Introduction to SciNet, Niagara & Mist

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Outline

- About SciNet
- Using Niagara and Mist
- Data management and I/O tips

About SciNet

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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.
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- 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.

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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 (SOSCIP)

Hardware, systems, etc..

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

- Chief Technical Officer: Daniel Gruner
- Information Systems Security: Shawn Winnington-Ball
- Business manager: Jackie Denholm

Niagara

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 #150)
- 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

Mist

- Niagara's little GPU sibling
  (Also a SOSCIP system.)
- 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.computecanada.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.

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2. Go to

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2. Go to

   https://ccdb.computecanada.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.

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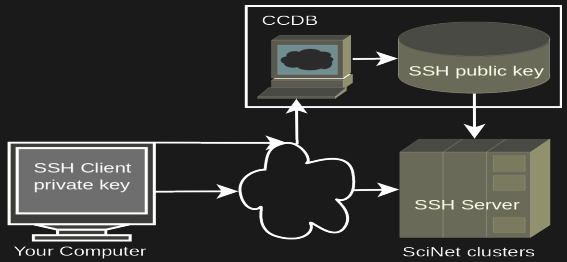
- The connection will get you to a Linux command line interface.
- Password doesn't work on Niagara and Mist! SSH keys must be used to authenticate.
- SSH keys come in a pair:
  - a **private key** which is kept on your own computer and used to connect
  - a **public key** that you upload to CCDB and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



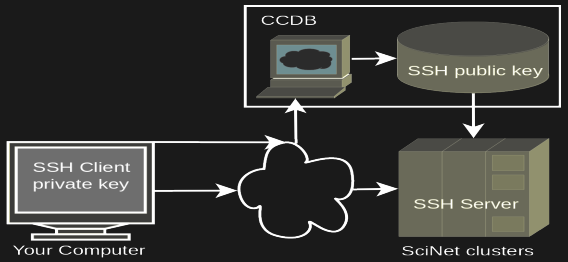
Note that you can use the same SSH keys for connecting to the other Alliance clusters as well.

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).
- Then generate a **ssh key pair** with the following command:

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

- That will prompt you to enter a **passphrase** to protect your private key.
  The passphrase does not leave your computer, it just 'unlocks' the 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.



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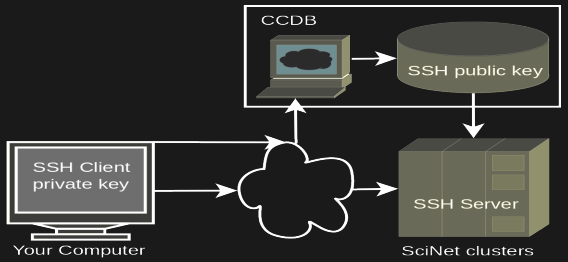

- `-f` option specifies the filename of the key file.
- (optional) `-C` option allows you to insert a comment into the key.

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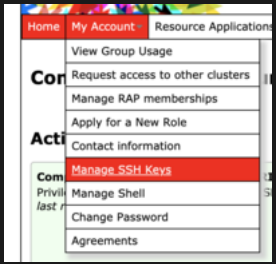
or via the CCDB menu:



Access: Uploading Your Public Key

- Step 2: Grab your SSH public key:

```
laptop> cat ~/.ssh/dra_ed25519.pub
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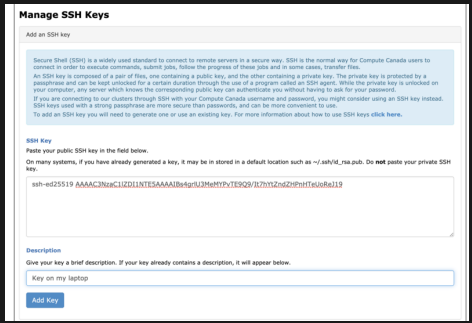
- Step 3: Paste the public key into the CCDB form and click "Add Key" button:

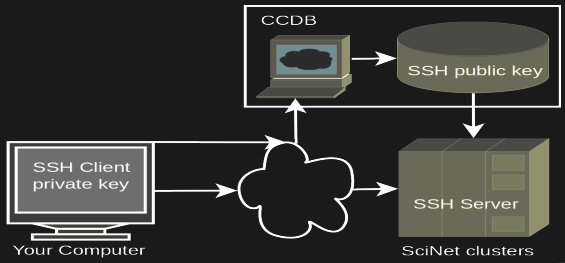


Access: Logging in

Wait a few minutes for your new uploaded public key to propagate to the systems and 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
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This will also make data transfer commands like `scp` and `rsync` work more easily.

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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.

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- Create one key pair for each different service, role or domain, and name them accordingly.
- Do not create key pairs in shared systems like HPC clusters.

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

Usage: login, compute, and datamovers nodes

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The *login nodes* are where you develop, edit, compile, prepare and submit jobs.

These login nodes are not part of the Niagara compute cluster, but have the same architecture, operating system, and software stack.
These nodes are shared, i.e., multiple users are on the same nodes.
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To run on Niagara's *compute nodes*, you must submit a batch job.

In a job script, you can specify how many nodes you need and for how long.
Once the job scheduler starts your job, it is the only thing running on its reserved nodes.

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For large data transfers, you can use the specialized *data mover nodes*.

All these nodes see the same shared file system.

Usage: Storage Systems and Locations

Home and scratch

You have a home and scratch directory on the shared file systems, whose locations are given by

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

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

Use these convenient variables!

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

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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

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- Backup means a recent snapshot, not an achive of all data that ever was.

Moving data

Move amounts less than 10GB through 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
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- These commands must be given on your computer.
- For rsync to use your ssh key, give it the '`-e "ssh -i ~/.ssh/YOURKEY"`' option.
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Move amounts larger than 10GB through 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.

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Moving 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 spider shows the available software.

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```
nia-login07:~$ module spider
----------------------------------------
The following is a list of the modules..
----------------------------------------
  CCEnv: CCEnv
    Compute Canada software modules. Mus
    modules in 'module spider'.
  NiaEnv: NiaEnv/2018a, NiaEnv/2019b
    Software modules for Niagara. Must b
    'module spider' (loaded by default).
  antlr: antlr/2.7.7
    ANTLR, ANother Tool for Language Rec
    language tool that provides a framew
  ...
```

