## MINICLUSTER TOOLS DOCUMENTATION

Repo: https://github.com/coyleej/MiniClusterTools

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### Operating system and shell

These scripts were developed to work with both the server and desktop versions of **Ubuntu 18.04** and the bash shell. If you are using a different operating system or a different version of Ubuntu, you will likely need to make modifications. My goal is to maintain POSIX compliance in all of the shell scripts, but I make no promises.

#### Documentation notes

This documentation automatically pulls relevant information from a larger, actively updated document. As a result, some internal references point to information that is not included. A few broken links seemed a reasonable compromise to ensure up-to-date documentation.

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## Setup Scripts

### 1.1 sshd\_setup.sh

This setup is automated in the sshd\_setup.sh file from MiniClusterTools repository.

- 1. Install fail2ban and openssh-server with apt. fail2ban will ban IPs that exceed 5 failed tries in 10 minutes. (Never modify /etc/fail2ban/jail.conf! Copy it into jail.local and modify that.)
- 2. We're required to display a banner message (option A) on the servers prior to login. It will be activated in a few steps. For now, we're just creating it.
  - (a) Create the login banner file: sudo touch /etc/ssh/sshd\_banner
  - (b) Add the warning found in the MiniClusterTools repo.
- 3. Open /etc/ssh/sshd\_config and change some ssh settings.

The convention in this file is to have default settings commented out and to only uncomment something if you change the value! Note: We are making an exception to this convention for values the higher ups have explicitly requested.

- (a) Specify that all ssh access to the servers must use protocol 2 by adding the following right below the line #Port 22. (Completely unnecessary for openssh 7.6+, but including anyway.)
   Protocol 2
- (b) Change LoginGraceTime to 1m

  This changes the allowable time between typing ssh <server> and entering a password.
- (c) Change PermitRootLogin to no
- (d) Uncomment StrictModes to yes (default value)
- (e) Change MaxAuthTries to 3

  This allows three password attempts after typing ssh <server> before resetting.
- (f) Restrict who is allowed to remotely access the server. Add these lines below MaxSessions:

DenyUsers root DenyGroups root AllowGroups users slurm

Only groups users and slurm are able to ssh or sftp. All (human) users should be placed in group users when creating their accounts! See chapter ?? for managing group membership. Technically the Deny... statements are redundant. root is already forbidden from using ssh because its password is disabled and locked.

- (g) Change IgnoreUserKnownHosts to yes
- (h) Uncomment PermitEmptyPasswords to no (default value)
- (i) Uncomment X11Forwarding to yes (default value)
- (j) Have it print the last login for \$USER (NOTE: While the convention would suggest that yes is the default, someone typo'd. The default is actually no.)
  - PrintLastLog yes
- (k) Uncomment PermitUserEnvironment to no (default value)
- (l) Uncomment Compression to delayed (default value)
- (m) Change ClientAliveInterval to 600
- (n) Change ClientAliveCountMax to 1
- (o) Display the banner text in between typing ssh <user>@<server> and password entry Banner /etc/ssh/sshd\_banner
- (p) UsePrivilegeSeparation sandbox is depricated starting from openssh 7.5! Privilege separation is now mandatory. Because it is depricated and results in a warning when checking the configuration, we are not adding this line to the config file.
- 4. Check that sshd\_config is valid and error-free:

```
sudo sshd -t
```

5. Reload the daemon:

```
sudo systemctl restart sshd
```

6. The code will remind you to manually add users to the ssh-approved group:

```
sudo usermod -a -G <ssh-users> <username>
```

7. Test by logging in again.

## 1.2 login\_banner.sh

You must configure gdm3 as described below. These changes are automated in the login\_banner.sh file.

1. NVidia and Wayland will not get along if you modify the default gdm settings (read: you can't log in and the NVidia drivers get corrupted). Open /etc/gdm3/custom.conf and set:

```
WaylandEnable=false
```

2. Create the following files and directories:

```
sudo touch /etc/dconf/profile/gdm
sudo mkdir /etc/dconf/db/gdm.d
sudo touch /etc/dconf/db/gdm.d/01-banner-message
```

3. Open /etc/dconf/profile/gdm and add the following:

```
user-db:user
system-db:gdm
file-db:/usr/share/gdm/greeter-dconf-defaults
```

4. Open /etc/dconf/db/gdm.d/01-banner-message and add the following:

```
[org/gnome/login-screen]
banner-message-enable=true
banner-message-text='I have read & consent to terms in IS user agreement.'
```

5. Reconfigure gdm3 and dconf.

```
sudo dconf update
sudo dpkg-reconfigure gdm3
```

6. Restart your computer for the changes to take effect.

### 1.3 unattended\_upgrades.sh

Ubuntu is set to automatically download and install security updates, but not security upgrades. We will use unattended-upgrades to automate upgrades. I recommend that users automate security upgrades and check for other upgrades manually. Automating everything is fine, but apt occasionally attempts to install or remove other packages. If you do automate everything and encounter dependency issues, refer to section ??. (Security upgrades are far less likely to cause problems.)

Automatic upgrades must be set up manually. While there are several ways to do this, we will use unnattended-upgrades. It's preinstalled and can be configured in two different ways. Both are automated in the set\_unattended\_upgrades.sh file:

- Run sudo dpkg-reconfigure unattended-upgrades and follow the prompts. The whole process should take about a minute. Automate all upgrades if you want but be aware of the warning above. Detailed documentation can be found here.
- Configure it manually by editing /etc/apt/apt.conf.d/50unattended-upgrades. The setup for our servers is described below. Additional details can be found at these locations: 1, 2, 3, and 4.

#### Manual setup:

- 1. Install bsd-mailx. In the installation process, pick "local only" and use "\$HOSTNAME" as the mail server host. (Substitute the name of your machine for "\$HOSTNAME".)
- 2. Navigate to /etc/apt/apt.conf.d/.
- 3. Copy 50unattended-upgrades to 50unattended-upgrades.backup.

Open 50unattended-upgrades and make the following changes:

- (a) Uncomment Unattended-Upgrade:: Mail and change the address to <admin\_account>.
- (b) Set it to send you mail only when there are errors. (The default is sending mail every time it updates.) Messages are placed in /var/mail. Uncomment the following:
  Unattended-Upgrade::MailOnlyOnError "true"
- (c) All other items are left as the defaults.
- 4. Copy 20auto-upgrades to 20auto-upgrades.backup.

