



OpenHPC (v1.3.4) Cluster Building Recipes

SLES12SP3 Base OS

Warewulf/PBS Professional Edition for Linux* (aarch64)

Document Last Update: 2018-04-02

Document Revision: 520a42f

Legal Notice

Copyright © 2016-2018, OpenHPC, a Linux Foundation Collaborative Project. All rights reserved.



This documentation is licensed under the Creative Commons Attribution 4.0 International License. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0>.

Intel, the Intel logo, and other Intel marks are trademarks of Intel Corporation in the U.S. and/or other countries.
Altair, the Altair logo, PBS Professional, and other Altair marks are trademarks of Altair Engineering, Inc. in the U.S. and/or other countries.

*Other names and brands may be claimed as the property of others.

Contents

| | | |
|----------|--|-----------|
| 1 | Introduction | 5 |
| 1.1 | Target Audience | 5 |
| 1.2 | Requirements/Assumptions | 5 |
| 1.3 | Inputs | 6 |
| 2 | Install Base Operating System (BOS) | 7 |
| 3 | Install OpenHPC Components | 7 |
| 3.1 | Enable OpenHPC repository for local use | 7 |
| 3.2 | Installation template | 8 |
| 3.3 | Add provisioning services on <i>master</i> node | 8 |
| 3.4 | Add resource management services on <i>master</i> node | 9 |
| 3.5 | Complete basic Warewulf setup for <i>master</i> node | 9 |
| 3.6 | Define <i>compute</i> image for provisioning | 10 |
| 3.6.1 | Build initial BOS image | 10 |
| 3.6.2 | Add OpenHPC components | 10 |
| 3.6.3 | Customize system configuration | 12 |
| 3.6.4 | Additional Customization (<i>optional</i>) | 12 |
| 3.6.4.1 | Enable forwarding of system logs | 12 |
| 3.6.4.2 | Add Nagios monitoring | 13 |
| 3.6.4.3 | Add Ganglia monitoring | 14 |
| 3.6.4.4 | Add ClusterShell | 15 |
| 3.6.4.5 | Add <i>genders</i> | 15 |
| 3.6.4.6 | Add ConMan | 16 |
| 3.6.4.7 | Add NHC | 16 |
| 3.6.5 | Import files | 16 |
| 3.7 | Finalizing provisioning configuration | 17 |
| 3.7.1 | Assemble bootstrap image | 17 |
| 3.7.2 | Assemble Virtual Node File System (VNFS) image | 17 |
| 3.7.3 | Register nodes for provisioning | 17 |
| 3.7.4 | Optional kernel arguments | 18 |
| 3.7.5 | Optionally configure stateful provisioning | 18 |
| 3.8 | Boot compute nodes | 19 |
| 4 | Install OpenHPC Development Components | 20 |
| 4.1 | Development Tools | 20 |
| 4.2 | Compilers | 20 |
| 4.3 | MPI Stacks | 20 |
| 4.4 | Performance Tools | 21 |
| 4.5 | Setup default development environment | 21 |
| 4.6 | 3rd Party Libraries and Tools | 21 |
| 5 | Resource Manager Startup | 22 |
| 6 | Run a Test Job | 23 |
| 6.1 | Interactive execution | 23 |
| 6.2 | Batch execution | 25 |

| | |
|--|-----------|
| Appendices | 26 |
| A Installation Template | 26 |
| B Upgrading OpenHPC Packages | 27 |
| B.1 New component variants | 27 |
| C Integration Test Suite | 29 |
| D Customization | 31 |
| D.1 Adding local Lmod modules to OpenHPC hierarchy | 31 |
| D.2 Rebuilding Packages from Source | 32 |
| E Package Manifest | 33 |
| F Package Signatures | 44 |

1 Introduction

This guide presents a simple cluster installation procedure using components from the OpenHPC software stack. OpenHPC represents an aggregation of a number of common ingredients required to deploy and manage an HPC Linux* cluster including provisioning tools, resource management, I/O clients, development tools, and a variety of scientific libraries. These packages have been pre-built with HPC integration in mind while conforming to common Linux distribution standards. The documentation herein is intended to be reasonably generic, but uses the underlying motivation of a small, 4-node stateless cluster installation to define a step-by-step process. Several optional customizations are included and the intent is that these collective instructions can be modified as needed for local site customizations.

Base Linux Edition: this edition of the guide highlights installation without the use of a companion configuration management system and directly uses distro-provided package management tools for component selection. The steps that follow also highlight specific changes to system configuration files that are required as part of the cluster install process.

1.1 Target Audience

This guide is targeted at experienced Linux system administrators for HPC environments. Knowledge of software package management, system networking, and PXE booting is assumed. Command-line input examples are highlighted throughout this guide via the following syntax:

```
[sms]# echo "OpenHPC hello world"
```

Unless specified otherwise, the examples presented are executed with elevated (root) privileges. The examples also presume use of the BASH login shell, though the equivalent commands in other shells can be substituted. In addition to specific command-line instructions called out in this guide, an alternate convention is used to highlight potentially useful tips or optional configuration options. These tips are highlighted via the following format:

Tip

To find yourself, think for yourself. –Socrates

1.2 Requirements/Assumptions

This installation recipe assumes the availability of a single head node *master*, and four *compute* nodes. The *master* node serves as the overall system management server (SMS) and is provisioned with SLES12SP3 and is subsequently configured to provision the remaining *compute* nodes with Warewulf in a stateless configuration. The terms *master* and SMS are used interchangeably in this guide. For power management, we assume that the compute node baseboard management controllers (BMCs) are available via IPMI from the chosen master host. For file systems, we assume that the chosen master server will host an NFS file system that is made available to the compute nodes.

An outline of the physical architecture discussed is shown in Figure 1 and highlights the high-level networking configuration. The *master* host requires at least two Ethernet interfaces with *eth0* connected to the local data center network and *eth1* used to provision and manage the cluster backend (note that these interface names are examples and may be different depending on local settings and OS conventions). Two



Figure 1: Overview of physical cluster architecture.

logical IP interfaces are expected to each compute node: the first is the standard Ethernet interface that will be used for provisioning and resource management. The second is used to connect to each host's BMC and is used for power management and remote console access. Physical connectivity for these two logical IP networks is often accommodated via separate cabling and switching infrastructure; however, an alternate configuration can also be accommodated via the use of a shared NIC, which runs a packet filter to divert management packets between the host and BMC.

1.3 Inputs

As this recipe details installing a cluster starting from bare-metal, there is a requirement to define IP addresses and gather hardware MAC addresses in order to support a controlled provisioning process. These values are necessarily unique to the hardware being used, and this document uses variable substitution (`${variable}`) in the command-line examples that follow to highlight where local site inputs are required. A summary of the required and optional variables used throughout this recipe are presented below. Note that while the example definitions above correspond to a small 4-node compute subsystem, the compute parameters are defined in array format to accommodate logical extension to larger node counts.

- `${sms_name}` # Hostname for SMS server
- `${sms_ip}` # Internal IP address on SMS server
- `${sms_eth_internal}` # Internal Ethernet interface on SMS
- `${eth_provision}` # Provisioning interface for computes
- `${internal_netmask}` # Subnet netmask for internal network
- `${ntp_server}` # Local ntp server for time synchronization
- `${bmc_username}` # BMC username for use by IPMI
- `${bmc_password}` # BMC password for use by IPMI
- `${num_computes}` # Total # of desired compute nodes
- `${c_ip[0]}, ${c_ip[1]}, ...` # Desired compute node addresses
- `${c_bmc[0]}, ${c_bmc[1]}, ...` # BMC addresses for computes
- `${c_mac[0]}, ${c_mac[1]}, ...` # MAC addresses for computes
- `${c_name[0]}, ${c_name[1]}, ...` # Host names for computes
- `${compute_regex}` # Regex matching all compute node names (e.g. "c*")
- `${compute_prefix}` # Prefix for compute node names (e.g. "c")

Optional:

- `${kargs}` # Kernel boot arguments
- `${nagios_web_password}` # Nagios web access password

2 Install Base Operating System (BOS)

In an external setting, installing the desired BOS on a *master* SMS host typically involves booting from a DVD ISO image on a new server. With this approach, insert the SLES12SP3 DVD, power cycle the host, and follow the distro provided directions to install the BOS on your chosen *master* host. Alternatively, if choosing to use a pre-installed server, please verify that it is provisioned with the required SLES12SP3 distribution.

Prior to beginning the installation process of OpenHPC components, several additional considerations are noted here for the SMS host configuration. First, the installation recipe herein assumes that the SMS host name is resolvable locally. Depending on the manner in which you installed the BOS, there may be an adequate entry already defined in `/etc/hosts`. If not, the following addition can be used to identify your SMS host.

```
[sms]# echo ${sms_ip} ${sms_name} >> /etc/hosts
```

While it is theoretically possible to enable SELinux on a cluster provisioned with Warewulf, doing so is beyond the scope of this document. Even the use of permissive mode can be problematic and we therefore recommend disabling SELinux on the *master* SMS host. If SELinux components are installed locally, the `selinuxenabled` command can be used to determine if SELinux is currently enabled. If enabled, consult the distro documentation for information on how to disable.

Finally, provisioning services rely on DHCP, TFTP, and HTTP network protocols. Depending on the local BOS configuration on the SMS host, default firewall rules may prohibit these services. Consequently, this recipe assumes that the local firewall running on the SMS host is disabled. If installed, the default firewall service can be disabled as follows:

```
[sms]# systemctl disable SuSEfirewall12
[sms]# systemctl stop SuSEfirewall12
```

3 Install OpenHPC Components

With the BOS installed and booted, the next step is to add desired OpenHPC packages onto the *master* server in order to provide provisioning and resource management services for the rest of the cluster. The following subsections highlight this process.

3.1 Enable OpenHPC repository for local use

To begin, enable use of the OpenHPC repository by adding it to the local list of available package repositories. Note that this requires network access from your *master* server to the OpenHPC repository, or alternatively, that the OpenHPC repository be mirrored locally. In cases where network external connectivity is available, OpenHPC provides an `ohpc-release` package that includes GPG keys for package signing and repository enablement. The example which follows illustrates installation of the `ohpc-release` package directly from the OpenHPC build server.

```
[sms]# rpm -ivh http://build.openhpc.community/OpenHPC:/1.3/SLE_12/aarch64/ohpc-release-1.3-1.sle12.aarch64.rpm
```

Tip

Many sites may find it useful or necessary to maintain a local copy of the OpenHPC repositories. To facilitate this need, standalone tar archives are provided – one containing a repository of binary packages as well as any available updates, and one containing a repository of source RPMS. The tar files also contain a simple bash script to configure the package manager to use the local repository after download. To use, simply unpack the tarball where you would like to host the local repository and execute the `make_repo.sh` script. Tar files for this release can be found at <http://build.openhpc.community/dist/1.3.4>

In addition to the OpenHPC package repository, the *master* host also requires access to the standard distro repositories in order to resolve necessary dependencies. For SLES12SP3, the requirements are to have access to both the base and SDK repositories. In addition, add-on modules are needed to resolve dependencies for certain optional components. A summary of these requirements is as follows:

- SLES12
- SLES12-SDK
- [Web and Scripting Module](#) (*only required for nagios/ganglia)
- [Server Monitoring Software](#) (*only required for nagios/ganglia)
- [Python development packages](#) (*only required for Spack)

3.2 Installation template

The collection of command-line instructions that follow in this guide, when combined with local site inputs, can be used to implement a bare-metal system installation and configuration. The format of these commands is intended to be usable via direct cut and paste (with variable substitution for site-specific settings). Alternatively, the OpenHPC documentation package (`docs-ohpc`) includes a template script which includes a summary of all of the commands used herein. This script can be used in conjunction with a simple text file to define the local site variables defined in the previous section (§ 1.3) and is provided as a convenience for administrators. For additional information on accessing this script, please see Appendix A.

