

Introduction to SciNet

DON'T PANIC

Outline

1. About SciNet

- SciNet is ...
- How to get access
- Useful sites
- SciNet systems

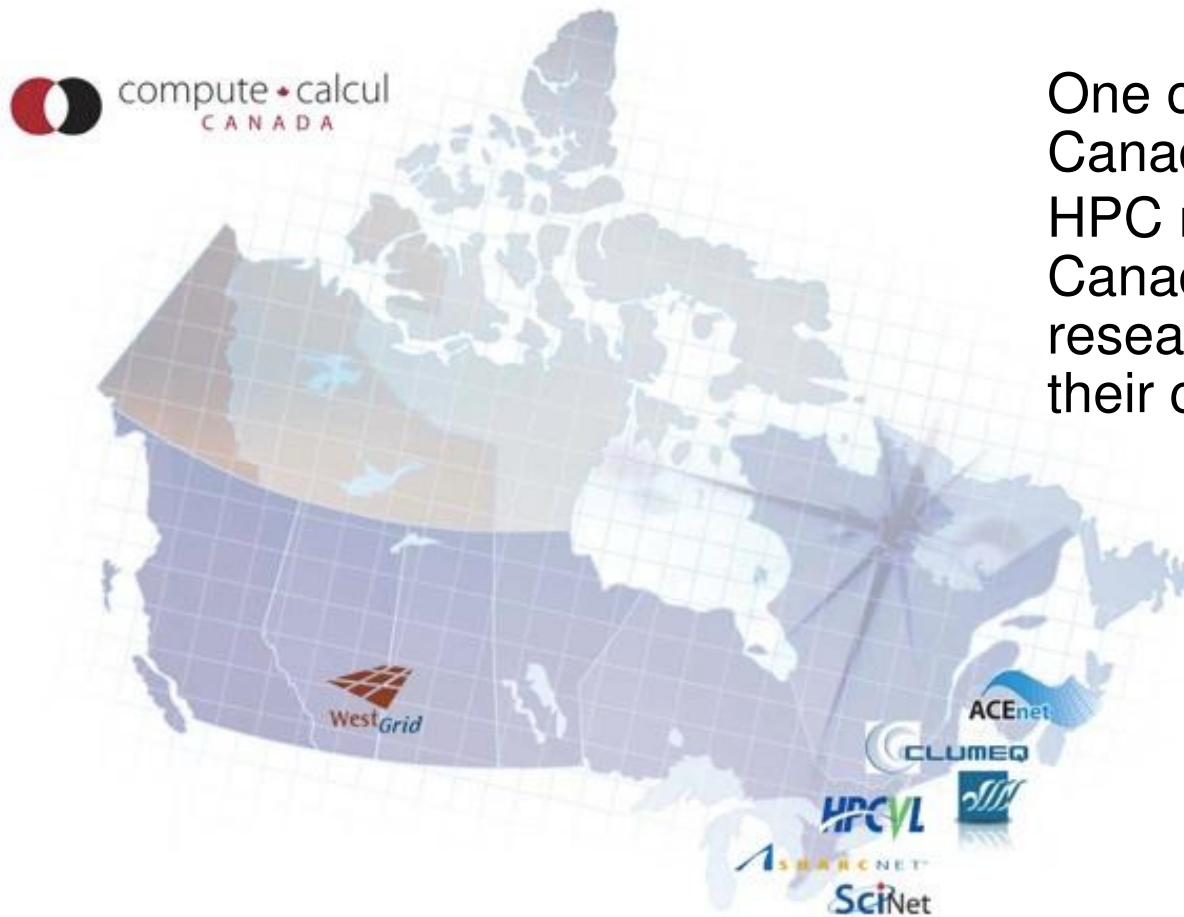
2. Using SciNet

- Software/Libraries
- Compilers
- Job submission
- Final tips

PART 1 — ABOUT SCINET

SciNet is ...

