Bright Cluster Manager 7.0

# User Manual

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# Preface

Welcome to the *User Manual* for the Bright Cluster Manager 7.0.

## 0.1 About This Manual

This manual is intended for the end users of a cluster running Bright Cluster Manager, and tends to see things from a user perspective. It covers the basics of using the Bright Cluster Manager user environment to run compute jobs on the cluster. Although it does cover some aspects of general Linux usage, it is by no means comprehensive in this area. Readers are expected to have some familiarity with the basics of a Linux environment from the regular user point of view.

Regularly updated production versions of the 7.0 manuals are available on updated clusters by default at `/cm/shared/docs/cm`. The latest updates are always online at `http://support.brightcomputing.com/manuals`.

The manuals constantly evolve to keep up with the development of the Bright Cluster Manager environment and the addition of new hardware and/or applications. The manuals also regularly incorporate customer feedback. Administrator and user input is greatly valued at Bright Computing. So any comments, suggestions or corrections will be very gratefully accepted at `manuals@brightcomputing.com`.

## 0.2 Getting User-Level Support

A user is first expected to refer to this manual or other supplementary site documentation when dealing with an issue. If that is not enough to resolve the issue, then support for an end-user is typically provided by the cluster administrator, who is often a unix or Linux system administrator with some cluster experience. Commonly, the administrator has configured and tested the cluster beforehand, and therefore has a good idea of its behavior and quirks. The initial step when calling in outside help is thus often to call in the cluster administrator.

# 1

# Introduction

This manual is intended for cluster users who need a quick introduction to the Bright Cluster Manager, which manages a Beowulf cluster configuration. It explains how to use the MPI and batch environments, how to submit jobs to the queueing system, and how to check job progress. The specific combination of hardware and software installed may differ depending on the specification of the cluster, which means that parts of this manual may not be relevant to the user's particular cluster.

## 1.1 What Is A Beowulf Cluster?

### 1.1.1 Background And History

In the history of the English language, Beowulf is the earliest surviving epic poem written in English. It is a story about a hero with the strength of many men who defeated a fearsome monster called Grendel.

In computing, a Beowulf class cluster computer is a multiprocessor architecture used for parallel computations, i.e., it uses many processors together so that it has the brute force to defeat certain "fearsome" number-crunching problems.

The architecture was first popularized in the Linux community when the source code used for the original Beowulf cluster built at NASA was made widely available. The Beowulf class cluster computer design usually consists of one head node and one or more regular nodes connected together via Ethernet or some other type of network. While the original Beowulf software and hardware has long been superseded, the name given to this basic design remains "Beowulf class cluster computer", or less formally "Beowulf cluster".

### 1.1.2 Brief Hardware And Software Description

On the hardware side, commodity hardware is generally used in Beowulf clusters to keep costs down. These components are usually x86-compatible processors produced at the Intel and AMD chip foundries, standard Ethernet adapters, InfiniBand interconnects, and switches.

On the software side, free and open-source software is generally used in Beowulf clusters to keep costs down. For example: the Linux operating system, the GNU C compiler collection and open-source implementations of the Message Passing Interface (MPI) standard.

The head node controls the whole cluster and serves files and information to the nodes. It is also the cluster's console and gateway to the

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outside world. Large Beowulf clusters might have more than one head node, and possibly other nodes dedicated to particular tasks, for example consoles or monitoring stations. In most cases compute nodes in a Beowulf system are dumb—in general, the dumber the better—with the focus on the processing capability of the node within the cluster, rather than other abilities a computer might generally have. A node may therefore have

- one or more processing elements. The processors may be standard CPUs, as well as GPUs, FPGAs, MICs, and so on.
- enough local memory—memory contained in a single node—to deal with the processes passed on to the node
- a connection to the rest of the cluster

Nodes are configured and controlled by the head node, and do only what they are told to do. One of the main differences between Beowulf and a Cluster of Workstations (COW) is the fact that Beowulf behaves more like a single machine rather than many workstations. In most cases, the nodes do not have keyboards or monitors, and are accessed only via remote login or possibly serial terminal. Beowulf nodes can be thought of as a CPU + memory package which can be plugged into the cluster, just like a CPU or memory module can be plugged into a motherboard to form a larger and more powerful machine. A significant difference is that the nodes of a cluster have a relatively slower interconnect.

## 1.2 Brief Network Description

A Beowulf Cluster consists of a login, compile and job submission node, called the head, and one or more compute nodes, often referred to as worker nodes. A second (fail-over) head node may be present in order to take control of the cluster in case the main head node fails. Furthermore, a second fast network may also have been installed for high-performance low-latency communication between the (head and the) nodes (see figure 1.1).

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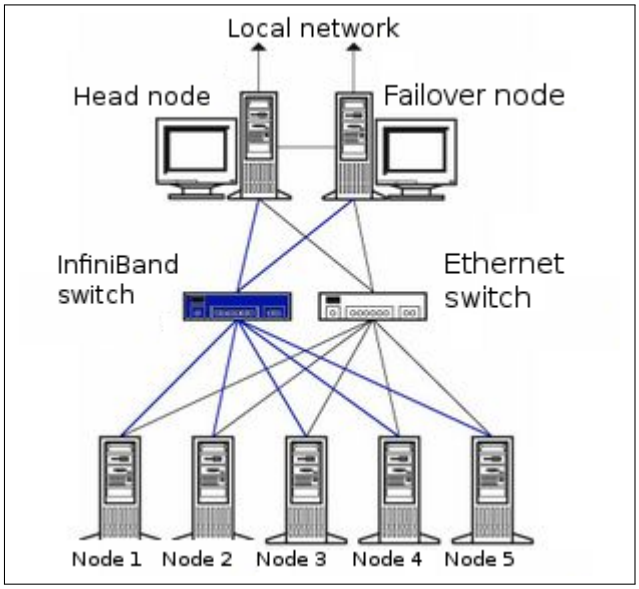


Figure 1.1: Cluster layout

The login node is used to compile software, to submit a parallel or batch program to a job queueing system and to gather/analyze results. Therefore, it should rarely be necessary for a user to log on to one of the nodes and in some cases node logins are disabled altogether. The head, login and compute nodes usually communicate with each other through a gigabit Ethernet network, capable of transmitting information at a maximum rate of 1000 Mbps. In some clusters 10 gigabit Ethernet (10GE, 10GBE, or 10GigE) is used, capable of up to 10 Gbps rates.

Sometimes an additional network is used by the cluster for even faster communication between the compute nodes. This particular network is mainly used for programs dedicated to solving large scale computational problems, which may require multiple machines and could involve the exchange of vast amounts of information. One such network topology is InfiniBand, commonly capable of transmitting information at a maximum effective data rate of about 124Gbps and about 1.2$\mu$s end-to-end latency on small packets, for clusters in 2013. The commonly available maximum transmission rates will increase over the years as the technology advances.

Applications relying on message passing benefit greatly from lower latency. The fast network is usually complementary to a slower Ethernet-based network.

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# 2

# Cluster Usage

## 2.1 Login To The Cluster Environment

The login node is the node where the user logs in and works from. Simple clusters have a single login node, but large clusters sometimes have multiple login nodes to improve the reliability of the cluster. In most clusters, the login node is also the head node from where the cluster is monitored and installed. On the login node:

- applications can be developed
- code can be compiled and debugged
- applications can be submitted to the cluster for execution
- running applications can be monitored

To carry out an ssh login to the cluster, a terminal session can be started from Unix-like operating systems:

**Example**

```
$ ssh myname@cluster.hostname
```

On a Windows operating system, an SSH client such as for PuTTY (`http://www.putty.org`) can be downloaded. Another standard possibility is to run a Unix-like environment such as Cygwin (`http://www.cygwin.com`) within the Windows operating system, and then run the SSH client from within it.

A Mac OS X user can use the Terminal application from the Finder, or under `Application/Utilities/Terminal.app`. X11 must be installed from the Mac OS X medium, or alternatively, XQuartz can be used instead. XQuartz is an alternative to the official X11 package, and is usually more up-to-date and less buggy.

When using the SSH connection, the cluster's address must be added. When the connection is made, a username and password must be entered at the prompt.

If the administrator has changed the default SSH port from 22 to something else, the port can be specified with the `-p <port>` option:

```
$ ssh -X -p <port> <user>@<cluster>
```

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The -X option can be dropped if no X11-forwarding is required. X11-forwarding allows a GUI application from the cluster to be displayed locally.

Optionally, after logging in, the password used can be changed using the `passwd` command:

```
$ passwd
```

## 2.2 Setting Up The User Environment

By default, each user uses the bash shell interpreter. In that case, each time a user login takes place, a file named `.bashrc` is executed to set up the shell environment for the user. The shell and its environment can be customized to suit user preferences. For example,

- the prompt can be changed to indicate the current username, host, and directory, for example: by setting the prompt string variable:

  ```
  PS1="[\u@\h:\w ] $"
  ```

- the size of the command history file can be increased, for example: `export HISTSIZE=100`
- aliases can be added for frequently used command sequences, for example: `alias lart='ls -alrt'`
- environment variables can be created or modified, for example: `export MYVAR=MYSTRING`
- the location of software packages and versions that are to be used by a user (the path to a package) can be set.

Because there is a huge choice of software packages and versions, it can be hard to set up the right environment variables and paths for software that is to be used. Collisions between different versions of the same package and non-matching dependencies on other packages must also be avoided. To make setting up the environment easier, Bright Cluster Manager provides preconfigured environment modules (section 2.3).

## 2.3 Environment Modules

It can be quite hard to set up the correct environment to use a particular software package and version.

For instance, managing several MPI software packages on the same system or even different versions of the same MPI software package is quite difficult for most users on a standard SUSE or Red Hat system because many software packages use the same names for executables and libraries.

A user could end up with the problem of never being quite sure which libraries have been used for the compilation of a program as multiple libraries with the same name may be installed. Very often a user would like to test new versions of a software package before permanently installing the package. Within a Red Hat or SuSE setup without special utilities, this would be quite a complex task to achieve. Environment modules, using the `module` command, are a special utility to make this task much easier.

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### 2.3.1 Available commands

```
$ module --help

  Modules Release 3.2.10 2012-12-21 (Copyright GNU GPL v2 1991):

  Usage: module [ switches ] [ subcommand ] [subcommand-args ]

Switches:
        -H|--help               this usage info
        -V|--version            modules version & configuration options
        -f|--force              force active dependency resolution
        -t|--terse              terse    format avail and list format
        -l|--long               long     format avail and list format
        -h|--human              readable format avail and list format
        -v|--verbose            enable  verbose messages
        -s|--silent             disable verbose messages
        -c|--create             create caches for avail and apropos
        -i|--icase              case insensitive
        -u|--userlvl <lvl>      set user level to (nov[ice],exp[ert],adv[anced])
  Available SubCommands and Args:
        + add|load              modulefile [modulefile ...]
        + rm|unload             modulefile [modulefile ...]
        + switch|swap           [modulefile1] modulefile2
        + display|show          modulefile [modulefile ...]
        + avail                 [modulefile [modulefile ...]]
        + use [-a|--append]     dir [dir ...]
        + unuse                 dir [dir ...]
        + update
        + refresh
        + purge
        + list
        + clear
        + help                  [modulefile [modulefile ...]]
        + whatis                [modulefile [modulefile ...]]
        + apropos|keyword       string
        + initadd               modulefile [modulefile ...]
        + initprepend           modulefile [modulefile ...]
        + initrm                modulefile [modulefile ...]
        + initswitch            modulefile1 modulefile2
        + initlist
        + initclear
```

### 2.3.2 Changing The Current Environment

The modules loaded into the user's environment can be seen with:

```
$ module list
```

Modules can be loaded using the `add` or `load` options. A list of modules can be added by spacing them:

```
$ module add shared open64 openmpi/open64
```

The `shared` module is special. If it is to be loaded, it is usually placed first in a list before the other modules, because the other modules often depend on it. The `shared` module is described further shortly.

The "`module avail`" command lists all modules that are available for loading (some output elided):

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**Example**

```
[fred@bright70 ~]$ module avail

--------------------------- /cm/local/modulefiles ----------------------
cluster-tools/7.0dot               module-info       use.own
cmd                freeipmi/1.2.6    null               version
cmsh               ipmitool/1.8.12   openldap
cmsub/7.0        module-git        shared

--------------------------- /cm/shared/modulefiles ---------------------
acml/gcc/64/5.3.1                     hwloc/1.7
acml/gcc/fma4/5.3.1                   intel-cluster-checker/2.0
acml/gcc/mp/64/5.3.1                  intel-cluster-runtime/ia32/3.5
acml/gcc/mp/fma4/5.3.1                intel-cluster-runtime/intel64/3.5
acml/gcc-int64/64/5.3.1               intel-cluster-runtime/mic/3.5
acml/gcc-int64/fma4/5.3.1             intel-tbb-oss/ia32/41_20130314oss
...
```

In the list there are two kinds of modules:

- **local modules**, which are specific to the node, or head node only
- **shared modules**, which are made available from a shared storage, and which only become available for loading after the `shared` module is loaded.

The `shared` module is obviously a useful local module, and is therefore usually configured to be loaded for the user by default.

Although version numbers are shown in the "`module avail`" output, it is not necessary to specify version numbers, unless multiple versions are available for a module[1].

To remove one or more modules, the "`module unload`" or "`module rm`" command is used.

To remove all modules from the user's environment, the "`module purge`" command is used.

The user should be aware that some loaded modules can conflict with others loaded at the same time. For example, loading `openmpi/gcc/64/` without removing an already loaded `openmpi/gcc/64/` can result in confusion about what compiler `opencc` is meant to use.

### 2.3.3 Changing The Default Environment

The initial state of modules in the user environment can be set as a default using the "`module init*`" subcommands. The more useful ones of these are:

- `module initadd`: add a module to the initial state
- `module initrm`: remove a module from the initial state
- `module initlist`: list all modules loaded initially

[1]For multiple versions, when no version is specified, the alphabetically-last version is chosen. This usually is the latest, but can be an issue when versions move from, say, 9, to 10. For example, the following is sorted in alphabetical order: v1 v10 v11 v12 v13 v2 v3 v4 v5 v6 v7 v8 v9.

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- `module initclear`: clear all modules from the list of modules loaded initially

**Example**

```
$ module initclear
$ module initlist
bash initialization file $HOME/.bashrc loads modules:
        null
$ module initadd shared gcc/4.8.1 openmpi/gcc sge
$ module initlist
bash initialization file $HOME/.bashrc loads modules:
   null shared gcc/4.8.1 openmpi/gcc/64/1.6.5 sge/2011.11p1
```

In the preceding example, the newly defined initial state module environment for the user is loaded from the next login onwards.

If the user is unsure about what the module does, it can be checked using "`module whatis`":

```
$ module whatis sge
sge                  : Adds sge to your environment
```

The `man` pages for `module` gives further details on usage.

