HPC

BAS4 for Xeon

User's Guide

REFERENCE
86 A2 91ET 02

HPC

BAS4 for Xeon

User's Guide

Software

December 2007

BULL CEDOC
357 AVENUE PATTON
B.P.20845
49008 ANGERS CEDEX 01
FRANCE

REFERENCE
86 A2 91ET 02

Printed in France

Suggestions and criticisms concerning the form, content, and presentation of this book are invited. A form is provided at the end of this book for this purpose.

To order additional copies of this book or other Bull Technical Publications, you are invited to use the Ordering Form also provided at the end of this book.

Trademarks and Acknowledgements

We acknowledge the rights of the proprietors of the trademarks mentioned in this manual.

All brand names and software and hardware product names are subject to trademark and/or patent protection.

Quoting of brand and product names is for information purposes only and does not represent trademark misuse.

Preface

Scope and Objectives

The purpose of this guide is to describe the tools and libraries available as part of the **Bull BAS4 for Xeon** delivery which allow the development and testing of application programs on the **Bull High Performance Computing (HPC)** clusters. In addition various open source and proprietary tools are described.

Intended Readers

This guide is for users and developers of HPC applications.

Prerequisites

The installation of all hardware and software components of the HPC must have been completed. The HPC administrator must have performed basic administration tasks (creation of users, definition of the file systems, network configuration, etc).

See the Bull HPC BAS4 for Xeon *Administrator's Guide* (86 A2 83ET) for more details.

Structure

This guide is organized as follows:

Chapter 1. *Introduction to the HPC Environment.*
Provides a general introduction to Bull's HPC software environment.

Two types of programming libraries are used when developing programs for the HPC environment: Parallel libraries and Mathematical libraries. These are described in the chapters 2 and 3:

Chapter 2. *Parallel Libraries.*
Describes the Message Passing Interface (MPI) libraries to be used when parallel programming.

Chapter 3. *Scientific Libraries.*
Describes the scientific libraries and scientific functions delivered with the Bull HPC XBAS delivery and how these should be invoked. Some of Intel's proprietary libraries are also described.

Chapter 4. *Compilers.*
Describes the compilers available and how to use them.

Chapter 5. *The User's Environment.*
Describes the user's environment on Bull HPC clusters, how the clusters are accessed and the use of the file systems. A description of Modules follows. These can be used to change and compare environments.

Chapter 6. *Resource Management using SLURM*
Describes the SLURM Resource Management utilities and commands.

Chapter 7. *Batch Management and Launching an Application*
Describes how to use the PBS Professional Batch Manager.

Chapter 8. *Debugging Tools.*
Describes Debugging Tools.

Appendix A A *Troubleshooting guide* which enables you to diagnose some common problems.

Glossary and Acronyms
Provides a Glossary and lists the Acronyms used in the manual.

Bibliography

- Bull HPC BAS4 for Xeon *Installation and Configuration Guide* (86 A2 82ET)
- Bull HPC BAS4 for Xeon *Administrator's Guide* (86 A2 83ET)
- Bull HPC BAS4 for Xeon *Maintenance Guide* (86 A2 92ET)
- The Bull HPC BAS4 for Xeon *Software Release Bulletin* (SRB) (86 A2 54EJ) provides release-specific information and details of restrictions resulting from known problems.
- Bull *Voltaire Switches Documentation CD* (86 A2 79ET 01)
- StoreWay *Optima 1200 Quick Start Guide* (86 A1 34ET)
- StoreWay *Optima 1200 Installation and User Guide* (86 A1 35ET)
- StoreWay *Master User Guide* (86 A1 38ET)
- *NovaScale Master* documentation

For clusters which use the **PBS Pro** Batch Manager:

- PBS Professional 9.0 *Administrator's Guide* (on PBS Pro CD-ROM)
- PBS Professional 9.0 User's Guide (on PBS Pro CD-ROM)

Web Links

http://www.bull.com/novascale/hpc.html

http://www.linuxhpc.org/

http://www.intel.com/products/server/processors/index.htm

Highlighting

- Commands entered by the user are in a frame in "Courier" font. Example:

```
mkdir /var/lib/newdir
```

- Commands, files, directories and other items whose names are predefined by the system are in "Bold". Example:
  The **/etc/sysconfig/dump** file.
- Text and messages displayed by the system to illustrate explanations are in "Courier New" font. Example:
  `BIOS Intel`
- Text for values to be entered in by the user is in "`Courier New`". Example:
  `COM1`
- *Italics* Identifies referenced publications, chapters, sections, figures, and tables.
- < > identifies parameters to be supplied by the user. Example:
  `<node_name>`

Warning

A Warning notice indicates an action that could cause damage to a program, device, system, or data.

Table of Contents

List of Figures

List of Tables

Chapter 1. Introduction to the HPC Environment

The term HPC (High Performance Computing) describes the development of large scientific applications and programs, which require a powerful computation facility that can process enormous amounts of data to give highly precise results.

Bull BAS4 for Xeon is a software suite that is used to operate and manage a Bull HPC cluster of Xeon-based nodes. These clusters are based on Bull NovaScale platforms using **InfiniBand** stacks with **Voltaire** switches or with a **Gigabit Ethernet** network. **BAS4 for Xeon** includes both Bull proprietary and Open Source software, which provides the infrastructure for optimal interconnect performance.

The Bull HPC cluster includes an administrative network based on a 10/100 Mbit or a Gigabit Ethernet network, and a separate console management network.

The Bull HPC delivery also provides a full environment for development, including optimized scientific libraries, FORTRAN and C/C++ compilers, MPI libraries, as well as debugging and performance optimization tools.

This manual describes these software components, and explains how to work within the BAS4 for Xeon environment.

1.1 Software Configuration

1.1.1 Operating System and Installation

BAS4 for Xeon is based on a standard Linux distribution, combined with a number of Open Source applications that exploit the best from the Open Systems community. This combined with technology from Bull and its partners, results in a powerful, complete solution for the development, execution, and management of parallel and serial applications simultaneously.

Its key features are:

- Strong manageability, through Bull's systems management suite that is linked to state-of-the-art workload management software.
- High-bandwidth, low-latency interconnect networks.
- Scalable high performance file systems, both distributed and parallel.

All cluster nodes use the same Linux distribution. Parallel commands are provided to supply users and system administrators with single-system attributes, these make it easier to manage and to use cluster resources.

Software installation is carried out by first creating an image on a node, loading this image onto the Management Node, and then distributing it to the other nodes using the **Image Building and Deployment** (KSIS) utility. This distribution is performed via the administration network.

1.2 Program Execution Environment

When a user logs onto the **BAS4 for Xeon** system, the login session is directed to one of several nodes. Upon logging onto the system, the users may then develop and execute their applications. Applications can be executed on other cluster nodes apart from the user login system. For development, the environment consists of:

- Standard Linux tools such as **GCC** (a collection of free compilers that can compile C/C++ and FORTRAN), **GDB Gnu Debugger**, and other third-party tools including the Intel FORTRAN Compiler, the Intel C Compiler and Intel Debugger **IDB**.
- Optimized parallel libraries that are part of the **BAS4 for Xeon** software suite. These libraries include the **Bull_MPI2** message-passing library. **Bull_MPI2** complies with the MPI1 and 2 standards and is a high performance, high quality native implementation. **Bull_MPI2** exploits shared memory for intra-node communication. It includes a trace and profiling tool, enabling data to be tracked.
- **Modules** software provides a means for predefining and changing environments. Each one includes a compiler, a debugger and library releases which are compatible with each other. So it is easy to invoke one given environment in order to perform tests and then compare the results with other environments.

1.2.1 Resource Management

The resource manager is responsible for the allocation of resources to jobs. The resources are provided by nodes that are designated as compute resources. Processes of the job are assigned to and executed on these allocated resources.

Both **Gigabit Ethernet** and **InfiniBand BAS4 for Xeon** clusters use the **SLURM** (Simple Linux Utility for Resource Management) open-source, highly scalable cluster management and job scheduling system. **SLURM** has the following functions.

- It allocates compute resources, in terms of processing power and Computer Nodes to jobs for specified periods of time. If required the resources may be allocated exclusively with priorities set for jobs.
- It is also used to launch and monitor jobs on sets of allocated nodes, and will also resolve any resource conflicts between pending jobs.
- It helps to exploit the parallel processing capability of a cluster.

See the Bull HPC BAS4 for Xeon *Administrator's Guide* and *Chapter 6* in this manual for more information on **SLURM**

1.2.2 Batch Management

Different possibilities exist for handling batch jobs for **BAS4 for Xeon** clusters **PBS-Professional**, a sophisticated, scalable, robust Batch Manager from **Altair Engineering** is supported as a standard. **PBS Pro** can also be integrated with the **MPI** libraries.

See the PBS-Professional *Administrator's Guide* and *User's Guide* available on the **PBS-Pro CD-ROM** delivered for the clusters which use PBS-Pro, and the PBS-Pro web site http://www.pbsgridworks.com.

Important

PBS Pro does not work with **SLURM** and should only be installed on clusters which do not use **SLURM.**

1.2.3 Parallel processing and MPI libraries

A common approach to parallel programming is to use a message passing library, where a process uses library calls to exchange messages (information) with another process. This message passing allows processes running on multiple processors to cooperate.

Simply stated, a **MPI** (Message Passing Interface) provides a standard for writing message-passing programs. A **MPI** application is a set of autonomous processes, each one running its own code, and communicating with each other through calls to subroutines of the MPI library.

Bull provides different MPI libraries for use in the HPC environment.

- **Bull_MPI2,** Bull's second generation MPI library, is included in the **Bull BAS4 for Xeon** delivery. This library enables dynamic communication with different device libraries, including InfiniBand **(IB)** interconnects, socket Ethernet/IB/EIB devices or single machine devices. **Bull_MPI2** is fully integrated with the **SLURM** resource manager.
- Third party MPI libraries are also available. **MPICH_Ethernet** is provided to allow applications to run using Ethernet interconnects. **BAS4 for Xeon** also uses **Voltaire MPI**, which in turn uses **MVAPICH**, an open-source MPI software library designed for **InfiniBand** clusters, which helps to ensure high performance and scalability for MPI applications.

See *Chapter 2* for more information on MPI Libraries

1.2.4 Data and Files

Application file I/O operations may be performed using locally mounted storage devices, or alternatively, on remote storage devices using either **Lustre** or the **NFS** file systems. By using a separate interconnect for administration and I/O operations, the Bull cluster system administrator is able to isolate user application traffic from administrative operations and monitoring. With this separation, application I/O performance and process communication can be made more predictable while still enabling administrative operations to proceed.

Chapter 2. Parallel Libraries

This chapter describes the following topics:

- 2.1 *Overview of Parallel Libraries*
- 2.2 *MPIBull2*
- 2.3 *mpibull2-params*
- 2.4 *Third party MPI libraries*
- *2.5 Managing your MPI environment*
- *2.6 Profiling with mpianalyser*

2.1 Overview of Parallel Libraries

A common approach to parallel programming is to use a message passing library, where a process uses library calls to exchange messages (information) with another process. This message passing allows processes running on multiple processors to cooperate.

Simply stated, a **MPI** (Message Passing Interface) provides a standard for writing message-passing programs. A MPI application is a set of autonomous processes, each one running its own code, and communicating with each other through calls to subroutines of the MPI library.

2.1.1 MPI Versions

Bull provides different MPI libraries for use in the HPC environment.

- The second generation MPI library is **MPIBull2**. This library enables dynamic communication with different device libraries, including InfiniBand **(IB)** interconnects, socket Ethernet/IB/EIB devices or single machine devices. See the MPIBull2 documentation for more information
- Third party MPI libraries are also available. MPICH_Ethernet is provided to allow applications to run in an Ethernet environment.

Programming with MPI

It is not in the scope of the present guide to describe how to program with MPI. Please, refer to the Web, where you will find complete information. For example, you can refer to the following site: http://www.idris.fr for information in French.

2.2 MPIBull2

MPIBull2 conforms to the MPI-2 standard.

2.2.1 Quick Start for MPIBull2

MPIBULL2 is usually installed in the **/opt/mpi/mpibull2-<version>** directory. The environmental variables **MPI_HOME, PATH, LD_LIBRARY_PATH, MAN_PATH, PYTHON_PATH** will need to be set or updated. These variables should not be set by the user. Use the **setenv_mpibull2.{sh,csh}** environment setting file, which may be sourced from the ${mpibull2_**install_path}/share** directory by a user or added to the profile for all users by the administrator.

2.2.2 MPIBull2 Compilers

The MPIBull2 library has been compiled with the latest Intel compilers, which, according to Bull's test farms, are the fastest ones available for the IA64 architecture. Bull uses Intel **Icc** and **Ifort** compilers to compile the MPI libraries. It is possible for the user to use their own compilers to compile their applications for example **gcc,** however see below.

