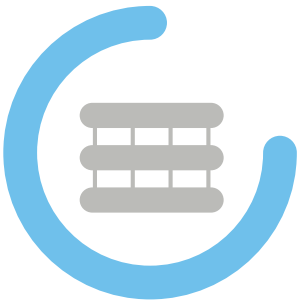

OpenHPC (v4.2)

Cluster Building Recipes

AlmaLinux 10 Base OS
xCAT/Slurm Edition for Linux* (x86_64)



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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 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:

```
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

Life is a tale told by an idiot, full of sound and fury signifying nothing. –Willy Shakes

1.2 Requirements/Assumptions

This installation recipe assumes the availability of a single *head node*, and four *compute* nodes. The *head node* serves as the overall system management server (SMS) and is provisioned with AlmaLinux 10 and is subsequently configured to provision the remaining *compute* nodes with xCAT in either a stateless or a stateful configuration. For power management, we assume that the compute node baseboard management controllers (BMCs) are available via IPMI from the chosen *head node*. For file systems, we assume that the chosen *head node* will host an NFS file system that is made available to the compute nodes.

Installation information is also discussed to optionally mount a parallel file system and in this case, the parallel file system is assumed to exist previously.

An outline of the physical architecture discussed is shown in the figure above and highlights the high-level networking configuration. The *head node* 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

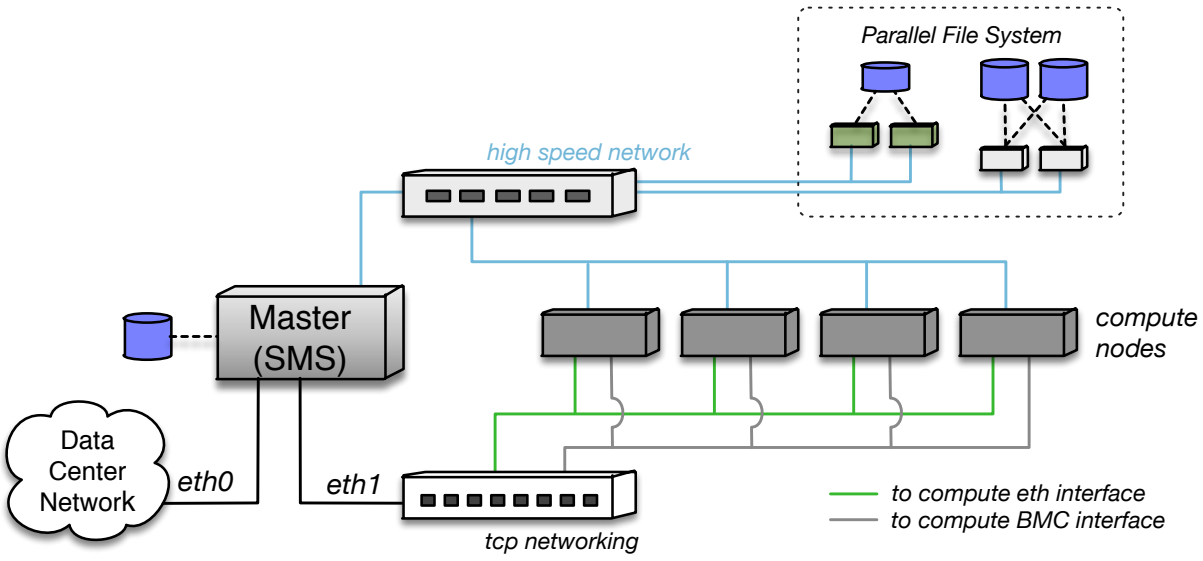

Figure 1: Overview of physical cluster architecture

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. Independent of the actual networking configuration it is recommended to have additional security boundaries like a firewall to protect the network interfaces from the Internet.

In addition to the IP networking, there is an optional high-speed network (InfiniBand or Omni-Path in this recipe) that is also connected to each of the hosts. This high speed network is used for application message passing and optionally for parallel file system connectivity as well (e.g. to existing Lustre or BeeGFS storage targets).

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.

Required variables:

- `${sms_name}` - Hostname for head node
- `${sms_ip}` - Internal IP address on head node
- `${sms_eth_internal}` - Internal Ethernet interface on head node
- `${internal_network}` - Subnet network address for internal network

- `${internal_netmask}` - Subnet netmask for internal network
- `${dns_domain}` - DNS domain name for cluster (e.g. `local`)
- `${ntp_server}` - Local ntp server for time synchronization
- `${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`)
- `iso_path` - location of compute node base os dvd iso (default: `AlmaLinux-10-latest-x86_64-dvd.iso`)
- `iso_url` - ISO download base URL (optional; overrides default upstream location)

Optional variables:

- `${modules_package}` - Module tool installed on the head node and the computes: `lmod-ohpc` (Lmod, the default) or `environment-modules-ohpc` (Environment Modules)
- `${sysmgmtd_host}` - BeeGFS System Management host name
- `${mgs_fs_name}` - Lustre MGS mount name
- `${sms_ipoib}` - IPoIB address for head node
- `${ipoib_dev}` - IPoIB interface name on head node and computes (e.g. `ib0`, or `ibp3s0` with predictable interface naming)
- `${ipoib_netmask}` - Subnet netmask for internal IPoIB
- `${ipoib_prefix_length}` - Subnet prefix length for internal IPoIB (e.g. `16`; must be consistent with `${ipoib_netmask}`)
- `${c_ipoib[0]}`, `${c_ipoib[1]}`, ... - IPoIB addresses for computes

1.4 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 (see Requirements/Assumptions) and is provided as a convenience for administrators. For additional information on accessing this script, please see the Automation Appendix.

2 Install Base Operating System

2.1 Install OS

In an external setting, installing the desired Base OS on a *head node* typically involves booting from a DVD ISO image on a new server. With this approach, insert the AlmaLinux 10 DVD, power cycle the host, and follow the distro provided directions to install the Base OS on your chosen *head node*. Alternatively, if choosing to use a pre-installed server, please verify that it is provisioned with the required AlmaLinux 10 distribution.

Prior to beginning the installation process of OpenHPC components, several additional considerations are noted here for the head node configuration. First, the installation recipe herein assumes that the head node name is resolvable locally. Depending on the manner in which you installed the Base OS, there may be an adequate entry already defined in `/etc/hosts`. If not, add one so the head node resolves itself by name (this guide relies on it for name-based commands):

```
echo ${sms_ip} ${sms_name} >> /etc/hosts
```

While it is theoretically possible to enable SELinux on a cluster provisioned with xCAT, 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 *head node*. 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.

2.2 Configure HTTPS Proxy (Optional)

If your environment requires an HTTPS caching proxy for external network access, configure it here before installing any packages.

2.3 Enable EL Package Repositories

In addition to the OpenHPC package repository, the *head node* also requires access to the standard base OS distro repositories in order to resolve necessary dependencies. For AlmaLinux 10, the requirements are to have access to the BaseOS, Appstream, Extras, CRB, and EPEL repositories for which mirrors are freely available online:

- AlmaLinux-10 (e.g. https://repo.almalinux.org/almalinux/10/)
- EPEL 10 (e.g. http://download.fedoraproject.org/pub/epel/10/)

Although the public EPEL repository would be enabled automatically upon installation of the `ohpc-release` package, we install it now. Note that this does depend on the AlmaLinux 10 Extras repository, which is shipped with AlmaLinux 10 and is typically enabled by default. In contrast, the CRB repository is typically disabled in a standard install, but can be enabled from EPEL as follows:

```
dnf -y install epel-release dnf-plugins-core
dnf config-manager --set-enabled crb
```

2.4 Configure Firewall

Provisioning services rely on DHCP, TFTP, and HTTP network protocols. Depending on the local Base OS configuration on the head node, default firewall rules may prohibit these services. Consequently, this

recipe assumes that the local firewall running on the head node is disabled (it is still recommended to have additional security boundaries like a firewall to protect the cluster from the Internet). If installed, the default firewall service can be disabled as follows:

```
systemctl disable --now firewalld.service || true
```

2.5 Configure NTP

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 head node with a specific server `${ntp_server}`, and allow this server to serve as a local time server for the cluster, issue the following:

```
dnf -y install chrony
systemctl enable chronyd.service
echo "local stratum 10" >> /etc/chrony.conf
echo "server ${ntp_server}" >> /etc/chrony.conf
echo "allow all" >> /etc/chrony.conf
systemctl restart chronyd.service
```

Tip

Note: Note that the "allow all" option specified for the chrony time daemon allows all servers on the local network to be able to synchronize with the head node. Alternatively, you can restrict access to fixed IP ranges and an example config line allowing access to a local class B subnet is as follows:

```
allow 192.168.0.0/16
```

2.6 Generate SSH Key Pair

An SSH key pair on the *head node* enables passwordless access to compute nodes and is useful for automating cluster configuration tasks.

If an ed25519 key does not already exist, generate one:

```
[[ -f ~/.ssh/id_ed25519 ]] || ssh-keygen -t ed25519 -f ~/.ssh/id_ed25519 -N ''
```

Tip

Note: The key is generated without a passphrase (`-N ''`) to allow unattended use in scripts and automated workflows. Ensure that access to the head node is appropriately restricted.

2.7 Setup NFS Server

Here we set up NFS mounting of a `$HOME` file system and the public OpenHPC install path (`/opt/ohpc/pub`) that will be hosted by the *head node* in this example configuration.

```
# Install and Start NFS server
dnf -y install nfs-utils
systemctl start nfs-server.service

# Create OpenHPC public packages directory
mkdir -p /opt/ohpc/pub

# Export /home and OpenHPC public packages from head node
echo "/home *(rw,no_subtree_check,fsid=10,no_root_squash)" >> /etc/exports
echo "/opt/ohpc/pub *(ro,no_subtree_check,fsid=11)" >> /etc/exports
exportfs -a

# Restart and enable nfs server
systemctl restart nfs-server.service
systemctl enable nfs-server.service
```

2.8 Optionally add InfiniBand support services on *head node*

The following command adds OFED and PSM support using base distro-provided drivers to the chosen *head node*.