3.3 Add provisioning services on *master* node

With the OpenHPC repository enabled, we can now begin adding desired components onto the *master* server. This repository provides a number of aliases that group logical components together in order to help aid in this process. For reference, a complete list of available group aliases and RPM packages available via OpenHPC are provided in Appendix E. To add support for provisioning services, the following commands illustrate addition of a common base package followed by the Warewulf provisioning system.

```
# Install base meta-packages
[sms]# zypper -n install ohpc-base
[sms]# zypper -n install ohpc-warewulf
```

Tip

Many server BIOS configurations have PXE network booting configured as the primary option in the boot order by default. If your compute nodes have a different device as the first in the sequence, the `ipmitool` utility can be used to enable PXE.

```
[sms]# ipmitool -E -I lanplus -H ${bmc_ipaddr} -U root chassis bootdev pxe options=persistent
```


HPC systems rely on synchronized clocks throughout the system and the NTP protocol can be used to facilitate this synchronization. To enable NTP services on the SMS host with a specific server `${ntp_server}`, issue the following:

```
[sms]# systemctl enable ntpd.service
[sms]# echo "server ${ntp_server}" >> /etc/ntp.conf
[sms]# systemctl restart ntpd
```

3.4 Add resource management services on *master* node

OpenHPC provides multiple options for distributed resource management. The following command adds the PBS Professional workload manager server components to the chosen *master* host. Note that client-side components will be added to the corresponding compute image in a subsequent step.

```
[sms]# zypper -n install pbspro-server-ohpc
```

Other versions of this guide are available that describe installation of other resource management systems, and they can be found in the `docs-ohpc` package.

3.5 Complete basic Warewulf setup for *master* node

At this point, all of the packages necessary to use Warewulf on the *master* host should be installed. Next, we need to update several configuration files in order to allow Warewulf to work with SLES12SP3 and to support local provisioning using a second private interface (refer to Figure 1).

Tip

By default, Warewulf is configured to provision over the `eth1` interface and the steps below include updating this setting to override with a potentially alternatively-named interface specified by `${sms_eth_internal}`.

```
# Configure Warewulf provisioning to use desired internal interface
[sms]# perl -pi -e "s/device = eth1/device = ${sms_eth_internal}/" /etc/warewulf/provision.conf

# Configure DHCP server to use desired internal interface
[sms]# perl -pi -e "s/^DHCPD_INTERFACE=\\S+/DHCPD_INTERFACE=${sms_eth_internal}/" /etc/sysconfig/dhcpd

# Enable tftp service for compute node image distribution
[sms]# perl -pi -e "s/^\\s+disable\\s+= yes/ disable = no/" /etc/xinetd.d/tftp

# Configure Warewulf to use the default SLES tftp location
[sms]# perl -pi -e "s/#tftpd\\s*= /var/lib/#tftpd\\s*= /srv/" /etc/warewulf/provision.conf

# Update Warewulf http configuration to use the SLES version of Apache modules
[sms]# export MODFILE=/etc/apache2/conf.d/warewulf-httpd.conf
[sms]# perl -pi -e "s#modules/mod_perl.so\\$#/usr/lib64/apache2/mod_perl.so#" $MODFILE
[sms]# perl -pi -e "s#modules/mod_version.so\\$#/usr/lib64/apache2/mod_version.so#" $MODFILE

# Enable internal interface for provisioning
[sms]# ifconfig ${sms_eth_internal} ${sms_ip} netmask ${internal_netmask} up

# Restart/enable relevant services to support provisioning
[sms]# systemctl restart xinetd
[sms]# systemctl enable mysql.service
[sms]# systemctl restart mysql
```

```
[sms]# systemctl enable apache2.service
[sms]# systemctl restart apache2
[sms]# systemctl enable dhcpd.service
```

3.6 Define *compute* image for provisioning

With the provisioning services enabled, the next step is to define and customize a system image that can subsequently be used to provision one or more *compute* nodes. The following subsections highlight this process.

3.6.1 Build initial BOS image

The OpenHPC build of Warewulf includes specific enhancements enabling support for SLES12SP3. The following steps illustrate the process to build a minimal, default image for use with Warewulf. We begin by creating a directory structure on the *master* host that will represent the root filesystem of the compute node. The default location for this example is in `/opt/ohpc/admin/images/sles12sp3`.

Tip

Note that Warewulf requires access to a zypper repository during the `wwmkchroot` process. The easiest way to provide this is to mount the SUSE-SLE-12-SP3-Server ISO image on a web server that can communicate with the *master* host, set the `${BOS_MIRROR}` environment variable to that URL, and update the template file *prior* to running the `wwmkchroot` command below. For example:

```
# Override default OS repository - set BOS_MIRROR variable to desired repo location
[sms]# perl -pi -e "s#^ZYP_MIRROR=(\S+)#ZYP_MIRROR=${BOS_MIRROR}#" \
    /usr/lib/warewulf/wwmkchroot/sles-12.tpl
```

```
# Define chroot location
[sms]# export CHROOT=/opt/ohpc/admin/images/sles12sp3

# Build initial chroot image
[sms]# mkdir -p -m 755 $CHROOT                # create chroot housing dir
[sms]# mkdir -m 755 $CHROOT/dev              # create chroot /dev dir
[sms]# mknod -m 666 $CHROOT/dev/zero c 1 5    # create /dev/zero device
[sms]# wwmkchroot sles-12 $CHROOT             # create base image
```

3.6.2 Add OpenHPC components

The `wwmkchroot` process used in the previous step is designed to provide a minimal SLES12SP3 configuration. Next, we add additional components to include resource management client services, NTP support, and other additional packages to support the default OpenHPC environment. This process augments the chroot-based install performed by `wwmkchroot` to modify the base provisioning image and will access the BOS and OpenHPC repositories to resolve package install requests. We begin by installing a few common base packages:

```
# Install compute node base meta-package
[sms]# zypper -n --root $CHROOT install ohpc-base-compute
```

To access the remote repositories by hostname (and not IP addresses), the chroot environment needs to be updated to enable DNS resolution. Assuming that the *master* host has a working DNS configuration in place, the chroot environment can be updated with a copy of the configuration as follows:

```
[sms]# cp -p /etc/resolv.conf $CHROOT/etc/resolv.conf
```

Now, we can include additional components to the compute instance using **zypper** to install into the chroot location defined previously:

```
# Import GPG keys for chroot repository usage
[sms]# zypper -n --root $CHROOT --no-gpg-checks --gpg-auto-import-keys refresh

# Add PBS Professional client support
[sms]# zypper -n --root $CHROOT install pbspro-execution-ohpc
[sms]# perl -pi -e "s/PBS_SERVER=\S+/PBS_SERVER=${sms_name}/" $CHROOT/etc/pbs.conf
[sms]# echo "PBS_LEAF_NAME=${sms_name}" >> /etc/pbs.conf
[sms]# chroot $CHROOT opt/pbs/libexec/pbs_habitat
[sms]# perl -pi -e "s/\$clienthost \S+/\$clienthost ${sms_name}/" $CHROOT/var/spool/pbs/mom_priv/config
[sms]# echo "\$usecp *:home /home" >> $CHROOT/var/spool/pbs/mom_priv/config
[sms]# chroot $CHROOT systemctl enable pbs

# Provide udev rules to enable /dev/iplath access for InfiniPath devices
[sms]# cp /opt/ohpc/pub/examples/udev/60-iplath.rules $CHROOT/etc/udev/rules.d/

# Add Network Time Protocol (NTP) support
[sms]# zypper -n --root $CHROOT install ntp

# Add kernel drivers
[sms]# zypper -n --root $CHROOT install kernel-default

# Include modules user environment
[sms]# zypper -n --root $CHROOT install lmod-ohpc

# Enable ssh access
[sms]# chroot $CHROOT systemctl enable sshd.service

# Remove default hostname to allow WW to provision network names
[sms]# mv $CHROOT/etc/hostname $CHROOT/etc/hostname.orig
```

3.6.3 Customize system configuration

Prior to assembling the image, it is advantageous to perform any additional customization within the chroot environment created for the desired *compute* instance. The following steps document the process to add a local *ssh* key created by Warewulf to support remote access, identify the resource manager server, configure NTP for compute resources, and enable NFS mounting of a *\$HOME* file system and the public OpenHPC install path (*/opt/ohpc/pub*) that will be hosted by the *master* host in this example configuration.

```
# Initialize warewulf database and ssh_keys
[sms]# wwininit database
[sms]# wwininit ssh_keys

# Add NFS client mounts of /home and /opt/ohpc/pub to base image
[sms]# echo "${sms_ip}:/home /home nfs nfsvers=3,nodev,nosuid,noatime 0 0" >> $CHROOT/etc/fstab
[sms]# echo "${sms_ip}:/opt/ohpc/pub /opt/ohpc/pub nfs nfsvers=3,nodev,noatime 0 0" >> $CHROOT/etc/fstab

# Export /home and OpenHPC public packages from master server
[sms]# echo "/home *(rw,no_subtree_check,fsid=10,no_root_squash)" >> /etc/exports
[sms]# echo "/opt/ohpc/pub *(ro,no_subtree_check,fsid=11)" >> /etc/exports
[sms]# exportfs -a
[sms]# systemctl restart nfs-server
[sms]# systemctl enable nfs-server

# Enable NTP time service on computes and identify master host as local NTP server
[sms]# chroot $CHROOT systemctl enable ntpd
[sms]# echo "server ${sms_ip}" >> $CHROOT/etc/ntp.conf
[sms]# cp /etc/ntp.keys $CHROOT/etc/ntp.keys
```

3.6.4 Additional Customization (*optional*)

This section highlights common additional customizations that can *optionally* be applied to the local cluster environment. These customizations include:

- Enable syslog forwarding
- Add Nagios Core monitoring
- Add Ganglia monitoring
- Add Sensys monitoring
- Add ClusterShell
- Add *mrsh*
- Add *genders*
- Add ConMan

Details on the steps required for each of these customizations are discussed further in the following sections.

