 to December 31, 2007 period. Proposals submitted subsequent to the deadlines are accepted, but have a lower priority.

Technical information and user support

Technical user support information including lists of available software for the IBM and SGI supercomputers can be found at:

www.msi.umn.edu/user_support/

In addition, you may obtain technical information and user support by contacting the Supercomputing Institute User Support Staff by phone at (612) 626-0802, via email at help@msi.umn.edu, or at:

www.msi.umn.edu/consult.html

Requesting resources and adding new users

Information pertaining to the use of the Supercomputing Institute's resources to start a research project, add new users to already existing projects, and comply with reporting requirements for those participating in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/resources.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Basic Sciences Computing Laboratory

Description

The Basic Sciences Computing Laboratory (BSCL) is in room 1-280 of Nils Hasselmo Hall located at the corner of Church Street S.E. and Washington Avenue on the East Bank of the University of Minnesota Twin Cities campus. This laboratory provides researchers with access to a unique mixture of computational servers, workstations, visualization tools, software, and technical support.

Detailed information about hardware available at the BSCL can be found at:

www.msi.umn.edu/bscl/hardware

A list of software resources available at the BSCL can be found at:

www.msi.umn.edu/bscl/software

Eligibility

Access to these resources is available to all faculty members of the University of Minnesota for their own use and that of their research groups.

Review procedures

Requests for access to or priority use of the Basic Sciences Computing Laboratory resources are peer reviewed by the Basic Sciences Computing Laboratory Steering Committee. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

To expedite supercomputing research, there is no deadline for submission of laboratory access requests at this time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Basic Sciences Computing Laboratory is available at:

www.msi.umn.edu/bscl/

In addition, you may obtain technical user support or additional technical information by contacting the laboratory's manager, Dr. Benjamin Lynch, at (612) 624-4122 or blynch@msi.umn.edu.

Requesting resources and adding new users

Information regarding obtaining access to the Basic Sciences Computing Laboratory, adding new users to existing projects, and complying with reporting requirements for participants in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/bscl.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Computational Genetics Laboratory

Description

The Computational Genetics Laboratory (CGL) is an initiative created in conjunction with the Microbial and Plant Genomics Institute and the Biomedical Genomics Center. The home of the laboratory is in St. Paul, in Room 138 of the Cargill Microbial and Plant Genomics Building. In addition, the laboratory has a secondary home in Nils Hasselmo Hall. The laboratory is designed to meet the emerging computational needs of the computational biology community, especially in the areas of bioinformatics, computational genomics/genetics, and proteomics.

For more information on the CGL, see:

www.msi.umn.edu/cgl/

Eligibility

Registration for use of the laboratory's resources is available to all faculty members of the University of Minnesota for their own use and that of their research groups.

Review procedures

The Computational Genetics Laboratory resources are prioritized by the Computational Genetics Laboratory Steering Committee. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

To expedite supercomputing research, access requests are accepted at any time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Computational Genetics Laboratory can be found at:

www.msi.umn.edu/cgl/

In addition, you may obtain technical user support or additional technical information by contacting any of the following persons:

Dr. Zheng Jin Tu, Computational Genetics Laboratory Manager and Computational Biology Consultant, (612) 624-9504, ztu@msi.umn.edu

Dr. Wayne Xu, Computational Genomics Consultant, (612) 624-1447, wxu@msi.umn.edu

Ms. Wen Dong, Web Interface Programmer, (612) 624-0969, wdong@msi.umn.edu

Requesting resources or technical support and adding new users

Information regarding becoming a registered researcher in the Computational Genetics Laboratory, adding new users to existing projects, and complying with reporting requirements for participants in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/cgl.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Related Web sites

For more information on computational biology and genomics at the Supercomputing Institute, see:

www.msi.umn.edu/user_support/compgen/

See also the one-stop portal for computational biology and bioinformatics at the University of Minnesota:

www.compbio.umn.edu/

A list of research reports in computational biology may be found at:

<http://www.msi.umn.edu/cb>

Digital Technology Computational Biology Laboratory

Description

The Digital Technology Computational Biology Laboratory provides computing resources to faculty members involved in computational biology at the University of Minnesota. While computational biology faculty have full access to all Institute resources, this laboratory is dedicated to computational biology in a way that allows special and focused stimulation of interdisciplinary and interdepartmental digital technology collaborations among University of Minnesota faculty and their research groups. The goal of the laboratory is to encourage collaboration and high-performance computing research within the computational biology community at the University of Minnesota.

Currently the laboratory is equipped with an 8-processor Compaq ES40. The processor speed is 500 MHz with 8 GB of memory.

Eligibility

Access to these resources is available to all faculty members of the University of Minnesota for their own use and that of their research groups on projects involving computational biology.