... a consortium for High-Performance Computing consisting of researchers at U. of T. and its associated hospitals.



One of 7 consortia in Canada that provide HPC resources to Canadian academic researchers and their collaborators.

SciNet is ...

... home to the first and third largest supercomputers in Canada.



SciNet is ...

... 4 technical analysts who can work directly with you to use our resources to produce good science.

- Jonathan Dursi
- Scott Northrup
- Ramses van Zon
- Daniel Gruner

+ 7 people that make sure everything runs smoothly.

- Jaime Pinto
- Joseph Chen
- Jason Chong
- Ching-Hsing Yu
- Neil Knecht
- Leslie Groer
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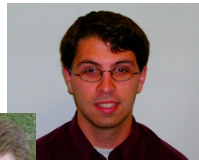
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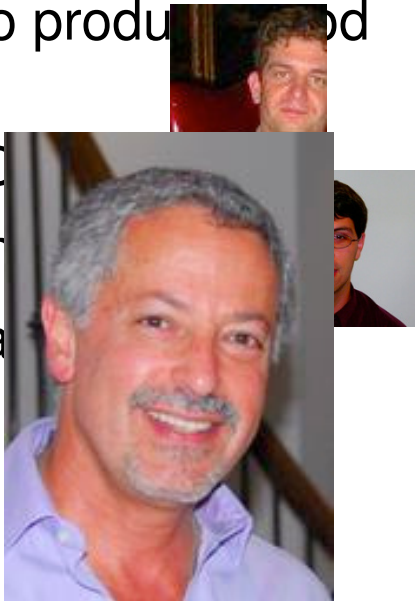
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How to get access

Any qualified researcher at a Canadian university can get a SciNet account through this two-step process:



- Register for a Compute Canada Database (CCDB) account
- Non-faculty need a sponsor (supervisor's CCRI number), who has to have a SciNet account already.
- Login to CCDB and apply for a SciNet account (click *Apply* beside SciNet on the *Consortium Accounts* page)

How to get access

Compute Canada: Please sign in

https://ccdb.compute canada.org/security/login

UTLib gScholar APJ WPR ISI NA @ UofT gCalendar astro-ph new TWiAF TWiCA Sci SciNetWiki Scotia SciNet Other

 compute  calcul
CANADA

Français || English
Login

FAQ

This site hosts the Compute Canada Database (CCDB) that is the central repository of information about users of high-performance computing equipment funded under CFI's National Platform Fund (NPF). It allows information to be shared between Compute Canada consortia and provides a means of associating usage with particular research groups as required for reporting purposes.

In order to register with the CCDB you either need to be a faculty member at a Canadian university or be sponsored by a faculty member at a Canadian university that is registered with the CCDB. People who can be sponsored include graduate students and research staff that report to the sponsoring faculty member.

All groups applying for allocations through the National Resource Allocation Committee (NRAC) must be registered in the CCDB. In the near future, all users will need to be registered in order to gain access to CFI NPF-funded equipment.

Please sign in

Email:

Password:

|| **Forgot Password** || **Register**

How to get access

Compute Canada: Consortium X

https://ccdb.compute canada.org/me/facilities

UTLib gScholar APJ WPR ISI NA @ UofT gCalendar astro-ph new TWIAF TWICA Sci SciNetWiki Scotia SciNet

compute + calcul CANADA

Logged in as Jonathan Dursi (CCI: idi-10)

> My Account < Resource Allocations FAQ Browse Database Pending Approvals Translation

Consortium Accounts

Use this page to apply for new consortium accounts using your Compute Canada Identifier (CCI), or to link existing consortium accounts with your CCI.

Security note: the convenience buttons below pass information in a POST request for security reasons. Security software may detect this as a Cross-Site Scripting (XSS) attempt. You may need to reconfigure your security software to permit it.