## 2.4 Compiling Applications

Compiling an application is usually done on the head node or login node. Typically, there are several compilers available on the head node, which provide different levels of optimization, standards conformance, and support for accelerators. For example: GNU compiler collection, Open64 compiler, Intel compilers, Portland Group compilers. The following table summarizes the available compiler commands on the cluster:

| Language | GNU | Open64 | Portland | Intel |
|---|---|---|---|---|
| C | `gcc` | `opencc` | `pgcc` | `icc` |
| C++ | `g++` | `openCC` | `pgCC` | `icc` |
| Fortran77 | `gfortran` | `openf90 -ff77` | `pgf77` | `ifort` |
| Fortran90 | `gfortran` | `openf90` | `pgf90` | `ifort` |
| Fortran95 | `gfortran` | `openf95` | `pgf95` | `ifort` |

GNU compilers are the de facto standard on Linux and are installed by default. They are provided under the terms of the GNU General Public License. AMD's Open64 is also installed by default on Bright Cluster Manager. Commercial compilers by Portland and Intel are available as packages via the Bright Cluster Manager YUM repository, and require the purchase of a license to use them. To make a compiler available to be used in a user's shell commands, the appropriate environment module (section 2.3) must be loaded first. On most clusters two versions of GCC are available:

1. The version of GCC that comes along with the Linux distribution. For example, for CentOS 6.x:

   **Example**

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```
[fred@bright70 ~]$ which gcc; gcc --version | head -1
/usr/bin/gcc
gcc (GCC) 4.4.7 20120313 (Red Hat 4.4.7-3)
```

2. The latest version suitable for general use that is packaged as a module by Bright Computing:

   **Example**

```
[fred@bright70 ~]$ module load gcc
[fred@bright70 ~]$ which gcc; gcc --version | head -1
/cm/shared/apps/gcc/4.8.1/bin/gcc
gcc (GCC) 4.8.1
```

To use the latest version of GCC, the `gcc` module must be loaded. To revert to the version of GCC that comes natively with the Linux distribution, the `gcc` module must be unloaded.

The compilers in the preceding table are ordinarily used for applications that run on a single node. However, the applications used may fork, thread, and run across as many nodes and processors as they can access if the application is designed that way.

The standard, structured way of running applications in parallel is to use the MPI-based libraries, which link to the underlying compilers in the preceding table. The underlying compilers are automatically made available after choosing the parallel environment (MPICH, MVAPICH, Open MPI, etc.) via the following compiler commands:

| Language | C | C++ | Fortran77 | Fortran90 | Fortran95 |
|---|---|---|---|---|---|
| **Command** | `mpicc` | `mpiCC` | `mpif77` | `mpif90` | `mpif95` |

### 2.4.1 Open MPI And Mixing Compilers

Bright Cluster Manager comes with multiple Open MPI packages corresponding to the different available compilers. However, sometimes mixing compilers is desirable. For example, C-compilation may be preferred using `icc` from Intel, while Fortran90-compilation may be preferred using `openf90` from Open64. In such cases it is possible to override the default compiler path environment variable, for example:

```
[fred@bright70 ~]$ module list
Currently Loaded Modulefiles:
  1) null                    3) gcc/4.4.7              5) sge/2011.11
  2) shared                  4) openmpi/gcc/64/1.4.5
[fred@bright70 ~]$ mpicc --version --showme; mpif90 --version --showme
gcc --version
gfortran --version
[fred@bright70 ~]$ export OMPI_CC=icc; export OMPI_FC=openf90
[fred@bright70 ~]$ mpicc --version --showme; mpif90 --version --showme
icc --version
openf90 --version
```

Variables that may be set are OMPI_CC, OMPI_FC, OMPI_F77, and OMPI_CXX. More on overriding the Open MPI wrapper settings is documented in the man pages of `mpicc` in the environment section.

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# 3

# Using MPI

The Message Passing Interface (MPI) is a standardized and portable message passing system designed by a group of researchers from academia and industry to function on a wide variety of parallel computers. The standard defines the syntax and semantics of a core of library routines useful to a wide range of users writing portable message-passing programs in Fortran or the C programming language. MPI libraries allow the compilation of code so that it can be used over a variety of multiprocessor systems from SMP nodes to NUMA (non-Uniform Memory Access) systems and interconnected cluster nodes .

The available MPI implementation for the variant MPI-3 is MPICH (version 3). Open MPI supports both variants. These MPI libaries can be compiled with GCC, Open64, Intel, or PGI.

Depending on the cluster hardware, the interconnect available may be: Ethernet (GE), InfiniBand (IB), or Myrinet (MX).

Depending on the cluster configuration, MPI implementations for different compilers can be loaded. By default MPI implementations that are installed are compiled and made available using both GCC and Open64.

The interconnect and compiler implementation can be worked out from looking at the module and package name. The modules available can be searched through for the compiler variant, and then the package providing it can be found:

**Example**

```
[fred@bright70 ~]$ # search for modules starting with the name openmpi
[fred@bright70 ~]$ module -l avail 2>&1 | grep ^openmpi
openmpi/gcc/64/1.6.5                            2013/09/05 22:01:44
openmpi/intel/64/1.6.5                          2013/09/05 21:23:57
openmpi/open64/64/1.6.5                         2013/09/05 22:28:37
[fred@bright70 ~]$ rpm -qa | grep ^openmpi
openmpi-geib-open64-64-1.6.5-165_cm7.0.x86_64
openmpi-geib-gcc-64-1.6.5-165_cm7.0.x86_64
openmpi-ge-intel-64-1.6.5-165_cm7.0.x86_64
```

Here, for example,

```
openmpi-geib-open64-64-1.6.5-165_cm7.0.x86_64
```

implies: Open MPI version `1.6.5` compiled for both Gigabit Ethernet (`ge`) and InfiniBand (`ib`), with the Open64 (`open64`) compiler for a 64-bit

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architecture, packaged as a cluster manager (cm) package for version 7.0 of Bright Cluster Manager, for the x86_64 architecture.

## 3.1 Interconnects

Jobs can use particular networks for intra-node communication.

### 3.1.1 Gigabit Ethernet

Gigabit Ethernet is the interconnect that is most commonly available. For Gigabit Ethernet, no additional modules or libraries are needed. The Open MPI, MPICH implementations will work over Gigabit Ethernet.

### 3.1.2 InfiniBand

InfiniBand is a high-performance switched fabric which is characterized by its high throughput and low latency. Open MPI, MVAPICH and MVAPICH2 are suitable MPI implementations for InfiniBand.

## 3.2 Selecting An MPI implementation

Once the appropriate compiler module has been loaded, the MPI implementation is selected along with the appropriate library modules. The following list, <*compiler*> indicates a choice of gcc, intel, open64, or pgi:

- mpich/ge/<*compiler*>
- mvapich/<*compiler*>
- mvapich2/<*compiler*>
- openmpi/<*compiler*>

After the appropriate MPI module has been added to the user environment, the user can start compiling applications. The mpich and openmpi implementations may be used on Ethernet. On InfiniBand, mvapich, mvapich2 and openmpi may be used. Open MPI's openmpi implementation will first attempt to use InfiniBand, but will revert to Ethernet if InfiniBand is not available.

## 3.3 Example MPI Run

This example covers an MPI run, which can be run inside and outside of a queuing system.

To use mpirun, the relevant environment modules must be loaded. For example, to use the mpich over Gigabit Ethernet (ge) GCC implementation:

```
$ module add mpich/ge/gcc
```

or to use the openmpi Open MPI GCC implementation:

```
$ module add openmpi/gcc
```

Similarly, to use the mvapich InfiniBand Open64 implementation:

```
$ module add mvapich/open64
```

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Depending on the libraries and compilers installed on the system, the availability of these packages might differ. To see a full list on the system the command "`module avail`" can be typed.

### 3.3.1 Compiling And Preparing The Application

The code must be compiled with MPI libraries and an underlying compiler. The correct library command can be found in the following table:

| Language | C | C++ | Fortran77 | Fortran90 | Fortran95 |
|---|---|---|---|---|---|
| **Command** | `mpicc` | `mpiCC` | `mpif77` | `mpif90` | `mpif95` |

An MPI application `myapp.c`, built in C, could then be compiled as:

```
$ mpicc myapp.c
```

The `a.out` binary that is created can then be executed using the `mpirun` command (section 3.3.3).

### 3.3.2 Creating A Machine File

A machine file contains a list of nodes which can be used by MPI programs.

The workload management system creates a machine file based on the nodes allocated for a job when the job is submitted with the workload manager job submission tool. So if the user chooses to have the workload management system allocate nodes for the job then creating a machine file is not needed.

However, if an MPI application is being run "by hand" outside the workload manager, then the user is responsible for creating a machine file manually. Depending on the MPI implementation, the layout of this file may differ.

Machine files can generally be created in two ways:

- Listing the same node several times to indicate that more than one process should be started on each node:

```
node001
node001
node002
node002
```

- Listing nodes once, but with a suffix for the number of CPU cores to use on each node:

```
node001:2
node002:2
```

### 3.3.3 Running The Application

#### A Simple Parallel Processing Executable

A simple "hello world" program designed for parallel processing can be built with MPI. After compiling it, it can be used to send a message about how and where it is running:

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```
[fred@bright70 ~]$ cat hello.c
#include <stdio.h>
#include <mpi.h>

int main (int argc, char *argv[])
{
    int id, np, i;
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    int processor_name_len;

    MPI_Init(&argc, &argv);

    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &id);
    MPI_Get_processor_name(processor_name, &processor_name_len);

    for(i=1;i<2;i++)
    {printf(
    "Hello world from process %03d out of %03d, processor name %s\n",
    id, np, processor_name
    );}

    MPI_Finalize();
    return 0;
}
[fred@bright70 ~]$ module add openmpi/gcc   #or as appropriate
[fred@bright70 ~]$ mpicc hello.c -o hello
[fred@bright70 ~]$ ./hello
Hello world from process 000 out of 001, processor name bright70.cm.cluster
```

However, it still runs on a single processor unless it is submitted to the system in a special way.

#### Running An MPI Executable In Parallel Without A Workload Manager

**Compute node environment provided by user's `.bashrc`:** After the relevant module files are chosen (section 3.3) for MPI, an executable compiled with MPI libraries runs on nodes in parallel when submitted with `mpirun`. The executable running on other nodes loads environmental modules on those other nodes by sourcing the `.bashrc` file of the user (section 2.3.3). It is therefore important to ensure that the environmental module stack used on the compute node is clean and consistent.

**Example**

Supposing the `.bashrc` loads two MPI stacks—the `mpich` stack, followed by the Open MPI stack—then that can cause errors because the compute node may use parts of the wrong MPI implementation.

The environment of the user from the interactive shell prompt is not normally carried over automatically to the compute nodes during an `mpirun` submission. That is, compiling and running the executable will normally work only on the local node without a special treatment. To have the executable run on the compute nodes, the right environment modules for the job must be made available on the compute nodes too, as part of the user login process to the compute nodes for that job. Usually

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the system administrator takes care of such matters in the default user configuration by setting up the default user environment (section 2.3.3), with reasonable `initrm` and `initadd` options. Users are then typically allowed to set up their personal default overrides to the default administrator settings, by placing their own `initrm` and `initadd` options to the `module` command according to their needs.

**Running `mpirun` outside a workload manager:** When using `mpirun` manually, outside a workload manager environment, the number of processes (`-np`) as well as the number of hosts (`-machinefile`) should be specified. For example, on a cluster with 2 compute-nodes and a machine file as specified in section 3.3.2:

**Example**

```
[fred@bright70 ~]$ module initclear; module initadd openmpi/gcc
[fred@bright70 ~]$ module add openmpi/gcc   #or as appropriate
[fred@bright70 ~]$ mpirun -np 4 -machinefile mpirun.hosts hello
Hello world from process 002 out of 004, processor name node002.cm.cluster
Hello world from process 003 out of 004, processor name node001.cm.cluster
Hello world from process 000 out of 004, processor name node002.cm.cluster
Hello world from process 001 out of 004, processor name node001.cm.cluster
```

The output of the preceding program is actually printed in random order. This can be modified as follows, so that only process 0 prints to the standard output, and other processes communicate their output to process 0:

```
#include "mpi.h"
#include "string.h"
#include <stdio.h>

int main( int argc, char *argv[] )
{
    int  numprocs, myrank, namelen, i;
    char processor_name[MPI_MAX_PROCESSOR_NAME];
    char greeting[MPI_MAX_PROCESSOR_NAME + 80];
    MPI_Status status;

    MPI_Init( &argc, &argv );
    MPI_Comm_size( MPI_COMM_WORLD, &numprocs );
    MPI_Comm_rank( MPI_COMM_WORLD, &myrank );
    MPI_Get_processor_name( processor_name, &namelen );

    sprintf( greeting, "Hello world, from process %d of %d on %s",
             myrank, numprocs, processor_name );

    if ( myrank == 0 ) {
        printf( "%s\n", greeting );
        for ( i = 1; i < numprocs; i++ ) {
            MPI_Recv( greeting, sizeof( greeting ), MPI_CHAR,
                      i, 1, MPI_COMM_WORLD, &status );
            printf( "%s\n", greeting );
        }
    }
```

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```
    else {
        MPI_Send( greeting, strlen( greeting ) + 1, MPI_CHAR,
                  0, 1, MPI_COMM_WORLD );
    }

    MPI_Finalize( );
    return 0;
}
```

```
fred@bright70 ~]$ module add mvapich/gcc   #or as appropriate
fred@bright70 ~]$ mpirun -np 4 -machinefile mpirun.hosts hello
Hello world from process 0 of 4 on node001.cm.cluster
Hello world from process 1 of 4 on node002.cm.cluster
Hello world from process 2 of 4 on node001.cm.cluster
Hello world from process 3 of 4 on node002.cm.cluster
```

Running the executable with `mpirun` outside the workload manager as shown does not take the resources of the cluster into account. To handle running jobs with cluster resources is of course what workload managers such as Slurm are designed to do. Workload managers also typically take care of what environment modules should be loaded on the compute nodes for a job, via additions that the user makes to a job script.

Running an application through a workload manager via a job script is introduced in Chapter 4.

Appendix A contains a number of simple MPI programs.

### 3.3.4 Hybridization

OpenMP is an implementation of multi-threading. This is a method of parallelizing whereby a parent thread—a series of instructions executed consecutively—forks a specified number of child threads, and a task is divided among them. The threads then run concurrently, with the runtime environment allocating threads to different processors and accessing the shared memory of an SMP system.

MPI can be mixed with OpenMP to achieve high performance on a cluster/supercomputer of multi-core nodes or servers. MPI creates processes that reside on the level of node, while OpenMP forks threads on the level of a core within an SMP node. Each process executes a portion of the overall computation, while inside each process, a team of threads is created through OpenMP directives to further divide the problem. This kind of execution makes sense due to:

- the ease of programming that OpenMP provides
- OpenMP might not require copies of data structure, which allows for designs that overlap computation and communication
- overcoming the limits of parallelism within the SMP node is of course still possible by using the power of other nodes via MPI.

#### Example

```
#include<mpi.h>
#include <omp.h>
#include <stdio.h>
#include<stdlib.h>
```

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```
int main(int argc , char** argv) {
  int size, myrank,namelength;
  char processor_name[MPI_MAX_PROCESSOR_NAME];
  MPI_Init(&argc,&argv);
  MPI_Comm_rank(MPI_COMM_WORLD,&myrank);
  MPI_Comm_size(MPI_COMM_WORLD,&size);
  MPI_Get_processor_name(processor_name,&namelength);
  printf("Hello I am Processor %d on %s of %d\n",myrank,processor_name,\
size);
    int tid = 0;  int n_of_threads = 1;
    #pragma omp parallel default(shared) private(tid, n_of_threads)
    {
    #if defined (_OPENMP)
          n_of_threads= omp_get_num_threads();
          tid = omp_get_thread_num();
    #endif
    printf("Hybrid Hello World: I am thread # %d out of %d\n", tid, n_o\
f_threads);
    }
 MPI_Finalize();
 return 0;
}
```

To compile the program:

```
fred@bright70 ~]$ mpicc -o hybridhello omphello.c -fopenmp
```

To specify the number of OpenMP threads per MPI task the environment variable `OMP_NUM_THREADS` must be set.

**Example**

```
fred@bright70 ~]$ export OMP_NUM_THREADS=3
```

The number of threads specified by the variable can then be run over the hosts specified by the `mpirun.hosts` file:

```
fred@bright70 ~]$ mpirun -np 2 -hostfile mpirun.hosts ./hybridhello
Hello I am Processor 0 on node001 of 2
Hello I am Processor 1 on node002 of 2
Hybrid Hello World: I am thread # 0 out of 3
Hybrid Hello World: I am thread # 2 out of 3
Hybrid Hello World: I am thread # 1 out of 3
Hybrid Hello World: I am thread # 0 out of 3
Hybrid Hello World: I am thread # 2 out of 3
Hybrid Hello World: I am thread # 1 out of 3
```

#### Benefits And Drawbacks Of Using OpenMP

The main benefit to using OpenMP is that it can decrease memory requirements, with usually no reduction in performance. Other benefits include:

- Potential additional parallelization opportunities besides those exploited by MPI.
- Less domain decomposition, which can help with load balancing as well as allowing for larger messages and fewer tasks participating in MPI collective operations.

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- OpenMP is a standard, so any modifications introduced into an application are portable and appear as comments on systems not using OpenMP.
- By adding annotations to existing code and using a compiler option, it is possible to add OpenMP to a code somewhat incrementally, almost on a loop-by-loop basis. The vector loops in a code that vectorize well are good candidates for OpenMP.

There are also some potential drawbacks:

- OpenMP can be hard to program and/or debug in some cases.
- Effective usage can be complicated on NUMA systems due to locality considerations
- If an application is network- or memory- bandwidth-bound, then threading it is not going to help. In this case it will be OK to leave some cores idle.
- In some cases a serial portion may be essential, which can inhibit performance.
- In most MPI codes, synchronization is implicit and happens when messages are sent and received. However, with OpenMP, much synchronization must be added to the code explicitly. The programmer must also explicitly determine which variables can be shared among threads and which ones cannot (parallel scoping). OpenMP codes that have errors introduced by incomplete or misplaced synchronization or improper scoping can be difficult to debug because the error can introduce race conditions which cause the error to happen only intermittently.

### 3.3.5 Support Thread Levels

MPI defines four "levels" of thread safety. The maximum thread support level is returned by the `MPI_Init_thread` call in the "provided" argument.

An environment variable `MPICH_MAX_THREAD_SAFETY` can be set to different values to increase the thread safety:

| MPICH_MAX_THREAD_SAFETY | Supported Thread Level |
|---|---|
| not set | MPI_THREAD_SINGLE |
| single | MPI_THREAD_SINGLE |
| funneled | MPI_THREAD_FUNNELED |
| serialized | MPI_THREAD_SERIALIZED |
| multiple | MPI_THREAD_MULTIPLE |

### 3.3.6 Further Recommendations

Users face various challenges with running and scaling large scale jobs on peta-scale production systems. For example: certain applications may not have enough memory per core, the default environment variables may need to be adjusted, or I/O may dominate run time.

