Introduction to SciNet, Niagara & Mist

Alexey Fedoseev (SciNet)

March 9, 2022





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

SCINet

SciNet is a consortium for high-performance computing of the U. of Toronto and associated hospitals.

- We run massively parallel computers to meet the needs of researchers across Canada.
- 5 similar consortia in Canada also provide academic Advanced Research Computing (ARC) resources.
- These consortia maintain and support a network of resources available to researchers across Canada, under a national allocation system.

National research computing clusters

- Four heterogeneous ("general purpose") clusters:
 - Cedar (Simon Fraser University)
 - Graham (University of Waterloo)
 - Béluga (Montréal, Québec)
 - Narval (Montréal, Québec)

- One homogeneous ("large parallel") 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



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



Software, user support, training, etc..

- Mike Nolta
- Erik Spence
- Ramses van Zon
- Bruno Mundim
- Alexey Fedoseev
- James Willis
- Fei Mao (SOSCIP)
- Yohai Meiron (SOSCIP)
- Chief Technical Officer: Daniel Gruner

Hardware, systems, etc..

- Joseph Chen
- Ching-Hsing Yu
- Leslie Groer
- Jaime Pinto
- Marco Saldarriaga
- Vladimir Slavnic
- Ram Sharma
- Information Systems Security: Raphaelle Gauriau
- Business manager: Jackie Denholm

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

Niagara





Niagara

- 80,960 x86-64 cores.
- 2,024 *Lenovo SD530* nodes
- Per node:
 - 40 Intel SkyLake/CascadeLake cores @ 2.4GHz
 - 188 GiB RAM per node (> 4 GiB per core)
- 3.6 PFlops sustained (6.25 PFlops theoretical).
 #59 on the Nov 2018 TOP500 (now #127)
- Operating system: Linux CentOS 7.
- Interconnect: InfiniBand Dragonfly+ 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, for 70%, 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).
- Operating system: Red Hat Enterprise 8.
- Interconnect: 1:1 InfiniBand Dragonfly+
- Same parallel shared file systems as Niagara





Register with the Compute Canada Database (CCDB)

https://ccdb.computecanada.ca/account_application

If you're not a PI and your PI does not have a CC account, they have to get one first, so they can sponsor your account.

The approval process typically takes 1-2 business days.

🛛 Go to

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

and click on the "Join" button next to Niagara and Mist.

After a business day or two (typically less), you get an email confirming your access to Niagara and Mist.

Using Niagara and Mist: Secure Login

- As with all SciNet and Compute Canada systems, access is via ssh only.
- Password authentication is disabled on Niagara and Mist, which means
 SSH keys must be used for authentication on Niagara and Mist.
- 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.







Using Niagara and Mist: SSH key setup before first login SCNet

- 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 ccf" -f ~/.ssh/ccf_ed25519

- That will prompt you to enter a passphrase to protect your private key.
 Choose 15 characters or more. Two short sentences meaningful to you, for example.
- A private key, ccf_ed25519, and a public key, ccf_ed25519.pub are then created in the directory ".ssh" in your home directory.



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



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 Compute Canada credentials to visit the following site:

https://ccdb.computecanada.ca/ssh_authorized_keys

or via the CCDB menu:



Using Niagara and Mist: Uploading Your Public Key



• Step 2: Grab your SSH public key:

laptop> cat ~/.ssh/ccf_ed25519.pub
ssh-ed25519 AAAAC3NzaC11ZDI1NTE5AAAAIEpDf+Wcvtru6pUcBgJQo/3+cmI4+MisfNE3U46/CDkx
USERNAME@MYLAPTOP ccf

• Step 3: Paste the public key into the CCDB form and click "Add Key" button:

Manage SSH Keys							
Add an SSH key							
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Add Key							

Using Niagara and Mist: 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/ccf_ed25519 USERNAME@niagara.computecanada.ca
Enter passphrase for ccf_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*.



• First time? Check host key fingerprints against

https://docs.computecanada.ca/wiki/SSH_host_keys



Connecting more conveniently: save ssh options and keys Schet

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

```
Host niagara
HostName niagara.computecanada.ca
User USERNAME
IdentityFile ~/.ssh/ccf_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/ccf_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.



- Do not share your private keys!
- Never copy your private key to other systems!
- Always protect it with a strong passphrase!
- Create one key pair for each computer you use to access our systems.
- 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.computecanada.ca/wiki/SSH_Keys



There are three types of nodes on Niagara:

• 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.

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

• 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.

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

All these nodes see the same shared file system.



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

nia-login07:~\$ cd \$SCRATCH

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



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Project

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Burst Buffer

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

Storage Limits on Niagara



					backed		
location	quota	#files	block size	expiration	up	on login	compute
\$HOME	100 GB	250K	1 MB		yes	yes	read-only
\$SCRATCH	1 25 TB	6M	16 MB	2 months	no	yes	yes
\$PROJECT	Tby group allocation	depends	16 MB		yes	yes	yes
\$BBUFFEF \$ARCHIVE	R10TB, by request by group allocation		1 MB	48 hours	no dual-copy	yes no	yes 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 CC RAC allocation competition.

Moving data



Move amounts less than 10GB through the login nodes.

Use scp or rsync to and from niagara.computecanada.ca.

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

laptop> scp -i ~/.ssh/ccf_ed25519 this USERNAME@niagara.computecanada.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 10GB.

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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.

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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- module spider shows the available software.