In order to check the configuration and the compilers used to compile the MPI libraries the following command may be used.

```
${mpibull2_install_path}/share/doc/compilers_version
```

MPI applications should be compiled using the MPIBull2 MPI wrapper to compilers:

C programs:	mpicc your-code.c
C++ programs:	mpiCC your-code.cc
	or
	mpic++ your-code.cc (for case-insensitive file systems)
F77 programs:	mpif77 your-code.f
F90 programs:	mpif90 your-code.f90

Wrappers to compilers simply add various command line flags and invoke a back-end compiler; they are not compilers in themselves.

The command below is used to override the compiler type used by the wrapper. **–cc**, **-fc -**, and **cxx** and used for C, Fortran and C++ wrappers.

```
mpi_user >>> mpicc -cc=gcc prog.c -o prog
```

2.2.3 Configuring MPIBull2

MPIBull2 may be used for different architectures including standalone **SMP**s, **Ethernet**, **Infiniband** or **Quadrics** Clusters.

You have to select the device that will use **MPIBull2** before launching an application withMPIBull2.

The list of possible devices available is as follows:

- **osock** is the default device. This uses sockets to communicate and is the device of choice for **Ethernet** clusters.
- **oshm** should be used on a standalone machines, communication is through shared memory.
- **ibmr_gen2**, otherwise known as **InfiniBand multi-rail gen2**. This works over **InfiniBand**'s verbs interface.
- **elanbull2** works with **Quadrics**' libelan interface.

The device is selected by using the **mpibull2-devices** command with the **–d** switch, for example, enter the command below to use the shared memory device:

```
mpi_user >>> mpibull2-devices –d=oshm
```

For more information on the **mpibull2-devices** command, see section 2.2.7.

2.2.4 Running MPIBull2

The MPI application requires a launching system in order to spawn the processes onto the cluster. **Bull** provides the **SLURM** Resource Manager as well as the **MPD** subsystem.

For **MPIBull2** to communicate with **SLURM** and **MPD**, the **PMI** interface has to be defined. By default, **MPIBull2** is linked with **MPD**'s **PMI** interface.

If you are using **SLURM**, you must ensure that **MPIBULL2_PRELIBS** includes **-lpmi** so that your **MPI** application can be linked with **SLURM**'s **PMI** library.

Notes:

- For more information on **SLURM**, see chapter 6.
- For more information on **MPD**, see section 2.2.6.3
- For more information on batch managers and launching jobs on BAS4 for Xeon clusters, see chapter 7.

2.2.5 MPIBull2_1.2.x features

MPIBull2_1.2.x includes the following features:

- It only has to be compiled once, supports the NovaScale architecture and is compatible with the more powerful interconnects.
- It is designed so that both development and testing times are reduced and it delivers high performance on **NovaScale** architectures
- Fully compatible with **MPICH2 MPI** libraries. Just set the library path to get all the **MPIBull2** features
- Supports both MPI 1.2 and MPI 2 standard functionalities including
  - Dynamic processes (**osock** only)
  - One-sided communications
  - Extended collectives
  - Thread safety (see the *Thread-Safety* Section below)
  - **ROMIO** including the latest patches developed by Bull
- Multi-device functionality: delivers high performance with an accelerated multi-device support layer for fast interconnects. The library supports:
  - Sockets-based messaging (for **Ethernet, SDP, SCI** and **EIP**)
  - Hybrid shared memory-based messaging for shared memory
  - InfiniBand architecture multirails driver Gen2
- Easy Runtime Selection: makes it easy and cost-effective to support multiple platforms. With MPIBull2 Library, both users and developers can select drivers at runtime easily, without modifying the application code. The application is built once and works for all interconnects supported by Bull.
- Ensures that the applications achieve a high performance with a high degree of interoperability with standard tools and architectures.
- Common feature for all devices:
  - **FUTEX** (Fast User mode muTEX) mechanism in user mode

2.2.6 Advanced features

2.2.6.1 MPIBull2 Linking Strategies

Designed to reduce development and testing time, **MPIBull2** includes two linking strategies for users.

Firstly, the user can choose to build his application and link dynamically, leaving the choice of the **MPI** driver until later, according to which resources are available. For instance, if a small **Ethernet** cluster is the only resource available, the user compiles and links dynamically, using an **osock** driver, whilst waiting for access to a bigger cluster via a different **InfiniBand** interconnect and which uses the **ibmr_gen2** driver at runtime.

Secondly, the User might want to use an out-of-the-box application, designed for a specified **MPI** device. Bull provides the combination of a **MPI** Core and all its supported devices, which enables the static libraries to be linked by the User's application.

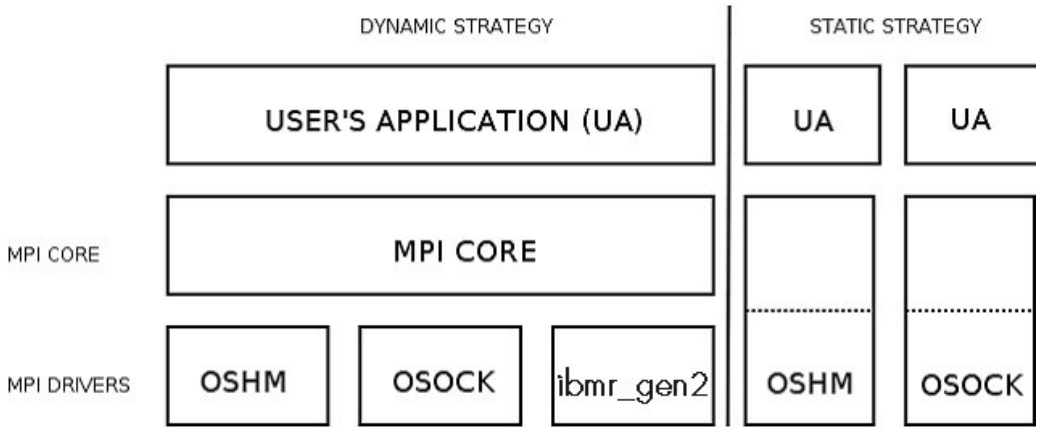


Figure 2-1. MPIBull2 Linking Strategies

2.2.6.2 Thread-safety

If the application needs an **MPI** Library which provides **MPI_THREAD_MULTIPLE** thread-safety level, then choose a device which supports **thread safety** and select a ***_ts device.** Use the **mpibull2-device** commands.

Note:

Thread-safety within the MPI Library requires data locking. Linking with such a library may impact performance. A loss of around 10 to 30% has been observed on microbenchmarks

Not all MPI Drivers are delivered with a thread-safe version. Devices known to support **MPI_THREAD_MULTIPLE** include **osock, oshm** and **ibmr_gen2**.

2.2.6.3 Using MPD

MPD is a simple launching system from **MPICH-2**.

To use it, you need to launch the **MPD** daemons on Compute hosts.

If you have a single machine, just launch **mpd &** and your **MPD** setup is complete.

If you need to spawn **MPI** processes across several machines, you must use **mpdboot** to create a launching ring on the cluster. This is as follows:

Create the hosts list:

```
mpi_user >>> export cluster_machines="host1 host2 host3 host4"
```

- Create the file used to store host information:

```
mpi_user >>> for i in $cluster_machines; do echo "$i" >> machinefiles; done
```

- Boot the MPD system on all the hosts:

```
mpi_user >>> mpdboot -n $(cat $clustermachines | wc -l) -f machinefiles
```

- Check if everything is OK:

```
mpi_user >>> mpdtrace
```

- Run the application or try hostname:

```
mpi_user >>> mpiexec -n 4 ./your_application
```

MPI Process Daemons (MPD) run on all nodes in a ring like structure and may be used in order to manage the launch of the different processes. **MPIBull2** library is **PMI** compliant which means it can interact with any other **PMI PM.** This software has been developed by **ANL**. In order to set up the system the **MPD** ring must firstly be knitted, by following the procedure below:

- At the $HOME prompt edit the .**mpd.conf** file by adding something like **MPD_SECRETWORD=your_password** and `chmod 600` to the file.
- Create a boot sequence file. Any type of file may be used. The **MPD** system will by default use the **mpd.hosts** file in your **$HOME** directory if a specific file is not specified in the boot sequence. This contains a list of hosts, separated by carriage returns. Semi-colons can be added to the host to specify the number of CPUS for the host, for example.

```
host1:4
host2:8
```

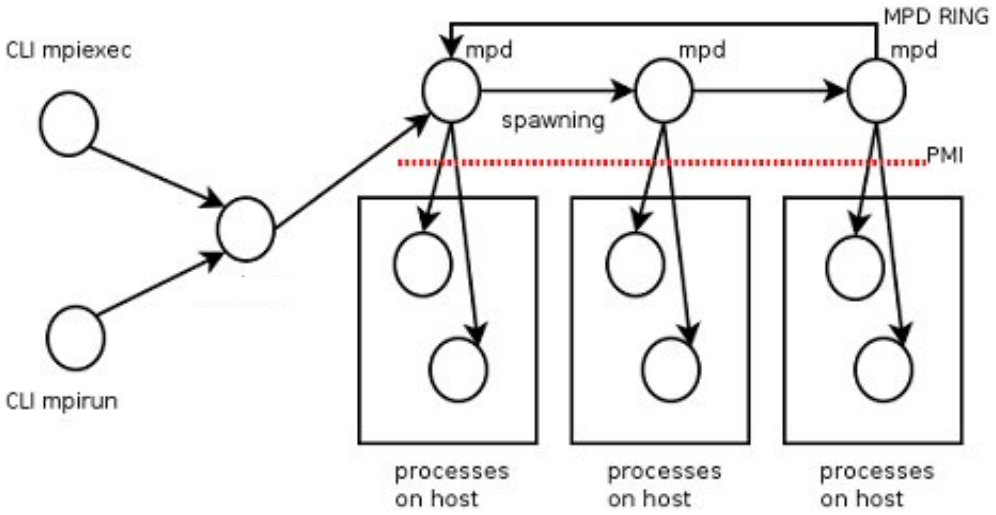


Figure 2-2. MPD ring

- Boot the ring by using the **mpdboot** command, and specify the number of hosts to be included in the ring.

```
mpdboot -n 2 -f myhosts_file
```

Check that the ring is functioning correctly by using the **mpdtrace** or **mpdringtest** commands. If everything is okay, then jobs may be run on the cluster.

2.2.7 MPIBull2 Tools

2.2.7.1 MPIBull2-devices

This tool may be used to change the user's preferences. It can also be used to disable a library. For example, if the program has already been compiled and the intention is to use dynamic MPI Devices which have already been linked with the MPI Core, then it is now possible to specify a particular runtime device with this tool. The following options are available with **MPIBULL2-devices**

-dl Provides list of drivers. This is also supported by MPI wrappers.

-dlv Provides list of drivers with versions of the drivers.

```
mpi_user >>> mpibull2-devices -dl
MPIBULL2 Communication Devices :
+ Original Devices :
*oshm    : Shared Memory device, to be used on a single machine [static][dynamic]
*osock   : Socket protocol (can be used over IPoIB, SDP, SCI...) [static][dynamic]
******
```

-c Obtains details of the user's configuration.

```
mpi_user >>> mpibull2-devices -c
MPIBULL2 home : /install_path
User prefs    :
  \__ Directory                  : /home_nfs/mpi_user/.MPIBull2/
  \__ Custom devices             : /home_nfs/mpi_user/.MPIBull2//site_libs
  \__ MPI Core flavor            : Standard / Error detection on
  \__ MPI Communication Driver   : oshm (Shared Memory device, to be used on a
single machine) [static][dynamic]
```

-d=xxx Sets the specified communication device driver.

```
mpi_user >>> mpibull2-devices -d=ibmr_gen2
```

2.2.7.2 mpibull2-launch

This is a meta-launcher which connects to whatever process manager is specified by the user. It is used to ensure compatibility between different process manager launchers, and also to allow users to specify their custom key bindings.

The purpose of **mpibull2-launch** is to help users to retain their launching commands **Mpibull2-launch** also interprets user's special keybindings, in order to allow the user to retain their preferences, regardless of the cluster and the **MPI** library. This means that the user's scripts will not need changing, except for those environment variables which are required.

The **mpibull2-launch** tool provides default keybindings. The user can check them using the **--metahelp** option. If the user wishes to check some of the **CPM** (Cluster Process Manager) special commands, they should use **--options** with the **CPM** launch name command (e.g. **--options srun**)

Some tool commands and 'device' functionalities rely on the implementation of the **MPI** components. This simple tool maps keybindings to the underlying **CPM**. Therefore, a unique command can be used to launch a job on a different CPM, using the same syntax. **mpibull2-launch** system takes in account the fact that a user might want to choose their own keybindings. A template file, named **keylayout.tmp1**, may be found in the tools rpm which may be used to construct individual keybinding preferences.

Launching a job on a cluster using mpibull2-launch

For a **SLURM CPM** use a command similar to the one below and set **MPIBULL2_LAUNCHER=srun** to make this command compatible with the **SLURM CPM**.

```
mpibull2-launch -n 16 -N 2 -ptest ./job
```

Example for a user who wants to use the Y key for the partition

```
PM Partition to use+Y:+partition:
```

The user should edit a file using the format found in the example template, and then add custom bindings using the **–custom_keybindings** option. The + sign is used to separate the fields. The first field is the name of the command, the second the short option, with a colon if an argument is needed, and the third field is the long option.

