

Introduction to SciNet, Niagara & Mist

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Outline

- About SciNet
- Using Niagara and Mist
 - ▶ Setting up an account
 - ▶ Logging in via SSH
 - ▶ Available software and libraries
 - ▶ Submitting jobs to the scheduler
- Data management and I/O tips

About SciNet



About SciNet

SciNet is a centre for high-performance computing at the University of Toronto.

- We run massively parallel computers to meet the needs of researchers across Canada.
- 5 other HPC centres in Canada also provide academic **Advanced Research Computing** resources.
- These centres maintain and support a network of resources available to researchers across Canada, under a national allocation system administered by the **Digital Research Alliance of Canada**.

National research computing clusters

- Four general purpose clusters:
 - ▶ [Cedar](#) (Simon Fraser University)
 - ▶ [Graham](#) (University of Waterloo)
 - ▶ [Béluga](#) (Montréal, Québec)
 - ▶ [Narval](#) (Montréal, Québec)
- One large parallel cpu cluster:
 - ▶ [Niagara](#) (University of Toronto)
- One homogeneous gpu cluster:
 - ▶ [Mist](#) (University of Toronto)
- Several [cloud](#) systems (Sherbrooke, Victoria, Waterloo).

What does SciNet do?

Systems

We host one of the largest supercomputers in Canada available to academics.

- [Niagara](#) CPU cluster



Plus some smaller ones

- [Mist](#) GPU cluster
- Rouge AMD GPU cluster
- Teach

And a longer-term storage facility

- [HPSS](#)

What else does SciNet do?

Training

- Intro to SciNet and Niagara, Linux Shell
- Scientific and Parallel Programming (C, C++, Fortran, R, Python, CUDA)
- Grad Courses on Scientific Computing , Data Analysis, and BioStatistics
- Data management, Parallel I/O, Databases, Machine learning, AI
- Ontario HPC summer school
- International HPC summer school (together with PRACE, XSEDE, RIKEN)

For full list see: <https://education.scinet.utoronto.ca>

Research

<https://www.scinet.utoronto.ca/research-scinet>

SciNet people

Reach all of us at once at support@scinet.utoronto.ca

Software, user support, training, etc..

- Mike Nolta
- Erik Spence
- Ramses van Zon
- Bruno Mundim
- Alexey Fedoseev
- James Willis
- Yohai Meiron

- Chief Technical Officer: Daniel Gruner
- Information Systems Security: Shawn Winnington-Ball

Hardware, systems, etc..

- Joseph Chen (Associate CTO)
- Ching-Hsing Yu
- Leslie Groer
- Jaime Pinto
- Marco Saldarriaga
- Vladimir Slavnic
- Ram Sharma
- Norbert Krawiec

- Business manager: Jackie Denholm

Niagara

- 80,960 x86-64 cores.
- 2,024 *Lenovo SD530* nodes
- Per node:
 - ▶ 40 Intel SkyLake/CascadeLake cores @ 2.4GHz
 - ▶ 188 GiB RAM
- 3.6 PFlops sustained (6.25 PFlops theoretical).
#59 on the Nov 2018 TOP500* (now #177)
- InfiniBand Dragonfly+ network
1:1 up to 432 nodes, 2:1 beyond that.
- Parallel shared file system for home, scratch, project
- Burst Buffer for fast I/O



Mist

- Niagara's little GPU sibling
- 54 IBM Power-9 nodes with 4 GPUs.
- Per node:
 - ▶ 32 Power-9 cores @ 2.4GHz
 - ▶ 256 GB RAM per node
 - ▶ 4 NVIDIA "Volta" GPUs with 32GB
- 1 PFlops peak (1.6 PFlops theoretical).
- Interconnect: 1:1 InfiniBand Dragonfly+
- Same parallel shared file systems as Niagara



Using Niagara and Mist



Access

- 1 Register with the Alliance CCDB

https://ccdb.alliancecan.ca/account_application

PIs have to get an account one first, so they can sponsor your account at no cost.