Consortium	Create New Account	Link Existing Account
ACEnet (Atlantic Computational Excellence Network)	(Coming soon)	(Coming soon)
CLUMEQ (Consortium Laval, Université du Québec, McGill and Eastern Quebec)	Apply	(Coming soon)
HPCVL (High Performance Computing Virtual Laboratory)	Apply	Link Account
RQCHP (Réseau québécois de calcul de haute performance)	Apply	(Automatic)
SciNet (SciNet)	Apply	Link Account
SHARCNET (Shared Hierarchical Academic Research Computing Network)	Apply	Link Account
WestGrid (WestGrid)	Apply	Link Account

Copyright © 2009 Compute Canada || [email webmaster](#)

How to get access

Getting more resources on SciNet

- Users who will be needing more than the default amount of resources must have their PI apply for it through the competitively awarded.
- Resource competition occurs in the fall of each year.
- Without such an allocation, a user may still use up to 32 GPC nodes at a times at low priority.

Now what?

Portal: <https://portal.scinet.utoronto.ca>

SciNet usage reports

Change password, default allocation, maillist subscriptions

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The screenshot shows a web browser window displaying the SciNet User Support Library wiki. The browser's address bar shows the URL https://support.scinet.utoronto.ca/wiki/index.php/SciNet_User_Support_Library. The page features a sidebar on the left with a search bar and a navigation menu. The main content area includes a welcome message, a system status section indicating 'Normal', and two columns of links: 'QuickStart Guides' and 'What's New On The Wiki'. The 'QuickStart Guides' column lists various topics like login essentials, GPC, TCS, data management, software, job scheduling, performance, and tutorials. The 'What's New On The Wiki' column lists recent updates and announcements, including a class schedule announcement, a tutorial update, SSH keys, disk space information, and hyperthreading with Gromacs. At the bottom, there are sections for 'User-Supplied Content' and 'News and Recent Events'.

SciNet User Support Library

Welcome to the SciNet User Support wiki. Here you will find up-to-date manuals put together by SciNet staff and users, as well as links to external resources, to help you make use of SciNet resources for computational scientific discovery. Navigate using the links in the grid style presentation below, or using the menu on the left.

System Status: Normal

message last updated on: Mon Aug 16 13:12:08 EDT 2010
(Previous messages)

QuickStart Guides

- » Login essentials
- » GPC: General Purpose Cluster
- » TCS: Tightly Coupled System
- » Data management
- » Software and libraries
- » Job scheduling system (Moab)
- » Performance primer, and performance tools for GPC and TCS
- » Tutorials and Manuals
- » FAQ (frequently asked questions)
- » SciNet User Tutorial **UPDATED!**
- » Usage policy
- » Acknowledging SciNet

What's New On The Wiki

- » SciNet class schedule announced (rzon, 30 August)
- » Updated and improved SciNet User Tutorial (rzon, 28 August)
- » SSH keys and SciNet (jdsuri, 19 August)
- » How to find out how much disk space you're using and how much you have left (pinto, 10 August)
- » Hyperthreading with Gromacs (cneale, 9 August)

Previous new stuff can be found in the [What's new archive](#).

User-Supplied Content

News and Recent Events

SciNet Class Schedule

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To learn about SciNet courses and sign up.

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The screenshot shows the SciNet Courses website interface. At the top, there's a navigation bar with links: All Classes (by date), SNUG Meetings, Short Courses, and Courses Forum. Below this is the SciNet logo and the text "SciNet Courses - High Performance Education".

On the left side, there's a "User login" section with fields for "Username:" and "Password:", and a "Log in" button. Below that is an "Event Calendar" for September 2010, showing a grid of days with some dates highlighted in red.

In the center, there's a "Welcome to the SciNet Courses Website!" message dated "Wed, 2010-09-01 14:47" by "admin". It mentions upcoming classes, meetings, RSS feed, calendar, Wiki, and mailing list. Below this is a link to "admin's blog".