Possible ways to deal with these are:

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- Trying out various compilers and compiler flags, and finding out which options are best for particular applications.
- Changing the default MPI rank ordering. This is a simple, yet sometimes effective, runtime tuning option that requires no source code modification, recompilation or re-linking. The default MPI rank placement on the compute nodes is SMP style. However, other choices are round-robin, folded rank, and custom ranking.
- Using fewer cores per node is helpful when more memory per process than the default is needed. Having fewer processes to share the memory and interconnect bandwidth is also helpful in this case. For NUMA nodes, extra care must be taken.
- Hybrid MPI/OpenMP reduces the memory footprint. Overlapping communication with computation in hybrid MPI/OpenMP can be considered.
- Some applications may perform better when large memory pages are used.

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# 4

# Workload Management

## 4.1 What Is A Workload Manager?

A workload management system (also known as a queueing system, job scheduler or batch submission system) manages the available resources such as CPUs, GPUs, and memory for jobs submitted to the system by users.

Jobs are submitted by the users using *job scripts*. Job scripts are constructed by users and include requests for resources. How resources are allocated depends upon policies that the system administrator sets up for the workload manager.

## 4.2 Why Use A Workload Manager?

Workload managers are used so that users do not manually have to keep track of node usage in a cluster in order to plan efficient and fair use of cluster resources.

Users may still perhaps run jobs on the compute nodes outside of the workload manager, if that is administratively permitted. However, running jobs outside a workload manager tends to eventually lead to an abuse of the cluster resources as more people use the cluster, and thus inefficient use of available resources. It is therefore usually forbidden as a policy by the system administrator on production clusters.

## 4.3 How Does A Workload Manager Function?

A workload manager uses policies to ensure that the resources of a cluster are used efficiently, and must therefore track cluster resources and jobs. A workload manager is therefore generally able to:

- Monitor:
  - the node status (up, down, load average)
  - all available resources (available cores, memory on the nodes)
  - the jobs state (queued, on hold, deleted, done)
- Modify:
  - the status of jobs (freeze/hold the job, resume the job, delete the job)

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- the priority and execution order for jobs
- the run status of a job. For example, by adding checkpoints to freeze a job.
- (optional) how related tasks in a job are handled according to their resource requirements. For example, a job with two tasks may have a greater need for disk I/O resources for the first task, and a greater need for CPU resources during the second task.

Some workload managers can adapt to external triggers such as hardware failure, and send alerts or attempt automatic recovery.

## 4.4 Job Submission Process

Whenever a job is submitted, the workload management system checks on the resources requested by the job script. It assigns cores, accelerators, local disk space, and memory to the job, and sends the job to the nodes for computation. If the required number of cores or memory are not yet available, it queues the job until these resources become available. If the job requests resources that are always going to exceed those that can become available, then the job accordingly remains queued indefinitely.

The workload management system keeps track of the status of the job and returns the resources to the available pool when a job has finished (that is, been deleted, has crashed or successfully completed).

## 4.5 What Do Job Scripts Look Like?

A job script looks very much like an ordinary shell script, and certain commands and variables can be put in there that are needed for the job. The exact composition of a job script depends on the workload manager used, but normally includes:

- commands to load relevant modules or set environment variables
- directives for the workload manager to request resources, control the output, set email addresses for messages to go to
- an execution (job submission) line

When running a job script, the workload manager is normally responsible for generating a machine file based on the requested number of processor cores (np), as well as being responsible for the allocation any other requested resources.

The executable submission line in a job script is the line where the job is submitted to the workload manager. This can take various forms.

**Example**

For the Slurm workload manager, the line might look like:

```
srun --mpi=mpich1_p4 ./a.out
```

**Example**

For Torque or PBS Pro it may simply be:

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```
mpirun ./a.out
```

**Example**

For SGE it may look like:

```
mpirun -np 4 -machinefile $TMP/machines ./a.out
```

## 4.6 Running Jobs On A Workload Manager

The details of running jobs through the following workload managers is discussed later on, for:

- Slurm (Chapter 5)
- SGE (Chapter 6)
- Torque (with Maui or Moab) and PBS Pro (Chapter 7)

## 4.7 Running Jobs In Cluster Extension Cloud Nodes Using `cmsub`

Extra computational power from cloud service providers such as the Amazon Elastic Compute Cloud (EC2) can be used by an appropriately configured cluster managed by Bright Cluster Manager.

If the head node is running outside a cloud services provider, and at least some of the compute nodes are in the cloud, then this "hybrid" cluster configuration is called a Cluster Extension cluster, with the compute nodes in the cloud being the cloud extension of the cluster.

For a Cluster Extension cluster, job scripts to a workload manager should be submitted using Bright Cluster Manager's `cmsub` utility. This allows the job to be considered for running on the extension (the cloud nodes). Jobs that are to run on the local regular nodes (not in a cloud) are not dealt with by `cmsub`.

The environment module (section 2.3) `cmsub` is typically configured by the system administrator to load by default on the head node. It must be loaded for the `cmsub` utility to work.

The basic usage for `cmsub` is:

```
cmsub [options] script
```

Options details are given in the man page for `cmsub(1)`.

Users that are used to running jobs as root should note that the root user cannot usefully run a job with `cmsub`.

The user can submit some cloud-related values as options to `cmsub` on the command line, followed by the job script.

**Example**

```
$ cat myscript1
#!/bin/sh
hostname

$ cmsub --regions=eu-west-1 myscript1
  Upload job id: 1
    User job id: 2
Download job id: 3
```

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All cmsub command line options can also be specified in a job-directive style format in the job script itself, using the "#CMSUB" tag to indicate an option.

**Example**

```
$ cat myscript2
#!/bin/sh
#CMSUB --regions=us-west-2,eu-west-1
#CMSUB --input-list=/home/user/myjob.in
#CMSUB --output-list=/home/user/myjob.out
#CMSUB --remote-output-list=/home/user/file-which-will-be-created
#CMSUB --input=/home/user/onemoreinput.dat
#CMSUB --input=/home/user/myexec
myexec

$ cmsub myscript2
  Upload job id: 4
    User job id: 5
Download job id: 6
```

## 4.8 Configuring Passwordless Login To Cloud Nodes

Logging in to a cloud node is possible, in a similar way to regular nodes. There is however a minor initial complication—passwordless ssh login to the cloud node or cloud director is not configured by default. This is because passwordless ssh uses certificate-based authentication, and the cloud director thus needs to have the ssh public key certificate of the user in the home directory of that user, in the cloud director. Since the home directory of the user in the cloud director is only created after the first login of the user to the cloud director, there can be no ssh public key certificate in that location to begin with.

This existential issue can be dealt with with the following one-time actions:

- The user, after logging in, generates an ssh key pair on the head node with an empty passphrase.
- The user runs the ssh-copy-id command to copy the public key over to the cloud director instance using the usual password for authentication.

After this, the user can carry out a passwordless login from the head node to the cloud director or the cloud node.

For example, after logging into the head node using the standard login with a password, a user galt can generate an ssh private and public certificate with ssh-keygen as follows:

**Example**

```
[galt@bright70 ~]$ #user galt already exists and has password
[galt@bright70 ~]$ ssh-keygen
Generating public/private rsa key pair.
Enter file in which to save the key (/home/galt/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
```

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```
Enter same passphrase again:
Your identification has been saved in /home/galt/.ssh/id_rsa.
Your public key has been saved in /home/galt/.ssh/id_rsa.pub.
The key fingerprint is:
7a:31:d1:f7:93:d5:96:bd:5a:6f:a1:11:b3:c2:d1:14 galt@bright70
The key's randomart image is:
+--[ RSA 2048]----+
|             E.  |
|         .  o   +|
|        . ...+ .=|
|         .....++.|
|        S  o o++ |
|       . o  . =.o|
|      . .    o  o|
|       .       . |
|                 |
+-----------------+
```

The user can then copy the public key over to the cloud director, `eu-west-1-director` in the following example, using `ssh-copy-id`:

**Example**

```
[galt@bright70 ~]$ ssh-copy-id eu-west-1-director
galt@eu-west-1-director's password:
Now try logging into the machine, with "ssh 'eu-west-1-director'",
and check in:

  .ssh/authorized_keys

to make sure we haven't added extra keys that you weren't expecting.

[galt@bright70 ~]$ ssh cnode001
Last login: Tue May 27 08:24:07 2014 from master.cm.cluster
[galt@cnode001 ~]$
```

If the user is able to login to a cloud node, `cnode001` in the preceding example, then it implies that the user can login to the cloud director anyway, so the user should now be correctly configured with passwordless authentication to the cloud nodes.

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# 5

# Slurm

Slurm is a workload management system developed originally at the Lawrence Livermore National Laboratory. Slurm used to stand for Simple Linux Utility for Resource Management. However Slurm has evolved since then, and its advanced state nowadays means that the acronym is obsolete.

Slurm has both a graphical interface and command line tools for submitting, monitoring, modifying and deleting jobs. It is normally used with *job scripts* to submit and execute jobs. Various settings can be put in the job script, such as number of processors, resource usage
and application specific variables.

The steps for running a job through Slurm are to:

- Create the script or executable that will be handled as a job
- Create a job script that sets the resources for the script/executable
- Submit the job script to the workload management system

The details of Slurm usage depends upon the MPI implementation used. The description in this chapter will cover using Slurm's Open MPI implementation, which is quite standard. Slurm documentation can be consulted (`http://slurm.schedmd.com/mpi_guide.html`) if the implementation the user is using is very different.

## 5.1 Loading Slurm Modules And Compiling The Executable

In section 3.3.3 an MPI "Hello, world!" executable that can run in parallel is created and run in parallel outside a workload manager.

The executable can be run in parallel using the Slurm workload manager. For this, the Slurm module should first be loaded by the user on top of the chosen MPI implementation, in this case Open MPI:

**Example**

```
[fred@bright52 ~]$ module list
Currently Loaded Modulefiles:
  1) gcc/4.4.6                3) shared
  2) openmpi/gcc/64/1.4.2     4) cuda40/toolkit/4.0.17
[fred@bright52 ~]$ module add slurm; module list
```

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```
Currently Loaded Modulefiles:
  1) gcc/4.4.6               3) shared                  5) slurm/2.2.4
  2) openmpi/gcc/64/1.4.2    4) cuda40/toolkit/4.0.17
```

The "hello world" executable from section 3.3.3 can then be compiled and run for one task outside the workload manager, on the local host, as:

```
mpicc hello.c -o hello
mpirun -np 1 hello
```

## 5.2 Running The Executable With salloc

Running it as a job managed by Slurm can be done interactively with the Slurm allocation command, salloc, as follows

```
[fred@bright52 ~]$ salloc mpirun hello
```

Slurm is more typically run as a batch job (section 5.3). However execution via salloc uses the same options, and it is more convenient as an introduction because of its interactive behavior.

In a default Bright Cluster Manager configuration, Slurm auto-detects the cores available and by default spreads the tasks across the cores that are part of the allocation request.

To change how Slurm spreads the executable across nodes is typically determined by the options in the following table:

| Short Option | Long Option | Description |
|---|---|---|
| -N | --nodes= | Request this many nodes on the cluster.<br>Use all cores on each node by default |
| -n | --ntasks= | Request this many tasks on the cluster.<br>Defaults to 1 task per node. |
| -c | --cpus-per-task= | request this many CPUs per task,<br>(not implemented by Open MPI yet) |
| (none) | --ntasks-per-node= | request this number of tasks per node . |

The full options list and syntax for salloc can be viewed with "man salloc".

The requirement of specified options to salloc must be met before the executable is allowed to run. So, for example, if --nodes=4 and the cluster only has 3 nodes, then the executable does not run.

### 5.2.1 Node Allocation Examples

The following session illustrates and explains some node allocation options and issues for Slurm using a cluster with just 1 compute node and 4 CPU cores:

**Default settings:** The hello MPI executable with default settings of Slurm runs successfully over the first (and in this case, the only) node that it finds:

```
[fred@bright52 ~]$ salloc mpirun hello
salloc: Granted job allocation 572
Hello world from process 0 out of 4, host name node001
Hello world from process 1 out of 4, host name node001
Hello world from process 2 out of 4, host name node001
Hello world from process 3 out of 4, host name node001
salloc: Relinquishing job allocation 572
```

The preceding output also displays if -N1 (indicating 1 node) is specified, or if -n4 (indicating 4 tasks) is specified.

The node and task allocation is almost certainly not going to be done by relying on defaults. Instead, node specifications are supplied to Slurm along with the executable.

To understand Slurm node specifications, the following cases consider and explain where the node specification is valid and invalid.

**Number of nodes requested:** The value assigned to the -N|--nodes= option is the number of nodes from the cluster that is requested for allocation for the executable. In the current cluster example it can only be 1. For a cluster with, for example, 1000 nodes, it could be a number up to 1000.

A resource allocation request for 2 nodes with the --nodes option causes an error on the current 1-node cluster example:

```
[fred@bright52 ~]$ salloc -N2 mpirun hello
salloc: error: Failed to allocate resources: Node count specification in\
valid
salloc: Relinquishing job allocation 573
```

**Number of tasks requested per cluster:** The value assigned to the -n|--ntasks option is the number of tasks that are requested for allocation from the cluster for the executable. In the current cluster example, it can be 1 to 4 tasks. The default resources available on a cluster are the number of available processor cores.

A resource allocation request for 5 tasks with the --ntasks option causes an error because it exceeds the default resources available on the 4-core cluster:

```
[fred@bright52 ~]$ salloc -n5 mpirun hello
salloc: error: Failed to allocate resources: More processors requested t\
han permitted
```

Adding and configuring just one more node to the current cluster would allows the resource allocation to succeed, since an added node would provide at least one more processor to the cluster.

**Number of tasks requested per node:** The value assigned to the --ntasks-per-node option is the number of tasks that are requested for allocation from each node on the cluster. In the current cluster example, it can be 1 to 4 tasks. A resource allocation request for 5 tasks per

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node with --ntasks-per-node fails on this 4-core cluster, giving an output like:

```
[fred@bright52 ~]$ salloc --ntasks-per-node=5 mpirun hello
salloc: error: Failed to allocate resources: More processors requested t\
han permitted
```

Adding and configuring another 4-core node to the current cluster would still not allow resource allocation to succeed, because the request is for at least 5 cores per node, rather than per cluster.

**Restricting the number of tasks that can run per node:** A resource allocation request for 2 tasks per node with the --ntasks-per-node option, and simultaneously an allocation request for 1 task to run on the cluster using the --ntasks option, runs successfully, although it uselessly ties up resources for 1 task per node:

```
[fred@bright52 ~]$ salloc --ntasks-per-node=2 --ntasks=1 mpirun hello
salloc: Granted job allocation 574
Hello world from process 0 out of 1, host name node005
salloc: Relinquishing job allocation 574
```

The other way round, that is, a resource allocation request for 1 task per node with the --ntasks-per-node option, and simultaneously an allocation request for 2 tasks to run on the cluster using the --ntasks option, fails because on the 1-cluster node, only 1 task can be allocated resources on the single node, while resources for 2 tasks are being asked for on the cluster:

```
[fred@bright52 ~]$ salloc --ntasks-per-node=1 --ntasks=3 mpirun hello
salloc: error: Failed to allocate resources: Requested node configuratio\
n is not available
salloc: Job allocation 575 has been revoked.
```

## 5.3 Running The Executable As A Slurm Job Script

Instead of using options appended to the salloc command line as in section 5.2, it is usually more convenient to send jobs to Slurm with the sbatch command acting on a job script.

A job script is also sometimes called a batch file. In a job script, the user can add and adjust the Slurm options, which are the same as the salloc options of section 5.2. The various settings and variables that go with the application can also be adjusted.

### 5.3.1 Slurm Job Script Structure

A job script submission for the Slurm batch job script format is illustrated by the following:

```
[fred@bright52 ~]$ cat slurmhello.sh
#!/bin/sh
#SBATCH -o my.stdout
#SBATCH --time=30     #time limit to batch job
#SBATCH -N 4
#SBATCH --ntasks=16
#SBATCH --ntasks-per-node=4
```

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```
module add shared openmpi/gcc/64/1.4.2 slurm
mpirun hello
```

The structure is:

**shebang line:** shell definition line.

**SBATCH lines:** optional job script *directives* (section 5.3.2).

**shell commands:** optional shell commands, such as loading necessary modules.

**application execution line:** execution of the MPI application using `sbatch`, the Slurm submission wrapper.

In SBATCH lines, "`#SBATCH`" is used to submit options. The various meanings of lines starting with "`#`" are:

| Line Starts With | Treated As |
|---|---|
| `#` | Comment in shell and Slurm |
| `#SBATCH` | Comment in shell, option in Slurm |
| `# SBATCH` | Comment in shell and Slurm |

After the Slurm job script is run with the `sbatch` command (Section 5.3.4), the output goes into file `my.stdout`, as specified by the "`-o`" command.

If the output file is not specified, then the file takes a name of the form "`slurm-<`*jobnumber*`>.out`", where <*jobnumber*> is a number starting from 1.

The command "`sbatch --usage`" lists possible options that can be used on the command line or in the job script. Command line values override script-provided values.