The approval process typically takes 1-2 business days.

- 2 Go to

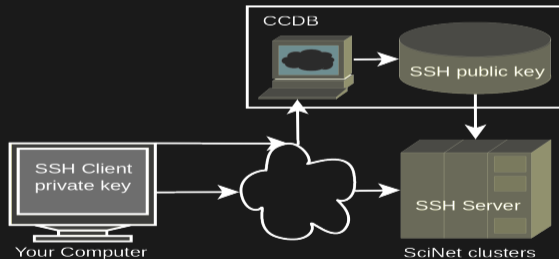
https://ccdb.alliancecan.ca/services/opt_in

and click on the “Join” button next to Niagara and Mist.

- 3 After a business day or two, you get an email confirming your access to Niagara and Mist.

Access: Secure Login

- As with all SciNet and Alliance systems, access is via **ssh** only.
- The connection will get you to a Linux command line interface.
- Password doesn't work on Niagara and Mist! **SSH keys** must be used to authenticate.
- SSH keys come in a **pair**:
 - ▶ a **private key** which is kept on your own computer and used to **connect**
 - ▶ a **public key** that you upload to CCDB and which then propagates to the clusters.



The same SSH keys will work for connecting to the other Alliance clusters.

Access: SSH key setup for first login

- To access SciNet systems for the first time, open a local terminal window on your computer (e.g. MobaXTerm on Windows).
- Then generate a **ssh key pair** with the following command:

```
laptop> ssh-keygen -t ed25519 -C "USERNAME@MYLAPTOP dra" -f ~/.ssh/dra_ed25519
```

- Enter a **passphrase** to protect your private key.
- A private key, `dra_ed25519`, and a public key, `dra_ed25519.pub` are then created in the directory `“.ssh”` in your home directory.
- `-f` option specifies the filename of the key file.
- (optional) `-C` option allows you to insert a comment into the key.

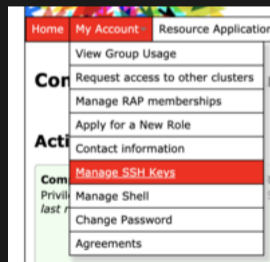
Access: Uploading Your Public Key

Once you created your ssh key pair, you need to make Niagara/Mist aware of the public part of your key.

- Step 1: Use your Alliance/CCDB credentials to visit the following site:

https://ccdb.alliancecan.ca/ssh_authorized_keys

or via the CCDB menu:



Access: Uploading Your Public Key

- Step 2: Grab your SSH public key:

```
laptop> cat ~/.ssh/dra_ed25519.pub  
ssh-ed25519 AAAAC3NzaC1lZDI1NTE5AAAAIEpDf+Wcvtru6pUcBgJQo/3+cmI4+MisfNE3U46/CDkx  
USERNAME@MYLAPTOP dra
```

- Step 3: Paste the public key into the CCDB form and click “Add Key” button:

Manage SSH Keys

Add an SSH key

Secure Shell (SSH) is a widely used standard to connect to remote servers in a secure way. SSH is the normal way for Compute Canada users to connect in order to execute commands, submit jobs, follow the progress of these jobs and in some cases, transfer files.

An SSH key is composed of a pair of files, one containing a public key, and the other containing a private key. The private key is protected by a passphrase and can be kept unlocked for a certain duration through the use of a program called an SSH agent. Unless the private key is unlocked on your computer, any server which knows the corresponding public key can authenticate you without having to ask for your password.

If you are connecting to our clusters through SSH with your Compute Canada username and password, you might consider using an SSH key instead. SSH keys used with a strong passphrase are more secure than passwords, and can be more convenient to use.

To add an SSH key you will need to generate one or use an existing key. For more information about how to use SSH keys [click here](#).

SSH Key

Paste your public SSH key in the field below.

On many systems, if you have already generated a key, it may be stored in a default location such as `~/.ssh/id_rsa.pub`. Do **not** paste your private SSH key.

Description

Give your key a brief description. If your key already contains a description, it will appear below.

