



OpenHPC (v3.5)

Cluster Building Recipes

openEuler 22.03 SP4 Base OS

Warewulf/OpenPBS Edition for Linux* (x86_64)



Document Last Update: 2026-06-08

Document Revision: 3add67899f534bf296d1759599fcc625ea5c05ed

Legal Notice

Copyright © 2016-2026, OpenHPC, a Linux Foundation Collaborative Project. All rights reserved.

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



Intel, the Intel logo, and other Intel marks are trademarks of Intel Corporation in the U.S. and/or other countries.

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

Contents

Legal Notice	2
1 Introduction	6
1.1 Target Audience	6
1.2 Requirements/Assumptions	6
1.3 Inputs	7
1.4 Installation Template	8
2 Install Base Operating System	8
2.1 Install OS	8
2.2 Configure HTTPS Proxy (Optional)	9
2.3 Configure Firewall	9
2.4 Add Hostname	9
2.5 Configure NTP	9
2.6 Generate SSH Key Pair	10
2.7 Setup NFS Server	10
2.8 Optionally add InfiniBand support services on <i>head node</i>	11
2.9 Optionally add Omni-Path support services on <i>head node</i>	11
3 Install OpenHPC Components	12
3.1 Enable OpenHPC Repository	12
3.2 Install OpenHPC Base Packages	13
4 Install OpenPBS	13
4.1 Add OpenPBS on Head Node	13
5 Install Warewulf Provisioner	13
5.1 Install Warewulf on <i>Head Node</i>	13
5.2 Configure Warewulf	13
5.3 Define <i>Compute</i> Image for Provisioning	14
5.3.1 Build Initial Base OS Image	14
5.4 Add OpenHPC Components	15
5.5 Customize System Configuration	15
5.6 Import Files	16

6	Additional Customization	16
6.1	Enable InfiniBand drivers	16
6.2	Enable Omni-Path drivers	16
6.3	Increase locked memory limits	17
6.4	GPU Drivers	17
6.5	Enable System Log Forwarding	18
6.6	Cluster Admin Tools	18
6.6.1	Add ClusterShell	18
6.6.2	Add genders	19
6.6.3	Add ConMan	19
6.6.4	Add NHC	19
6.7	Add Magpie	20
6.8	Charliecloud	20
7	Deploy Cluster	20
7.1	Finalize Provisioning Configuration	20
7.1.1	Assemble Bootstrap Image	20
7.1.2	Assemble VNFS Image	20
7.2	Register Compute Nodes for Provisioning	21
7.3	Start OpenPBS	21
7.4	Boot Compute Nodes	22
8	Install OpenHPC Development Components	22
8.1	Development Tools	22
8.2	Compilers	23
8.3	MPI Stacks	23
8.4	Performance Tools	24
8.5	Setup default development environment	24
8.6	3rd Party Libraries and Tools {#3rd-party-libraries-and-tools}	24
9	Post Provisioning	26
9.1	Check Cluster Status	26
9.2	Add User	26
9.3	Update NHC	26
10	Test Cluster	26
10.1	Run a Test Job	26
10.2	Interactive Execution	27
10.3	Batch execution	28

Appendices	29
A Installation Template	29
B Upgrading OpenHPC Packages	30
C Integration Test Suite	31
D Customization	34
D.1 Adding local Lmod modules to OpenHPC hierarchy	34
D.2 Rebuilding Packages from Source	35
E Package Manifest	36
E.1 Available OpenHPC Meta-packages	36
E.2 RPM Packages	38
E.2.1 Administrative Tools	39
E.2.2 Resource Management	40
E.2.3 Compiler Families	41
E.2.4 MPI Families / Communication Libraries	41
E.2.5 Development Tools	41
E.2.6 Performance Analysis Tools	42
E.2.7 IO Libraries	42
E.2.8 Distro Packages	43
E.2.9 Runtimes	43
E.2.10 Serial/Threaded Libraries	43
E.2.11 Parallel Libraries	44
F Package Signatures	45

