Introduction to SciNet

SciNet HPC Consortium
Compute Canada

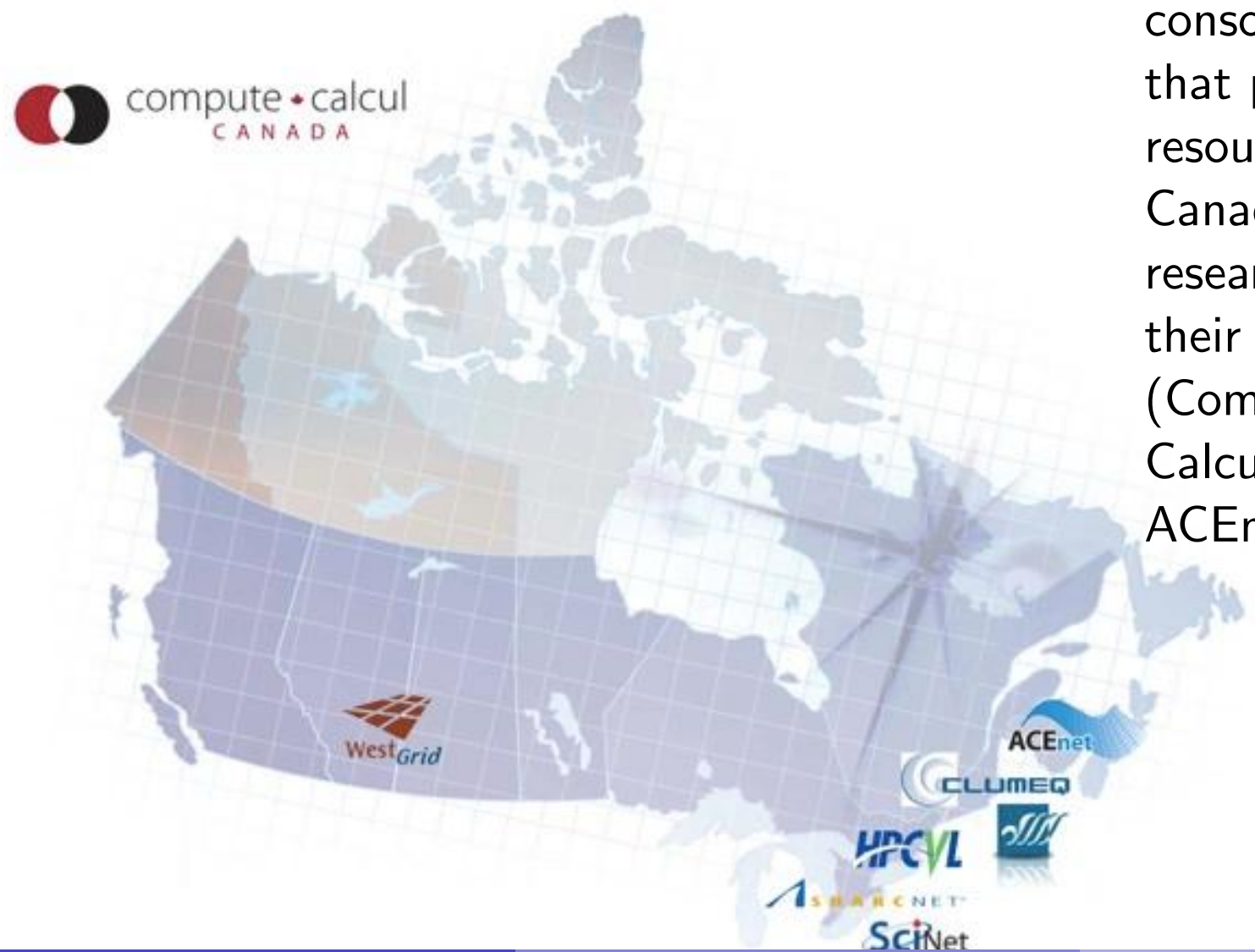
May 6, 2016

Part I

ABOUT SCINET

SciNet is ...

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



There are 4 regional consortia in Canada that provide HPC resources to Canadian academic researchers and their collaborators (Compute Ontario, Calcul Quebec, ACEnet, WestGrid).

SciNet
compute • calcul
CANADA

SciNet is ...

. . . where to take courses on computational topics, e.g.

- Parallel programming courses
- GPGPU with CUDA
- Parallel I/O
- Research Computing with Python
- Scientific Programming with Modern FORTRAN
- Scientific Computing Course (credit for physics/chemistry/astro grads)
- Intro to SciNet
- Linux Shell
- Ontario HPC Summerschool (July 11-15)

https://support.scinethpc.ca/education

SciNet is ...

... where to meet other users at the SciNet User Group meetings.