[Add Key](#)

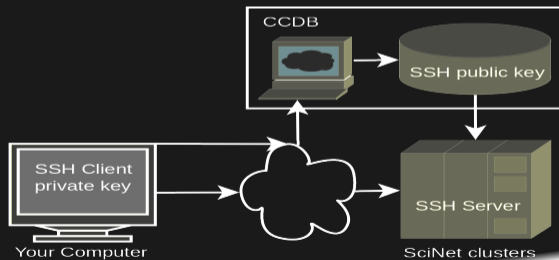
Access: Logging in

Wait a few minutes for your new uploaded public key to propagate to the systems.

Then ssh into the Niagara [login nodes](#) specifying the corresponding ssh private key:

```
laptop> ssh -Y -i ~/.ssh/dra_ed25519 USERNAME@niagara.scinet.utoronto.ca
Enter passphrase for dra_ed25519:
nia-login07:~$
```

- The optional `-Y` is needed to open windows from the Niagara command-line onto your local X server.
- `-i` option selects a file from which the identity (private key) for key authentication is read.
- For *Mist*, replace *niagara* with *mist*.



Connecting more conveniently: ssh options and keys

Once you've logged in successfully, you can save the ssh options in `~/.ssh/config`:

```
Host niagara
  HostName niagara.scinet.utoronto.ca
  User USERNAME
  IdentityFile ~/.ssh/dra_ed25519
  IdentitiesOnly yes
```

Now you can access Niagara by simply typing (in addition to your passphrase):

```
laptop> ssh niagara
```

This will also make data transfer commands like `scp` and `rsync` work more easily.

You can use the `ssh-agent` to hold your key for you by typing:

```
laptop> ssh-add ~/.ssh/dra_ed25519
```

This will ask for the passphrase, and then save that key so you do not have to type the passphrase again during the session.

Ssh Key Best Practices

- Do not share or copy your private key.
- Always protect it with a strong passphrase.
- Create a separate key pair for each computer you use to access our systems.
- Do not create key pairs on shared systems like HPC clusters.

A reference to help you troubleshooting: https://docs.alliancecan.ca/wiki/SSH_Keys

- If you get a warning “REMOTE HOST IDENTIFICATION HAS CHANGED”, check the list of fingerprints on https://docs.alliancecan.ca/wiki/SSH_host_keys.

Usage: login, compute, and datamovers nodes

There are three types of nodes on Niagara:

Login nodes

These are where you develop, edit, compile, prepare and submit jobs.

These nodes are shared, i.e., multiple users are on the same nodes.

These nodes have limits in terms of how long you can run and the memory your applications can use.

Compute nodes

To do computations on Niagara, you must submit a **batch job**. In a **job script**, you can specify how many compute nodes you need and for how long.

Once the job scheduler starts your job, that is the only thing running on its reserved nodes.

Datamover nodes

Meant for large data transfers from, to or on Niagara.

Usage: Storage Systems and Locations

Home and scratch

```
$HOME=/home/g/groupname/username
```

```
$SCRATCH=/scratch/g/groupname/username
```

Use these convenient variables!

```
nia-login07:~$ pwd
/home/s/scinet/myusername

nia-login07:~$ cd $SCRATCH

nia-login07:myusername$ pwd
/scratch/s/scinet/myusername
```

Project

Users from groups with a RAC allocation will also have a [project](#) directory.

```
$PROJECT=/project/g/groupname/username
```

Burst Buffer

Groups with heavy I/O can request access to a smaller, faster parallel file system called [burst buffer](#).

```
$BBUFFER=/bb/g/groupname/username
```

Usage: Storage Limits

location	quota	#files	block size	expiration	backed up	on login	compute
\$HOME	100 GB	250K	1 MB		yes	yes	read-only
\$SCRATCH	25 TB	6M	16 MB	2 months	no	yes	yes
\$PROJECT	by group allocation	depends	16 MB		yes	yes	yes
\$BBUFFER	10TB, by request		1 MB	48 hours	no	yes	yes
\$ARCHIVE	by group allocation				dual-copy	no	no

- Compute nodes do not have local storage, but they have a lot of memory, which you can use as if it is local disk (`$SLURM_TMPDIR`)
- `$ARCHIVE` space, also called [nearline](#) storage or HPSS, is not mounted on login or compute nodes.
- Storage space on project and HPSS is allocated through the annual [Alliance RAC allocation competition](#).
- Backup means a recent snapshot, not an archive of all data that ever was.

