Introduction
Making better infrastructure nodes
Making better compute nodes
Managing system complexity
Configuring Slurm policies

# OpenHPC: Beyond the Install Guide for PEARC24

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## Acknowledgments and shameless plugs

- OpenHPC especially Tim Middelkoop (Internet2) and Chris Simmons (Massachusetts Green High Performance Computing Center). They have a BOF at 1:30 Wednesday. You should go to it.
- Jetstream2 especially Jeremy Fischer, Mike Lowe, and Julian Pistorius. Jetstream2 has a tutorial at the same time as this one. Please stay here.
  - NSF CC\* for the equipment that led to some of the lessons we're sharing today (award #2127188).
  - ACCESS current maintainers of the project formerly known as the XSEDE Compatible Basic Cluster.

Configuring Slurm policies

#### Where we're starting from

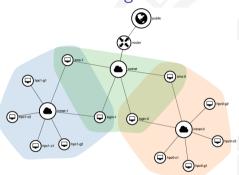


Figure 1: Two example HPC networks for the tutorial

#### You:

- have installed OpenHPC before
- have been issued a (basically) out-of-the-box OpenHPC cluster for this tutorial

#### Cluster details:

- Rocky Linux 9 (x86\_64)
- OpenHPC 3.1. Warewulf 3. Slurm 23.11.6
- 2 non-GPU nodes
- 2 GPU nodes (currently without GPU drivers, so: expensive non-GPU nodes)
- 1 management node (SMS)
- 1 unprovisioned login node

## Where we're starting from

We used the OpenHPC automatic installation script from Appendix A with a few variations:

- 1. Installed s-nail to have a valid MailProg for slurm.conf.
- 2. Created user1 and user2 accounts with password-less sudo privileges.
- 3. Changed CHROOT from /opt/ohpc/admin/images/rocky9.3 to /opt/ohpc/admin/images/rocky9.4.
- 4. Enabled slurmd and munge in CHROOT.
- 5. Added nano and yum to CHROOT.
- 6. Removed a redundant ReturnToService line from /etc/slurm/slurm.conf.
- 7. Stored all compute/GPU nodes' SSH host keys in /etc/ssh/ssh known hosts.

# Where we're going

- 1. A login node that's practically identical to a compute node (except for where it needs to be different)
- 2. A slightly more secured SMS and login node
- GPU drivers on the GPU nodes.
- 4. Using node-local storage for the OS and/or scratch
- 5. De-coupling the SMS and the compute nodes (e.g., independent kernel versions)
- 6. Easier management of node differences (GPU or not, diskless/single-disk/multi-disk, Infiniband or not, etc.)
- 7. Slurm configuration to match some common policy goals (fair share, resource limits, etc.)

#### Assumptions

- 1. We have a VM named login, with no operating system installed.
- 2. The eth0 network interface for login is attached to the internal network, and eth1 is attached to the external network.
- 3. The eth0 MAC address for login is known—check the **Login server** section of your handout for that. It's of the format aa:bb:cc:dd:ee:ff.
- 4. We're logged into the SMS as user1 or user2 that has sudo privileges.

# Create a new login node

Working from section 3.9.3 of the install guide:

```
[user1@sms ~]$ sudo wwsh -y node new login --netdev eth0 \
    --ipaddr=172.16.0.2 --hwaddr=__:__:__:__:__:
[user1@sms ~]$ sudo wwsh -y provision set login \
    --vnfs=rocky9.4 --bootstrap=`uname -r` \
    --files=dynamic_hosts, passwd, group, shadow, munge.key, network
```

Make sure to replace the \_\_ with the characters from your login node's MAC address!

Ever since login was powered on, it's been stuck in a loop trying to PXE boot. What's the usual PXE boot process for a client in an OpenHPC environment?

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- 4. iPXE makes a second DHCP request and this time, it gets a URL (by default, http://SMS\_IP/WW/ipxe/cfg/\${client\_mac}) for an iPXE config file.

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- 4. iPXE makes a second DHCP request and this time, it gets a URL (by default, http://SMS\_IP/WW/ipxe/cfg/\${client\_mac}) for an iPXE config file.
- 5. The config file contains the URL of a Linux kernel and initial ramdisk, plus multiple kernel parameters available after initial bootup for getting the node's full operating system contents.