- SNUGs every 2nd Wednesday of the Month (next one May 11).
- 1 or more TechTalks
- Free pizza!
- https://support.scinet.utoronto.ca/education

... where you go for SciNet Developer Seminars

SciNet people

Analysts

- Daniel Gruner (CTO)
- Mike Nolta
- Scott Northrup
- Marcelo Ponce
- Erik Spence
- Ramses van Zon

Hardware and Systems

- Joseph Chen
- Jason Chong
- Leslie Groer
- Chris Loken (CTO)
- Jaime Pinto
- Ching-Hsing Yu

And

- Technical director
  Prof. Richard Peltier
- Business manager
  Teresa Henriques
- Project coordinator
  Jillian Dempsey (Alex Dos Santos)

Part II

SCINET SYSTEMS

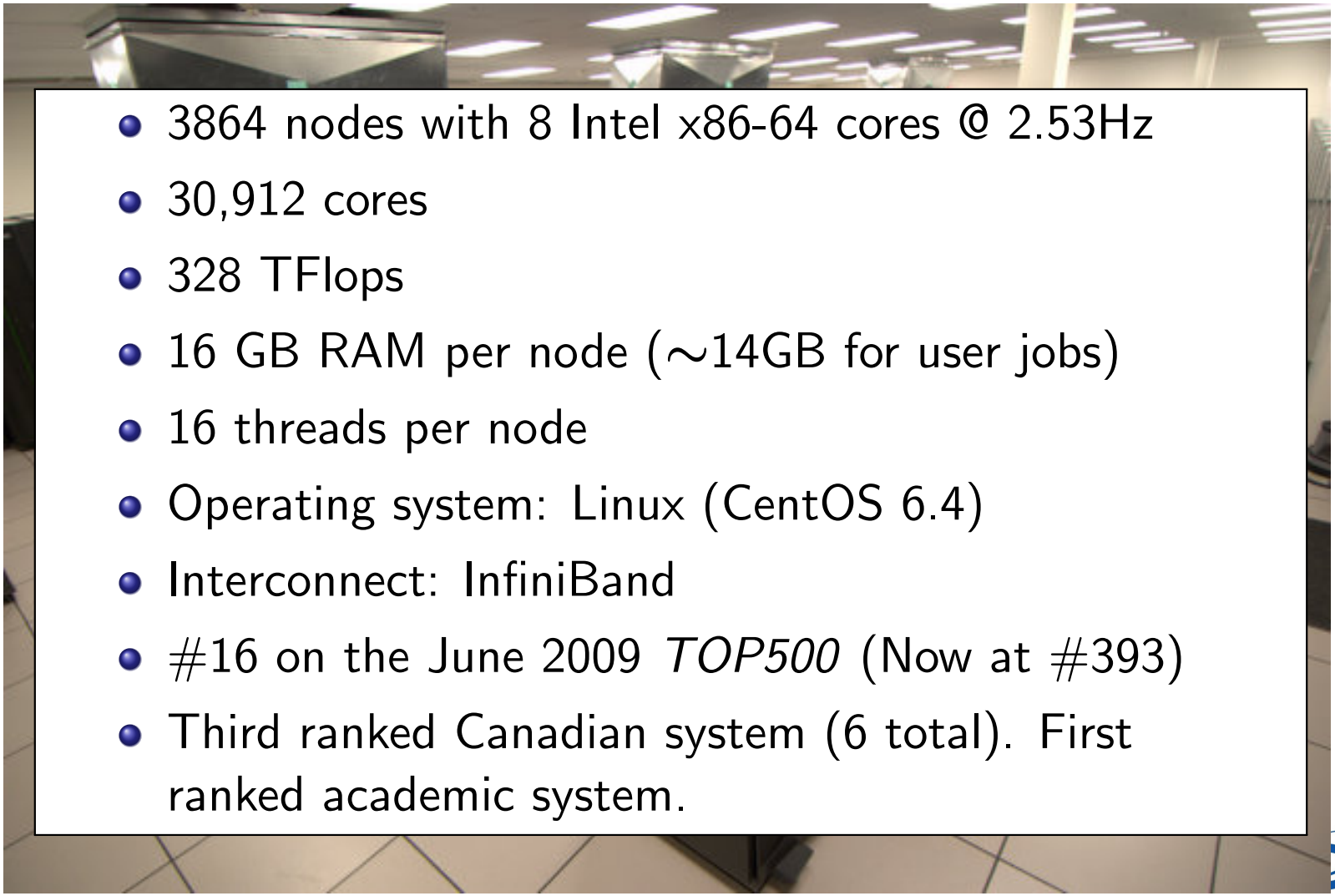
Compute Resources at SciNet

General Purpose Cluster (GPC)

http://wiki.scinethpc.ca/wiki/index.php/GPC_Quickstart

Compute Resources at SciNet

General Purpose Cluster (GPC)



- 3864 nodes with 8 Intel x86-64 cores @ 2.53Hz
- 30,912 cores
- 328 TFlops
- 16 GB RAM per node (∼14GB for user jobs)
- 16 threads per node
- Operating system: Linux (CentOS 6.4)
- Interconnect: InfiniBand
- #16 on the June 2009 *TOP500* (Now at #393)
- Third ranked Canadian system (6 total). First ranked academic system.

http://wiki.scinethpc.ca/wiki/index.php/GPC_Quickstart

Other Compute Resources at SciNet

Tightly Coupled System (TCS)

Power 7 Linux Cluster (P7)

GPU Nodes (Gravity)

Blue Gene/Q

Storage Resources at SciNet

Disk space

- 1.4 PB of storage in 1790 drives
- Two controllers each delivering 4-5 GB/s (r/w)
- *Shared* file system GPFS on all systems
- Your files go in /home/g/group/user ($HOME) and /scratch/g/group/user ($SCRATCH).