1 Introduction

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

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

1.1 Target Audience

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

```
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 openEuler 22.03 SP4 and is subsequently configured to provision the remaining *compute nodes* with warewulf3 in a stateless 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

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

Optional variables:

- `${sysmgmt_host}` - BeeGFS System Management host name
- `${mgs_fs_name}` - Lustre MGS mount name
- `${sms_ipoib}` - IPoIB address for head node
- `${ipoib_netmask}` - Subnet netmask for internal IPoIB
- `${c_ipoib[0]}`, `${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 openEuler 22.03 SP4 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 openEuler 22.03 SP4 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, the following addition can be used to identify your head node.

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

While it is theoretically possible to enable SELinux on a cluster provisioned with warewulf3, 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.

By default all repositories use <http://repo.openeuler.org>. For better network speed it could be replaced with any of the mirrors listed [here](#).

2.3 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 || true
```

2.4 Add Hostname

Add the head node name to `/etc/hosts` so we can make API calls by hostname.

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

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
```

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
systemctl enable nfs-server
```

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 openEuler 22.03 SP4 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. OpenHPC provides a template configuration file to aid in setting up an *ib0* interface on the *head node*. To use, copy the template provided and update the `${sms_ipoib}` and `${ipoib_netmask}` entries to match local desired settings (alter *ib0* naming as appropriate if system contains dual-ported or multiple HCAs).

```
cp /opt/ohpc/pub/examples/network/centos/ifcfg-ib0 \
  /etc/sysconfig/network-scripts

# Define local IPoIB address and netmask
sed -i "s/master_ipoib/${sms_ipoib}/" \
  /etc/sysconfig/network-scripts/ifcfg-ib0
sed -i "s/ipoib_netmask/${ipoib_netmask}/" \
  /etc/sysconfig/network-scripts/ifcfg-ib0

# configure NetworkManager to *not* override local /etc/resolv.conf
echo "[main]" > /etc/NetworkManager/conf.d/90-dns-none.conf
echo "dns=none" >> /etc/NetworkManager/conf.d/90-dns-none.conf
# Start up NetworkManager to initiate ib0
systemctl start NetworkManager
```

2.9 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 openEuler 22.03 SP4 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/3/openEuler_22.03/x86_64/\
ohpc-release-3-1.oe2203.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/3.5>

3.2 Install OpenHPC Base Packages

Now OpenHPC packages can be installed. To add the base package on the head node issue the following:

```
dnf -y install ohpc-base
```

4 Install OpenPBS

4.1 Add OpenPBS on Head Node

OpenHPC provides multiple options for distributed resource management. The following command adds the OpenPBS 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.

```
# Install OpenPBS server meta-package
dnf -y install openpbs-server-ohpc
```

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

5 Install Warewulf Provisioner

5.1 Install Warewulf on *Head Node*

To add support for provisioning services, we install the Warewulf provisioning system packages. Then the main Warewulf configuration files are edited to reflect the environment.

```
# Make sure required variables are set
: "${sms_eth_internal:?ERROR: sms_eth_internal not set}"

# Install Warewulf
dnf -y install ohpc-warewulf
```

5.2 Configure Warewulf

With Warewulf installed, the next step is to update the configuration to allow Warewulf to work with openEuler 22.03 SP4 and to support local provisioning using a second private interface.

