MINICLUSTER TOOLS DOCUMENTATION

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

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Important notes

These scripts were developed to work with the following operating system and shell. If you are using a different operating system or a different version of Ubuntu, you will likely need to make modifications. I tried to maintain POSIX compliance with the shell scripts, but I make no promises.

Operating System Ubuntu 18.04

Shell bash

Documentation

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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Chapter 1

Setup Scripts

1.1 sshd_setup

This setup is automated in the sshd_setup.sh file from MiniClusterTools repository.

- 1. Install fail2ban and openssh-server with apt. We'll use the default: ban IP addresses 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 here).
- 3. Open /etc/ssh/sshd_config and change some ssh settings.

The convention in this file is to have default settings commented out. Only uncomment something if you are changing the value from the default! Note: We are making an exception to this convention for the values the base has 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.

Protocol 2

- (b) Change LoginGraceTime to ${\tt lm}$
 - 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 with openssh 7.5! We are using openssh 7.6. Privilege separation is now mandatory. Including this line results in a warning when checking the configuration.
- 4. Check that sshd_config is valid and error-free:

```
sudo sshd -t
```

5. Reload the daemon:

```
sudo systemctl restart sshd
```

6. Test by logging in again.

1.2 login_banner

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

Ubuntu is set to automatically download and install security updates, but not security upgrades. The base requires us to automate security upgrades, so we will use the unattended-upgrades package. These changes are automated in the set_unattended_upgrades.sh file.

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 which may cause dependency issues. Security upgrades are far less likely to cause dependency issues. If you do automate everything and happen to run into problems, refer to section ??.

Automatic upgrades must be set up manually. While there are several ways to do this, we will all use unnattended-upgrades. It comes preinstalled and can be configured in two different ways:

- 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 apt logs: /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. To view the default values:

```
cat /lib/systemd/system/apt-daily.timer
```

2. If you wish to change the values, do **NOT** modify the default file. Instead, you should override it. Create a new file:

```
/etc/systemd/system/apt-daily-upgrade.timer.d/override.conf
```

Add something like the following (run once a day at 6:00, randomized delay of <4 hours):

```
[Timer]
OnCalendar=*-*-* 6:00
RandomizedDelaySec=4h
```

3. Reload and restart the daemons:

sudo systemctl daemon-reload && sudo systemctl restart apt-daily.timer

1.4 set_password_policy

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
```

1.4.2 HBSS

We must install HBSS and update the policies. The installation script (install.sh) is included in Mini-ClusterTools and called as part of set_passwd_policy.sh. It can be called separately with the following:

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

1.5 auto_user_setup

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

Chapter 2

Installation scripts

2.1 repo_download_w_some_install

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: Although MANTIS can (and will if you use the script) be installed prior to S4, S4 is a required dependency of MANTIS. 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 repos (pybind11, OpenBLAS, 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.

Chapter 3

Monitoring scripts

3.1 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.

Chapter 4

Slurm setup and administration

This setup works on Ubuntu 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

4.1 Reference materials

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

Slurm admin quick-start

Slurm official documentation

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

4.2 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 correct timezone and confirm that your system clock is correct:

sudo timedatectl set-timezone America/New_York
timedatectl

- (c) Check that nvidia-driver-418 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-418.
 - iii. Use apt to install nvidia-driver-418 if neither it nor a newer version are present.
- (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

- (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 file.
- 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

 $\label{eq:def:Add-cgroup} Add\ \texttt{cgroup_enable=memory}\ \ \texttt{swapaccount=1}\ \ \texttt{to}\ \ \texttt{GRUB_CMDLINE_LINUX}\ \ \texttt{line}.$

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. 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.
- xii. 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
- xiii. 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
- xiv. Modify slurm.conf so that the nodes can be rebooted while slurm is running. Change the reboot program to RebootProgram="/sbin/reboot".
- xv. Check that StateSaveLocation=/var/spool/slurm/ctld. This directory should already exist, but doublecheck to make sure.
- xvi. Check that FastSchedule=1 and SchedulerType=sched/backfill (default settings).
- xvii. Set the consumable resources (1 and 2): SelectType=select/cons_res
- xviii. 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.

- xix. 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.
- xx. 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
- xxi. 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.)

- xxii. 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 will be the same, so all that will be required is copy/pasting the node and partition information between files. You need to add NodeAddr=<IP> to all of the compute nodes. Add this just after NodeName=<name>.
 - (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.