```
dnf -y groupinstall "InfiniBand Support"
# Load IB services
udevadm trigger --type=devices --action=add
systemctl restart rdma-load-modules@infiniband.service
```

Tip

Note: InfiniBand networks require a subnet management service that can typically be run on either an administrative node, or on the switch itself. The optimal placement and configuration of the subnet manager is beyond the scope of this document, but AlmaLinux 10 provides the `opensm` package should you choose to run it on the *head node*.

With the InfiniBand drivers included, you can also enable (optional) IPoIB functionality which provides a mechanism to send IP packets over the IB network. If you plan to mount a Lustre file system over InfiniBand, then having IPoIB enabled is a requirement for the Lustre client. The following creates a NetworkManager connection for the IPoIB interface `${ipoib_dev}` on the *head node*, with the address `${sms_ipoib}` and subnet prefix `${ipoib_prefix_length}`. Set `${ipoib_dev}` to the name the system gives the interface, for example `ibp3s0` under predictable interface naming, and add one connection per port if the system contains dual-ported or multiple HCAs.

```
# Define the local IPoIB interface, address, and subnet prefix
nmcli connection add type infiniband con-name ipoib ifname "${ipoib_dev}" \
    ipv4.method manual ipv4.addresses "${sms_ipoib}/${ipoib_prefix_length}"

# Bring up the IPoIB interface
nmcli connection up ipoib
```

2.9 Optionally add RoCE support on *head node*

RoCE (RDMA over Converged Ethernet) runs RDMA over Ethernet NICs that support it, for example NVIDIA ConnectX "Dx" models. It uses the same distro-provided RDMA stack as InfiniBand, but it needs no subnet manager and no IPoIB: RDMA traffic is addressed by the Ethernet interface's own IP address. This recipe runs RoCE over the internal cluster network. The following command adds the RDMA stack to the *head node*. If you enabled InfiniBand above, the stack is already installed and the script skips this step.

```
dnf -y groupinstall "InfiniBand Support"
# Load the RDMA drivers for the RoCE NIC
udevadm trigger --type=devices --action=add
systemctl restart rdma-load-modules@rdma.service
```

RoCE takes its own MTU (up to 4096 bytes) from the Ethernet MTU: the largest that fits with room for headers. An Ethernet MTU of 1500 gives RoCE 1024, and exactly 4096 gives only 2048; about 4200 or more (9000 is common) gives the full 4096. RoCE works at the default MTU, and a larger one adds a little bandwidth. Every host and switch port on the network must carry the larger frames.

This recipe leaves the MTU unchanged. To use a larger one, set the same value on the *head node*'s internal interface and on the computes' interfaces in your xCAT network configuration.

2.10 Optionally add Omni-Path support services on *head node*

The following command adds Omni-Path support using base distro-provided drivers to the chosen *head node*.

```
dnf -y install opa-basic-tools
```

Tip

Note: OmniPath networks require a subnet management service that can typically be run on either an administrative node, or on the switch itself. The optimal placement and configuration of the subnet manager is beyond the scope of this document, but AlmaLinux 10 provides the `opa-fm` package should you choose to run it on the *head node*.

Tip

Note: 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.

```
ipmitool -E -I lanplus -H ${bmc_ipaddr} -U root chassis \
    bootdev pxe options=persistent
```

3 Install OpenHPC Components

3.1 Enable OpenHPC Repository

With the Base OS installed and booted, the next step is to add desired OpenHPC packages onto the *head node* in order to provide provisioning and resource management services for the rest of the cluster.

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 *head node* 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 enabling the repository. The example which follows illustrates installation of the `ohpc-release` package directly from the OpenHPC build server.

```
dnf -y install http://repos.openhpc.community/OpenHPC/4/EL_10/x86_64/\
ohpc-release-4-1.el10.x86_64.rpm
```

Tip

Note: 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://repos.openhpc.community/dist/4.2

3.2 Install OpenHPC Base Packages

Now OpenHPC packages can be installed. The `ohpc-base` meta-package requires a module tool to manage the user environment, and OpenHPC provides two of them: Lmod in the `lmod-ohpc` package and Environment Modules in the `environment-modules-ohpc` package. Both read the OpenHPC module hierarchy and provide the `module` command. The `${modules_package}` variable in `input.local` selects the one installed on the head node and, later in this guide, on the compute nodes; it defaults to `lmod-ohpc`. To add the base package and the module tool on the head node issue the following:

```
dnf -y install ohpc-base ${modules_package:-lmod-ohpc}
```

Tip

Naming the module tool keeps the choice explicit; `ohpc-base` alone normally pulls in Lmod, which it suggests. The two tools can also be installed side by side: the startup scripts `/etc/profile.d/modules.sh` and `modules.csh`, which define the `module` command, and `/usr/bin/modulecmd` are links managed with `alternatives`, and `environment-modules-ohpc` takes precedence over `lmod-ohpc` when both are present. Run `alternatives --config modules.sh` to select the active tool.

4 Install Slurm

4.1 Add Slurm on Head Node

The following command adds the Slurm workload manager server components to the chosen *head node*. Note that client-side components will be added to the corresponding compute image in a subsequent step. Note that Slurm leverages the use of the *munge* library to provide authentication services and this daemon also needs to be running on all hosts within the resource management pool.

```
# Install slurm server meta-package
dnf -y install ohpc-slurm-server

# Use ohpc-provided file for starting SLURM configuration
cp /etc/slurm/slurm.conf.ohpc /etc/slurm/slurm.conf

# Setup default cgroups file
cp /etc/slurm/cgroup.conf.example /etc/slurm/cgroup.conf

# Identify resource manager hostname on head node
sed -i "s/SlurmctldHost=\S\+/SlurmctldHost=${sms_name}/" \
    /etc/slurm/slurm.conf
```

There are a wide variety of configuration options and plugins available for Slurm and the example config file illustrated above targets a fairly basic installation. In particular, job completion data will be stored in a text file (`/var/log/slurm_jobcomp.log`) that can be used to log simple accounting information. Sites who desire more detailed information, or want to aggregate accounting data from multiple clusters, will likely want to enable the database accounting back-end. This requires a number of additional local modifications (on top of installing `slurm-slurmdbd-ohpc`), and users are advised to consult the online documentation for more detailed information on setting up a database configuration for Slurm.

Tip

Note: SLURM requires enumeration of the physical hardware characteristics for compute nodes under its control. In particular, three configuration parameters combine to define consumable compute resources: *Sockets*, *CoresPerSocket*, and *ThreadsPerCore*. The default configuration file provided via OpenHPC assumes the nodes are named c1-c4 and are dual-socket, 8 cores per socket, and two threads per core for this 4-node example. If this does not reflect your local hardware, please update the configuration file at `/etc/slurm/slurm.conf` accordingly to match your nodes names and particular hardware. Be sure to run `scontrol reconfigure` to notify SLURM of the changes. Note that the SLURM project provides an easy-to-use online configuration tool that can be accessed here.

5 Install xCAT Provisioner

This guide provisions compute nodes in **stateful** (*diskful*) mode: a base OS is installed onto each node's local disk and the OpenHPC components are installed in the same provisioning pass. Nodes keep their state across reboots. Following the xCAT model, the OpenHPC package list and configuration are staged on the head node and applied automatically by xCAT when each node installs and first boots – there is no configuration over a live-node shell. The nodes are booted later, in the deploy chapter.

5.1 Enable xCAT Repository

Enable the xCAT package repositories. xCAT ships an `xCAT-release` package that configures the `xcat-core` (main xCAT packages) and `xcat-dep` (OS/arch dependencies) repositories and installs the package-signing key – the same pattern as the `ohpc-release` package used earlier:

```
dnf -y install \
  https://xcat.org/files/xcat/repos/yum/latest/xcat-core/xCAT-release-latest.noarch.rpm
```

5.2 Install xCAT on *Head Node*

With the OpenHPC and xCAT repositories enabled, install the xCAT provisioning system:

```
# Install xCAT
dnf -y install xCAT
```

Source the environment script to make the xCAT tools available in the current shell (new login shells pick this up automatically):

```
. /etc/profile.d/xcat.sh
```

5.3 Complete Basic xCAT Setup for *Head Node*

With xCAT installed, register the internal provisioning interface with xCAT for DHCP service. The head node serves DNS to the cluster (`makedns`, below), so it is the compute nodes' name server and forwards other lookups to `${dns_servers}`. Then set the cluster domain name used for system-wide name resolution; `makedns` requires the head node to resolve by its name in that domain, so add it to `/etc/hosts`.