Tip

By default, Warewulf is configured to provision over the `eth1` interface. The steps below update this setting to use the interface specified by ``${sms_eth_internal}``.

```
# Configure Warewulf provisioning to use desired internal interface
sed -i "s/device = eth1/device = ${sms_eth_internal}/" \
/etc/warewulf/provision.conf

# Configure MariaDB to handle large VNFS images
sed -i "/\[mysqld\]/a max_allowed_packet=32M" /etc/my.cnf.d/mysql-server.cnf
sed -i "s/^# database chunk size.*/database chunk size = 16777216/" \
/etc/warewulf/database.conf
systemctl enable mysqld
systemctl restart mysqld

systemctl enable httpd.service
systemctl restart httpd

systemctl enable dhcpd.service
systemctl enable tftp.socket
systemctl start tftp.socket
```

5.3 Define *Compute* Image for Provisioning

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

5.3.1 Build Initial Base OS Image

The OpenHPC build of Warewulf includes specific enhancements enabling support for openEuler 22.03 SP4. The following steps illustrate the process to build a minimal, default image for use with Warewulf. We begin by defining a directory structure on the *head node* that will represent the root filesystem of the compute node. The default location for this example is `/opt/ohpc/admin/images/openeuler22.03`.

Tip

Warewulf is configured by default to access an external repository during the `wwmkchroot` process. If the head node cannot reach the public openEuler 22.03 SP4 mirrors, set the `YUM_MIRROR_BASE` environment variable to your desired mirror base URL prior to running `wwmkchroot`.

```
# Define chroot location
export CHROOT=/opt/ohpc/admin/images/openeuler22.03

# Build initial chroot image
wwmkchroot -v openeuler-22.03 $CHROOT
```

```
# Enable OpenHPC and distro repos inside chroot
dnf -y --installroot="$CHROOT" install openEuler-release
cp -p /etc/yum.repos.d/OpenHPC*.repo $CHROOT/etc/yum.repos.d
```

5.4 Add OpenHPC Components

Next, we add additional components to include resource management client services, NTP support, and other additional packages to support the default OpenHPC environment. This process augments the chroot-based install performed by `wmmkchroot` and will access the Base OS and OpenHPC repositories to resolve package install requests.

We begin by installing a few common base packages:

```
# Copy DNS configuration from head node
cp -L --remove-destination /etc/resolv.conf $CHROOT/etc/resolv.conf

# Install compute node base meta-package
dnf -y --installroot="$CHROOT" install ohpc-base-compute
```

Now, we can include additional required components to the compute instance including resource manager client, NTP, and development environment modules support.

```
# Add OpenPBS client support
dnf -y --installroot="$CHROOT" install openpbs-execution-ohpc
sed -i "s/PBS_SERVER=\S\+/PBS_SERVER=${sms_name}/" $CHROOT/etc/pbs.conf
echo "PBS_LEAF_NAME=${sms_name}" >> /etc/pbs.conf

chroot $CHROOT opt/pbs/libexec/pbs_habitat
sed -i "s/\\\$clienthost \S\+/\\\$clienthost ${sms_name}/" \
    $CHROOT/var/spool/pbs/mom_priv/config
echo "\$usecp *:/home /home" >> $CHROOT/var/spool/pbs/mom_priv/config
chroot $CHROOT systemctl enable pbs

# Add Network Time Protocol (NTP) support
dnf -y --installroot="$CHROOT" install chrony

# Identify head node as local NTP server
echo "server ${sms_ip} iburst" >> $CHROOT/etc/chrony.conf

# Add kernel drivers

dnf -y --installroot="$CHROOT" install kernel-$(uname -r)

# Include modules user environment
dnf -y --installroot="$CHROOT" install lmod-ohpc
```

5.5 Customize System Configuration

Prior to assembling the image, it is advantageous to perform additional customization within the chroot environment. The following steps add a local `ssh` key created by Warewulf to support remote access, and

enable NFS mounting of the `$HOME` file system and the public OpenHPC install path (`/opt/ohpc/pub`) hosted by the *head node*.

```
# Initialize warewulf database and ssh_keys
wwinit database
wwinit ssh_keys

# Add NFS client mounts of /home and /opt/ohpc/pub to base image
echo "${sms_ip}:/home /home nfs nfsvers=4,nodev,nosuid 0 0" \
    >> $CHROOT/etc/fstab
echo "${sms_ip}:/opt/ohpc/pub /opt/ohpc/pub nfs nfsvers=4,nodev 0 0" \
    >> $CHROOT/etc/fstab

# 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

systemctl restart nfs-server
```