3.6.4.1 Enable forwarding of system logs It is often desirable to consolidate system logging information for the cluster in a central location, both to provide easy access to the data, and to reduce the impact of storing data inside the stateless compute node's memory footprint. The following commands highlight the steps necessary to configure compute nodes to forward their logs to the SMS, and to allow the SMS to accept these log requests.

```
# Configure SMS to receive messages and reload rsyslog configuration
[sms]# perl -pi -e "s/\\#\\$ModLoad imudp/\\$ModLoad imudp/" /etc/rsyslog.conf
[sms]# perl -pi -e "s/\\#\\$UDPServerRun 514/\\$UDPServerRun 514/" /etc/rsyslog.conf
[sms]# systemctl restart rsyslog

# Define compute node forwarding destination
[sms]# echo ".* @${sms_ip}:514" >> $CHROOT/etc/rsyslog.conf

# Disable most local logging on computes. Emergency and boot logs will remain on the compute nodes
```

```
[sms]# perl -pi -e "s/^*\.\.info/\\#\.\.info/" $CHROOT/etc/rsyslog.conf
[sms]# perl -pi -e "s/^authpriv/\\#\authpriv/" $CHROOT/etc/rsyslog.conf
[sms]# perl -pi -e "s/^mail/\\#\mail/" $CHROOT/etc/rsyslog.conf
[sms]# perl -pi -e "s/^cron/\\#\cron/" $CHROOT/etc/rsyslog.conf
[sms]# perl -pi -e "s/^uucp/\\#\uucp/" $CHROOT/etc/rsyslog.conf
```

3.6.4.2 Add Nagios monitoring Nagios is an open source infrastructure monitoring package that monitors servers, switches, applications, and services and offers user-defined alerting facilities. As provided by OpenHPC, it consists of a base monitoring daemon and a set of plug-ins for monitoring various aspects of an HPC cluster. The following commands can be used to install and configure a Nagios server on the *master* node, and add the facility to run tests and gather metrics from provisioned *compute* nodes.

```
# Install Nagios meta-package on master host
[sms]# zypper -n install ohpc-nagios

# Install plugins into compute node image
[sms]# zypper -n --root $CHROOT install nagios-plugins-all-ohpc nrpe-ohpc

# Enable and configure NRPE in compute image
[sms]# chroot $CHROOT systemctl enable nrpe
[sms]# perl -pi -e "s/^allowed_hosts=/# allowed_hosts=/" $CHROOT/etc/nagios/nrpe.cfg
[sms]# echo "nrpe 5666/tcp # NRPE" >> $CHROOT/etc/services
[sms]# echo "nrpe : ${sms_ip} : ALLOW" >> $CHROOT/etc/hosts.allow
[sms]# echo "nrpe : ALL : DENY" >> $CHROOT/etc/hosts.allow
[sms]# chroot $CHROOT /usr/sbin/useradd -c "NRPE user for the NRPE service" -d /var/run/nrpe \
-r -g nrpe -s /sbin/nologin nrpe
[sms]# chroot $CHROOT /usr/sbin/groupadd -r nrpe

# Configure remote services to test on compute nodes
[sms]# mv /etc/nagios/conf.d/services.cfg.example /etc/nagios/conf.d/services.cfg

# Define compute nodes as hosts to monitor
[sms]# mv /etc/nagios/conf.d/hosts.cfg.example /etc/nagios/conf.d/hosts.cfg
[sms]# for ((i=0; i<$num_compute; i++)) ; do
    perl -pi -e "s/HOSTNAME${(i+1)}/${c_name[$i]}/ || s/HOST${(i+1)}_IP/${c_ip[$i]}/" \
    /etc/nagios/conf.d/hosts.cfg
done

# Update location of mail binary for alert commands
[sms]# perl -pi -e "s/ \/\bin\/mail/ \/\usr\/bin\/mailx/g" /etc/nagios/objects/commands.cfg

# Update email address of contact for alerts
[sms]# perl -pi -e "s/nagios@localhost/root@${sms_name}/" /etc/nagios/objects/contacts.cfg

# Add check_ssh command for remote hosts
[sms]# echo command[check_ssh]=/usr/lib64/nagios/plugins/check_ssh localhost \
>> $CHROOT/etc/nagios/nrpe.cfg

# define password for nagiosadmin to be able to connect to web interface
[sms]# htpasswd -bc /etc/nagios/passwd nagiosadmin ${nagios_web_password}

# Enable Nagios on master, and configure
[sms]# chkconfig nagios on
[sms]# systemctl start nagios
[sms]# chmod u+s `which ping`
```

3.6.4.3 Add Ganglia monitoring Ganglia is a scalable distributed system monitoring tool for high-performance computing systems such as clusters and grids. It allows the user to remotely view live or historical statistics (such as CPU load averages or network utilization) for all machines running the *gmond* daemon. The following commands can be used to enable Ganglia to monitor both the *master* and *compute* hosts.

```
# Install Ganglia meta-package on master
[sms]# zypper -n install ohpc-ganglia

# Install Ganglia compute node daemon
[sms]# zypper -n --root $CHROOT install ganglia-gmond-ohpc

# Use example configuration script to enable unicast receiver on master host
[sms]# cp /opt/ohpc/pub/examples/ganglia/gmond.conf /etc/ganglia/gmond.conf
[sms]# perl -pi -e "s/<sms>/${sms_name}/" /etc/ganglia/gmond.conf

# Add configuration to compute image and provide gridname
[sms]# cp /etc/ganglia/gmond.conf $CHROOT/etc/ganglia/gmond.conf
[sms]# echo "gridname MySite" >> /etc/ganglia/gmetad.conf

# Start and enable Ganglia services
[sms]# systemctl enable gmond
[sms]# systemctl enable gmetad
[sms]# systemctl start gmond
[sms]# systemctl start gmetad
[sms]# chroot $CHROOT systemctl enable gmond

# Restart web server
[sms]# systemctl try-restart httpd
```

Once enabled and running, Ganglia should provide access to a web-based monitoring console on the *master* host. Read access to monitoring metrics will be enabled by default and can be accessed via a web browser. When running a web browser directly on the *master* host, the Ganglia top-level overview is available at <http://localhost/ganglia>. When accessing remotely, replace *localhost* with the chosen name of your master host (`${sms_name}`).

3.6.4.4 Add ClusterShell ClusterShell is an event-based Python library to execute commands in parallel across cluster nodes. Installation and basic configuration defining three node groups (*adm*, *compute*, and *all*) is as follows:

```
# Install ClusterShell
[sms]# zypper -n install clustershell-ohpc

# Setup node definitions
[sms]# cd /etc/clustershell/groups.d
[sms]# mv local.cfg local.cfg.orig
[sms]# echo "adm: ${sms_name}" > local.cfg
[sms]# echo "compute: ${compute_prefix}[1-${num_computes}]" >> local.cfg
[sms]# echo "all: @adm,@compute" >> local.cfg
```

3.6.4.5 Add *genders* *genders* is a static cluster configuration database or node typing database used for cluster configuration management. Other tools and users can access the *genders* database in order to make decisions about where an action, or even what action, is appropriate based on associated types or "*genders*". Values may also be assigned to and retrieved from a *gender* to provide further granularity. The following example highlights installation and configuration of two genders: *compute* and *bmc*.

```
# Install genders
[sms]# zypper -n install genders-ohpc

# Generate a sample genders file
[sms]# echo -e "${sms_name}\tsms" > /etc/genders
[sms]# for ((i=0; i<$num_computes; i++)) ; do
    echo -e "${c_name[$i]}\tcompute,bmc=${c_bmc[$i]}"
done >> /etc/genders
```

3.6.4.6 Add ConMan ConMan is a serial console management program designed to support a large number of console devices and simultaneous users. It supports logging console device output and connecting to compute node consoles via IPMI serial-over-lan. Installation and example configuration is outlined below.

```
# Install conman to provide a front-end to compute consoles and log output
[sms]# zypper -n install conman-ohpc

# Configure conman for computes (note your IPMI password is required for console access)
[sms]# for ((i=0; i<$num_computes; i++)) ; do
    echo -n 'CONSOLE name='${c_name[$i]}'" dev="ipmi:${c_bmc[$i]}"' '
    echo 'ipmiopts="'U:${bmc_username},P:${IPMI_PASSWORD:-undefined},W:solpayloadsize'"
done >> /etc/conman.conf

# Enable and start conman
[sms]# systemctl enable conman
[sms]# systemctl start conman
```

Note that an additional kernel boot option is typically necessary to enable serial console output. This option is highlighted in §3.7.4 after compute nodes have been registered with the provisioning system.

3.6.4.7 Add NHC Resource managers provide for a periodic "node health check" to be performed on each compute node to verify that the node is working properly. Nodes which are determined to be "unhealthy" can be marked as down or offline so as to prevent jobs from being scheduled or run on them. This helps increase the reliability and throughput of a cluster by reducing preventable job failures due to misconfiguration, hardware failure, etc. OpenHPC distributes NHC to fulfill this requirement.

In a typical scenario, the NHC driver script is run periodically on each compute node by the resource manager client daemon. It loads its configuration file to determine which checks are to be run on the current node (based on its hostname). Each matching check is run, and if a failure is encountered, NHC will exit with an error message describing the problem. It can also be configured to mark nodes offline so that the scheduler will not assign jobs to bad nodes, reducing the risk of system-induced job failures.

```
# Install NHC on master and compute nodes
[sms]# zypper -n install nhc-ohpc
[sms]# zypper -n --root $CHROOT install nhc-ohpc

# Generate NHC configuration file based on compute node environment
[sms]# pdsh -w c1 "/usr/sbin/nhc-genconf -H '*' -c -" | dshbak -c > /etc/nhc/nhc.conf.new
```

3.6.5 Import files

The Warewulf system includes functionality to import arbitrary files from the provisioning server for distribution to managed hosts. This is one way to distribute user credentials to *compute* nodes. To import local file-based credentials, issue the following:

```
[sms]# wwsh file import /etc/passwd
[sms]# wwsh file import /etc/group
[sms]# wwsh file import /etc/shadow
```


3.7 Finalizing provisioning configuration

Warewulf employs a two-stage boot process for provisioning nodes via creation of a bootstrap image that is used to initialize the process, and a virtual node file system capsule containing the full system image. This section highlights creation of the necessary provisioning images, followed by the registration of desired compute nodes.

3.7.1 Assemble bootstrap image

The bootstrap image includes the runtime kernel and associated modules, as well as some simple scripts to complete the provisioning process. The following commands highlight the inclusion of additional drivers and creation of the bootstrap image based on the running kernel.

```
# (Optional) Include drivers from kernel updates; needed if enabling additional kernel modules on computes
[sms]# export WW_CONF=/etc/warewulf/bootstrap.conf
[sms]# echo "drivers += updates/kernel/" >> $WW_CONF

# (Optional) Include overlayfs drivers; needed by Singularity
[sms]# echo "drivers += overlay" >> $WW_CONF

# Build bootstrap image
[sms]# wwbootstrap `uname -r`
```

3.7.2 Assemble Virtual Node File System (VNFS) image

With the local site customizations in place, the following step uses the `wwvnfs` command to assemble a VNFS capsule from the chroot environment defined for the *compute* instance.

```
[sms]# wwvnfs --chroot $CHROOT
```

3.7.3 Register nodes for provisioning

In preparation for provisioning, we can now define the desired network settings for four example compute nodes with the underlying provisioning system and restart the `dhcp` service. Note the use of variable names for the desired compute hostnames, node IPs, and MAC addresses which should be modified to accommodate local settings and hardware. By default, Warewulf uses network interface names of the `eth#` variety and adds kernel boot arguments to maintain this scheme on newer kernels. Consequently, when specifying the desired provisioning interface via the `$eth_provision` variable, it should follow this convention. Alternatively, if you prefer to use the predictable network interface naming scheme (e.g. names like `en4s0f0`), additional steps are included to alter the default kernel boot arguments and take the `eth#` named interface down after bootstrapping so the normal init process can bring it up again using the desired name.

