

# SHARCNET Literacy: *User / Introduction*

## *Supercomputing Environment at Your Institution and Beyond*

Via AccessGrid, April 23, 2007

### Agenda

- What is SHARCNET
- Where to find Information
- SHARCNET essentials
- Support
- Parallel Computation using MPI
- Parallel and Concurrent Computation using OpenMP

SHARCNET Weekly Online Seminar  
The University of Western Ontario, April 23, 2007



*The largest HPC facility in Canada.*

*It enables computational tasks  
that otherwise impossible or not  
feasible...*

*You can access up to over 8,000  
processors/cores across southwest  
Ontario and work together as if they  
were next to each other...*

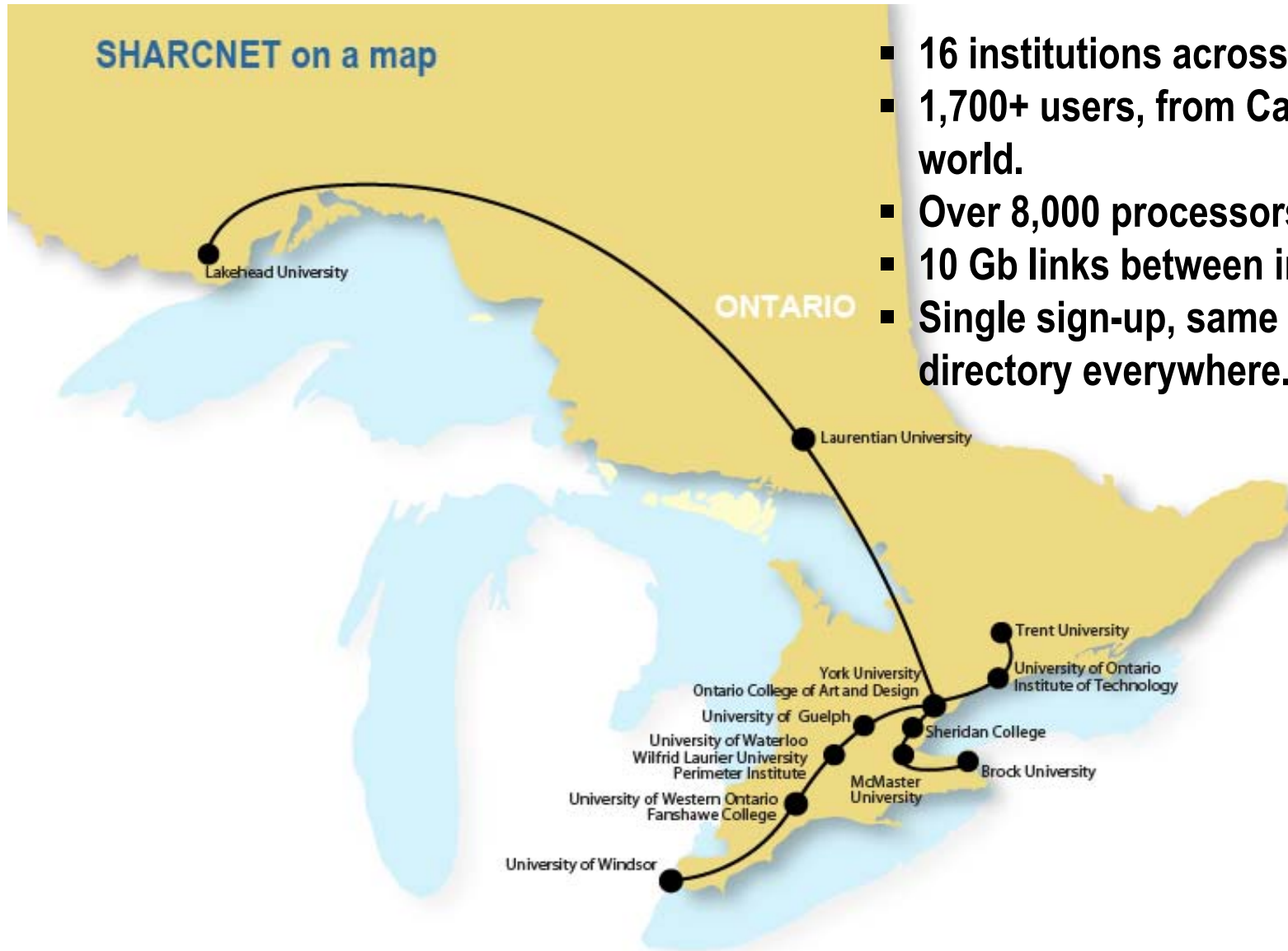
*SHARCNET also enables face to face  
collaboration via AccessGrid over the  
10 Gb high speed network.*

# What is SHARCNET

- A consortium
- A cluster of clusters of high performance, networked supercomputer systems
- Visions and missions



# SHARCNET Is A Supercomputing Consortium...



- 16 institutions across Ontario.
- 1,700+ users, from Canada and world.
- Over 8,000 processors.
- 10 Gb links between institutions.
- Single sign-up, same home directory everywhere.

# Vision, Mission and Goals

## ■ The SHARCNET Vision

- *To become a world leading, academic high-performance computing consortium enabling forefront research and innovation.*

## ■ The SHARCNET Mission

- *To promote and facilitate the use of high performance computational techniques among researchers in all fields and to create a new generation of computationally-aware individuals.*

## ■ General Goals

- provision of otherwise unattainable compute resources
- reduce time to science
- remote collaboration

# Founding Members, Partners since 2001

## Founding members (2001.06)

- The University of Western Ontario
- University of Guelph
- McMaster University
- Wilfrid Laurier University
- University of Windsor
- Fanshawe College
- Sheridan College

## New Partners (2005.12)

- Trent University
- Laurentian University
- Lakehead University

## New Partners (2006.03)

- Ontario College of Art and Design
- Perimeter Institute for Theoretical Physics

## New Partners (2003.06)

- University of Waterloo
- Brock University
- University of Ontario Institute of Technology
- York University