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- 3. The node name, --netdev, --ipaddr, --hwaddr parameters all go into kernel parameters accessible from the provisioning software.
- 4. During the initial bootup, the --hwaddr parameter is passed to a CGI script on the SMS to identify the correct VNFS for the provisioning software to download (set by the --vnfs parameter).

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- 2. The --bootstrap parameter defines the kernel and ramdisk for the iPXE configuration.
- 3. The node name, --netdev, --ipaddr, --hwaddr parameters all go into kernel parameters accessible from the provisioning software.
- 4. During the initial bootup, the --hwaddr parameter is passed to a CGI script on the SMS to identify the correct VNFS for the provisioning software to download (set by the --vnfs parameter).
- 5. After downloading the VNFS, the provisioning software will also download files from the SMS set by the --files parameter.

# Did it work? So far, so good.

```
[user1@sms ~]$ sudo ssh login
[root@login ~]# df -h
Filesystem
...
172.16.0.1:/home
172.16.0.1:/opt/ohpc/pub
```

#### Did it work? Not entirely.

```
[root@login ~]# sinfo
sinfo: error: resolve_ctls_from_dns_srv: res_nsearch error:
   Unknown host
sinfo: error: fetch_config: DNS SRV lookup failed
sinfo: error: _establish_config_source: failed to fetch config
sinfo: fatal: Could not establish a configuration source
```

systemctl status slurmd is more helpful, with

fatal: Unable to determine this slurmd's NodeName. So how do we fix this one?

So there's no entry for login in the SMS slurm.conf. To fix that:

1. Run slurmd -C on the login node to capture its correct CPU specifications. Copy that line to your laptop's clipboard.

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- 2. On the SMS, run nano /etc/slurm/slurm.conf and make a new line of all the slurmd -C output from the previous step (pasted from your laptop clipboard).

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- 3. Save and exit nano by pressing Ctrl-X and then Enter.

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- 4. Reload the new Slurm configuration everywhere (well, everywhere functional) with sudo scontrol reconfigure on the SMS.

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- 2. On the SMS, run nano /etc/slurm/slurm.conf and make a new line of all the slurmd -C output from the previous step (pasted from your laptop clipboard).
- 3. Save and exit nano by pressing Ctrl-X and then Enter.
- 4. Reload the new Slurm configuration everywhere (well, everywhere functional) with sudo scontrol reconfigure on the SMS.
- 5. ssh back to the login node and restart slurmd, since it wasn't able to respond to the scontrol reconfigure from the previous step (sudo ssh login systemctl restart slurmd on the SMS).

Now an sinfo should work on the login node:

```
[root@login ~]# sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 idle c1
```

#### Option 2: why are we running slurmd anyway?

The slurmd service is really only needed on systems that will be running computational jobs, and the login node is not in that category.

Running slurmd like the other nodes means the login node can get all its information from the SMS, but we can do the same thing with a very short customized slurm.conf with two lines from the SMS' slurm.conf:

```
ClusterName=cluster
SlurmctldHost=sms
```

#### Interactive test

- 1. On the login node as root, temporarily stop the slurmd service with systemctl stop slurmd
- On the login node as root, edit /etc/slurm/slurm.conf with nano /etc/slurm/slurm.conf
- 3. Add the two lines to the right, save and exit nano by pressing Ctrl-X and then Enter.

/etc/slurm/slurm.conf on login node

ClusterName=cluster SlurmctldHost=sms

Verify that sinfo still works without slurmd and with the custom /etc/slurm/slurm.conf.

```
[root@login ~]# sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 idle c1
```

# Make permanent changes from the SMS

Let's reproduce the changes we made interactively on the login node in the Warewulf settings on the SMS.

For the customized slurm.conf file, we can keep a copy of it on the SMS and add it to the Warewulf file store.

We've done that previously for files like the shared munge.key for all cluster nodes (see section 3.8.5 of the OpenHPC install guide).

We also need to make sure that file is part of the login node's provisioning settings.

#### Make permanent changes from the SMS

#### On the SMS:

Now the file is available, but we need to ensure the login node gets it. That's handled with wwsh provision.