Storage space

- HPSS: Tape-backed storage expansion solution.

  1-2TB per group if they ask *(more by allocation)*

  http://wiki.scinethpc.ca/wiki/index.php/HPSS

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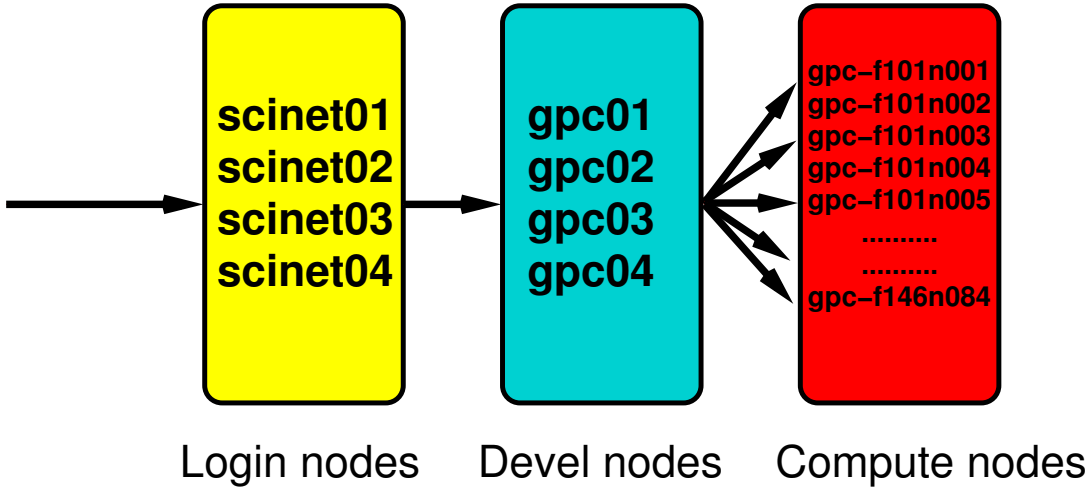
Part III

USING SCINET

Using SciNet



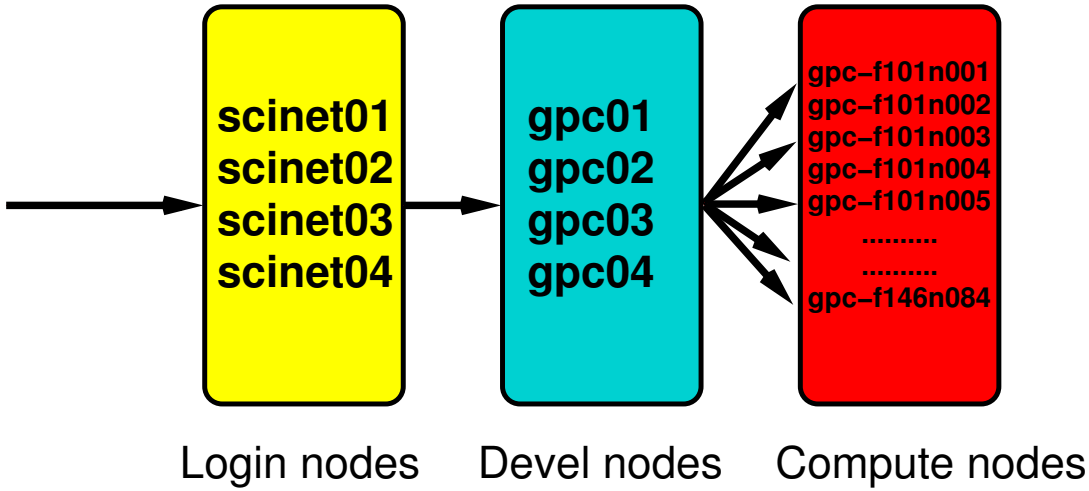
1. Access systems: login.scinet.utoronto.ca

First ssh to login (not part of clusters):

```
ssh <username>@login.scinet.utoronto.ca [-Y]
```

The login nodes are gateways:
- only to be used for small data transfer
- and to proceed logging into one of the devel nodes.
- `-Y` specifies that you want your graphics display forwarded.