## Affiliated Partners

- Robarts Research Institute
- Fields Institute for Mathematical Sciences



# Industry and Government Partners

## ■ Industry

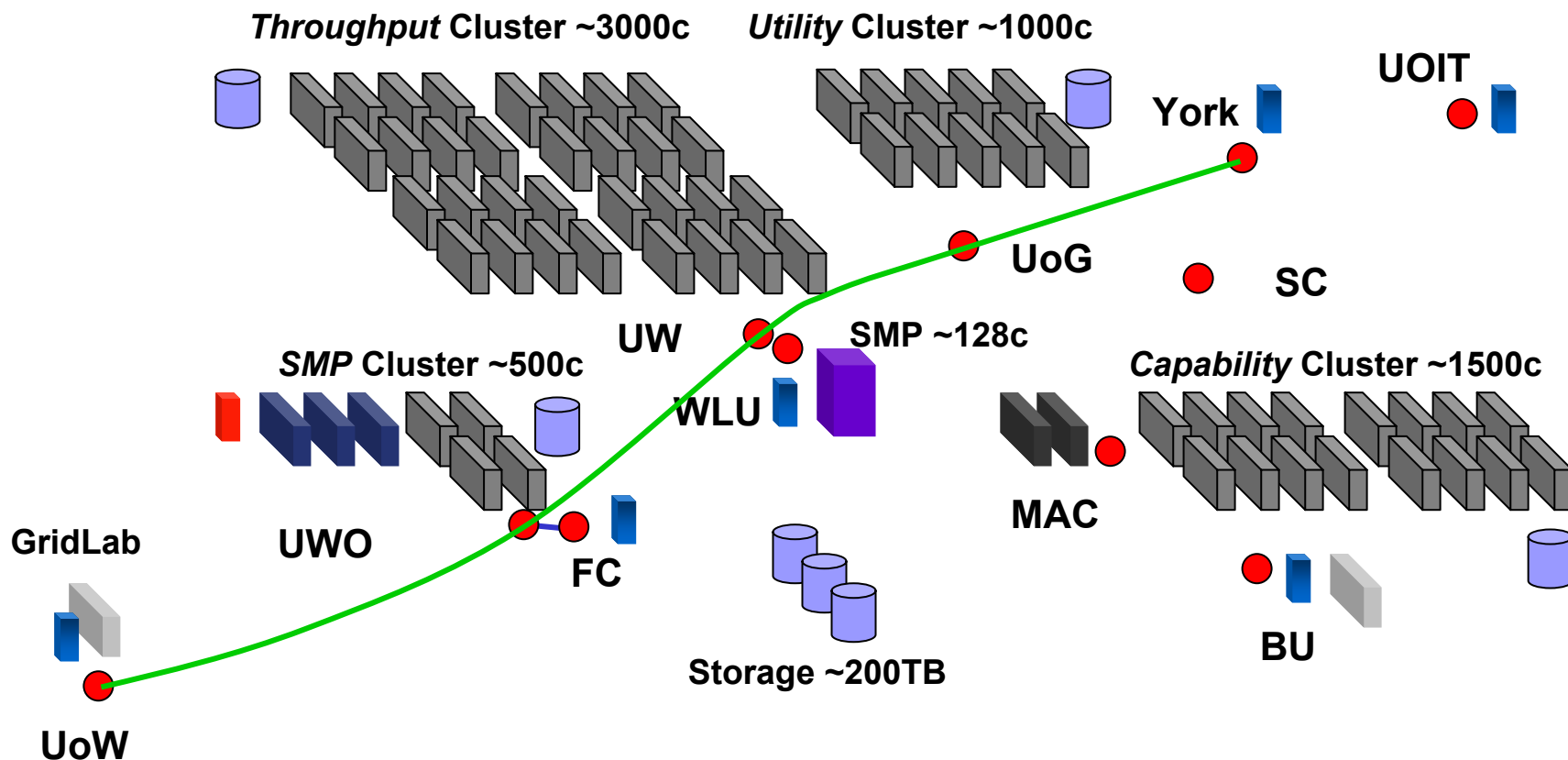
- Hewlett Packard
- SGI
- Quadrics Supercomputing World
- Platform Computing
- Nortel Networks
- Bell Canada

## ■ Government

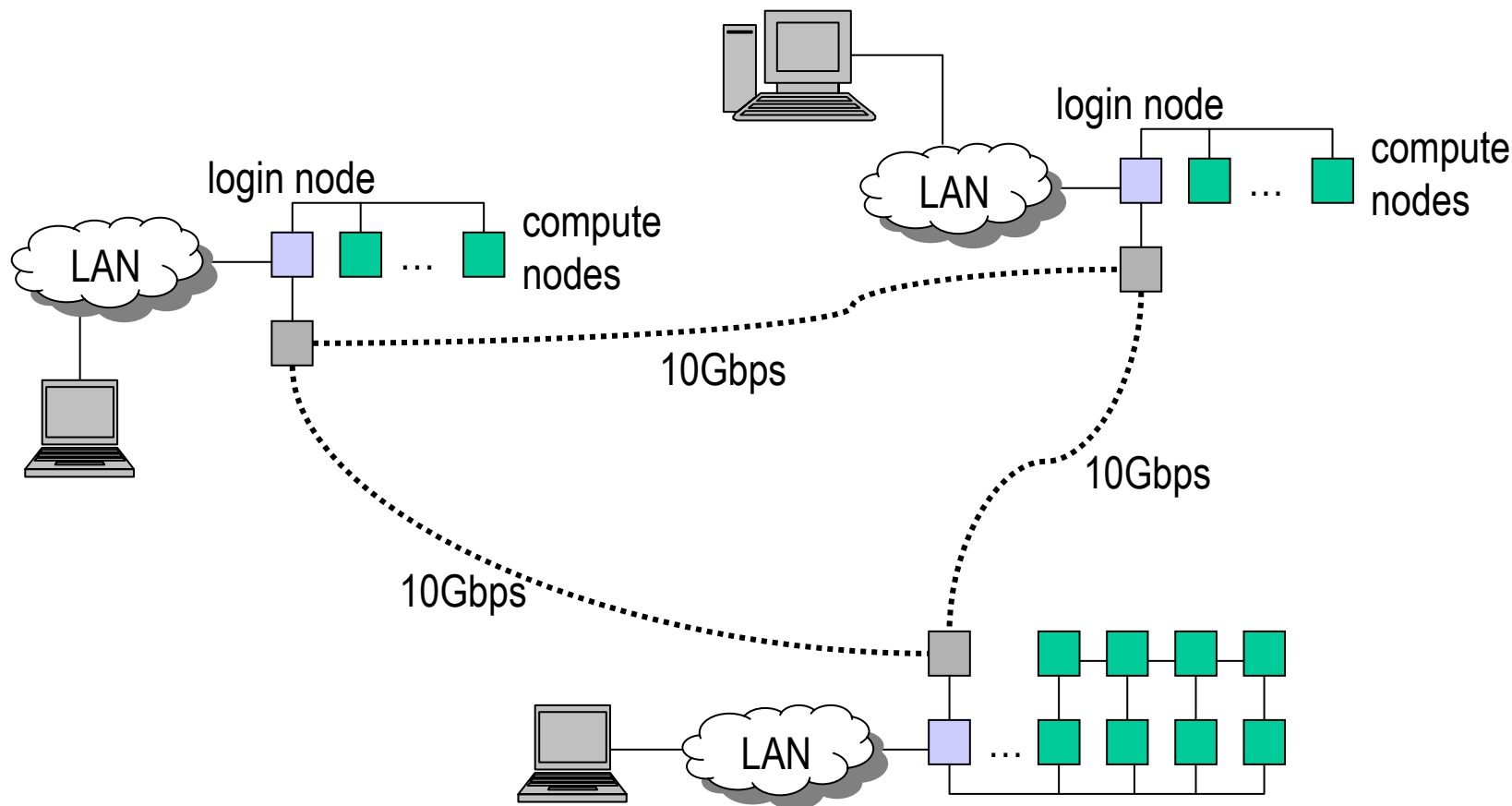
- Canada Foundation for Innovation
- Ontario Innovation Trust
- Ontario R&D Challenge Fund
- Optical Regional Advanced Network of Ontario (ORANO)

# Resources at A Glance

- Over 8,000 processors deployed on 11 sites since 2005.



# Cluster of Clusters



# SHARCNET Facilities

## ■ Computers

- Clusters (**distributed memory**): for parallel and serial programs
  - Super fast interconnect
  - Fast interconnect
  - Fast interconnect and SMP nodes
  - Serial farm
- Symmetric multiprocessing (SMP) systems (**shared memory**): for parallel, threaded applications.

## ■ Visualization Clusters

- Being deployed at some institutions.

## ■ Access Grid Rooms (Multi-media)

- Video conference, cross site workshops, etc.

# SHARCNET Basics

- **FREE to academic researchers**
  
- **Compute-Intensive Problems**
  - The resources are provided to enable HPC and are not intended as a replacement for a researcher's desktop or lab machines.
  - SHARCNET users can productively conduct HPC research on a variety of SHARCNET systems each optimally designed for specific HPC tasks
  
- **Academic HPC research**
  - The research can be business-related, but must be done in collaboration with an academic researcher
  
- **Fairness access**
  - Users have access to all systems
  - Clusters are designed for certain type of jobs
  - Job runs in batch mode (scheduling system) with fairshare

# Online Resource Discovery


SHARCNET: Facilities - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://www.sharcnet.ca/Facilities/index.php

Customize Links Free Hotmail Windows Marketplace Windows Media Windows

Shared Hierarchical Academic Research Computing Network

 SHARCNET™

Facilities > Systems Login by: jemmyhu

**Main Menu**

- Home
- About
- Research
- Facilities
  - Systems
  - Network
  - Statistics
  - Contributions
  - Software
  - Policies
  - Photo Gallery
  - Performance
- Help
- FAQs
- Contact
- Media
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**Personal**

- My Login Page
- Submit Problems
- View Problems
- My Account
- My Profile
- My Projects
- My Publications
- My Mailing Lists