#### A quick look at wwsh provision

What are the provisioning settings for compute node c1?

```
[user1@sms ~] $ wwsh provision print c1
c1: MASTER
                  = UNDEF
c1: BOOTSTRAP
                  = 6.1.96-1.el9.elrepo.x86_64
c1: VNFS
                  = rockv9.4
c1: VALIDATE
                  = FALSE
c1: FILES
                  = dynamic_hosts, group, munge.key, network,
  passwd, shadow
c1: KARGS
                  = "net.ifnames=0 biosdevname=0 quiet"
c1: BOOTLOCAL
                  = FALSE
```

#### A quick look at wwsh provision

What are the provisioning settings for node login?

```
[user1@sms ~] $ wwsh provision print login
login: MASTER
                  = UNDEF
login: BOOTSTRAP = 6.1.96-1.el9.elrepo.x86_64
login: VNFS
                  = rockv9.4
login: VALIDATE = FALSE
login: FILES
                  = dynamic_hosts, group, munge.key, network,
  passwd, shadow
login: KARGS
                  = "net.ifnames=0 biosdevname=0 quiet"
login: BOOTLOCAL
                  = FALSE
```

#### A quick look at wwsh provision

The provisioning settings for c1 and login are identical, but there's a lot to read in there to be certain about it.

We could run the two outputs through diff, but every line contains the node name, so no lines are literally identical.

Let's simplify and filter the wwsh provision output to make it easier to compare.

## Filter the wwsh provision output

▶ I only care about the lines containing = signs, so

```
wwsh provision print c1 | grep =
```

is a start.

#### Filter the wwsh provision output

▶ I only care about the lines containing = signs, so

is a start.

▶ Now all the lines are prefixed with c1:, and I want to keep everything after that, so

```
wwsh provision print c1 | grep = | cut -d: -f2-
```

will take care of that.

#### Filtered result

```
wwsh provision print c1 | grep = | cut -d: -f2-
```

```
MASTER
                    UNDEF
BOOTSTRAP
                   = 6.1.96-1.el9.elrepo.x86 64
VNFS
                    rockv9.4
VALIDATE
                   = FALSE
FILES
                   = dynamic_hosts,group,munge.key,network,
  passwd, shadow
. . .
KARGS
                   = "net.ifnames=0 biosdevname=0 quiet"
BOOTLOCAL
                   = FALSE
```

Much more useful.

#### Make a function for this

We may be typing that command pipeline a lot, so let's make a shell function to cut down on typing:

```
[user1@sms ~]$ function proprint() {
  wwsh provision print $@ | grep = | cut -d: -f2- ; }
[user1@sms ~]$ proprint c1
  MASTER = UNDEF
  BOOTSTRAP = 6.1.96-1.el9.elrepo.x86_64
...
```

#### diff the outputs

We could redirect a proprint c1 and a proprint login to files and diff the resulting files, or we can use the shell's <() operator to treat command output as a file:

```
[user1@sms ~]$ diff -u <(proprint c1) <(proprint login)
[user1@sms ~]$</pre>
```

Either of those shows there are zero provisioning differences between a compute node and the login node.

#### Add the custom slurm.conf to the login node

Add a file to login's FILES property with:

```
[user1@sms ~]$ sudo wwsh -y provision set login \
  --fileadd=slurm.conf.login
```

(refer to section 3.9.3 of the install guide for previous examples of --fileadd).

# Check for provisioning differences

```
[user10sms ~]$ diff -u <(proprint c1) <(proprint login)
--- /dev/fd/63 2024-07-06 11:11:07.682959677 -0400
+++ /dev/fd/62 2024-07-06 11:11:07.683959681 -0400
00 - 2.7 + 2.7 00
 BOOTSTRAP
                   = 6.1.96-1.el9.elrepo.x86_64
 VNFS
                    = rocky9.4
 VALIDATE
                   = FALSE
 FILES
                    = dynamic hosts, group, munge.key, network,
 passwd, shadow
+ FILES
                    = dynamic hosts, group, munge.key, network,
 passwd, shadow, slurm.conf.login
 PRESHELL.
                   = FALSE
 POSTSHELL
                   = FALSE
  POSTNETDOWN
                   = FALSE
```

#### Ensure slurmd doesn't run on the login node

To disable the slurmd service on just the login node, we can take advantage of conditions in the systemd service file. Back on the login node as root:

```
[user1@sms ~]$ sudo ssh login
[root@login ~]# systemctl edit slurmd
```

Insert three lines between the lines of ### Anything between here... and
### Lines below this comment...:

```
[Unit]
ConditionHost=|c*
ConditionHost=|g*
```

This will only run the service on nodes whose hostnames start with c or g.