```
# Verify required variables are set
: "${sms_eth_internal:?ERROR: sms_eth_internal not set}"
: "${sms_ip:?ERROR: sms_ip not set}"

# Register internal provisioning interface with xCAT for DHCP
chdef -t site dhcpinterfaces="xcatmn|${sms_eth_internal}"

# Point provisioning services at the internal interface address. Without
# this, a multi-homed head node may auto-select its external address.
# The head node is the cluster's name server; it forwards other names upstream.
chdef -t site master=${sms_ip} nameservers=${sms_ip} forwarders=${dns_servers}

# Define local domain name; makedns needs the head node's name in this domain
chdef -t site domain=${dns_domain:-local}
echo "${sms_ip} ${sms_name}.${dns_domain:-local}" >> /etc/hosts
```

xCAT installs the same ssh host keys, generated in `/etc/xcat/hostkeys` during the xCAT installation, on every compute node, but only configures `root` on the head node to accept them. Add them to the system-wide known hosts so that all users can reach the compute nodes with ssh (e.g. via `pdsh`) while host key checking stays enabled:

```
awk -v hosts="${compute_prefix}*" '{print hosts, $1, $2}' \
    /etc/xcat/hostkeys/ssh_host_*_key.pub >> /etc/ssh/ssh_known_hosts
```

5.4 Define Compute Image for Provisioning

The following steps import the distribution installation media for use with xCAT. A local copy of the distribution ISO is required; for this recipe the ISO is `AlmaLinux-10-latest-x86_64-dvd.iso`, available from the AlmaLinux 10 download page and expected at `${iso_path}`. If it is not already present there, it is downloaded first.

`copycds` names the OS images after the distribution it finds inside the ISO, including the minor release (for example a Rocky 10.0 x86_64 ISO creates `rocky10.0-x86_64-{install,netboot,statelite}-compute`). Read that name from the ISO, import it, and select the `install` image this stateful recipe uses:

```
: "${iso_path:=AlmaLinux-10-latest-x86_64-dvd.iso}"
iso_url="${iso_url:=https://repo.almalinux.org/almalinux/10/isos/x86_64}"
[[ -f "${iso_path}" ]] || \
    curl -fo "${iso_path}" "${iso_url}/AlmaLinux-10-latest-x86_64-dvd.iso"

# Read the distribution name (e.g. alma10.2) that copycds names the images after
xcat_osver=$(copycds -i "${iso_path}" | awk -F: '/^DISTNAME/{print $2}')
copycds "${iso_path}"

# Select the install compute image (set xcat_osimage in input.local to override)
xcat_osimage=${xcat_osimage:-${xcat_osver}-x86_64-install-compute}
lsdef -t osimage -o ${xcat_osimage}
```

5.5 Add Compute Nodes into xCAT Database

Add compute nodes and define their properties as objects in the xCAT database. Hosts are grouped into a group named *compute* to allow group-level commands later in the recipe. Note the use of variable names for

hostnames, node IPs, MAC addresses, and BMC login credentials — adjust to match local hardware.

```
for ((i=0; i<num_computes; i++)) ; do
    mkdef -t node ${c_name[$i]} \
        groups=compute,all \
        ip=${c_ip[$i]} \
        mac=${c_mac[$i]} \
        netboot=xnba \
        arch=x86_64 \
        bmc=${c_bmc[$i]} \
        bmcusername=${bmc_username} \
        bmcpassword=${bmc_password} \
        mgt=ipmi \
        cons=ipmi \
        serialport=0 \
        serialspeed=115200
done
```

5.6 Optionally configure IPoIB on *compute nodes*

To use IPoIB on the compute nodes (required if planning to mount Lustre/BeeGFS over IB; see Optionally add InfiniBand support services on *head node*), give each compute its own address `${c_ipoib[i]}` on the IPoIB interface `${ipoib_dev}`, with the `${ipoib_netmask}` netmask (`${ipoib_prefix_length}` prefix). These are per-node settings, so they belong in the xCAT node definitions:

xCAT configures the interface on each node from its `nic*` attributes, applied by the `confignetwork` postscript at boot (`confignics` is deprecated and no longer configures anything):

```
# Define the IPoIB network
chdef -t network -o ipoib mask=${ipoib_netmask} net=${c_ipoib[0]}

# Register desired IPoIB IPs per compute
for ((i=0; i<num_computes; i++)) ; do
    chdef "${c_name[$i]}" \
        nicips."${ipoib_dev}"="${c_ipoib[$i]}" \
        nictypes."${ipoib_dev}"="InfiniBand" \
        nicnetworks."${ipoib_dev}"=ipoib
done
```

The postscript that applies these attributes is registered in Stage the Compute Configuration, after `ohpc-config`: the InfiniBand packages that create `${ipoib_dev}` are installed there.

5.7 Complete the Network Services

Generate the host, network, DNS, and DHCP configuration from the node definitions:

```
# Generate /etc/hosts and network definitions from the node defs
makehosts
makenetworks

# makedns must run before makedhcp: xCAT's Kea DHCP-DDNS integration
# requires the DDNS key material that makedns generates
makedns -n
makedhcp -n
```

5.8 Identify Files for Synchronization

xCAT includes functionality to synchronize files from the head node to managed hosts via *synclists*. This is one way to distribute user credentials to compute nodes. The default `syncfiles` postscript applies the synclist during the install, and changes can be pushed on demand afterwards with `updatenode`. Enable the synclist feature and register credential files:

```
# Synclists are registered per image type
xcat_synclist_dir="/install/custom/install"

# Define path for xCAT synclist file
mkdir -p ${xcat_synclist_dir}
chdef -t osimage -o ${xcat_osimage} \
    synclists="${xcat_synclist_dir}/compute.synclist"

# Add credential files to synclist
echo "/etc/passwd  -> /etc/passwd"  >  ${xcat_synclist_dir}/compute.synclist
echo "/etc/group   -> /etc/group"   >> ${xcat_synclist_dir}/compute.synclist
echo "/etc/shadow  -> /etc/shadow"  >> ${xcat_synclist_dir}/compute.synclist
echo "/etc/munge/munge.key -> /etc/munge/munge.key" \
    >> ${xcat_synclist_dir}/compute.synclist
```

The `updatenode compute -F` command distributes changes made to any defined synchronization files. Use the uppercase `-F` flag; lowercase `-f` targets service nodes.

5.9 Disk Layout and Root Password

The install applies a default disk layout to the first detected disk (a 1 GiB `/boot` plus an LVM volume group holding swap and a `/` volume grown to fill the disk). Sites requiring a different layout can register a custom partition file in kickstart syntax with `chdef -t osimage ${xcat_osimage} partitionfile=<file>`; consult the xCAT documentation for details.

The kickstart generated for stateful installs reads the compute root password from the xCAT `passwd` table, so the entry must exist before the provisioning image is associated with the nodes. Administrative access relies on the head node root ssh keys that xCAT installs during provisioning, so the randomly generated password below is intentionally throwaway; sites that want interactive (console) root logins should substitute a chosen password for the `openssl rand` call. Store the password as a hash:

```
chtab key=system passwd.username=root \
    passwd.password="$(openssl passwd -6 "$(openssl rand -base64 12)")"
```

5.10 Stage the Compute Configuration

In stateful mode OpenHPC is added in the same provisioning pass as the base OS, the xCAT-native way, rather than by logging in to the running nodes. Two things are staged on the head node and applied automatically when a node installs:

- an **otherpkgs pkglist** – the OpenHPC packages xCAT installs into the node, from the OpenHPC, EPEL, and CRB repositories named by `otherpkgdir`; and
- a **postscript** (`ohpc-config`) – the configuration commands xCAT runs on the node at first boot, after those packages are installed.

The customization chapters later in this guide add to both through the same compute macros used by every provisioner, so no step is xCAT-specific: a package step appends a name to the pkglist, a configuration step appends a command to the postscript. Both files are created fresh here, so working through the guide yields the same result each time.

The postscript's commands append to and edit node files directly, written for a single run on a freshly installed node. Re-applying it to an already-configured node – with `updatenode -P`, or by enabling `runbootscripts` – repeats those edits, so review the assembled script (see the deploy chapter) before using it that way.

```
# Locations of the staged package list and configuration postscript
OHPC_OTHERPKGS=/install/custom/install/almalinux/ohpc.otherpkgs.pkglist
OHPC_POSTSCRIPT=/install/postscripts/ohpc-config
export OHPC_OTHERPKGS OHPC_POSTSCRIPT

# OpenHPC packages to install on the compute nodes
mkdir -p "$(dirname "${OHPC_OTHERPKGS}")"
cat > "${OHPC_OTHERPKGS}" << 'EOF'
ohpc-base-compute
ohpc-slurm-client
chrony
nfs-utils
EOF
# Module tool, the same one as on the head node (see input.local)
echo "${modules_package:-lmod-ohpc}" >> "${OHPC_OTHERPKGS}"

# OpenHPC (base + updates), EPEL, and CRB repositories that provide the packages
# above. The base OS repositories are served from the head node's /install tree
# automatically. EPEL is the tree for the image's EL minor release (e.g. 10.2),
# the one epel-release selects on the head node.
epel_release=${xcat_osver##*[a-z]}
chdef -t osimage ${xcat_osimage} \
    otherpkglist="${OHPC_OTHERPKGS}" \
    otherpkgdir="http://repos.openhpc.community/OpenHPC/4/EL_10/,\
http://repos.openhpc.community/OpenHPC/4/updates/EL_10/,\
https://download.fedoraproject.org/pub/epel/${epel_release}/Everything/x86_64/,\
https://repo.almalinux.org/almalinux/10/CRB/x86_64/os/"

# Create the compute configuration postscript; the "Configure OpenHPC on the
# Compute Nodes" step below and the customization chapters append to it.
cat > "${OHPC_POSTSCRIPT}" << 'EOF'
#!/bin/sh
# OpenHPC compute configuration -- generated by the install recipe, run by xCAT.
EOF
chmod 0755 "${OHPC_POSTSCRIPT}"

# Run the postscript on every compute node at provisioning (after the default
# otherpkgs postbootscript, so the packages it configures are present).
chdef compute -p postbootscripts=ohpc-config
```

```
# Apply the IPoIB nic* attributes after the postscript above has installed the
# InfiniBand packages; until then the IPoIB interface does not exist.
chdef compute -p postbootscripts=confignetwork

# confignetwork reuses the IPoIB connection the OS installer created, which does
# not start at boot, and leaves it that way; turn autoconnect on so IPoIB comes
# back after a reboot. (Workaround until xCAT's configib sets it.)
cat > /install/postscripts/ohpc-ipoib-autoconnect << EOF
#!/bin/sh
nmcli connection modify ${ipoib_dev} connection.autoconnect yes
EOF
chmod 0755 /install/postscripts/ohpc-ipoib-autoconnect
chdef compute -p postbootscripts=ohpc-ipoib-autoconnect
```

The head node exports `/home` and `/opt/ohpc/pub`; disable the xCAT-managed `/tftpboot` and `/install` export entries so they do not conflict:

```
sed -i "s|/tftpboot|#/tftpboot|" /etc/exports
sed -i "s|/install|#/install|"   /etc/exports
exportfs -a
```

5.11 Configure OpenHPC on the Compute Nodes

Apply the baseline compute-node configuration: disable the firewall, point chrony at the head node, add the NFS client mounts, and enable the cluster services. The service enables come last – a stateful node runs this configuration after boot with no further restart, so the settings must be in place before the services start. The scheduler's own configuration follows in the next section.