Using SciNet



2. Go to the right cluster: ssh to the devel nodes

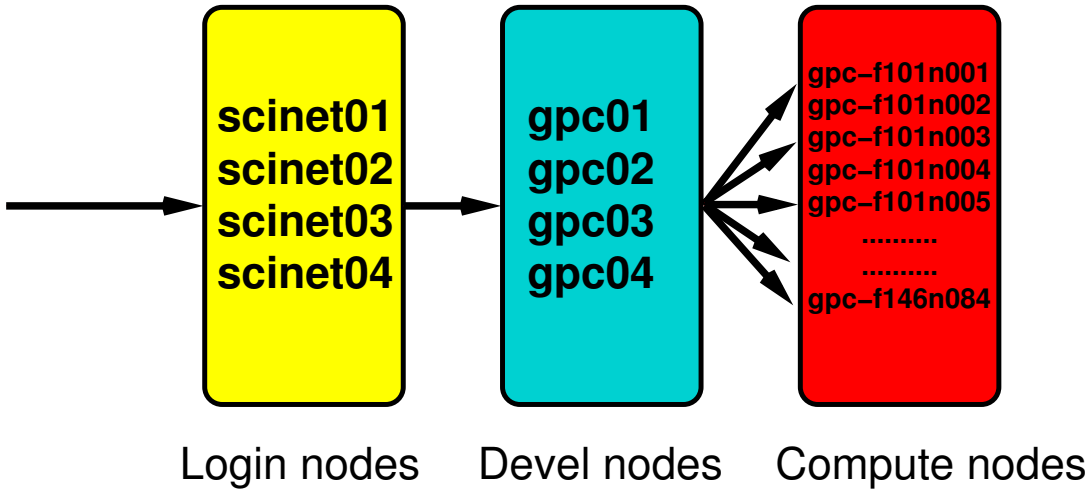
Pick a devel node. On the GPC that means: gpc01, ..., gpc08, e.g.:

```
ssh gpc04
```

Or you can let us randomly pick a node for you:

```
ssh gpc
```

Using SciNet



3. Submit a job to the compute nodes

E.g.

```
cd $SCRATCH/jobdir
qsub jobscript.sh
```

Wait, didn't we skip some steps?

Software and Libraries (1)

Once you log into devel nodes, what software is already installed?

- Other than essentials, all software installed using `module` commands.
- sets environment variables `(LD_LIBRARY_PATH, PATH, ...)`
- Allows multiple, conflicting versions of package to be available.
- More on *Software and Libraries* page of wiki.

http://wiki.scinethpc.ca/wiki/index.php/Software_and_Libraries

Software and Libraries (1)

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- Allows multiple, conflicting versions of package to be available.
- More on *Software and Libraries* page of wiki.

```
gpc-f103n084-$ module avail
------/scinet/gpc/Modules6/Modules/versions-----
3.2.8  3.2.9
------/scinet/gpc/Modules6/Modules/3.2.9/modulef
dot                 modules           use.own
module-cvs          use.deprecated
module-info         use.experimental
-------/scinet/gpc/Modules6/Modules/modulefiles-
ImageMagick/6.6.7(default)
R/2.13.1(default)
R/2.14.1
ROOT/5.30.03(default)
ROOT/5.32.00
Xlibraries/X11-64
abyss/1.3.2
adios/131-openmpi-gcc(default)
amber/10.0.30
antlr/2.7.7
autoconf/2.68
automake/1.11.2
blast/2.2.23+
...
```

http://wiki.scinethpc.ca/wiki/index.php/Software_and_Libraries

Software and Libraries (2)

`module load <module-name>`	use particular software
`module purge`	remove currently loaded modules
`module avail`	list available software packages
`module list`	list loaded modules
`module help <module-name>`	describe a module

- We don't recommend loading modules in your .bashrc file. It can lead to very confusing behaviour under certain circumstances.
- Instead, load modules inside your job submission script.
- Short name gives default (e.g. `intel` → `intel/12.1.3`). However, the defaults are not updated, so they're very old at this point.

Software and Libraries (3)

Dependencies

- Modules sometimes require other modules to be loaded first.

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Example

Software and Libraries (3)

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Example

```
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```

Software and Libraries (3)

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Example

```
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Software and Libraries (3)

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Example

```
gpc-f103n084$ module purge
gpc-f103n084$ module load python
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Software and Libraries (3)

Dependencies

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Example

```
gpc-f103n084$ module purge
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the module(s) '4.8.1 gcc/4.7.2 gcc/4.7.0 gcc/4.6.1 gcc/4.4.6'
python/2.7.2(11):ERROR:102:  Tcl command execution failed:  prereq gcc
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Software and Libraries (3)

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Software and Libraries (3)

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Software and Libraries (3)

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Software and Libraries (3)

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Software and Libraries (3)

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python/2.7.2(11):ERROR:102:  Tcl command execution failed:  prereq intel
gpc-f103n084$ module load gcc intel python
gpc-f103n084$ module list
Currently Loaded Modulefiles:
     1) gcc/4.6.1      2) intel/12.1.3      3) python/2.7.2
```

Software and Libraries (4)

Commercial Software?

- SciNet has an extremely large and broad user base (∼1000 users)
- The only commercial software that SciNet installs is software that can benefit everyone:
  Compilers, math libraries and debuggers.
- No Matlab, Gaussian, IDL, ...
- Octave, Python are available.
- We can help you to install software for which you have a license.

Compiling on SciNet (1): GPC

- From `login.scinet.utoronto.ca`, ssh to one of the eight devel nodes.