### 5.3.2 Slurm Job Script Options

Options, sometimes called "directives", can be set in the job script file using this line format for each option:

```
#SBATCH {option} {parameter}
```

Directives are used to specify the resource allocation for a job so that Slurm can manage the job optimally. Available options and their descriptions can be seen with the output of `sbatch --help`. The more overviewable usage output from `sbatch --usage` may also be helpful.

Some of the more useful ones are listed in the following table:

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| Directive Description | Specified As |
|---|---|
| Name the job <*jobname*> | `#SBATCH -J <jobname>` |
| Request at least <*minnodes*> nodes | `#SBATCH -N <minnodes>` |
| Request <*minnodes*> to <*maxnodes*> nodes | `#SBATCH -N <minnodes>-<maxnodes>` |
| Request at least <*MB*> amount of temporary disk space | `#SBATCH --tmp <MB>` |
| Run the job for a time of <*walltime*> | `#SBATCH -t <walltime>` |
| Run the job at <*time*> | `#SBATCH --begin <time>` |
| Set the working directory to <*directorypath*> | `#SBATCH -D <directorypath>` |
| Set error log name to <*jobname.err*>* | `#SBATCH -e <jobname.err>` |
| Set output log name to <*jobname.log*>* | `#SBATCH -o <jobname.log>` |
| Mail <*user@address*> | `#SBATCH --mail-user <user@address>` |
| Mail on any event | `#SBATCH --mail-type=ALL` |
| Mail on job end | `#SBATCH --mail-type=END` |
| Run job in partition | `#SBATCH -p <destination>` |
| Run job using GPU with ID <*number*>, as described in section 8.5.2 | `#SBATCH --gres=gpu:<number>` |

*By default, both standard output and standard error go to a file "`slurm-<%j>.out`", where <%*j*> is the job number.

### 5.3.3 Slurm Environment Variables

Available environment variables include:

```
SLURM_CPUS_ON_NODE - processors available to the job on this node
SLURM_JOB_ID - job ID of executing job
SLURM_LAUNCH_NODE_IPADDR - IP address of node where job launched
SLURM_NNODES - total number of nodes
SLURM_NODEID - relative node ID of current node
SLURM_NODELIST - list of nodes allocated to job
SLURM_NTASKS - total number of processes in current job
SLURM_PROCID - MPI rank (or relative process ID) of the current process
SLURM_SUBMIT_DIR - directory from with job was launched
SLURM_TASK_PID - process ID of task started
SLURM_TASKS_PER_NODE - number of task to be run on each node.
CUDA_VISIBLE_DEVICES - which GPUs are available for use
```

Typically, end users use `SLURM_PROCID` in a program so that an input of a parallel calculation depends on it. The calculation is thus spread across processors according to the assigned `SLURM_PROCID`, so that each processor handles the parallel part of the calculation with different values.

More information on environment variables is also to be found in the man page for `sbatch`.

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### 5.3.4 Submitting The Slurm Job Script

Submitting a Slurm job script created like in the previous section is done by executing the job script with `sbatch`:

```
[fred@bright52 ~]$ sbatch slurmhello.sh
Submitted batch job 703
[fred@bright52 ~]$ cat slurm-703.out
Hello world from process 001 out of 004, processor name node001
...
```

Queues in Slurm terminology are called "partitions". Slurm has a default queue called `defq`. The administrator may have removed this or created others.

If a particular queue is to be used, this is typically set in the job script using the `-p` or `--partition` option:

```
#SBATCH --partition=bitcoinsq
```

It can also be specified as an option to the `sbatch` command during submission to Slurm.

### 5.3.5 Checking And Changing Queued Job Status

After a job has gone into a queue, the queue status can be checked using the `squeue` command. The job number can be specified with the `-j` option to avoid seeing other jobs. The man page for `squeue` covers other options.

Jobs can be canceled with "`scancel <job number>`".

The `scontrol` command allows users to see and change the job directives while the job is still queued. For example, a user may have specified a job, using the `--begin` directive, to start at 10am the next day by mistake. To change the job to start at 10pm tonight, something like the following session may take place:

```
[fred@bright52 ~]$ scontrol show jobid=254 | grep Time
   RunTime=00:00:04 TimeLimit=UNLIMITED TimeMin=N/A
   SubmitTime=2011-10-18T17:41:34 EligibleTime=2011-10-19T10:00:00
   StartTime=2011-10-18T17:44:15 EndTime=Unknown
   SuspendTime=None SecsPreSuspend=0
```

The parameter that should be changed is "`EligibleTime`", which can be done as follows:

```
[fred@bright52 ~]$ scontrol update jobid=254 EligibleTime=2011-10-18T22:00:00
```

An approximate GUI Slurm equivalent to `scontrol` is the `sview` tool. This allows the job to be viewed under its jobs tab, and the job to be edited with a right click menu item. It can also carry out many other functions, including canceling a job.

Webbrowser-accessible job viewing is possible from the workload tab of the `User Portal` (section 10.2).

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# 6

# SGE

Sun Grid Engine (SGE) is a workload management and job scheduling system first developed to manage computing resources by Sun Microsystems. SGE has both a graphical interface and command line tools for submitting, monitoring, modifying and deleting jobs.

SGE uses *job scripts* to submit and execute jobs. Various settings can be put in the job script, such as number of processors, resource usage and application specific variables.

The steps for running a job through SGE are to:

- Create a job script
- Select the directives to use
- Add the scripts and applications and runtime parameters
- Submit it to the workload management system

## 6.1 Writing A Job Script

A binary cannot be submitted directly to SGE—a job script is needed for that. A job script can contain various settings and variables to go with the application. A job script format looks like:

```
#!/bin/bash
#$ Script options  # Optional script directives
shell commands     # Optional shell commands
application        # Application itself
```

### 6.1.1 Directives

It is possible to specify options ('directives') to SGE by using "`#$`" in the script. The difference in the meaning of lines that start with the "`#`" character in the job script file should be noted:

| Line Starts With | Treated As |
|---|---|
| `#` | Comment in shell and SGE |
| `#$` | Comment in shell, directive in SGE |
| `# $` | Comment in shell and SGE |

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### 6.1.2 SGE Environment Variables

Available environment variables:

```
$HOME - Home directory on execution machine
$USER - User ID of job owner
$JOB_ID - Current job ID
$JOB_NAME - Current job name; (like the -N option in qsub, qsh, qrsh, q\
login and qalter)
$HOSTNAME - Name of the execution host
$TASK_ID - Array job task index number
```

### 6.1.3 Job Script Options

Options can be set in the job script file using this line format for each option:

```
#$ {option} {parameter}
```

Available options and their descriptions can be seen with the output of `qsub -help`:

*Table 6.1.3: SGE Job Script Options*

| Option and parameter | Description |
|---|---|
| `-a date_time` | request a start time |
| `-ac context_list` | add context variables |
| `-ar ar_id` | bind job to advance reservation |
| `-A account_string` | account string in accounting record |
| `-b y[es]\|n[o]` | handle command as binary |
| `-binding [env\|pe\|set] exp\|lin\|str` | binds job to processor cores |
| `-c ckpt_selector` | define type of checkpointing for job |
| `-ckpt ckpt-name` | request checkpoint method |
| `-clear` | skip previous definitions for job |
| `-cwd` | use current working directory |
| `-C directive_prefix` | define command prefix for job script |
| `-dc simple_context_list` | delete context variable(s) |
| `-dl date_time` | request a deadline initiation time |
| `-e path_list` | specify standard error stream path(s) |
| `-h` | place user hold on job |
| `-hard` | consider following requests "hard" |
| `-help` | print this help |
| `-hold_jid job_identifier_list` | define jobnet interdependencies |
| `-hold_jid_ad job_identifier_list` | define jobnet array interdependencies |
| `-i file_list` | specify standard input stream file(s) |
| `-j y[es]\|n[o]` | merge stdout and stderr stream of job |
| `-js job_share` | share tree or functional job share |

...continued

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*Table 6.1.3: SGE Job Script Options...continued*

| Option and parameter | Description |
|---|---|
| -jsv jsv_url | job submission verification script to be used |
| -l resource_list | request the given resources |
| -m mail_options | define mail notification events |
| -masterq wc_queue_list | bind master task to queue(s) |
| -notify | notify job before killing/suspending it |
| -now y[es]\|n[o] | start job immediately or not at all |
| -M mail_list | notify these e-mail addresses |
| -N name | specify job name |
| -o path_list | specify standard output stream path(s) |
| -P project_name | set job's project |
| -p priority | define job's relative priority |
| -pe pe-name slot_range | request slot range for parallel jobs |
| -q wc_queue_list | bind job to queue(s) |
| -R y[es]\|n[o] | reservation desired |
| -r y[es]\|n[o] | define job as (not) restartable |
| -sc context_list | set job context (replaces old context) |
| -shell y[es]\|n[o] | start command with or without wrapping <loginshell> -c |
| -soft | consider following requests as soft |
| -sync y[es]\|n[o] | wait for job to end and return exit code |
| -S path_list | command interpreter to be used |
| -t task_id_range | create a job-array with these tasks |
| -tc max_running_tasks | throttle the number of concurrent tasks (experimental) |
| -terse | tersed output, print only the job-id |
| -v variable_list | export these environment variables |
| -verify | do not submit just verify |
| -V | export all environment variables |
| -w e\|w\|n\|v\|p | verify mode (error\|warning\|none\|just verify\|poke) for jobs |
| -wd working_directory | use working_directory |
| -@ file | read commandline input from file |

More detail on these options and their use is found in the man page for `qsub`.

### 6.1.4 The Executable Line

In a job script, the executable line is launched with the job launcher command after the directives lines have been dealt with, and after any other shell commands have been carried out to set up the execution environment.

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#### Using `mpirun` In The Executable Line

The `mpirun` job-launcher command is used for executables compiled with MPI libraries. Executables that have not been compiled with MPI libraries, or which are launched without any specified number of nodes, run on a single free node chosen by the workload manager.

The executable line to run a program `myprog` that has been compiled with MPI libraries is run by placing the job-launcher command `mpirun` before it as follows:

```
mpirun myprog
```

#### Using `cm-launcher` With `mpirun` In The Executable Line

For SGE, for some MPI implementations, jobs sometimes leave processes behind after they have ended. A default Bright Cluster Manager installation provides a cleanup utility that removes such processes. To use it, the user simply runs the executable line using the `cm-launcher` wrapper before the `mpirun` job-launcher command:

```
cm-launcher mpirun myprog
```

The wrapper tracks processes that the workload manager launches. When it sees processes that the workload manager is unable to clean up after a job is over, it carries out the cleanup instead. Using `cm-launcher` is recommended if jobs that do not get cleaned up correctly are an issue for the user or administrator.

### 6.1.5 Job Script Examples

Some job script examples are given in this section. Each job script can use a number of variables and directives.

#### Single Node Example Script

An example script for SGE:

```
noob@sgecluster:~$ cat application
#!/bin/sh
#$ -N sleep
#$ -S /bin/sh
# Make sure that the .e and .o file arrive in the
# working directory
#$ -cwd
#Merge the standard out and standard error to one file
#$ -j y
sleep 60
echo Now it is: `date`
```

#### Parallel Example Script

For parallel jobs the `-pe` (parallel environment) option must be assigned to the script. Depending on the interconnect, there may be a choice between a number of parallel environments such as MPICH (Ethernet) or MVAPICH (InfiniBand).

```
#!/bin/sh
#
# Your job name
#$ -N My_Job
```

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```
#
# Use current working directory
#$ -cwd
#
# Join stdout and stderr
#$ -j y
#
# pe (Parallel environment) request. Set your number of requested slots here.
#$ -pe mpich 2
#
# Run job through bash shell
#$ -S /bin/bash

# If modules are needed, source modules environment:
. /etc/profile.d/modules.sh

# Add any modules you might require:

module add shared mpich/ge/gcc/64/3.1

# The following output will show in the output file. Used for debugging.

echo "Got $NSLOTS processors."
echo "Machines:"
cat machines

# Use MPIRUN to run the application
mpirun -machinefile machines ./application
```

The number of available slots can be set by the administrator to an arbitrary value. However, it is typically set so that it matches the number of cores in the cluster, for efficiency reasons. More slots can be set than cores, but most administrators prefer not to do that.

In a job script, the user can request slots from the available slots. Requesting multiple slots therefore typically means requesting multiple cores. In the case of an environment that is not set up as a parallel environment, the request for slots is done with the `-np` option. For jobs that run in a parallel environment, the `-pe` option is used. Mixed jobs, running in both non-MPI and parallel environments are also possible if the administrator has allowed it in the complex attribute slots settings.

Whether the request is granted is decided by the workload manager policy set by the administrator. If the request exceeds the number of available slots, then the request is not granted.

If the administrator has configured the cluster to use cloud computing with `cm-scale-cluster` (section 7.9.2 of the *Administrator Manual*), then the total number of slots available to a cluster changes over time automatically, as nodes are started up and stopped dynamically.

## 6.2 Submitting A Job

The SGE module must be loaded first so that SGE commands can be accessed:

```
$ module add shared sge
```

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With SGE a job can be submitted with `qsub`. The `qsub` command has the following syntax:

```
qsub [ options ] [ jobscript | -- [ jobscript args ]]
```

After completion (either successful or not), output is put in the user's current directory, appended with the job number which is assigned by SGE. By default, there is an error and an output file.

```
myapp.e#{JOBID}
myapp.o#{JOBID}
```

### 6.2.1 Submitting To A Specific Queue

Some clusters have specific queues for jobs which run are configured to house a certain type of job: long and short duration jobs, high resource jobs, or a queue for a specific type of node.

To see which queues are available on the cluster the `qstat` command can be used:

```
qstat -g c
CLUSTER QUEUE   CQLOAD   USED    RES  AVAIL  TOTAL aoACDS  cdsuE
--------------------------------------------------------------------
long.q          0.01      0      0    144    288      0    144
default.q       0.01      0      0    144    288      0    144
```

The job is then submitted, for example to the `long.q` queue:

```
qsub -q long.q sleeper.sh
```

## 6.3 Monitoring A Job

The job status can be viewed with `qstat`. In this example the `sleeper.sh` script has been submitted. Using `qstat` without options will only display a list of jobs, with no queue status options:

```
$ qstat
job-ID  prior   name       user   state submit/start at     queue  slots
-----------------------------------------------------------------------
    249 0.00000 Sleeper1   root   qw    12/03/2008 07:29:00         1
    250 0.00000 Sleeper1   root   qw    12/03/2008 07:29:01         1
    251 0.00000 Sleeper1   root   qw    12/03/2008 07:29:02         1
    252 0.00000 Sleeper1   root   qw    12/03/2008 07:29:02         1
    253 0.00000 Sleeper1   root   qw    12/03/2008 07:29:03         1
```

More details are visible when using the `-f` (for full) option:

- The Queuetype `qtype` can be Batch (B) or Interactive (I).
- The `used/tot` or `used/free` column is the count of used/free slots in the queue.
- The `states` column is the state of the queue.

```
$ qstat -f
queuename                qtype used/tot. load_avg arch          states
---------------------------------------------------------------------
all.q@node001.cm.cluster   BI    0/16      -NA-     lx26-amd64    au
```

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```
---------------------------------------------------------------------------
all.q@node002.cm.cluster   BI    0/16      -NA-     lx26-amd64    au

############################################################################
PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS - PENDING JOBS
############################################################################
    249 0.55500 Sleeper1   root         qw    12/03/2008 07:29:00     1
    250 0.55500 Sleeper1   root         qw    12/03/2008 07:29:01     1
```

Job state can be:

- d(eletion)
- E(rror)
- h(old)
- r(unning)
- R(estarted)
- s(uspended)
- S(uspended)
- t(ransfering)
- T(hreshold)
- w(aiting)

The queue state can be:

- u(nknown) if the corresponding `sge_execd` cannot be contacted
- a(larm) - the load threshold is currently exceeded
- A(larm) - the suspend threshold is currently exceeded
- C(alendar suspended) - see `calendar_conf`
- s(uspended) - see qmod
- S(ubordinate)
- d(isabled) - see qmod
- D(isabled) - see `calendar_conf`
- E(rror) - `sge_execd` was unable to locate the `sge_shepherd` - use qmod to fix it.
- o(rphaned) - for queue instances

By default the `qstat` command shows only jobs belonging to the current user, i.e. the command is executed with the option `-u $user`. To see jobs from other users too, the following format is used:

```
$ qstat -u ''*''
```

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## 6.4 Deleting A Job

A job can be deleted in SGE with the following command

```
$ qdel <jobid>
```

The job-id is the number assigned by SGE when the job is submitted using `qsub`. Only jobs belonging to the logged-in user can be deleted. Using `qdel` will delete a user's job regardless of whether the job is running or in the queue.

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# 7

# PBS Variants: Torque And PBS Pro

Bright Cluster Manager works with Torque and PBS Pro, which are two forks of Portable Batch System (PBS). PBS was a workload management and job scheduling system first developed to manage computing resources at NASA in the 1990s.

Torque and PBS Pro can differ significantly in the output they present when using their GUI visual tools. However because of their historical legacy, their basic design structure and job submission methods from the command line remain very similar for the user. Both Torque and PBS Pro are therefore covered in this chapter. The possible Torque schedulers (Torque's built-in scheduler, Maui, or Moab) are also covered when discussing Torque.