**Features**

- What's New
- Documents
- SHARCwiki

**SHARCNET Facilities at a Glance**

System	State	CPUs	Architecture	Nodes	Notices
<a href="#">bala</a>	Online	128	Cluster/Myrinet G2	Opteron	<a href="#">Aug 25 2006</a>
<a href="#">bruce</a>	Online	128	Cluster/Myrinet G2	Opteron	<a href="#">Aug 24 2006</a>
<a href="#">bull</a>	Online	384	Cluster/Quadrics Elan4	Opteron	<a href="#">Aug 04 2006</a>
<a href="#">cat</a>	Online	160	Cluster/Gigabit Ethernet	Xeon, Opteron	<a href="#">Jun 14 2006</a>
<a href="#">coral</a>	Offline	60	Cluster/Quadrics (Elan 3)	Itanium2	<a href="#">Jun 13 2005</a>
<a href="#">dolphin</a>	Online	128	Cluster/Myrinet G2	Opteron	<a href="#">Sep 08 2006</a>
<a href="#">goblin</a>	Online	54	Cluster/Gigabit Ethernet	Opteron	<a href="#">Jul 31 2006</a>
<a href="#">greatwhite</a>	Online	456	Cluster/Quadrics (Elan 3), Gigabit Ethernet	Alpha	<a href="#">Sep 07 2006</a>
<a href="#">gulper</a>	Offline	44	Cluster/Myrinet	Opteron	<a href="#">Jul 27 2006</a>
<a href="#">mako</a>	Testing	14	Cluster/Myrinet, Gigabit Ethernet	Xeon	<a href="#">Aug 30 2006</a>
<a href="#">megaladon</a>	Online	128	Cluster/Myrinet G2	Opteron	<a href="#">Sep 06 2006</a>
<a href="#">narwhal</a>	Online	1068	Cluster/Myrinet	Opteron	<a href="#">Aug 30 2006</a>
<a href="#">requin</a>	Online	1536	Cluster/Quadrics Elan4	Opteron	<a href="#">Sep 06 2006</a>
<a href="#">silky</a>	Online	128	SMP/NUMA	Itanium2	<a href="#">Aug 04 2006</a>
<a href="#">spinner</a>	Offline	70	Cluster/Gigabit Ethernet	Itanium2	<a href="#">Aug 22 2006</a>
<a href="#">tiger</a>	Offline	128	Cluster/Myrinet G2	Opteron	<a href="#">Jul 25 2006</a>
<a href="#">typhon</a>	Offline	16	SMP/SMP	Alpha	<a href="#">Feb 09 2006</a>
<a href="#">whale</a>	Online	3072	Cluster/Gigabit Ethernet	Opteron	<a href="#">Sep 11 2006</a>
<a href="#">wobbe</a>	Online	208	Cluster/Myrinet, Gigabit Ethernet	Opteron	<a href="#">Jun 14 2006</a>
<a href="#">zebra</a>	Online	128	Cluster/Myrinet G2	Opteron	<a href="#">Sep 05 2006</a>
Totals		8038			

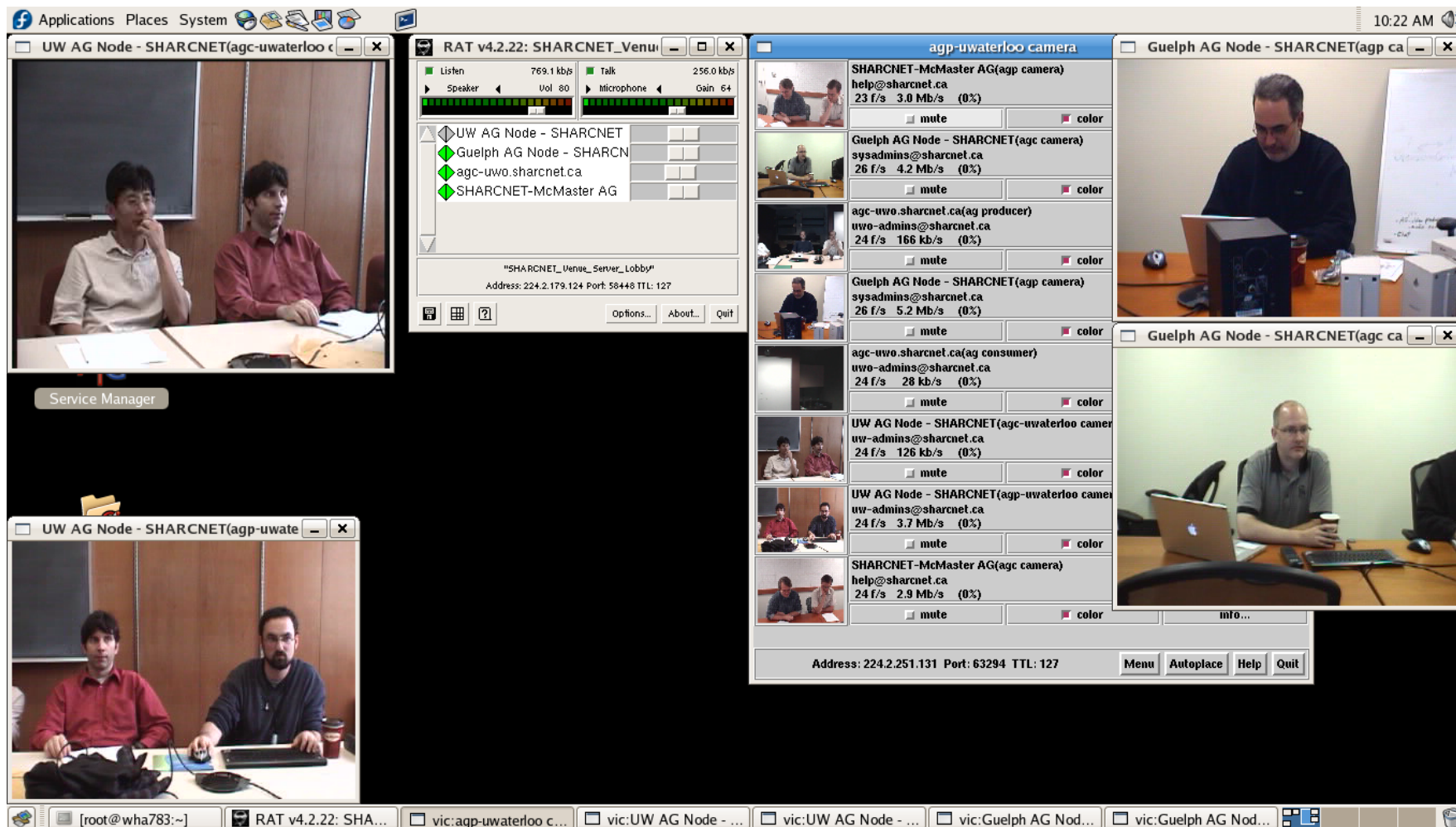
(Report a problem.)  
(List systems and sites.)

Done

# Examples of Systems

System	CPUs	Memory	Storage	Interconnect	Intend Use
requin (Capability)	1536	8 GB	70 TB	Quadrics	Large scale MPI
narwhal (Utility)	1068	8 GB	70 TB	Myrinet	MPI, SMP
whale (Throughput)	3072	4 GB	70 TB	GigE	Serial
bull (SMP-friendly)	384	32 GB	70 TB	Quadrics	High RAM/BW MPI & SMP
silky (SMP)	128	256 GB	4 TB	NUMAlink	OpenMP/threads, large memory SMP
PoPs (6x)	128	8 GB	4 TB	Myrinet	General purpose

# Collaboration via Access Grid



# SHARCNET's Position in The World

Position on Top 500 List	Installation Site	Computer Model	Number of processors	Rmax	Rmax/Rmax(10)	Area of Installation
66 (previously 51)	RQCHP (Sherbrooke)	3.6 GHz Xeon + Infiniband	1152	6888	0.19	Academic Research
80	SHARCNET (Waterloo)	2.2 GHz Opteron + Gigabit Ethernet	3072	6015	0.17	Academic Research
83	SHARCNET (McMaster)	2.6 GHz Opteron + Quadrics	1536	5746	0.16	Academic Research
146 (previously 106)	WestGrid (UBC)	3.06 GHz Intel Xeon + Gigabit Ethernet	1680	3755	0.10	Academic Research
165 (previously 115)	Telco	3.2 GHz Intel Xeon + Gigabit Ethernet	1036	3755	0.10	Industrial
209	SHARCNET (Guelph)	2.2 GHz (Dual core) Opteron + Myrinet	1068 cores	3491	0.10	Academic Research
273 (previously 157)	RQCHP (Sherbrooke)	3.2 GHz Intel Xeon + Gigabit Ethernet	872	3064	0.09	Academic Research
385 (Previously 240)	Canadian Meteorological Centre, Dorval	IBM p690	960	2560	0.07	Research (Weather)





# Where to Find Information

- Account
- Resource discovery
- People



Home | About | Research | Facilities | Help | FAQs | Media/Visitor | Events | Career | Contact | Sign In/Up

**SHARCNET™**  
SHARED HIERARCHICAL ACADEMIC RESEARCH COMPUTING NETWORK

SHARCNET is a multi-institutional high performance computing network that spans 16 leading academic institutions in South central Ontario, Canada.