5.6 Import Files

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

```
wwsh file import /etc/passwd
wwsh file import /etc/group
wwsh file import /etc/shadow
```

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
dnf -y --installroot="$CHROOT" groupinstall "InfiniBand Support"
```

6.2 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
dnf -y --installroot="$CHROOT" install opa-basic-tools
dnf -y --installroot="$CHROOT" install libpsm2
```

6.3 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 '* soft memlock unlimited' >> \
"$CHROOT/etc/security/limits.d/40-ohpc-limits.conf"
echo '* hard memlock unlimited' >> \
"$CHROOT/etc/security/limits.d/40-ohpc-limits.conf"
```

6.4 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 SMS 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.

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

# Add NVIDIA GPU driver repository to the compute nodes
dnf -y --installroot="$CHROOT" install cuda-repo-ohpc

# Install the GPU driver on the compute nodes
dnf -y --installroot="$CHROOT" install nvidia-driver:latest-dkms

# Enable DKMS service to automatically rebuild driver
chroot $CHROOT /bin/sh -c \
"systemctl enable dkms"

# Install the toolkit on the head node
dnf -y --installroot="$CHROOT" install cuda-devel-ohpc nvidia-driver-cuda
```

6.5 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

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

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

6.6 Cluster Admin Tools

6.6.1 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
```

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

6.6.3 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_compute; 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
systemctl start conman
```

6.6.4 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
dnf -y --installroot="$CHROOT" install nhc-ohpc
```

6.7 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
```

6.8 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 Finalize Provisioning Configuration

Warewulf employs a two-stage boot process: a bootstrap image initializes the process, and a Virtual Node File System (VNFS) capsule contains the full system image.

7.1.1 Assemble Bootstrap Image

The bootstrap image includes the runtime kernel and associated modules, as well as some simple scripts to complete the provisioning process.

```
# Optionally include drivers from kernel updates; add virtio drivers for VM support
export WW_CONF=/etc/warewulf/bootstrap.conf
echo "drivers += updates/kernel/" >> $WW_CONF
echo "modprobe += virtio_pci, virtio_net" >> $WW_CONF

# Build bootstrap image
wwbootstrap $(uname -r)
```

7.1.2 Assemble VNFS Image

With the local site customizations in place, the following step assembles a VNFS capsule from the chroot environment defined for the *compute* instance.

```
wwvnfs --chroot $CHROOT
```

7.2 Register Compute Nodes for Provisioning

In preparation for provisioning, we define the desired network settings for the example compute nodes and restart the `dhcp` service. Note the use of variable names for the desired compute hostnames, node IPs, and MAC addresses which should be modified to accommodate local settings and hardware.

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

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

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

```
# Define provisioning image for hosts
wwsh -y provision set "${compute_regex}" \
    --vnfs=openeuler22.03 \
    --bootstrap=$(uname -r) \
    --files=dynamic_hosts,password,group,shadow,network

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

7.3 Start OpenPBS

In an earlier section, the OpenPBS 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 PBS daemons on head node
systemctl enable pbs
systemctl start pbs
```

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

```
# Initialize PBS path
. /etc/profile.d/pbs.sh
# Enable user environment propagation (needed for modules support)
qmgr -c "set server default_qsub_arguments= -V"
# Enable uniform multi-node MPI task distribution
qmgr -c "set server resources_default.place=scatter"
# Enable support for job accounting
qmgr -c "set server job_history_enable=True"
# Register compute hosts with PBS
for ((i=0; i<num_computes; i++)); do
    qmgr -c "create node ${c_name[$i]}"
done
```