The final step in this process associates the VNFS image assembled in previous steps with the newly defined compute nodes, utilizing the user credential files and munge key that were imported in §3.6.5.

```
# Set provisioning interface as the default networking device
[sms]# echo "GATEWAYDEV=${eth_provision}" > /tmp/network.$$
[sms]# wwsh -y file import /tmp/network.$$ --name network
[sms]# wwsh -y file set network --path /etc/sysconfig/network --mode=0644 --uid=0

# Add nodes to Warewulf data store
[sms]# for ((i=0; i<num_computes; i++)) ; do
    wwsh -y node new ${c_name[i]} --ipaddr=${c_ip[i]} --hwaddr=${c_mac[i]} -D ${eth_provision}
done
```

```
# Additional step required if desiring to use predictable network interface
# naming schemes (e.g. en4s0f0). Skip if using eth# style names.
[sms]# wwsh provision set "${compute_regex}" --kargs "net.ifnames=1,biosdevname=1"
[sms]# wwsh provision set --postnetdown=1 "${compute_regex}"
```

```
# Define provisioning image for hosts
[sms]# wwsh -y provision set "${compute_regex}" --vnfs=sles12sp3 --bootstrap='uname -r` \
--files=dynamic_hosts,passwd,group,shadow,network
```

Tip

Warewulf includes a utility named `wwnodescan` to automatically register new compute nodes versus the outlined node-addition approach which requires hardware MAC addresses to be gathered in advance. With `wwnodescan`, nodes will be added to the Warewulf database in the order in which their DHCP requests are received by the master, so care must be taken to boot nodes in the order one wishes to see preserved in the Warewulf database. The IP address provided will be incremented after each node is found, and the utility will exit after all specified nodes have been found. Example usage is highlighted below:

```
[sms]# wwnodescan --netdev=${eth_provision} --ipaddr=${c_ip[0]} --netmask=${internal_netmask} \
--vnfs=sles12sp3 --bootstrap='uname -r` --listen=${sms_eth_internal} ${c_name[0]}-${c_name[3]}
```

```
# Restart dhcp / update PXE
[sms]# systemctl restart dhcpd
[sms]# wwsh pxe update
```

3.7.4 Optional kernel arguments

If you chose to enable ConMan in §3.6.4.6, additional boot-time kernel arguments are needed to enable serial console redirection. An example provisioning setting which adds to any other kernel arguments defined in `${kargs}` is as follows:

```
# Define node kernel arguments to support SOL console
[sms]# wwsh -y provision set "${compute_regex}" --console=ttyS1,115200
```

3.7.5 Optionally configure stateful provisioning

Warewulf normally defaults to running the assembled VNFS image out of system memory in a *stateless* configuration. Alternatively, Warewulf can also be used to partition and format persistent storage such that the VNFS image can be installed locally to disk in a *stateful* manner. This does, however, require that a boot loader (GRUB) be added to the image as follows:

```
# Add GRUB2 bootloader and re-assemble VNFS image
[sms]# zypper -n --root $CHROOT install grub2
[sms]# wwnfs --chroot $CHROOT
```

Enabling stateful nodes also requires additional site-specific, disk-related parameters in the Warewulf configuration, and several example partitioning scripts are provided in the distribution.

```
# Select (and customize) appropriate parted layout example
[sms]# cp /etc/warewulf/filesystem/examples/gpt_example.cmds /etc/warewulf/filesystem/gpt.cmds
[sms]# wwsh provision set --filesystem=gpt "${compute_regex}"
[sms]# wwsh provision set --bootloader=sda "${compute_regex}"
```

Tip

Those provisioning compute nodes in UEFI mode will install a slightly different set of packages in to the VNFS. Warewulf also provides an example EFI filesystem layout.

```
# Add GRUB2 bootloader and re-assemble VNFS image
[sms]# zypper -n --root $CHROOT install grub2-efi grub2-efi-modules
[sms]# cp /etc/warewulf/filesystem/examples/efi_example.cmds /etc/warewulf/filesystem/efi.cmds
[sms]# wwsh provision set --filesystem=efi "${compute_regex}"
[sms]# wwsh provision set --bootloader=sda "${compute_regex}"
```

Upon subsequent reboot of the modified nodes, Warewulf will partition and format the disk to host the desired VNFS image. Once the image is installed to disk, warewulf can be configured to use the nodes' local storage as the boot device.

```
# Boot the node from the local disk
[sms]# wwsh provision set --bootlocal=normal "${compute_regex}"
```

3.8 Boot compute nodes

At this point, the *master* server should be able to boot the newly defined compute nodes. Assuming that the compute node BIOS settings are configured to boot over PXE, all that is required to initiate the provisioning process is to power cycle each of the desired hosts using IPMI access. The following commands use the `ipmitool` utility to initiate power resets on each of the four compute hosts. Note that the utility requires that the `IPMI_PASSWORD` environment variable be set with the local BMC password in order to work interactively.

```
[sms]# for ((i=0; i<${num_computes}; i++)) ; do
    ipmitool -E -I lanplus -H ${c_bmc[$i]} -U ${bmc_username} chassis power reset
done
```

Once kicked off, the boot process should take less than 5 minutes (depending on BIOS post times) and you can verify that the compute hosts are available via ssh, or via parallel ssh tools to multiple hosts. For example, to run a command on the newly imaged compute hosts using `pdsh`, execute the following:

```
[sms]# pdsh -w c[1-4] uptime
c1 05:03am up 0:02, 0 users, load average: 0.20, 0.13, 0.05
c2 05:03am up 0:02, 0 users, load average: 0.20, 0.14, 0.06
c3 05:03am up 0:02, 0 users, load average: 0.19, 0.15, 0.06
c4 05:03am up 0:02, 0 users, load average: 0.15, 0.12, 0.05
```

Tip

While the `pxelinux.0` and `lpxelinux.0` files that ship with Warewulf to enable network boot support a wide range of hardware, some hosts may boot more reliably or faster using the BOS versions provided via the `syslinux` package. If you encounter PXE issues, consider replacing the `pxelinux.0` and `lpxelinux.0` files supplied with `warewulf-provision-ohpc` with versions from `syslinux`.

4 Install OpenHPC Development Components

The install procedure outlined in §3 highlighted the steps necessary to install a *master* host, assemble and customize a *compute* image, and provision several compute hosts from bare-metal. With these steps completed, additional OpenHPC-provided packages can now be added to support a flexible HPC development environment including development tools, C/C++/Fortran compilers, MPI stacks, and a variety of 3rd party libraries. The following subsections highlight the additional software installation procedures.

4.1 Development Tools

To aid in general development efforts, OpenHPC provides recent versions of the GNU autotools collection, the Valgrind memory debugger, EasyBuild, and Spack. These can be installed as follows:

```
# Install autotools meta-package
[sms]# zypper -n install ohpc-autotools

[sms]# zypper -n install EasyBuild-ohpc
[sms]# zypper -n install hwloc-ohpc
[sms]# zypper -n install spack-ohpc
[sms]# zypper -n install valgrind-ohpc
```

4.2 Compilers

OpenHPC presently packages the GNU compiler toolchain integrated with the underlying modules-environment system in a hierarchical fashion. The modules system will conditionally present compiler-dependent software based on the toolchain currently loaded.

```
[sms]# zypper -n install gnu7-compilers-ohpc
```

The llvm compiler toolchains are also provided as a standalone additional compiler family (ie. users can easily switch between gcc/clang environments), but we do not provide the full complement of downstream library builds.

```
[sms]# zypper -n install llvm5-compilers-ohpc
```

4.3 MPI Stacks

For MPI development and runtime support, OpenHPC provides pre-packaged builds for two MPI families that are compatible with ethernet fabrics. These MPI stacks can be installed as follows:

```
[sms]# zypper -n install openmpi3-gnu7-ohpc mpich-gnu7-ohpc
```

4.4 Performance Tools

OpenHPC provides a variety of open-source tools to aid in application performance analysis (refer to Appendix E for a listing of available packages). This group of tools can be installed as follows:

```
# Install perf-tools meta-package
[sms]# zypper -n install ohpc-gnu7-perf-tools
```

4.5 Setup default development environment

System users often find it convenient to have a default development environment in place so that compilation can be performed directly for parallel programs requiring MPI. This setup can be conveniently enabled via modules and the OpenHPC modules environment is pre-configured to load an `ohpc` module on login (if present). The following package install provides a default environment that enables autotools, the GNU compiler toolchain, and the OpenMPI stack.

```
[sms]# zypper -n install lmod-defaults-gnu7-openmpi3-ohpc
```

Tip

If you want to change the default environment from the suggestion above, OpenHPC also provides the GNU compiler toolchain with the MPICH stack:

- `lmod-defaults-gnu7-mpich-ohpc`

4.6 3rd Party Libraries and Tools

OpenHPC provides pre-packaged builds for a number of popular open-source tools and libraries used by HPC applications and developers. For example, OpenHPC provides builds for FFTW and HDF5 (including serial and parallel I/O support), and the GNU Scientific Library (GSL). Again, multiple builds of each package are available in the OpenHPC repository to support multiple compiler and MPI family combinations where appropriate. Note, however, that not all combinatorial permutations may be available for components where there are known license incompatibilities. The general naming convention for builds provided by OpenHPC is to append the compiler and MPI family name that the library was built against directly into the package name. For example, libraries that do not require MPI as part of the build process adopt the following RPM name:

```
package-<compiler_family>-ohpc-<package_version>-<release>.rpm
```

Packages that do require MPI as part of the build expand upon this convention to additionally include the MPI family name as follows:

```
package-<compiler_family>-<mpi_family>-ohpc-<package_version>-<release>.rpm
```

To illustrate this further, the command below queries the locally configured repositories to identify all of the available PETSc packages that were built with the GNU toolchain. The resulting output that is included shows that pre-built versions are available for each of the supported MPI families presented in §4.3.

```
[sms]# zypper search -t package petsc-gnu7-*--ohpc
Loading repository data...
Reading installed packages...
```

| S | Name | Summary |
|---|--------------------------|--|
| | petsc-gnu7-mpich-ohpc | Portable Extensible Toolkit for Scientific Computation package |
| | petsc-gnu7-openmpi3-ohpc | Portable Extensible Toolkit for Scientific Computation package |

Tip

OpenHPC-provided 3rd party builds are configured to be installed into a common top-level repository so that they can be easily exported to desired hosts within the cluster. This common top-level path (`/opt/ohpc/pub`) was previously configured to be mounted on *compute* nodes in §3.6.3, so the packages will be immediately available for use on the cluster after installation on the *master* host.