Torque and PBS Pro both offer a graphical interface and command line tools for submitting, monitoring, modifying and deleting jobs.

For submission and execution of jobs, both workload managers use PBS "job scripts". The user puts values into a job script for the resources being requested, such as the number of processors, memory. Other values are also set for the runtime parameters and application-specific variables.

The steps for running a job through a PBS job script are:

- Creating an application to be run via the job script
- Creating the job script, adding directives, applications, runtime parameters, and application-specific variables to the script
- Submitting the script to the workload management system

This chapter covers the using the workload managers and job scripts with the PBS variants so that users can get a basic understanding of how they are used, and can get started with typical cluster usage.

In this chapter:

- section 7.1 covers the components of a job script and job script examples
- section 7.2.1 covers submitting, monitoring, and deleting a job with a job script

More depth on using these workload managers is to be found in the PBS Professional User Guide and in the online Torque documentation at `http://www.adaptivecomputing.com/resources/docs/`.

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## 7.1 Components Of A Job Script

To use Torque or PBS Pro, a batch job script is created by the user. The job script is a shell script containing the set of commands that the user wants to run. It also contains the resource requirement directives and other specifications for the job. After preparation, the job script is submitted to the workload manager using the `qsub` command. The workload manager then tries to make the job run according to the job script specifications.

A job script can be resubmitted with different parameters (e.g. different sets of data or variables).

### 7.1.1 Sample Script Structure

A job script in PBS Pro or Torque has a structure illustrated by the following basic example:

**Example**

```
#!/bin/bash
#
#PBS -l walltime=1:00:00
#PBS -l nodes=4
#PBS -l mem=500mb
#PBS -j oe

cd ${HOME}/myprogs
mpirun myprog a b c
```

The first line is the standard "shebang" line used for scripts.

The lines that start with `#PBS` are PBS directive lines, described shortly in section 7.1.2.

The last two lines are an example of setting remaining options or configuration settings up for the script to run. In this case, a change to the directory `myprogs` is made, and then run the executable `myprog` with arguments `a b c`. The line that runs the program is called the executable line (section 7.1.3).

To run the executable file in the executable line in parallel, the job launcher `mpirun` is placed immediately before the executable file. The number of nodes the parallel job is to run on is assumed to have been specified in the PBS directives.

### 7.1.2 Directives

**Job Script Directives And `qsub` Options**

A job script typically has several configurable values called job script directives, set with job script directive lines. These are lines that start with a "`#PBS`". Any directive lines beyond the first executable line are ignored.

The lines are comments as far as the shell is concerned because they start with a "`#`". However, at the same time the lines are special commands when the job script is processed by the `qsub` command. The difference is illustrated by the following:

- The following shell comment is only a comment for a job script processed by `qsub`:

  ```
  # PBS
  ```

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- The following shell comment is also a job script directive when processed by `qsub`:

```
#PBS
```

Job script directive lines with the "`#PBS `" part removed are the same as options applied to the `qsub` command, so a look at the `man` pages of `qsub` describes the possible directives and how they are used. If there is both a job script directive and a `qsub` command option set for the same item, the `qsub` option takes precedence.

Since the job script file is a shell script, the shell interpreter used can be changed to another shell interpreter by modifying the first line (the "`#!`" line) to the preferred shell. Any shell specified by the first line can also be overridden by using the "`#PBS -S`" directive to set the shell path.

#### Walltime Directive

The workload manager typically has default walltime limits per queue with a value limit set by the administrator. The user sets walltime limit by setting the "`#PBS -l walltime`" directive to a specific time. The time specified is the maximum time that the user expects the job should run for, and it allows the workload manager to work out an optimum time to run the job. The job can then run sooner than it would by default.

If the walltime limit is exceeded by a job, then the job is stopped, and an error message like the following is displayed:

`=» PBS: job killed: walltime <runningtime> exceeded limit <settime>`

Here, <*runningtime*> indicates the time for which the job actually went on to run, while <*settime*> indicates the time that the user set as the walltime resource limit.

#### Resource List Directives

Resource list directives specify arguments to the `-l` directive of the job script, and allow users to specify values to use instead of the system defaults.

For example, in the sample script structure earlier, a job walltime of one hour and a memory space of at least 500MB are requested (the script requires the size of the space be spelled in lower case, so "`500mb`" is used).

If a requested resource list value exceeds what is available, the job is queued until resources become available.

For example, if nodes only have 2000MB to spare and 4000MB is requested, then the job is queued indefinitely, and it is up to the user to fix the problem.

Resource list directives also allow, for example, the number of nodes (`-l nodes`) and the virtual processor cores per nodes (`-l ppn`) to be specified. If no value is specified, the default is 1 core per node.

If 8 cores are wanted, and it does not matter how the cores are allocated (e.g. 8 per node or 1 on 8 nodes) the directive used in Torque is:

```
#PBS -l nodes=8
```

For PBS Pro v11 this also works, but is deprecated, and the form "`#PBS -l select=8`" is recommended instead.

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Further examples of node resource specification are given in a table on page 47.

#### Job Directives: Job Name, Logs, And IDs

If the name of the job script file is `jobname`, then by default the output and error streams are logged to `jobname.o<number>` and `jobname.e<number>` respectively, where <*number*> indicates the associated job number. The default paths for the logs can be changed by using the `-o` and `-e` directives respectively, while the base name (`jobname` here) can be changed using the `-N` directive.

Often, a user may simply merge both logs together into one of the two streams using the -j directive. Thus, in the preceding example, "`-j oe`" merges the logs to the output log path, while "`-j eo`" would merge it to error log path.

The job ID is an identifier based on the job number and the FQDN of the login node. For a login node called `bright52.cm.cluster`, the job ID for a job number with the associated value <*number*> from earlier, would by default be <*number*>.bright52.cm.cluster, but it can also simply be abbreviated to <*number*>.

#### Job Queues

Sending a job to a particular job queue is sometimes appropriate. An administrator may have set queues up so that some queues are for very long term jobs, or some queues are for users that require GPUs. Submitting a job to a particular queue <*destination*> is done by using the directive "`#PBS -q <destination>`".

#### Directives Summary

A summary of the job directives covered, with a few extras, are shown in the following table:

| Directive Description | Specified As |
|---|---|
| Name the job <*jobname*> | `#PBS -N <jobname>` |
| Run the job for a time of <*walltime*> | `#PBS -l <walltime>` |
| Run the job at <*time*> | `#PBS -a <time>` |
| Set error log name to <*jobname.err*> | `#PBS -e <jobname.err>` |
| Set output log name to <*jobname.log*> | `#PBS -o <jobname.log>` |
| Join error messages to output log | `#PBS -j eo` |
| Join output messages to error log | `#PBS -j oe` |
| Mail to <*user@address*> | `#PBS -M <user@address>` |
| Mail on <*event*> | `#PBS -m <event>` |
| where <*event*> takes the | `(a)bort` |
| value of the letter in | `(b)egin` |
| the parentheses | `(e)nd` |
| | `(n) do not send email` |
| Queue is <*destination*> | `#PBS -q <destination>` |
| Login shell path is <*shellpath*> | `#PBS -S <shellpath>` |

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#### Resource List Directives Examples

Examples of how requests for resource list directives work are shown in the following table:

| Resource Example Description | "#PBS -l" Specification |
|---|---|
| Request 500MB memory | `mem=500mb` |
| Set a maximum runtime of 3 hours 10 minutes and 30 seconds | `walltime=03:10:30` |
| 8 nodes, anywhere on the cluster | `nodes=8*` |
| 8 nodes, anywhere on the cluster | `select=8**` |
| 2 nodes, 1 processor per node | `nodes=2:ppn=1` |
| 3 nodes, 8 processors per node | `nodes=3:ppn=8` |
| 5 nodes, 2 processors per node and 1 GPU per node | `nodes=5:ppn=2:gpus=1*` |
| 5 nodes, 2 processors per node, and 1 GPU per node | `select=5:ncpus=2:ngpus=1**` |
| 5 nodes, 2 processors per node, 3 virtual processors for MPI code | `select=5:ncpus=2:mpiprocs=3**` |
| 5 nodes, 2 processors per node, using any GPU on the nodes | `select=5:ncpus=2:ngpus=1**` |
| 5 nodes, 2 processors per node, using a GPU with ID 0 from nodes | `select=5:ncpus=2:gpu_id=0**` |

*For Torque 2.5.5
**For PBS Pro 11

Some of the examples illustrate requests for GPU resource usage. GPUs and the CUDA utilities for NVIDIA are introduced in Chapter 8. In the Torque and PBS Pro workload managers, GPU usage is treated like the attributes of a resource which the cluster administrator will have pre-configured according to local requirements.

For further details on resource list directives, the Torque and PBS Pro user documentation should be consulted.

### 7.1.3 The Executable Line

In the job script structure (section 7.1.1), the executable line is launched with the job launcher command after the directives lines have been dealt with, and after any other shell commands have been carried out to set up the execution environment.

#### Using `mpirun` In The Executable Line

The `mpirun` command is used for executables compiled with MPI libraries. Executables that have not been compiled with MPI libraries, or which are launched without any specified number of nodes, run on a single free node chosen by the workload manager.

The executable line to run a program `myprog` that has been compiled with MPI libraries is run by placing the job-launcher command `mpirun` before it as follows:

```
mpirun myprog
```

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#### Using `cm-launcher` With `mpirun` In The Executable Line

For Torque, for some MPI implementations, jobs sometimes leave processes behind after they have ended. A default Bright Cluster Manager installation provides a cleanup utility that removes such processes. To use it, the user simply runs the executable line using the `cm-launcher` wrapper before the `mpirun` job-launcher command:

```
cm-launcher mpirun myprog
```

The wrapper tracks processes that the workload manager launches. When it sees processes that the workload manager is unable to clean up after the job is over, it carries out the cleanup instead. Using `cm-launcher` is recommended if jobs that do not get cleaned up correctly are an issue for the user or administrator.

### 7.1.4 Example Batch Submission Scripts

#### Node Availability

The following job script tests which out of 4 nodes requested with "`-l nodes`" are made available to the job in the workload manager:

**Example**

```
#!/bin/bash
#PBS -l walltime=1:00
#PBS -l nodes=4
echo -n "I am on: "
hostname;

echo finding ssh-accessible nodes:
for node in $(cat ${PBS_NODEFILE}) ; do
    echo -n "running on: "
    /usr/bin/ssh $node hostname
done
```

The directive specifying `walltime` means the script runs at most for 1 minute. The `${PBS_NODEFILE}` array used by the script is created and appended with hosts by the queueing system. The script illustrates how the workload manager generates a `${PBS_NODEFILE}` array based on the requested number of nodes, and which can be used in a job script to spawn child processes. When the script is submitted, the output from the log will look like:

```
I am on: node001
finding ssh-accessible nodes:
running on: node001
running on: node002
running on: node003
running on: node004
```

This illustrates that the job starts up on a node, and that no more than the number of nodes that were asked for in the resource specification are provided.

The list of all nodes for a cluster can be found using the `pbsnodes` command (section 7.2.6).

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#### Using InfiniBand

A sample PBS script for InfiniBand is:

```
#!/bin/bash
#!
#! Sample PBS file
#!
#! Name of job

#PBS -N MPI

#! Number of nodes (in this case 8 nodes with 4 CPUs each)
#! The total number of nodes passed to mpirun will be nodes*ppn
#! Second entry: Total amount of wall-clock time (true time).
#! 02:00:00 indicates 02 hours

#PBS -l nodes=8:ppn=4,walltime=02:00:00

#! Mail to user when job terminates or aborts
#PBS -m ae

# If modules are needed by the script, then source modules environment:
. /etc/profile.d/modules.sh

# Add any modules you might require:
module add shared mvapich/gcc torque maui pbspro

#! Full path to application + application name
application="<application>"

#! Run options for the application
options="<options>"

#! Work directory
workdir="<work dir>"

###############################################################
### You should not have to change anything below this line ####
###############################################################

#! change the working directory (default is home directory)

cd $workdir

echo Running on host $(hostname)
echo Time is $(date)
echo Directory is $(pwd)
echo PBS job ID is $PBS_JOBID
echo This job runs on the following machines:
echo $(cat $PBS_NODEFILE | uniq)

mpirun_command="mpirun $application $options"

#! Run the parallel MPI executable (nodes*ppn)
echo Running $mpirun_command
eval $mpirun_command
```

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In the preceding script, no machine file is needed, since it is automatically built by the workload manager and passed on to the `mpirun` parallel job launcher utility. The job is given a unique ID and run in parallel on the nodes based on the resource specification.

### 7.1.5 Links To Other Resources About Job Scripts In Torque And PBS Pro

A number of useful links are:

- Torque examples:
  `http://bmi.cchmc.org/resources/software/torque/examples`
- PBS Pro script files:
  `http://www.ccs.tulane.edu/computing/pbs/pbs.phtml`

## 7.2 Submitting A Job

### 7.2.1 Preliminaries: Loading The Modules Environment

To submit a job to the workload management system, the user must ensure that the following environment modules are loaded:

- If using Torque with no external scheduler:

```
$ module add shared torque
```

- If using Torque with Maui:

```
$ module add shared torque maui
```

- If using Torque with Moab:

```
$ module add shared torque moab
```

- If using PBS Pro:

```
$ module add shared pbspro
```

Users can pre-load particular environment modules as their default using the "`module init*`" commands (section 2.3.3).

### 7.2.2 Using `qsub`

The command `qsub` is used to submit jobs to the workload manager system. The command returns a unique job identifier, which is used to query and control the job and to identify output. The usage format of `qsub` and some useful options are listed here:

```
USAGE: qsub [<options>] <job script>

Option  Hint    Description
------  ----    -----------
-a      at      run the job at a certain time
-l      list    request certain resource(s)
-q      queue   job is run in this queue
-N      name    name of job
-S      shell   shell to run job under
-j      join    join output and error files
```

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For example, a job script called `mpirun.job` with all the relevant directives set inside the script, may be submitted as follows:

**Example**

```
$ qsub mpirun.job
```

A job may be submitted to a specific queue `testq` as follows:

**Example**

```
$ qsub -q testq mpirun.job
```

The `man` page for `qsub` describes these and other options. The options correspond to PBS directives in job scripts (section 7.1.1). If a particular item is specified by a `qsub` option as well as by a PBS directive, then the `qsub` option takes precedence.

### 7.2.3 Job Output

By default, the output from the job script <*scriptname*> goes into the home directory of the user for Torque, or into the current working directory for PBS Pro.

By default, error output is written to <*scriptname*>`.e`<*jobid*> and the application output is written to <*scriptname*>`.o`<*jobid*>, where <*jobid*> is a unique number that the workload manager allocates. Specific output and error files can be set using the `-o` and `-e` options respectively. The error and output files can usefully be concatenated into one file with the `-j oe` or `-j eo` options. More details on this can be found in the `qsub` man page.

### 7.2.4 Monitoring A Job

To use the commands in this section, the appropriate workload manager module must be loaded. For example, for Torque, `torque` module needs to be loaded:

```
$ module add torque
```

**`qstat` Basics**

The main component is `qstat`, which has several options. In this example, the most frequently used options are discussed.

In PBS/Torque, the command "`qstat -an`" shows what jobs are currently submitted or running on the queuing system. An example output is:

```
[fred@bright52 ~]$ qstat -an
bright52.cm.cluster:
                                                  Req'd  Req'd   Elap
Job ID          User     Queue  Jobname SessID NDS TSK Memory Time  S Time
--------------- -------- ------ ------- ------ --- --- ------ ----- - -----
78.bright52     fred     shortq tjob     10476   1   1  555mb 00:01 R 00:00
79.bright52     fred     shortq tjob       --    1   1  555mb 00:01 Q   --
```

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The output shows the Job ID, the user who owns the job, the queue, the job name, the session ID for a running job, the number of nodes requested, the number of CPUs or tasks requested, the time requested (`-l walltime`), the job state (S) and the elapsed time. In this example, one job is seen to be running (R), and one is still queued (Q). The `-n` parameter causes nodes that are in use by a running job to display at the end of that line.