On the right side, there's an "Upcoming events" section listing several events with their durations:

- Intro To SciNet (3 hours)
- September SNUG - TechTalk: GPFS (5 days)
- Intro To SciNet (7 days)
- Intro to Parallel Programming (19 days)
- Parallel I/O (33 days)
- October SNUG - TechTalk: Version Control (40 days)

At the bottom, there's a "November SNUG - TechTalk: Debuggers" event dated "Mon, 2010-08-30 22:15" by "admin", with a "Start: 2010-11-10 12:00".



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For further questions, mail our system administrators and technical analysts.

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Login: login.scinet.utoronto.ca

Access SciNet systems: `ssh` to login (not part of clusters)

`ssh -l <username> login.scinet.utoronto.ca`



Overview of the SciNet Systems

Systems

General Purpose Cluster (GPC)



Systems

General Purpose Cluster (GPC)

- 3780 nodes with two 2.53GHz quad-core Intel Xeon 5500 (*Nehalem*) x86-64 processors
- 16GB RAM per node
- Gigabit ethernet network on all nodes for management, disk I/O, boot, etc.
- InfiniBand network on 1/4 of the nodes only used for job communication
- 306 TFlops
- #16 on the June 2009 *TOP500* supercomputer sites
- #1 in Canada

Systems

Tightly Coupled System (TCS)



Systems

Tightly Coupled System (TCS)

- 104 nodes of 16 dual-core 4.7GHz P6 processors.
- 128GB RAM per node
- Interconnected by full non-blocking InfiniBand
- 62 TFlops
- #80 on the June 2009 *TOP500* supercomputer sites
- #3 in Canada

Systems

Tightly Coupled System (TCS)

- 104 nodes of 16 dual-core 4.7GHz P6 processors.
- 128GB RAM per node
- Interconnected by full non-blocking InfiniBand
- 62 TFlops
- #80 on the June 2009 *TOP500* supercomputer sites
- #3 in Canada

Access disabled by default. For access, email us explaining the nature of your work. Your application should scale well to over 32 procs.