Moving data

To move amounts less than 20GB, use the [login nodes](#)

Use scp or rsync to and from niagara.scinet.utoronto.ca.

- For scp to use your ssh key, give it the '-i ~/.ssh/YOURKEY' option. *E.g.*

```
laptop> scp -i ~/.ssh/dra_ed25519 this USERNAME@niagara.scinet.utoronto.ca:that
```

- These commands must be given on your computer.
- For rsync to use your ssh key, give it the '-e "ssh -i ~/.ssh/YOURKEY"' option.
- This will time out for amounts larger than about 20GB.

To move amounts larger than 20GB, use the [datamover nodes](#).

- Use scp or rsync with nia-datamover1.scinet.utoronto.ca or nia-datamover2.scinet.utoronto.ca.
- If you do this often, consider using [Globus](#), a web-based tool for data transfer.

To move data to HPSS/Archive/Nearline

- [HPSS](#) is a tape-based storage solution, and is SciNet's [nearline](#) a.k.a. [archive](#) facility.
- Store and recall using [scheduled jobs](#) or [Globus](#).

Usage: Software and Libraries

Once you are on one of the login nodes, what software is already installed?

- Other than essentials, all installed software is made available using `module` commands.
- These set environment variables (PATH, etc.)
- Allows multiple, conflicting versions of a given package to be available.
- `module overview` shows the available software.

```
nia-login07:~$ module overview
----- /scinet/niagara/.../base -----
apptainer      (2)  meson      (1)
arm-forge     (1)  mii        (1)
autotools     (2)  mpfr       (1)
bedtools      (2)  muscle     (1)
bowtie2       (1)  namd       (1)
bwa-mem2      (1)  nano       (1)
bwa           (1)  ncl        (1)
cereal        (1)  ncvview    (1)
cget          (1)  ninja      (1)
...
----- /scinet/niagara/stacks -----
CCEnv (1)  NiaEnv (3)
```


Usage: Software and Libraries, continued

Module subcommands

- `module load <module-name>`
use particular software
- `module purge`
remove currently loaded modules
- `module spider`
(or `module spider <module-name>`)
list available software packages
- `module list`
list loaded modules

On Niagara, there are a few **distinct software stacks** whose modules do not mix.

```
module load NiaEnv/2022a
module load NiaEnv/2019b
```

```
module load CCEnv StdEnv
```

Stacks compiled for Niagara
(newer)
(default, but old)

Software stack as on the
Alliance's general purpose
clusters.

On Mist, there is one, system-specific stack,
with modules like `cuda`, `pgi`, `xl`.

Usage: Module examples

```
nia-login07:~$ module load openmpi
```

```
Lmod has detected the following error: These module(s) or extension(s) exist but
cannot be loaded as requested: "openmpi"
```

```
Try: "module spider openmpi" to see how to load the module(s).
```

```
nia-login07:~$ module spider openmpi
openmpi:
```

Description:

The Open MPI Project is an open source MPI-2 implementation

Versions:

openmpi/3.1.3

openmpi/4.0.1

openmpi/4.0.3

For detailed information about a specific "openmpi" module use the full name.