  ```
  ssh gpc04 [-Y]
  ```

- We recommend Intel compilers, which are

  ```
  icc, icpc, ifort
  ```

  for C, C++, and Fortran, respectively (from the module `intel`)
- Optimize code for the GPC machine using of at least

  ```
  -O3 -xhost
  ```

- Add `-fopenmp` to the command line for OpenMP
- Compile MPI code with `mpif77/mpif90/mpicc/mpicxx`.
  1. OpenMPI, in module `openmpi` (v1.4.4 , 1.6.4)
  2. Intel MPI, in module `intelmpi` (v4.0.3, 4.1.0, 4.1.1)

Compiling on SciNet (2): library modules

- Libraries are rarely installed in 'standard locations'.
- The name of the base directory for the library you need to access is

  `-I${SCINET_[shortmodulename]_BASE}`

- To compile code that uses that a library from a module, add

  `-I${SCINET_[shortmodulename]_INC}`

  to the compile command.
- To link to the libraries, add

  `-L${SCINET_[shortmodulename]_LIB}`

  to the link command.

Compiling on SciNet (3): library modules

Example

```
scinet04$ ssh -Y gpc03
gpc-f103n084$ module list
No Modulefiles Currently Loaded.
gpc-f103n084$ pwd
/home/s/scinet/rzon
gpc-f103n084$ ls
main.c module.c
gpc-f103n084$ module load intel gsl
gpc-f103n084$ module list
Currently Loaded Modulefiles:
1) intel/12.1.3 2) gsl/1.13-intel
gpc-f103n084$ icc -c -O3 -xHost -o main.o main.c
gpc-f103n084$ icc -c -O3 -xHost -I$SCINET_GSL_INC -o module.o module.c
gpc-f103n084$ icc -o main module.o main.o -L$SCINET_GSL_LIB -lgsl -mkl
gpc-f103n084$ ./main
```

Testing

Why test?

- Computations are run by the job scheduler:
  - Not interactive.
  - Gets queued, i.e. does not run immediately.

  So one cannot catch obvious bugs quickly.
- You need to test your job's requirements and scaling behaviour, so you know what to request from the scheduler.
- Best to start small and work your way up.

How to test:

- Small test jobs can be run on the devel nodes. Rule of thumb: couple of minutes, taking at most about 1-2GB of memory.
- You can run the ddt debugger (or gdb or ddd) on the devel nodes.
- Short tests that do not fit on a development node, or for which you need a dedicated node, can be run through the debug queue.

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Submitting jobs

Every job must be submitted to a batch queue (scheduler).

- You submit jobs from a devel node in the form of a script
- Scheduling is by node. You need to use all 8 cores on the node!
- Must run from the scratch directory (home=read-only)
- Copy essential results out after runs have finished.

Limits:

- Group based limits:
  possible for your colleagues to exhaust group limits
- Talk to us first to run massively parallel jobs ($>$ 2048 cores)
- While their resources last, jobs will run at a higher priority than others for groups with an allocation.

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GPC queues

queue	min.time	max.time	max jobs	max cores
batch	15m	48h	32/1000	256/8000
debug		2h/30m	1	16/64
largemem	15m	48h	1	16

- Submit to these queues from a GPC devel node with

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

- Common options (usually in script):

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

```
-l nodes=2:ppn=8,walltime=1:00:00
```

  `-q`: specifies the queue, e.g.

```
-q batch
-q debug
-q largemem
```

  `-I` specifies that you want an interactive session.

GPC queues

- The debug queue is used for testing: highly recommended!
- 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. Use GNU Parallel†.
- Remember: submit your job from a devel node, NOT the login node!

† O. Tange (2011): GNU Parallel - The Command-Line Power Tool, *;login: The USENIX Magazine,* February 2011:42-47.

GPC job script example

```
#!/bin/bash
#PBS -l nodes=1:ppn=8
#PBS -l walltime=1:00:00
#PBS -N simple-openmp-job
cd $PBS_O_WORKDIR
export OMP_NUM_THREADS=8
./openmp_example > output
```

