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OpenHPC: Beyond the Install Guide

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.

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Where we're starting from

Figure 1: Two example HPC networks

31 HPC clusters (2 shown) with:

1. Rocky Linux 9
2. OpenHPC 3
3. Warewulf 3
4. Slurm
5. 2 non-GPU nodes
6. 2 GPU nodes (currently without GPU drivers, so: expensive non-GPU nodes)
7. 1 management node (SMS)
8. 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 nodes' SSH host keys in `/etc/ssh/ssh_known_hosts`.

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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
3. 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.)

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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.

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Working from section 3.9.3 of the install guide:

```
[user1@sms-0 ~]$ sudo wwsh -y node new login --netdev eth0 \
    --ipaddr=172.16.0.2 --hwaddr=__:__:__:__:__:__
[user1@sms-0 ~]$ 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!

What'd we just do?

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?

1. The client network card tries to get an IP address from a DHCP server (the SMS) by broadcasting its MAC address.

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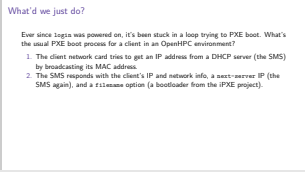
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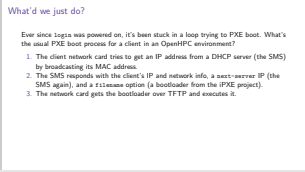
x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3. The network card gets the bootloader over TFTP and executes it.
4. iPXE makes a second DHCP request and this time, it gets a URL (by default, `http://SMS_IP/WW/ipxe/cfg/${client_mac}`) for an iPXE config file.

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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.

What'd we just do?

1. The node name, `--bmaddr`, and `--ipaddr` parameters go into the SMS DHCP server settings.

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What'd we just do?

1. The node name, `--bmaddr`, and `--ipaddr` parameters go into the SMS DHCP server settings.
2. The `--bootstrap` parameter defines the kernel and ramdisk for the iPXE configuration.

What'd we just do?

1. The node name, `--hwaddr`, and `--ipaddr` parameters go into the SMS DHCP server settings.
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.

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What'd we just do?

1. The node name, `--hwaddr`, and `--ipaddr` parameters go into the SMS DHCP server settings.
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).

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What'd we just do?

1. The node name, `--hwaddr`, and `--ipaddr` parameters go into the SMS DHCP server settings.
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@smc-0 ~]$ sudo ssh login
[root@login ~]# df -h
Filesystem
...
172.16.0.1:/home
172.16.0.1:/opt/ohpc/pub
```

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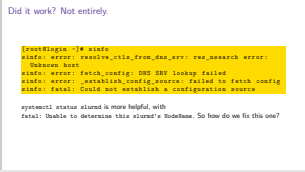
Did it work? Not entirely.
[root@login ~]# sinfo
sinfo: error: resolve_ctls_from_dns_srv: res_nsearch error: Unknown host
sinfo: error: fetch_config: DNS SRV lookup failed
sinfo: error: _establish_config_source: failed to fetch config
sinfo: fatal: Could not establish a configuration source
systemctl status slurmd is more helpful, with
fatal: Unable to determine this slurmd's NodeName. So how do we fix this one?

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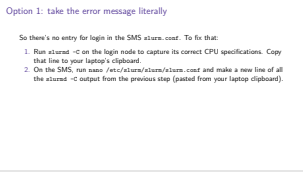
Option 1: take the error message literally

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.

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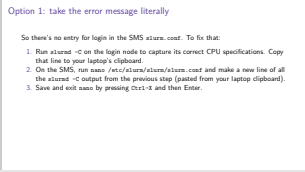
x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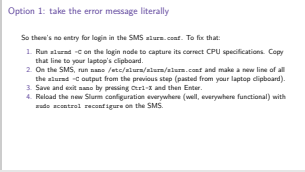
3. Save and exit nano by pressing Ctrl-X and then Enter.

x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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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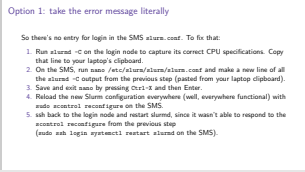
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4. Reload the new Slurm configuration everywhere (well, everywhere functional) with sudo scontrol reconfigure on the SMS.
5. ssh back to the login node and restart slurmd, since it wasn't able to respond to the scontrol reconfigure from the previous step (sudo ssh login systemctl restart slurmd on the SMS).