```
# Disable the firewall on the compute nodes
echo "systemctl disable --now firewalld.service" \
  >> "$OHPC_POSTSCRIPT"

# Point time synchronization at the head node
echo "echo server ${sms_ip} iburst >> /etc/chrony.conf" \
  >> "$OHPC_POSTSCRIPT"

# NFS client mounts of /home and the OpenHPC public tree
echo "echo ${sms_ip}:/home /home nfs nfsvers=4,nodev,nosuid >> /etc/fstab" \
  >> "$OHPC_POSTSCRIPT"
echo "echo ${sms_ip}:/opt/ohpc/pub /opt/ohpc/pub nfs nfsvers=4,nodev >> /etc/fstab" \
  >> "$OHPC_POSTSCRIPT"
echo "mkdir -p /opt/ohpc/pub" \
  >> "$OHPC_POSTSCRIPT"
echo "mount -a" \
  >> "$OHPC_POSTSCRIPT"

# Enable the cluster services
echo "systemctl enable --now munge.service" \
  >> "$OHPC_POSTSCRIPT"
echo "systemctl enable --now chronyd.service" \
  >> "$OHPC_POSTSCRIPT"
```

5.12 Configure Slurm on the Compute Nodes

Point each compute node's `slurmd` at the head node (configless mode) and enable it. The setting is written before the service is enabled, so a stateful node that applies this after boot starts `slurmd` with it already in place.

```
# Register the Slurm server with the computes (configless mode)
echo "echo SLURMD_OPTIONS=--conf-server ${sms_ip} > /etc/sysconfig/slurmd" \
  >> "$OHPC_POSTSCRIPT"
echo "systemctl enable --now slurmd.service" \
  >> "$OHPC_POSTSCRIPT"
```

6 Additional Customization

This chapter highlights common additional customizations that can *optionally* be applied to the local cluster environment. Details on the steps required for each of these customizations are discussed further in the following sections.

6.1 Enable InfiniBand drivers

If your compute resources support InfiniBand, the following commands add OFED and PSM support using base distro-provided drivers to the compute image.

```
# Add IB support and enable
echo "dnf -y groupinstall 'InfiniBand Support'" \
  >> "$OHPC_POSTSCRIPT"
```

6.2 Enable RoCE drivers

If your compute resources support RoCE, the following commands add the same RDMA stack to the compute image. If you enabled InfiniBand drivers above, the stack is already there and the script skips the install.

```
# Add RDMA support
echo "dnf -y groupinstall 'InfiniBand Support'" \
  >> "$OHPC_POSTSCRIPT"
```

To run MPI over RoCE, select the RDMA device and port for UCX, for example `UCX_NET_DEVICES=mlx5_1:1`; `rdma link` lists each RDMA device with its network interface.

6.3 Enable Omni-Path drivers

If your compute resources support Omni-Path, the following commands add OPA support using base distro-provided drivers to the compute image.

```
# Add OPA support and enable
printf '%s\n' opa-basic-tools \
  >> "$OHPC_OTHERPKGS"
printf '%s\n' libpsm2 \
  >> "$OHPC_OTHERPKGS"
```

6.4 Increase locked memory limits

In order to utilize InfiniBand or Omni-Path as the underlying high speed interconnect, it is generally necessary to increase the locked memory settings for system users. This can be accomplished by adding the `/etc/security/limits.d/40-ohpc-limits.conf` file and this should be performed on all job submission hosts. In this recipe, jobs are submitted from the *head node*, and the following commands can be used to update the maximum locked memory settings on both the *head node* and compute nodes:

```
# Update memlock settings on head node
echo '* soft memlock unlimited' >> \
  /etc/security/limits.d/40-ohpc-limits.conf
echo '* hard memlock unlimited' >> \
  /etc/security/limits.d/40-ohpc-limits.conf

# Update memlock settings on compute
echo "echo '* soft memlock unlimited' >> \
'/etc/security/limits.d/40-ohpc-limits.conf'" >> "$OHPC_POSTSCRIPT"
echo "echo '* hard memlock unlimited' >> \
'/etc/security/limits.d/40-ohpc-limits.conf'" >> "$OHPC_POSTSCRIPT"
```

6.5 Enable ssh control via resource manager

An additional optional customization that is recommended is to restrict `ssh` access on compute nodes to only allow access by users who have an active job associated with the node. This can be enabled via the use of a pluggable authentication module (PAM) provided as part of the Slurm package installs. To enable this feature on *compute* nodes, issue the following:

```
echo "echo 'account    required     pam_slurm.so' >> \
'/etc/pam.d/sshd'" >> "$OHPC_POSTSCRIPT"
```

6.6 NVIDIA GPU Drivers

To add the optional NVIDIA GPU driver to the compute nodes, an additional external dnf repository provided by NVIDIA must be configured. Once the repository is configured, the GPU driver needs to be installed on the compute image and the corresponding toolkit installed on the head node.

OpenHPC provides a convenience package to enable the NVIDIA repository locally along with compatibility packages that integrate the NVIDIA HPC SDK within the standard OpenHPC user environment.

Tip

Note: The driver is NVIDIA's open GPU kernel module (`kmod-nvidia-open-dkms`), the only kernel module in NVIDIA's EL10 repository. It supports GPUs of the Turing architecture and newer.

```
# Add NVIDIA GPU driver repository to the head node
dnf -y install cuda-repo-ohpc

# Add NVIDIA GPU driver repository to the compute nodes
printf '%s\n' cuda-repo-ohpc \
  >> "$OHPC_OTHERPKGS"

# Install the GPU driver on the compute nodes
printf '%s\n' nvidia-driver-cuda kmod-nvidia-open-dkms \
  >> "$OHPC_OTHERPKGS"

# Build the driver for the image's kernel (DKMS otherwise targets the running kernel)
echo "dkms autoinstall -k \$(ls /lib/modules | sort -V | tail -n 1)" \
  >> "$OHPC_POSTSCRIPT"

# Enable DKMS service to automatically rebuild driver
echo "systemctl enable --now dkms.service" \
  >> "$OHPC_POSTSCRIPT"

# Install the toolkit on the head node
dnf -y install cuda-devel-ohpc
```

6.7 AMD GPU Drivers

AMD Instinct GPUs use the `amdgpu` kernel driver included in the AlmaLinux kernel, so no additional kernel module is needed. The compute image does need the GPU firmware (`amd-gpu-firmware`, from the distribution's AppStream repository); without it, `amdgpu` cannot initialize the GPUs. The ROCm runtime and tools come from EPEL: the runtime on the compute nodes, and the HIP development tools on the head node for building applications. EPEL's HIP runtime package requires the HIP compiler, so the compute image also gains the ROCm compiler toolchain; together these packages add about 900 MB to the image.

The distribution's udev rules give all users access to the GPU devices (`/dev/kfd` and `/dev/dri/renderD*`), so users need no additional group membership to run GPU jobs.

```
# Install the GPU firmware and the ROCm runtime on the compute nodes
printf '%s\n' amd-gpu-firmware rocm-hip rocminfo rocm-smi \
  >> "$OHPC_OTHERPKGS"

# Install the ROCm HIP development tools on the head node
dnf -y install rocm-hip-devel hipcc rocminfo
```

Tip

Tip: Once the compute nodes boot, `rocminfo` on a compute node lists each GPU as an agent (e.g. `gfx908` for an Instinct MI100), and `rocm-smi` shows their temperature, power and utilization.

When the head node has no GPU, `hipcc` cannot detect the target and builds for a default architecture that may not run on the compute nodes' GPUs. Name the GPU architecture and link the HIP runtime explicitly, e.g. `hipcc --offload-arch=gfx908 -o app app.hip -lamdhip64` for an Instinct MI100.

6.8 Enable System Log Forwarding

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 compute node's memory footprint if it is stateless. The following commands highlight the steps necessary to configure compute nodes to forward their logs to the head node, and to allow the head node to accept these log requests.