```
$ qsub scriptname.pbs
```

GPC job script example

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- In this case, scheduler looks for one node with 8 cores for 1 hour.

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- It gives this job the name `simple-openmp-job`.

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- Once the scheduler has found such a node, it runs the script there.

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- In this case, scheduler looks for one node with 8 cores for 1 hour.
- It gives this job the name `simple-openmp-job`.
- Once the scheduler has found such a node, it runs the script there.
  - Change directory to that from which the script was submitted.
  - Setting an environment variable
  - Running the `openmp_example` application.

GPC queues

Monitoring

Once the job is incorporated into the queue (this takes a minute),
Command you can use:

- `qstat` to show your jobs in the queue;
- `showstart -e hist JOBID` to get an estimate for when it will run;
- `checkjob JOBID` to get information on the job (quite verbose);
- `canceljob JOBID` to cancel the job.

GPC queues

Jobs can be in one of three states:

1. Running: great, all is well (at least from a scheduler point-of-view).
2. Idle: waiting in the queue for resource. All is well (at least from a scheduler point-of-view).
3. Blocked: too many jobs submitted at the same time; scheduler will not consider these until some of the idle ones have been scheduled.

More serious errors (such as asking for a node with 16 cores), will lead to a rejection, and you will get an error with a more-or-less cryptic explanation. See the FAQ on the wiki for some typical cases and their explanation.

Example 1 (GPC)

```
gpc-f101n084-$
```

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```
gpc-f101n084-$ module load intel openmpi
gpc-f101n084-$
```

Example 1 (GPC)

```
gpc-f101n084-$ module load intel openmpi
gpc-f101n084-$ mpif90 -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$
```

Example 1 (GPC)

```
gpc-f101n084-$ module load intel openmpi
gpc-f101n084-$ mpif90 -O3 -xhost mycode.f90 -o mycode
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gpc-f101n084-$
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gpc-f101n084-$
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gpc-f101n084-$ cp mycode $SCRATCH/example1
gpc-f101n084-$ cd $SCRATCH/example1
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=8:ppn=8,walltime=1:00:00
     #PBS -N JobName
     cd $PBS_O_WORKDIR
     module load intel openmpi
     mpirun -np 64 ./mycode > out
gpc-f101n084-$
```

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     #PBS -N JobName
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gpc-f101n084-$ qsub myjob.pbs
     2961983.gpc-sched
gpc-f101n084-$
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gpc-f101n084-$ cd $SCRATCH/example1
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=8:ppn=8,walltime=1:00:00
     #PBS -N JobName
     cd $PBS_O_WORKDIR
     module load intel openmpi
     mpirun -np 64 ./mycode > out
gpc-f101n084-$ qsub myjob.pbs
     2961983.gpc-sched
gpc-f101n084-$ qstat
```

(or **checkjob 2961983**, or **showq -u $USER**)

Example 1 (GPC)

```
gpc-f101n084-$ module load intel openmpi
gpc-f101n084-$ mpif90 -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example1
gpc-f101n084-$ cp mycode $SCRATCH/example1
gpc-f101n084-$ cd $SCRATCH/example1
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=8:ppn=8,walltime=1:00:00
     #PBS -N JobName
     cd $PBS_O_WORKDIR
     module load intel openmpi
     mpirun -np 64 ./mycode > out
gpc-f101n084-$ qsub myjob.pbs
     2961983.gpc-sched
gpc-f101n084-$ qstat    (or checkjob 2961983, or showq -u $USER)
     Job id              Name             User Time Use S Queue
     ----------------- -------------- ---- -------- - --------
     2961983.gpc-sched JobName        rzon         0 Q batch
gpc-f101n084-$
```

Example 1 (GPC)

```
gpc-f101n084-$ module load intel openmpi
gpc-f101n084-$ mpif90 -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example1
gpc-f101n084-$ cp mycode $SCRATCH/example1
gpc-f101n084-$ cd $SCRATCH/example1
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=8:ppn=8,walltime=1:00:00
     #PBS -N JobName
     cd $PBS_O_WORKDIR
     module load intel openmpi
     mpirun -np 64 ./mycode > out
gpc-f101n084-$ qsub myjob.pbs
     2961983.gpc-sched
gpc-f101n084-$ qstat    (or checkjob 2961983, or showq -u $USER)
     Job id              Name             User Time Use S Queue
     ------------------- ---------------- ---- -------- - --------
     2961983.gpc-sched JobName          rzon            0 Q batch
gpc-f101n084-$ ls
     JobName.e2961983   JobName.o2961983   mycode   myjob.pbs
     out
```

Example 2 (GPC)