#### Ensure slurmd doesn't run on the login node

Once that file is saved, try to start the slurmd service with systemctl start slurmd and check its status with systemctl status slurmd:

```
o slurmd.service - Slurm node daemon
...
Condition: start condition failed at Sat 2024-07-06 18:12:17
EDT; 4min 22s ago
...
Jul 06 17:14:16 login systemd[1]: Stopped Slurm node daemon.
Jul 06 18:12:17 login systemd[1]: Slurm node daemon was skipped because of an unmet condition check (ConditionHost=c*).
```

#### Make the changes permanent

The systemctl edit command resulted in a file /etc/systemd/system/slurmd.service.d/override.conf. Let's:

- make a place for it in the chroot on the SMS, and
- copy the file over from the login node.

```
[user1@sms ~]$ export CHROOT=/opt/ohpc/admin/images/rocky9.4
[user1@sms ~]$ sudo mkdir -p \
    ${CHROOT}/etc/systemd/system/slurmd.service.d/
[user1@sms ~]$ sudo scp \
    login:/etc/systemd/system/slurmd.service.d/override.conf \
    ${CHROOT}/etc/systemd/system/slurmd.service.d/
override.conf 100% 23 36.7KB/s 00:00
```

## Make the changes permanent

#### Finally, we'll:

- rebuild the VNFS, and
- reboot both the login node and a compute node to test the changes.

```
[user1@sms ~]$ sudo wwvnfs --chroot=${CHROOT}
Using 'rocky9.4' as the VNFS name
...
Total elapsed time
: 84.45 s
[user1@sms ~]$ sudo ssh login reboot
[user1@sms ~]$ sudo ssh c1 reboot
```

#### Verify the changes on the login node

Verify that the login node doesn't start slurmd, but can still run sinfo without any error messages.

```
[user1@sms ~]$ sudo ssh login systemctl status slurmd
o slurmd.service - Slurm node daemon
...
Jul 06 18:26:23 login systemd[1]: Slurm node daemon was
    skipped because of an unmet condition check
    (ConditionHost=c*).
[user1@sms ~]$ sudo ssh login sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 idle c1
```

## Verify the changes on a compute node

Verify that the compute node still starts slurmd (it can also run sinfo).

```
[user1@sms ~] $ sudo ssh c1 systemctl status slurmd
o slurmd.service - Slurm node daemon
. . .
Jul 06 19:03:22 c1 systemd[1]: Started Slurm node daemon.
Jul 06 19:03:22 c1 slurmd[1082]: slurmd: CPUs=2 Boards=1
 Sockets=2 Cores=1 Threads=1 Memory=5912 TmpDisk=2956
 Uptime = 28  CPUSpecList = (null) FeaturesAvail = (null)
 FeaturesActive=(null)
[user1@sms ~]$ sudo ssh c1 sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 down c1
```

(Yes, c1 is marked down—we'll fix that shortly.)

#### Problem: the login node doesn't let users log in

What if we ssh to the login node as someone other than root?

```
[user1@sms ~]$ ssh login
Access denied: user user1 (uid=1001) has no active jobs on this
  node.
Connection closed by 172.16.0.2 port 22
```

which makes this the exact opposite of a login node for normal users. Let's fix that.

# Make the login node function as a login node

- ► The Access denied is caused by the pam\_slurm.so entry at the end of /etc/pam.d/sshd, which is invaluable on a normal compute node, but not on a login node.
- On the SMS, you can also do a diff -u /etc/pam.d/sshd \${CHROOT}/etc/pam.d/sshd
- ▶ You'll see that the pam\_slurm.so line is the only difference between the two files.