For convenience, OpenHPC provides package aliases for these 3rd party libraries and utilities that can be used to install available libraries for use with the GNU compiler family toolchain. For parallel libraries, aliases are grouped by MPI family toolchain so that administrators can choose a subset should they favor a particular MPI stack. Please refer to Appendix E for a more detailed listing of all available packages in each of these functional areas. To install all available package offerings within OpenHPC, issue the following:

```
# Install 3rd party libraries/tools meta-packages built with GNU toolchain
[sms]# zypper -n install ohpc-gnu7-serial-libs
[sms]# zypper -n install ohpc-gnu7-io-libs
[sms]# zypper -n install ohpc-gnu7-python-libs
[sms]# zypper -n install ohpc-gnu7-runtimes
```

```
# Install parallel lib meta-packages for all available MPI toolchains
[sms]# zypper -n install ohpc-gnu7-mpich-parallel-libs
[sms]# zypper -n install ohpc-gnu7-openmpi3-parallel-libs
```

5 Resource Manager Startup

In section §3, the PBS Professional workload manager was installed and configured for use on both the *master* host and *compute* node instances. With the cluster nodes up and functional, we can now startup the resource manager services on the *master* host in preparation for running user jobs.

The following command can be used to startup the necessary services to support resource management under PBS Professional.

```
# start pbspro daemons on master host
[sms]# systemctl enable pbs
[sms]# systemctl start pbs
```

In the default configuration, the *compute* hosts have not been added to the PBS Professional resource manager. To add the *compute* hosts, execute the following to register each host and apply several key global configuration options.

```
# initialize PBS path
[sms]# . /etc/profile.d/pbs.sh
# enable user environment propagation (needed for modules support)
[sms]# qmgr -c "set server default_qsub_arguments= -V"
# enable uniform multi-node MPI task distribution
[sms]# qmgr -c "set server resources_default.place=scatter"
# enable support for job accounting
[sms]# qmgr -c "set server job_history_enable=True"
# register compute hosts with pbspro
[sms]# for host in "${c_name[@]}; do
    qmgr -c "create node $host"
done
```

6 Run a Test Job

With the resource manager enabled for production usage, users should now be able to run jobs. To demonstrate this, we will add a “test” user on the *master* host that can be used to run an example job.

```
[sms]# useradd -m test
```

Warewulf installs a utility on the compute nodes to automatically synchronize known files from the provisioning server at five minute intervals. In this recipe, recall that we previously registered credential files with Warewulf (e.g. `passwd`, `group`, and `shadow`) so that these files would be propagated during compute node imaging. However, with the addition of a new “test” user above, the files have been outdated and we need to update the Warewulf database to incorporate the additions. This re-sync process can be accomplished as follows:

```
[sms]# wwsh file resync passwd shadow group
```

Tip

After re-syncing to notify Warewulf of file modifications made on the *master* host, it should take approximately 5 minutes for the changes to propagate. However, you can also manually pull the changes from compute nodes via the following:

```
[sms]# pdsh -w $compute_prefix[1-4] /warewulf/bin/wwgetfiles
```

OpenHPC includes a simple “hello-world” MPI application in the `/opt/ohpc/pub/examples` directory that can be used for this quick compilation and execution. OpenHPC also provides a companion job-launch utility named `prun` that is installed in concert with the pre-packaged MPI toolchains. This convenience script provides a mechanism to abstract job launch across different resource managers and MPI stacks such that a single launch command can be used for parallel job launch in a variety of OpenHPC environments. It also provides a centralizing mechanism for administrators to customize desired environment settings for their users.

6.1 Interactive execution

To use the newly created “test” account to compile and execute the application *interactively* through the resource manager, execute the following (note the use of `mpiexec` for parallel job launch which summarizes

the underlying native job launch mechanism being used):

```
# Switch to "test" user
[sms]# su - test

# Compile MPI "hello world" example
[test@sms ~]$ mpicc -O3 /opt/ohpc/pub/examples/mpi/hello.c

# Submit interactive job request and use prun to launch executable
[test@sms ~]$ qsub -I -l select=2:mpiprocs=4

[test@c1 ~]$ prun ./a.out

[prun] Master compute host = c1
[prun] Resource manager = pbspro
[prun] Launch cmd = mpiexec.hydra -rmk pbs ./a.out

Hello, world (8 procs total)
--> Process # 0 of 8 is alive. -> c1
--> Process # 1 of 8 is alive. -> c1
--> Process # 2 of 8 is alive. -> c1
--> Process # 3 of 8 is alive. -> c1
--> Process # 4 of 8 is alive. -> c2
--> Process # 5 of 8 is alive. -> c2
--> Process # 6 of 8 is alive. -> c2
--> Process # 7 of 8 is alive. -> c2
```

Tip

The following table provides approximate command equivalences between PBS Pro and SLURM:

| Command | PBS Pro | SLURM |
|----------------------------------|----------------------|------------------------------|
| Submit <i>batch</i> job | qsub [job script] | sbatch [job script] |
| Request <i>interactive</i> shell | qsub -I /bin/bash | srun -pty /bin/bash |
| Delete job | qdel [job id] | scancel [job id] |
| Queue status | qstat -q | sinfo |
| Job status | qstat -f [job id] | scontrol show job [job id] |
| Node status | pbsnodes [node name] | scontrol show node [node id] |

6.2 Batch execution

For batch execution, OpenHPC provides a simple job script for reference (also housed in the `/opt/ohpc/pub/examples` directory). This example script can be used as a starting point for submitting batch jobs to the resource manager and the example below illustrates use of the script to submit a batch job for execution using the same executable referenced in the previous interactive example.

```
# Copy example job script
[test@sms ~]$ cp /opt/ohpc/pub/examples/pbspro/job.mpi .

# Examine contents (and edit to set desired job sizing characteristics)
[test@sms ~]$ cat job.mpi
#!/bin/bash
#-----
# Job name
#PBS -N test

# Name of stdout output file
#PBS -o job.out

# Total number of nodes and MPI tasks/node requested
#PBS -l select=2:mpiprocs=4

# Run time (hh:mm:ss) - 1.5 hours
#PBS -l walltime=01:30:00
#-----

# Change to submission directory
cd $PBS_O_WORKDIR

# Launch MPI-based executable
prun ./a.out

# Submit job for batch execution
[test@sms ~]$ qsub job.mpi
5.master
```

Appendices

A Installation Template

This appendix highlights the availability of a companion installation script that is included with OpenHPC documentation. This script, when combined with local site inputs, can be used to implement a starting recipe for bare-metal system installation and configuration. This template script is used during validation efforts to test cluster installations and is provided as a convenience for administrators as a starting point for potential site customization.

Tip

Note that the template script provided is intended for use during initial installation and is not designed for repeated execution. If modifications are required after using the script initially, we recommend running the relevant subset of commands interactively.

The template script relies on the use of a simple text file to define local site variables that were outlined in §1.3. By default, the template installation script attempts to use local variable settings sourced from the `/opt/ohpc/pub/doc/recipes/vanilla/input.local` file, however, this choice can be overridden by the use of the `${OHPC_INPUT_LOCAL}` environment variable. The template install script is intended for execution on the SMS *master* host and is installed as part of the `docs-ohpc` package into `/opt/ohpc/pub/doc/recipes/vanilla/recipe.sh`. After enabling the OpenHPC repository and reviewing the guide for additional information on the intent of the commands, the general starting approach for using this template is as follows:

1. Install the `docs-ohpc` package

```
[sms]# zypper -n install docs-ohpc
```

2. Copy the provided template input file to use as a starting point to define local site settings:

```
[sms]# cp /opt/ohpc/pub/doc/recipes/sles12/input.local input.local
```

3. Update `input.local` with desired settings
4. Copy the template installation script which contains command-line instructions culled from this guide.

```
[sms]# cp -p /opt/ohpc/pub/doc/recipes/sles12/aarch64/warewulf/pbspro/recipe.sh .
```

5. Review and edit `recipe.sh` to suite.
6. Use environment variable to define local input file and execute `recipe.sh` to perform a local installation.

```
[sms]# export OHPC_INPUT_LOCAL=./input.local
[sms]# ./recipe.sh
```

B Upgrading OpenHPC Packages

As newer OpenHPC releases are made available, users are encouraged to upgrade their locally installed packages against the latest repository versions to obtain access to bug fixes and newer component versions. This can be accomplished with the underlying package manager as OpenHPC packaging maintains versioning state across releases. Also, package builds available from the OpenHPC repositories have “-ohpc” appended to their names so that wild cards can be used as a simple way to obtain updates. The following general procedure highlights a method for upgrading existing installations. When upgrading from a minor release older than v1.3, you will first need to update your local OpenHPC repository configuration to point against the v1.3 release (or update your locally hosted mirror). Refer to §3.1 for more details on enabling the latest repository. In contrast, when upgrading between micro releases on the same branch (e.g. from v1.3 to 1.3.2), there is no need to adjust local package manager configurations when using the public repository as rolling updates are pre-configured.

1. (Optional) Ensure repo metadata is current (on head node and in chroot location(s)). Package managers will naturally do this on their own over time, but if you are wanting to access updates immediately after a new release, the following can be used to sync to the latest.

```
[sms]# zypper clean -a
[sms]# zypper --root $CHROOT clean
```

2. Upgrade master (SMS) node

```
[sms]# zypper -n up "*-ohpc"
```

3. Upgrade packages in compute image

```
[sms]# zypper -n --root $CHROOT up "*-ohpc"
```

4. Rebuild image(s)

```
[sms]# wvwnfs --chroot $CHROOT
```

In the case where packages were upgraded within the chroot compute image, you will need to reboot the compute nodes when convenient to enable the changes.

B.1 New component variants

As newer variants of key compiler/MPI stacks are released, OpenHPC will periodically add toolchains enabling the latest variant. To stay consistent throughout the build hierarchy, minimize recompilation requirements for existing binaries, and allow for multiple variants to coexist, unique delimiters are used to distinguish RPM package names and module hierarchy.