```
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$ cd $SCRATCH/example2
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$ cd $SCRATCH/example2
gpc-f101n084-$ cat > joblist.txt
   mkdir run1; cd run1; ../mycode 1 > out
   mkdir run2; cd run2; ../mycode 2 > out
   mkdir run3; cd run3; ../mycode 3 > out
   ...
   mkdir run64; cd run64; ../mycode 64 > out
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$ cd $SCRATCH/example2
gpc-f101n084-$ cat > joblist.txt
   mkdir run1; cd run1; ../mycode 1 > out
   mkdir run2; cd run2; ../mycode 2 > out
   mkdir run3; cd run3; ../mycode 3 > out
   ...
   mkdir run64; cd run64; ../mycode 64 > out
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=1:ppn=8,walltime=24:00:00
     #PBS -N ASerialJob
     cd $PBS_O_WORKDIR
     module load intel gnu-parallel
     parallel -j 8 < joblist.txt
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$ cd $SCRATCH/example2
gpc-f101n084-$ cat > joblist.txt
   mkdir run1; cd run1; ../mycode 1 > out
   mkdir run2; cd run2; ../mycode 2 > out
   mkdir run3; cd run3; ../mycode 3 > out
   ...
   mkdir run64; cd run64; ../mycode 64 > out
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=1:ppn=8,walltime=24:00:00
     #PBS -N ASerialJob
     cd $PBS_O_WORKDIR
     module load intel gnu-parallel
     parallel -j 8 < joblist.txt
gpc-f101n084-$ qsub myjob.pbs
     2961985.gpc-sched
gpc-f101n084-$
```

Example 2 (GPC)