Possible job states are:

| Job States | Description |
|---|---|
| C | Job is completed (regardless of success or failure) |
| E | Job is exiting after having run |
| H | Job is held |
| Q | job is queued, eligible to run or routed |
| R | job is running |
| S | job is suspend |
| T | job is being moved to new location |
| W | job is waiting for its execution time |

The command "`qstat -q`" shows what queues are available. In the following example, there is one job running in the `testq` queue and 4 are queued.

```
$ qstat -q

server: master.cm.cluster

Queue            Memory CPU Time Walltime Node  Run Que Lm  State
---------------- ------ -------- -------- ----  --- --- --  -----
testq              --      --    23:59:59   --    1   4 --   E R
default            --      --    23:59:59   --    0   0 --   E R
                                                ----- -----
                                                    1     4
```

`showq` **From Maui**

If the Maui scheduler is running, and the Maui module loaded (`module add maui`), then Maui's `showq` command displays a similar output. In this example, one dual-core node is available (1 node, 2 processors), one job is running and 3 are queued (in the `Idle` state).

```
$ showq
ACTIVE JOBS----------
JOBNAME    USERNAME    STATE   PROC  REMAINING   STARTTIME

45         cvsupport   Running 2     1:59:57     Tue Jul 14 12:46:20

     1 Active Job        2 of   2 Processors Active (100.00%)
                         1 of   1 Nodes Active      (100.00%)

IDLE JOBS------------
JOBNAME    USERNAME    STATE   PROC  WCLIMIT     QUEUETIME

46         cvsupport   Idle    2     2:00:00     Tue Jul 14 12:46:20
```

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```
47          cvsupport   Idle    2     2:00:00     Tue Jul 14 12:46:21
48          cvsupport   Idle    2     2:00:00     Tue Jul 14 12:46:22

3 Idle Jobs

BLOCKED JOBS----------
JOBNAME    USERNAME    STATE   PROC  WCLIMIT     QUEUETIME


Total Jobs: 4   Active Jobs: 1   Idle Jobs: 3   Blocked Jobs: 0
```

**Viewing Job Details With `qstat` And `checkjob`**

**Job Details With `qstat`** With `qstat -f` the full output of the job is displayed. The output shows what the jobname is, where the error and output files are stored, and various other settings and variables.

```
$ qstat -f
Job Id: 19.mascm4.cm.cluster
    Job_Name = TestJobPBS
    Job_Owner = cvsupport@mascm4.cm.cluster
    job_state = Q
    queue = testq
    server = mascm4.cm.cluster
    Checkpoint = u
    ctime = Tue Jul 14 12:35:31 2009
    Error_Path = mascm4.cm.cluster:/home/cvsupport/test-package/TestJobPBS
    .e19
    Hold_Types = n
    Join_Path = n
    Keep_Files = n
    Mail_Points = a
    mtime = Tue Jul 14 12:35:31 2009
    Output_Path = mascm4.cm.cluster:/home/cvsupport/test-package/TestJobPB
    S.o19
    Priority = 0
    qtime = Tue Jul 14 12:35:31 2009
    Rerunable = True
    Resource_List.nodect = 1
    Resource_List.nodes = 1:ppn=2
    Resource_List.walltime = 02:00:00
    Variable_List = PBS_O_HOME=/home/cvsupport,PBS_O_LANG=en_US.UTF-8,
    PBS_O_LOGNAME=cvsupport,
    PBS_O_PATH=/usr/kerberos/bin:/usr/local/bin:/bin:/usr/bin:/sbin:/usr/
    sbin:/home/cvsupport/bin:/cm/shared/apps/torque/2.3.5/bin:/cm/shar
    ed/apps/torque/2.3.5/sbin,PBS_O_MAIL=/var/spool/mail/cvsupport,
    PBS_O_SHELL=/bin/bash,PBS_SERVER=mascm4.cm.cluster,
    PBS_O_HOST=mascm4.cm.cluster,
    PBS_O_WORKDIR=/home/cvsupport/test-package,PBS_O_QUEUE=default
    etime = Tue Jul 14 12:35:31 2009
    submit_args = pbs.job -q default
```

**Job Details With `checkjob`** The `checkjob` command (only for Maui) is particularly useful for checking why a job has not yet executed. For a job that has an excessive memory requirement, the output looks something like:

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```
[fred@bright52 ~]$ checkjob 65

checking job 65

State: Idle
Creds:  user:fred  group:fred  class:shortq  qos:DEFAULT
WallTime: 00:00:00 of 00:01:00
SubmitTime: Tue Sep 13 15:22:44
  (Time Queued  Total: 2:53:41  Eligible: 2:53:41)

Total Tasks: 1

Req[0]  TaskCount: 1  Partition: ALL
Network: [NONE]  Memory >= 0  Disk >= 0  Swap >= 0
Opsys: [NONE]  Arch: [NONE]  Features: [NONE]
Dedicated Resources Per Task: PROCS: 1  MEM: 495M

IWD: [NONE]  Executable:  [NONE]
Bypass: 0  StartCount: 0
PartitionMask: [ALL]
Flags:       RESTARTABLE

PE:  1.01  StartPriority:  173
job cannot run in partition DEFAULT (idle procs do not meet requirement\
s : 0 of 1 procs found)
idle procs:   3  feasible procs:   0

Rejection Reasons: [CPU          :    3]
```

The `-v` option gives slightly more detail.

### 7.2.5 Deleting A Job

An already submitted job can be deleted using the `qdel` command:

```
$ qdel <jobid>
```

The job ID is printed to the terminal when the job is submitted. To get the job ID of a job if it has been forgotten, the following can be used:

```
$ qstat
```

or

```
$ showq
```

### 7.2.6 Monitoring Nodes In Torque And PBS Pro

The nodes that the workload manager knows about can be viewed using the `pbsnodes` command.

The following output is from a cluster made up of 2-core nodes, as indicated by the value of 2 for `ncpu` for Torque and PBS Pro. If the node is available to run scripts, then its state is `free` or `time-shared`. When a node is used exclusively (section 8.5.2) by one script, the state is `job-exclusive`.

For Torque the display resembles (some output elided):

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```
[fred@bright52 ~]$ pbsnodes -a
node001.cm.cluster
     state = free
     np = 3
     ntype = cluster
     status = rectime=1317911358,varattr=,jobs=96...ncpus=2...
     gpus = 1

node002.cm.cluster
     state = free
     np = 3
     ...
     gpus = 1

     ...
```

For PBS Pro the display resembles (some output elided):

```
[fred@bright52 ~]$ pbsnodes -a
node001.cm.cluster
     Mom = node001.cm.cluster
     ntype = PBS
     state = free
     pcpus = 3
     resources_available.arch = linux
     resources_available.host = node001
     ...
     sharing = default_shared

node002.cm.cluster
     Mom = node002.cm.cluster
     ntype = PBS
     state = free
     ...

     ...
```

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# 8

# Using GPUs

GPUs (Graphics Processing Units) are chips that provide specialized parallel processing power. Originally, GPUs were designed to handle graphics processing as part of the video processor, but their ability to handle non-graphics tasks in a similar manner has become important for general computing. GPUs designed for general purpose computing task are commonly called General Purpose GPUs, or GPGPUs.

A GPU is suited for processing an algorithm that naturally breaks down into a process requiring many similar calculations running in parallel. GPUs cores are able to rapidly apply the instruction on multiple data points organized in a 2-D, and more recently, 3-D, image. The image is placed in a framebuffer. In the original chips, the data points held in the framebuffer were intended for output to a display, thereby accelerating image generation.

The similarity between multicore CPU chips and modern GPUs makes it at first sight attractive to use GPUs for general purpose computing. However, the instruction set on GPGPUs is used in a component called the *shader pipeline*. This is, as the name suggests, to do with a limited set of graphics operations, and so is by its nature rather limited. Using the instruction set for problems unrelated to shader pipeline manipulations requires that the problems being processed map over to a similar manipulation. This works best for algorithms that naturally break down into a process requiring an operation to be applied in the same way on many independent vertices and pixels. In practice, this means that 1-D vector operations are an order of magnitude less efficient on GPUs than operations on triangular matrices.

Modern GPGPU implementations have matured so that they can now sub-divide their resources between independent processes that work on independent data, and they provide programmer-friendlier ways of data transfer between the host and GPU memory.

Physically, one GPU is typically a built-in part of the motherboard of a node or a board in a node, and consists of several hundred processing cores. There are also dedicated standalone units, commonly called GPU Units, consisting of several GPUs in one chassis. Several of these can be assigned to particular nodes, typically via PCI-Express connections, to increase the density of parallelism even further.

Bright Cluster Managerhas several tools that can be used to set up and program GPUs for general purpose computations.

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## 8.1 Packages

A number of different GPU-related packages are included in Bright Cluster Manager. For CUDA these are:

- `cuda50-driver`: Provides the GPU driver
- `cuda50-libs`: Provides the libraries that come with the driver (libcuda etc)
- `cuda50-toolkit`: Provides the compilers, cuda-gdb, and math libraries
- `cuda50-tools`: Provides the CUDA tools SDK
- `cuda50-profiler`: Provides the CUDA visual profiler
- `cuda50-sdk`: Provides additional tools, development files and source examples

CUDA versions 4.2, and 5.0 are also provided by Bright Cluster Manager. The exact implementation depends on how the system administrator has configured CUDA.

## 8.2 Using CUDA

After installation of the packages, for general usage and compilation it is sufficient to load just the CUDA<*version*>/toolkit module, where <*version*> is a number, `42` or `50`, indicating the version.

```
module add cuda50/toolkit
```

Also available are several other modules related to CUDA:

- `cuda50/blas`: Provides paths and settings for the CUBLAS library.
- `cuda50/fft`: Provides paths and settings for the CUFFT library.

The toolkit comes with the necessary tools and the NVIDIA compiler wrapper to compile CUDA C code.

Extensive documentation on how to get started, the various tools, and how to use the CUDA suite is in the `$CUDA_INSTALL_PATH/doc` directory.

## 8.3 Using OpenCL

OpenCL functionality is provided with the `cuda`<*version*>`/toolkit` environment module, where <*version*> is a number, `42`, or `50`.

Examples of OpenCL code can be found in the `$CUDA_SDK/OpenCL` directory.

## 8.4 Compiling Code

Both CUDA and OpenCL involve running code on different *platforms*:

- `host`: with one or more CPUs
- `device`: with one or more CUDA enabled GPUs

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Accordingly, both the host and device manage their own memory space, and it is possible to copy data between them. The CUDA and OpenCL Best Practices Guides in the `doc` directory, provided by the CUDA toolkit package, have more information on how to handle both platforms and their limitations.

The `nvcc` command by default compiles code and links the objects for both the host system and the GPU. The `nvcc` command distinguishes between the two and it can hide the details from the developer. To compile the host code, `nvcc` will use `gcc` automatically.

```
nvcc [options] <inputfile>
```

A simple example to compile CUDA code to an executable is:

```
nvcc testcode.cu -o testcode
```

The most used options are:

- `-g` or `-debug <level>`: This generates debug-able code for the host
- `-G` or `-device-debug <level>`: This generates debug-able code for the GPU
- `-o` or `-output-file <file>`: This creates an executable with the name <*file*>
- `-arch=sm_13`: This can be enabled if the CUDA device supports compute capability 1.3, which includes double-precision

If double-precision floating-point is not supported or the flag is not set, warnings such as the following will come up:

```
warning : Double is not supported. Demoting to float
```

The `nvcc` documentation manual, "*The CUDA Compiler Driver NVCC*" has more information on compiler options.

The CUDA SDK has more programming examples and information accessible from the file `$CUDA_SDK/C/Samples.html`.

For OpenCL, code compilation can be done by linking against the OpenCL library:

```
gcc test.c -lOpenCL
g++ test.cpp -lOpenCL
nvcc test.c -lOpenCL
```

## 8.5 Available Tools

### 8.5.1 CUDA gdb

The CUDA debugger can be started using: `cuda-gdb`. Details of how to use it are available in the "*CUDA-GDB (NVIDIA CUDA Debugger)*" manual, in the `doc` directory. It is based on GDB, the GNU Project debugger, and requires the use of the "`-g`" or "`-G`" options compiling.

#### Example

```
nvcc -g -G testcode.cu -o testcode
```

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### 8.5.2 nvidia-smi

The NVIDIA System Management Interface command, `nvidia-smi`, can be used to allow exclusive access to the GPU. This means only one application can run on a GPU. By default, a GPU will allow multiple running applications.
Syntax:

```
nvidia-smi [OPTION1 [ARG1]] [OPTION2 [ARG2]] ...
```

The steps for making a GPU exclusive:

- List GPUs
- Select a GPU
- Lock GPU to a compute mode
- After use, release the GPU

After setting the compute rule on the GPU, the first application which executes on the GPU will block out all others attempting to run. This application does not necessarily have to be the one started by the user that set the exclusivity lock on the GPU!

To list the GPUs, the `-L` argument can be used:

```
$ nvidia-smi -L
GPU 0: (05E710DE:068F10DE)  Tesla T10 Processor  (S/N: 706539258209)
GPU 1: (05E710DE:068F10DE)  Tesla T10 Processor  (S/N: 2486719292433)
```

To set the ruleset on the GPU:

```
$ nvidia-smi -i 0 -c 1
```

The ruleset may be one of the following:

- 0 - Default mode (multiple applications allowed on the GPU)
- 1 - Exclusive thread mode (only one compute context is allowed to run on the GPU, usable from one thread at a time)
- 2 - Prohibited mode (no compute contexts are allowed to run on the GPU)
- 3 - Exclusive process mode (only one compute context is allowed to run on the GPU, usable from multiple threads at a time)

To check the state of the GPU:

```
$ nvidia-smi -i 0 -q
COMPUTE mode rules for GPU 0: 1
```

In this example, GPU0 is locked, and there is a running application using GPU0. A second application attempting to run on this GPU will not be able to run on this GPU.

```
$ histogram  --device=0
main.cpp(101) : cudaSafeCall() Runtime API error :
no CUDA-capable device is available.
```

After use, the GPU can be unlocked to allow multiple users:

```
nvidia-smi -i 0 -c 0
```

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### 8.5.3 CUDA Utility Library

CUTIL is a simple utility library designed for use in the CUDA SDK samples. There are 2 parts for CUDA and OpenCL. The locations are:

- $CUDA_SDK/C/lib
- $CUDA_SDK/OpenCL/common/lib

Other applications may also refer to them, and the toolkit libraries have already been pre-configured accordingly. However, they need to be compiled prior to use. Depending on the cluster, this might have already have been done.

```
[fred@demo ~] cd
[fred@demo ~] cp -r $CUDA_SDK
[fred@demo ~] cd $(basename $CUDA_SDK); cd C
[fred@demo C] make
[fred@demo C] cd $(basename $CUDA_SDK); cd OpenCL
[fred@demo OpenCL] make
```

CUTIL provides functions for:

- parsing command line arguments
- read and writing binary files and PPM format images
- comparing data arrays (typically used for comparing GPU results with CPU results)
- timers
- macros for checking error codes
- checking for shared memory bank conflicts

### 8.5.4 CUDA "Hello world" Example

A hello world example code using CUDA is:

**Example**

```
/*
  CUDA example
  "Hello World" using shift13, a rot13-like function.
  Encoded on CPU, decoded on GPU.

  rot13 cycles between 26 normal alphabet characters.

  shift13 shifts 13 steps along the normal alphabet characters
  So it translates half the alphabet into non-alphabet characters

  shift13 is used because it is simpler than rot13 in c
  so we can focus on the point

  (c) Bright Computing
  Taras Shapovalov <taras.shapovalov@brightcomputing.com>
 */
```

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```
#include <cuda.h>  \* remove this line in CUDA 6 onwards *\
#include <cutil_inline.h> \* remove this line in CUDA 6 onwards *\
#include <stdio.h>

// CUDA kernel definition: undo shift13
__global__ void helloWorld(char* str) {
  int idx = blockIdx.x * blockDim.x + threadIdx.x;
  str[idx] -= 13;
}

int main(int argc, char** argv )
{
  char s[] = "Hello World!";
  printf("String for encode/decode: %s\n", s);

  // CPU shift13
  int len = sizeof(s);
  for (int i = 0; i < len; i++) {
    s[i] += 13;
  }
  printf("String encoded on CPU as: %s\n", s);

  // Allocate memory on the CUDA device
  char *cuda_s;
  cudaMalloc((void**)&cuda_s, len);

  // Copy the string to the CUDA device
  cudaMemcpy(cuda_s, s, len, cudaMemcpyHostToDevice);

  // Set the grid and block sizes  (dim3 is a type)
  // and "Hello World!" is 12 characters, say 3x4
  dim3 dimGrid(3);
  dim3 dimBlock(4);

  // Invoke the kernel to undo shift13 in GPU
  helloWorld<<< dimGrid, dimBlock >>>(cuda_s);

  // Retrieve the results from the CUDA device
  cudaMemcpy(s, cuda_s, len, cudaMemcpyDeviceToHost);

  // Free up the allocated memory on the CUDA device
  cudaFree(cuda_s);

  printf("String decoded on GPU as: %s\n", s);
  return 0;
}
```

The preceding code example may be compiled and run with:

```
[fred@bright52 ~]$ nvcc hello.cu -o hello
[fred@bright52 ~]$ module add shared openmpi/gcc/64/1.4.4 slurm
[fred@bright52 ~]$ salloc -n1 --gres=gpu:1 mpirun hello
salloc: Granted job allocation 2263
String for encode/decode: Hello World!
String encoded on CPU as: Uryy|-d|yq.
```