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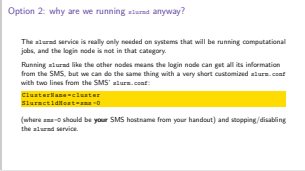
Option 1: take the error message literally

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
```

x


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-0
```

(where sms-0 should be **your** SMS hostname from your handout) and stopping/disabling the slurmd service.

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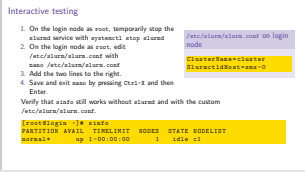
Interactive testing
1. On the login node as root, temporarily stop the slurmd service with systemctl stop slurmd
2. On the login node as root, edit /etc/slurm/slurm.conf with nano /etc/slurm/slurm.conf
3. Add the two lines to the right.
4. Save and exit nano by pressing Ctrl-X and then Enter.
/etc/slurm/slurm.conf on login node
ClusterName=cluster
SlurmctldHost=vnm-0
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

Making 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.

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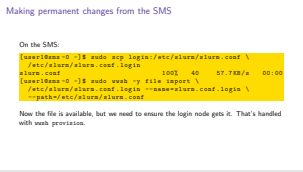
Making permanent changes from the SMS
On the SMS:
[user1@smx-0 ~]$ sudo scp login:/etc/slurm/slurm.conf \
/etc/slurm/slurm.conf.login
slurm.conf 100% 40 57.7KB/s 00:00
[user1@smx-0 ~]$ sudo wwsh -y file import \
/etc/slurm/slurm.conf.login --name=slurm.conf.login \
--path=/etc/slurm/slurm.conf
Now the file is available, but we need to ensure the login node gets it. That's handled
with wwsh provision.

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A quick look at wwsh provision

What are the provisioning settings for compute node c1?

```
[user1@sms-0 ~]$ wwsh provision print c1
#### c1 ########################################################################
c1: MASTER              = UNDEF
c1: BOOTSTRAP           = 6.1.96-1.el9.elrepo.x86_64
c1: VNFS                = rocky9.4
c1: VALIDATE            = FALSE
c1: FILES               = dynamic_hosts,group,munge.key,network,
  passwd,shadow
...
c1: KARGS               = "net.ifnames=0 biosdevname=0 quiet"
c1: ROOTLOCAL           = FALSE
```

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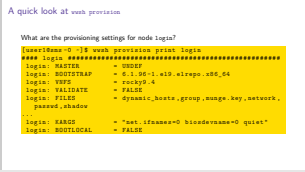
A quick look at wwsh provision
What are the provisioning settings for node login?
[user1@sms-0 ~]$ wwsh provision print login
login
login: MASTER = UNDEF
login: BOOTSTRAP = 6.1.96-1.el9.elrepo.x86_64
login: VNFS = rocky9.4
login: VALIDATE = FALSE
login: FILES = dynamic_hosts,group,munge.key,network,
passwd,shadow
...
login: KARGS = "net.ifnames=0 biosdevname=0 quiet"
login: BOOTLOCAL = FALSE

x

A quick look at `wwsh provision`

The provisioning settings for `c1` and `login` are identical, but there's a lot to read in them 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.

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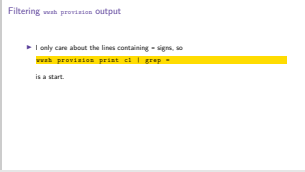
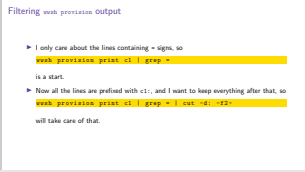

Filtering wwsh provision output
I only care about the lines containing = signs, so
wwsh provision print c1 | grep =
is a start.


Filtering wwsh provision output
I only care about the lines containing = signs, so
wwsh provision print c1 | grep =
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.

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A bit more security for the SMS

(going to talk about fail2ban here, maybe also firewalld)

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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)

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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.)

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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)

└Configuring Slurm policies

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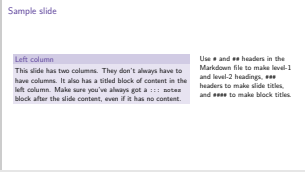
Configuring Slurm policies

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.



This is my note.

- It can contain Markdown
- like this list