For example:

```
$ module spider openmpi/4.0.3
```

Usage: Module examples, continued

```
nia-login07:~$ module spider openmpi/4.0.1
```

```
-----  
openmpi: openmpi/4.0.1  
-----
```

Description:

The Open MPI Project is an open source MPI-2 implementation
You will need to load all module(s) on any one of the lines below before the "ope

```
gcc/8.3.0
```

```
gcc/9.2.0
```

```
intel/2019u3
```

```
intel/2019u4
```

Help:

```
Description
```

```
=====
```

```
The Open MPI Project is an open source MPI-2 implementation.
```

```
More information
```

```
=====
```

```
- Homepage: https://www.open-mpi.org/
```

Usage: Module examples, continued

```
nia-login07:~$ module load intel/2019u4  
nia-login07:~$ module load openmpi/4.0.1
```

```
nia-login07:~$ module list  
Currently Loaded Modules:  
  1) NiaEnv/2019b (S)   2) intel/2019u4   3) openmpi/4.0.1
```

Usage: Tips for loading modules

- We advise *against* loading modules in your `.bashrc` file.
This could lead to very confusing behaviour under certain circumstances.
- Instead, load modules by hand when needed, or by sourcing a separate script.
- Load run-specific modules inside your job submission script.
- Short names give default versions; e.g. `intel` → `intel/2019u4`.
It is usually better to be explicit about the versions, for future reproducibility.

Can I Run Commercial Software?

- Possibly, but you have to **bring your own license** for it.
- SciNet and the Digital Research Alliance of Canada have an extremely large and broad user base of thousands of users, so we cannot provide licenses for everyone's favorite software.
- Thus, the only commercial software installed on Niagara is software that can benefit everyone, i.e. compilers and debuggers.
- Open source alternatives like Octave, Python, R, Julia are available.
- We are happy to help you to install commercial software for which you have a license.
- In some cases, if you have a license, you can use software in the CCEnv stack.

Usage: Python modules

- Several python versions are available as modules.
- These comes with optimized Numpy, SciPy, ...
- Further packages for Python and R are not installed in modules; These need to be installed in users' home directories.
- For installing packages for Python, use [virtual environments](#):

```
nia-login07:~$ module load python/3.9.8
nia-login07:~$ virtualenv --system-site-packages ~/myenv
nia-login07:~$ source ~/myenv/bin/activate
(myenv) nia-login07:~$ pip install THISPACKAGE
```

If you want, use the “venv2jup” command to use your virtual environment in the JupyterHub.

If at all possible, do not use conda environments.

Usage: R modules

- Several R versions are available as modules, but you first need to load a gcc module

```
$ module load gcc
$ module -r avail ^r/
----- /scinet/niagara/software/2019b/modules/gcc-8.3.0 -----
      r/3.5.3      r/3.6.1      r/3.6.3 (D)      r/4.0.3      r/4.1.2
$ module load r/4.1.2
```

- To install R packages, use the R command “install.packages(...)”
- The first time you do this, you’ll be asked if you are okay with installing in your home directory (hint: you are).

Usage: Compiling on Niagara

Suppose you have to compile your own C, C++ or Fortran code.

- Not a problem: Niagara has GNU compilers as well as Intel compilers installed in **modules**.
- Need an MPI library? Not a problem either: Niagara has openmpi and intelmpi libraries as **modules**.
- We recommend that you use the intel compilers with openmpi libraries.
- Use `-march=native` (gcc) or `-xhost` (intel) compilation flags to get the most out of Niagara's cpus.
- Need libraries? "module load" them.

Example

```
nia-login07:~$ module load intel/2019u4 gsl/2.5
nia-login07:~$ ls
main.c module.c
nia-login07:~$ icc -c -O3 -xHost -o main.o main.c
nia-login07:~$ icc -c -O3 -xHost -o module.o module.c
nia-login07:~$ icc -o main module.o main.o -lgsl -mkl
```

Usage: Testing

- Small test jobs can be run on the login nodes.
Rule of thumb: couple of minutes, taking at most about 1-2GB of memory, couple of cores, ≤ 1 gpu.
- You can run the the `ddt` debugger after `module load ddt`.
- The `ddt` module also gives you the `map` performance profiler.
- Short tests on Niagara that do not fit on a login node, or for which you need a dedicated node, request an `interactive debug job` with the `debugjob` command

```
nia-login07:~$ debugjob N
```

where N is the number of nodes. The duration of your interactive debug session can be at most one hour, can use at most N=4 nodes, and each user can only have one such session at a time.