7.4 Boot Compute Nodes

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

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

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

```
pdsh -w ${compute_prefix}[1-${num_computes}] uptime
c1 05:03am up 0:02, 0 users, load average: 0.20, 0.13, 0.05
c2 05:03am up 0:02, 0 users, load average: 0.20, 0.14, 0.06
c3 05:03am up 0:02, 0 users, load average: 0.19, 0.15, 0.06
c4 05:03am up 0:02, 0 users, load average: 0.15, 0.12, 0.05
```

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 Lmod modules system in a hierarchical fashion. The modules system will conditionally present compiler-dependent software based on the toolchain currently loaded.

```
dnf -y install gnu15-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-gnu15-ohpc mpich-ofi-gnu15-ohpc
```

Note that OpenHPC 2.x introduces the use of two related transport layers for the MPICH and OpenMPI builds that support 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-gnu15-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/gnu15-----
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-gnu15-ohpc
```

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

```
dnf -y install mvapich2-psm2-gnu15-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-gnu15-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 lmod-defaults-gnu15-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:

- `lmod-defaults-gnu15-mpich-ofi-ohpc`
- `lmod-defaults-gnu15-mpich-ucx-ohpc`
- `lmod-defaults-gnu15-mvapich2-ohpc`

8.6 3rd Party Libraries and Tools {#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-gnu15 ohpc
Loaded plugins: fastestmirror
Loading mirror speeds from cached hostfile
===== N/S matched: petsc-gnu15, ohpc =====
petsc-gnu15-mpi-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Computation
petsc-gnu15-mpich-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Computation
petsc-gnu15-mvapich2-ohpc.x86_64 : Portable Extensible Toolkit for Scientific Comp...
petsc-gnu15-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-gnu15-serial-libs
dnf -y install ohpc-gnu15-io-libs
dnf -y install ohpc-gnu15-python-libs
dnf -y install ohpc-gnu15-runtimes
```

```
# Install parallel lib meta-packages for all available MPI toolchains
dnf -y install ohpc-gnu15-mpich-parallel-libs
dnf -y install ohpc-gnu15-openmpi5-parallel-libs
```

9 Post Provisioning

9.1 Check Cluster Status

After this, check status of the nodes within OpenPBS by using the `pbsnodes` command. All compute nodes should be in a *free* state. If a node is not responding, the following may help diagnose the issue:

```
pbsnodes -a
```

In case of additional OpenPBS issues, ensure that the `pbs` service is running on both the head node and compute nodes, and that the `PBS_SERVER` value in `/etc/pbs.conf` on the compute nodes matches the head node hostname.

9.2 Add User

We will now add a new user to the cluster. This will be used later to run a test job.

```
useradd -m test
```

Warewulf installs a utility on the compute nodes to automatically synchronize known files from the provisioning server at five minute intervals. With the addition of the new “test” user, we need to update the Warewulf database to incorporate the additions:

```
wwsh file resync passwd shadow group
```

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

```
pdsh -w "${compute_prefix}[1-${num_computes}]" /warewulf/bin/wwgetfiles
```

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, we will add a “test” user on the **head** node that 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 ~]$ qsub -I -l select=2:mpiprocs=4

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

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

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

Tip

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

Command	OpenPBS	SLURM
Submit <i>batch</i> job	qsub [job script]	sbatch [job script]
Request <i>interactive</i> 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/openpbs/job.mpi .

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

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

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

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

# Change to submission directory
cd $PBS_O_WORKDIR

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

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

Appendices

A Installation Template

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

Tip

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

The template script relies on the use of a simple text file to define local site variables that were outlined in 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/openEuler22.03/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/openEuler22.03/x86_64/warewulf3/openpbs/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 v3, you will first need to update your local OpenHPC repository configuration to point against the v3 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 v3 to 3.2), there is no need to adjust local package manager configurations when using the public repository as rolling updates are pre-configured.

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