Usage: Software and Libraries, continued

- `module load <module-name>`

  use particular software

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  remove currently loaded modules

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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).
```

Usage: Module examples

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cannot be loaded as requested: "openmpi"
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```

```
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
```

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:

  Vendor compilers (Intel, IBM) and parallel debuggers.
- That means no MATLAB, Gaussian, IDL, ...
- 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 Alliance 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.
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```
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
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If you want, use the "venv2jup" command to use your virtual environment in the JupyterHub.

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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
```

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```

- To install R packages, use the R command "install.packages(...)"

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```

- 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).

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

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- 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.

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- 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.

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Keep in mind:

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

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nia-login07:scratch$ sbatch omp_job.sh
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- In this case, SLURM looks for one node with 40 cores to be run inside one task, for 1 hour.

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- 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
```

Example submission script (MPI)

```
#!/bin/bash
#SBATCH --nodes=2
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#SBATCH --time=3:00:00
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- Submit from /scratch, so output can be written.
- Once it found nodes, the script is run:
  - Loads modules;
  - Runs the `mpi_app` application.

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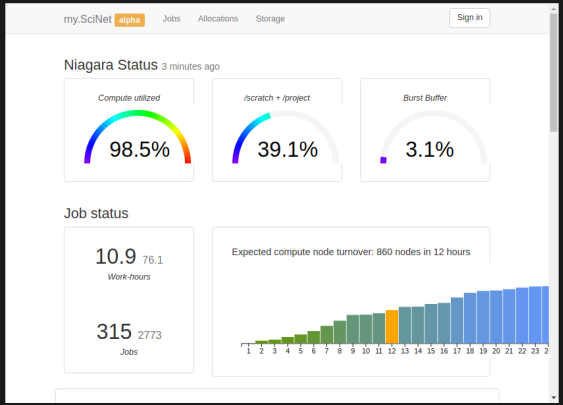
- SLURM documentation: https://docs.scinet.utoronto.ca/index.php/Slurm

Usage: my.scinet.utoronto.ca

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



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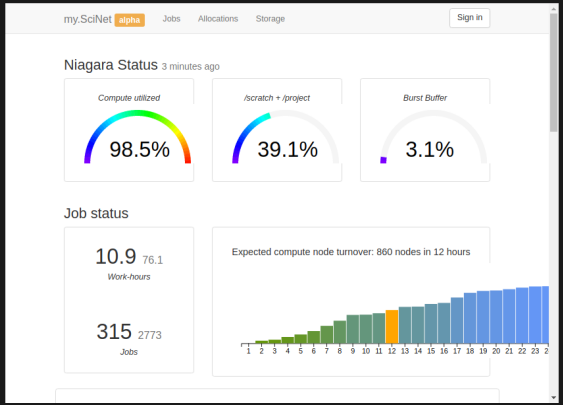

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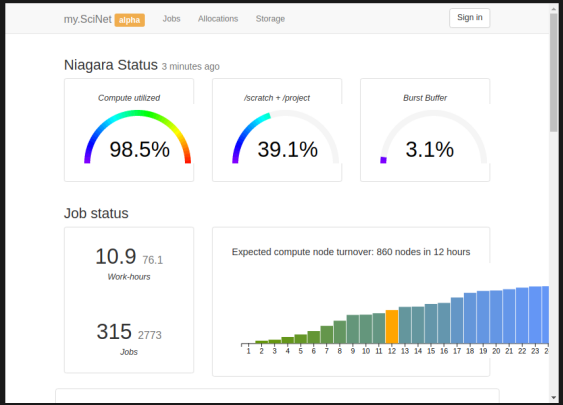