2.2.7.3 mpiexec

This is a launcher which connects to the MPD ring.

2.2.7.4 mpirun

This is a launcher which connects to the MPD ring.

2.2.7.5 mpicc, mpiCC, mpicxx, mpif77 and mpif90

These are all compiler wrappers and are available, for C, C++, Fortran 77 and Fortran 90 languages. These allow the user to concentrate on developing the application without having to think about the internal mechanics of MPI. The man page files provide more details about wrappers.

When using compiling tools, they need to know which communication device and a linking strategy they should use. The compiling tools parse as long as some of the following conditions have been met:

- The device and linking strategy has been specified in the command line using the **-sd** options.

- The environment variables **DEF_MPIDEV, DEF_MPIDEV_LINK** (required to ensure compatibility), **MPIBULL2_COMM_DRIVER,** and **MPIBULL2_LINK_STRATEGY** have been set.
- The preferences have already been set up; the tools will use the device they find in the environment using the **MPIBULL2-devices** tool.
- The tools take the system default, using dynamic socket device.

Note:
One can obtain better performance using the **–fast/-static** options to link statically with one of the dependent libraries using the commands below.

```
mpicc –static prog.c
mpicc –fast prog.c
```

2.2.8 MPIBull2 – Example of use

2.2.8.1 Setting up the devices

When compiling an application the user may wish to keep those makefiles and build files which have already been generated. Bull has taken this into account. The code and build files can be kept as they are. All the user needs to do is to set up a few variables or use the **MPIBULL2-devices** tool.

During the installation process, the **/etc/profile.d/mpibull2.sh** file will have been modified by the System Administrator according to the user's needs. This file determines the default settings (by default the rpm sets the **osock** socket/TCP/IP driver). It is possible to override these settings by using environment variables – this is practical as it avoids modifying makefiles - or by using the tools options. For example, the user can statically link their application against a static driver as shown below. The default linking is dynamic, and this enables drive modification during runtime. Linking statically, as shown below, overrides the user's preferences but does not change them.

```
mpi_user >>> mpicc -sd=ibmr_gen2 prog.c -o prog
mpicc : Linking statically MPI library with device (ibmr_gen2)
```

The following environment variables may also be used

MPIBULL2_COMM_DRIVER	Specifies the default device to be linked against
MPIBULL2_LINK_STRATEGY	Specifies the link strategy (the default is dynamic) (required to ensure compatibility)
MPIBULL2_MPITOOLS_VERBOSE	Provides information when building (the default is verbose off)

```
mpi_user >>> export DEF_MPIDEV=ibmr_gen2
mpi_user >>> export MPIBULL2_MPITOOLS_VERBOSE=1
mpi_user >>> mpicc prog.c -o prog
mpicc : Using environment MPI variable specifications
mpicc : Linking dynamically MPI library with device (ibmr_gen2)
```

2.2.8.2 Submitting a job

If a user wants to submit a job, then according to the process management system, they can use **MPIEXEC**, **MPIRUN, SRUN or MPIBULL2-LAUNCH** to launch the processes on the cluster (the online man pages gives details of all the options for these launchers)

2.2.9 Debugging

2.2.9.1 Parallel gdb

With the **mpiexec** launching tool it is possible to add the Gnu DeBugger in the global options by using **-gdb**. All the **gdb** outputs are then aggregated, indicating when there are differences between processes. The **-gdb** option is very useful as it helps to pinpoint faulty code very quickly without the need of intervention by external software.

Refer to the **gdb** man page for more details about the options which are available.

2.2.9.2 Totalview

Totalview is a proprietary software application and is not included in the **BAS4 for Xeon** distribution. See chapter 7 for more details.

It is possible to submit jobs using the **SLURM** resource manage with a command similar to the format below or via MPD.

```
totalview srun -a <args> ./prog <progs_args>
```

Alternatively, it is possible to use MPI process daemons (**MPD**) and to synchronize **Totalview** with the processes running on the MPD ring.

```
mpiexec -tv <args> ./prog <progs_args>
```

2.2.9.3 MARMOT MPI Debugger

MARMOT is an **MPI** debugging library. **MARMOT** surveys and automatically checks the correct usage of the MPI calls and their arguments made during runtime. It does not replace classical debuggers, but is used in addition to them.
The usage of the MARMOT library will be specified when linking and building an application. This library will be linked to the application and to the **MPIBULL2** library.
It is possible to specify the usage of this library manually by using the **MPIBULL2_USE_MPI_MARMOT** environment variable, as shown in the example below;

```
export MPIBULL2_USE_MPI_MARMOT=1
mpicc bench.c -o bench
```

or by using the **-marmot** option with the MPI compiler wrapper, as shown below:

```
mpicc -marmot bench.c -o bench
```

See the documentation in the share section of the marmot package, or go to http://www.hlrs.de/organization/amt/projects/marmot/ for more details on Marmot.

2.3 mpibull2-params

mpibull2-params is a tool that is used to list/modify/save/restore the environment variables that are used by the **mpibull2** library and/or by the communication device libraries (**InfiniBand**, **Quadrics**, etc.). The behaviour of the **mpibull2** MPI library may be modified using environment variable parameters to meet the specific needs of an application. The purpose of the **mpibull2-params** tool is to help **mpibull2** users to manage different sets of parameters. For example, different parameter combinations can be tested separately on a given application, in order to find the combination that is best suited to its needs. This is facilitated by the fact that **mpibull2-params** allow parameters to be set/unset dynamically.

Once a specific combination of parameters has been tested and found to be good for a particular context, they can be saved into a file by a mpibull2 user. Using the **mpibull2-params** tool, this file can then be used to restore the set of parameters, combined in exactly the same way, at a later date.

Notes:

- The effectiveness of a set of parameters will vary according to the application. For instance, a particular set of parameters may ensure low latency for an application, but reduce the bandwidth. By carefully defining the parameters for an application the optimum, in terms of both latency and bandwidth, may be obtained.
- Some parameters are located in the **/proc** file system and only super users can modify them.

The entry point of the **mpibull2-params** tool is an internal function of the environment. This function calls an executable to manage the MPI parameter settings and to create two temporary files. According to which shell is being used, one of these two files will be used to set the environment and the two temporary files will then be removed. To update your environment automatically with this function, please source either the **$MPI_HOME/bin/setenv_mpibull2.sh** file or the **$MPI_HOME/bin/setenv_mpibull2.csh** file, according to which shell is used.

2.3.1 The mpibull2-params command

SYNOPSIS

```
mpibull2-params <operation_type> [options]
```

Actions

The following actions are possible for **mpibull2-params** command:

-l List the MPI parameters and their values

-f List families of parameters

-m Modify a MPI parameter

-d Display all modified parameters

-s Save the current configuration into a file

-r Restore a configuration from a file

-h Show help message and exit

Options

The following options and arguments are possible for the **mpibull2-params** command.

Note: The options shown can be combined, for example, **-li** or can be listed separately, for example **–l –i.** The different option combinations for each argument are shown below.

-l [iv] [PNAME]

List current default values of all MPI parameters. Use the PNAME argument (this could be a list) to specify a precise MPI parameter name or just a part of a name. Use the **-v** (verbose) option to also display all possible values, including the default. Use the **-i** option to list all information.

Examples

- This command will list all the parameters with the string 'all' or 'shm' in their name. **mpibull2-params -l | grep -e all -e shm** will return the same result.

```
mpibull2-params -l all shm
```

- This command will display all information - possible values, family, purpose, etc. for each parameter name which includes the string 'all'. This command will also indicate when the current value has been returned by **getenv()** i.e. the parameter has been modified in the current environment.

```
mpibull2-params -li all
```

- This command will display current and possible values for each parameter name which includes the string 'rom'. It is practical to run this command before a parameter is modified.

```
mpibull2-params -lv rom
```

-f [l[iv]] [FNAME]

List all the default family names. Use the FNAME argument (this could be a list) to specify a precise family name or just a part of a name. Use the **-l** option to list all parameters for the family specified. **–l**, **-v** and **-i** options are as described above.

Examples

- This command will list all family names with the string 'band' in their names.

```
mpibull2-params -f band
```

- For each family name with the string 'band' inside, this command will list all the parameters and current values.

```
mpibull2-params -fl band
```

-m [v] [PARAMETER VALUE]

Modify a MPI PARAMETER with VALUE. The exact name of the parameter should be used to modify a parameter. The parameter is set in the environment, independently of the shell syntax (**ksh/csh**) being used. The keyword 'default' should be used to restore the parameter to its original value. If necessary, the parameter can then be unset in its environment. The **-m** operator lists all the modified MPI parameters by comparing all the MPI parameters with their default values. If none of the MPI parameters have been modified then nothing is displayed. The **–m** operator is like the **-d** option. Use the **-v** option for a verbose mode.

Examples

- This command will set the ROMIO_LUSTRE parameter in the current environment.

```
mpibull2-params -m mpibull2_romio_lustre true
```

- This command will unset the ROMIO_LUSTRE parameter in the environment in which it is running and returns it to its default value.

```
mpibull2-params -m mpibull2_romio_lustre default
```

-d [v]

This will display the difference between the current and the default configurations. Displays all modified MPI parameters by comparing all MPI parameters with their default values.

-s [v] [FILE]

This will save all modified MPI parameters into FILE. It is not possible to overwrite an existing file, an error will be returned if one exists. Without any specific arguments, this file will create a file named with the date and time of the day in the current directory. This command works silently by default. Use the **-v** option to list all modified MPI parameters in a standard output.

Example

- This command will, for example, try to save all the MPI parameters into the file named Thu_May_10_15_50_28_2007.

```
mpibull2-params -sv
```

- Output Example:

```
save the current setting :
mpibull2_mpid_xxx=1
1 parameter(s) saved.
```

-r [v] [FILE]

Restore all the MPI parameters found in FILE and set the environment. Without any arguments, this will restore all modified MPI parameters to their default value. This command works silently, in the background, by default. Use the **-v** option to list all restored parameters in a standard output.

Example

- This command will restore all modified parameters to default.

```
mpibull2-params -r
```

-h

Displays the help page

2.3.2 Family names

The command **mpibull2-params –f** will list the parameter family names which are possible for a particular cluster environment.

Some of the parameter family names which are possible for Bull **BAS4 for Xeon** are listed below.

LK_Ethernet_Core_driver
LK_IPv4_route
LK_IPv4_driver
OpenFabrics_IB_driver
Marmot_Debugging_Library
MPI_Collective_Algorithms
MPI_Errors
CH3_drivers
CH3_drivers_Shared_Memory
Execution_Environment
Infiniband_RDMA_IMBR_mpibull2_driver
Infiniband_Gen2_mpibull2_driver
UDAPL_mpibull2_driver
IBA-VAPI_mpibull2_driver
MPIBull2_Postal_Service
MPIBull2_Romio

Run the command **mpibull2-params <fl> <family>** to see the list of individual parameters that are included in the parameter families used within your cluster environment.

2.4 Third party MPI libraries

2.4.1 MPICH_Ethernet

Bull supplies **MPICH_Ethernet** (version 1.2.6), this is to be used with Ethernet interconnects.

Modify the file **/opt/mpi/mpich_ethernet-1.2.6/share/machines.LINUX** in order to set the host name of the corresponding interface (Administration Network or Dedicated Network) and the number of processors for each machine. For example:

```
ns0:4
ns1:4
ns2:4
ns3:4
```

The program which uses **MPICH_Ethernet** must be compiled using the appropriate wrapping tool, for example **mpicc**, **mpif77**, etc. Launch the program with the following command where **np** is the number of processes, and **appli.exe** is the name of the application using MPI:

```
$mpirun -np 4 ./appli.exe
```

For more details, see the *Installation and User's Guide to MPICH, a portable implementation of MPI* for the device ch_p4 which is available from http://www-unix.mcs.anl.gov/mpi/mpich/

2.4.2 Voltaire MPI

BAS4 for Xeon uses **Voltaire MPI** which in turn uses **MVAPICH**, an open-source MPI software library designed for **InfiniBand** clusters, which helps to ensure high performance and scalability for MPI applications.

Refer to the *MVAPICH User Guide* available from http://mvapich.cse.ohio-state.edu/support/ for more information on installing, configuring, managing and tuning MPI applications over an **InfiniBand** stack using MVAPICH.

This document also includes details of using **MVAPICH** with the **TotalView** debugger, tuning performance on large clusters, and a description of the **MVAPICH** parameters.

2.5 Managing your MPI environment

Bull provides different MPI libraries for the different requirements of users. In order to help users manage different environment configurations, Bull also ships modules and these can be used to switch from one MPI library environment to another. This relies on the module software – see chapter 5.

The directory used to store the module files is **/opt/mpi/modulefiles/**, into which the different module files that include the **mpich_ethernet, vltmpi** libraries for **Voltaire InfiniBand,** and **MPIBull2** environments are placed.