Review procedures

Requests for access to the Digital Technology Computational Biology Laboratory resources are peer reviewed by the Digital Technology Computational Biology Laboratory Steering Committee. Priority will be given to projects that promote initiatives in computational biology, especially interdisciplinary and interdepartmental activities. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

Deadlines

To expedite supercomputing research, there is no deadline for submission of laboratory access requests at this time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Digital Technology Computational Biology Laboratory is available at:

www.msi.umn.edu/cbl/

You may contact the user support staff by clicking on the help request form, by sending email to help@msi.umn.edu, or by calling (612) 626-0802 (8:30 a.m.–5:00 p.m. Monday through Friday). You may also use these mechanisms to report problems with the systems.

Requesting resources or technical information and adding new users

Information regarding becoming a registered researcher in the Digital Technology Computational Biology Laboratory, adding new users to existing projects, and complying with reporting requirements for participants in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/cbl.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Medicinal Chemistry-Supercomputing Institute Visualization/Workstation Laboratory

Description

The Medicinal Chemistry/Supercomputing Institute Visualization-Workstation Laboratory is in room 7-123 of Weaver-Densford Hall located at the corner of Washington Avenue and Harvard Street S.E. on the East Bank of the University of Minnesota Twin Cities campus. This laboratory provides University researchers with access to workstations, software, and technical support for scientific computation and visualization.

Eligibility

Access to these resources is available to all faculty members of the University of Minnesota for their own use and that of their research groups.

Review procedures

Requests for access to or priority use of the laboratory's resources are peer reviewed by the laboratory's steering committee. The review criteria for this program are at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

To expedite supercomputing research, there is no deadline for submission of laboratory access requests at this time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Visualization-Workstation Laboratory are available at:

www.msi.umn.edu/vwl/

In addition, you may obtain technical user support or additional technical information by contacting the laboratory's manager, Dr. Yuk Sham, at (612) 624-0783 or by sending email to shamy@msi.umn.edu.

Requesting resources and adding new users

Information regarding obtaining access to the Visualization-Workstation Laboratory, adding new users to existing projects, and complying with reporting requirements for participants in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/vwl.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Scientific Data Management Laboratory

Description

The Scientific Data Management Laboratory (SDML) is designed to meet the evolving data-management demands of University faculty and researchers. The SDML provides access to software, computational, and storage resources necessary to develop and support high profile research-related data applications. This centralized data/database infrastructure is available for all applicable research projects.

The SDML currently houses a database server, a computing server, a Web server, an interactive login server for database and Web interface development, and about 20 TB of disk space. The available hardware will continue to evolve with demand.

The SDML provides users access to a variety of database management systems including MySQL, ORACLE, and DB2. Other database management systems and related software can be installed upon request, dependent on availability.

For more information on the DSML: see:

www.msi.umn.edu/sdml/

Eligibility

Access to these resources is available to all faculty members of the University of Minnesota for their own use and that of their research groups.

Review procedures

Requests for access to the SDML's resources are peer reviewed by the laboratory's steering committee. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

To expedite supercomputing research, there is no deadline for submission of laboratory access requests at this time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Scientific Data Management Laboratory are available at:

www.msi.umn.edu/sdml/

In addition, you may obtain technical user support or additional technical information by contacting the laboratory's manager, Dr. Zheng Jin Tu, at (612) 624-9504 or

ztu@msi.umn.edu, or by contacting the Manager of User Support, Dr. H. Biralı Runesha, at (612) 624-8857 or runesha@msi.umn.edu.

Requesting resources and adding new users

Information regarding obtaining access to the Scientific Data Management Laboratory, adding new users to existing projects, and complying with reporting requirements for participants in the Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/sdml.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Scientific Development and Visualization Laboratory

Description

The Supercomputing Institute Scientific Development and Visualization Laboratory is located on the fifth floor of Walter adjacent to the Institute's systems and user support staff. It provides Institute researchers with access to SGI, Sun, and LINUX workstations, an 8-processor system with PQS nodes known as QuantumCube, Macintosh workstations, PCs, a three-dimensional LCD panel for autostereo display, hardware and software for the production of short videos, and associated software and technical support.

Eligibility

Access to these resources is available to faculty members of the University of Minnesota or other accredited institutions of post-secondary education in the state of Minnesota for their own use and that of their research groups.

Review procedures

Access is provided upon request to all researchers who apply for and receive competitively reviewed Supercomputing Institute supercomputer resource allocations on core machines. Laboratory access is also available by separate proposal. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

To expedite supercomputing research, there is no deadline for submission of laboratory access requests at this time. For continuing projects, a new or updated abstract and user group list are required every six months.

Technical information and user support

Technical and user support information regarding the Scientific Development and Visualization Laboratory can be found at:

www.msi.umn.edu/sdvl/

In addition, you may obtain technical user support or additional technical information by contacting the laboratory's manager, Ms. Seema Jaisinghani, at (612) 626-3541 or via email at seemaj@msi.umn.edu.