```
# Configure head node to receive messages and reload rsyslog configuration
echo 'module(load="imudp")' >> /etc/rsyslog.d/ohpc.conf
echo 'input(type="imudp" port="514")' >> /etc/rsyslog.d/ohpc.conf
systemctl restart rsyslog.service

# Define compute node forwarding destination
echo "echo '*.* @${sms_ip}:514' > /etc/rsyslog.d/ohpc-forward.conf" \
  >> "$OHPC_POSTSCRIPT"

# Disable most local logging on computes.
# Emergency and boot logs will remain on the compute nodes
echo "sed -i 's/^\*\.info/#\*\.info/' \
'/etc/rsyslog.conf'" >> "$OHPC_POSTSCRIPT"
echo "sed -i 's/^authpriv/#authpriv/' \
'/etc/rsyslog.conf'" >> "$OHPC_POSTSCRIPT"
echo "sed -i 's/^mail/#mail/' \
'/etc/rsyslog.conf'" >> "$OHPC_POSTSCRIPT"
echo "sed -i 's/^cron/#cron/' \
'/etc/rsyslog.conf'" >> "$OHPC_POSTSCRIPT"
echo "sed -i 's/^uucp/#uucp/' \
'/etc/rsyslog.conf'" >> "$OHPC_POSTSCRIPT"

# Let the compute nodes pick up the new configuration
echo "systemctl restart rsyslog.service" \
  >> "$OHPC_POSTSCRIPT"
```

6.9 Intel oneAPI Compiler Runtime

If planning to install the Intel® oneAPI compiler runtime (see Optional Development Tool Builds), register the following additional path (`/opt/intel`) to share with computes:

```
# (Optional) Setup NFS mount for /opt/intel if planning to install oneAPI packages
mkdir -v /opt/intel
echo "/opt/intel *(ro,no_subtree_check,fsid=12)" >> /etc/exports
echo "echo '${sms_ip}:/opt/intel /opt/intel nfs nfsvers=4,nodev 0 0' >> \
'/etc/fstab'" >> "$OHPC_POSTSCRIPT"
```

6.10 Cluster Admin Tools

6.10.1 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
dnf -y install clustershell

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

6.10.2 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
dnf -y install genders-ohpc

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

6.10.3 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
dnf -y install conman-ohpc

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

# Enable and start conman
systemctl enable conman.service
systemctl start conman.service
```

6.10.4 Add NHC

Resource managers often 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 head and compute nodes
dnf -y install nhc-ohpc
printf '%s\n' nhc-ohpc \
  >> "$OHPC_OTHERPKGS"
```

```
# Register as SLURM's health check program
echo "HealthCheckProgram=/usr/sbin/nhc" >> /etc/slurm/slurm.conf

# execute every five minutes
echo "HealthCheckInterval=300" >> /etc/slurm/slurm.conf
```

6.11 Add Magpie

Magpie contains a number of scripts to aid in running a variety of big data software frameworks within HPC queuing environments. Examples include Hadoop, Spark, Hbase, Storm, Pig, Mahout, Phoenix, Kafka, Zeppelin, and Zookeeper. Consult the online repository for more information on using these scripts; basic installation is outlined as follows:

```
# Install magpie
dnf -y install magpie-ohpc
```

6.12 Charliecloud

Typical Charliecloud workflows are based around Docker containers, but it is not strictly necessary to install Docker itself on the HPC resource. A common pattern is to build the Docker container on a laptop or VM and upload the result to the cluster for use with Charliecloud. More information can be found at https://hpc.github.io/charliecloud/

7 Deploy Cluster

7.1 Start Slurm

In an earlier section, the Slurm resource manager was installed and configured for use on both the *head node* and *compute* node instances. With the cluster nodes up and functional, we can now startup the resource manager services in preparation for running user jobs.

```
# Start munge and slurm controller on head node
systemctl enable --now munge.service
systemctl enable --now slurmctld.service
```

Running systems may need to restart `slurmctld` to pickup any changes.

7.2 Provision the Compute Nodes

Everything the compute nodes need was staged on the head node during the provisioner chapter: the install image, the OpenHPC package list (`otherpkglist`/`otherpkgdir`), and the `ohpc-config` postscript. Provisioning now applies all of it in a single pass – associate the install image with the *compute* group and boot the nodes, and xCAT installs the base OS onto local disk, installs the OpenHPC packages from the staged repositories, runs the configuration postscript, and reboots each node into a ready state.

The OpenHPC packages are pulled from the OpenHPC, EPEL, and CRB repositories named by `otherpkgdir`, so the nodes must be able to reach them during the install. By default xCAT points the compute default route at the head node; ensure this provides a path to those repositories (for example via NAT on the head node or a site gateway registered in the xCAT `networks` table), or host a local mirror on the head node and name it in `otherpkgdir` instead.

The `${OHPC_POSTSCRIPT}` configuration script is now complete: the provisioner chapter created it and the customization chapters appended to it. Review it before provisioning – it is a plain shell script, and this is the point to confirm it holds what you expect (its commands are appended in order and are not de-duplicated, so if you re-ran earlier steps, check for repeated lines):

```
# Associate provisioning image for compute group
nodeset compute osimage=${xcat_osimage}
```

Before power cycling, mark the OS that is currently running, if any. `/run` is a tmpfs, so the marker cannot survive a reboot. The wait further below refuses any node that still carries it, which stops a slow BMC reset from letting the system that is about to be replaced satisfy the check when nodes are being reinstalled rather than installed for the first time.

```
# Set compute group to boot from network on next boot
rsetboot compute net

# Boot compute nodes (power on if off, reset if on; `reset` skips nodes that are off)
rpower compute boot
```

`rsetboot compute net` applies to the next boot only, and the boot into the installer uses it up. When the installation finishes, a node whose firmware prefers the network would boot from the network again instead of starting the new system. Once every compute node reports the `installing` status, set the next boot to the local disk:

```
# Every compute node should report status=installing
lsdef compute -i status -c

# Boot from the local disk when the installation finishes
rsetboot compute hd
```

Without a BMC, the site's reset handler must also leave the nodes booting from their disk.

The stateful installation typically completes in 5 to 10 minutes, depending on BIOS post times and disk speed. Monitor provisioning with the `rcons` command, which displays the serial console for a selected node;

the escape sequence to exit `rcons` is `Ctrl-e c .` typed sequentially. Deployment progress can also be queried with `nodestat compute`, which reports the installation state of each node until an `sshd` response indicates the node is up.

Wait until every compute node has completed the installation and finished booting before proceeding. `sshd` starts before the rest of the boot completes, so waiting only for it lets the configuration steps below run against a node that still refuses logins and has not finished starting systemd. The loop below therefore requires every node to positively report a finished boot *and* to have lost the pre-reset marker, so that neither an unreachable node nor one still running the previous OS counts as ready. It gives up after `${install_timeout}` seconds (two hours by default) rather than waiting forever on an installation that failed:

Once installed, verify access with a parallel command across the compute nodes using `xdsh`, xCAT's native distributed shell:

```
xdsh compute uptime
c1:  12:56:50 up  4 min,  0 users,  load average: 0.00, 0.01, 0.04
c2:  12:56:50 up  3 min,  0 users,  load average: 0.00, 0.02, 0.05
```

7.3 Check Slurm on the Compute Nodes

Once provisioning is complete every compute node has installed the base OS and OpenHPC, run the configuration postscript, and started `munge` and `slurmd`. Check the nodes with `sinfo`; all should report *idle* (without an asterisk). If a node is shown as *unknown*, `scontrol update partition=normal state=idle` will clear it.

8 Install OpenHPC Development Components

The install procedure outlined in Install OpenHPC Components highlighted the steps necessary to install a *head node*, 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.

8.1 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
dnf -y install ohpc-autotools
dnf -y install EasyBuild-ohpc
dnf -y install hwloc-ohpc
dnf -y install spack-ohpc
dnf -y install valgrind-ohpc
```

8.2 Compilers

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

```
dnf -y install gnu16-compilers-ohpc
```

8.3 MPI Stacks

For MPI development and runtime support, OpenHPC provides pre-packaged builds for a variety of MPI families and transport layers. Currently available options and their applicability to various network transports are summarized in the Available MPI variants table below. The command that follows installs a starting set of MPI families that are compatible with both ethernet and high-speed fabrics.

Table: Available MPI variants

	Ethernet (TCP)	InfiniBand	Intel Omni-Path
MPICH (ofi)	✓	✓	✓
MPICH (ucx)	✓	✓	✓
MVAPICH2		✓	
MVAPICH2 (psm2)			✓
OpenMPI (ofi/ucx)	✓	✓	✓

```
dnf -y install openmpi5-pmix-gnu16-ohpc mpich-ofi-gnu16-ohpc
```

Note that the MPICH and OpenMPI builds support two related transport layers for a variety of underlying fabrics: UCX (Unified Communication X) and OFI (OpenFabrics interfaces). In the case of OpenMPI, a monolithic build is provided which supports both transports and end-users can customize their runtime preferences with environment variables. For MPICH, two separate builds are provided and the example above highlighted installing the `ofi` variant. However, the packaging is designed such that both versions can be installed simultaneously and users can switch between the two via normal module command semantics. Alternatively, a site can choose to install the `ucx` variant instead as a drop-in MPICH replacement:

```
dnf -y install mpich-ucx-gnu16-ohpc
```

In the case where both MPICH variants are installed, two modules will be visible in the end-user environment and an example of this configuration is highlighted is below.

```
module avail mpich

-------------------- /opt/ohpc/pub/moduledeps/gnu16---------------------
   mpich/3.4.3-ofi    mpich/3.4.3-ucx (D)
```

If your system includes InfiniBand and you enabled underlying support in InfiniBand support and Enable Infiniband Drivers, an additional MVAPICH2 family is available for use:

```
dnf -y install mvapich2-gnu16-ohpc
```

Alternatively, if your system includes Intel Omni-Path, use the (`psm2`) variant of MVAPICH2 instead:

```
dnf -y install mvapich2-psm2-gnu16-ohpc
```

8.4 Performance Tools

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

```
# Install perf-tools meta-package
dnf -y install ohpc-gnu16-perf-tools
```

8.5 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.

```
dnf -y install modules-defaults-gnu16-openmpi5-ohpc
```

Tip

If you want to change the default environment from the suggestion above, OpenHPC also provides the GNU compiler toolchain with the MPICH and MVAPICH2 stacks:

- modules-defaults-gnu16-mpich-ofi-ohpc
- modules-defaults-gnu16-mpich-ucx-ohpc
- modules-defaults-gnu16-mvapich2-ohpc

8.6 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 MPI Stacks.

```
dnf search petsc-gnu16 ohpc
Loaded plugins: fastestmirror
Loading mirror speeds from cached hostfile
============================ N/S matched: petsc-gnu16, ohpc ============================
petsc-gnu16-impi-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Computation
petsc-gnu16-mpich-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Computation
petsc-gnu16-mvapich2-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Comp...
petsc-gnu16-openmpi5-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Comp...
```

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 an earlier section, so the packages will be immediately available for use on the cluster after installation on the **head node**.