## Computing tomorrow's solutions

[Detailed Map](#)

**Message from the Scientific Director**

*"All of this infrastructure is available to all users irrespective of where the equipment is located."*  
[ more... ]

Total CPU performance  
**17505 GFLOPS**

**SHARCNET in the news**

- » Student paper on hydrological modelling using SHARCNET wins commendation (06.07.25)
- » Solving the world's problems with tech (06.06.30)
- » SHARCNET chooses Allinea Tools for Debugging Codes (06.06.28)
- » SHARCNET II fast-tracking research (06.06.08)

**Events at SHARCNET**

- » TECC Summit 2006: A C3.ca Technical Symposium, Building the National Platform for HPC in Canada (06.10.23)
- » SHARCNET Fall Workshop 2006 (06.10.16)
- » SHARCNET September Seminars (06.09.19)

[ RSS ] -- Retrieving updates...

# Getting An Account

- **Apply for an account online**
  - Account must be applied online
  - Students, postdoc, visiting fellows must have a **sponsor** who has an account.
- **Account approval:**
  - Faculty accounts are approved by the **site leader**
  - Students/postdoc/fellows require a faculty **sponsor**, who shall approve such accounts
  - Non-SHARCNET institution accounts are approved by the **Scientific Director**
- You will have a ***webportal account*** that allows you to access information/files, submit requests and manage your own profile.

# One Account, Access to All Systems!

## ■ Login to systems

- Siteless login – single username/password for all systems.
- Same user home directory across all systems.
- Systems are designed and deployed for different purposes:
  - **parallel applications**,
  - **serial applications**, e.g. large number of **serial case runs**,
  - **threaded applications** that make use of shared memory by threads, etc

## ■ Login to web

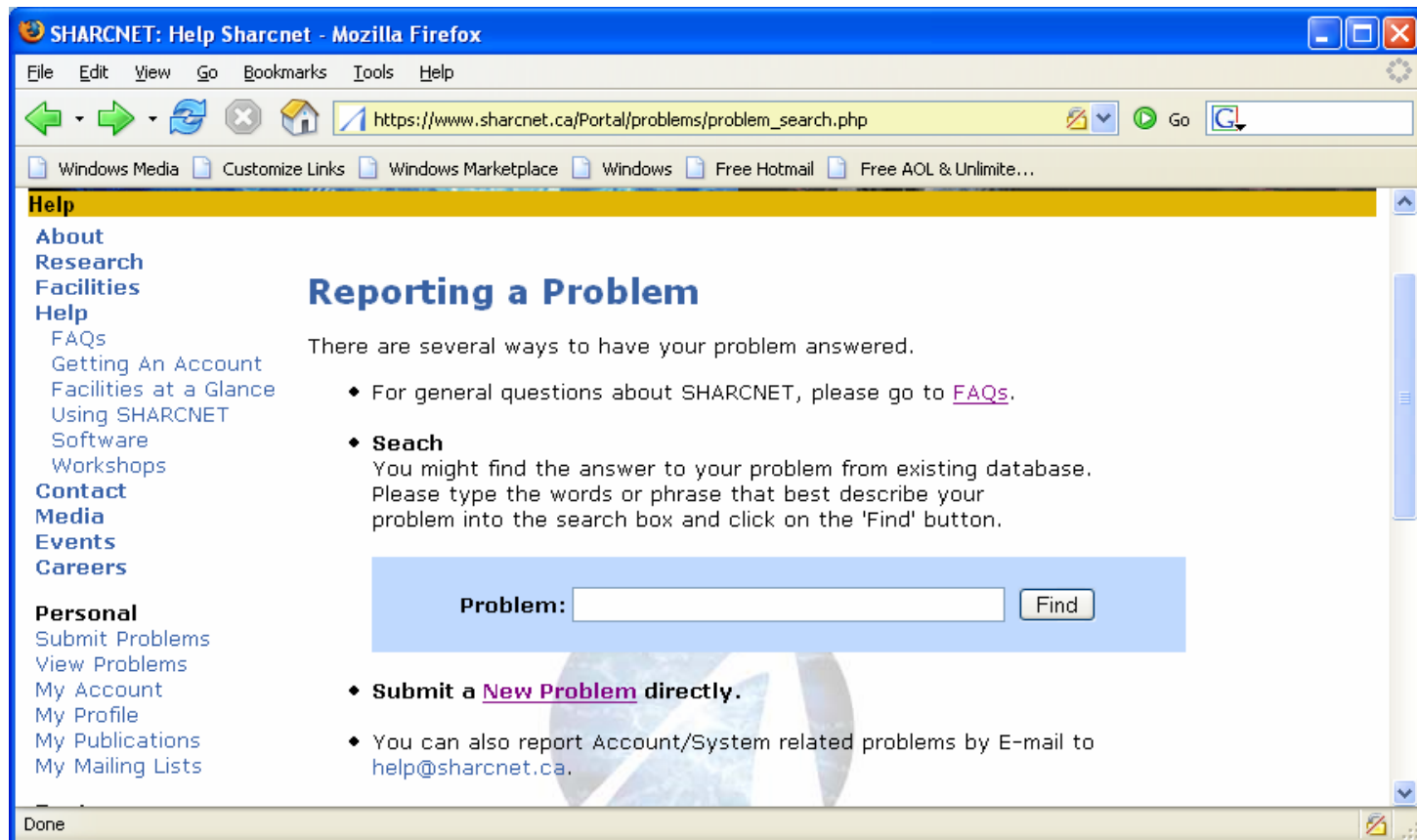
- Discovery resources.
- See statistics.
- Users can change password on the web.
- Report and keep track of problems.

# Where to Look for Information

- **FAQs** are on the web. Go to SHARCNET web site
- **Weekly online seminars** on every Monday
- **Education Online** – slide, examples from past workshops are also available on the web on the **Help** page.
- Information on individual systems are available on the web on the **Facilities** page.

# How to Contact Us

- E-mail us. Our contact info is listed on the **Contact** page at
- Call us.
- Use **Problem Tracking** in the web portal.



The screenshot shows a Mozilla Firefox browser window with the title "SHARCNET: Help Sharcnet - Mozilla Firefox". The address bar shows the URL "https://www.sharcnet.ca/Portal/problems/problem\_search.php". The page content includes a left-hand navigation menu with categories like "Help", "Contact", and "Personal". The main content area is titled "Reporting a Problem" and contains a search form with a "Problem:" label, a text input field, and a "Find" button. Below the form, there are several bullet points providing instructions on how to report a problem.

**Help**  
 About  
 Research  
 Facilities  
 Help  
 FAQs  
 Getting An Account  
 Facilities at a Glance  
 Using SHARCNET  
 Software  
 Workshops  
**Contact**  
 Media  
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 Submit Problems  
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## Reporting a Problem

There are several ways to have your problem answered.

- For general questions about SHARCNET, please go to [FAQs](#).
- **Seach**  
 You might find the answer to your problem from existing database. Please type the words or phrase that best describe your problem into the search box and click on the 'Find' button.