Important

It is recommended that a file is created, for example **99-mpimodules.sh** and **99-mpimodules.sh .csh,** and this is added to the **/etc/profile.d/** directory. The line below should be pasted into this file. This will make the configuration environment available to all users.

```
module use -a /opt/mpi/modulefiles
```

1. To check the modules which are available run the following command:

```
module av
```

   This will give output similar to that below:

```
------------------- /opt/mpi/modulefiles ------------------

mpibull2/1.2.8-1.t      mpich/1.2.7-p1          vltmpi/24-1
```

2. To see which modules are loaded run the command:

```
module li
```

   This will give output similar to that below:

```
-------------------------------------------------------------
Currently Loaded Modulefiles:
  1) oscar-modules/1.0.3
-------------------------------------------------------------
```

3. To change MPI environments run the following commands according to your needs:

```
module load mpich
module li
```

```
-------------------------------------------------------------
Currently Loaded Modulefiles:
  1) oscar-modules/1.0.3   2) mpich/1.2.7-p1
-------------------------------------------------------------
```

4. To check which MPI environment is loaded run the command below:

```
which mpicc
```

This will give output similar to that below:

```
/opt/mpi/mpich-1.2.7-p1/bin/mpicc
```

5. To remove a module (e.g. mpich) run the command below:

```
module rm mpich
```

6. Then load the new MPI environment by running the load command, as below:

```
module load mpibull2
```

2.6 Profiling with mpianalyser

mpianalyser is a profiling tool, developed by Bull for its own **MPI_Bull** implementation. This is a non-intrusive tool which allows the display of data from counters that has been logged when the application is run.

Chapter 3. Scientific Libraries

This chapter describes the following topics:

Important
See the BAS4 for Xeon System Release Bulletin for details of the Scientific Libraries included with your delivery.

3.1 Overview

Scientific Libraries are sets of tested, validated and optimized functions which spare users the need to develop such subprograms themselves.
The advantages of these scientific libraries are:

- Portability
- Support for different types of data (real, complex, double precision, etc.)
- Support for different kinds of storage (banded matrix, symmetrical, etc.)

Delivery

The scientific libraries **BLACS**, **SCALAPACK**, **FFTW**, **Blocksolve95**, **SuperLU**, **PETSC** use **MPI** (Message Passing Interface). They are delivered in different environmental versions according to the implementation to be used. **BAS4 for Xeon** uses the following implementations:

- **MPICH_Ethernet** for clusters using Gigabit Ethernet interconnects.
- **MPIBull2** for clusters using InfiniBand interconnects.

Interdependence of BLAS, BLACS, PBLAS, LAPACK, SCALAPACK

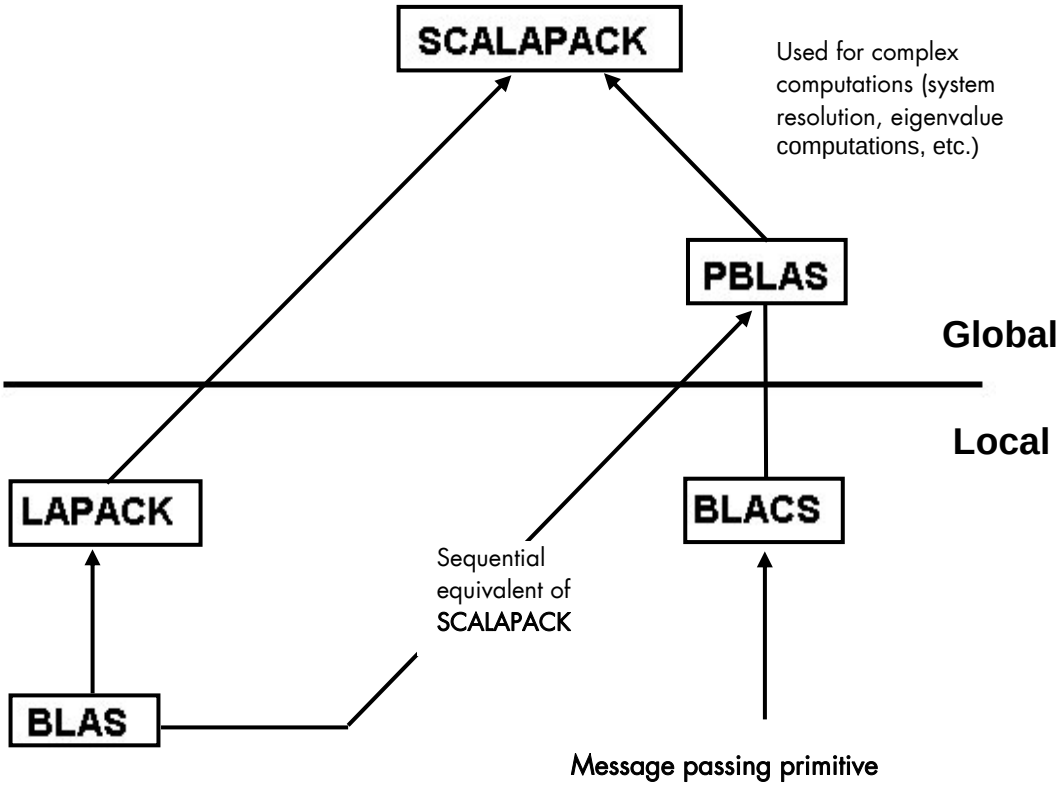


Figure 3-1. Interdependence of some mathematical libraries

3.2 Intel Math Kernel Library (MKL)

The Intel Math Kernel Library, which has been optimized by **Intel** for its processors, contains among other things, the following libraries: **BLAS**, **LAPACK** and **FFT**.

The Intel **MKL** is a fully thread-safe library.

An installation notice is provided by Bull with the library delivery.

The Intel MKL library is located in the **/opt/intel/mkl<release_nb>/** directory.

To use it, the environment has to be set by updating the **LD_LIBRARY_PATH** variable:

```
export LD_LIBRARY_PATH=/opt/intel/mkl<release_nb>/lib/64:$LD_LIBRARY_PATH
```

Example for **MKL** 7.2:

```
export LD_LIBRARY_PATH=/opt/intel/mkl72/lib/64:$LD_LIBRARY_PATH
```

3.3 Intel Cluster Math Kernel Library (CMKL)

The Intel Cluster Math Kernel Library contains all the highly optimized math functions of Math Kernel Library plus **ScaLAPACK** for Linux Clusters.

The Intel Cluster MKL is a fully thread-safe library and provides **C** and **Fortran** interfaces.

An installation notice is provided by Bull with the library delivery.

The Cluster MKL library is located in the **/opt/intel/mkl<release_nb>cluster/** directory.

3.4 BLAS

BLAS stands for Basic Linear Algebra Subprograms.

This library contains linear algebraic operations that include matrixes and vectors. Its functions are separated into three parts:

- Level 1 routines to represent vectors and vector/vector operations.
- Level 2 routines to represent matrixes and matrix/vector operations.
- Level 3 routines mainly for matrix/matrix operations.

This library is included in the Intel MKL package.

For more information see:

www.netlib.org/blas

3.5 BLACS

BLACS stands for Basic Linear Algebra Communication Subprograms.

BLACS is a specialized communications library (using message passing). After defining a process chart, it exchanges vectors, matrices and blocks and so on. It can be compiled on top of **MPI** or **PVM** systems.

BLACS uses MPI and thus it is delivered in two releases, corresponding to the two available MPIs.

For more information see:

www.netlib.org/blacs/index.html

3.5.1 Using BLACS

There are multiple versions of BLACS. One uses the mpich and one uses mpibull2. These libraries are located in the following directories:

- **/usr/lib/blacs/blacs_mpich_ethernet-<versions>/**
- **/usr/lib/blacs/blacs_mpibull2-<version>**

The libraries include the following:

libblacsCinit_MPI-LINUX-0.a
libblacsF77init_MPI-LINUX-0.a
libblacs_MPI-LINUX-0.a

3.5.2 Testing BLACS

You may test the installation of the library with the provided tests found under the following directory:

- **/usr/lib/blacs/blacs_<mpibull or mpich>/tests**

First you must set up your environment. To do this you need to setup the MPI_HOME and LD_LIBRARY_PATH variables to point to the MPI libraries you would like to test. In the example below, we use the mpich library.

```
export MPI_HOME=/opt/mpi/mpich_ethernet/
export PATH=$MPI_HOME/bin:$PATH
export LD_LIRARY_PATH=$MPI_HOME/lib:$LD_LIRARY_PATH
```

Now you can run the tests:

```
mpirun -np 4 xCbtest_MPI-LINUX-0
mpirun -np 4 xFbtest_MPI-LINUX-0
```

Note:
These tests require a machine file, which contains your system names and number of processors. The default is: **/usr/mpi/mpich_ethernet<version>/machines.LINUX**
For example:

```
Bass:4
Molson:8
```

3.6 PBLAS

PBLAS stands for Parallel Basic Linear Algebra Subprograms.

PBLAS is the parallelized version of **BLAS** for distributed memory machines. It requires cyclic distribution by matrix block that the BLACS library offers.

This library is included in the Intel **MKL** package.

3.7 LAPACK

LAPACK stands for Linear Algebra PACKage.

This is a set of Fortran 77 routines used to resolve linear algebra problems such as the resolution of linear systems, eigenvalue computations, matrix computations, etc. However, it is not written for a parallel architecture.

This library is included in the Intel **MKL** package.

3.8 SCALAPACK

SCALAPACK stands for: SCAlable Linear Algebra PACKage.

This library is the scalable version of **LAPACK**. Both libraries use block partitioning to reduce data exchanges between the different memory levels to a minimum. **SCALAPACK** is above all used for eigenvalue problems and factorizations (LU, Cholesky and QR). Matrices are distributed using **BLACS**.

For more information see:

www.netlib.org/scalapack/index.html

Using SCALAPACK

Local component routines are called by a single process with arguments residing in local memory.

Global component routines are synchronous and parallel. They are called with arguments that are matrices or vectors distributed over all the processes.

SCALAPACK uses MPI and thus it is delivered in two releases, corresponding to the two available MPIs.

The default installation of these two libraries is the following:

- **/usr/lib/scalapack/scalapack_mpibull2<version>**
- **/usr/lib/scalapack/scalapack_mpich_ethernet<version>**

The library proved is:

Libscalapack.a

Some tests are provided in the following directory:

/usr/lib/scalapack/scalapack_<version>/tests

3.9 Blocksolve95

BlockSolve95 is a scalable parallel software library primarily intended for the solution of sparse linear systems that arise from physical models, especially problems involving multiple degrees of freedom at each node.

BlockSolve95 uses MPI and thus it is delivered in two releases, corresponding to the two available MPIs.

The default installations of these two libraries are the following:

- **/usr/lib/BlockSolve95/BlockSolve95_mpich_ethernet<version>/lib/lib0/linux**
- **/usr/lib/BlockSolve95/BlockSolve95_mpibull2<version>/lib/lib0/linux**

The library provided is the following:

libBS95.a

Some examples are also provided in the following directory:

/usr/lib/BlockSolve95/BlockSolve95_<version>/examples

For more information see:

http://www.mcs.anl.gov/sumaa3d/BlockSolve/index.html

3.10 SuperLU

The SuperLU libraries are for the direct solution of large, sparse, nonsymmetrical systems of linear equations on high performance machines. The routines will perform an LU decomposition with partial pivoting and triangular systems solves through forward and back substitution. The factorization routines can handle non-square matrices but the triangular solves are performed only for square matrices. The matrix commands may be pre ordered either though library or user supplied routines. This preordering for sparsely is completely separate from the factorization. Working precision iterative refinement subroutines are provided for improved backward stability. Routines are also provided to equilibrate the system, estimate the condition number, calculate the relative backward error and estimate error bounds for the refined solutions. SuperLU_Dist is for distributed memory

For more information see:

http://crd.lbl.gov/~xiaoye/SuperLU/#superlu_dist

The following SuperLU libraries are provided:

- **/usr/lib/SuperLU/SuperLU_DIST_mpibull2<version>/superlu_lnx_x86_64.a**
- **/usr/lib/SuperLU/SuperLU_DIST_mpibull2<version>/superlu_lnx_x86_64.a**
- **/usr/lib/SuperLU/SuperLU-SEQ2-2.0/superlu_lnx_x86_64.a**
- **/usr/lib/SuperLU/SuperLU-SEQ-3.0/superlu_lnx_x86_64.a**
- **/usr/lib/SuperLU/SuperLU-SMP-1.0 /superlu_mt_PTHREAD.a**

Tests are provided for each library under the following directory:

/usr/lib/Super/<versions>/test

3.11 FFTW

FFTW stands for Fastest Fourier Transform in the West. **FFTW** is a C subroutine library for computing a discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and with both real and complex data.
There are three versions of FFTW in this distribution. They are located in the following directories:

- **/usr/lib/FFTW3-3.1.2/lib**
- **/usr/lib/FFTW_mpibull2-<version>/lib**
- **/usr/lib/FFTW_mpich_ethernet-<version>/lib**

Tests are also available in the following directory:

/usr/lib/<version>/test

For more information see: www.fftw.org/

3.12 PETSc

PETSc stands for Portable, Extensible Toolkit for Scientific Computation. **PETSc** is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It employs the MPI standard for all message-passing communication (see http://www.mcs.anl.gov/mpi for more details).