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 the Package Manifest appendix 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
dnf -y install ohpc-gnu16-serial-libs
dnf -y install ohpc-gnu16-io-libs
dnf -y install ohpc-gnu16-python-libs
dnf -y install ohpc-gnu16-runtimes
```

```
# Install parallel lib meta-packages for all available MPI toolchains
dnf -y install ohpc-gnu16-mpich-parallel-libs
dnf -y install ohpc-gnu16-openmpi5-parallel-libs
```

8.7 Optional Development Tool Builds

In addition to the 3rd party development libraries built using the open source toolchains mentioned in an earlier section, OpenHPC also provides **optional** compatible builds for use with the compilers and MPI stack included in newer versions of the Intel(R) oneAPI HPC Toolkit (using the **classic** compiler variants). These packages provide a similar hierarchical user environment experience as other compiler and MPI families present in OpenHPC.

To take advantage of the available builds, OpenHPC provides a convenience package to enable the oneAPI repository locally along with compatibility packages that integrate oneAPI-generated compiler and MPI modulefiles within the standard OpenHPC user environment. To enable the Intel(R) oneAPI repository and install minimum compiler and MPI requirements for OpenHPC packaging, issue the following:

```
# Enable Intel oneAPI and install OpenHPC compatibility packages
dnf -y install intel-oneapi-toolkit-release-ohpc
rpm --import \
    https://yum.repos.intel.com/intel-gpg-keys/GPG-PUB-KEY-INTEL-SW-PRODUCTS.PUB
dnf -y install intel-compilers-devel-ohpc
dnf -y install intel-mpi-devel-ohpc
```

Tip

As noted in an earlier section, the default installation path for OpenHPC (`/opt/ohpc/pub`) is exported over NFS from the **head node** to the compute nodes, but the Intel(R) oneAPI HPC Toolkit packages install to a top-level path of `/opt/intel`. To make the Intel(R) compilers available to the compute nodes one must add an additional NFS export for `/opt/intel` that is mounted on desired compute nodes.

To enable all 3rd party builds available in OpenHPC that are compatible with the Intel(R) oneAPI classic compiler suite, issue the following:

```
# Optionally, choose the Omni-Path enabled build for MVAPICH2.
# Otherwise, skip to retain IB variant
dnf -y install mvapich2-psm2-intel-ohpc
```

```
# Install 3rd party libraries/tools meta-packages built with Intel toolchain
dnf -y install openmpi5-pmix-intel-ohpc
dnf -y install ohpc-intel-serial-libs
dnf -y install ohpc-intel-io-libs
dnf -y install ohpc-intel-perf-tools
dnf -y install ohpc-intel-python3-libs
dnf -y install ohpc-intel-mpich-parallel-libs
dnf -y install ohpc-intel-mvapich2-parallel-libs
dnf -y install ohpc-intel-openmpi5-parallel-libs
dnf -y install ohpc-intel-impi-parallel-libs
```

9 Post Provisioning

9.1 Check Cluster Status

After this, check status of the nodes within Slurm by using the `sinfo` command. All compute nodes should be in an *idle* state (without asterisk). If the state is reported as *unknown*, the following might help:

```
scontrol update partition=normal state=idle
```

In case of additional Slurm issues, ensure that the configuration file fits your hardware and that it is identical across the nodes. Also, verify that the Slurm user id is the same on the head node and *compute* nodes. You may also consult Slurm Troubleshooting Guide.

9.2 Add User

Add a new user to the cluster. Distribute the updated credentials to compute nodes using `updatenode`:

```
useradd -m test

# Push updated credentials to compute nodes
updatenode compute -F
```

9.3 Update NHC

Generate NHC configuration file based on compute node environment

```
pdsh -w c1 "/usr/sbin/nhc-genconf -H '*' -c -" | dshbak -c
```

10 Test Cluster

We now run some simple tests on the cluster to ensure it is operational.

10.1 Run a Test Job

With the resource manager enabled for production usage, users should now be able to run jobs. To demonstrate this, the "test" user added in the Post Provisioning section can be used to run an example job.

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.

10.2 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 `prun` for parallel job launch which summarizes the underlying native job launch mechanism being used):

```
# Switch to "test" user
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 ~]$ salloc -n 8 -N 2

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

[prun] Master compute host = c1
[prun] Resource manager = slurm
[prun] Launch cmd = mpiexec.hydra -bootstrap slurm ./a.out

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

Tip

The following table provides approximate command equivalences between SLURM and OpenPBS:

Command	OpenPBS	SLURM
Submit *batch* job	qsub [job script]	sbatch [job script]
Request *interactive* shell	qsub -I /bin/bash	salloc
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]

10.3 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/slurm/job.mpi .

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

#SBATCH -J test              # Job name
#SBATCH -o job.%j.out        # Name of stdout output file (%j expands to %jobId)
#SBATCH -N 2                 # Total number of nodes requested
#SBATCH -n 16                # Total number of mpi tasks #requested
#SBATCH -t 01:30:00          # Run time (hh:mm:ss) - 1.5 hours

# Launch MPI-based executable

prun ./a.out

# Submit job for batch execution
[test@sms ~]$ sbatch job.mpi
Submitted batch job 339
```

Tip

The use of the `%j` option in the example batch job script shown is a convenient way to track application output on an individual job basis. The `%j` token is replaced with the Slurm job allocation number once assigned (job #339 in this example).

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 the Inputs section. 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 **head node** 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

```
dnf -y install docs-ohpc
```

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

```
cp /opt/ohpc/pub/doc/recipes/almalinux10/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.

```
cp -p /opt/ohpc/pub/doc/recipes/almalinux10/x86_64/xcat_stateful/slurm/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.

```
export OHPC_INPUT_LOCAL=./input.local
./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 v4, you will first need to update your local OpenHPC repository configuration to point against the v4 release (or update your locally hosted mirror). Refer to an earlier section for more details on enabling the latest repository. In contrast, when upgrading between micro releases on the same branch (e.g. from v4 to 4.2), 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 the head node and in the compute environment). 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. The compute-side command depends on how the cluster was provisioned. The helper functions defined while installing are not available in a later shell, so the commands are spelled out in full here.

```
dnf clean expire-cache
```

For a stateful cluster, act on the running compute nodes:

```
xdsh compute dnf clean expire-cache
```

For a stateless cluster, act on the image chroot, re-deriving its location:

```
# Read the image the compute nodes were provisioned with
xcat_osimage=${xcat_osimage:-$(lsdef compute -i provmethod | \
    awk -F= '/provmethod=/{print $2; exit}')}
rootimgdir=$(lsdef -t osimage -o ${xcat_osimage} -i rootimgdir \
    | awk -F= '/rootimgdir=/{print $2}')
CHROOT=${rootimgdir}/rootimg
dnf --installroot="${CHROOT}" clean expire-cache
```

2. Upgrade head node

```
dnf -y upgrade "*-ohpc"

# Any new Base OS provided dependencies can be installed by
# updating the ohpc-base metapackage
dnf -y upgrade "ohpc-base"
```

3. Upgrade packages in the compute environment

   For a stateful cluster, upgrade the running compute nodes. Note that to update running services such as a resource manager, a service restart is required on the compute nodes.

```
xdsh compute dnf -y upgrade "*-ohpc"

# Any new compute-node Base OS provided dependencies can be installed by
# updating the ohpc-base-compute metapackage
xdsh compute dnf -y upgrade "ohpc-base-compute"
```

For a stateless cluster, upgrade the image chroot, re-deriving its location if it is not already set in the current shell:

```
# Read the image the compute nodes were provisioned with
xcat_osimage=${xcat_osimage:-$(lsdef compute -i provmethod | \
    awk -F= '/provmethod=/{print $2; exit}')}
rootimgdir=$(lsdef -t osimage -o ${xcat_osimage} -i rootimgdir \
    | awk -F= '/rootimgdir=/{print $2}')
CHROOT=${rootimgdir}/rootimg

dnf -y --installroot="${CHROOT}" upgrade "*-ohpc"

# Any new compute-node Base OS provided dependencies can be installed by
# updating the ohpc-base-compute metapackage
dnf -y --installroot="${CHROOT}" upgrade "ohpc-base-compute"
```

4. Rebuild and redeploy the stateless image

   This step applies to stateless provisioning only. In stateful mode the upgrade above already ran on the compute nodes and there is no image to rebuild. Reboot the compute nodes when convenient to pick up the new image.

```
rm -f ${CHROOT}/etc/munge/munge.key
packimage --nosyncfiles ${xcat_osimage}
nodeset compute osimage=${xcat_osimage}
```

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.

```
dnf -y 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 SLURM 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. By default, the test suite will endeavor to run tests for multiple MPI stacks where applicable. To restrict tests to only a subset of MPI families, use the `--with-mpi-families` option (e.g. `--with-mpi-families="openmpi4"`). Example output is shown below (some output is omitted for the sake of brevity).