```
sudo systemctl start slurmctld # Control node
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):

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

```
#SBATCH --job-name=example
#SBATCH --cpus-per-task=1
#SBATCH --nodes=1
#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
sudo systemctl enable slurmd # Compute nodes
```

4.3 Database setup

1. If you followed the basic slurm install instructions in section 4.2, 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]

 ${\tt skip-networking=0}$

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.
```

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 ??

4.4 Slurm plugins

Do not change the default Slurm plugin location in slurm.conf! Default location: /usr/lib/x86_64-linux-gnu/slurm-wlm

4.4.1 Node health check

4.5 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

scontrol reboot [ASAP] [Nodelist] Reboots nodes, see documentation
scontrol shutdown Shuts down the slurm daemons
sacctmgr shutdown Shuts 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 View and modify slurm account info sacctmgr add <entity> <specs> Add cluster, accounts, users; identical to create sacctmgr list <entity> [specs] Displays information about the specified entity sdiag Scheduling diagnostic tool Failure management suport tool smdsreport [options] [command] Generates reports of job usage and cluster utilization Display various status information sstat Graphical user interface to view and modify slurm sview

• 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 4.6).

systemctld enable <daemon> Enable daemons to start on boot; will not start a stopped daesystemctld 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 Stops daemon manually, does not disable the daemon systemctld stop <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

4.6 Adjusting configuration files

When changing configuration files (e.g. slurm.conf, cgroup.conf), the change must first be distributed to all compute and login nodes. After copying the new configuration files to all nodes, use scontrol reconfigure on the control node to force all slurm daemons to re-read the configuration file. The slurm controller (slurmctld) forwards the request to all other daemons (e.g. slurmd). Depending on the changes, you may also have to restart the slurm daemons. From the scontrol man page about the reconfigure option:

- 1. If you modify settings like Epilog, Prolog, SlurmctldLogFile, SlurmdLogFile, etc.), all you need to do is run scontrol reconfigure. 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.

4.6.1 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.

Reboot and shutdown nodes 4.7

4.7.1Reboot

Nodes may need to be rebooted after firmware or kernel upgrades. Reboot them as they become idle using the RebootProgram as configured in slurm.conf. Be mindful of slurm downtime behavior (section 4.7.3).

```
scontrol reboot [ASAP] [NodeList]
                                               # comma-separated, slurm 17.11.2
scontrol reboot [ASAP] [nextstate=<RESUME|DOWN>] [reason=<reason>] [NodeList] # newer
```

Explanation: ASAP will prevent initiation of new jobs, otherwise the system will wait until it is idle to reboot. Job scheduling is still allowed. Node state will be REBOOT until rebooted or the reboot is cancelled. NOTE: Behavior of ASAP is sometime wonky in slurm 17.11.2.

Newer versions of slurm also include nextstate, which specifies the state of the node after reboot, and reason, shows users the reason the node is unavailable.

To cancel a reboot, use one of the following

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

4.7.2 Shutdown

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

4.7.3 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) during an upgrade, nodes may be marked DOWN and their jobs killed. You can either increase the timeout values during an upgrade or ensure that the slurmd daemons on compute nodes are not down for longer than SlurmdTimeout.

4.8 Backup and restore database

(source for the following)

In order to backup the entire database to a different location (for disaster recovery or migration), the following files must be backed up. 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>
```

4.9 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.