The PETSc library is available under the following directories for both MPI:

- **/opt/scilibs/PETSC/PETSc-2.3.3-p0/mpich_ethernet/lib/linux-intel-opt/**
- **/opt/scilibs/PETSC/PETSc-2.3.3-p0/mpibull2/lib/linux-intel-opt/**

For more information see: http://www-unix.mcs.anl.gov/petsc/petsc-2/

3.13 NETCDF

NetCDF (Network Common Data Form) allows the management of data input/output. **NetCDF** is an interface for array-oriented data access and is a library that provides an implementation of the interface. The **netCDF** library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data.

The library is located in the following directories:

- **/usr/bin**
- **/usr/include**
- **/usr/lib**
- **/usr/man**

For more information see:

http://www.unidata.ucar.edu/software/netcdf/
http://trac.mcs.anl.gov/projects/parallel-netcdf

3.14 METIS and PARMETIS

METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms implemented in **METIS** are based on the multilevel recursive-bisection, multilevel *k*-way, and multi-constraint partitioning schemes developed in our lab.

ParMETIS is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices. **ParMETIS** extends the functionality provided by METIS and includes routines that are especially suited for parallel Adaptive Mesh Refinement computations and large scale numerical simulations.

The libraries for ParmMETIS are located in the following directory:

- **/opt/parmetis/parmetis_mpibull2-3.1/lib**

For more information see:

http://www-users.cs.umn.edu/~karypis/metis/

3.15 SciPort

SCIPORT is a portable implementation of **CRAY SCILIB** that provides both single and double precision object libraries. **SCIPORTS** provides single precision and **SCIPORTD** provides double precision.

The libraries for SCIPORT are located in the following directory:

- **/opt/scilibs/sciport/sciport-1.0/lib/**

For more information see:

http://www.netlib.org/scilib/sciport

Chapter 4. Compilers

This chapter describes the following topics:

- 4.1 *Overview*
- 4.2 *Intel® Fortran Compiler Professional Edition for Linux*
- 4.3 *Intel® C++ Compiler Professional Edition for Linux*
- 4.4 *Intel Compiler Licenses*
- 4.5 *Intel Math Kernel Library Licenses*
- 4.6 *GNU Compilers*

4.1 Overview

Compilers play an essential role in exploiting the full potential of Xeon® processors. Bull therefore recommends the use of Intel® C/C++ and Intel® Fortran compilers.

GNU compilers are also available. However, these compilers are unable to compile/link any program which uses **MPI_Bull**. For **MPI_Bull** programs it is essential that Intel compilers are used.

4.2 Intel® Fortran Compiler Professional Edition for Linux

The current version of the Intel® Fortran compiler is version 10. This supports the Fortran 95, Fortran 90, Fortran 77, Fortran IV standards whilst including many features from the Fortran 2003 language standard.

The main features of this compiler are:

- Advanced optimization features including auto-vectorization, High-Performance Parallel Optimizer (HPO), Interprocedural Optimization (IPO), Profile Guided Optimization (PGO) and Optimized Code Debugging.
- Multi-threaded Application Support including OpenMP and Auto Parallelization to convert serial applications into parallel applications to fully exploit the processing power that is available
- Data preloading
- Loop unrolling

The Professional Edition includes the **Intel® Math Kernel Library (Intel® MKL)** with its optimized functions for maths processing. It is also compatible with GNU products.

It also supports big endian encoded files. Finally, this compiler allows the execution of applications which combine programs written in C and Fortran.

For more details of these features, see the Intel web site www.intel.com.

Different versions of the compiler may be installed to ensure compatibility with the compiler version used to compile the libraries and applications on your system.

Note:
It may be necessary to contact the System Administrator to ascertain the location of the compilers on your system. The paths shown in the examples below may vary.

To specify a particular environment use the command below.

```
source /opt/intel/fce/<package_id>/bin/ifortvars.sh
```

For example:

- To use version 10.0.025 of the Fortran compiler:

```
source /opt/intel/fce/10.0.025/bin/ifortvars.sh
```

- To display the version of the active compiler, enter:

```
ifort --version
```

- To obtain the documentation of the compiler:

```
/opt/intel/fce/10.0.025/doc
```

Remember that if you are using **MPI_Bull** then a compiler version has to be used which is compatible with the compiler originally used to compile the MPI library.

4.3 Intel® C++ Compiler Professional Edition for Linux

The current version of the Intel C++ compiler is version 10.

The main features of this compiler are:

- Advanced optimization features including auto-vectorization, High-Performance Parallel Optimizer (HPO), Interprocedural Optimization (IPO), Profile Guided Optimization (PGO) and Optimized Code Debugging.
- Multi-threaded Application Support including OpenMP and Auto Parallelization to convert serial applications into parallel applications to fully exploit the processing power that is available
- Data preloading
- Loop unrolling

The Professional Edition includes **Intel® Threading Building Blocks (Intel® TBB), Intel Integrated Performance Primitives (Intel® IPP)** and the **Intel® Math Kernel Library (Intel® MKL)** with its optimized functions for maths processing. It is also compatible with GNU products.

For more details on these libraries, visit the Intel web site www.intel.com.

Different versions of the compiler may be installed to ensure compatibility with the compiler version used to compile the libraries and applications on your system.

Note:
It may be necessary to contact the System Administrator to ascertain the location of the compilers on your system. The paths shown in the examples below may vary.

To specify a particular environment use the command below:

```
source /opt/intel/cce/<package_id>/bin/iccvars.sh
```

For example:

- To use version 10.0.025 of the C/C++ compiler:

```
source /opt/intel/cce/10.0.025/bin/iccvars.sh
```

- To display the version of the active compiler, enter:

```
icc --version
```

- To obtain the documentation of the compiler:

```
/opt/intel/cce/10.0.025/doc
```

Remember that if you are using **MPI_Bull** then a compiler version has to be used which is compatible with the compiler originally used to compile the MPI library.

4.4 Intel Compiler Licenses

Three types of Intel ® compiler licenses are available:

- **Single User:** allows one user to operate the product on multiple computers as long as only one copy is in use at any given time.
- **Node-Locked:** locked to a node, allows any user who has access to this node to operate the product concurrently with other users, limited to the number of licenses purchased.
- **Floating:** locked to a network, allows any user who has access to the network server to operate the product concurrently with other users, limited to the number of licenses purchased.

The node-locked and floating licenses are managed by **FlexLM** from **Macrovision.**

License installation, and **FlexLM** configuration, may differ according to your compiler, the license type, the number of licenses purchased, and the period of support for your product. Please check the Bull Product Designation document delivered with your compiler and follow the instructions contained therein.

4.5 Intel Math Kernel Library Licenses

Intel Math Kernel Library licenses are required for each Node on which you compile with MKL. However, the runtime libraries which are used on the compute nodes do not require a license fee.

4.6 GNU Compilers

GCC, a collection of free compilers that can compile both C/C++ and Fortran, is part of the installed Linux distribution.

Chapter 5. The User's Environment

This chapter describes how to access the HPC environment, how to use file systems, and how to use the modules package to switch and compare environments:

- *5.1 Cluster Access and Security*
- *5.2 Global File Systems*
- *5.3 Environment Modules*
- *5.4 Module Files*
- *5.5 The Module Command*

5.1 Cluster Access and Security

Typically, users connect to and use a HPC cluster as described below:

- Users log on to the HPC platform either through Service Nodes or through the Login Node when the configuration includes these special Login Node(s). Once logged on to a node, users can then launch their jobs.
- Compilation is possible on all nodes which have compilers installed on them. The best approach is that compilers reside on Login Nodes, so that they do not interfere with performance on the Compute Nodes.

5.1.1 ssh (Secure Shell)

The **ssh** command is used to access a cluster node.

Syntax:

```
ssh [-l login_name] hostname | user@hostname [command]

ssh [-afgknqstvxACNTX1246] [-b bind_address] [-c cipher_spec]
    [-e escape_char] [-i identity_file] [-l login_name] [-m mac_spec]
    [-o option] [-p port] [-F configfile] [-L port:host:hostport]
    [-R port:host:hostport] [-D port] hostname | user@hostname [command]
```

ssh (ssh client) can also be used as a command to log onto a remote machine and to execute commands on it. It replaces **rlogin** and **rsh**, and provides secure encrypted communications between two untrusted hosts over an insecure network. X11 connections and arbitrary TCP/IP ports can also be forwarded over the secure channel. **ssh** connects and logs onto the specified hostname. The user must verify his/her identity, using the appropriate protocol, before being granted access to the remote machine.

5.2 Global File Systems

The Bull BAS4 for Xeon software uses **NFS** distributed file system.

5.3 Environment Modules

Environment modules provide a great way to customize your shell environment easily, particularly on the fly.

For instance an environment can consist of one set of compatible products including a defined release of a FORTRAN compiler, a C compiler, a debugger and mathematical libraries. In this way you can easily reproduce trial conditions, or use only proven environments.

The Modules environment is a program that can read and list module files returning commands; suitable for the shell to interpret, and most importantly for the **eval** command. Modulefiles is a kind of flat database which uses files.

In UNIX a child process can not modify its parent environment.
So how does Modules do this? Modules parses the given modules file and produces the appropriate shell commands to **set/unset/append/un-append** onto an environment variable. These commands are eval'd by the shell. Each shell provides some mechanism where commands can be executed and the resulting output can, in turn, be executed as shell commands. In the C-shell & Bourne shell and derivatives this is the **eval** command.

This is the only way that a child process can modify the parent's (login shell) environment. Hence the module command itself is a shell alias or function that performs these operations. To the user, it looks just like any other command.

The module command is only used in the development environment and not in other environments such as that for administration node.

More details are available at http://modules.sourceforge.net/

5.3.1 Using Modules

The following command gives the list of available modules on a cluster.

```
module avail
------------------------ /opt/modules/version -----------------------
3.1.6

------------------- /opt/modules/3.1.6/modulefiles -------------------
dot         module-info null
module-cvs  modules     use.own

---------------------- /opt/modules/modulefiles ----------------------
oscar-modules/1.0.3 (default)
```

Modules available for the user are listed under the line **/opt/modules/modulefiles**.

The command to load a module is:

```
module load module_name
```

The command to verify the loaded modules list is:

```
module list
```

Using the `avail` command it is possible that some modules will be marked *(default)*:

```
module avail
```

These modules are those which have been loaded without the user specifying a module version number. For example the following commands are the same:

```
module load configuration
module load configuration/2
```

The **module unload** command unloads a module.

The **module purge** command clears all the modules from the environment.

```
module purge
```

It is not possible to load modules which include different versions of **intel_cc** or **intel_fc** at the same time because they cause conflicts.

Module Configuration Examples

Note:
The examples shown below are examples only. The module configurations possible for **BAS4** for **Xeon** will differ.

Configuration/1	intel_fc –version 8.0.046 intel_cc –version 8.0.066 intel_db –version 8.1.3 intel_mkl –version 7.0.017
Configuration/2	intel_fc –version 8.0.049 intel_cc –version 8.0.071 intel_db –version 8.1.3 intel_mkl –version 7.0.017
Configuration/3	intel_fc –version 8.0.061 intel_cc –version 8.0.071 intel_db –version 8.1.3 intel_mkl –version 7.0.017
Configuration/4	intel_fc –version 8.0.019 intel_cc –version 8.0.022 intel_db –version 8.1.3 intel_mkl –version 7.0.017

Table 5-1. Examples of different module configurations

5.3.2 Setting Up the Shell RC Files

Here's a quick tutorial on Shell rc (run-command) files. When a user logs in and if they **have /bin/csh(/bin/sh)** as their shell, the first **rc** fire to be parsed by the shell is **/etc/csh.login** & **/etc/csh.cshrc (/etc/profile)** (the order is implementation dependent), and then the user's $HOME/.cshrc ($HOME/.kshenv) and finally $HOME/.login ($HOME/.profile).

All the other login shells are based on **/bin/csh** and **/bin/sh** with additional features and **rc** files. Certain environment variables and aliases (functions) need to be set for Modules to work correctly. This is handled by the Module init files in **/opt/modules /default/init**, which contains separate init files for each of the various supported shells, where the default is a symbolic link to a module command version.

Skeleton Shell RC ("Dot'') Files

The skeleton files provide a "default'' environment for new users when they are added to your system, this can be used if you do not have the time to set them up individually. The files are usually placed in **/etc/skel** (or wherever you specified with the --with-skel-path=<path> option to the configuration script), and contains a minimal set of "dot'' files and directories that every new user should start with.