```
dnf clean expire-cache
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 compute image

```
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 image(s)

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

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 OPENPBS 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 ..... : OPENPBS
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 (OPENPBS/gnu9/mpich)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (OPENPBS/gnu9/mpich)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (OPENPBS/gnu9/mpich)
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (OPENPBS/gnu9/mvapich2)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (OPENPBS/gnu9/mvapich2)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (OPENPBS/gnu9/...
PASS rm_execution (exit status: 0)
1..3
ok 1 [libs/FFTW] Serial C binary runs under resource manager (OPENPBS/gnu9/openmpi4)
ok 2 [libs/FFTW] MPI C binary runs under resource manager (OPENPBS/gnu9/openmpi4)
ok 3 [libs/FFTW] Serial Fortran binary runs under resource manager (OPENPBS/gnu9/...
PASS rm_execution (exit status: 0)

```

D Customization

D.1 Adding local Lmod 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 `lmod` application should pick them up automatically.

```
# 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-gnu15-openmpi5-ohpc

# Download SRPM from OpenHPC repository and install locally
dnf download --source fftw-gnu15-openmpi5-ohpc
rpm -i ./fftw-gnu15-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/$(uname -m)/fftw-gnu15-openmpi5-static-ohpc-*.$(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-gnu12-geopm	Global Extensible Open Power Manager for use with GNU compiler toolchain.
ohpc-gnu12-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu12-mpich-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu12-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu12-mpich-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu12-openmpi4-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu12-openmpi4-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu12-openmpi4-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu12-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu12-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu12-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu12-python3-libs	Collection of python3 related library builds for use with GNU compiler toolchain.
ohpc-gnu12-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu12-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.
ohpc-gnu13-geopm	Global Extensible Open Power Manager for use with GNU compiler toolchain.
ohpc-gnu13-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu13-mpich-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu13-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu13-mpich-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu13-openmpi5-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu13-openmpi5-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.

Group Name	Description
ohpc-gnu13-openmpi5-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu13-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu13-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu13-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu13-python3-libs	Collection of python3 related library builds for use with GNU compiler toolchain.
ohpc-gnu13-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu13-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.
ohpc-gnu14-geopm	Global Extensible Open Power Manager for use with GNU compiler toolchain.
ohpc-gnu14-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu14-mpich-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu14-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu14-mpich-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu14-openmpi5-io-libs	Collection of IO library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu14-openmpi5-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu14-openmpi5-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu14-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu14-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu14-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu14-python3-libs	Collection of python3 related library builds for use with GNU compiler toolchain.
ohpc-gnu14-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu14-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.
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.

Group Name	Description
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.
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	3.4.0	OpenHPC documentation. https://github.com/openhpc/ohpc
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	1.6.0	Temporary workspace management. https://github.com/holgerBerger/hpc-workspace
lmod-defaults-gnu12-mpich	2.0	OpenHPC default login environments. https://github.com/openhpc/ohpc
lmod-defaults	2.0	OpenHPC default login environments. https://github.com/openhpc/ohpc
lmod	9.2	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