```
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
```

• 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 avail

list loadable software packages that require no other modules to be loaded first.

• module list

list loaded modules



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Alexey Fedoseev (SciNet)

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 A Niagara software stack tuned and compiled for this machine. This stack is available by default, but if not, can be loaded with

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 The same software stack available on Compute Canada's general purpose clusters. For the Béluga/Narval stack:
 module load CCEnv StdEnv

For the Graham and Cedar stack:

module load CCEnv arch/avx2 StdEnv



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For the Graham and Cedar stack:

module load CCEnv arch/avx2 StdEnv

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

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).

Module examples



```
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
```

Module examples, continued

Alexev Fedoseev (SciNet)



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```
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
      _____
        Homenage · https://www.open-mpi org/
```

Introduction to SciNet, Niagara & Mist


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



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



• 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 Compute 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: Intel compilers, math libraries 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 Compute Canada stack.

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:

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- 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.



• 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).

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.

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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 -03 -xHost -o main.o main.c
nia-login07:~$ icc -c -03 -xHost -o module.o module.c
nia-login07:~$ icc -o main module.o main.o -lgsl -mkl
```





• 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, \leq 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

Submitting jobs



- 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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- 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 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.

Hyperthreading: Logical CPUs vs. cores



- 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.

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On Niagara, hyperthreading is actually fairly easy to use:

- Ask for a certain number of nodes N for your jobs.
- You know that you get 40×N cores, so you will get to use a total of 40×N MPI processes or threads. (mpirun, srun, and the OS will automatically spread these over the real cores)
- But you should also test if running 80xN MPI processes or threads gives you any speedup.
- Regardless, your usage will be counted as 40×N×(walltime in years).



```
#!/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

• First line indicates that this is a bash script.



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- Lines starting with #SBATCH go to SLURM.



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module load NiaEnv/2019b intel/2019u4
OMP_NUM_THREADS=\$SLURM_CPUS_PER_TASK
export OMP_NUM_THREADS

./omp_example # or 'srun ./omp_example'

- 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).



```
#!/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'

- 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.



```
#!/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'

- 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.



```
#!/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'

- 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.

```
#!/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 gnu-parallel

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





```
#!/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 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.



```
#!/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 gnu-parallel
```

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

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.



```
#!/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 gnu-parallel
```

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

- 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).



```
#!/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 gnu-parallel
```

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

- 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 tasks to be run for 3 hours.



```
#!/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 gnu-parallel
```

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

- 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 tasks to be run for 3 hours.
- Submit from /scratch, as /home is read-only.



```
#!/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 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 (which it gives the name omp_job).
- 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
 - Uses gnu-parallel to load-balance 99 tasks over the 40 cores on the node.

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

Alexey Fedoseev (SciNet)

```
#!/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'





```
#!/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<u>/4.0.1</u>

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

nia-login07:scratch\$ sbatch mpi_job.sh

First line indicates that this is a bash script.



```
#!/bin/bash
```

```
#SBATCH --ntasks-per-node=40
```

```
#SDATOII IICASKS PET IIOUE--
```

```
#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'

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.



```
#!/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'

- 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)



```
#!/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'

- 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.



```
#!/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'

- 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.



```
#!/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'

- 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.
Monitoring jobs - command line



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

- squeue to show the job queue (squeue --me for just your jobs or watch squeue --me);
- squeue -j JOBID to get information on a specific job

(alternatively, scontrol show job JOBID, which is more verbose).

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









Features

- Niagara cpu and storage utilization
- Status of the login nodes
- Niagara and Mist job history





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.



my.SciNet alpha	Jobs	Allocations	Storage	Users	TestJobs	Sign out rzon
Job 824361: m	pi jo	b				
Statu Partition / QO: Alloctre Nodelis StarTime Maxdisiveri Maxdisiveri Maxdisiveri Maxdisiveri MaxVisiz MaxVis	RUN RUN Comp Comp	VINING suite / bigprio 160, node=2, billi 437, 1417] 0:00 -01-14 14:16:19 3:44 /fs0/scratch/s/sc 0:00 ut of 24m (0.0%	ng=80 .000000 inet/rzor/mp	iexample		

Features

- Niagara cpu and storage utilization
- Status of the login nodes
- 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.

Monitoring jobs online - my.scinet



my.SciNet alpha	Jobs	Allocations	Storage	Users	TestJobs		Sign out rzon				
Job 824361: mpi_job											
State Partition / QOS Alloctre: Nodelis Timelimi StartTim. Walltim Waxdiskread Maxdiskread Maxdiskread Maxdiskread MaxVMSiz TotalCPU UserCPU Queue time CPU time	e RUN e RUN S computing s cpu= t nia[0 t 01:00 e 2019 e 00:02 r /gfs d - e - S - e - J 00:00 J - e 0m o e 0m o	NING ute / bigprio 160,node=2,bill 437,1417] 0:00 -01-14 14:16:15 9:44 ffs0/scratch/s/sc 0:00 ut of 24m (0.0% ut of 31h 39m (i	ng=80 .000000 :inet/rzon/mp .) 0.0%)	iexample							

Monitoring jobs online - my.scinet





Alexey Fedoseev (SciNet)

Monitoring jobs online - my.scinet



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

Data Management and I/O Tips



- \$HOME, \$SCRATCH, and \$PROJECT all use the parallel file system called GPFS.
- Your files can be seen on all Niagara login and compute nodes.
- GPFS is a high-performance file system which provides rapid reads and writes to large data sets in parallel from many nodes.
- But 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.
- Many small files on the system would waste space and would be slower to access, read and write.
- 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.computecanada.ca/wiki/Niagara_Quickstart
- Mist: https://docs.scinet.utoronto.ca/index.php/Mist
- Other Compute Canada clusters or general topics: https://docs.computecanada.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 support@scinet.utoronto.ca or to niagara@computecanada.ca