The skeleton files are copied to the new user's $HOME directory with the "**-m**'' option added to the "**useradd**'' command. A set of sample "dot'' files are located in **./etc/skel**. Copy everything but the .*.in and CVS files and directories to the skeleton directory. Edit and tailor for your system.

If you have a pre-existing set of skeleton files, then make sure the following minimum set exists: **.cshrc, .login, .kshenv, .profile**. These can be automatically updated with the command:

```
env HOME=/etc/skel/opt/modules/default/bin/add.modules
```

Inspect the new "dot'' files and if they are OK, then remove all the .*.old (original) files. An alternative way of setting-up the users' dot files can be found in ./ext.
This model can be used with the --with-dot-ext configure option.

User Shell RC ("Dot'') Files

The final step for a functioning modules environment is to modify the user "dot'' files to source the right files. One way to do this is to put a message in the **/etc/motd** telling each user to run the command:

```
/opt/modules/default/bin/add.modules
```

This is a script that parses their existing "dot'' files prepending the appropriate commands to initialize the Modules environment.

The user can re-run this script and it will find and remember what modules they initially loaded and then strip out the previous module initialization and restore it with an upgraded one.

If the user lacks a necessary "dot'' file, the script will copy one over from the skeleton directory. The user will have to logout and login for it to come into effect.
Another way is for the system administrator to "su - username" to each user and run it interactively. The process can be semi-automated with a single line command that obviates the need for direct interaction:

```
su - username -c "yes | /opt/modules/modules/default/bin/add.modules"
```

Power users can create a script to directly parse the **/etc/passwd** file to perform this command. Otherwise, just copy the passwd file and edit it to execute this command for each valid user.

5.4 Module Files

Once the above steps have been performed, then it is important to have module files in each of the modulefiles directories. For example, the following module files will be installed:

```
--------- /opt/modules/3.0.9-rko/modulefiles ----------
dot         module-info modules     null        use.own
```

If you do not have your own module files in **/opt/modules/modulefiles** then copy "null'' to that directory. On some systems an empty modulefiles directory will cause a core dump, whilst on other systems there will be no problem. Use **/opt/modules/default/modulefiles/modules** as a template for creating your own module files.

For more information run:

```
module load modules
```

You will then have ready access to the module(1) modulefile(4) man pages, as well as the versions directory. Study the man pages carefully.
The version directory may look something like this:

```
---------------- /opt/modules/versions ----------------
3.0.5-rko 3.0.6-rko 3.0.7-rko 3.0.8-rko 3.0.9-rko
```

The model you should use for modulefiles is "name/version''. For example, **/opt/modules/modulefiles** directory may have a directory named "netscape'' which contains the following module files: 301, 405c, 451c, etc.
When it's displayed with "module avail'' it looks something like this:

```
netscape/301
netscape/405c
netscape/451c(default)
netscape/45c
netscape/46
```

The default is established with **.version** file in the netscape directory and it looks something like this:

```
#%Module1.0#####################################################
####
##
## version file for Netscape
##
set ModulesVersion      "451c"
```

If the user does "module load netscape'', then the default netscape/451c will be used. The default can be instantly changed by editing the **.version** file to point to a different module file in that directory. If no **.version** file exists then Modules will just use the last module in the alphabetical ordered directory listing as the default.

5.4.1 Upgrading via the Modules Command

The theory is that Modules should use a similar package/version locality as the package environments it helps to define. Switching between versions of the module command should be as easy as switching between different packages via the module command. Suppose there is a change from 3.0.5-rko to version 3.0.6-rko. The goal is to semi-automate the changes to the user "dot'' files so that the user is oblivious to the change.

The first step is to install the new module command & files to **/opt/modules/3.0.6-rko/.** Test it out by loading with "module load modules 3.0.6-rko". You may get an error like: 3.0.6-rko (25):ERROR:152: Module 'modules' is currently not loaded. This is OK and should not appear with future versions.

Make sure you have the new version with "module --version". If it seems stable enough, then advertise it to your more adventurous users. Once you are satisfied that it appears to work adequately well, then go into **/opt/modules** remove the old "default" symbolic link to the new versions.

For example:

```
cd /opt/modules
rm default; ln -s 3.0.6-rko default
```

This new version is now the default and will be referenced by all the users that log in and by those that have not loaded a specific module command version.

5.5 The Module Command

Synopsis

```
module [ switches ] [ sub-command ] [ sub-command-args ]
```

The **Module** command provides a user interface to the Modules package. The Modules package provides for the dynamic modification of the user's environment via *modulefiles*.

Each *modulefile* contains the information needed to configure the shell for an application. Once the Modules package is initialized, the environment can be modified on a per-module basis using the module command which interprets *modulefiles*. Typically *modulefiles* instruct the **module** command to alter or to set shell environment variables such as PATH, MANPATH, etc. *modulefiles* may be shared by many users on a system and users may have their own collection to supplement or replace the shared *modulefiles*.

The *modulefiles* are added to and removed from the current environment by the user. The environment changes contained in a *modulefile* can be summarized through the module command as well. If no arguments are given, a summary of the module usage and sub-commands are shown.

The action for the module command to take is described by the sub-command and its associated arguments.

5.5.1 modulefiles

modulefiles are the files containing **TCL** code for the Modules package.

modulefiles are written in the Tool Command Language, **TCL**(3) and are interpreted by the modulecmd program via the module(1) user interface. **modulefiles** can be loaded, unloaded, or switched on-the-fly while the user is working.

A modulefile begins with the magic cookie, '#%Module'. A version number may be placed after this string. The version number is useful as the format of **modulefiles** may change. If a version number doesn't exist, then modulecmd will assume the modulefile is compatible with the latest version. The current version for **modulefiles** will be 1.0. Files without the magic cookie will not be interpreted by modulecmd.

Each modulefile contains the changes to a user's environment needed to access an application. **TCL** is a simple programming language which permits **modulefiles** to be arbitrarily complex, depending on the needs of the application and the modulefile writer. If support for extended tcl (tclX) has been configured for your installation of modules, you may use all the extended commands provided by tclX, too. **modulefiles** can be used to implement site policies regarding the access and use of applications.

A typical **modulefiles** file is a simple bit of code that sets or adds entries to the PATH, MANPATH, or other environment variables. **TCL** has conditional statements that are evaluated when the modulefile is loaded. This is very effective for managing path or environment changes due to different OS releases or architectures. The user environment information is encapsulated into a single modulefile kept in a central location. The same modulefile is used by all users independent of the machine. So, from the user's perspective, starting an application is exactly the same regardless of the machine or platform they are on.

modulefiles also hide the notion of different types of shells. From the user's perspective, changing the environment for one shell looks exactly the same as changing the environment for another shell. This is useful for new or novice users and eliminates the need for statements such as "if you're using the C Shell do this ..., otherwise if you're using the Bourne shell do this ..." Announcing and accessing new software is uniform and independent of the user's shell. From the modulefile writer's perspective, this means one set of information will take care of all types of shells.

5.5.2 Modules Package Initialization

The Modules package and the module command are initialized when a shell-specific initialization script is sourced into the shell. The script creates the module command as either an alias or function, creates Modules environment variables, and saves a snapshot of the environment in ${HOME }/.modulesbeginenv. The module alias or function executes the modulecmd program located in ${MODULESHOME }/bin and has the shell evaluate the command's output. The first argument to modulecmd specifies the type of shell.

The initialization scripts are kept in ${MODULESHOME }/init/shellname where shellname is the name of the sourcing shell. For example, a C Shell user sources the ${MODULESHOME }/init/csh script. The **sh, csh, tcsh, bash, ksh**, and **zsh** shells are all supported by **modulecmd**. In addition, python and perl "shells" are supported which writes the environment changes to stdout as python or perl code.

5.5.3 Examples of Initialization

In the following examples, replace ${MODULESHOME } with the actual directory name.

C Shell initialization (and derivatives)

```
source ${MODULESHOME }/init/csh module load modulefile modulefile
```

Bourne Shell (sh) (and derivatives)

```
${MODULESHOME }/init/sh module load modulefile modulefile
```

Perl

```
require "${MODULESHOME }/init/perl"; &module("load modulefile modulefile ");
```

5.5.4 Modulecmd Startup

Upon invocation modulecmd sources **rc** files which contain global, user and *modulefile* specific setups. These files are interpreted as **modulefiles.**

Upon invocation of modulecmd module RC files are sourced in the following order:

1. Global RC file as specified by ${MODULERCFILE } or ${MODULESHOME }/etc/rc
2. User specific module RC file ${HOME }/.modulerc
3. All .module rc and .version files found during modulefile searches.

5.5.5 Module Command Line Switches

The module command accepts command line switches as its first parameter. These may be used to control output format of all information displayed and the module behavior in the case of locating and interpreting module files.

All switches may be entered either in short or long notation. The following switches are accepted:

--force, -f

Force active dependency resolution. This will result in modules found on a prereq command inside a module file being loaded automatically. Unloading module files using this switch will result in all required modules which have been loaded automatically using the -f switch being unloaded. This switch is experimental at the moment.

--terse, -t

Display avail and list output in short format.

--long, -l

Display avail and list output in long format.

--human, -h

Display short output of the avail and list commands in human readable format.

--verbose, -v

Enable verbose messages during module command execution.

--silent, -s

Disable verbose messages. Redirect **stderr** to **/dev/null** if **stderr** is found not to be a **tty**. This is a useful option for module commands being written into **.cshrc** , **.login** or .profile files, because some remote shells (e.g. **rsh** (1)) and remote execution commands (e.g. **rdist**) get confused if there is output on **stderr**.

--create, -c

Create caches for module **avail** and module **apropos** . You must be granted write access to the ${MODULEHOME }/*modulefiles/* directory if you try to invoke module with the -c option.

--icase, -i

This is a case insensitive module parameter evaluation. Currently only implemented for the module apropos command.

--userlvl <lvl>, -u <lvl>

Set the user level to the specified value. The argument of this option may be one of:

novice	nov Novice
expert	exp Experienced module user
advanced	adv Advanced module user

5.5.6 Module Sub-Commands

Print the use of each sub-command. If an argument is given, print the Module specific help information for the *modulefile*.

```
help [modulefile...]
```

Load **modulefile** into the shell environment.

```
load modulefile [modulefile...]
add modulefile [modulefile...]
```

Remove *modulefile* from the shell environment.

```
unload modulefile [modulefile...]
rm modulefile [modulefile...]
```

Switch loaded *modulefile*1 with *modulefile*2.

```
switch modulefile1 modulefile2
swap modulefile1 modulefile2
```

Display information about a *modulefile*. The display sub-command will list the full path of the *modulefile* and all (or most) of the environment changes the *modulefile* will make when loaded. (It will not display any environment changes found within conditional statements).

```
display modulefile [modulefile...]
```

List loaded modules.

```
show modulefile [modulefile...]
list
avail [path...]
```

List all available *modulefiles* in the current MODULEPATH. All directories in the MODULEPATH are recursively searched for files containing the *modulefile* magic cookie. If an argument is given, then each directory in the MODULEPATH is searched for *modulefiles* whose pathname match the argument. Multiple versions of an application can be supported by creating a subdirectory for the application containing *modulefiles* for each version.

```
use directory [directory...]
```

Prepend directory to the MODULEPATH environment variable. The --append flag will append the directory to MODULEPATH.

```
use [-a|--append] directory [directory...]
```

Remove directory from the MODULEPATH environment variable.

```
unuse directory [directory...]
```

Attempt to reload all loaded *modulefiles*. The environment will be reconfigured to match the saved ${HOME }**/.modulesbeginenv** and the *modulefiles* will be reloaded. The `update` command will only change the environment variables that the *modulefiles* set.

```
update
```

Force the Modules Package to believe that no modules are currently loaded.

```
clear
```

Unload all loaded *modulefiles*.

```
purge
```

Display the *modulefile* information set up by the module-`whatis` commands inside the specified *modulefiles*. If no *modulefiles* are specified, all the whatis information lines will be shown.

```
whatis [modulefile [modulefile...]]
```

Searches through the `whatis` information of all *modulefiles* for the specified string. All module `whatis` information matching the search string will be displayed.

```
apropos string
keyword string
```

Add *modulefile* to the shell's initialization file in the user's home directory. The startup files checked are .cshrc, .login, and .csh_variables for the C Shell; .profile for the Bourne and Korn Shells; **.bashrc, .bash_env**, and .**bash_profile** for the GNU Bourne Again Shell; **.zshrc, .zshenv**, and .**zlogin** for zsh. The .modules file is checked for all shells. If a 'module load' line is found in any of these files, the *modulefile*(s) is(are) appended to any existing list of *modulefiles*. The 'module load' line must be located in at least one of the files listed above for any of the 'init' sub-commands to work properly. If the 'module load' line is found in multiple shell initialization files, all of the lines are changed.

```
initadd modulefile [modulefile...]
```

Does the same as initadd but prepends the given modules to the beginning of the list. initrm *modulefile* [*modulefile*...] Remove *modulefile* from the shell's initialization files.

```
initprepend modulefile [modulefile...]
```

Switch *modulefile*1 with *modulefile*2 in the shell's initialization files.

```
initswitch modulefile1 modulefile2
```

List all of the *modulefiles* loaded from the shell's initialization file.

```
initlist
```

Clear all of the *modulefiles* from the shell's initialization files.

```
initclear
```

5.5.7 Modules Environment Variables

Environment variables are unset when unloading a *modulefile*. Thus, it is possible to load a *modulefile* and then unload it without having the environment variables return to their prior state.