- For short single-gpu tests on Mist use

```
mist-login01:~$ debugjob -g 1
```

Usage: Submitting jobs to the Compute Nodes

- Niagara and Mist use **SLURM** as the job scheduler.
- You submit jobs from a login node by passing a script to the **sbatch** command:

```
nia-login07:~$ sbatch jobscript.sh
```

- This puts the job in the queue. It will run on the compute nodes in due course.
- Jobs will run under their group's RRG allocation, or, if the group has none, under a RAS (or “default”) allocation.

Keep these in mind when submitting jobs

- Niagara scheduling is **by node**, so in multiples of 40-cores. *Use all cores!*
- Mist scheduling is **by single gpu** or **by whole node** (multiple of 4 gpus). *Use all GPUs!*
- Maximum walltime is **24 hours**.
- Jobs must write to your scratch or project directory (**home is read-only** on compute nodes).
- Compute nodes have **no internet access**.

Example submission script (Many serial jobs)

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=40
#SBATCH --time=3:00:00
#SBATCH --job-name serialjob
#SBATCH --output=serial_output_%j.txt
#SBATCH --mail-type=FAIL
module load NiaEnv/2019b
module load python/3
module load gnu-parallel

source ~/myenv/bin/activate
parallel python serial.py ::: {0..99}
```

```
nia-login07:scratch$ sbatch serialjob.sh
```

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.
- `sbatch` reads these lines as a job request
- In this case, SLURM looks for one node with 40 tasks to be run for 3 hours.
- Submit from `/scratch`, as `/home` is read-only.
- Once it found such a node, script is run:
 - ▶ Loads modules
 - ▶ Activates python environment
 - ▶ Has gnu-parallel load-balance 99 tasks over 40 cores.

https://docs.scinet.utoronto.ca/index.php/Running_Serial_Jobs_on_Niagara

Example submission script (OpenMP)

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --cpus-per-task=40
#SBATCH --time=1:00:00
#SBATCH --job-name omp_job
#SBATCH --output=omp_output_%j.txt
#SBATCH --mail-type=FAIL
module load NiaEnv/2019b intel/2019u4

OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
export OMP_NUM_THREADS

./omp_example # or 'srun ./omp_example'

nia-login07:scratch$ sbatch omp_job.sh
```

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.
- `sbatch` reads these lines as a job request (which it gives the name `omp_job`).
- In this case, SLURM looks for one node with 40 cores to be run inside one task, for 1 hour.
- Submit from `/scratch`, as `/home` is read-only.
- Once it found such a node, script is run:
 - ▶ Loads modules;
 - ▶ Sets an environment variable;
 - ▶ Runs the `omp_example` application.

Example submission script (MPI)

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=40
#SBATCH --time=3:00:00
#SBATCH --job-name mpi_job
#SBATCH --output=mpi_output_%j.txt
#SBATCH --mail-type=FAIL
module load NiaEnv/2019b
module load intel/2019u4
module load openmpi/4.0.1