In the case of a fresh install, OpenHPC recipes default to installation of the latest toolchains available in a given release branch. However, if upgrading a previously installed system, administrators can *opt-in* to enable new variants as they become available. To illustrate this point, consider the previous OpenHPC 1.3.2 release as an example which contained an “openmpi” MPI variant providing OpenMPI 1.10.x along with runtimes and libraries compiled with this toolchain. That release also contained the “llvm4” compiler family which was updated to “llvm5” in OpenHPC 1.3.3. In the case where an admin would like to enable the newer “openmpi3” toolchain, installation of these additions is simplified with the use of OpenHPC’s meta-packages (see Table 1 in Appendix E). The following example illustrates adding the complete “openmpi3” toolchain. Note that we leverage the convenience meta-packages containing MPI-dependent builds, and we also update the modules environment to make it the default.

```
# Update default environment
[sms]# zypper -n remove lmod-defaults-gnu7-openmpi-ohpc
[sms]# zypper -n install lmod-defaults-gnu7-openmpi3-ohpc

# Install OpenMPI 3.x-compiled meta-packages with dependencies
[sms]# zypper -n install ohpc-gnu7-perf-tools \
                        ohpc-gnu7-io-libs \
                        ohpc-gnu7-python-libs \
                        ohpc-gnu7-runtimes \
                        ohpc-gnu7-openmpi3-parallel-libs

# Install LLVM/Clang 5.x
[sms]# zypper -n install llvm5-compilers-ohpc
```

C Integration Test Suite

This appendix details the installation and basic use of the integration test suite used to support OpenHPC releases. This suite is not intended to replace the validation performed by component development teams, but is instead, devised to confirm component builds are functional and interoperable within the modular OpenHPC environment. The test suite is generally organized by components and the OpenHPC CI workflow relies on running the full suite using [Jenkins](#) to test multiple OS configurations and installation recipes. To facilitate customization and running of the test suite locally, we provide these tests in a standalone RPM.

```
[sms]# zypper -n install test-suite-ohpc
```

The RPM installation creates a user named `ohpc-test` to house the test suite and provide an isolated environment for execution. Configuration of the test suite is done using standard GNU autotools semantics and the [BATS](#) shell-testing framework is used to execute and log a number of individual unit tests. Some tests require privileged execution, so a different combination of tests will be enabled depending on which user executes the top-level `configure` script. Non-privileged tests requiring execution on one or more compute nodes are submitted as jobs through the PBS Professional resource manager. The tests are further divided into “short” and “long” run categories. The short run configuration is a subset of approximately 180 tests to demonstrate basic functionality of key components (e.g. MPI stacks) and should complete in 10-20 minutes. The long run (around 1000 tests) is comprehensive and can take an hour or more to complete.

Most components can be tested individually, but a default configuration is setup to enable collective testing. To test an isolated component, use the `configure` option to disable all tests, then re-enable the desired test to run. The `--help` option to `configure` will display all possible tests. Example output is shown below (some output is omitted for the sake of brevity).

```
[sms]# su - ohpc-test
[test@sms ~]$ cd tests
[test@sms ~]$ ./configure --disable-all --enable-fftw
checking for a BSD-compatible install... /bin/install -c
checking whether build environment is sane... yes
...
----- SUMMARY -----
Package version..... : test-suite-1.3.0

Build user..... : ohpc-test
Build host..... : sms001
Configure date..... : 2017-03-24 15:41
Build architecture..... : aarch64
Compiler Families..... : gnu
MPI Families..... : mpich mvapich2 openmpi
Resource manager ..... : PBS Professional
Test suite configuration..... : short
...
Libraries:
  Adios ..... : disabled
  Boost ..... : disabled
  Boost MPI..... : disabled
  FFTW..... : enabled
  GSL..... : disabled
  HDF5..... : disabled
  HYPRE..... : disabled
...
```

Many OpenHPC components exist in multiple flavors to support multiple compiler and MPI runtime permutations, and the test suite takes this in to account by iterating through these combinations by default.

If `make check` is executed from the top-level test directory, all configured compiler and MPI permutations of a library will be exercised. The following highlights the execution of the FFTW related tests that were enabled in the previous step.

```
[test@sms ~]$ make check
make --no-print-directory check-TESTS
PASS: libs/fftw/ohpc-tests/test_mpi_families
=====
Testsuite summary for test-suite 1.3.0
=====
# TOTAL: 1
# PASS: 1
# SKIP: 0
# XFAIL: 0
# FAIL: 0
# XPASS: 0
# ERROR: 0
=====
[test@sms ~]$ cat libs/fftw/tests/family-gnu-*/rm_execution.log
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (PBS Professional/gnu/mpich)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (PBS Professional/gnu/mpich)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (PBS Professional/gnu/mpich)
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (PBS Professional/gnu/mvapich2)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (PBS Professional/gnu/mvapich2)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (PBS Professional/gnu/mvapich2)
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (PBS Professional/gnu/openmpi)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (PBS Professional/gnu/openmpi)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (PBS Professional/gnu/openmpi)
PASS rm_execution (exit status: 0)
```

D Customization

D.1 Adding local Lmod modules to OpenHPC hierarchy

Locally installed applications can easily be integrated in to OpenHPC systems by following the Lmod convention laid out by the provided packages. Two sample module files are included in the `examples-ohpc` package—one representing an application with no compiler or MPI runtime dependencies, and one dependent on OpenMPI and the GNU toolchain. Simply copy these files to the prescribed locations, and the `lmod` application should pick them up automatically.

```
[sms]# mkdir /opt/ohpc/pub/modulefiles/example1
[sms]# cp /opt/ohpc/pub/examples/example.modulefile \
/opt/ohpc/pub/modulefiles/example1/1.0
[sms]# mkdir /opt/ohpc/pub/moduledeps/gnu7-openmpi3/example2
[sms]# cp /opt/ohpc/pub/examples/example-mpi-dependent.modulefile \
/opt/ohpc/pub/moduledeps/gnu7-openmpi3/example2/1.0
[sms]# module avail
```

```
----- /opt/ohpc/pub/moduledeps/gnu7-openmpi3 -----
adios/1.12.0  imb/2018.0      netcdf-fortran/4.4.4  ptscotch/6.0.4    sionlib/1.7.1
boost/1.65.1  mpi4py/2.0.0    netcdf/4.4.1.1       scalapack/2.0.2   slepc/3.7.4
example2/1.0  mpiP/3.4.1      petsc/3.7.6          scalasca/2.3.1    superlu_dist/4.2
fftw/3.3.6    mumps/5.1.1     phdf5/1.10.1         scipy/0.19.1      tau/2.26.1
hybre/2.11.2  netcdf-cxx/4.3.0  pnetcdf/1.8.1        scorep/3.1        trilinos/12.10.1

----- /opt/ohpc/pub/moduledeps/gnu7 -----
R/3.4.2      metis/5.1.0     ocr/1.0.1            pdttoolkit/3.24   superlu/5.2.1
gsl/2.4      mpich/3.2       openblas/0.2.20      plasma/2.8.0
hdf5/1.10.1  numpy/1.13.1    openmpi3/3.0.0 (L)   scotch/6.0.4

----- /opt/ohpc/admin/modulefiles -----
spack/0.10.0

----- /opt/ohpc/pub/modulefiles -----
EasyBuild/3.4.1  cmake/3.9.2  hwloc/1.11.8  pmix/1.2.3  valgrind/3.13.0
autotools (L)    example1/1.0 (L)  llvm5/5.0.0  prun/1.2 (L)
clustershell/1.8  gnu7/7.2.0 (L)  ohpc (L)    singularity/2.4

Where:
L: Module is loaded

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

D.2 Rebuilding Packages from Source

Users of OpenHPC may find it desirable to rebuild one of the supplied packages to apply build customizations or satisfy local requirements. One way to accomplish this is to install the appropriate source RPM, modify the specfile as needed, and rebuild to obtain an updated binary RPM. A brief example using the FFTW library is highlighted below. Note that the source RPMs can be downloaded from the community build server at <https://build.openhpc.community> via a web browser or directly via `rpm` as highlighted below. The OpenHPC build system design leverages several keywords to control the choice of compiler and MPI families for relevant development libraries and the `rpmbuild` example illustrates how to override the default `mpi_family`.

```
# Install rpm-build package from base OS distro
[sms ~]# zypper -n install rpm-build

# Download SRPM from OpenHPC repository and install locally
[sms ~]# zypper source-install fftw-gnu7-openmpi3-ohpc

# Modify spec file as desired
[sms ~]# cd ~/rpmbuild/SPECS
[sms ~/rpmbuild/SPECS]# perl -pi -e "s/enable-static=no/enable-static=yes/" fftw.spec

# Increment RPM release so package manager will see an update
[sms ~/rpmbuild/SPECS]# perl -pi -e "s/Release: 28.11/Release: 29.1/" fftw.spec

# Rebuild binary RPM. Note that additional directives can be specified to modify build
[sms ~/rpmbuild/SPECS]# rpmbuild -bb --define "mpi_family mpich" fftw.spec