MODULESHOME

This is the location of the master Modules package file directory containing module command initialization scripts, the executable program modulecmd, and a directory containing a collection of master *modulefiles*.

MODULEPATH

This is the path that the module command searches when looking for *modulefiles*. Typically, it is set to the master *modulefiles* directory, ${MODULESHOME }/*modulefiles*, by the initialization script. MODULEPATH can be set using 'module use' or by the module initialization script to search group or personal *modulefile* directories before or after the master *modulefile* directory.

LOADEDMODULES

A colon separated list of all loaded *modulefiles*.

_LOADED_MODULEFILES_

A colon separated list of the full pathname for all loaded *modulefiles*.

MODULESBEGINENV

The filename of the file containing the initialization environment snapshot.

Files

/opt

The MODULESHOME directory.

${MODULESHOME}/etc/rc

The system-wide modules rc file. The location of this file can be changed using the MODULERCFILE environment variable as described above.

${HOME}/.modulerc

The user specific modules rc file.

${MODULESHOME}/*modulefiles*

The directory for system-wide *modulefiles*. The location of the directory can be changed using the MODULEPATH environment variable as described above.

${MODULESHOME}/bin/modulecmd

The *modulefile* interpreter that gets executed upon each invocation of a module.

${MODULESHOME}/init/shellname

The Modules package initialization file sourced into the user's environment.

${MODULESHOME}/init/.modulespath

The initial search path setup for module files. This file is read by all shell init files.

${MODULEPATH}/.moduleavailcache

File containing the cached list of all *modulefiles* for each directory in the MODULEPATH (only when the avail cache is enabled).

${MODULEPATH}/.moduleavailcachedir

File containing the names and modification times for all sub-directories with an avail cache.

${HOME}/.modulesbeginenv

A snapshot of the user's environment taken when Modules are initialized. This information is used by the module update sub-command.

Chapter 6. Resource Management using SLURM

6.1 SLURM Resource Management Utilities

As a cluster resource manager, SLURM has three key functions. First, it allocates exclusive and/or non-exclusive access to resources (compute nodes) to users for some duration of time so they can perform work. Second, it provides a framework for starting, executing, and monitoring work (normally a parallel job) on the set of allocated nodes. Finally, it arbitrates conflicting requests for resources by managing a queue of pending work.

Users interact with **SLURM** through various command line utilities:

- **SRUN** for submitting a job for execution and optionally controlling it interactively.
- **SBCAST** to transmit a file to all nodes running a job.
- **SCANCEL** for terminating a pending or running job.
- **SQUEUE** for monitoring job queues.
- **SINFO** for monitoring partition and overall system state.
- **SACCT** displays data for all jobs and job steps in the SLURM accounting log.
- **Global Accounting API** for merging the data from a **LSF** accounting file and the SLURM accounting file into a single record.

Note:
LSF (**Load Sharing Facility** from **Platform Computing**) is proprietary software and is not included in the BAS4 for Xeon delivery.

Important
SLURM does not work with **PBS Professional** Resource Manager and should only be installed on clusters which do not use **PBS PRO.**

6.2 SRUN

SRUN submits jobs to run under **SLURM** management. **SRUN** can:

- Submit a batch job and then terminate
- Submit an interactive job and then persist to shepherd the job as it runs
- Allocate resources to a shell and then spawn that shell for use in running subordinate jobs.

SLURM associates every set of parallel tasks ("*job steps*") with the **SRUN** instance that initiated that set, and SRUN provides comprehensive control over node choice and I/O redirection for the parallel job.

6.2.1 SRUN Roles and Modes

SRUN executes tasks ("*jobs*") in parallel on multiple compute nodes at the same time (on machines where SLURM manages the resources). **SRUN** options allow the User to both:

- Specify the parallel environment for job(s), such as the number of nodes used, node partition, distribution of processes among nodes, and total time.
- Control the behavior of a parallel job as it runs, such as by redirecting or labeling its output, sending it signals, or specifying its reporting verbosity.

Because it performs several different roles, SRUN can be used in four distinct ways or "**modes**". These modes are described in the following table.

Mode	Description
INTERACTIVE	The simplest way to use SRUN is to distribute execution of a serial program (such as a UNIX utility) across a specified number or range of compute nodes. For example, `srun -N 8 cp ~/data1 /var/tmp/data1` copies (CP) file data1 from a common home directory to local disk space on each of eight compute nodes. SRUN allows relevant environment variables to be set on its own execute line. In interactive mode, SRUN submits job to the local SLURM job controller, then initiates all processes on the specified nodes and blocks until the requested resources become available. Many control options are available to change the details of this general pattern.
BATCH	SRUN can also directly submit complex scripts to the job queue(s) managed by SLURM for later execution, when needed resources become available and when no higher priority jobs are pending. For example, `srun -N 16 -b myscript.sh` uses the -b option of SRUN to place myscript.sh into the queue to later run on 16 nodes. Scripts in turn normally contain either MPI programs or other *simple* invocations of SRUN itself (as shown above). Thus, the -b option of SRUN supports basic, local-batch service.

ALLOCATE	The SRUN "allocate" mode can be used to combine the job complexity of scripts with the immediacy of interactive execution. For example, `srun -A -N 4 myscript.sh` uses the SRUN (uppercase) -A option to allocate specified resources (in this case, four nodes), spawn a subshell with access to those resources, and then run multiple subsequent jobs using *simple* SRUN commands within the specified script (here, **myscript.sh**) that the **subshell** immediately starts to execute.
ATTACH	To monitor or intervene in an already running SRUN job, either batch (started with -b) or interactive ("allocated", started with -A), execute SRUN again and "attach"(-a, lowercase) to that job. For example, `srun -a 6543 -j` forwards the standard output and error messages from the running job with SLURM ID 6543 to the attaching SRUN to reveal the job's current status, and (with -j, lowercase) also "joins" the job so that you can send it signals as if this SRUN had initiated the job. Omit -j for read-only attachments. Because you are attaching to a running job whose resources have already been allocated, SRUN's resource-allocation options (such as -N) are incompatible with -a.

Table 6-1. SRUN Modes

6.2.2 SRUN Signal Handling

Signals sent to SRUN are automatically forwarded to the tasks that SRUN controls, with a few special cases. SRUN handles the sequence CTRL-C in different ways, depending on how many it receives in one second:

```
CTRL-Cs within one second
-------------------------
First    reports the state of all tasks
         associated with SRUN.
Second   sends SIGINT signal to all
         associated SRUN tasks.
Third    terminates the job at once,
         without waiting for remote
         tasks to exit.
```

6.2.3 SRUN Run-Mode Options

This section explains the ***mutually exclusive*** SRUN options that enable its different run modes. Each option has a one-character (UNIX) and a longer (Linux) alternative syntax.

NAME

SRUN - run parallel jobs

SYNOPSIS

```
srun [OPTIONS...] executable [args...]
srun --batch [OPTIONS...] job_script
srun --allocate [OPTIONS...] [job_script]
srun --attach=jobid
```

DESCRIPTION

Allocate resources and optionally initiate parallel jobs on clusters managed by SLURM.

6.2.4 Parallel Run Options

`-n, --ntasks=ntasks`

Specify the number of processes to run. Request that SRUN allocate ntasks processes. The default is one process per node, but note that the **-c** parameter will change this default.

`-c, --cpus-per-task=ncpus`

Request that ncpus be allocated per process. This may be useful if the job is multithreaded and requires more than one CPU per task for optimal performance. The default is one CPU per process. If **-c** is specified without **-n** as many tasks will be allocated per node as possible while satisfying the **-c** restriction.

`-N, --nodes=minnodes[-maxnodes]`

Request that a minimum of minnodes nodes be allocated to this job. The scheduler may decide to launch the job on more than minnodes nodes. A limit on the maximum node count may be specified with maxnodes (e.g. "--nodes=2-4"). The minimum and maximum node count may be the same in order that a specific number of nodes are specified (e.g. "--nodes=2-2" will ask for two and ONLY two nodes).

Note:

The specified minimum is exceeded ONLY IF a maximum is specified.

The partition's node limits supersede those of the job. If the node limits of a job are outside the range permitted for its associated partition, the job will be left in a PENDING state. This permits possible execution at a later time, when the partition limit is changed. If the node limits of a job exceed the number of nodes configured in the partition, the job will be rejected. Note that the environment variable SLURM_NNODES will be set to the count of nodes actually allocated to the job. See the ENVIRONMENT VARIABLES section for more information. If **-N** is not specified, the default behavior is to allocate enough nodes to satisfy the requirements of the -n and -c options.

`-r, --relative=n`

Run a job step relative to node n of the current allocation. This option may be used to spread several job steps out among the nodes of the current job. If -r is used, the current job step will begin at node n of the allocated nodelist, where the first node is considered node 0. The **-r** option is not permitted along with **-w** or **-x**, and will be silently ignored when not running within a prior allocation (i.e. when SLURM_JOBID is not set). If the **–r** is used without prior allocation an error message is displayed, as in the following example:

```
srun -r1 my_script
```

```
error: Unable to create job step: Requested node
configuration is not available
```

The default for n is 0. If the value of **--nodes** exceeds the number of nodes identified with the **--relative** option, a warning message will be printed and the **--relative** option will take precedence.

`-p, --partition=partition`
Request resources from partition "partition." The SLURM administrator creates the partitions, and also identifies one of those partitions as the default.

`-P, --dependency=jobid`
Defer initiation of this job until the specified jobid has completed execution. Many jobs can share the same dependency and these jobs may belong to different users. The value may be changed after job submission using the SCONTROL command.

`--nice[=adjustment]`
Run the job with an adjusted scheduling priority within SLURM. With no adjustment value, the scheduling priority is decreased by 100. The adjustment range is from -10000 (highest priority) to 10000 (lowest priority). Only privileged users can specify a negative adjustment. Note that this option is presently ignored if SchedulerType=sched/wiki.

`--multi-prog`
Run a job with different programs and different arguments for each task. In this case, the executable program specified is actually a configuration file specifying the executable and the arguments for each task. See MULTIPLE PROGRAM CONFIGURATION below for details about the configuration file contents.

`--begin=time`
Defer initiation of this job until the specified time. It accepts times of the form HH:MM:SS to run a job at a specific time of day (seconds are optional). (If that time is already past, the next day is assumed.) It is also possible to specify midnight, noon, or teatime (4pm) and have a time-of-day appended with AM or PM, for running in the morning or the evening. Additionally, it is possible to specify the day on which the job will be run, by giving a date in the form MMDDYY, MM/DD/YY, or MM.DD.YY. Another option is to give times like now + count time-units, where the time-units can be minutes, hours, days, or weeks and SLURM can be told to run the job today with the keyword today, or to run the job tomorrow with the keyword tomorrow. The value may be changed after job submission using the SCONTROL command.

Notes for date/time specifications:

- Although the 'seconds' field of the HH:MM:SS time specification is allowed by the code, the poll time of the SLURM scheduler is not precise enough to guarantee dispatch of the job on the exact second. The job will be eligible to start on the next poll following the specified time. The exact poll interval depends on the SLURM scheduler (e.g. 60 seconds with the default **sched/builtin**).
- If no time (HH:MM:SS) is specified, the default is (00:00:00).
- If a date is specified without a year (e.g. MM/DD) then the current year is assumed, unless the combination of MM/DD and HH:MM:SS has already passed for that year, in which case the next year is used.

`-U, --account=account`
Change resource use by this job to specified account. The account is an arbitrary string. The account may be changed after job submission using the SCONTROL command.

`-t, --time=minutes`
Establish a time limit to terminate the job after the specified number of minutes. If the job's time limit exceeds the partition's time limit, the job will be left in a PENDING state. The default value is the partition's time limit. When the time limit is reached, the job's processes are sent SIGTERM followed by SIGKILL. The interval between signals is specified by the SLURM configuration parameter KillWait. Time limit of 0 minutes indicates that an infinite timelimit should be used.

`-D, --chdir=path`
Have the remote processes do a **chdir** to path before beginning execution. The default is to chdir to the current working directory of the SRUN process.

`-I, --immediate`
Exit if resources are not immediately available. By default, `--immediate` is off, and SRUN will block until resources become available.

`-k, --no-kill`
Do not automatically terminate a job if one of the nodes it has been allocated fails. This option is only recognized on a job allocation, not for the submission of individual job steps. The job will assume all responsibilities for fault-tolerance. The active job step (MPI job) will almost certainly suffer a fatal error, but subsequent job steps may be run if this option is specified. The default action is to terminate the job upon node failure. Note that -batch jobs will be re-queued if a node failure occurs in the process of initiating it.

