Minnesota Supercomputing Institute
Introduction to MSI for Physical Scientists

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Goals

- Introduction to MSI resources
- Show you how to access our systems
- Highlight resources of particular use to physical scientists
- Point you to where to go for help
- Ensure that you are not overwhelmed
- Encourage you to ask questions of MSI staff to get what you need
MSI At a Glance

- Operates 3 large and several smaller/experimental HPC (High Performance Computing) systems
- Manages approximately 400 software packages and 50 research databases.
- Main data center in Walter Library.
- MSI operates five laboratories on campus, open to all MSI users.

- Serves more than 500 PI groups with 3000+ users.
- MSI is an academic unit of the University of Minnesota (under OVPR) with about 45 full time employees.
- Dedicated resources for serial workflows, database management, and cloud access.
MSI Resources

HPC Resources
- Koronis
- Itasca
- Calhoun
- Cascade
- GPUT

Laboratories
- BMSDL
- BSCL
- CGL
- SDVL
- LMVL

Software
- Chemical and Physical Sciences
- Engineering
- Graphics and Visualization
- Life Sciences
- Development Tools

User Services
- Consulting
- Tutorials
- Code Porting
- Parallelization
- Visualization

University of Minnesota

Minnesota Supercomputing Institute
The Machines at MSI
HPC Resources

Koronis: SGI Altix
1140 Intel Nehalem Cores
2.96 TB of memory

Itasca: Hewlett-Packard 3000BL
9480 Intel Nehalem Cores
31.3 TB of memory

Calhoun: SGI Altix XE 1300
1440 Intel Xeon Clovertown Cores
2.8 TB of memory

Heterogeneous Computing
Cascade:
8 Dell Compute Nodes  8 Kepler Nodes
32 Nvidia M2070 GPGPUs  2 Phi Nodes

GPUT:
16 Nvidia GeForce GTX 480 GPUs
Machine Type: Cluster

Machine Type: Cluster

• Clusters at MSI
  - Itasca
    - 1,091 HP ProLiant blade servers, each with two quad-core 2.8 GHz Intel Xeon X5560 "Nehalem EP" processors sharing 24 GiB of system memory. 40-gigabit QDR InfiniBand (IB) interconnect. In total, Itasca consists of 8,728 compute cores and 24 TiB of main memory.
    - itasca.msi.umn.edu
  - Calhoun
    - SGI Altix XE 1300 cluster with 180 compute nodes, each with 16 GB of memory. The nodes are interconnected with a 20-gigabit DDR InfiniBand (IB) network.
    - calhoun.msi.umn.edu
Machine Type: Heterogeneous

Source: http://electronicdesign.com/digital-ics/gpu-architecture-improves-embedded-application-support
Machine Type: Heterogeneous

- **Cascade**
  - 32 M2070 Telsa GPUs (4 per node, 8 nodes), 8 K20 Kepler GPUs (2 per node, 4 nodes), 2 Xeon Phi co-processors (1 per node, 2 nodes)
  - cascade.msi.umn.edu
Machine Types: Programming Complexity

General View:

Simplest: Shared Memory (OpenMP)
Medium: Cluster (MPI)
Complex: Heterogeneous (CUDA, special statements)
Laboratories

Scientific Development and Visualization
- Application development
- Computational Physics
- Workshops

Basic Sciences Computing
- Structural Biology
- Batch processing
- Stereo Projection system

Computational Genetics
- Bioinformatics
- Genomics
- Proteomics

Biomedical Modeling, Simulation, and Design
- Drug Design
- Molecular Modeling
- Computational chemistry

LCSE-MSI Visualization
- Virtual reality
- Large screen
- Remote visualization
MSI Labs and Lab Servers

https://www.msi.umn.edu/labs

- Labs at 5 locations
  - Labs machines use the MSI software environment
  - Special high definition and 3D visualization equipment
- Labs Servers for small jobs
  - lab.msi.umn.edu
  - Many software packages.
  - Some special hardware such as liquid cooled overclocked nodes.
Interacting with MSI Systems
Connecting to MSI

https://www.msi.umn.edu/remote-access

• SSH is usually the best choice
  • ssh -X <username>@login.msi.umn.edu
  • ssh -X itasca
  • Windows SSH options include PuTTY and Cygwin

• Remote desktop options include NX and VNC client
  • See above page for details

• Most systems require you to connect first to:
  login.msi.umn.edu
MSI Computing Environment

https://www.msi.umn.edu/resources/computing-environment

• MSI systems are mostly Linux compute clusters running CentOS
• Software is managed via a system of environment modules
• Jobs are run via a batch scheduling system
High Performance Primary Storage

Home directories are unified across all Linux systems (except for Koronis).

Each group has a disk quota which can be viewed with the command: `groupquota`

Panasas ActivStor 14: 1.28PB storage, capable of 30 GB/sec read/write, and 270,000 IOPS
Software Management

Software is managed via a module system

- `module load modulename` loads a software module
- `module show modulename` shows the actions of a module
- `module avail` shows all available modules
- `module list` shows a list of currently loaded modules
- `module unload modulename` unloads a software module
- `module purge` unloads all software modules
Job Scheduling

Jobs are scheduled using the Portable Batch System (PBS) queueing system.

To schedule a job first make a PBS job script:

```bash
#!/bin/bash -l
#PBS -l walltime=8:00:00,nodes=3:ppn=8,pmem=1000mb
#PBS -m abe
#PBS -M sample_email@umn.edu

cd ~/program_directory
module load intel
module load ompi/intel
mpirun -np 24 program_name < inputfile > outputfile
```

https://www.msi.umn.edu/resources/job-submission-and-scheduling-pbs-scripts
https://www.msi.umn.edu/resources/job-queues
Interactive Jobs

Nodes may be requested for interactive use using the command:

```
qsub -I -l walltime=1:00:00,nodes=1:ppn=8
```

The job waits in the queue like all jobs, and when it begins the terminal returns control.
Jobs on the high performance computing (HPC) systems consume Service Units (SUs), which roughly correspond to processor time.

Each research group is given a service unit allocation at the beginning of the year. To view the number of service units remaining use the command: acctinfo

If a group is using service units faster than the "fairshare target", then the group's jobs will have lower queue priority. [https://www.msi.umn.edu/hpc/fairshare](https://www.msi.umn.edu/hpc/fairshare)
Important Software
Problem Solving

MSI has resources available to help solve job problems.

https://www.msi.umn.edu/services/user-support

https://www.msi.umn.edu/resources/job-problem-solving

https://www.msi.umn.edu/support/faq

https://www.msi.umn.edu/resources/debugging

Help can be requested by emailing: help@msi.umn.edu