# Install the new package
[sms ~]# zypper -n install ~/rpmbuild/RPMS/aarch64/fftw-gnu7-mpich-ohpc-3.3.6-29.1.aarch64.rpm
```


E Package Manifest

This appendix provides a summary of available meta-package groupings and all of the individual RPM packages that are available as part of this OpenHPC release. The meta-packages provide a mechanism to group related collections of RPMs by functionality and provide a convenience mechanism for installation. A list of the available meta-packages and a brief description is presented in Table 1.

Table 1: Available OpenHPC Meta-packages

| Group Name | Description |
|----------------------------------|--|
| ohpc-autotools | Collection of GNU autotools packages. |
| ohpc-base | Collection of base packages. |
| ohpc-base-compute | Collection of compute node base packages. |
| ohpc-ganglia | Collection of Ganglia monitoring and metrics packages. |
| ohpc-gnu7-io-libs | Collection of IO library builds for use with GNU compiler toolchain. |
| ohpc-gnu7-mpich-io-libs | Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime. |
| ohpc-gnu7-mpich-parallel-libs | Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime. |
| ohpc-gnu7-mpich-perf-tools | Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime. |
| ohpc-gnu7-openmpi3-io-libs | Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime. |
| ohpc-gnu7-openmpi3-parallel-libs | Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime. |
| ohpc-gnu7-openmpi3-perf-tools | Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime. |
| ohpc-gnu7-parallel-libs | Collection of parallel library builds for use with GNU compiler toolchain. |
| ohpc-gnu7-perf-tools | Collection of performance tool builds for use with GNU compiler toolchain. |
| ohpc-gnu7-python-libs | Collection of python related library builds for use with GNU compiler toolchain. |
| ohpc-gnu7-python2-libs | Collection of python2 related library builds for use with GNU compiler toolchain. |
| ohpc-gnu7-python3-libs | Collection of python3 related library builds for use with GNU compiler toolchain. |
| ohpc-gnu7-runtimes | Collection of runtimes for use with GNU compiler toolchain. |
| ohpc-gnu7-serial-libs | Collection of serial library builds for use with GNU compiler toolchain. |
| ohpc-nagios | Collection of Nagios monitoring and metrics packages. |
| ohpc-slurm-client | Collection of client packages for SLURM. |
| ohpc-slurm-server | Collection of server packages for SLURM. |
| ohpc-warewulf | Collection of base packages for Warewulf provisioning. |

What follows next in this Appendix is a series of tables that summarize the underlying RPM packages available in this OpenHPC release. These packages are organized by groupings based on their general functionality and each table provides information for the specific RPM name, version, brief summary, and the web URL where additional information can be obtained for the component. Note that many of the 3rd party community libraries that are pre-packaged with OpenHPC are built using multiple compiler and MPI families. In these cases, the RPM package name includes delimiters identifying the development environment for which each package build is targeted. Additional information on the OpenHPC package naming scheme is presented in §4.6. The relevant package groupings and associated Table references are as follows:

- Administrative tools (Table 2)
- Provisioning (Table 3)
- Resource management (Table 4)
- Compiler families (Table 5)
- MPI families (Table 6)
- Development tools (Table 7)
- Performance analysis tools (Table 8)
- Distro support packages and dependencies (Table 9)
- IO Libraries (Table 10)
- Runtimes (Table 11)
- Serial/Threaded Libraries (Table 12)
- Parallel Libraries (Table 13)

Table 2: Administrative Tools

| RPM Package Name | Version | Info/URL |
|----------------------------------|---------|--|
| clustershell-ohpc | 1.8 | Python framework for efficient cluster administration. http://clustershell.sourceforge.net |
| conman-ohpc | 0.2.8 | ConMan: The Console Manager. http://dun.github.io/conman |
| docs-ohpc | 1.3.4 | OpenHPC documentation. https://github.com/openhpc/ohpc |
| examples-ohpc | 1.5 | Example source code and templates for use within OpenHPC environment. https://github.com/openhpc/ohpc |
| ganglia-ohpc | 3.7.2 | Distributed Monitoring System. http://ganglia.sourceforge.net |
| genders-ohpc | 1.22 | Static cluster configuration database. https://github.com/chaos/genders |
| lmod-defaults-gnu-mpich-ohpc | 1.2 | OpenHPC default login environments. https://github.com/openhpc/ohpc |
| lmod-defaults-gnu-openmpi-ohpc | | |
| lmod-defaults-gnu7-mpich-ohpc | | |
| lmod-defaults-gnu7-openmpi-ohpc | 1.3.1 | |
| lmod-defaults-gnu7-openmpi3-ohpc | 1.3.3 | |
| lmod-ohpc | 7.7.14 | Lua based Modules (lmod). https://github.com/TACC/Lmod |
| losf-ohpc | 0.55.0 | A Linux operating system framework for managing HPC clusters. https://github.com/hpsi/losf |
| mrsh-ohpc | 2.12 | Remote shell program that uses munge authentication. https://github.com/chaos/mrsh |
| nagios-plugins-ohpc | 2.2.1 | Host/service/network monitoring program plugins for Nagios. https://www.nagios-plugins.org |
| nagios-ohpc | 4.3.4 | Host/service/network monitoring program. http://www.nagios.org |
| ndoutils-ohpc | 2.1.3 | Stores all configuration and event data from Nagios in a database. http://www.nagios.org/download/addons |
| nhc-ohpc | 1.4.2 | LBNL Node Health Check. https://github.com/mej/nhc |
| nrpe-ohpc | 3.2.0 | Host/service/network monitoring agent for Nagios. http://www.nagios.org |
| ohpc-release | 1.3 | OpenHPC release files. https://github.com/openhpc/ohpc |
| pdsh-ohpc | 2.33 | Parallel remote shell program. http://sourceforge.net/projects/pdsh |
| prun-ohpc | 1.2 | Convenience utility for parallel job launch. https://github.com/openhpc/ohpc |
| test-suite-ohpc | 1.3.4 | Integration test suite for OpenHPC. https://github.com/openhpc/ohpc/tests |

Table 3: **Provisioning**

| RPM Package Name | Version | Info/URL |
|--------------------------------|---------|---|
| warewulf-common-ohpc | 3.8pre | A suite of tools for clustering. http://warewulf.lbl.gov |
| warewulf-ipmi-ohpc | 3.8pre | IPMI Module for Warewulf. http://warewulf.lbl.gov |
| warewulf-cluster-node-ohpc | 3.8pre | Tools used for clustering with Warewulf. http://warewulf.lbl.gov |
| warewulf-cluster-ohpc | 3.8pre | Tools used for clustering with Warewulf. http://warewulf.lbl.gov |
| warewulf-vnfs-ohpc | 3.8pre | Warewulf VNFS Module. http://warewulf.lbl.gov |
| warewulf-provision-ohpc | 3.8pre | Warewulf - Provisioning Module. http://warewulf.lbl.gov |
| warewulf-provision-server-ohpc | 3.8pre | Warewulf - Provisioning Module - Server. http://warewulf.lbl.gov |

Table 4: Resource Management

| RPM Package Name | Version | Info/URL |
|----------------------------|---------|--|
| munge-ohpc | 0.5.13 | MUNGE authentication service. http://dun.github.io/munge |
| pbspro-execution-ohpc | 14.1.2 | PBS Professional for an execution host. https://github.com/PBSPRO/pbspro |
| pbspro-client-ohpc | 14.1.2 | PBS Professional for a client host. https://github.com/PBSPRO/pbspro |
| pbspro-server-ohpc | 14.1.2 | PBS Professional for a server host. https://github.com/PBSPRO/pbspro |
| pmix-ohpc | 2.1.1 | An extended/exascale implementation of PMI. https://pmix.github.io/pmix |
| slurm-devel-ohpc | 17.11.5 | Development package for Slurm. https://slurm.schedmd.com |
| slurm-example-configs-ohpc | 17.11.5 | Example config files for Slurm. https://slurm.schedmd.com |
| slurm-sview-ohpc | 17.11.5 | Graphical user interface to view and modify Slurm state. https://slurm.schedmd.com |
| slurm-pam_slurm-ohpc | 17.11.5 | PAM module for restricting access to compute nodes via Slurm. https://slurm.schedmd.com |
| slurm-perlapi-ohpc | 17.11.5 | Perl API to Slurm. https://slurm.schedmd.com |
| slurm-contribs-ohpc | 17.11.5 | Perl tool to print Slurm job state information. https://slurm.schedmd.com |
| slurm-ohpc | 17.11.5 | Slurm Workload Manager. https://slurm.schedmd.com |
| slurm-slurmd-ohpc | 17.11.5 | Slurm compute node daemon. https://slurm.schedmd.com |
| slurm-slurmdctld-ohpc | 17.11.5 | Slurm controller daemon. https://slurm.schedmd.com |
| slurm-slurmdbd-ohpc | 17.11.5 | Slurm database daemon. https://slurm.schedmd.com |
| slurm-libpmi-ohpc | 17.11.5 | Slurm's implementation of the pmi libraries. https://slurm.schedmd.com |
| slurm-torque-ohpc | 17.11.5 | Torque/PBS wrappers for transition from Torque/PBS to Slurm. https://slurm.schedmd.com |
| slurm-openlava-ohpc | 17.11.5 | openlava/LSF wrappers for transition from OpenLava/LSF to Slurm. https://slurm.schedmd.com |

Table 5: **Compiler Families**

| RPM Package Name | Version | Info/URL |
|----------------------|---------|--|
| gnu-compilers-ohpc | 5.4.0 | The GNU C Compiler and Support Files. http://gcc.gnu.org |
| gnu7-compilers-ohpc | 7.3.0 | The GNU C Compiler and Support Files. http://gcc.gnu.org |
| llvm4-compilers-ohpc | 4.0.1 | The LLVM Compiler Infrastructure. http://www.llvm.org |
| llvm5-compilers-ohpc | 5.0.1 | The LLVM Compiler Infrastructure. http://www.llvm.org |

Table 6: **MPI Families**

| RPM Package Name | Version | Info/URL |
|-------------------------------|---------|--|
| mpich-gnu-ohpc | 3.2 | MPICH MPI implementation. http://www.mpich.org |
| mpich-gnu7-ohpc | 3.2.1 | |
| openmpi-gnu-ohpc | 1.10.6 | A powerful implementation of MPI. http://www.open-mpi.org |
| openmpi-gnu7-ohpc | 1.10.7 | |
| openmpi3-gnu7-ohpc | 3.0.0 | A powerful implementation of MPI. http://www.open-mpi.org |
| openmpi3-pmix-slurm-gnu7-ohpc | | |

Table 7: Development Tools

| RPM Package Name | Version | Info/URL |
|-----------------------------------|---------|---|
| EasyBuild-ohpc | 3.5.3 | Build and installation framework. http://easybuilders.github.io/easybuild |
| R_base-ohpc | 3.3.2 | R is a language and environment for statistical computing and graphics (S-Plus like). http://www.r-project.org |
| automake-ohpc | 1.15 | A GNU tool for automatically creating Makefiles. http://www.gnu.org/software/automake |