# Test a PAM change to the login node

- ► Temporarily comment out the last line of the login node's /etc/pam.d/ssh and see if you can ssh into the login node as a normal user (i.e., ssh user1@login).
- ► Your user should be able to log in now.
- ▶ In case the PAM configuration won't let root log in, **don't panic**! Instructors can reboot your login node from its console to put it back to its original state.

# Make the change permanent

- ▶ We want to ensure that the login node gets the same /etc/pam.d/sshd that the SMS uses.
- ▶ We'll follow the same method we used to give the login node a custom slurm.conf:

```
[user1@sms ~]$ sudo wwsh -y file import /etc/pam.d/sshd \
    --name=sshd.login
[user1@sms ~]$ wwsh file list
...
sshd.login : rw-r--r-- 1 root root 727 /etc/pam.d/sshd
```

#### Make the change permanent

(refer to section 3.9.3 of the install guide for previous examples of --fileadd).

# Test the change

Reboot the login node and let's see if we can log in as a regular user.

```
[user1@sms ~]$ sudo ssh login reboot
[user1@sms ~]$ ssh login
[user1@login ~]$
```

## A bit more security for the login node

- narrative about brute-force SSH activity
- verify what ports are listening on login (should really just be SSH)
- enabling firewalld
- enabling fail2ban
- realizing that the default wwbootstrap kernel is lacking, and rebuilding it

#### A bit more security for the login node

Not too long after your SMS and/or login nodes are booted, you'll see messages in the SMS /var/log/secure like:

because people who want to break into computers for various reasons have Internet connections.

## A bit more security for the login node

There's a lot of things that can be done to secure things, including:

- 1. Placing the SMS and login node external interfaces on protected network segment.
- 2. Allowing only administrative users to SSH into the SMS.
- 3. Replacing password-based authentication with key-based authentication.

Though #3 will eliminate brute-force password guessing attacks, it's usually not practical for a login node. So let's mitigate that differently with fail2ban.

#### How fail2ban works

- 1. Monitor /var/log/secure and other logs for indicators of brute-force attacks (invalid users, failed passwords, etc.)
- 2. If indicators from a specific IP address happen often enough over a period of time, block all access from that address for a period of time.
- 3. Once that period has expired, remove the IP address from the block list.

This reduces the effectiveness of brute-force password guessing by orders of magnitude ( $\sim$ 10 guesses per hour versus  $\sim$ 100 or  $\sim$ 1000 guesses per hour).

#### Test installing fail2ban on the login node

Install the fail2ban packages on the login node with

```
[user1@sms ~]$ sudo yum install --installroot=${CHROOT} \
  fail2ban
[user1@sms ~]$ sudo chroot ${CHROOT} systemctl enable \
  fail2ban firewalld
```

(this will also install firewalld).

Add the following to the chroot's sshd.local file with sudo nano \${CHROOT}/etc/fail2ban/jail.d/sshd.local:

```
[sshd]
enabled = true
```

Add drivers  $+= \frac{\text{kernel/net/}}{\text{to /etc/warewulf/bootstrap.conf}}$  and rerun wwbootstrap.

#### Test installing fail2ban on the login node

Befoer we go further, check if there's anything in /var/log/secure on the login node:

```
[user1@sms ~]$ sudo ssh login ls -l /var/log/secure -rw----- 1 root root 0 Jul 7 03:14 /var/log/secure
```

Nope. Let's fix that, too.

- ► Looking in /etc/rsyslog.conf, we see a bunch of things commented out, including the line #authpriv.\* /var/log/secure.
- ► Rather than drop in an entirely new rsyslog.conf file that we'd have to maintain, rsyslog will automatically include any \*.conf files in /etc/rsyslog.d.
- Let's make one of those for the chroot.