```
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-2.0.0

Build user................... : ohpc-test
Build host................... : sms001
Configure date............... : 2020-10-05 08:22
Build architecture........... : x86_64
Compiler Families............ : gnu9
MPI Families................. : mpich mvapich2 openmpi4
Python Families.............. : python3
Resource manager ............ : SLURM
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 2.0.0
============================================================================
# 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 (SLURM/gnu9/mpich)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (SLURM/gnu9/mpich)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (SLURM/gnu9/mpich)
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (SLURM/gnu9/mvapich2)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (SLURM/gnu9/mvapich2)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (SLURM/gnu9/...
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (SLURM/gnu9/openmpi4)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (SLURM/gnu9/openmpi4)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (SLURM/gnu9/...
PASS rm_execution (exit status: 0)
```

D Customization

D.1 Adding local environment modules to OpenHPC hierarchy

Administrators may wish to add locally built software packages to the OpenHPC module hierarchy. This can be accomplished by creating module files in the appropriate locations under `/opt/ohpc/pub/moduledeps` or `/opt/ohpc/pub/modulefiles`. 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 `module` command should pick them up automatically. The example output below is from Lmod; Environment Modules lists the same modules in its own format.

```
# Create a simple example module
mkdir /opt/ohpc/pub/modulefiles/example1
cp /opt/ohpc/pub/examples/example.modulefile \
    /opt/ohpc/pub/modulefiles/example1/1.0

# Create an example module with a dependency
mkdir /opt/ohpc/pub/moduledeps/gnu7-openmpi3/example2
cp /opt/ohpc/pub/examples/example-mpi-dependent.modulefile \
    /opt/ohpc/pub/moduledeps/gnu7-openmpi3/example2/1.0

# Show modules
module avail
```

Example Output

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

--------------------------- /opt/ohpc/pub/moduledeps/gnu7 ---------------------------
   R/3.4.2        metis/5.1.0     ocr/1.0.1              pdtoolkit/3.24
   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
   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

OpenHPC packages can be rebuilt from source using the source RPMs available from the OpenHPC repository. This allows administrators to customize package builds for their specific needs. One way to accomplish this is to install the appropriate source RPM, modify the spec file as needed, and rebuild to obtain an updated binary RPM. OpenHPC spec files contain macros to facilitate local customizations of compiler, compilation flags and MPI family. A brief example using the FFTW library is highlighted below. Note that the source RPMs can be downloaded from the community repository server at http://repos.openhpc.community via a web browser or directly via dnf as highlighted below. In this example we make an explicit change to FFTW's configuration, as well as modifying the CFLAGS environment variable. The package is also tagged with an additional delimiter to allow easy co-installation and use.

```
# Install rpm-build package and dnf tools from base OS distro
sudo dnf -y install rpm-build dnf-plugins-core

# Install FFTW's build dependencies
sudo dnf builddep fftw-gnu16-openmpi5-ohpc

# Download SRPM from OpenHPC repository and install locally
dnf download --source fftw-gnu16-openmpi5-ohpc
rpm -i ./fftw-gnu16-openmpi5-ohpc-*.rpm

# Modify spec file as desired
cd ~/rpmbuild/SPECS
sed -i "s/enable-static=no/enable-static=yes/" fftw.spec

# Increment RPM release so the package manager will see an update
sed -i "s/Release:   400.ohpc.3.1/Release:   400.ohpc.3.2/" fftw.spec

# Rebuild binary RPM. Note that additional directives can be specified to modify build
rpmbuild -bb --define "OHPC_CFLAGS '-O3 -mtune=native'" \
        --define "OHPC_CUSTOM_DELIM static" fftw.spec

# Install the new package
sudo dnf -y install \
        ../RPMS/$(uname -m)/fftw-gnu16-openmpi5-static-ohpc-*.$(uname -m).rpm
```

The new module file now appears along side the default.