Problem:

- **Submit a [New Problem](#) directly.**
- You can also report Account/System related problems by E-mail to [help@sharcnet.ca](mailto:help@sharcnet.ca).

# SHARCNET Essentials

- Computing environment
- Moving, editing files
- Compiling programmes
- Software and libraries
- Running programmes in batch mode - Queuing system and commonly used commands

# Computing Environment

- **Systems** – Cluster and SMPs.
- **Operating systems** – Linux, Tru64, all 64-bit.
- **Languages** – Fortran, C/C++, Java, Matlab, etc.
- **Compilers**
  - SHARCNET unified compilation environment: **cc**, **c++**, **f77/90**, **mpicc**, **mpif90**.
  - Underlying compilers: **PathScale**, **PGI**, **Intel**, **Compaq**, **gcc**, **g++** and **gfortran**.
- **Key parallel development support**
  - MPI (hp-MPI, SGI MPI, Quadric MPI, MPICH, OpenMPI, etc.)
  - Pthreads, OpenMP
- **Batch scheduling**
  - **sq** - SHARCNET unified batch execution environment.
  - Underlying scheduler: **LSF** – Platform's *Load Sharing Facility*

## Facilities: Intended Use

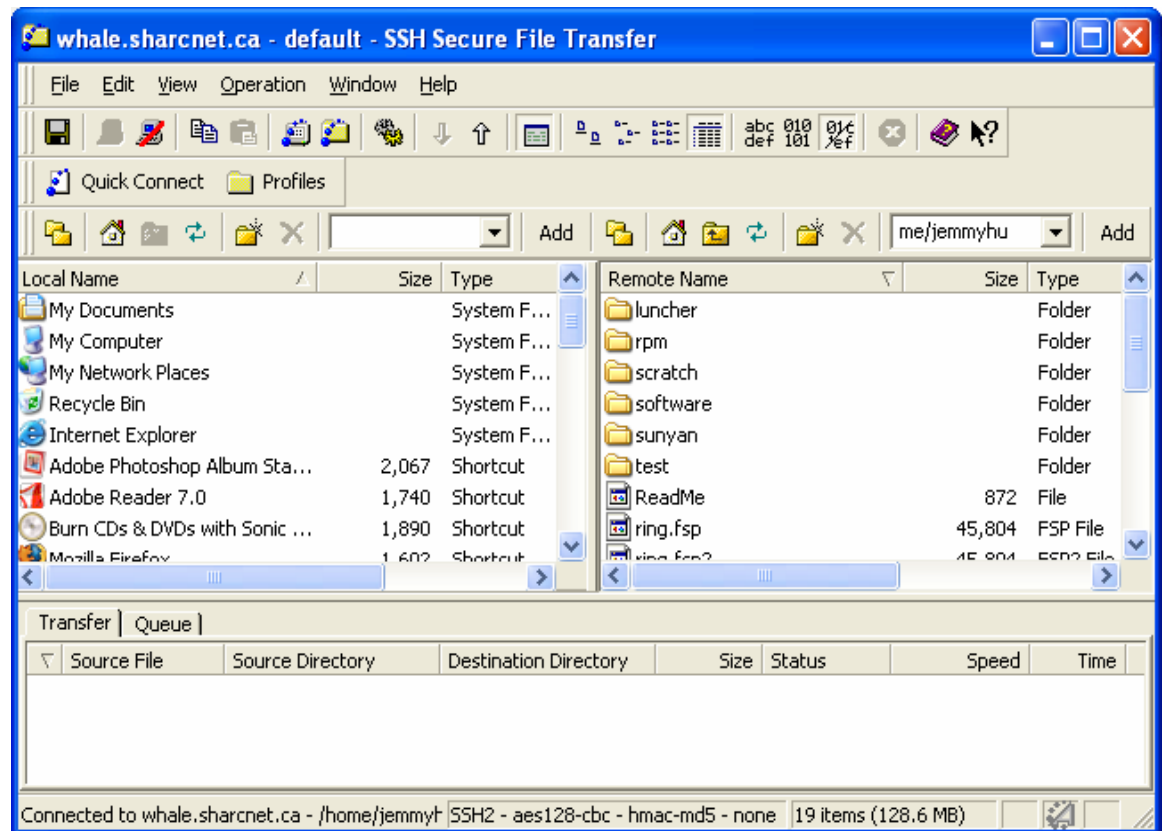
Cluster	CPUs	RAM /node	Storage	Interconnect	Intended Use
<b>requin</b> (Capability)	1536	8 GB	70 TB	Quadrics	Resource intensive MPI (fine grained, large mem.)
<b>narwhal</b> (Utility)	1068	8 GB	70 TB	Myrinet (GM)	MPI, small-scale SMP
<b>whale</b> (Throughput)	3072	4 GB	70 TB	GigE	Serial
<b>bull</b> (SMP-friendly)	384	32 GB	70 TB	Quadrics	High RAM/BW MPI & small-scale SMP
<b>silky</b> (SMP)	128	256 GB	4 TB	NUMALink	large memory/medium-scale SMP
<b>bala, bruce, dolphin, megaladon, tiger, zebra</b>	128	8 GB	4 TB	Myrinet (GM)	General purpose
<b>mako</b>	16	2GB	200GB	Myrinet (MX)	Development/testbed

# How One Typically Works

- Login to a system via SSH, you see familiar UNIX environment.
- Edit source code and/or change the input data/configuration file(s).
- Compile source code.
- Submit a program (or many) to batch queuing system.
- Check results in two days 😊

# File Transfer from/to Your Desktop

- UNIX
  - User **scp** or **sftp**
- Windows
  - User **putty**, or
  - **SSH Secure File Transfer/Shell**



# Compiling Programmes

- SHARCNET provides a unified compiling environment that chooses the right underlying compiler, options and libraries for you! Use them always unless you know better.

Command	Language	Extension	Example
<b>cc</b>	C	c	<b>cc</b> code.c -o code.exe
<b>CC, c++, cxx</b>	C++	.C, .cc, .cpp, .cxx, c++	<b>CC</b> code.cpp -o code.exe
<b>f77</b>	Fortran 77	.f, .F	<b>f77</b> Fcode.f -o Fcode.exe
<b>f90/f95</b>	Fortran	.f90, .f95, .F90, F95	<b>f90</b> Fcode.f90 -o Fcode.exe
<b>mpicc</b>	C	c	<b>mpicc</b> mpicode.c -o mpicode.exe
<b>mpiCC</b>	C++	C++	<b>mpiCC</b> mpicode.cc -o mpicode.exe
<b>mpif77</b>	Fortran 77	f77	<b>mpif77</b> mpicode.f -o mpicode.exe
<b>mpif90/mpif95</b>	Fortran	f90/f95	<b>mpif90</b> mpicode.f90 -o mpicode.exe

# Common Compiler Options

- There are minor differences between compilers (see man page for details), e.g. Pathscale:

<b>-c</b>	Do not link, generate object file only.
<b>-o file</b>	Write output to specified <i>file</i> instead of default.
<b>-Ipath</b>	Add <i>path</i> to search path for include files.
<b>-llibrary</b>	Search the library named <i>library.a</i> or <i>library.so</i> such as <code>-lmpi</code> , <code>-lacml</code>
<b>-Lpath</b>	Add <i>path</i> to search path for libraries
<b>-g[N]</b>	Specify the level of debugging support produced by the compiler
<b>-g0</b>	No debugging information for symbolic debugging is produced. This is the default.
<b>-g2</b>	Produce additional debugging information for symbolic debugging.
<b>-O[n]</b>	Optimization level <i>n</i> =0 to 3. Default is <b>-O2</b> .
<b>-O0</b>	Turns off all optimizations.
<b>-O1</b>	Turns on local optimizations that can be done quickly.
<b>-O2</b>	Turns on extensive optimization. This is the default
<b>-O3</b>	Turns on aggressive optimization (e.g. loop nest optimizer).
<b>-Ofast</b>	Equivalent to <code>-O3 -ipa -OPT:Ofast -fno-math-errno</code>
<b>-pg</b>	Generate extra code to profile information suitable for the analysis program <a href="#">pathprof</a>
<b>-Wall</b>	Enable most warning messages.