Open 20auto-upgrades and make sure that it contains the following (time intervals are in days):

```
APT::Periodic::Update-Package-Lists "1";
APT::Periodic::Download-Upgradeable-Packages "1";
APT::Periodic::AutocleanInterval "7";
APT::Periodic::Unattended-Upgrade "1";
```

- 5. Test: sudo unattended-upgrades --dry-run --debug
- 6. If the dry run worked: sudo rm \*.backup

If things ever go wrong, you may need to check the log files: /var/log/unattended-upgrades/unattended-upgrades.log/var/log/apt

unattended-upgrades runs randomly within a twelve hour block to smooth out demand on the mirrors. This is fine for our purposes and does not need modification.

### 1.4 set\_password\_policy.sh

#### 1.4.1 Password policy

Passwords must be at least 15 characters long, with at least two upper case letters, two lower case letters, two numbers, and two special characters. They must expire after 60 days and contain at least two characters not in the previous password. Running set\_passwd\_policy.sh will automatically change these settings.

1. Change the password expiration settings. Open /etc/login.defs and set these variables:

```
PASS_MAX_DAYS 60
PASS_WARN_AGE 7
```

2. Set the password requirements. Open /etc/security/pwquality.conf. Negative values indicate that that number of the thing be present in a new password.

```
difok = 2
minlen = 15
dcredit = -2
ucredit = -2
lcredit = -2
ocredit = -2
minclass = 4
maxrepeat = 2
usercheck = 1
```

3. Changes to /etc/login.defs only affect new users (source). You must also apply these changes to existing users: sudo chage -M <days> <user>

The following code automates these changes (you can confirm changes with sudo chage -1 <user>):

```
userlist=$(grep "10[0-9][0-9]" /etc/passwd | cut -d ":" -f 1)
for user in $userlist; do
    sudo chage -M 60 $user
    sudo chage -l $user | grep "Pass.*expire"
done
```

#### 1.4.2 HBSS

We must install HBSS and update the policies. The installation script is called in set\_passwd\_policy.sh. Contact me for the current installation script. If you wish to call it separately, do so with the following:

sudo bash <install>.sh -i && /opt/McAfee/cma/bin/cmdagent -c

## 1.5 auto\_user\_setup.sh

REMOVED in latest commit. (This works on test files. It has not been used for actual setup as of now, so I cannot guarantee full functionality.)

## ML installation scripts

### 2.1 repo\_download\_w\_some\_install.sh

Downloads all of the necessary machine learning repos (pybind11, OpenBLAS, S4, MANTIS, and signac) and installs both MANTIS and Signac. Users must compile the other packages themselves.

#### 2.1.1 **MANTIS**

Note: MANTIS can (and will if you use the script) be installed prior to S4, but S4 is a required dependency. MANTIS will not work properly unless S4 is installed.

1. Clone MANTIS from github:

```
cd /home/<admin>/Code
git clone https://github.com/harperes/MANTIS.git
```

2. Make sure that the system pip is installed. If you skip this bit, then sudo won't find pip3...

```
sudo apt install python3-pip
```

3. Install MANTIS to /opt

```
cd MANTIS
sudo pip3 install . --target="/opt" --no-deps --no-dependencies
```

4. Open /etc/environment:

Prepend /opt/MANTIS to the system path.

Make sure that /opt has been added to PYTHONPATH.

- 5. Create or activate an s4py environment.
- 6. Test the install. Navigate to the MANTIS tests directory and type: python -m unittest

### 2.1.2 Signac

Setup is automated in repo\_download\_w\_some\_setup.sh.

1. Clone Signac from github and check out the develop branch:

```
cd /home/<admin>/Code
git clone https://bitbucket.org/glotzer/signac.git
cd signac
git checkout develop
```

- 2. Make sure that the system pip is installed. If you skip this bit, then sudo won't find pip3... sudo apt install python3-pip
- 3. Install MANTIS to /opt sudo pip3 install . --target="/opt" --no-deps --no-dependencies
- 4. Open /etc/environment:

  Make sure that /opt has been added to PYTHONPATH.

### 2.1.3 S4

repo\_download\_w\_some\_setup.sh downloads the necessary machine learning repositories (pybind11, Open-BLAS, and S4), but compiling is left to the user.

Please refer to Eric Harper's S4 installation instructions. If you have access to the MANTIS folder, you can direct your browser to file:///home/<User>/<PathToSyncFolder>/MANTISBIBLE/S4Documentation/html/install.html. If not, please see the harperes S4 repository on github.

# Monitoring scripts

## 3.1 check\_passwd\_expiry.sh

Returns a warning if the user's password expires in 7 or fewer days.

## 3.2 downtime.py

Used for monitoring downtime. It is a modified version of script created by waleedahmad. The original version can be found on waleedahmad's github page.

## 3.3 Syncthing

### 3.3.1 Summarize syncthing usage

The synthing\_usage.sh script in the MiniClusterTools repository reports the size of all directories in the synching folder. It reports on all directories but does *not* message users.

### 3.3.2 Automated messages about syncthing usage

- 1. Copy syncthing-warning into /usr/share on the servers. Add eye-catching ASCII art if desired.
- 2. Open /etc/bash.bashrc and append the following.

## **Files**

Descriptions of all files in the files directory. Other sections cover the usage of each where relevant.

### 4.1 banner\_text\*.txt

The long and short versions of the banner text displayed when logging in. Which message is displayed depends on the login method. See sections 1.1 and 1.2 for details.

## 4.2 cgroup.conf

A cgroup.conf example file in case install\_slurm.sh fails to properly make it's own.

## 4.3 s4py.yml

Used to create the s4py environment in conda. Contains all the packages required to install our ML tools (chapter 2).

### 4.4 test\_sbatch.sh

Test if slurm is working properly by submitting a simple job with sbatch. Contains the sleep command to keep it in the queue longer.