| autoconf-ohpc | 2.69 | A GNU tool for automatically configuring source code. http://www.gnu.org/software/autoconf |
| cmake-ohpc | 3.10.2 | CMake is an open-source, cross-platform family of tools designed to build, test and package software. https://cmake.org |
| hwloc-ohpc | 1.11.9 | Portable Hardware Locality. http://www.open-mpi.org/projects/hwloc |
| libtool-ohpc | 2.4.6 | The GNU Portable Library Tool. http://www.gnu.org/software/libtool |
| python-scipy-gnu-mpich-ohpc | 0.19.0 | Scientific Tools for Python. http://www.scipy.org |
| python-scipy-gnu-openmpi-ohpc | | |
| python-scipy-gnu7-mpich-ohpc | 1.0.0 | Scientific Tools for Python. http://www.scipy.org |
| python-scipy-gnu7-openmpi3-ohpc | | |
| python3-scipy-gnu7-mpich-ohpc | 1.0.0 | Scientific Tools for Python. http://www.scipy.org |
| python3-scipy-gnu7-openmpi3-ohpc | | |
| python-numpy-gnu-ohpc | 1.11.1 | NumPy array processing for numbers, strings, records and objects. http://sourceforge.net/projects/numpy |
| python-numpy-gnu7-ohpc | 1.14.2 | |
| python3-numpy-gnu7-ohpc | 1.14.2 | NumPy array processing for numbers, strings, records and objects. http://sourceforge.net/projects/numpy |
| python-mpi4py-gnu7-mpich-ohpc | 3.0.0 | Python bindings for the Message Passing Interface (MPI) standard. https://bitbucket.org/mpi4py/mpi4py |
| python-mpi4py-gnu7-openmpi3-ohpc | | |
| python3-mpi4py-gnu7-mpich-ohpc | 3.0.0 | Python bindings for the Message Passing Interface (MPI) standard. https://bitbucket.org/mpi4py/mpi4py |
| python3-mpi4py-gnu7-openmpi3-ohpc | | |
| spack-ohpc | 0.11.2 | HPC software package management. https://github.com/LLNL/spack |
| valgrind-ohpc | 3.13.0 | Valgrind Memory Debugger. http://www.valgrind.org |

Table 8: Performance Analysis Tools

| RPM Package Name | Version | Info/URL |
|---|---------|---|
| imb-gnu-mpich-ohpc imb-gnu-openmpi-ohpc imb-gnu7-openmpi-ohpc | 4.1 | Intel MPI Benchmarks (IMB). https://software.intel.com/en-us/articles/intel-mpi-benchmarks |
| imb-gnu7-mpich-ohpc imb-gnu7-openmpi3-ohpc | 2018.1 | |
| mpiP-gnu-mpich-ohpc mpiP-gnu-openmpi-ohpc mpiP-gnu7-mpich-ohpc mpiP-gnu7-openmpi-ohpc mpiP-gnu7-openmpi3-ohpc | 3.4.1 | mpiP: a lightweight profiling library for MPI applications. http://mpip.sourceforge.net |
| pdtoolkit-gnu-ohpc | 3.23 | PDT is a framework for analyzing source code. http://www.cs.uoregon.edu/Research/pdt |
| pdtoolkit-gnu7-ohpc | 3.25 | |
| scalasca-gnu-mpich-ohpc scalasca-gnu-openmpi-ohpc scalasca-gnu7-mpich-ohpc scalasca-gnu7-openmpi-ohpc scalasca-gnu7-openmpi3-ohpc | 2.3.1 | Toolset for performance analysis of large-scale parallel applications. http://www.scalasca.org |
| scorep-gnu-mpich-ohpc scorep-gnu-openmpi-ohpc | 3.0 | Scalable Performance Measurement Infrastructure for Parallel Codes. http://www.vi-hps.org/projects/score-p |
| scorep-gnu7-mpich-ohpc scorep-gnu7-openmpi-ohpc scorep-gnu7-openmpi3-ohpc | 3.1 | |
| sionlib-gnu-mpich-ohpc sionlib-gnu-openmpi-ohpc | 1.7.0 | Scalable Performance Measurement Infrastructure for Parallel Codes. http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SIONlib/_node.html |
| tau-gnu-mpich-ohpc tau-gnu-openmpi-ohpc tau-gnu7-openmpi-ohpc | 2.26.1 | Tuning and Analysis Utilities Profiling Package. http://www.cs.uoregon.edu/research/tau/home.php |
| tau-gnu7-mpich-ohpc tau-gnu7-openmpi3-ohpc | 2.27 | |

Table 9: Distro Support Packages/Dependencies

| RPM Package Name | Version | Info/URL |
|---------------------|---------|---|
| lua-bit-ohpc | 1.0.2 | Module for Lua which adds bitwise operations on numbers. http://bitop.luajit.org |
| lua-filesystem-ohpc | 1.6.3 | Lua library to Access Directories and Files. http://keplerproject.github.com/luafs |
| lua-posix-ohpc | 33.2.1 | POSIX library for Lua. https://github.com/luaposix/luaposix |

Table 10: IO Libraries

| RPM Package Name | Version | Info/URL |
|-----------------------------------|---------|--|
| adios-gnu-mpich-ohpc | 1.11.0 | The Adaptable IO System (ADIOS). http://www.olcf.ornl.gov/center-projects/adios |
| adios-gnu-openmpi-ohpc | | |
| adios-gnu7-openmpi-ohpc | 1.12.0 | |
| adios-gnu7-mpich-ohpc | 1.13.0 | |
| adios-gnu7-openmpi3-ohpc | | |
| hdf5-gnu-ohpc | 1.8.17 | A general purpose library and file format for storing scientific data. http://www.hdfgroup.org/HDF5 |
| hdf5-gnu7-ohpc | 1.10.1 | |
| netcdf-cxx-gnu-mpich-ohpc | 4.3.0 | C++ Libraries for the Unidata network Common Data Form. http://www.unidata.ucar.edu/software/netcdf |
| netcdf-cxx-gnu-openmpi-ohpc | | |
| netcdf-cxx-gnu7-mpich-ohpc | | |
| netcdf-cxx-gnu7-openmpi-ohpc | | |
| netcdf-cxx-gnu7-openmpi3-ohpc | | |
| netcdf-gnu-mpich-ohpc | 4.4.1.1 | C Libraries for the Unidata network Common Data Form. http://www.unidata.ucar.edu/software/netcdf |
| netcdf-gnu-openmpi-ohpc | | |
| netcdf-gnu7-openmpi-ohpc | | |
| netcdf-fortran-gnu-mpich-ohpc | 4.4.4 | |
| netcdf-fortran-gnu-openmpi-ohpc | | |
| netcdf-fortran-gnu7-mpich-ohpc | | |
| netcdf-fortran-gnu7-openmpi-ohpc | | |
| netcdf-fortran-gnu7-openmpi3-ohpc | | |
| netcdf-gnu7-mpich-ohpc | 4.5.0 | |
| netcdf-gnu7-openmpi3-ohpc | | |
| phdf5-gnu-mpich-ohpc | 1.8.17 | A general purpose library and file format for storing scientific data. |
| phdf5-gnu-openmpi-ohpc | | |
| phdf5-gnu7-mpich-ohpc | 1.10.1 | http://www.hdfgroup.org/HDF5 |
| phdf5-gnu7-openmpi-ohpc | | |
| phdf5-gnu7-openmpi3-ohpc | | |
| pnetcdf-gnu7-mpich-ohpc | 1.8.1 | A Parallel NetCDF library (PnetCDF). http://cucis.ece.northwestern.edu/projects/PnetCDF |
| pnetcdf-gnu7-openmpi-ohpc | | |
| pnetcdf-gnu7-openmpi3-ohpc | | |
| sionlib-gnu7-mpich-ohpc | 1.7.1 | Scalable I/O Library for Parallel Access to Task-Local Files. http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/SIONlib/_node.html |
| sionlib-gnu7-openmpi-ohpc | | |
| sionlib-gnu7-openmpi3-ohpc | | |

Table 11: **Runtimes**

| RPM Package Name | Version | Info/URL |
|-------------------------------|---------|--|
| ocr-gnu-ohpc ocr-gnu7-ohpc | 1.0.1 | Open Community Runtime (OCR) for shared memory. https://xstack.exascale-tech.com/wiki |
| singularity-ohpc | 2.4.5 | Application and environment virtualization. http://singularity.lbl.gov |

Table 12: **Serial/Threaded Libraries**

| RPM Package Name | Version | Info/URL |
|---|------------------|---|
| R-gnu7-ohpc | 3.4.4 | R is a language and environment for statistical computing and graphics (S-Plus like). http://www.r-project.org |
| gsl-gnu-ohpc gsl-gnu7-ohpc | 2.2.1 2.4 | GNU Scientific Library (GSL). http://www.gnu.org/software/gsl |
| metis-gnu-ohpc metis-gnu7-ohpc | 5.1.0 | Serial Graph Partitioning and Fill-reducing Matrix Ordering. http://glaros.dtc.umn.edu/gkhome/metis/metis/overview |
| openblas-gnu-ohpc openblas-gnu7-ohpc | 0.2.19 0.2.20 | An optimized BLAS library based on GotoBLAS2. http://www.openblas.net |
| plasma-gnu7-ohpc | 2.8.0 | Parallel Linear Algebra Software for Multicore Architectures. https://bitbucket.org/icl/plasma |
| scotch-gnu7-ohpc | 6.0.4 | Graph, mesh and hypergraph partitioning library. http://www.labri.fr/perso/pelegrin/scotch |
| superlu-gnu-ohpc superlu-gnu7-ohpc | 5.2.1 | A general purpose library for the direct solution of linear equations. http://crd.lbl.gov/~xiaoye/SuperLU |

Table 13: **Parallel Libraries**

| RPM Package Name | Version | Info/URL |
|---------------------------------|---------|--|
| boost-gnu-mpich-ohpc | 1.63.0 | Boost free peer-reviewed portable C++ source libraries. http://www.boost.org |
| boost-gnu-openmpi-ohpc | | |
| boost-gnu7-openmpi-ohpc | | |
| boost-gnu7-mpich-ohpc | 1.66.0 | |
| boost-gnu7-openmpi3-ohpc | | |
| fftw-gnu-mpich-ohpc | | |
| fftw-gnu-openmpi-ohpc | | |
| fftw-gnu7-openmpi-ohpc | 3.3.6 | |
| fftw-gnu7-mpich-ohpc | | 3.3.7 |
| fftw-gnu7-openmpi3-ohpc | | |
| hypre-gnu-mpich-ohpc | 2.11.1 | |
| hypre-gnu-openmpi-ohpc | | |
| hypre-gnu7-openmpi-ohpc | | 2.11.2 |
| hypre-gnu7-mpich-ohpc | 2.13.0 | |
| hypre-gnu7-openmpi3-ohpc | | |
| mfem-gnu7-mpich-ohpc | | 3.3.2 |
| mfem-gnu7-openmpi3-ohpc | | |
| mumps-gnu-mpich-ohpc | 5.0.2 | |
| mumps-gnu-openmpi-ohpc | | |
| mumps-gnu7-openmpi-ohpc | | 5.1.1 |
| mumps-gnu7-mpich-ohpc | 5.1.2 | |
| mumps-gnu7-openmpi3-ohpc | | |
| petsc-gnu-mpich-ohpc | | 3.7.5 |
| petsc-gnu-openmpi-ohpc | | |
| petsc-gnu7-openmpi-ohpc | 3.7.6 | |
| petsc-gnu7-mpich-ohpc | | 3.8.3 |
| petsc-gnu7-openmpi3-ohpc | | |
| ptscotch-gnu7-mpich-ohpc | 6.0.4 | |
| ptscotch-gnu7-openmpi-ohpc | | |
| ptscotch-gnu7-openmpi3-ohpc | | |
| slepc-gnu7-openmpi-ohpc | 3.7.4 | A library for solving large scale sparse eigenvalue problems. http://www.grycap.upv.es/slepc |
| slepc-gnu7-mpich-ohpc | 3.8.2 | |
| slepc-gnu7-openmpi3-ohpc | | |
| superlu_dist-gnu-mpich-ohpc | | 4.2 |
| superlu_dist-gnu-openmpi-ohpc | | |
| superlu_dist-gnu7-openmpi-ohpc | 5.3.0 | |
| superlu_dist-gnu7-mpich-ohpc | | |
| superlu_dist-gnu7-openmpi3-ohpc | | |
| trilinos-gnu-mpich-ohpc | 12.10.1 | |
| trilinos-gnu-openmpi-ohpc | | |
| trilinos-gnu7-openmpi-ohpc | | 12.12.1 |
| trilinos-gnu7-mpich-ohpc | | |
| trilinos-gnu7-openmpi3-ohpc | | |

F Package Signatures

All of the RPMs provided via the OpenHPC repository are signed with a GPG signature. By default, the underlying package managers will verify these signatures during installation to ensure that packages have not been altered. The RPMs can also be manually verified and the public signing key fingerprint for the latest repository is shown below:

Fingerprint: DD5D 8CAA CB57 364F FCC2 D3AE C468 07FF **26CE 6884**

The following command can be used to verify an RPM once it has been downloaded locally by confirming if the package is signed, and if so, indicating which key was used to sign it. The example below highlights usage for a local copy of the `docs-ohpc` package and illustrates how the *key ID* matches the fingerprint shown above.

```
[sms]# rpm --checksig -v docs-ohpc-*.rpm
docs-ohpc-1.0-1.1.x86_64.rpm:
  Header V3 RSA/SHA256 Signature, key ID 26ce6884: OK
  Header SHA1 digest: OK (c3873bf495c51d2ea6d3ef23ab88be105983c72c)
  V3 RSA/SHA256 Signature, key ID 26ce6884: OK
  MD5 digest: OK (43d067f33fb370e30a39789439ead238)
```