# Development Tools

## ■ Libraries

- ACML, ATLAS, CXML, ScaLAPACK, MKL (Intel), MLIB (hp), IMSL (VNI), etc.
- PETSc.
- ...*requested by users.*

## ■ Application Packages

- Blast, Gromacs, NWChem, Octave, R, ...

## ■ Commercial Packages

- Gaussian (several places, site license required).
- Fluent.

## ■ Development tools

- Debugging: DDT, gdb, ...
- Profiling/Optimization: OPT, Altix toolkit (SGI), gprof,

# File System Basics

## ■ Policy

- Same username/password across all systems, and web account.
- Common home directory across SHARCNET (exceptions: wobbe, cat)
- Common SHARCNET wide software are in /opt/sharcnet
- /home backup

## ■ File system

pool	quota	expiry	purpose
/home	200 GB	none	Source, small configuration files
/scratch	None	none	Active data files, binaries
/work	none	none	Active data files
/tmp	160 GB	10 days	Node-local scratch

- /scratch and /work are cluster dependant, backup by users
- **Important:** run jobs on /scratch or /work

# The Batch Scheduling System

- All access to resources managed by queuing system.
- Programs are submitted to queues to run using **sqsub** command:  
**sqsub -q *qname* [ options ] ./myprog [ arg1 [,...] ]**
- By default results will be mailed to you afterwards. But you may choose to have all outputs be saved in a disk file with an **-o *output*** option. This is strongly encouraged.

# Queues

- Specific job queues have different priorities and constraints (**bqueues** command):
  - **mpi** – for parallel jobs.
  - **serial** – for serial jobs.
  - **threaded** – for jobs that use threads.
  - **test** – for test purpose.
  - *special queues* on some systems for running special packages, such as **GAUSSIAN, FLUENT**.

# Commonly Used Batch Commands

- **bqueues** – list available queues.
- **sqsub** – submit a program (“job”) to a specific queue.
- **sqjobs** – list the status of submitted jobs.
- **sqkill** – kill a program by job ID.
- **bhist** – list history of jobs.

- **bqueues** – list available queues

```
[bge@nar316 ~]$ bqueues
```

QUEUE_NAME	PRIO	STATUS	MAX	JL/U	JL/P	JL/H	NJOBS	PEND	RUN	SUSP
staff	150	Open:Active	-	-	-	-	0	0	0	0
test	100	Open:Active	-	-	-	-	0	0	0	0
threaded	80	Open:Active	-	-	-	-	6	0	6	0
mpi	80	Open:Active	-	-	-	-	1972	914	994	64
serial	40	Open:Active	-	-	-	-	25	0	10	15

- **sqsub** – submit a program (job) to a queue, which will be executed later by the scheduler.

```
[bge@nar316 ~]$ sqsub -q serial hostname  
Job <136670> is submitted to queue <serial>.
```

```
[bge@nar316 ~]$ sqsub -q mpi -n 20 -o my_mpi_prog.stdout ./my_mpi_prog  
Job <136671> is submitted to queue <mpi>.
```

- **sqsub -t** – submit a program (job) to the test queue, which will be started sooner (< 60 seconds), for **short**, test runs.

```
[bge@nar316 ~]$ sqsub -q serial -t hostname  
Job <136670> is submitted to queue <serial>.
```

```
[bge@nar316 ~]$ sqsub -q mpi -t -n 20 -o my_mpi_prog.stdout ./my_mpi_prog  
Job <136671> is submitted to queue <mpi>.
```

- **sqsub -man** – display command options

- **sqjobs** – list the status of submitted jobs.

```
[bge@nar316 ~]$ sqjobs
 jobid user queue state ncpus time command
-----
136671 bge  mpi     R     20  0s  ./my_mpi_prog
1060 CPUs total, 30 idle, 1030 busy; 43 jobs running; 16 suspended, 12 queued.
```

- **sqkill** – kill a job in the queue that you want to stop.

```
[bge@nar316 ~]$ sqjobs
 jobid user queue state ncpus time command
-----
136672 bge  mpi    Q     1   0s  ./my_mpi_prog
1060 CPUs total, 50 idle, 1010 busy; 42 jobs running; 16 suspended, 13 queued.
```

```
[bge@nar316 ~]$ sqkill 136672
Job <136672> is being terminated
```

- **bhist** – list jobs history

**bhist** [-a | -d | -p | -r | -s] [-b | -w ] [-l ] [-t ] ...

Options:

- a displays finished and unfinished jobs (over-rides -d, -p, -s and -r)
- b brief format; if used with -s option, shows reason why jobs were suspended
- d only display finished jobs
- l long format; displays additional information
- u user display jobs submitted by specified user

- **bhist** – A snapshot of command output

```
nar317:~/pub/exercises% bhist -a
```

```
Summary of time in seconds spent in various states:
```

JOBID	USER	JOB_NAME	PEND	PSUSP	RUN	USUSP	SSUSP	UNKWN	TOTAL
134177	dbm	*o_mpi_c	8	0	37	0	0	0	45
134227	dbm	*o_mpi_c	10	0	10	0	0	0	20

```
nar317:~/pub/exercises% bhist -l 134177
```

```
Job <134177>, User <dbm>, Project <dbm>, Job Group </dbm/dbm>,
```

```
Command </opt/hpmpi/bin/mpirun -srun -o mpi_hello.log ./
mpi_hello>
```

```
Fri Sep 15 13:06:08: Submitted from host <wha780>, to Queue <test>, CWD <${HOME}/
scratch/examples>, Notify when job ends, 4 Processors Requ
ested, Requested Resources <type=any>;
```

```
Fri Sep 15 13:06:16: Dispatched to 4 Hosts/Processors <4*lsfhost.localdomain>;
```

```
Fri Sep 15 13:06:16: slurm_id=318135;ncpus=4;slurm_alloc=wha2;
```

```
Fri Sep 15 13:06:16: Starting (Pid 29769);
```

```
Fri Sep 15 13:06:17: Running with execution home </home/dbm>, Execution CWD
</scratch/dbm/examples>, Execution Pid <29769>;
```

```
Fri Sep 15 13:06:53: Done successfully. The CPU time used is 0.3 seconds;
```

```
Fri Sep 15 13:06:57: Post job process done successfully;
```

```
Summary of time in seconds spent in various states by Fri Sep 15 13:06:57
```

PEND	PSUSP	RUN	USUSP	SSUSP	UNKWN	TOTAL
8		0	37	0	0	45

## Debugging Tools: gdb, idb, DDT

- DDT is a powerful debugger for parallel programs with GUI
  - works best with MPI programs, but can also be used for threaded and serial jobs
  - supports with C, C++ and many flavours of Fortran (77, 90, 95)
  
- Installed on requin, narwhal, bull and six PoP clusters
  
- To use DDT:
  - **ddt program [arguments]**
  - then choose number of processes to run and press “Submit”
  - DDT itself involves the scheduler using the test queue
  - The debugging session starts almost immediately, but has a 1 hour time limit

Session Select Search View Help

Current Group: All [▶] [⏸] [↶] [↷] [↵] [↶] [↷] [↵]

All [0] [1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15]

Root [0]

Workers [1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15]

Project Files | Fortran Modules

- home
  - syam
    - Gadget
      - P-Gadget
        - accel.c
        - allocate.c
        - allvars.c
        - begrun.c
        - cooling.c
        - density.c
          - double INLINE\_FUNC periodic(doc)
          - void density(void)
          - void determine\_interior(void)
          - void ensure\_neighbours(int mode)
        - dissolvegas.c
        - domain.c
        - endrun.c
        - world.c

main.c

```

6
7 #include "allvars.h"
8 #include "proto.h"
9
10
11
12 /*
13  * This function initializes the MPI communication packages,
14  * and sets cpu-time counters to 0.
15  * Then begun() is called, which sets up the simulation
16  * either from IC's or from restart files.
17  * Finally, run() is started, the main simulation loop,
18  * which iterates over the timesteps.
19  */
20 int main(int argc, char **argv)
21 {
22     double t0, t1;
23
24     MPI_Init(&argc, &argv);
25     MPI_Comm_rank(MPI_COMM_WORLD, &ThisTask);
26     MPI_Comm_size(MPI_COMM_WORLD, &NTask);
27
28     if(NTask<=1)
29     {
30         if(ThisTask==0)
31             printf("Number of processors MUST be a power of 2\n");
32     }
33 }
    
```