## Slurm setup and administration

### This setup works on Ubuntu 18.04 and Ubuntu Server 18.04.

SchedMD recommends a separate database server if possible. It may be on the same server as slurmctld, but this may impact performance. You should consider optimizing the database performance by mounting the MariaDB or MySQL database directory on a dedicated high-speed file system. Ideally this would be a PCIe SSD disk drive (e.g. Intel SSD P3700 series or Kingston E1000 series), but SSD SAS/SATA will also work. Drives must be qualified for high-volume random small read/write operations, and should be built with the Non-Volatile Memory Express (NVMe) storage interface standard for reliability and performance. A disk size of 200 GB or 400 GB should be sufficient. Consider installing 2 disk drives in a RAID-1 configuration.

The following will be installed in this setup guide:

• MPI : OpenMPI version 2

• Slurm 17.11.2-1

• Authentication and digital signatures: MUNGE

• Database : MariaDB

### 5.1 Reference materials

This guide was constructed from the following references and my own experiences:

Slurm admin quick-start

Slurm official documentation

man slurm-wlm-doc for Slurm 17.11.2-1build1

Slurm man pages and configuration file index

Slurm multi-core support

Slurm download and addons list

Slurm configuration (Niflheim)

Slurm database (Niflheim)

Slurm-gpu github

## 5.2 Basic Slurm set up

- 1. If you intend to set up a database on its own high speed drive, mount the drive now.
- 2. Make sure that OpenMPI is installed. If not, install it with sudo apt install libopenmpi2 libopenmpi-dev openmpi-common openmpi-doc
- 3. Download the MiniClusterTools repo if you haven't already. It contains a slurm installation script. git clone https://github.com/coyleej/MiniClusterTools.git

- 4. Run install\_slurm.sh. It automates much of the setup. The following explains what it does. bash install\_slurm.sh
  - (a) Create Munge user with uid and gid of 399. (Can be any *unused* value between SYS\_UID\_MIN and SYS\_UID\_MAX, which are defined in /etc/login.defs).

mungeuid=399
sudo groupadd -g \$mungeUID munge
sudo useradd -r -u \$mungeUID -g \$mungeUID munge
sudo usermod -d /nonexistent munge

- (b) Make sure the system clock is set to the proper timezone and that your system clock is correct: sudo timedatectl set-timezone America/New\_York timedatectl
- (c) Check that nvidia-driver-430 or newer is installed so that slurm can find the GPUs.
  - i. Check that we're using the Ubuntu graphics-drivers PPA. If we aren't: sudo add-apt-repository ppa:graphics-drivers/ppa sudo apt update
  - ii. Use apt to purge anything older than nvidia-driver-430.
  - iii. Use apt to install nvidia-driver-430 if you purged an older driver.
- (d) Install OpenMPI if it is not presently installed: sudo apt install libopenmpi2 libopenmpi-dev openmpi-common openmpi-doc
- (e) Install MUNGE, SLURM, MySQL, MariaDB, and cgroup-tools: apt install munge libmunge-dev libpam-slurm slurmd slurmdbd slurm-wlm-doc cgroup-tools mariadb-common mariadb-server
- (f) If the node in question is the control node or the backup control node: sudo apt install slurmctld slurm-wlm slurmdbd Otherwise: sudo apt install slurm-client
  - bado apo imbodii bidim oliono
- (g) User prompts will gather some information on GPUs.
- (h) Configure the control node, if applicable.
  - i. Make sure that /var/spool/slurmctld/ and /var/log/slurm-llnl/ exist. If not, create them with mkdir.
  - ii. Make sure that slurm is the owner of these directories. If not, use chown slurm: <dirname>
  - iii. Make sure that the permissions on these directories are set to 755. If not, use chmod.
  - iv. Check that /var/log/slurm-llnl/slurmctld.log exists and is owned by slurm. Otherwise, create it using touch and chown.
  - v. Create the Linux default accounting file. sudo touch /var/log/slurm-llnl/slurm\_jobacct.log

sudo chown slurm: /var/log/slurm-llnl/slurm\_jobacct.log
sudo touch /var/log/slurm-llnl/slurm\_jobcomp.log
sudo chown slurm: /var/log/slurm-llnl/slurm\_jobcomp.log

- (i) Configure the compute nodes. See this site for further details.
  - i. Create the slurmd spool directory with the correct ownership.

mkdir /var/spool/slurmd

chown slurm: /var/spool/slurmd chmod 755 /var/spool/slurmd

ii. Create the log files:

touch /var/log/slurmd.log

chown slurm: /var/log/slurmd.log

- iii. Create the pid files (only need slurmctld.pid on the control node):
   touch /var/log/slurm-llnl/slurmd.pid /var/log/slurm-llnl/slurmctld.pid
   chown slurm: /var/log/slurm-llnl/slurmd.pid /var/log/slurm-llnl/slurmctld.pid
- iv. View the physical configuration (sockets, cores, real memory, etc.) of each of the compute nodes with the command slurmd -C, and update this information in slurm.conf.
- v. Set the State of the node as UNKNOWN (slurm assigns BUSY or IDLE) or FUTURE.
- vi. It may be a good idea to assign weights to the compute nodes. All things being equal, jobs will be allocated the nodes with the lowest weight. The enables prioritization based upon hardware parameters such as GPUs, RAM, CPU clock speed, CPU core number, CPU generation. (more info)
- vii. It may be a good idea in the future to uncomment TmpFS= in slurm.conf. (/tmp is the default; can change to e.g. /scratch.) You can add TmpDisk=xxxxx to each compute node line, where xxxxx is the size of the temporary file system.
- (j) Create spool directories:

mkdir -p /var/spool/slurm/d
mkdir /var/spool/slurm/ctld

chown slurm: /var/spool/slurm /var/spool/slurm/d /var/spool/slurm/ctld

(k) Create a gres.conf file.

Inside this file, add a line for each GPU available on that node as follows: Name=gpu Type=<type> File=/dev/nvidia#. (Confirm numbers with ls -l /dev/nvidia\*.) See the documentation for more options.

- (l) Copy cgroup.conf.example into cgroup.conf and make the following changes:
  - i. ConstrainCores=no
  - ii. ConstrainRAMSpace=yes (change from no)
  - iii. You may also want to include MemSpecLimit and ContrainKmemSpace. (reference material)
- (m) Adjust the grub configuration. Open /etc/default/grub

 $\label{eq:condition} {\rm Add\ cgroup\_enable=memory\ swapaccount=1\ to\ GRUB\_CMDLINE\_LINUX\ line}.$ 

Run update-grub.