```
gpc-f101n084-$ module load intel
gpc-f101n084-$ ifort -O3 -xhost mycode.f90 -o mycode
gpc-f101n084-$ mkdir $SCRATCH/example2
gpc-f101n084-$ cp mycode $SCRATCH/example2
gpc-f101n084-$ cd $SCRATCH/example2
gpc-f101n084-$ cat > joblist.txt
   mkdir run1; cd run1; ../mycode 1 > out
   mkdir run2; cd run2; ../mycode 2 > out
   mkdir run3; cd run3; ../mycode 3 > out
   ...
   mkdir run64; cd run64; ../mycode 64 > out
gpc-f101n084-$ cat > myjob.pbs
     #!/bin/bash
     #PBS -l nodes=1:ppn=8,walltime=24:00:00
     #PBS -N ASerialJob
     cd $PBS_O_WORKDIR
     module load intel gnu-parallel
     parallel -j 8 < joblist.txt
gpc-f101n084-$ qsub myjob.pbs
     2961985.gpc-sched
gpc-f101n084-$ ls
     ASerialJob.e2961985  ASerialJob.o2961985  joblist.txt  mycode
     myjob.pbs            run1/                run2/        run3/
     ...
```

Part IV

DATA MANAGEMENT TIPS

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 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.
- 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 11GB max.
- Copy back from ramdisk at end of run.

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Storage Limits at SciNet

location	quota	block-size	time-limit	backup	devel	comp
/home	50GB	256kB	perpetual	yes	rw	ro
/scratch	20TB/1M	4MB	3 months	no	rw	rw

- Compute nodes do not have local hard drives.
- /home and /scratch are both part of the GPFS file system.
- GPFS is a high-performance file system which provides rapid reads and writes to large data sets in parallel from many nodes.
- Performs poorly accessing data sets which consist of many, small files.
- Avoid reading and writing lots of small amounts of data to disk.
- Many small files on the system would waste space and would be slower to access, read and write.

http://wiki.scinethpc.ca/wiki/index.php/Data_Management

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.
- Your machine must be reachable from the outside.

Moving data to HPSS

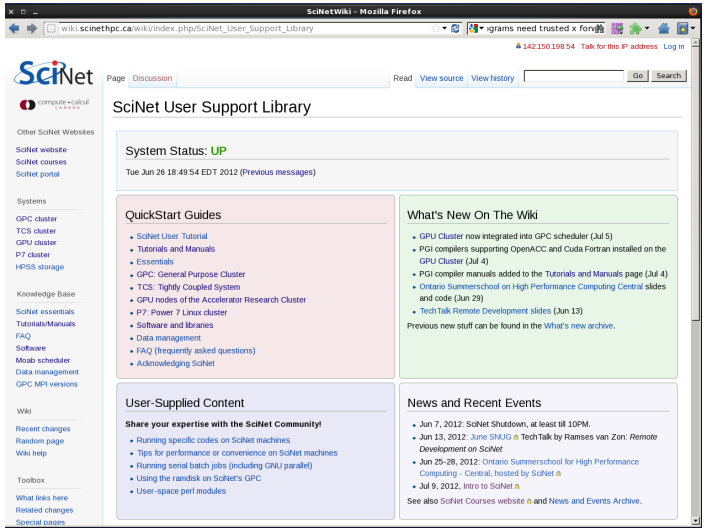
- HPSS is a tape-based storage solution.
- 1-2TB per group by default (more with special allocation).

Part V

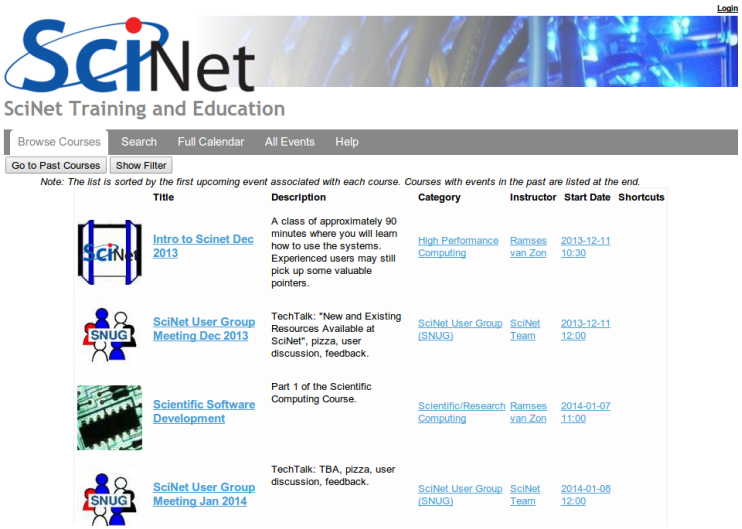
USEFUL SITES

www.scinethpc.ca

wiki.scinethpc.ca



https://support.scinet.utoronto.ca/education



https://portal.scinet.utoronto.ca

SciNet usage reports
Change password, default allocation, maillist subscriptions

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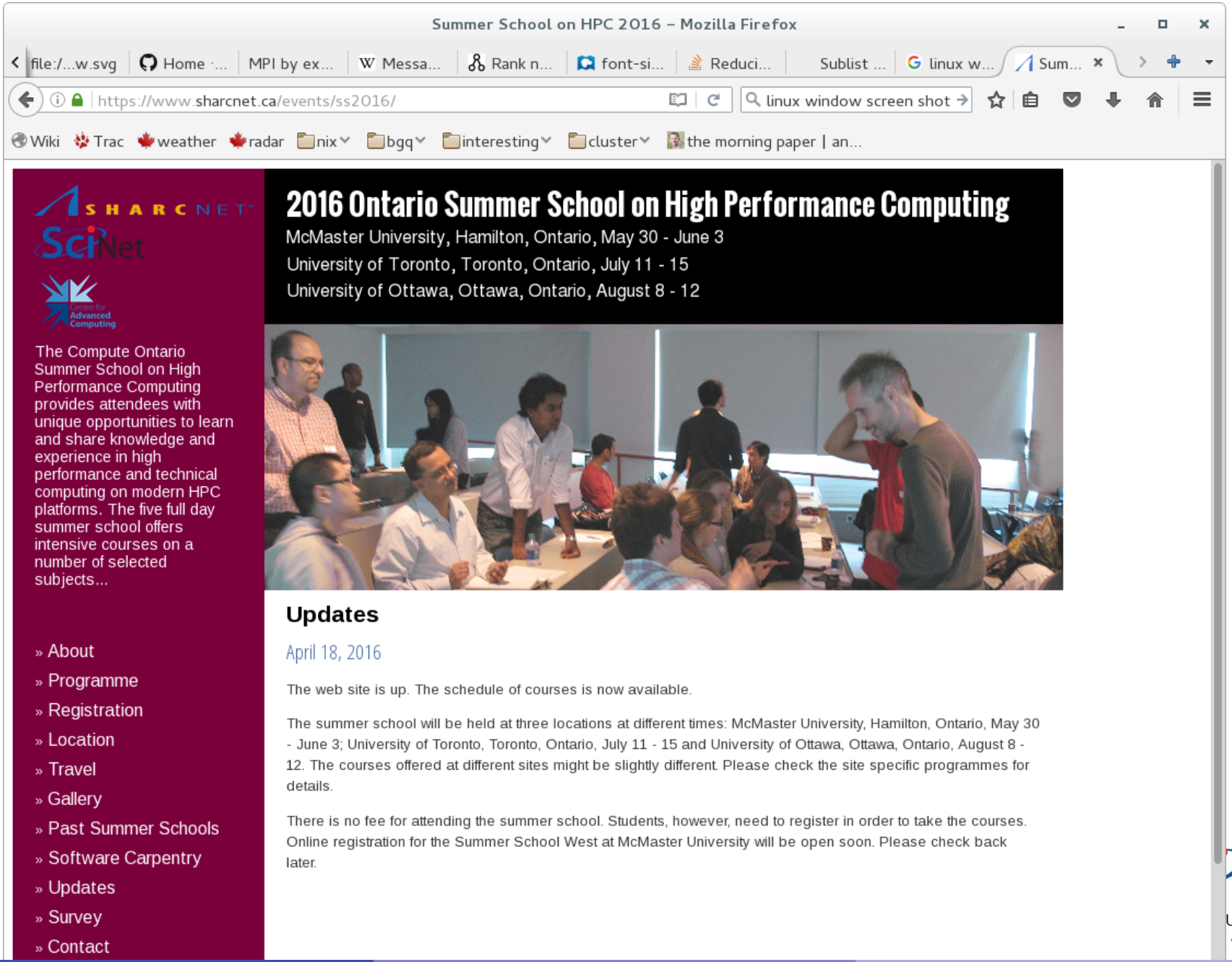
https://www.sharcnet.ca/events/ss2016/



Thanks!