Thread: 0: PID unknown

Stack: #0 main (argc=2, arg

Variables:

Variable Name	Value
ThisTask	0

Type: none selected

Stdout | Stderr | Stdin (to current group) | Breakpoints | Watches | Parallel Stack View

Procs	Function
16	main (main.c:25)

Evaluate:

Expression	Value
------------	-------

# Support

- People
- Problem tracking
- Research projects
- Education and training

# SHARCNET People

## ■ HPC Analysts

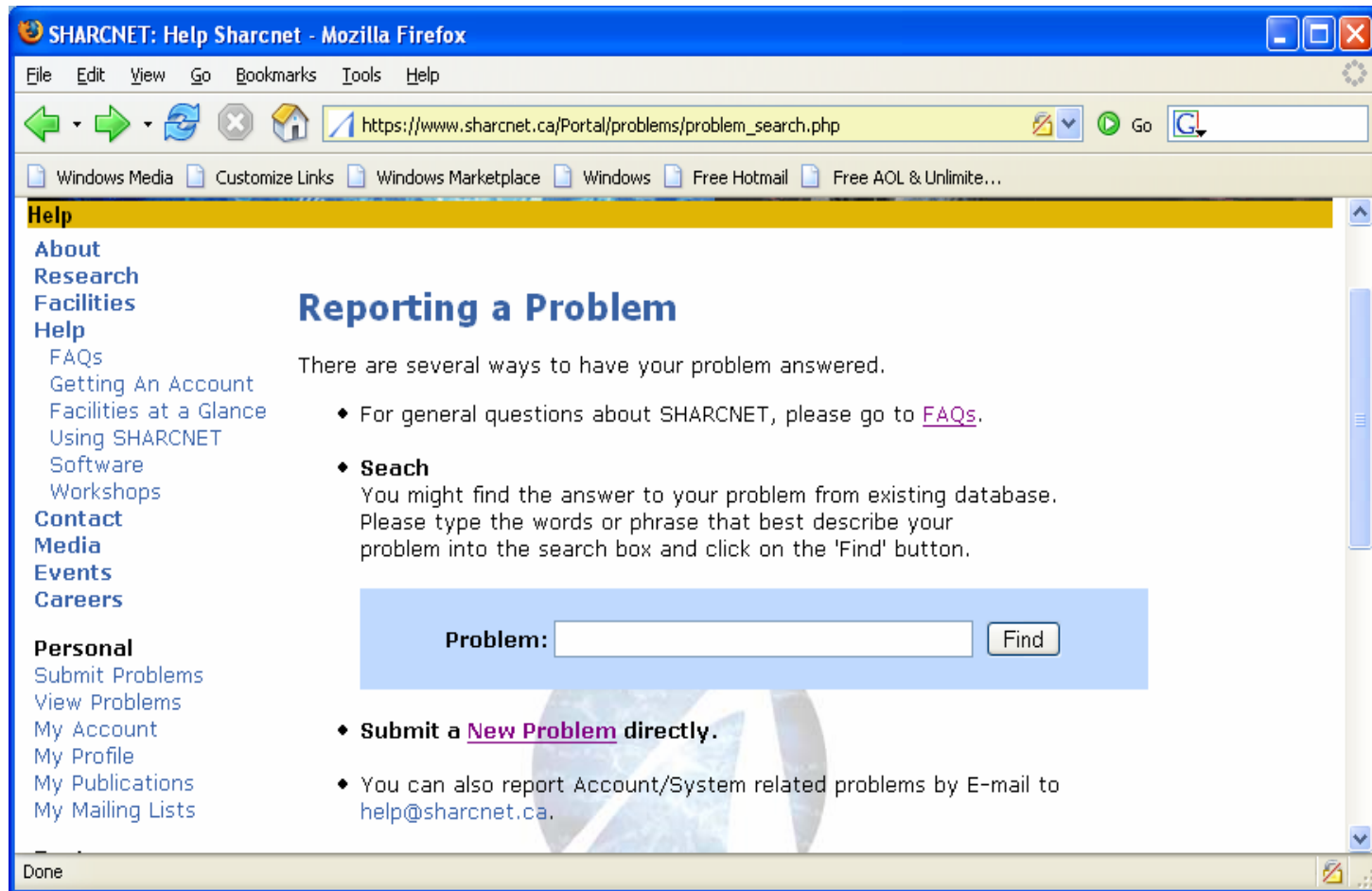
- A point of contact, central resource.
- Analysis of requirements.
- Development support, performance analysis.
- Training and education.
- Research computing consultations.

## ■ System Administrators

- User accounts.
- System software.
- Hardware and software maintenance.
- Research computing consultations.

# Webportal: Problem Tracking

- Use **Problem Tracking** in the web portal.



SHARCNET: Help Sharcnet - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

https://www.sharcnet.ca/Portal/problems/problem\_search.php

Windows Media Customize Links Windows Marketplace Windows Free Hotmail Free AOL & Unlimite...

**Help**

- About
- Research
- Facilities
- Help
  - FAQs
  - Getting An Account
  - Facilities at a Glance
  - Using SHARCNET
  - Software
  - Workshops
- Contact
- Media
- Events
- Careers

**Personal**

- Submit Problems
- View Problems
- My Account
- My Profile
- My Publications
- My Mailing Lists

## Reporting a Problem

There are several ways to have your problem answered.

- For general questions about SHARCNET, please go to [FAQs](#).
- Search**  
You might find the answer to your problem from existing database. Please type the words or phrase that best describe your problem into the search box and click on the 'Find' button.

Problem:  Find

- Submit a [New Problem](#) directly.
- You can also report Account/System related problems by E-mail to [help@sharcnet.ca](mailto:help@sharcnet.ca).

Done

# Research Project Consultation

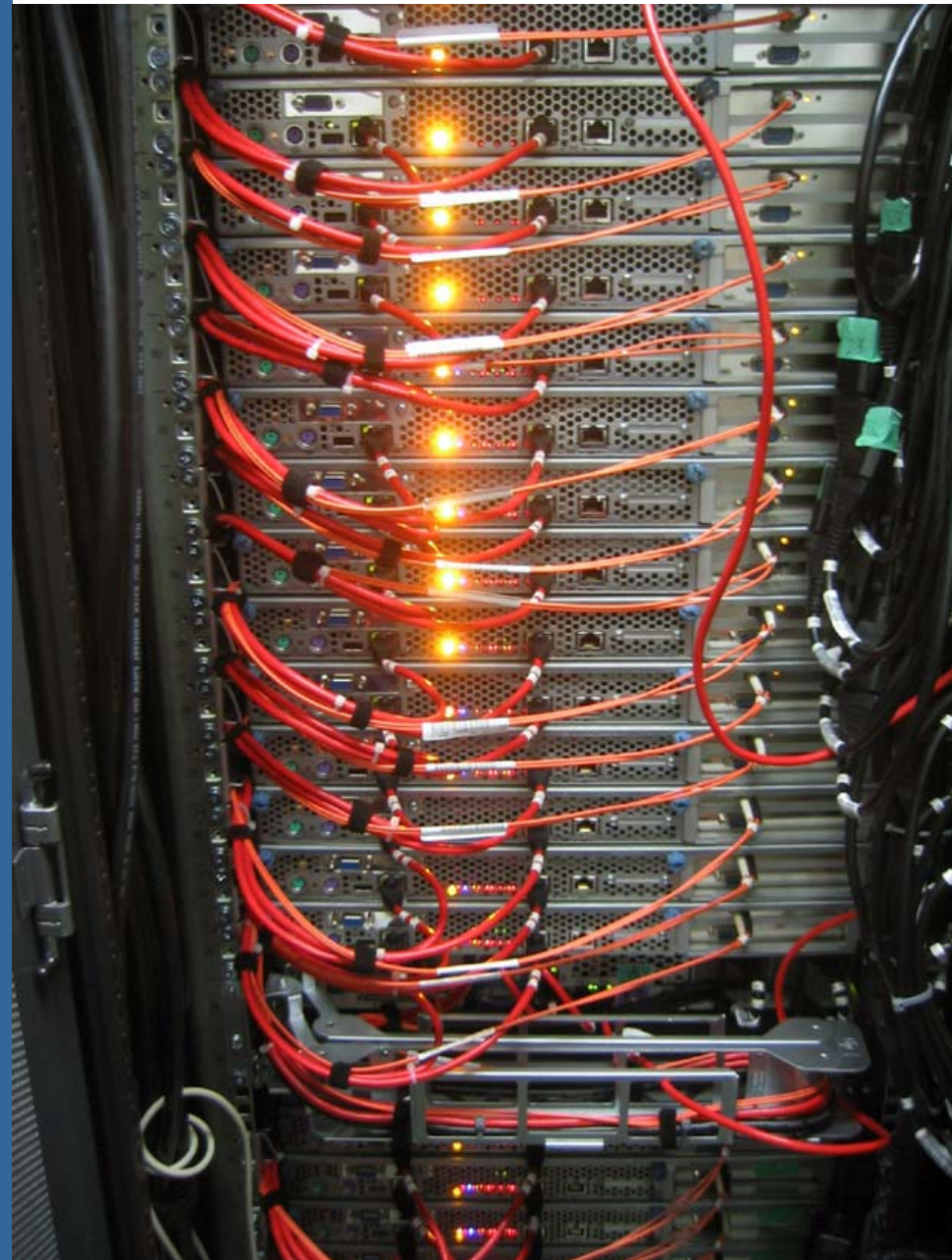
- HPTC people also do research consultation projects.