## Make an rsyslog.d file, rebuild the VNFS, reboot the login node

```
[user1@sms ~] $ echo "authpriv.* /var/log/secure" | \
    sudo tee ${CHROOT}/etc/rsyslog.d/authpriv-local.conf
authpriv.* /var/log/secure
[user1@sms ~] $ cat \
    ${CHROOT}/etc/rsyslog.d/authpriv-local.conf
authpriv.* /var/log/secure
[user1@sms ~] $ sudo wwvnfs --chroot=${CHROOT}
[user1@sms ~] $ sudo ssh login reboot
```

#### Post-reboot, how's fail2ban and firewalld on the login node?

```
[user1@sms ~] $ sudo ssh login systemctl status firewalld
[root@login ~]# systemctl status firewalld
x firewalld.service - firewalld - dynamic firewall daemon
     Loaded: loaded (/usr/lib/systemd/system/firewalld.service;
       enabled; preset>
     Active: failed (Result: exit-code) since Thu 2024-07-11
       16:49:47 EDT: 46mi>
. . .
Jul 11 16:49:47 login systemd[1]: firewalld.service: Main
 process exited, code=exited, status=3/NOTIMPLEMENTED
Jul 11 16:49:47 login systemd[1]: firewalld.service: Failed
 with result 'exit-code'.
```

#### Why was c1 marked as down?

You can return c1 to an idle state by running sudo scontrol update node=c1 state=resume on the SMS:

```
[user1@sms ~]$ sudo scontrol update node=c1 state=resume
[user1@sms ~]$ sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 idle c1
```

We should configure things so that we don't have to manually resume nodes every time we reboot them.

#### More seamless reboots of compute nodes

- ▶ Slurm doesn't like it when a node gets rebooted without its knowledge.
- ► There's an scontrol reboot option that's handy to have nodes reboot when system updates occur, but it requires a valid setting for RebootProgram in /etc/slurm/slurm.conf.
- ▶ By default, Slurm and OpenHPC don't ship with a default RebootProgram, so let's make one.

#### Adding a valid RebootProgram

## Informing all nodes of the changes and testing it out

```
[user1@sms ~]$ sudo scontrol reconfigure
[user1@sms ~]$ sudo scontrol reboot ASAP nextstate=RESUME c1
```

- scontrol reboot will wait for all jobs on a group of nodes to finish before rebooting the nodes.
- ▶ scontrol reboot ASAP will immediately put the nodes in a DRAIN state, routing all pending jobs to other nodes until the rebooted nodes are returned to service.
- scontrol reboot ASAP nextstate=RESUME will set the nodes to accept jobs after the reboot. nextstate=DOWN will lave the nodes in a DOWN state if you need to do more work on them before returning them to service.

#### Did it work?

TODO: verify what a successful "return to idle" looks like here, including an uptime of seconds to minutes rather than days.

```
[user1@sms ~]$ sudo ssh c1 uptime
  08:44:31 up 66 days, 17:24, 2 users, load average: 0.00, 0.04, 0.
[user1@sms ~]$ sinfo
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
normal* up 1-00:00:00 1 idle c1
```

# Decoupling kernels from the SMS

How to install kernels into the chroot and bootstrap from the chroot.

## Semi-stateful node provisioning

(talking about the gparted and filesystem-related pieces here.)

# Management of GPU drivers

(installing GPU drivers – mostly rsync'ing a least-common-denominator chroot into a GPU-named chroot, copying the NVIDIA installer into the chroot, mounting /proc and /sys, running the installer, umounting /proc and /sys, and building a second VNFS)

#### Configuration settings for different node types

(have been leading into this a bit with the wwsh file entries, systemd conditions, etc. But here we can also talk about nodes with two drives instead of one, nodes with and without Infiniband, nodes with different provisioning interfaces, etc.)

## Automation for Warewulf3 provisioning

(here we can show some sample Python scripts where we can store node attributes and logic for managing the different VNFSes)

Introduction
Making better infrastructure nodes
Making better compute nodes
Managing system complexity
Configuring Slurm policies

# Configuring Slurm policies

Can adapt a lot of Mike's CaRCC Emerging Centers talk from a couple years ago for this. Fair share, hard limits on resource consumption, QOSes for limiting number of GPU jobs or similar.

# Sample slide

#### Left column

This slide has two columns. They don't always have to have columns. It also has a titled block of content in the left column. Make sure you've always got a ::: notes block after the slide content, even if it has no content.

Use # and ## headers in the Markdown file to make level-1 and level-2 headings, ### headers to make slide titles, and #### to make block titles.