Systems

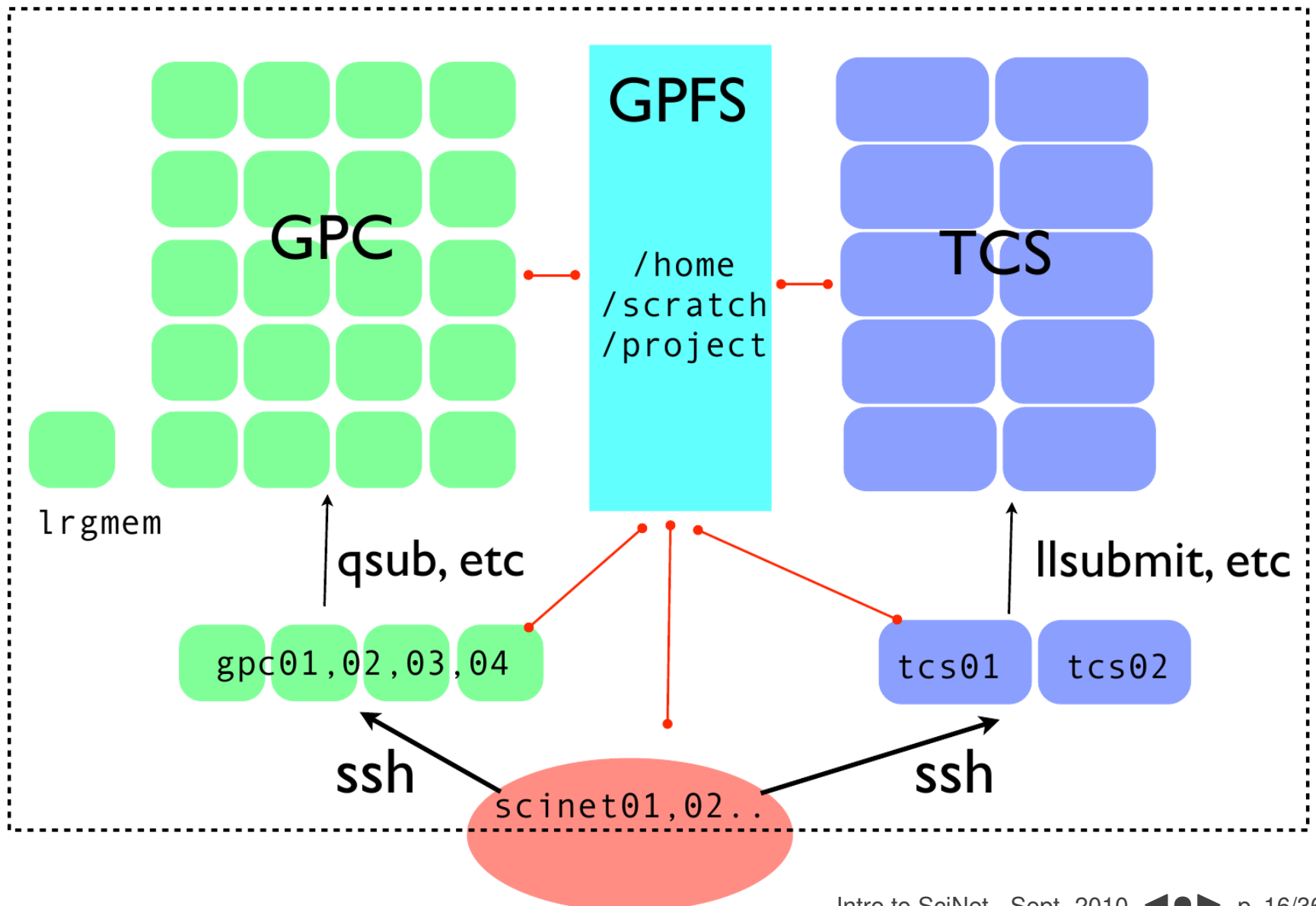


Disk space

- 1790 1TB disk drives, for a total of 1.4 PB of storage
- Two DCS9900 couplets, each delivering 4-5GB/s read/write access to the drives
- Single *GPFS* filesystem on both TCS and GPC
- I/O goes over Gb ethernet network on the GPC, and over the infiniband network on the TCS

location	quota	block-size	time-limit	backup	devel	comp
/home	10GB	256kB	perpetual	yes	rw	ro
/scratch	X TB	4MB	3 months	no	rw	rw

Systems



Systems

Moving large data

Moving less than 10GB through the login nodes

- Only login nodes visible from outside SciNet (1Gb/s link).
- Use scp or rsync.
- but datamover1 node is faster.

Moving more than 10GB through the datamover1 node

- Should be done from the datamover1 node (10Gb/s link).
- From any SciNet node, ssh to datamover1.
- Transfers must originate from datamover1.
Cannot copy files from the outside world to datamover1.
- Your machine must be reachable from the outside.

Systems

File system

- Compute nodes do not contain hard drives
- The available disk space, /home and /scratch, all part of the GPFS file system which runs over the network.
- GPFS is a high-performance file system which provides rapid reads and writes to large data sets in parallel from many nodes.
- It performs quite poorly at accessing data sets which consist of many, small files.
- Don't keep many small files on the system.
They waste space, and are slower to access, read and write.

I/O strategies

- Do not read and write lots of small amounts of data to disk. Reading data in from one 4MB file can be enormously faster than from 100 40KB files.
- Write your data out in binary. Faster and takes less space.
- Each process writing to a file of its own is not scalable. A directory gets locked by the first process accessing it, so the other processes have to wait for it.
- Consider using MPI-IO (part of the MPI-2 standard), NetCDF or HDF5.
- If you must read and write a lot to disk, use ramdisk if possible. The ramdisk can be accessed using `/dev/shm/` and is currently set to 8GB max.
- Copy back from ramdisk at end of run.