- (n) Check the node configuration as detected by slurm by typing slurmd -C into the command line. Adjust the appropriate line of the COMPUTE NODES section of the slurm.conf file to match.
- (o) Retrieve the configuration files:
  - i. Determine your version of slurm by typing dpkg -l | grep slurm. It should report version 17.11.2-1build1.
  - ii. Obtain the code directly from the command line with: wget https://github.com/SchedMD/slurm/archive/slurm-17-11-2-1.tar.gz
  - iii. Extract the files. The example configuration files are in <unzipped-slurm>/etc/. Copy all example config files into /etc/slurm-llnl/
- (p) Copy slurm.conf.example to slurm.conf and make the following changes (e.g. on thanos):
  - i. ClusterName=Marvel
  - ii. ControlMachine=magneto
  - iii. ProctrackType=proctrack/cgroup
  - iv. TaskPlugin=task/cgroup
  - v. InactiveLimit=600
  - vi. NodeName=thanos
  - vii. Nodes=thanos
  - viii. PartitionName=CEM
  - ix. Remove Procs=1 and replace it with CPUs=128. (On a multi-core/hyperthreaded system, slurm uses the number of threads as the number of CPUs)

- x. Add a RESOURCES section just above COMPUTE NODES with the following: GresTypes=gpu.
- xi. Also under the RESOURCES section, add LaunchParameters=send\_gids. This has slurmctld look up the user name and group ids instead of the individual nodes and prevents the "couldn't chdir" error. This is the default setting in newer versions of slurm.
- xii. In the COMPUTE NODES, add the following to each node containing one or more GPUs. # is the number of available GPUs on that node: Gres=gpu:#. Insert this just before State=UNKNOWN.
- xiii. In the SCHEDULING section, set the default memory per node at 1000 MB. (Slurm's default is ALL, which will not allow multiple jobs simultaneously.) DefMemPerNode=1000
- xiv. Change the location of the slurm PID files to the following: SlurmctldPidFile=/var/run/slurm-llnl/slurmctld.pid SlurmdPidFile=/var/run/slurm-llnl/slurmd.pid
- xv. Modify slurm.conf so that the nodes can be rebooted while slurm is running. Change the reboot program to RebootProgram="/sbin/reboot".
- xvi. Change when a DOWN node will be returned to service. The default (0) is that nodes will remain down until the admin manually changes the state. We will change this to 1, meaning that the nodes will be restored to service if it is reponding, has a valid configuration, and was not manually set as DOWN.

ReturnToService=1

- xvii. Check that StateSaveLocation=/var/spool/slurm/ctld. This directory should already exist, but doublecheck to make sure.
- xviii. Check that FastSchedule=1 and SchedulerType=sched/backfill (default settings).
- xix. Set the consumable resources (1 and 2): SelectType=select/cons\_res
- xx. You must also select what is allowed as consumable resources. In slurm.conf, set  $SelectTypeParameters=CR\_CPU\_Memory$ .

NOTE: If you use memory as a consumable resource, you *must* set the RealMemory parameter. NOTE: If CPUs are a consumable resource, Slurm has no notion of sockets, cores, or threads. On single- and multi-core systems, CPU refers to cores. On a multi-core/hyperthread system CPU refers to threads.

- xxi. Because both CPUs and Memory are consumable resources, you *must* set OverSubscribe=NO to prevent jobs from conflicting with one another. Strange behavior will occur if OverSubscribe=YES, as jobs will conflict with one another.
- xxii. Configure the partitions in slurm.conf, for example:

PartitionName=xeon8 Nodes=a[070-080] Default=YES DefaultTime=50:00:00 MaxTime=168:00:00 State=UNKNOWN

In the SCHEDULING section of the slurm.conf file, set EnforcePartLimits=YES. This will reject jobs that exceed a partition's size and/or time limits when they're submitted.

Things to keep in mind for the future (not setting these up):

- Partitions may overlap so that some nodes belong to several partitions.
- Access to partitions is configured in slurm.conf using AllowAccounts, AllowGroups, or AllowQos.
- If some partitions (e.g. big memory nodes) should have a higher priority, set this in slurm.conf using the multifactor plugin: PartitionName ... PriorityJobFactor=10 PriorityWeightPartition=1000
- xxiii. By default, slurm propagates all user limits from the submitting node (see ulimit -a to the batch jobs. Configure slurm.conf so that the locked memory limit isn't propagated by uncommenting and setting as follows:

#### PropagateResourceLimitsExcept=MEMLOCK

(We haven't done the following, but if you have imposed any non-default limits on the login nodes in /etc/security/limits.conf or /etc/security/limits.d/\*.conf, you probably want to prohibit these by setting: PropagateResourceLimitsExcept=ALL

See the slurm documentation for available options.)

- xxiv. Do NOT modify #PluginDir! Doing so causes slurm to crash. Slurm defaults to: usr/lib/x86\_64-linux-gnu/slurm-wlm
- (q) Start slurmd and, if applicable, slurmctld.

sudo systemctl start slurmd

sudo systemctl start slurmctld # if applicable

You will get a warning or error if slurmd -C failed and the code autofilled the laptop values.

- (r) Removes the extracted folder. The downloaded compressed folder is left untouched.
- (s) End of installation script.
- 5. Check that the NodeName line matches the output of slurmd -C. If slurmd -C fails to execute properly, install\_slurm.sh autofills with the values for an Oryx Pro.
- 6. Resolve any errors that popped up when running the installation script.
  - (a) If the daemon(s) failed to start, type systemctl status <daemon>. If slurm can't find nodes or a machine name, fix the slurm.conf and try again.
  - (b) If slurm complains that it doesn't have permissions to access a directory, you probably forgot sudo when starting slurm.
  - (c) If slurm isn't starting because it is missing directories, manually create those directories, set slurm as the owner, and try again.
  - (d) If slurm claims to be missing any configuration files (\*.conf), see if it exists in /etc/slurm-llnl as \*.conf.example. If it does, copy it, modify it, and try again. If it doesn't exist, refer to the source code on github for your version of slurm and copy it where it needs to go.
  - (e) If slurm can't find the GPUs, make sure that the system can see the GPUs and that you have an appropriate Nvidia driver.
  - (f) If it's still not working, start slurm manually (section ??) to see more detailed error messages.
- 7. At present the script only handles local setup.
  - (a) slurm.conf Nodes and partitions on remote machines must be added manually. The rest of the file is the same, so all that will be required is copy/pasting the node and partition information. Add NodeAddr=<IP> just after NodeName=<name> to all of the compute nodes.
  - (b) Copy the proper munge key into /etc/munge, then restart the munge and slurmd daemons.
- 8. If you installed slurm with install\_slurm.sh, cgroup.conf will be the same on all nodes and all the gres.conf files will be setup appropriately. If you did not use the script, make sure that cgroup.conf is the same on all compute nodes and add gres.conf files as necessary.
- 9. Restart the node.
- 10. Check that munge is setup properly.
  - (a) If munge is already running, stop it with systemctl stop munge.
  - (b) Check that the following files/directories are owned by munge instead of root: /etc/munge, /usr/bin/munge, /usr/sbin/munged, /var/lib/munge, /var/log/munge, /var/run/munge
  - (c) Create a munge key on the control node with sudo /usr/sbin/create-munge-key. (Ubuntu may have already done this for you.)
  - (d) On the controller, make sure the munge key (munge.key) is in /etc/munge/munge.key and change the owner to munge.