Requesting resources and adding new users

Information regarding establishing a research project with access to the Scientific Development and Visualization Laboratory, adding new users to existing projects, and

complying with reporting requirements for participants in Supercomputing Institute research programs is available at:

www.msi.umn.edu/general/Programs/obtain/sdvl.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Supercomputing Institute User Support

Description

The user support staff provides assistance with all aspects of scientific computing, data mining, informatics, and visualization. This assistance includes—but is not limited to—general user support, writing and porting serial and parallel codes to the supercomputers, development of scripts or user-friendly procedures to allow more productive use of the supercomputing resources, assistance with visualization or communications, assistance with software packages, tutorials on specialized topics or programs, user training, code optimization, parallel model building support, and assistance with workstations used to develop code for the supercomputers.

Each member of the user support staff can provide technical assistance in their area of expertise. The areas of expertise include 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.

Eligibility

The Supercomputing Institute provides user support to University researchers utilizing its computing and visualization resources, both hardware and software.

Contacting the user support group

User Support may be contacted by phone at (612) 626-0802, via email at help@msi.umn.edu, or at:

www.msi.umn.edu/consult.html

Please feel free to contact Dr. H. Birali Runesha, the Institute's Manager of User Support, at (612) 624-8857 or runesha@msi.umn.edu regarding any questions or suggestions you may have about user support or requests to arrange for assistance.

Research Scholarship Program

Description

The Supercomputing Institute provides grants for research scholarships for supercomputing research at the University of Minnesota. The upper limit on research scholarship grants is \$23,000 (including fringe benefits), with a required match of no less than 1:1 from non-state funds.

Eligibility

Nominations for research scholarships must be made by a University of Minnesota faculty member.

Review procedures

The Research Scholarship Peer Review Panel makes research scholarship awards based upon a competitive review of faculty-initiated nominations. Nominees for research scholarships are expected to hold the Ph.D. degree and usually are considered potential postdoctoral research associates. More senior visitors may also be nominated. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu. In addition, they are stated in the call for nominations.

Deadlines

The deadline for submitting a nomination is January 15 for scholarships in the following fiscal year (July 1 to June 30). Late nominations cannot be accepted.

Nomination forms

Research Scholarship Program nominating forms are available at:

www.msi.umn.edu/general/Programs/Forms/

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Travel Awards Program

Description

The Supercomputing Institute provides travel awards for the following types of travel: (i) travel by a University of Minnesota researcher to present supercomputing research results at a conference; (ii) travel by a University of Minnesota faculty member to seek external support for supercomputing research; and (iii) short-term visits of research collaborators or visiting research scholars to the University of Minnesota in order to perform collaborative supercomputing research with one or more university faculty members or in order to plan collaborative grant proposals. The upper limit on travel awards is \$2,000. Requests less than \$1,000 have the highest priority. A match of no less than 1:1 from non-state funds is required.

Eligibility

Faculty members of the University of Minnesota may apply for travel awards for their own use or that of their research groups and collaborators.

Review procedures

Travel awards are granted on the basis of competitive review. The review criteria for this program are available at:

www.msi.umn.edu/general/Programs/review.html

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Deadlines

The deadline is three months before the proposed travel. Earlier submission is encouraged when possible to facilitate planning. Late proposals may be considered, but as a lower priority.

Request form

The request form for the Travel Awards Program is available at:

www.msi.umn.edu/general/Programs/Forms/

or from Jane Zirbes, Research Programs Administrator, at (612) 625-0012 or zirbes@msi.umn.edu.

Undergraduate Internship Program

Description

The Supercomputing Institute for Digital Simulation and Advanced Computation conducts an internship program for undergraduates for 10 weeks every summer.

The focus of the program is the application of computational approaches and visualization methods to supercomputing research. This includes digital simulation and advanced computation and all aspects of high-performance computing and scientific modeling and simulation as well as graphics, visualization, informatics, and high-performance network communications.

Interns work with faculty members and their research groups on projects from a wide variety of disciplines. This research involves the use of high-performance computing environments to address problems in science and engineering that could not otherwise be attempted. This program provides an opportunity for a challenging and enriching educational experience for undergraduate students interested in pursuing graduate or professional education.

Eligibility—faculty

Faculty members at the University of Minnesota who are principal investigators of the Supercomputing Institute are encouraged to submit undergraduate internship projects. Projects should have a clear relation to some aspect of high-performance computing and/or visualization.

Eligibility—students

A recipient of an internship must be an undergraduate at the time the internship is held and must be a citizen or permanent resident of the United States or its possessions. Undergraduates from colleges and universities nationwide are eligible to apply.

Project submission by faculty

University of Minnesota faculty members interested in supervising an undergraduate internship project should contact Tracey Bartlett, the program's coordinator, at (612) 624-2330 or bartlett@msi.umn.edu. All Supercomputing Institute Principal Investigators are invited to submit potential projects.

Program details and application information for undergraduate students

More information regarding the Undergraduate Internship Program is available at:

www.msi.umn.edu/general/Programs/uip/

or by contacting Tracey Bartlett, the Undergraduate Internship Program Coordinator at uip@msi.umn.edu or (612) 624-2330.