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```
String decoded on GPU as: Hello World!
alloc: Relinquishing job allocation 2263
salloc: Job allocation 2263 has been revoked.
```

The number of characters displayed in the encoded string appear less than expected because there are unprintable characters in the encoding due to the cipher used being not exactly rot13.

### 8.5.5 OpenACC

OpenACC (`http://www.openacc-standard.org`) is a new open parallel programming standard aiming at simplifying the programmability of heterogeneous CPU/GPU computing systems. OpenACC allows parallel programmers to provide *OpenACC directives* to the compiler, identifying which areas of code to accelerate. This frees the programmer from carrying out time-consuming modifications to the original code itself. By pointing out parallelism to the compiler, directives get the compiler to carry out the details of mapping the computation onto the accelerator.

Using OpenACC directives requires a compiler that supports the OpenACC standard.

In the following example, where $\pi$ is calculated, adding the `#pragma` directive is sufficient for the compiler to produce code for the loop that can run on either the GPU or CPU:

#### Example

```
#include <stdio.h>
 #define N 1000000

 int main(void) {
 double pi = 0.0f; long i;
 #pragma acc parallel loop reduction(+:pi)
 for (i=0; i<N; i++) {
    double t= (double)((i+0.5)/N);
    pi +=4.0/(1.0+t*t);
 }
 printf("pi=%16.15f\n",pi/N);
 return 0;
 }
```

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# 9

# Using MICs

The hardware concept of the Intel MIC (Many Integrated Cores) architecture is to bundle many x86-like chips into a processor, currently implemented in the Intel Xeon Phi release. The MIC implementation is placed on a MIC card, which can be hosted inside a node using the PCIe bus. In this chapter, the word MIC on its own implies the MIC architecture or implementation.

Bright Cluster Manager deals with MIC cards as if they are regular nodes. If the Slurm workload manager is used, then the MIC cards become compute nodes in Slurm, because the Slurm compute daemon (slurmd) can be started inside a MIC card. MIC offloading is supported by an appropriate generic resource in the workload managers supported by Bright Cluster Manager. Both offloaded and native jobs are supported by Slurm.

This guide does not give details on how to write code for MIC, or what tools and libraries should be used to do so.

The next two sections give an overview of the native and offload modes under which MIC can be used.

## 9.1 Compiling Code In Native Mode

The simplest way to run applications on the Intel Xeon Phi coprocessor is in native mode. The native application can be compiled inside a coprocessor or on a host. In the second case the binary can then be copied to the coprocessor and has to be started there. Although the MIC and x86_64 architectures are very similar, the MIC native application cannot be run on an x86_64 core. The MIC assembly instruction set is highly, but not completely, x86-compatible, and also has some additional scalar and vector instructions not found elsewhere. Therefore, to run a distributed MPI application on MICs and on hosts at the same time, two versions of the application binary have to be built.

### 9.1.1 Using The GNU Compiler

Bright Cluster Manager provides a patched `gcc` which can be used to build a native MIC application. However, Intel recommends using the Intel Compiler (section 9.1.2), which can create a more-optimized k1om code for a better performance.

By default `gcc` with MIC support is in the following directory:

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```
/usr/linux-k1om-<version>
```

To build a native application on an x86_64 host, the compiler tools prefixed by `x86_64-k1om-linux-` have to be used:

**Example**

```
[user@bright70 ~]$ module load intel/mic/runtime
[user@bright70 ~]$ x86_64-k1om-linux-gcc ./test.c -o test
[user@bright70 ~]$
```

If the GNU autoconf tool is used, then the following shell commands can be used to build the application:

```
MIC_ARCH=k1om
GCC_VERSION=4.7
GCC_ROOT=/usr/linux-${MIC_ARCH}-${GCC_VERSION}
./configure \
  CXX="${GCC_ROOT}/bin/x86_64-${MIC_ARCH}-linux-g++"  \
  CXXFLAGS="-I${GCC_ROOT}/linux-${MIC_ARCH}/usr/include" \
  CXXCPP="${GCC_ROOT}/bin/x86_64-${MIC_ARCH}-linux-cpp" \
  CC="${GCC_ROOT}/bin/x86_64-${MIC_ARCH}-linux-gcc" \
  CFLAGS="-I${GCC_ROOT}/linux-${MIC_ARCH}/usr/include" \
  CPP="${GCC_ROOT}/bin/x86_64-${MIC_ARCH}-linux-cpp" \
  LDFLAGS="-L${GCC_ROOT}/linux-${MIC_ARCH}/usr/lib64" \
  LD="${GCC_ROOT}/bin/x86_64-${MIC_ARCH}-linux-ld" \
  --build=x86_64-redhat-linux \
  --host=x86_64-${MIC_ARCH}-linux \
  --target=x86_64-${MIC_ARCH}-linux
make
```

### 9.1.2 Using Intel Compilers

Intel Composer XE, version 2013 and higher, can also be used to compile a native application on Intel Xeon Phi coprocessors.

The compiler for this is at:

```
/opt/intel/composer_xe_<version>
```

The `-mmic` switch generates code for the MIC on the non-MIC host. For example:

```
[user@bright70 ~]$ module load intel/compiler/64/13.0
[user@bright70 ~]$ icc -mmic ./test.c -o test
[user@bright70 ~]$
```

If the GNU autoconf application is used instead, then the environment variables are like those defined earlier in section 9.1.1.

Detailed information on building a native application for the Intel Xeon Phi coprocessor using the Intel compilers can be found at `http://software.intel.com/en-us/articles/building-a-native-application-for-intel-xeon-phi-coprocessors`.

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## 9.2 Compiling Code In Offload Mode

MICs can also build user applications in offload (heterogeneous) mode. With this method, the application starts on a host platform. The Intel Compiler should be used, since the current stable version of the GNU Compiler does not support this mode. A special statement, #pragma, should be added to the C/C++ or Fortran code to mark regions of code that are to be offloaded to a MIC and run there. This directive approach ressembles that used by the PGI compiler, CAPS HMPP, or OpenACC, when these specify the offloading of code to GPUs.

In this case, all data transfer and synchronization are managed by the compiler and runtime. When an offload code region is encountered and a MIC is found on the host, the offload code and data are transferred and run on the MIC coprocessor. If no available MIC devices are found, then the offload code is run on the host CPU(s).

Offload statements can also be combined with OpenMP directives. The following "`hello_mic`" example shows how a system call is offloaded to the MIC. The example is used in other sections of this chapter:

**Example**

```
#include <stdio.h>
#include <stdlib.h>
#include <limits.h>
#include <unistd.h>

int main(void) {
  char hostname[HOST_NAME_MAX];
  #pragma offload target(mic)
  {
    gethostname(hostname, HOST_NAME_MAX);
    printf("My hostname is \%s\n", hostname);
  }
  exit(0);
}
```

Standard command line arguments, with no MIC-related switch required, compile the code. This is because offloading is enabled by default in Intel Compiler version 2013 and higher:

**Example**

```
[user@bright70 ~]$ module load intel/compiler/64/13.0
[user@bright70 ~]$ icc -O3 ./hello_mic.c -o hello_mic
[user@bright70 ~]$ module load intel/mic/runtime
[user@bright70 ~]$ ./hello_mic
My hostname is bright70-mic0
[user@bright70 ~]$
```

To get debug information when an offloaded region is executed, the `OFFLOAD_REPORT` environment variable can be used. Possible values, in order of increasing verbosity, are 1, 2, or 3. Setting the empty string disables debug messages:

**Example**

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```
[user@bright70 ~]$ module load intel/mic/runtime
[user@bright70 ~]$ export OFFLOAD_REPORT=2
[user@bright70 ~]$ ./hello_mic
[Offload] [MIC 0] [File]            ./hello_mic.c
[Offload] [MIC 0] [Line]            7
[Offload] [MIC 0] [Tag]             Tag0
[Offload] [MIC 0] [CPU Time]        0.000000 (seconds)
[Offload] [MIC 0] [CPU->MIC Data]   64 (bytes)
[Offload] [MIC 0] [MIC Time]        0.000134 (seconds)
[Offload] [MIC 0] [MIC->CPU Data]   64 (bytes)

My hostname is node001-mic0
[user@bright70 ~]$
```

More information on building applications in offload mode can be found at `http://software.intel.com/en-us/articles/the-heterogeneous-programming-model`.

## 9.3 Using MIC With Workload Managers

When a MIC is configured as a regular node, the user can start a native application inside the MIC. This can be done by logging into it directly using `ssh` or using a workload manager. The workload manager schedules jobs by determining the order in which the jobs will use the MIC cards. This is the recommended way to use MIC cards on a multiuser cluster, but currently only Slurm supports both the native and offload modes. All other workload managers support only offload mode, by using a preconfigured generic resource.

### 9.3.1 Using MIC Cards With Slurm

**Offload mode:** The user creates a job script and specifies a consumable resource "`mic`". For example, the following job script runs the `dgemm` test from the MIC binaries on a host where at least one MIC is available and free:

```
#!/bin/sh
#SBATCH --partition=defq
#SBATCH --gres=mic:1

module load intel-cluster-runtime/intel64
/opt/intel/mic/perf/bin/intel64/dgemm_cpu.x -i 2 -l 2048
```

The job is submitted as usual using the `sbatch` or `salloc/srun` commands of Slurm (chapter 5).

**Native mode—non-distributed job:** The user creates a job script and sets a constraint "`miccard`". For example, the following job script runs the `dgemm` test directly inside the MIC:

```
#!/bin/sh
#SBATCH --partition=micq
#SBATCH --constraint="miccard"

module load intel-cluster-runtime/intel-mic
/opt/intel/mic/perf/bin/mic/dgemm_mic.x -i 2 -l 2048
```

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**Native mode—MPI job:** The user creates a job script in the same way as for non-distributed job, but the `--nodes` parameter is specified. For example, the next job script executes the Intel IMB-MPI1 benchmark on two MICs using RDMA calls:

```
#!/bin/sh
#SBATCH --partition=micq
#SBATCH --constraint="miccard"
#SBATCH --nodes=2

SLURM_BIN=/cm/shared/apps/slurm/current/k1om-arch/bin
MPI_DIR=/cm/shared/apps/intel/mpi/current/mic
MPI_RUN=$MPI_DIR/bin/mpirun
APP=$MPI_DIR/bin/IMB-MPI1
APP_ARGS="PingPong"
MPI_ARGS="-genv I_MPI_DAPL_PROVIDER ofa-v2-scif0 -genv I_MPI_FABRICS=shm\
:dapl -perhost 1"

export LD_LIBRARY_PATH=/lib64:$MPI_DIR/lib:$LD_LIBRARY_PATH
export PATH=$SLURM_BIN:$MPI_DIR/bin/:$PATH
$MPI_RUN $MPI_ARGS $APP $APP_ARGS
```

The value of DAPL provider (the argument `I_MPI_DAPL_PROVIDER`) should be set to `ofa-v2-scif0` when an application needs MIC-to-MIC or MIC-to-HOST RDMA communication.

All Slurm job examples given here can be found on a cluster in the following directory:

```
/cm/shared/examples/workload/slurm/jobscripts/
```

### 9.3.2 Using MIC Cards With PBS Pro

PBS Pro version 12.0 and higher allows a special virtual node to be created, which represents a MIC coprocessor. This virtual node is a consumable resource, which can be allocated and released like any other resources, for example, like a GPU. A MIC coprocessor is represented as a virtual node, altough users cannot actually start a native job via PBS Pro. All nodes that show the property `resources_available.mic_id` as an output to the command `pbsnodes -av` are MICs.

Users can request a number of MICs for offload jobs as follows:

```
[user@bright70 ~]$ qsub -l select=1:ncpus=2+mic_id=1:ncpus=0 ./mic-offload-job
```

At the time of writing, PBS Pro (version 12.1) is not pinning tasks to a specific MIC device. That is, the `OFFLOAD_DEVICES` environment variable is not set for a job.

### 9.3.3 Using MIC Cards With TORQUE

TORQUE version 4.2 and higher detects MIC cards automatically and sets the `OFFLOAD_DEVICES` environment variable for a job. To find out how many MIC cards are detected by TORQUE and to find out their detected properties, the `pbsnodes` command can be run. For example:

```
[user@bright70 ~]$ pbsnodes node001 | grep mic
     mics = 1
     mic_status = mic[0]=mic_id=8796;num_cores=61;num_threads=244;phys\
```

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```
mem=8071106560;free_physmem=7796191232;swap=0;free_swap=0;max_frequenc\
y=1181;isa=COI_ISA_KNC;load=0.400000;normalized_load=0.006557
[user@bright70 ~]$
```

However, the `mics` consumable resource can be used only when TORQUE is used together with MOAB, otherwise the job is never scheduled. This behavior is subject to change, but has been verified on MAUI 3.3.1 and `pbs_sched` 4.2.2. When MOAB is used, then user can submit a job, with offload code regions, as shown in the following example:

**Example**

```
#!/bin/sh
#PBS -N TEST_MIC_OFFLOAD
#PBS -l nodes=1:mics=2

module load intel/mic/runtime
module load intel-cluster-runtime/intel-mic
module load intel-cluster-runtime/intel64

./hello_mic
```

These examples can be found in:

```
/cm/shared/examples/workload/torque/jobscripts/
```

### 9.3.4 Using MIC Cards With SGE

Bright Cluster Manager distributes a branch of SGE called Open Grid Scheduler (OGE). OGE, for which the current version is 2011.11p1, does not have native support of MIC devices, and the `OFFLOAD_DEVICES` environment variable will not be set for a job by default. However, the support can be emulated using consumable resources.

### 9.3.5 Using MIC Cards With `openlava`

openlava does not have a native support of MIC devices, and the `OFFLOAD_DEVICES` environment variable is not set for a job by default. However, the support can be emulated using a consumable resource.

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# 10

# User Portal

The user portal allows users to login via a browser and view the state of the cluster themselves. It is a read-only interface.

The first time a browser is used to login to the cluster portal, a warning about the site certificate being untrusted appears in a default Bright Cluster Manager configuration. This can safely be accepted.

## 10.1 Home Page

The default home page allows a quick glance to convey the most important cluster-related information for users (figure 10.1):

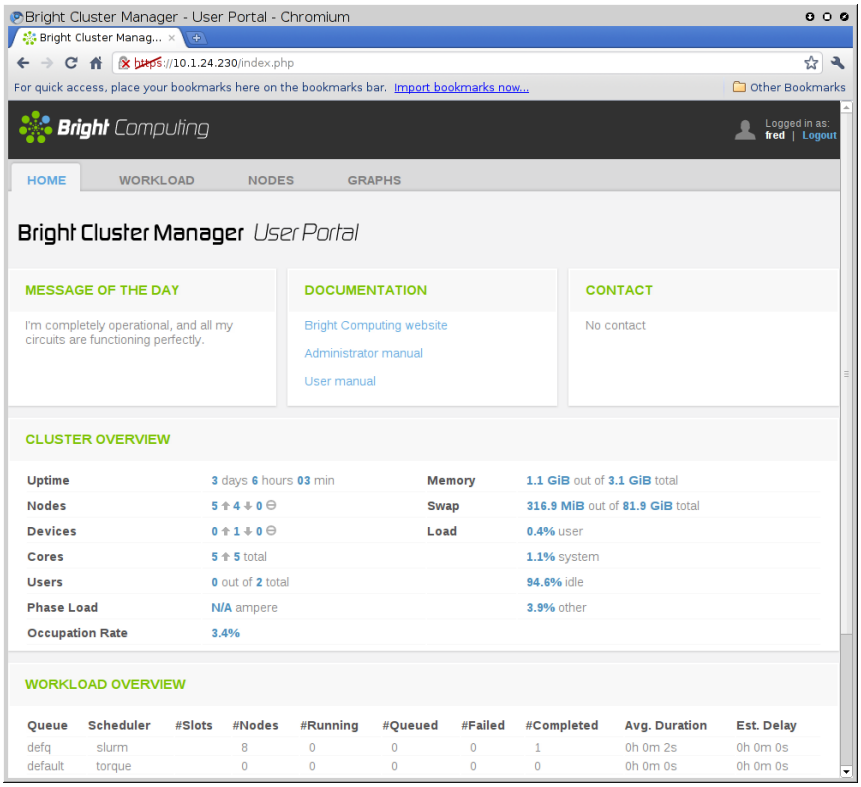


Figure 10.1: User Portal: Default Home Page

The following items are displayed on a default home page:

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- a Message Of The Day. The administrator may put up important messages for users here
- links to the documentation for the cluster
- contact information. This typically shows how to contact technical support
- an overview of the cluster state, displaying some cluster parameters
- a workload overview. This is a table displaying a summary of queues and their associated jobs

## 10.2 The WORKLOAD Tab

The page opened by clicking on the WORKLOAD tab allows a user to see workload-related information for the cluster (figure 10.2).