mpirun ./mpi_app # or 'srun ./mpi_app'
```

```
nia-login07:scratch$ sbatch mpi_job.sh
```

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.
- `sbatch` reads these lines as a job request (which it gives the name `mpi_job`)
- In this case, SLURM looks for 2 nodes with 40 cores on which to run 80 tasks, for 3 hours.
- Submit from `/scratch`, so output can be written.
- Once it found nodes, the script is run:
 - ▶ Loads modules;
 - ▶ Runs the `mpi_app` application.

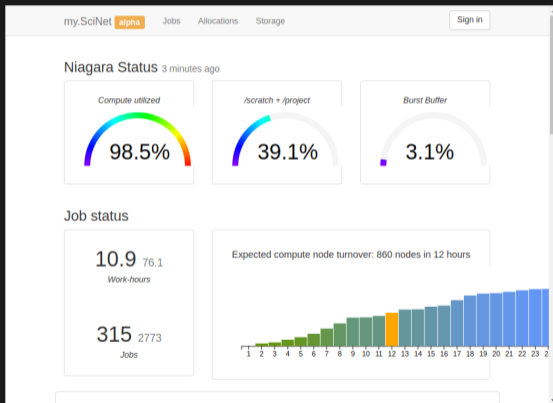
Usage: Monitoring jobs - command line

Once the job is in the queue, there are some commands you can use to monitor its progress:

- `squeue --me` to show your jobs in the queue (`squeue` for all jobs);
- `squeue -j JOBID` or `scontrol show job JOBID` to get information on a specific job.
- `squeue --start -j JOBID` to get an estimate for when a job will run.
- `jobperf JOBID` to get an instantaneous view of the cpu+memory usage of a running job's nodes.
- `scancel -i JOBID` to cancel the job.
- `scancel -u USERID` to cancel all your jobs (careful!).
- `sinfo -p compute` to look at available nodes.
- `sacct` to get information on your recent jobs.
- SLURM documentation: <https://docs.scinet.utoronto.ca/index.php/Slurm>

Usage: my.scinet.utoronto.ca

Check out <https://my.scinet.utoronto.ca> for past and present job info.

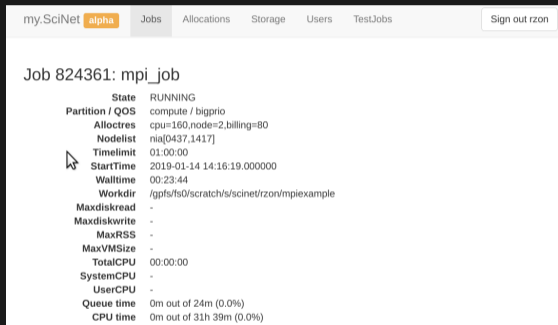


Features

- Niagara cpu and storage utilization
- Status of the login nodes
- Niagara and Mist job history
- Per job:
 - ▶ jobscript
 - ▶ environment
 - ▶ wall time
 - ▶ memory usage every 10 minutes.
 - ▶ cpu usage every 10 minutes.
 - ▶ GFlops/s every 10 minutes.
 - ▶ disk I/O usage every 10 minutes.

Usage: my.scinet.utoronto.ca

Check out <https://my.scinet.utoronto.ca> for past and present job info.



The screenshot shows the my.SciNet alpha web interface. The top navigation bar includes 'my.SciNet alpha', 'Jobs', 'Allocations', 'Storage', 'Users', 'TestJobs', and a 'Sign out rzon' button. The main content area displays 'Job 824361: mpi_job' with the following details:

State	RUNNING
Partition / QOS	compute / bigprio
Alloctres	cpu=160,node=2,billing=80
NodeList	nia[0437,1417]
Timelimit	01:00:00
StartTime	2019-01-14 14:16:19.000000
Walltime	00:23:44
Workdir	/gpfs/fs0/scratch/s/scinet/rzon/mpiexample
Maxdiskread	-
Maxdiskwrite	-
MaxRSS	-
MaxVMSize	-
TotalCPU	00:00:00
SystemCPU	-
UserCPU	-
Queue time	0m out of 24m (0.0%)
CPU time	0m out of 31h 39m (0.0%)

Features

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 - ▶ jobscript
 - ▶ environment
 - ▶ wall time
 - ▶ memory usage every 10 minutes.
 - ▶ cpu usage every 10 minutes.
 - ▶ GFlops/s every 10 minutes.
 - ▶ disk I/O usage every 10 minutes.

my.SciNet **alpha**

Jobs

Allocations

Storage

Users

TestJobs

Sign out rzon

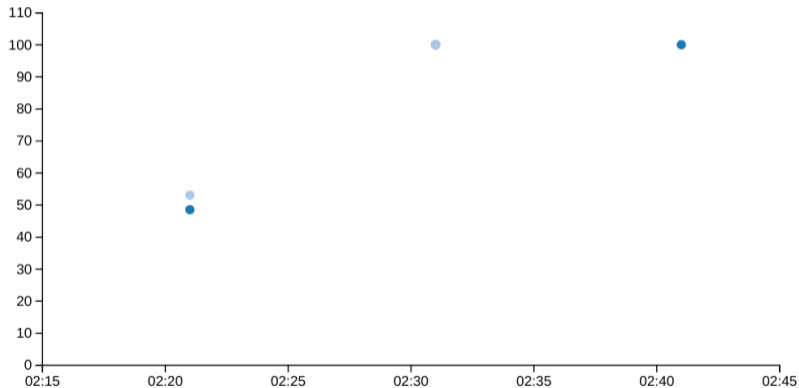
Job 824361: mpi_job

State	RUNNING
Partition / QOS	compute / bigprio
Alloctres	cpu=160,node=2,billing=80
Nodelist	nia[0437,1417]
Timelimit	01:00:00
StartTime	2019-01-14 14:16:19.000000
Walltime	00:23:44
Workdir	/gpfs/fs0/scratch/s/scinet/rzon/mpiexample
Maxdiskread	-
Maxdiskwrite	-
MaxRSS	-
MaxVMSize	-
TotalCPU	00:00:00
SystemCPU	-
UserCPU	-
Queue time	0m out of 24m (0.0%)
CPU time	0m out of 31h 39m (0.0%)

Usage: my.scinet.utoronto.ca

Performance

CPU Usage [%] ▾



Usage: my.scinet.utoronto.ca

Script

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks=80
#SBATCH --time=1:00:00
#SBATCH --job-name mpi_job
#SBATCH --output=mpi_output_%j.txt
#SBATCH --mail-type=FAIL

module load intel/2018.2
module load openmpi/3.1.0

mpirun ./mpi_example
```