PART 2 — USING SCINET

Software and Libraries

Modules

- Once you log into devel nodes, what's already installed?
- Other than essentials, all software installed as modules.
- modules set environment variables (LD_LIBRARY_PATH, PATH, ...) to include the appropriate package.
- Allows multiple versions of package to be available.
- More on *Software and Libraries* page of wiki.

```
gpc-f103n084-$ module avail
```

```
----- /scinet/gpc/Modules/version_index
3.2.6
```

```
----- /scinet/gpc/Modules/3.2.6/module
dot                modules                use.c
module-cvs         use.deprecated
module-info        use.experimental
```

```
----- /scinet/gpc/Modules/modulefiles
ROOT/5.26.00
Xlibraries/X11-32
Xlibraries/X11-64(default)
amber10/amber10
autoconf/autoconf-2.64
blast/2.2.23+
cmake/2.8.0
...
```

Software and Libraries

```
module load <module-name>
module purge
module avail
module list
module help <module-name>
```

use particular software
remove currently loaded modules
list available software packages
list loaded modules
describe a module

- Load frequently used modules in `.bashrc` in home directory.
- Short name preferred (`intel` not `intel/intel-v11.1.056`)
- To compile code that uses that package add
`-I${SCINET_[shortmodulename]_INC}`
- To link, add
`-L${SCINET_[shortmodulename]_LIB} -l[libname]`

Software and Libraries

Dependencies

- Modules sometimes require other modules to be loaded first.
- Module will let you know if you didn't.
- For example:

```
gpc-f103n084-$ module purge
```

```
gpc-f103n084-$ module load python
python/2.6.2(11):ERROR:151: Module
'python/2.6.2' depends on one of the
module(s) 'gcc/gcc-4.4.0'
python/2.6.2(11):ERROR:102: Tcl
command execution failed:  prereq gcc/
gcc-4.4.0
```

```
gpc-f103n084-$ module load gcc python
```

```
gpc-f103n084-$
```

Software and Libraries

Commercial Software?

- We have an extremely large and broad user base
- We cannot buy everyone's favourite commercial software package.
- Only commercial software we have installed is software that can benefit everyone:
 - GPC: intel compilers, MKL (both in module intel)
 - TCS: ibm compilers, ESSL
- No matlab, gaussian, idl, . . .
- Can work with you to get commercial software that you have license for installed.

Compiling

- **WARNING:**
The login machines are not the same architecture as either the GPC or TCS nodes, so you should not compile programs on the login machines.
- Compile on devel nodes:

```
gpc01, gpc02, gpc03, gpc04  
tcs01, tcs02
```

Also good for short, small scale tests.
- Test your job's requirements and scaling behaviour before submitting a large scale computation.
- Devel nodes are used by *everyone* who needs to use the SciNet systems, so be considerate.

Compiling

GPC compilation

- From `login.scinet.utoronto.ca`, ssh to one of the four GPC devel nodes, e.g.

```
ssh gpc04
```

- We recommend Intel compilers, which are `icc`, `icpc`, and `ifort` for C, C++, and Fortran, from the module `intel`.
- Optimize your code for the GPC machine using of at least the following compiler flags

```
-O3 -xhost
```

- Add `-openmp` to the command line for OpenMP
- Compile MPI code with `mpif77/mpif90/mpicc/mpicxx`.
 - Open MPI, in module `openmpi` (v1.4.1) default
 - Intel MPI, in module `intelmpi` (v4.0.0)

Compiling

TCS compilers

- ssh to tcs devel nodes
`ssh tcs01` or `ssh tcs02`
 - Use the IBM compilers on the TCS devel nodes. These are `xlc`, `xlC`, `xlf` for C, C++, and Fortran.
 - For OpenMP code, use `xlc_r`, `xlC_r`, `xlf_r`.
 - For MPI code, `mpicc`, `mpCC`, `mpxlf` are the mpi wrappers.
-
- We strongly suggest the compiler flags
`-q64 -O3 -qhot -qarch=pwr6 -qtune=pwr6`
supplemented by `-qsmp=omp` for OpenMP programs.
 - On the link line we suggest using
`-q64 -bdatapsize:64k -bstacksize:64k`
also supplemented by `-qsmp=omp` for OpenMP programs.