- (e) Copy the key from the control node to all existing compute nodes: sudo scp /etc/munge/munge.key admin@compute-node:/home/<admin>/
- (f) On the compute nodes, move the munge.key into /etc/munge. Make sure that it is owned by munge with file permissions 400.
- (g) Make sure that munge is enabled and (re)start it on all machines: sudo systemctl start munge
- (h) Check if munge is running by typing systemctl status munge.
- (i) Test munge:

Generate a credential on stdout:

munge -n

Check if a credential can be locally decoded:

munge -n | unmunge

Check if a credential can be remotely decoded:

munge -n | ssh <admin>@<node> unmunge

Run a quick benchmark:

remunge

11. Start slurm. Don't worry about enabling the daemons just yet; that will happen later.

```
# Control node
sudo systemctl start slurmctld
sudo systemctl start slurmd # Compute nodes
```

12. Test that the job submission is working. The submission command is sbatch <script-name>. To check the status of the job, type squeue. Output will be written in the same folder as the script. Refer to section ?? for an explanation of the SBATCH directives.

A very basic test script:

```
#!/bin/bash
#SBATCH --job-name="testjob"
#SBATCH --time=2:00:00
echo "running job"
sleep 120
echo "All done! :)"
```

A slightly less basic test script (%x is the job name and %j is the job number):

```
#SBATCH --job-name=example
#SBATCH --cpus-per-task=1
#SBATCH --nodes=1
```

#!/bin/bash

#SBATCH --ntasks-per-node=1

#SBATCH --time=10:00 #SBATCH --mem=1000

#SBATCH --partition=CEM

#SBATCH --output=%x.o%j

python temp.py sleep 120

Note: Both of these test scripts contain the sleep command specifically to keep the job "running" for a longer time; it is not necessary for actual jobs.

13. Stop the slurm daemons:

```
systemd: sudo systemctl stop <daemon>
Manual start: Ctrl-C
```

- 14. We are using the default Prolog and Epilog scripts. Refer to the documentation if this changes.
- 15. Restart the node.
- 16. Start slurm and test the queue to confirm that it can run multiple jobs simultaneously.
- 17. Enable slurm.

```
sudo systemctl enable slurmctld # Control node(s)
sudo systemctl enable slurmd # Compute nodes
```

### 5.3 Hyperthreading

Check for hyperthreading on your system with lscpu or lscpu | grep "per core". From the slurm documentation on hyperthreading:

If your nodes are configured with hyperthreading, then a CPU is equivalent to a hyperthread. Otherwise a CPU is equivalent to a core. You can determine if your nodes have more than one thread per core using the command "scontrol show node" and looking at the values of "ThreadsPerCore".

Note that even on systems with hyperthreading enabled, the resources will generally be allocated to jobs at the level of a core (see NOTE below). Two different jobs will not share a core except through the use of a partition OverSubscribe configuration parameter. For example, a job requesting resources for three tasks on a node with ThreadsPerCore=2 will be allocated two full cores. Note that Slurm commands contain a multitude of options to control resource allocation with respect to base boards, sockets, cores and threads.

(NOTE: An exception to this would be if the system administrator configured SelectType-Parameters=CR\_CPU and each node's CPU count without its socket/core/thread specification. In that case, each thread would be independently scheduled as a CPU. This is not a typical configuration.)

If SelectTypeParameters is set to CR\_CPU or CP\_CPU\_Memory, slurm will treat each thread as a CPU and completely disregard which core a thread is on. If it is set to CR\_Core or CR\_Core\_Memory, slurm can assign multiple threads to a core but will not assign multiple jobs to the same core. If it is set to CR\_ONE\_TASK\_PER\_CORE, then slurm will only assign one task per core regardless of the number of threads available.

You can also disable hyperthreading in the kernel using grub:

- 1. Create a backup copy of /etc/default/grub.
- Open /etc/default/grub and set the maximum number of CPUs the the number of physical cores:
   Find the line that begins with GRUB\_CMDLINE\_LINUX\_DEFAULT=. Append maxcpus=N after other options like quiet splash
- 3. Save the file, then run sudo update-grub
- 4. Reboot, then check for hyperthreading with lscpu | grep "per core".

We need to BENCHMARK to decide the best option. Benchmarking tests:

- 1. Use CR\_CPU\_Memory with hyperthreading enabled.
- 2. Use CR\_Core\_Memory with hyperthreading enabled.
- 3. Use CR\_ONE\_TASK\_PER\_CORE with hyperthreading enabled.
- 4. Use CR\_CPU\_Memory with hyperthreading disabled in the kernel.

### 5.4 Sharing StateSaveLocation

If you have two controllers (primary and backup) and the system was set up with NFS instead of Lustre with each controller as an NFS host, some rsync and ssh key trickery is required to make both controllers share the state save information. Each machine must check the other should one of them go offline.

(The choice of NFS was a good idea with the initial cluster. We did not originally expect to have two controllers. Not switching to Lustre as long as this kluge works.)

- 1. Use sudo -i to run as root.
- 2. Open root's crontab on both machines with crontab -e.