mrsh	2.12	Remote shell program that uses munge authentication. https://github.com/chaos/mrsh
nhc	1.4.3	LBNL Node Health Check. https://github.com/mej/nhc
ohpc-release	3	OpenHPC release files. https://github.com/openhpc/ohpc
pdsh	2.36	Parallel remote shell program. https://github.com/chaos/pdsh
prun	2.2	Convenience utility for parallel job launch. https://github.com/openhpc/ohpc
test-suite	3.5.0	Integration test suite for OpenHPC. https://github.com/openhpc/ohpc

E.2.2 Resource Management

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.github.io/pmix
slurm-contribs	25.11.4	Perl tool to print Slurm job state information. https://slurm.schedmd.com
slurm-devel	25.11.4	Development package for Slurm. https://slurm.schedmd.com
slurm-example-configs	25.11.4	Example config files for Slurm. https://slurm.schedmd.com
slurm-libpmi	25.11.4	Slurm's implementation of the pmi libraries. https://slurm.schedmd.com
slurm	25.11.4	Slurm Workload Manager. https://slurm.schedmd.com
slurm-openlava	25.11.4	openlava/LSF wrappers for transition from OpenLava/LSF to Slurm. https://slurm.schedmd.com
slurm-pam_slurm	25.11.4	PAM module for restricting access to compute nodes via Slurm. https://slurm.schedmd.com
slurm-perlapi	25.11.4	Perl API to Slurm. https://slurm.schedmd.com

RPM Package Name	Version	Info/URL
slurm-sackd	25.11.4	Slurm authentication daemon. https://slurm.schedmd.com
slurm-slurmctld	25.11.4	Slurm controller daemon. https://slurm.schedmd.com
slurm-slurmd	25.11.4	Slurm compute node daemon. https://slurm.schedmd.com
slurm-slurmdbd	25.11.4	Slurm database daemon. https://slurm.schedmd.com
slurm-sview	25.11.4	Graphical user interface to view and modify Slurm state. https://slurm.schedmd.com
slurm-torque	25.11.4	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
gnu12-compilers	12.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org
gnu13-compilers	13.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org
gnu14-compilers	14.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org
gnu15-compilers	15.2.0	The GNU C Compiler and Support Files. http://gcc.gnu.org

E.2.4 MPI Families / Communication Libraries

RPM Package Name	Version	Info/URL
libfabric	1.18.0	User-space RDMA Fabric Interfaces. http://www.github.com/ofiwg/libfabric
mpich	5.0.1	MPICH MPI implementation. http://www.mpich.org
mvapich2	4.1	OSU MVAPICH2 MPI implementation. http://mvapich.cse.ohio-state.edu
openmpi4	4.1.5	A powerful implementation of MPI/SHMEM. http://www.open-mpi.org
openmpi5	5.0.10	A powerful implementation of MPI/SHMEM. http://www.open-mpi.org
ucx	1.20.1	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	5.3.0	Software build and installation framework. https://easybuilders.github.io/easybuild
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	4.3.2	CMake is an open-source, cross-platform family of tools designed to build, test and package software. https://cmake.org
hwloc	2.13.0	Portable Hardware Locality. http://www.open-mpi.org/projects/hwloc

RPM Package Name	Version	Info/URL
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	1.26.4	NumPy array processing for numbers, strings, records and objects. https://github.com/numpy/numpy
python3-scipy	1.5.4	Scientific Tools for Python. http://www.scipy.org
spack	1.1.1	HPC software package management. https://github.com/spack/spack
valgrind	3.27.0	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	5.0.6	Extrae tool. https://tools.bsc.es
geopm	1.1.0	Global Extensible Open Power Manager. https://geopm.github.io
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	6.0.0	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	2.12.1	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

RPM Package Name	Version	Info/URL
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	3.2.4	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	0.44	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	4.6.0	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	0.3.33	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

RPM Package Name	Version	Info/URL
superlu	7.0.0	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	3.3.11	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
mfem	4.9	Lightweight, general, scalable C++ library for finite element methods. http://mfem.org
mumps	5.9.0	A MULTifrontal Massively Parallel Sparse direct Solver. https://mumps-solver.org
opencoarrays	2.10.2	ABI to leverage the parallel programming features of the Fortran 2018 DIS. http://www.opencoarrays.org
petsc	3.25.1	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	3.25.1	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: 6E19 BE11 D9A0 82C0 0A7D B41A 7AC0 5F09 **40A90CC8**

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 `ohpc-release` package and illustrates how the **key ID** matches the fingerprint shown above.

```
rpm --checksig -v ohpc-release-3-1.el9.x86_64.rpm
ohpc-release-3-1.el9.x86_64.rpm:
  Header V3 RSA/SHA256 Signature, key ID 40a90cc8: OK
  Header SHA256 digest: OK
  Header SHA1 digest: OK
  Payload SHA256 digest: OK
  V3 RSA/SHA256 Signature, key ID 40a90cc8: OK
  MD5 digest: OK
```