Submitting jobs

- To run a job, you must submit to a queue.
 - You submit jobs from a devel node in the form of a script
 - Best to run from the scratch directory (home=read-only)
 - Copy essential results out after your runs have finished.
-
- Group based allocation:
possible for your colleagues to exhaust group limits.
 - Talk to us first to run massively parallel jobs (over 2048 cores).
 - While their resources last, jobs will run at a higher priority than others for groups with an allocation.

Submitting jobs

GPC queues

queue	time(hrs)	max jobs	max cores
batch	48	32/1000	256/8000 (512/16000 threads)
debug	2/0.5	1	16/64 (32/128 threads)
largemem	48	1	16 (32 threads)

You submit to these queues with

```
qsub [options] <script>
```

Common options:

-l: specifies requested nodes and time, e.g.

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

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

-q: specifies the queue, e.g.

```
-q largemem
```

```
-q debug
```

-I specifies that you want an interactive session; no script needed

Mandatory number of nodes may be specified in script.

Submitting jobs

- GPC HyperThreading: Appears as if there are 16 processors rather than 8 per node. For OpenMP application, try setting `OMP_NUM_THREADS=16`. For MPI, try `-np 16`.
- *Always first test if this is beneficial and feasible!*
- Once the job is incorporated into the queue, you can use: `showq` to show the queue, and job-specific commands such as `showstart`, `checkjob`, `canceljob`
- There is no separate queue for infiniband nodes. You request these through the option `:ib`.
- Always request `ppn=8`, even with hyperthreading.
- The largemem queue is exceptional, in that it provides access to two nodes (only) that have 16 processors and 128GB of ram.
- There is no queue for serial jobs, so if you have serial jobs, **YOU** will have to bunch together 8 of them to use the node's full power.

Submitting jobs

TCS queue

queue	time(hrs)	max jobs	max cores
verylong	48	2/25	64/800 (128/1600 threads)

Submitting is done with

```
llsubmit <script>
```

and `llq` shows the queue.

- The POWER6 processors have Simultaneous Multi Threading. Similar to hyperthreading.
- Once your job is in the queue, you can use `llq` to show the queue, and job-specific commands such as `llcancel`, `llhold`, ...
- *Do not run serial jobs on the TCS!*
- To make your jobs start sooner, reduce the `wall_clock_limit` to be closer to the estimated run time (perhaps adding about 10 % to be sure). Shorter jobs are scheduled sooner than longer ones.

Submitting jobs

Example for GPC

```
#!/bin/bash
#PBS -l nodes=8:ppn=8,walltime=1:00:00
#PBS -N myInformativeJobName
cd $PBS_O_WORKDIR
#assume module load openmpi in .bashrc
mpirun -np 64 ./mycode > out
```

```
$ qsub myjob.pbs
```

```
$ qstat
```

Job id	Name	User	Time	Use	S	Queue
2961983.gpc-sched	myInformat...	rzon		0	Q	batch

Submitting jobs

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```
$ ls
```

myInformativeJobName.e2961983	mycode	out
myInformativeJobName.o2961983		

Final tips

- Use the right compilers and compile with optimization.
- Test your job's requirements and scaling behaviour. Start runs on a small scale and work your way up to larger scales.
- Accurately specify the walltime when you submit a job.
- Avoid reading and writing lots of small amounts of data to disk.
- Do not create lots of files.
- Do not submit single serial jobs.
- Do not keep lots of files in your directory (use `tar`).
- Read the SciNet user wiki at support.scinet.utoronto.ca/wiki
- Take SciNet classes: support.scinet.utoronto.ca/courses
- Email to support@scinet.utoronto.ca with any SciNet questions or problems.