Add the following lines to copy to the other machine once an hour (for testing, ultimately more frequently). (Slurm by default writes this state every 5 seconds.) Note: you must use the admin account for rsync. Running rsync from the root crontab with sudo [-i] -u <admin> rsync will be rejected by the remote servers.

- 3. Type exit to return to the admin account.
- 4. If ssh keys are already set up, skip to step 7. Otherwise, make ssh keys on each machine in the admin account. Modify the key name/location if desired, but you must leave the passphrase empty.

```
ssh-keygen [-f ~/.ssh/<custom_name>]
```

5. Copy the keys to the admin account on the other controller, then test the key.

```
ssh-copy-id <admin>0<remote>
ssh -i ~/.ssh/<local_id_rsa> <admin>0<remote>
```

6. Test that rsync works over ssh in the admin account.

```
rsync -a -e "ssh -i ~/.ssh/<local_id_rsa>" "<randomfile>" "<admin>0<remote>:~/"
```

7. Modify the admin crontab on each machine to copy to the remote machine once an hour.

- 8. Check /var/log/syslog or the log mailed by rsync to confirm that it works.
- 9. Each node needs to copy the state files from the other system *before* starting slurm. I could make this into a daemon that is required before slurmctld can start, but I'm going with the following for now.

NOTE: I've confirmed that this script works in isolation but have yet to properly test takeover on the controllers!

(a) Open the ~/.bashrc file on the admin account.
Append the following text:

```
# Slurmctld start if daemon test condition failed
# Daemon: /etc/systemd/system/multi-user.target.wants/slurmctld.service
if (! systemctl status slurmctld | grep "[Aa]ctive.*[Rr]unning" > /dev/null); then
    deltat=$(( $(date "+%s") - $(date "+%s" -r /var/spool/slurm/ctld/job_state) ))
```

- (b) Stop slurmctld for testing purposes.
- (c) Source ~/.bashrc.

fi

- (d) If you see Starting slurmctld... and no error messages, then the script works properly. Confirm that the daemon is running with systemctl status slurmctld.
- (e) Disable slurmctld. The daemon will only start when the admin logs in for the first time, but the slurm state will always be up to date when the system resumes.
- 10. Open the admin .bashrc on both controllers and alias a command that transfers the slurm state immediately prior to issuing the takeover command.
  - (a) Create a file called transfer\_slurm\_state.sh.

Guides to crazy ssh options: 1

Place the following text into the file:

- (b) Alias the following in .bash\_aliases (preferred) or .bashrc, then source .bashrc. alias state\_takeover='bash /Code/MiniClusterTools/transfer\_slurm\_state.sh; sudo scontrol takeover'
- 11. Switch from using cron to the systemd timers to run more frequently.

## 5.5 Database setup

1. If you followed the basic slurm install instructions in section 5.2, you should have downloaded the MiniClusterTools git repo. If not, do it now.

```
git clone https://github.com/coyleej/MiniClusterTools.git
```

2. Run slurmdb\_initial\_setup.sh. It automates much of the setup:

```
bash slurmdb_initial_setup.sh
```

Here's what the script does, with some explanation:

- (a) Create the log file:
  - touch /var/log/slurmdbd.log

chown slurm: /var/log/slurmdbd.log

- (b) Create the pid file:
  - touch /var/run/slurm-llnl/slurmdbd.pid

chown slurm: /var/run/slurm-llnl/slurmdbd.pid

- (c) In slurm.conf, make the following changes:
  - i. Uncomment:

JobAcctGatherType=jobacct\_gather/linux

JobAcctGatherFrequency=30

AccountingStorageType=accounting\_storage/slurmdbd

ii. Modify:

AccountingStorageHost=<IP or domain name>

AccountingStorageLoc=/var/lib/mysql

AccountingStoragePass=/var/run/munge/munge.socket.2 # munge daemon port

AccountingStoragePort=3306

AccountingStorageUser=slurm

iii. Add:

AccountingStoreJobComment=YES

AccountingStorageEnforce=associations

AccountingStorageTRES=gres/gpu,gres/gpu:gtx1080ti # by default billing, CPU, energy, and node are tracked

(d) Restart slurmctld, as required by some of these changes:

systemctl restart slurmctld

- (e) Copy slurmdbd.conf.example to slurmdbd.conf.
- (f) Open slurmdbd.conf
  - i. Change the following lines to the following:

DbdAddr=<magnetoIP>

DbdHost=magneto

PidFile=/var/run/slurm-llnl/slurmdbd.pid

ii. Modify the following:

StorageHost=magneto

StoragePort=3306 # the mysql default port

StoragePass=<password> # slurm's password in MariaDB StorageLoc=slurm\_acct\_db

iii. Add the following:

PurgeEventAfter=12months

PurgeJobAfter=12months

PurgeResvAfter=2months

PurgeStepAfter=2months

PurgeSuspendAfter=1month

PurgeTXNAfter=12months

PurgeUsageAfter=12months

- (g) Re-read the config files: scontrol reconfigure
- (h) We need to enable remote access to mariadb. Open /etc/mysql/my.cnf (it's symlinked to /etc/mysql/mariadb.cnf), and append the following to the end of the file:

[mysqld]

skip-networking=0

skip-bind-address

(i) Start MariaDB: systemctl start mariadb

3. Verify the setup with

scontrol show config | grep AccountingStorageHost

4. Troubleshoot the MariaDB daemon if it didn't start automatically in the script. Follow whatever error messages it gives, then restart the node and try again.

```
sudo systemctl start mariadb
```

If there have been multiple failed connection attempts, you may need to use the following to unblock the host IP:

sudo mysqladmin flush-hosts

- 5. Set up MariaDB:
  - (a) sudo mysql\_secure\_installation
  - (b) Set up the MariaDB root user password: Y
  - (c) Create root password: [redacted]
  - (d) Remove the anonymous user: Y
  - (e) Restrict root user access to the local machine: Y
  - (f) Remove the test database: Y
  - (g) Reload privilege tables: Y
- 6. Log in to the MariaDB server as the root user and add a slurm user. (MariaDB doesn't actually require the capitalization, but I'm including it to match their documentation.
  - (a) Open the database: sudo mysql
  - (b) Create the database:

```
MariaDB [(none)]> CREATE DATABASE slurm_acct_db;
Confirm with:
```

```
MariaDB [(none)]> SHOW DATABASES;
```

(c) Create a slurm user and grant database access (replace '<pass>' with the value in slurmdbd.conf):

GRANT ALL ON slurm\_acct\_db.\* TO 'slurm'@'," IDENTIFIED BY '<pass>' with grant option; Confirm with:

```
MariaDB [(none)]> SELECT user, host, plugin FROM mysql.user;
MariaDB [(none)]> SHOW GRANTS for slurm@localhost;
```

(d) Review the current setting for MySQL's innodb\_buffer\_pool\_size before running the slurmdbd for the first time.

```
MariaDB [(none)]> SHOW VARIABLES LIKE innodb_buffer_pool_size;
```

(e) Consider setting this value large enough to handle the size of the database. This helps when converting large tables over to the new database schema and when purging old records. Setting innodb\_lock\_wait\_timeout and innodb\_log\_file\_size to larger values than the default is also recommended. Note: The default buffer size is 128M.