```
$ module -t spider fftw
fftw/3.3.10-static
fftw/3.3.10
```

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 the table below.

E.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-flux-client	Collection of client packages for Flux.
ohpc-flux-server	Collection of server packages for Flux.
ohpc-gnu15-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu15-mpich-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu15-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu15-mpich-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu15-mvapich2-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu15-mvapich2-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu15-mvapich2-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu15-openmpi5-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu15-openmpi5-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu15-openmpi5-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu15-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu15-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu15-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu15-python3-libs	Collection of python3 related library builds for use with GNU compiler toolchain.
ohpc-gnu15-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu15-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.

Group Name	Description
ohpc-gnu16-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu16-mpich-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu16-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu16-mpich-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu16-mvapich2-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu16-mvapich2-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu16-mvapich2-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu16-openmpi5-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu16-openmpi5-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu16-openmpi5-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu16-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu16-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu16-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu16-python3-libs	Collection of python3 related library builds for use with GNU compiler toolchain.
ohpc-gnu16-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu16-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.
ohpc-intel-impi-io-libs	Collection of IO library builds for use with Intel(R) oneAPI Toolkit and Intel(R) MPI runtime.
ohpc-intel-impi-parallel-libs	Collection of parallel library builds for use with Intel(R) oneAPI Toolkit and the Intel(R) MPI Library.
ohpc-intel-impi-perf-tools	Collection of performance tool builds for use with Intel(R) oneAPI Toolkit compiler toolchain and the Intel(R) MPI runtime.
ohpc-intel-io-libs	Collection of IO library builds for use with Intel(R) oneAPI Toolkit.
ohpc-intel-mpich-io-libs	Collection of IO library builds for use with Intel(R) oneAPI Toolkit and MPICH runtime.
ohpc-intel-mpich-parallel-libs	Collection of parallel library builds for use with Intel(R) oneAPI Toolkit and the MPICH runtime.
ohpc-intel-mpich-perf-tools	Collection of performance tool builds for use with Intel(R) oneAPI Toolkit compiler toolchain and the MPICH runtime.
ohpc-intel-mvapich2-io-libs	Collection of IO library builds for use with Intel(R) oneAPI Toolkit and MVAPICH2 runtime.

Group Name	Description
ohpc-intel-mvapich2-parallel-libs	Collection of parallel library builds for use with Intel(R) oneAPI Toolkit and the MVAPICH2 runtime.
ohpc-intel-mvapich2-perf-tools	Collection of performance tool builds for use with Intel(R) oneAPI Toolkit compiler toolchain and the MVAPICH2 runtime.
ohpc-intel-openmpi5-io-libs	Collection of IO library builds for use with Intel(R) oneAPI Toolkit and OpenMPI runtime.
ohpc-intel-openmpi5-parallel-libs	Collection of parallel library builds for use with Intel(R) oneAPI Toolkit and the OpenMPI runtime.
ohpc-intel-openmpi5-perf-tools	Collection of performance tool builds for use with Intel(R) oneAPI Toolkit compiler toolchain and the OpenMPI runtime.
ohpc-intel-perf-tools	Collection of performance tool builds for use with Intel(R) oneAPI Toolkit.
ohpc-intel-python3-libs	Collection of python3 related library builds for use with Intel(R) oneAPI Toolkit.
ohpc-intel-serial-libs	Collection of serial library builds for use with Intel(R) oneAPI Toolkit.
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.

E.2 RPM Packages

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 Section 3rd Party Packages. The relevant package groupings and associated references are as follows:

- Administrative Tools
- Resource Management
- Compiler Families
- MPI Families / Communication Libraries
- Development Tools
- Performance Analysis Tools
- IO Libraries
- Distro Packages
- Runtimes
- Serial/Threaded Libraries
- Parallel Libraries

E.2.1 Administrative Tools

RPM Package Name	Version	Info/URL
conman	0.3.1	ConMan: The Console Manager. http://dun.github.io/conman
docs	4.0.0	OpenHPC documentation. https://github.com/openhpc/ohpc
docs	4.2.0	OpenHPC documentation. https://github.com/openhpc/ohpc
environment-modules	5.7.0	Provides dynamic modification of a user's environment. https://envmodules.io
examples	2.0	Example source code and templates for use within OpenHPC environment. https://github.com/openhpc/ohpc
genders	1.32	Static cluster configuration database. https://github.com/chaos/genders
hpc-workspace	1.6.3	Temporary workspace management. https://github.com/holgerBerger/hpc-workspace
lmod-defaults	2.0	OpenHPC default login environments. https://github.com/openhpc/ohpc
lmod	9.4.5	Lua based Modules (lmod). https://github.com/TACC/Lmod
losf	0.56.0	A Linux operating system framework for managing HPC clusters. https://github.com/hpcsi/losf
modules-defaults	2.1	OpenHPC default login environments. https://github.com/openhpc/ohpc
nhc	1.4.3	LBNL Node Health Check. https://github.com/mej/nhc
ohpc-release	4	OpenHPC release files. https://github.com/openhpc/ohpc
pdsh	2.36	Parallel remote shell program. https://github.com/chaos/pdsh
prun	3	Convenience utility for parallel job launch. https://github.com/openhpc/ohpc
test-suite	4.2.0	Integration test suite for OpenHPC. https://github.com/openhpc/ohpc

E.2.2 Resource Management

RPM Package Name	Version	Info/URL
flux-core	0.89.0	Core components of the Flux resource manager framework. https://github.com/flux-framework/flux-core
flux	0.7.1	PMIx support for the Flux resource manager. https://github.com/flux-framework/flux-pmix
flux-sched	0.55.0	Fluxion graph-based scheduler for the Flux resource manager. https://github.com/flux-framework/flux-sched
flux-security	0.15.0	Independent security component for the Flux resource manager. https://github.com/flux-framework/flux-security

RPM Package Name	Version	Info/URL
magpie	3.2	Scripts for running Big Data software in HPC environments. https://github.com/LLNL/magpie
openpbs-client	23.06.06	OpenPBS for a client host. http://www.openpbs.org
openpbs-execution	23.06.06	OpenPBS for an execution host. http://www.openpbs.org
openpbs-server	23.06.06	OpenPBS for a server host. http://www.openpbs.org
pmix	4.2.9	An extended/exascale implementation of PMI. https://pmix.org
slurm-contribs	26.05.5	Perl tool to print Slurm job state information. https://slurm.schedmd.com
slurm-devel	26.05.5	Development package for Slurm. https://slurm.schedmd.com
slurm-example-configs	26.05.5	Example config files for Slurm. https://slurm.schedmd.com
slurm-libpmi	26.05.5	Slurm's implementation of the pmi libraries. https://slurm.schedmd.com
slurm	26.05.5	Slurm Workload Manager. https://slurm.schedmd.com
slurm-openlava	26.05.5	openlava/LSF wrappers for transition from OpenLava/LSF to Slurm. https://slurm.schedmd.com
slurm-pam_slurm	26.05.5	PAM module for restricting access to compute nodes via Slurm. https://slurm.schedmd.com
slurm-perlapi	26.05.5	Perl API to Slurm. https://slurm.schedmd.com
slurm-sackd	26.05.5	Slurm authentication daemon. https://slurm.schedmd.com
slurm-slurmctld	26.05.5	Slurm controller daemon. https://slurm.schedmd.com
slurm-slurmd	26.05.5	Slurm compute node daemon. https://slurm.schedmd.com
slurm-slurmdbd	26.05.5	Slurm database daemon. https://slurm.schedmd.com
slurm-sview	26.05.5	Graphical user interface to view and modify Slurm state. https://slurm.schedmd.com
slurm-torque	26.05.5	Torque/PBS wrappers for transition from Torque/PBS to Slurm. https://slurm.schedmd.com

E.2.3 Compiler Families

RPM Package Name	Version	Info/URL
gnu15-compilers	15.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org
gnu16-compilers	16.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org
intel-compilers-devel	2026.0	OpenHPC compatibility package for Intel(R) oneAPI HPC Toolkit. https://github.com/openhpc/ohpc
intel-oneapi-toolkit-release	2026.0	Intel(R) oneAPI HPC Toolkit Repository Setup. https://github.com/openhpc/ohpc

E.2.4 MPI Families / Communication Libraries

RPM Package Name	Version	Info/URL
intel-mpi-devel	2026.0	OpenHPC compatibility package for Intel(R) oneAPI MPI Library. https://github.com/openhpc/ohpc
mpich	5.0.1	MPICH MPI implementation. http://www.mpich.org
mvapich2	4.1	OSU MVAPICH2 MPI implementation. http://mvapich.cse.ohio-state.edu
openmpi5	5.0.10	A powerful implementation of MPI/SHMEM. http://www.open-mpi.org
ucx	1.22.0	UCX is a communication library implementing high-performance messaging. http://www.openucx.org

E.2.5 Development Tools

RPM Package Name	Version	Info/URL
EasyBuild	5.4.1	Software build and installation framework. https://easybuild.io
autoconf	2.71	A GNU tool for automatically configuring source code. http://www.gnu.org/software/autoconf
automake	1.16.5	A GNU tool for automatically creating Makefiles. http://www.gnu.org/software/automake
cmake	4.4.4	CMake is an open-source, cross-platform family of tools designed to build, test and package software. https://cmake.org
cuda-devel	25.9	OpenHPC compatibility package for cuda. https://github.com/openhpc/ohpc
cuda-repo	25.9	Cuda toolkit online repository. https://github.com/openhpc/ohpc
hwloc	2.15.0	Portable Hardware Locality. http://www.open-mpi.org/projects/hwloc
libtool	2.4.6	The GNU Portable Library Tool. http://www.gnu.org/software/libtool
python3-mpi4py	4.1.1	Python bindings for the Message Passing Interface (MPI) standard. https://github.com/mpi4py/mpi4py
python3-numpy	2.4.4	NumPy array processing for numbers, strings, records and objects. https://github.com/numpy/numpy
spack	1.2.2	HPC software package management. https://github.com/spack/spack
valgrind	3.27.1	Valgrind Memory Debugger. http://www.valgrind.org

E.2.6 Performance Analysis Tools

RPM Package Name	Version	Info/URL
dimemas	5.5.0	Dimemas tool. https://tools.bsc.es
extrae	5.0.4	Extrae tool. https://tools.bsc.es

RPM Package Name	Version	Info/URL
imb	2021.11	Intel MPI Benchmarks (IMB). https://software.intel.com/en-us/articles/intel-mpi-benchmarks
likwid	5.5.1	Performance tools for the Linux console. https://github.com/RRZE-HPC/likwid
omb	7.5.2	OSU Micro-benchmarks. https://mvapich.cse.ohio-state.edu/benchmarks
papi	7.2.0	Performance Application Programming Interface. http://icl.cs.utk.edu/papi
paraver	4.12.0	Paraver. https://tools.bsc.es
pdtoolkit	3.25.1	PDT is a framework for analyzing source code. http://www.cs.uoregon.edu/Research/pdt
scalasca	2.6.2	Toolset for performance analysis of large-scale parallel applications. http://www.scalasca.org
scorep	9.4	Scalable Performance Measurement Infrastructure for Parallel Codes. http://www.vi-hps.org/projects/score-p
tau	2.35.1	Tuning and Analysis Utilities Profiling Package. http://www.cs.uoregon.edu/research/tau/home.php

E.2.7 IO Libraries

RPM Package Name	Version	Info/URL
adios2	2.12.0	The Adaptable IO System v2 (ADIOS2). https://adios2.readthedocs.io/en/latest/index.html
cubew	4.9.1	CUBE Uniform Behavioral Encoding generic presentation writer component. http://www.scalasca.org/software/cube-4.x/download.html
hdf5	2.1.1	A general purpose library and file format for storing scientific data. http://www.hdfgroup.org/HDF5
netcdf-cxx	4.3.1	C++ Libraries for the Unidata network Common Data Form. http://www.unidata.ucar.edu/software/netcdf
netcdf-fortran	4.6.2	Fortran Libraries for the Unidata network Common Data Form. http://www.unidata.ucar.edu/software/netcdf
netcdf	4.10.0	C Libraries for the Unidata network Common Data Form. http://www.unidata.ucar.edu/software/netcdf
otf2	3.1.1	Open Trace Format 2 library. http://score-p.org
phdf5	2.1.1	A general purpose library and file format for storing scientific data (parallel version). http://www.hdfgroup.org/HDF5
pnetcdf	1.14.1	A Parallel NetCDF library (PnetCDF). http://cucis.ece.northwestern.edu/projects/PnetCDF
sionlib	1.7.7	Scalable I/O Library for Parallel Access to Task-Local Files. https://apps.fz-juelich.de/jsc/sionlib/docu/index.html

E.2.8 Distro Packages

RPM Package Name	Version	Info/URL
python3-Cython	3.3.0	The Cython compiler for writing C extensions for the Python language. http://www.cython.org

E.2.9 Runtimes

RPM Package Name	Version	Info/URL
charliecloud	0.45.2	Lightweight user-defined software stacks for high-performance computing. https://charliecloud.io

E.2.10 Serial/Threaded Libraries

RPM Package Name	Version	Info/URL
R	4.5.3	R is a language and environment for statistical computing and graphics (S-Plus like). http://www.r-project.org
cubelib	4.9.1	CUBE Uniform Behavioral Encoding generic presentation library component. http://www.scalasca.org/software/cube-4.x/download.html
gotcha	1.0.8	A library for wrapping function calls to shared libraries. https://github.com/llnl/gotcha
gsl	2.8	GNU Scientific Library (GSL). http://www.gnu.org/software/gsl
metis	5.1.0	Serial Graph Partitioning and Fill-reducing Matrix Ordering. http://glaros.dtc.umn.edu/gkhome/metis/metis/overview
opari2	2.0.9	An OpenMP runtime performance measurement instrumenter. https://www.vi-hps.org/projects/score-p
openblas	0.3.32	An optimized BLAS library based on GotoBLAS2. http://www.openblas.net
plasma	25.5.27	Parallel Linear Algebra Software for Multicore Architectures. https://github.com/icl-utk-edu/plasma
scotch	7.0.11	Graph, mesh and hypergraph partitioning library. https://gitlab.inria.fr/scotch/scotch
superlu	7.0.1	A general purpose library for the direct solution of linear equations. http://crd.lbl.gov/~xiaoye/SuperLU

E.2.11 Parallel Libraries

RPM Package Name	Version	Info/URL
boost	1.90.0	Free peer-reviewed portable C++ source libraries. http://www.boost.org
fftw	3.3.10	A Fast Fourier Transform library. http://www.fftw.org
hypre	3.1.0	Scalable algorithms for solving linear systems of equations. http://www.llnl.gov/casc/hypre

RPM Package Name	Version	Info/URL
mfem	4.9	Lightweight, general, scalable C++ library for finite element methods. http://mfem.org
mumps	5.8.2	A MUltifrontal Massively Parallel Sparse direct Solver. https://mumps-solver.org
petsc	3.25.0	Portable Extensible Toolkit for Scientific Computation. http://www.mcs.anl.gov/petsc
ptscotch	7.0.11	Graph, mesh and hypergraph partitioning library using MPI. https://gitlab.inria.fr/scotch/scotch
scalapack	2.2.3	A subset of LAPACK routines redesigned for heterogeneous computing. https://netlib.org/scalapack
slepc	3.25.0	A library for solving large scale sparse eigenvalue problems. http://slepc.upv.es
superlu_dist	9.2.1	A general purpose library for the direct solution of linear equations. https://portal.nersc.gov/project/sparse/superlu
trilinos	17.0.0	A collection of libraries of numerical algorithms. https://trilinos.org

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: 5E33 3CA3 A1BD BBC9 DF14 9D74 09AD FAE4 **D722A692**
```

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.

```
rpm --checksig -v ohpc-release-4-1.el10.x86_64.rpm
ohpc-release-4-1.el10.x86_64.rpm:
    Header V3 RSA/SHA256 Signature, key ID d722a692: OK
    Header SHA256 digest: OK
    Header SHA1 digest: OK
    Payload SHA256 digest: OK
    V3 RSA/SHA256 Signature, key ID d722a692: OK
    MD5 digest: OK
```