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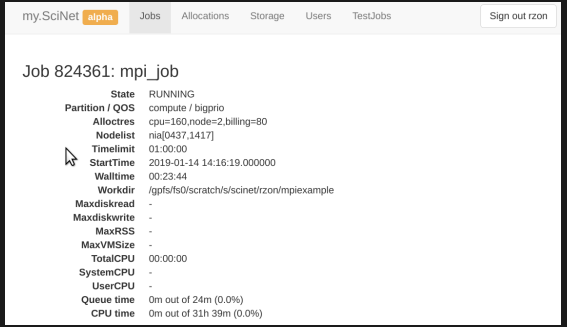

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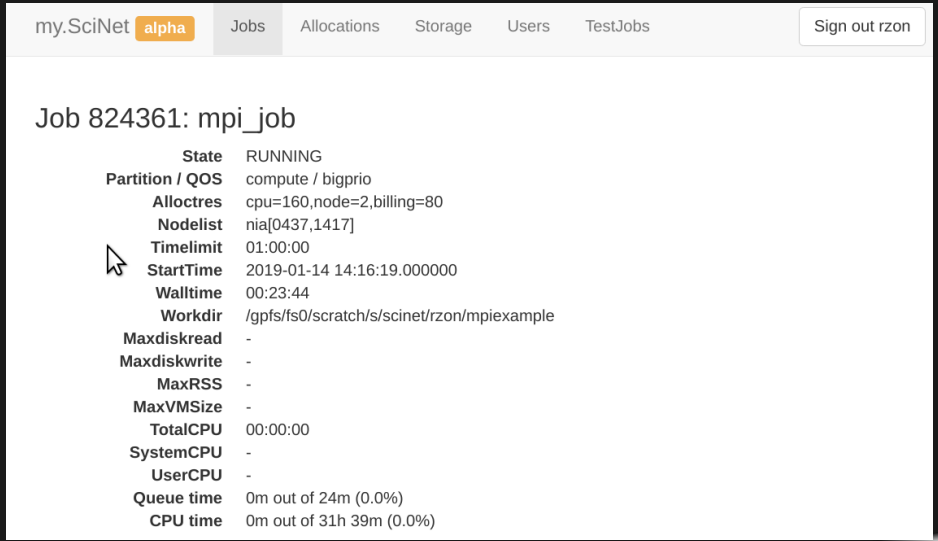

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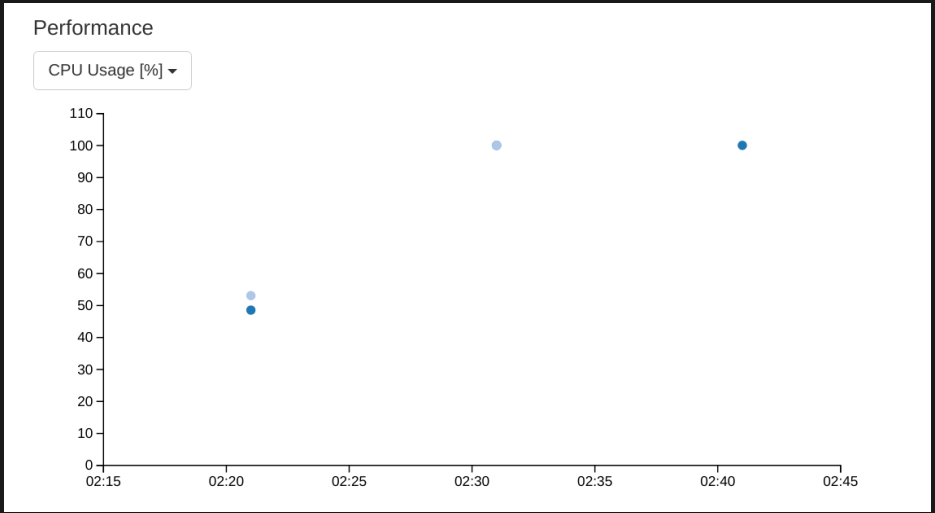

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Script

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --ntasks=80
#SBATCH --time=1:00:00
#SBATCH --job-name mpi_job
#SBATCH --output=mpi_output_%j.txt
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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.
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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 automaticallly spread processes over the real cores)
- Then **test** if running 80xN 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 40xNx(walltime in years).

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- So 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.

  Either (1) ask `support@scinet.utoronto.ca` for persistent burst buffer space

  or (2) use the temporary `$BB_JOB_DIR`.
- Even better, when it fits is to use `$SLURM_TMPDIR`, which lives in memory.

Further information

Useful sites

- SciNet: https://www.scinet.utoronto.ca
- 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

Questions? Need help?

Don't be afraid to contact us! We are here to help.

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