These variables can be changed in one of the following files (not sure which one, but I suspect it's the first one):

```
/etc/mysql/conf.d/mysql.cnf
/etc/mysql/mariadb.cnf
/etc/mysql/mariadb.conf.d/*.cnf
[mysqld]
innodb_buffer_pool_size=256M
innodb_log_file_size=256M
innodb_lock_wait_timeout=1800
```

To implement this change you must shut down the database and move/remove the log files:

```
sudo systemctl stop mariadb
sudo rm /var/lib/mysql/ib_logfile?
sudo systemctl start mariadb
```

Verify the new buffer setting using the following command in the MariaDB shell:

MariaDB [(none)]> SHOW VARIABLES LIKE innodb\_buffer\_pool\_size;

This has been left as the default for now (obviously).

(f) Exit MariaDB:

```
MariaDB [(none)]> QUIT;
```

7. Start slurmdbd, acting on any issues that may appear:

```
sudo systemctl start slurmdbd
```

One issue I encountered was fixed by manually changing the owner of the database directory, and reinstall mariadb:

```
sudo chown mysql: /var/lib/mysql
sudo apt install --reinstall mariadb-common mariadb-client mariadb-server
Try setting up the database again.
```

If it's still grumpy, install mysql-server-5.7 with apt, then try setting up the database again.

- 8. Enable mariadb and slurmdbd.
- 9. For job accounting to work, the database and accounting tools must be configured as explained in the official documentation. Use sacctmgr to create and manage these records.

Accounting records are maintained based on "associations" consisting of four elements: cluster, account, user names and an optional partition name. All accounting things are lower case. You must define clusters before you add accounts and you must add accounts before you add users.

(a) Add the cluster to the database: sacctmgr add cluster <clustername>

(b) Add accounts:

```
sacctmgr add account <account> [Cluster=<clustername>] [parent=<parent>] \
Description="<description>" Organization=<organization>
Omitting Cluster will add the account to all clusters. parent is only required if the new account is a sub-account of another account.
```

(c) Add users:

```
sacctmgr add user <username> [Account=<accounts>] [DefaultAccount=<account>]
Account can take a single account or a comma separated list. Not specifying Account will give the user access to all accounts on the cluster. DefaultAccount will set the default account for a user. At least one of the two options is required.
```

(d) Commands to view accounting information:

```
sacctmgr list cluster
sacctmgr list configuration
sacctmgr list stats
```

- 10. If other nodes than the slurmdbd node must be able to connect to the slurmdbd service, you must open the firewall to specific hosts. Please see the Slurm\_configuration page under the firewall section.
- 11. Make the following changes in slurmdbd.conf:

May want to set PrivateData

- 12. Currently have no need to set up WCkeys. (Workload characterization keys are an orthogonal way to do accounting against possibly unrelated accounts. This can be useful where users from different accounts are all working on the same project.)
- 13. QOS includes multifactor job priority and job preemption. View with sacctmgr. By default everything is assigned normal. Can create something with higher priority.
- 14. Job completion logging is redundant if using the accounting infrastructure.
- 15. Don't set up PAM with the configuration we currently have! As long as users must submit from the node they want to run on, this is counterproductive!! For future use, see this guide.
- 16. Enable and start all daemons: mariadb, slurmdbd, slurmctld, slurmd
- 17. If you wish to customize squeue output, refer to section ??

### 5.6 Adjusting configuration files

When changing configuration files (e.g. slurm.conf, cgroup.conf), the change must be distributed to all nodes before applying the changes. You may also have to restart the slurm daemons.

- 1. If you modify settings like Epilog, Prolog, SlurmctldLogFile, SlurmdLogFile, etc.), all you need to do is run scontrol reconfigure on the control node to force all slurm daemons to re-read the configuration files. The slurm controller (slurmctld) forwards the request to all other daemons (e.g. slurmd). Running jobs will continue execution.
- 2. Slurm daemons must be restarted if any of these parameters are changed: AccountingStorageEnforce, AuthType, BackupAddr, BackupController, ControlAddr, ControlMach, PluginDir, StateSaveLocation, SlurmctldPort, SlurmdPort.
- 3. Slurm daemons must be restarted if nodes are added to or removed from the cluster.

ControlMachine and ControlAddr are defunct in newer versions; use SlurmctldHost instead.

### 5.6.1 Adding/removing nodes

When adding/removing nodes, do the following:

- 1. Stop slurmctld
- 2. Add/remove nodes in slurm.conf
- 3. Restart slurmd on all nodes
- 4. Start slurmctld

It is also possible to add nodes to slurm.conf with state=FUTURE. The nodes will not be seen by slurm commands in this state. Make them available by changing their state in the slurm.conf file and update the node state using scontrol rather than restarting the slurmctld daemon.

## 5.7 Slurm plugins

Do not change the default Slurm plugin location in slurm.conf!

Default: /usr/lib/x86\_64-linux-gnu/slurm-wlm

### 5.8 Slurm admin commands

These are the most common admin-specific commands in addition to the ones listed in section ??. (Those commands can be run with sudo to affect any job.) For details, refer to man <command>.