Environment

```
SLURM_ACCOUNT=scinet
```

Usage: Hyperthreading

- **Hyperthreading** is a technology that leverages more of the physical hardware by pretending there are more logical cores than real ones.
- On Niagara, each physical core becomes 2 virtual cores, so nodes seem to have 80 cores.
- On Mist, each physical core becomes 4 virtual cores, so nodes appear to have 128 cores.

Using hyperthreading on Niagara

- First, ask for a certain number of nodes for your jobs and set `--ntasks-per-node=40`.
- This way you get to use all cores on the nodes, but without hyperthreading.
(mpirun, srun, and the OS will automatically spread processes over the real cores)
- Then **test** if running $80 \times N$ MPI processes or threads gives you any speedup by setting `--ntasks-per-node=80`.

Even when doing so, your usage will be counted (“billing”) as $40 \times N \times (\text{walltime in years})$.

Data Management



Data Management and I/O Tips

- \$HOME, \$SCRATCH, and \$PROJECT all use the parallel file system called GPFS. GPFS is a high-performance file system which provides **rapid reads and writes to large data sets in parallel** from many nodes.
- Accessing data sets which consist of **many, small files leads to poor performance**.
Avoid reading and writing lots of small amounts of data to disk!
- Write data out in **binary**. Faster and takes less space.
- **Burst buffer** is better for I/O heavy jobs and to speed up checkpoints.
Ask support@scinet.utoronto.ca for persistent burst buffer space.
- Even better, when it fits, use \$SLURM_TMPDIR, which lives in **memory**.

Further information

Useful sites

- Niagara: https://docs.alliancecan.ca/wiki/Niagara_Quickstart
- Mist: <https://docs.scinet.utoronto.ca/index.php/Mist>
- Other Alliance clusters or general topics: <https://docs.alliancecan.ca>
- System Status: <https://docs.scinet.utoronto.ca>
- Training: <https://education.scinet.utoronto.ca/>

Support

- Email to niagara@tech.alliancecan.ca or support@scinet.utoronto.ca
- Still need help? Request a one-to-one consultation (request via email).