# Education and Training

- SHARCNET offers different forms of education and training
  - Weekly online seminar: New users introduction and research topics;
  - Irregular and annual workshops. This year SHARCNET will hold a week long HPTC summer school;
  - Credit courses at undergraduate and graduate level.

# MPI Examples

- Hello world! – *All up*
- Send/receive
- Broadcast – A collective all



```
#include <stdio.h>
#include "mpi.h"

int main( int argc, char *argv[] )
{
    int nprocs, myrank, pnamelen;
    char pname[128];

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    MPI_Get_processor_name(pname, &pnamelen);

    if (0 == myrank)
        printf("Hello world from root on %s\n", pname);
    else
        printf("Hello world from %d on %s of %d\n", \
            myrank, pname, nprocs);

    MPI_Finalize();
    return 0;
}
```

```
program main
    implicit none
    include 'mpif.h'
    integer :: nprocs, myrank, ierr

    call MPI_Init(ierr)
    call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
    call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
    call MPI_Get_processor_name(pname, &pnamelen)

    if (0 == myrank) then
        print *, "Hello world from root on", pname
    else
        print *, "Proc", myrank, ": Hello world"
    end if

    call MPI_Finalize(ierr)
end program main
```

- Main

```
#include "mpi.h"
int main( int argc, char *argv[] )
{
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    if (0 != myrank)
        server();
    else
    {
        sleep(1);          /* Wait for servers to come up */
        client();
    }

    MPI_Finalize();
    return 0;
}
```

- Server

```
static void server( void )
{
    char sbuf[MSGSIZE+1], rbuf[MSGSIZE+1];
    MPI_Status status;

    while (1)
    {
        MPI_Recv(rbuf, MSGSIZE, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);
        if (strcasecmp("shutdown", rbuf) == 0) break;

        printf("Server %d: Received %d bytes (\"%s\")\n", myrank, MSGSIZE, rbuf);
        MPI_Send(rbuf, MSGSIZE, MPI_CHAR, 0, tag, MPI_COMM_WORLD);
    }

    return;
}
```

- Client

```
static void client( void )
{
    ... ..
    while (1)
    {
        printf("client>> ");
        fgets(sbuf, 256, stdin);

        for (ip = 1; ip < np; ip++)
            MPI_Send(sbuf, MSGSIZE, MPI_CHAR, ip, tag, MPI_COMM_WORLD);
        if (strcasecmp(sbuf, "shutdown") == 0) break;
        for (ip = 1; ip < np; ip++) {
            MPI_Recv(rbuf, MSGSIZE, MPI_CHAR, ip, tag, MPI_COMM_WORLD, &status);
            printf("Server %d echo: %s\n", ip, rbuf);
        }
    }
}
```

```
program mpi_avg
... ..
iseed = myid + MPI_WTIME(ierr)
call srand(iseed)
nlocal = 1 + n * rand(0)
do i = 1, nlocal
  mark = 100 * rand(0)
  print *, "(Proc ", myid, ")", mark
  myavg = (myavg * (i - 1) + mark) / i
end do
print *, "Average of class ", myid+1, ": ", myavg
myavg = myavg * nlocal
```

## ! Reduce the local count

```
call MPI_REDUCE(myavg, avg, 1, MPI_REAL8,&
  MPI_SUM, 0, MPI_COMM_WORLD, ierr)
call MPI_REDUCE(nlocal, ntotal, 1, MPI_INTEGER,&
  MPI_SUM, 0, MPI_COMM_WORLD, ierr)
```

## ! Announce the final results (master only)

```
if (myid .eq. 0) then
  avg = avg / ntotal
  print *, "Total number: ", ntotal
  print *, "Total average: ", avg
end if
```

```
call MPI_FINALIZE(ierr)
end program mpi_avg
```

## References

- MPI forum, [www.mpi-forum.org](http://www.mpi-forum.org)
- William Gropp, et al, ***Using MPI***, MIT, 1999.
- William Gropp, et al, ***Using MPI-2***, MIT, 1999.

# OpenMP Examples

- Hello world! – *All up*
- Fork/join
- Concurrent tasks



```
#include <stdio.h>
#include <string.h>
#include "omp.h"

int main(int argc, char *argv[ ])
{
    int thd, nth = 1;

    if (argc > 1) nth = atoi(argv[1]);
    omp_set_num_threads(nth);

    #pragma omp parallel
    {
        tid = omp_get_thread_num();
        printf("Hello world! thread %d of %d\n", tid+1, nth);
    }

    return 0;
}
```

# Example 1: Hello world! (Fortran)

```
program hello
implicit none
integer tid, nth/1/
integer omp_get_num_threads
integer omp_get_thread_num

C
read *, nth

C
call omp_set_num_threads(nth)

C
!$omp parallel
  tid = omp_get_thread_num()
  print *, "Hello world! from thread ", thid+1, " of ", nth
!$omp end parallel

C
stop
end
```

# Example 2: Loop parallelization

```
#include "omp.h"

int main( int argc, char *argv[] )
{
    ... ..
    omp_set_num_threads(nt);

    #pragma omp parallel for reduction(+:s)
    for (i = 0; i < n; i++)
    {
        s += a[i];
    #ifdef DEBUG
        tid = omp_get_thread_num();
        printf("Sum: %g (thread %d)\n", s, tid);
    #endif
    }

    printf("Sum = %g\n", s);
    return 0;
}
```

```
program reduce77
    ... ..
    call omp_set_num_threads(nt)
c
!$omp parallel do reduction(+:s)
    do 20 i = 1, n
        s = s + a(i)
    #ifdef DEBUG
        tid = omp_get_num_threads();
        print *, "Sum: ", s, " (thread ", tid, )"
    #endif
    20 continue
!$omp end parallel do
c
    print *, "Sum = ", s
c
    stop
end
```

- Independent sections of code are executed concurrently

```
#pragma omp parallel sections
{
    #pragma omp section
    task1( );
    #pragma omp section
    task2( );
    #pragma omp section
    task3( );
}
```

*omp barrier – no one shall proceed until all arrive at this point*

- By default there is a **barrier** at the end of **omp** sections, use **nowait** clause to turn off the barrier

## Reference

- OpenMP standard, [www.openmp.org](http://www.openmp.org)