• Setup and rebooting commands

scontroltakedownOrders switch to backup controllerscontrolreboot[ASAP][Nodelist]Reboots nodes, see documentationscontrolshutdownShuts down the slurm daemonssacctmgrshutdownShuts down the cluster

slurmd -C Displays the physical configuration of a node when run

on that specific node

scontrol reconfigure Makes running daemons re-read configuration files

• Selected management and accounting commands

sacct [options] Display accounting information for slurm jobs
sacctmgr add <entity> <specs> Add cluster, accounts, users; identical to create
sacctmgr list <entity> [specs] Displays information about the specified entity

sacctmgr list <entity> [specs] Displays information about the specified entity sdiag Scheduling diagnostic tool

smd Failure management suport tool

sreport [options] [command] Generates reports of job usage and cluster utilization

sstat Display various status information

sview Graphical user interface to view and modify slurm

• Daemon commands: slurmctld, slurmd, and slurmdbd are the master/control, compute, and database daemons, respectively. They may need to be restarted if configuration files are modified (section 5.6).

systemctld enable <daemon> Enable daemons to start on boot; will not start a stopped dae-

mon

systemctld disable <daemon > Disable daemon so that it will not start; will not stop a running

daemon

systemctld start <daemon> Starts daemon manually, does not enable the daemon systemctld stop <daemon> Stops daemon manually, does not disable the daemon

systemctld status <daemon> Reports status of daemon

<daemon> -Dvvvv
Manually starts the daemon; "D" runs in the foreground and

"v"s (can have 0 to 7 "v"s) indicates desired verbosity

### 5.9 Reboot and shutdown nodes

#### 5.9.1 Reboot

Nodes may need to be rebooted after firmware or kernel upgrades. Use the RebootProgram in slurm.conf to reboot nodes as they become idle. Be mindful of slurm downtime behavior (section 5.9.3).

If you are rebooting the primary controller, the switch should be automatic, but you can also instruct the backup controller to take over. The backup controller requests control from the primary and wait for its termination, then switches to controller mode if primary controller cannot be contacted. This speeds up the slurm controller fail-over mechanism and minimizes disruption when the primary control node is down. Note: the primary controller will take the control back at startup. To reboot nodes

```
# Force switch to the backup controller (primary controller only)
scontrol takeover
# All nodes
scontrol reboot [ASAP] [NodeList]  # slurm 17.11.2
scontrol reboot [ASAP] [nextstate=<RESUME|DOWN>] [reason=<reason>] [NodeList] # newer
```

Explanation: ASAP prevents initiation of new jobs. Otherwise the system waits until it is idle to reboot and job scheduling is still allowed. The node state will be DRAIN (17.11.2) or REBOOT (newer) until rebooted or the reboot is cancelled. Newer versions of slurm also include nextstate, which specifies the state of the node after reboot, and reason, which shows users the reason the node is unavailable.

To cancel a reboot, use one of the following

```
scontrol update NodeName=<nodename> State=RESUME # slurm 17.11.2
scontrol cancel_reboot <nodelist> # newer versions, e.g. 18.08
```

#### 5.9.2 Shutdown

Shut down slurm daemons with scontrol shutdown [options], and servers with sacctmgr shutdown.

#### 5.9.3 Slurm downtime behavior

Be mindful of your configured SlurmdTimeout and SlurmctldTimeout values. If the Slurm daemons are down for longer than the specified timeout (currently 5 minutes), nodes will be marked DOWN and their jobs killed. Either increase the timeout values during an upgrade or ensure that the compute node slurmd are not down for longer than SlurmdTimeout.

### 5.10 Backup and restore database

In order to backup the entire database to a different location (for disaster recovery or migration), the following files must be backed up. (source) Make a database mysqldump using this script /root/mysqlbackup (insert the correct root database password for PWD).

Write permission to \$BACKUPFILE is required.

Make regular database dumps, for example by a crontab job: 30 7 \* \* \* /root/mysqlbackup

Restore of a database backup: The database contents must be loaded from the backup. To restore a MySQL database see for example How do I restore a MySQL dump file?. As user root input the above created backup file:

```
mysql -u root -p < /root/mysql_dump</pre>
```

## 5.11 Upgrading slurm

Almost every new major release of Slurm (e.g. 16.05.x to 17.02.x) involves changes to the state files with new data structures, new options, etc. Slurm permits upgrades between any two versions whose major release numbers differ by two or less (e.g. 16.05.x or 17.02.x to 17.11.x) without loss of jobs or other state information. State information from older versions will not be recognized and will be discarded, resulting in loss of all running and pending jobs. State files are not recognized when downgrading and will be discarded. Create backup copies of state files before proceeding to later recover the jobs.

slurmdbd must be the same or higher major release as slurmctld. When changing the version to a higher release number (e.g. from 16.05.x to 17.02.x) always upgrade slurmdbd first. Database table changes

may be required for the upgrade. If the database contains a large number of entries, slurmdbd may require an hour or two to update the database and will be unresponsive during this time.

slurmctld must be upgraded before or at the same time as slurmd on the compute nodes. It is recommended to update all daemons at the same time.

The libslurm.so version is increased every major release. Packages with slurm integration (e.g. MPI libraries) should be recompiled. Sometimes symlinking old .so name(s) to the new one(s) may work, but this is not guaranteed.

If you built your own version of Slurm plugins, they will likely need modification to support a new version of Slurm. It is common for plugins to add new functions and function arguments during major updates. See the RELEASE\_NOTES file for details.

The recommended upgrade order is as follows:

- 1. Shutdown the slurmdbd daemon
- 2. Dump the Slurm database using mysqldump in case of possible failure
- 3. Increase innodb\_buffer\_size in my.cnf to 128M
- 4. Upgrade the slurmdbd daemon
- 5. Restart the slurmdbd daemon
- 6. Increase SlurmdTimeout and SlurmctldTimeout values and scontrol reconfigure to take effect
- 7. Shutdown the slurmctld daemon(s)
- 8. Shutdown the slurmd daemons on the compute nodes
- 9. Copy the contents of the configured StateSaveLocation directory in case of possible failure
- 10. Upgrade the slurmctld and slurmd daemons
- 11. Restart the slurmd daemons on the compute nodes
- 12. Restart the slurmctld daemon(s)
- 13. Validate proper operation
- 14. Restore original SlurmdTimeout and SlurmctldTimeout, and then scontrol reconfigure
- 15. Destroy backup copies of database and/or state files

Note: It is possible to update the slurmd daemons on a node-by-node basis after the slurmctld daemon(s) are upgraded, but make sure their down time is below the SlurmdTimeout value.