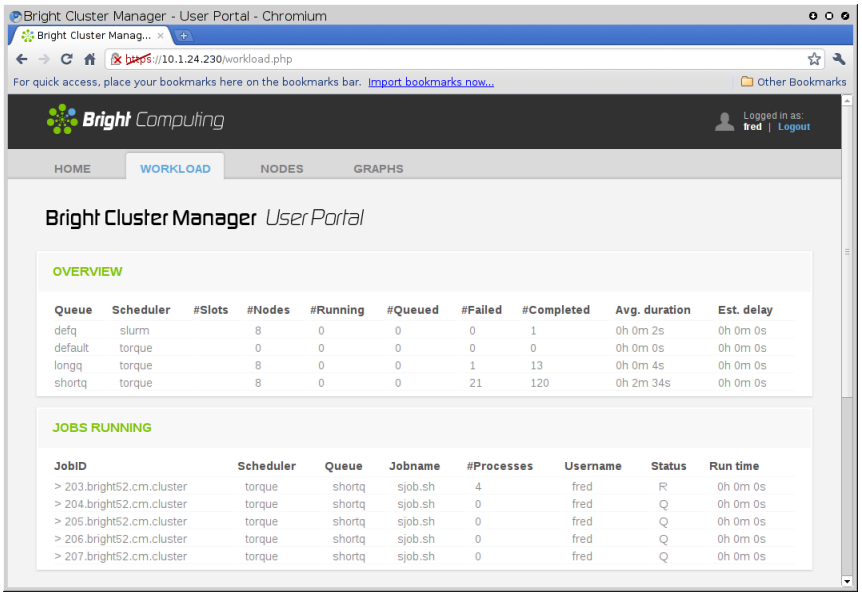


Figure 10.2: User Portal: Workload Page

The following two tables are displayed:

- A workload overview table (the same as the table in the home page).
- A table displaying the current jobs running on the cluster

## 10.3 The NODES Tab

The page opened by clicking on the NODES tab shows a list of nodes on the cluster (figure 10.3).

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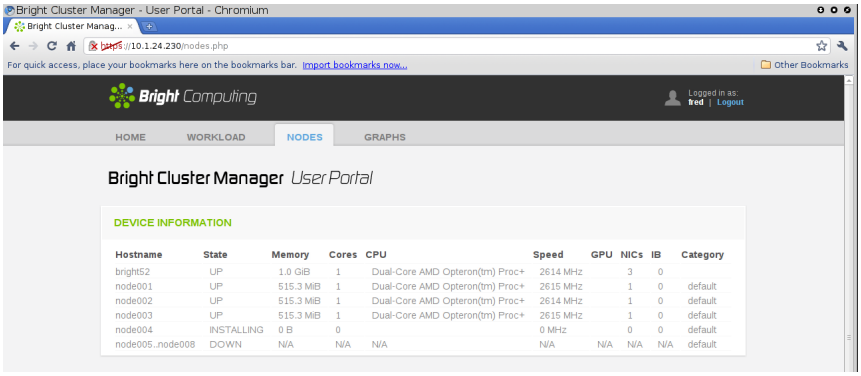


Figure 10.3: User Portal: Nodes Page

The following information about the head or regular nodes is presented:

- `Hostname`: the node name
- `State`: For example, `UP`, `DOWN`, `INSTALLING`
- `Memory`: RAM on the node
- `Cores`: Number of cores on the node
- `CPU`: Type of CPU, for example, Dual-Core AMD Opteron™
- `Speed`: Processor speed
- `GPU`: Number of GPUs on the node, if any
- `NICs`: Number of network interface cards on the node, if any
- `IB`: Number of InfiniBand interconnects on the node, if any
- Category: The node category that the node has been allocated by the administrator (by default it is `default`)

## 10.4 The GRAPHS Tab

By default the GRAPHS tab displays the cluster occupation rate for the last hour (figure 10.4).

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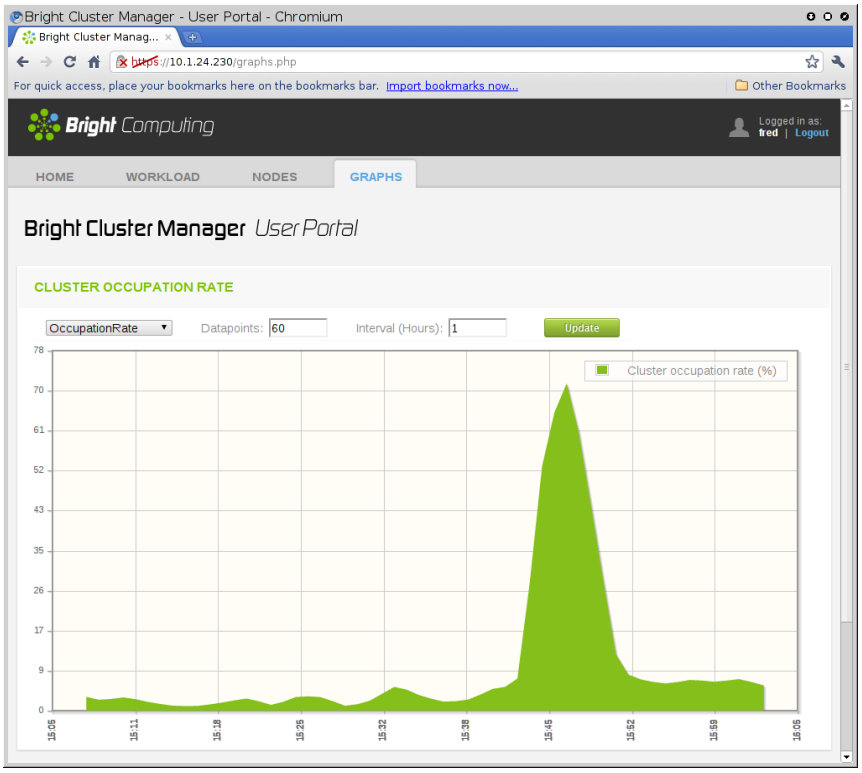


Figure 10.4: User Portal: Graphs Page

Selecting other values is possible for

- Workload Management Metrics. The following workload manager metrics can be viewed:
  - RunningJobs
  - QueuedJobs
  - FailedJobs
  - CompletedJobs
  - EstimatedDelay
  - AvgJobDuration
  - AvgExpFactor
- Cluster Management Metrics. The following metrics can be viewed
  - OccupationRate
  - NetworkBytesRecv
  - NetworkBytesSent
  - DevicesUp
  - NodesUp
  - TotalMemoryUsed
  - TotalSwapUsed
  - PhaseLoad
  - CPUCoresAvailable

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  - GPUAvailable
  - TotalCPUUser
  - TotalCPUSystem
  - TotalCPUIdle

- Datapoints: The number of points used for the graph can be specified. The points are interpolated if necessary
- Interval (Hours): The period over which the data points are displayed

The Update button must be clicked to display any changes made.

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# A

# MPI Examples

## A.1 "Hello world"

A quick application to test the MPI libraries and the network.

```
/*
 ``Hello World'' Type MPI Test Program
*/
#include <mpi.h>
#include <stdio.h>
#include <string.h>

#define BUFSIZE 128
#define TAG 0

int main(int argc, char *argv[])
{
  char idstr[32];
  char buff[BUFSIZE];
  int numprocs;
  int myid;
  int i;
  MPI_Status stat;

  /* all MPI programs start with MPI_Init; all 'N' processes exist thereafter */
  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD,&numprocs); /* find out how big the SPMD world is */
  MPI_Comm_rank(MPI_COMM_WORLD,&myid); /* and this processes' rank is */

  /* At this point, all the programs are running equivalently, the rank is used to
     distinguish the roles of the programs in the SPMD model, with rank 0 often used
     specially... */
  if(myid == 0)
  {
    printf("%d: We have %d processors\n", myid, numprocs);
    for(i=1;i<numprocs;i++)
    {
      sprintf(buff, "Hello %d! ", i);
      MPI_Send(buff, BUFSIZE, MPI_CHAR, i, TAG, MPI_COMM_WORLD);
    }
    for(i=1;i<numprocs;i++)
```

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```
    {
      MPI_Recv(buff, BUFSIZE, MPI_CHAR, i, TAG, MPI_COMM_WORLD, &stat);
      printf("%d: %s\n", myid, buff);
    }
  }
  else
  {
    /* receive from rank 0: */
    MPI_Recv(buff, BUFSIZE, MPI_CHAR, 0, TAG, MPI_COMM_WORLD, &stat);
    sprintf(idstr, "Processor %d ", myid);
    strcat(buff, idstr);
    strcat(buff, "reporting for duty\n");
    /* send to rank 0: */
    MPI_Send(buff, BUFSIZE, MPI_CHAR, 0, TAG, MPI_COMM_WORLD);
  }

  /* MPI Programs end with MPI Finalize; this is a weak
     synchronization point */
  MPI_Finalize();
  return 0;
}
```

## A.2 MPI Skeleton

The sample code below contains the complete communications skeleton for a dynamically load balanced head/compute node application. Following the code is a description of some of the functions necessary for writing typical parallel applications.

```
include <mpi.h>
#define WORKTAG     1
#define DIETAG     2
main(argc, argv)
int argc;
char *argv[];
{
        int         myrank;
        MPI_Init(&argc, &argv);   /* initialize MPI */
        MPI_Comm_rank(
        MPI_COMM_WORLD,   /* always use this */
        &myrank);      /* process rank, 0 thru N-1 */
        if (myrank == 0) {
                head();
        } else {
                computenode();
        }
        MPI_Finalize();       /* cleanup MPI */
}

head()
{
        int     ntasks, rank, work;
        double       result;
        MPI_Status     status;
        MPI_Comm_size(
```

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```
        MPI_COMM_WORLD,   /* always use this */
        &ntasks);          /* #processes in application */
/*
* Seed the compute nodes.
*/
        for (rank = 1; rank < ntasks; ++rank) {
                work = /* get_next_work_request */;
                MPI_Send(&work,         /* message buffer */
                1,              /* one data item */
                MPI_INT,        /* data item is an integer */
                rank,           /* destination process rank */
                WORKTAG,        /* user chosen message tag */
                MPI_COMM_WORLD);/* always use this */
        }



/*
* Receive a result from any compute node and dispatch a new work
* request work requests have been exhausted.
*/
        work = /* get_next_work_request */;
        while (/* valid new work request */) {
                MPI_Recv(&result,       /* message buffer */
                1,              /* one data item */
                MPI_DOUBLE,     /* of type double real */
                MPI_ANY_SOURCE, /* receive from any sender */
                MPI_ANY_TAG,    /* any type of message */
                MPI_COMM_WORLD, /* always use this */
                &status);       /* received message info */
                MPI_Send(&work, 1, MPI_INT, status.MPI_SOURCE,
                WORKTAG, MPI_COMM_WORLD);
                work = /* get_next_work_request */;
        }
/*
* Receive results for outstanding work requests.
*/
        for (rank = 1; rank < ntasks; ++rank) {
                MPI_Recv(&result, 1, MPI_DOUBLE, MPI_ANY_SOURCE,
                MPI_ANY_TAG, MPI_COMM_WORLD, &status);
        }
/*
* Tell all the compute nodes to exit.
*/
        for (rank = 1; rank < ntasks; ++rank) {
                MPI_Send(0, 0, MPI_INT, rank, DIETAG, MPI_COMM_WORLD);
        }
}

computenode()
{
        double              result;
        int                 work;
        MPI_Status          status;
        for (;;) {
                MPI_Recv(&work, 1, MPI_INT, 0, MPI_ANY_TAG,
```

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```
                MPI_COMM_WORLD, &status);
/*
* Check the tag of the received message.
*/
                if (status.MPI_TAG == DIETAG) {
                        return;
                }
                result = /* do the work */;
                MPI_Send(&result, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD);
        }
}
```

Processes are represented by a unique rank (integer) and ranks are numbered 0, 1, 2, ..., N-1. MPI_COMM_WORLD means all the processes in the MPI application. It is called a communicator and it provides all information necessary to do message passing. Portable libraries do more with communicators to provide synchronisation protection that most other systems cannot handle.

## A.3 MPI Initialization And Finalization

As with other systems, two functions are provided to initialize and clean up an MPI process:

```
MPI_Init(&argc, &argv);
MPI_Finalize( );
```

## A.4 What Is The Current Process? How Many Processes Are There?

Typically, a process in a parallel application needs to know who it is (its rank) and how many other processes exist.

A process finds out its own rank by calling:

```
MPI_Comm_rank( ):
Int myrank;
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
```

The total number of processes is returned by `MPI_Comm_size( )`:

```
int nprocs;
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
```

## A.5 Sending Messages

A message is an array of elements of a given data type. MPI supports all the basic data types and allows a more elaborate application to construct new data types at runtime. A message is sent to a specific process and is marked by a tag (integer value) specified by the user. Tags are used to distinguish between different message types a process might send/receive. In the sample code above, the tag is used to distinguish between work and termination messages.

```
MPI_Send(buffer, count, datatype, destination, tag, MPI_COMM_WORLD);
```

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## A.6 Receiving Messages

A receiving process specifies the tag and the rank of the sending process. `MPI_ANY_TAG` and `MPI_ANY_SOURCE` may be used optionally to receive a message of any tag and from any sending process.

```
MPI_Recv(buffer, maxcount, datatype, source, tag, MPI_COMM_WORLD, &status);
```

Information about the received message is returned in a status variable. The received message tag is `status.MPI_TAG` and the rank of the sending process is `status.MPI_SOURCE`. Another function, not used in the sample code, returns the number of data type elements received. It is used when the number of elements received might be smaller than `maxcount`.

```
MPI_Get_count(&status, datatype, &nelements);
```

## A.7 Blocking, Non-Blocking, And Persistent Messages

`MPI_Send` and `MPI_Receive` cause the running program to wait for non-local communication from a network. Most communication networks function at least an order of magnitude slower than local computations. When an MPI process has to wait for non-local communication CPU cycles are lost because the operating system has to block the process, then has to wait for communication, and then resume the process.

An optimal efficiency is usually best achieved by overlapping communication and computation. *Blocking* messaging functions only allow one communication to occur at a time. *Non-blocking* messaging functions allow the application to initiate multiple communication operations, enabling the MPI implementation to proceed simultaneously. *Persistent* non-blocking messaging functions allow a communication state to persist, so that the MPI implementation does not waste time on initializing or terminating a communication.

### A.7.1 Blocking Messages

In the following example, the communication implementation executes in a sequential fashion causing each process, `MPI_Recv`, then `MPI_Send`, to block while waiting for its neighbor:

**Example**

```
while (looping) {
  if (i_have_a_left_neighbor)
    MPI_Recv(inbuf, count, dtype, left, tag, comm, &status);
  if (i_have_a_right_neighbor)
    MPI_Send(outbuf, count, dtype, right, tag, comm);
  do_other_work();
}
```

MPI also has the potential to allow both communications to occur simultaneously, as in the following communication implementation example:

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### A.7.2 Non-Blocking Messages

**Example**

```
while (looping) {
  count = 0;
  if (i_have_a_left_neighbor)
    MPI_Irecv(inbuf, count, dtype, left, tag, comm, &req[count++]);
  if (i_have_a_right_neighbor)
    MPI_Isend(outbuf, count, dtype, right, tag, comm, &req[count++]);
  MPI_Waitall(count, req, &statuses);
  do_other_work();
}
```

In the example, `MPI_Waitall` potentially allows both communications to occur simultaneously. However, the process as show is blocked until both communications are complete.

### A.7.3 Persistent, Non-Blocking Messages

A more efficient use of the waiting time means to carry out some other work in the meantime that does not depend on that communication. If the same buffers and communication parameters are to be used in each iteration, then a further optimization is to use the MPI persistent mode. The following code instructs MPI to set up the communications once, and communicate similar messages every time:

**Example**

```
int count = 0;
if (i_have_a_left_neighbor)
  MPI_Recv_init(inbuf, count, dtype, left, tag, comm, &req[count++]);
if (i_have_a_right_neighbor)
  MPI_Send_init(outbuf, count, dtype, right, tag, comm, &req[count++]);
while (looping) {
 MPI_Startall(count, req);
  do_some_work();
  MPI_Waitall(count, req, &statuses);
 do_rest_of_work();
}
```

In the example, `MPI_Send_init` and `MPI_Recv_init` perform a persistent communication initialization.

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# B

# Compiler Flag Equivalence

The following table is an overview of some of the compiler flags that are equivalent or almost equivalent.

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| PGI | Pathscale | Cray | Intel | GCC | Explanation |
|---|---|---|---|---|---|
| `-fast` | `-O3` | default | default | `-O3 -ffast-math` | Produce high level of optimization |
| `-mp=nonuma` | `-mp` | `-Oomp` (default) | `-openmp` | `-fopenmp` | Activate OpenMP directives and pragmas in the code |
| `-byteswapio` | `-byteswapio` | `-h byteswapio` | `-convert big_endian` | `-fconvert=swap` | Read and write Fortran unformatted data files as big-endian |
| `-Mfixed` | `-fixedform` | `-f fixed` | `-fixed` | `-ffixed-form` | Process Fortran source using fixed form specifications. |
| `-Mfree` | `-freeform` | `-f free` | `-free` | `-ffree-form` | Process Fortran source using free form specifications. |
| `-V` | `-dumpversion` | `-V` | `--version` | `--version` | Dump version. |
| N/A | `-zerouv` | `-h zero` | N/A | `-finit-local-zero` | Zero fill all uninitialized variables. |
| | | `-e m` | | | Creates `.mod` files to hold Fortran90 module information for future compiles. |
| | | `-j` <*dir_name*> | | | Specifies the directory <*dir_name*> to which `.mod` files are written when the `-e m` option is specified |



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