`-K, --kill-on-bad-exit`
Terminate a job if any task exits with a non-zero exit code.

`-s, --share`
The job can share nodes with other running jobs. This may result in faster job initiation and higher system utilization, but lower application performance.

`-O, --overcommit`

Overcommit resources. Normally, SRUN will not allocate more than one process per CPU. Specifying `--overcommit` explicitly allows more than one process per CPU. However, no more than MAX_TASKS_PER_NODE tasks are permitted to execute per node.

`-T, --threads=nthreads`
Request that SRUN use nthreads to initiate and control the parallel job. The default value is the smallest of 10 or the number of nodes allocated.

`-l, --label`
Prefix task number to lines of stdout/err. Normally, stdout and stderr from remote tasks are line-buffered directly to the stdout and stderr of SRUN. The `--label` option will prefix lines of output with the remote task id.

`-u, --unbuffered`
Do not line buffer stdout from remote tasks. This option cannot be used with -label.

`-m, --distribution=(block|cyclic|hostfile)`
Specify an alternate distribution method for remote processes.

`block`
The block method of distribution will allocate processes in-order to the CPUs on a node. If the number of processes exceeds the number of CPUs on all of the nodes in the allocation then all nodes will be utilized. For example, consider an allocation of three nodes each with two CPUs. A four-process block distribution request will distribute those processes to the nodes with processes one and two on the first node, process three on the second node, and process four on the third node. Block distribution is the default behavior if the number of tasks exceeds the number of nodes requested.

`cyclic`
The cyclic method distributes processes in a round-robin fashion across the allocated nodes. That is, process one will be allocated to the first node, process two to the second, and so on. This is the default behavior if the number of tasks is not larger than the number of nodes requested.

`hostfile`
The hostfile method of distribution will allocate processes in the order in which they are listed in the file designated by the environment variable SLURM_HOSTFILE. If this variable is listed, it will override any other method specified. If not set, the method will default to block.

`-J, --job-name=jobname`
Specify a name for the job. The specified name will appear along with the job id number when querying running jobs on the system. The default is the supplied executable program's name.

`--mpi=mpi_type`
Identify the type of MPI to be used. This may result in unique initiation procedures.

`list`
Lists available MPI types from which to choose.

`lam`
Initiates one `lamb` process per node and establishes necessary environment variables for LAM/MPI.

`mpich-gm`
For use with Myrinet.

`mvapich`
For use with Infiniband.

`none`
No special MPI processing. This is the default and works with many other versions of MPI.

`--ctrl-comm-ifhn=addr`
Specify the address or hostname to be used for PMI communications only (task communication and synchronization primitives for MPCIH2). The default is hostname (response from getnodename function). Use of this is required if a DNS lookup cannot be performed on the hostname or if that address is blocked from the compute nodes.

`--jobid=id`
Initiate a job step under an already allocated job with job id id. Using this option will cause SRUN to behave exactly as if the SLURM_JOBID environment variable were set.

`-o, --output=mode`
Specify the mode for stdout redirection. By default, in interactive mode, SRUN collects stdout from all tasks, and line buffers this output to the attached terminal. With `--output` stdout may be redirected to a file, to one file per task, or to /dev/null. If the specified file already exists, it will be overwritten. If `--error` is not also specified on the command line, both stdout and stderr will be directed to the file specified by `--output`.

`-i, --input=mode`
Specify how stdin is to be redirected. By default, SRUN redirects stdin from the terminal to all tasks.

`-e, --error=mode`
Specify how stderr is to be redirected. By default in interactive mode, SRUN redirects stderr to the same file as stdout, if one is specified. The `--error` option is provided to allow stdout and stderr to be redirected to different locations. If the specified file already exists, it will be overwritten.

`-b, --batch`
Submit in "batch mode." SRUN will make a copy of the executable file (a script) and submit the request for execution when resources are available. SRUN will terminate after the request has been submitted. The executable file will run on the first node allocated to the job and must contain SRUN commands to initiate parallel tasks. **stdin** will be redirected from **/dev/null**, **stdout** and **stderr** will be redirected to a file with the name of **slurm-<jobid>.out**.

Example:
`slurm-2345.out`

Note that if the SLURM daemons are cold-started, jobid values will be reused. Plan accordingly to avoid over-writing output and error files. The executable must be specified using either a fully-qualified pathname, or its pathname will be treated as relative to the current working directory. The search path will not be used to locate the file. The executable will be interpreted by the users default shell unless the file begins with "#!" followed by the fully-qualified pathname of a valid shell. Note that batch jobs will be re-queued if a node fails while it is being initiated.

SRUN command-line options can also be inserted into the script by prefacing the option with #SLURM. Multiple options can be on one line or multiple lines. i.e.

```
#SLURM -N 2 -n 2
#SLURM --mpi=lam
```

This is running the script on 2 nodes, with 2 procs with mpi type lam. All command-line options are able to be set inside the script with the exception of the mode (which has already been set to run a batch script since the running mode is batch). Options on the command line take precedence over options in the batch script, which in turn take precedence over existing environment variables.

`-v, --verbose`
Verbose operation. Using the -v multiple times will further increase the verbosity of SRUN. By default, only errors will be displayed.

`-d, --slurmd-debug=level`
Specify a debug level for SLURMD. “level” may be an integer value between 0 [quiet, only errors are displayed] and 4 [verbose operation]. The SLURMD debug information is copied to the stderr of the job. By default, only errors are displayed.

`-W, --wait=seconds`
Specify how long to wait after the first task terminates before terminating all remaining tasks. A value of 0 indicates an unlimited wait (a warning will be issued after 60 seconds). The default value is set by the WaitTime parameter in the SLURM configuration file (see slurm.conf). This option can be useful to insure that a job is terminated in a timely fashion in the event that one or more tasks terminate prematurely.

`-q, --quit-on-interrupt`
Quit immediately on single SIGINT (Ctrl-C). Use of this option disables the status feature normally available when SRUN receives a single Ctrl-C and causes SRUN to instead immediately terminate the running job.

`-X, --disable-status`
Disable the display of task status when SRUN receives a single SIGINT (Ctrl-C). Instead, immediately forward the SIGINT to the running job. A second Ctrl-C in one second will forcibly terminate the job and SRUN will immediately exit. May also be set via the environment variable SLURM_DISABLE_STATUS.

`-Q, --quiet`
Quiet operation. Suppress informational messages. Errors will still be displayed.

`--mail-type=type`
Notify user by email when certain event types occur. Valid type values are BEGIN, END, FAIL, ALL (any state change). The user to be notified is indicated with `--mail-user`.

`--mail-user=user`
User to receive email notification of state changes as defined by `--mail-type`. The default value is the submitting user.

`--uid=user`
Attempt to submit and/or run a job as user instead of the invoking user id. The invoking user's credentials will be used to check access permissions for the target partition. User root may use this option to run jobs as a normal user in a RootOnly partition for example. If run as root, SRUN will drop its permissions to the uid specified after node allocation is successful. "user" may be the user name or numerical user ID.

`--gid=group`
If SRUN is run as root, and the `--gid` option is used, submit the job with group's group access permissions. **group** may be the group name or the numerical group ID.

`--core=type`
Adjust corefile format for parallel job. If possible, SRUN will set up the environment for the job such that a corefile format other than full core dumps is enabled. If run with type = "list", SRUN will print a list of supported corefile format types to stdout and exit.

`--propagate[=rlimits]`
Allows users to specify which of the modifiable (soft) resource limits to propagate to the compute nodes and apply to their jobs. If rlimits is not specified, then all resource limits will be propagated.

`--prolog=executable`
SRUN will run executable just before launching the job step. The command line arguments for executable will be the command and arguments of the job step. If executable is "none", then no prolog will be run. This parameter overrides the SrunProlog parameter in slurm.conf.

`--epilog=executable`
SRUN will run executable just after the job step completes. The command line arguments for executable will be the command and arguments of the job step. If executable is "none", then no epilog will be run. This parameter overrides the SrunEpilog parameter in slurm.conf.

`--task-prolog=executable`

The SLURMD daemon will run executable just before launching each task. This will be executed after any TaskProlog parameter in slurm.conf is executed. Besides the normal environment variables, this has SLURM_TASK_PID available to identify the process ID of the task being started. Standard output from this program of the form "export NAME=value" will be used to set environment variables for the task being spawned.

`--task-epilog=executable`
The SLURMD daemon will run executable just after each task terminates. This will be before any TaskEpilog parameter in slurm.conf is executed. This is meant to be a very short-lived program. If it fails to terminate within a few seconds, it will be killed along with any descendant processes.

6.2.5 Running the epilog, prolog, task-epilog and task-prolog scripts in batch mode

```
srun -b --epilog=myscript hostname
```

When the **srun** runs in the command above, the task is submitted in batch mode and **srun** submits the **hostname** request for execution when resources are available for it then once the request is submitted **srun** will terminate.

To execute the **epilog, prolog, task-epilog** and **task-prolog** options in batch mode, use a script file similar to the **batch-epilog.sh** example shown below:

```
cat batch-epilog.sh
```

```
----------------------------------------------------------------
srun --epilog=myscript hostname
```

```
srun -b batch-epilog.sh
```

```
----------------------------------------------------------------
srun: jobid 7 submitted
```

6.2.6 Allocate Options

`-A, --allocate`
Allocate resources and spawn a shell. When `--allocate` is specified to SRUN, no remote tasks are started. Instead a subshell is started that has access to the allocated resources. Multiple jobs can then be run on the same CPUs from within this subshell. See Allocate Mode below.

`--no-shell`
Immediately exit after allocating resources instead of spawning a shell when used with the -A, `--allocate` option.

6.2.7 Attach Option

`-a, --attach=id`
This option will attach SRUN to a running job with job id = id. Provided that the calling user has access to that running job, stdout and stderr will be redirected to the current session (assuming that the tasks' stdout and stderr are not connected directly to files). stdin is not connected to the remote tasks, and signals are not forwarded unless the `--join` parameter is also specified.

`-j, --join`
Used in conjunction with `--attach` to specify that stdin should also be connected to the remote tasks (assuming that the remote tasks' stdin are not directly connected to files), and signals sent to SRUN will be forwarded to the remote tasks.


Note:
See section 6.2.16 Attaching To a Running Job for more information.

6.2.8 Constraint Options

The following options all put constraints on the nodes that may be considered for the job:

`--mincpus=n`
Specify minimum number of CPUs per node.

`--mem=MB`
Specify a minimum amount of real memory.

`--tmp=MB`
Specify a minimum amount of temporary disk space.

`-C, --constraint=list`
Specify a list of constraints. The constraints are features that have been assigned to the nodes by the SLURM administrator. The list of constraints may include multiple features separated by commas, in which case all nodes must have all listed features (i.e. the features are ANDed together). Alternately, the features may be separated by a vertical bar (|), in which case all nodes must have at least one of the listed features (i.e. the features are ORed together). If no nodes have the requested features, then the SLURM job manager will reject the job.

`--contiguous`
Demand a contiguous range of nodes. The default is "yes". Specify `--contiguous=no` if a contiguous range of nodes is not a constraint.

`-w, --nodelist=host1,host2,... or filename`
Request a specific list of hosts. The job will contain at least these hosts. The list may be specified as a comma-separated list of hosts, a range of hosts (host[1-5,7,...] for example), or a filename. The host list will be assumed to be a filename if it contains a "/" character.

`-x, --exclude=host1,host2,... or filename`
Request that a specific list of hosts not be included in the resources allocated to this job. The host list will be assumed to be a filename if it contains a "/"character.

6.2.9 Affinity/Multi-core Options with task/affinity or task/numa plug-in

These options are used when the **task/affinity** or **task/numa plug-in** is enabled.

`--cpu_bind=[{quiet,verbose},]type`
Bind tasks to CPUs

`q[uiet],`
quietly bind before task runs (default)

`v[erbose],`
verbosely report binding before task runs

`no[ne]`
do not bind tasks to CPUs (default)

`rank`
bind by task rank

`map_cpu:<list>`
bind by mapping CPU IDs to tasks as specified where <list> is <cpuid1>,<cpuid2>,...<cpuidN>. CPU IDs are interpreted as decimal values unless they are preceded with "x" in which case they are interpreted as hexadecimal values.

`mask_cpu:<list>`
bind by setting CPU masks on tasks as specified where <list> is <mask1>,<mask2>,...<maskN>. CPU masks are always interpreted as hexadecimal values but can be preceded with an optional "x".

To have SLURM always report on the selected CPU binding for all SRUN commands executed in a shell, enable verbose mode separately from the command line with:

```
setenv SLURM_CPU_BIND verbose
```

SLURM_CPU_BIND will not propagate into the tasks environment (binding by default only affects the first SRUN). To propagate `--cpu_bind` to successive SRUN commands, first do the following in each task:

```
setenv SLURM_CPU_BIND \
${SLURM_CPU_BIND_VERBOSE},${SLURM_CPU_BIND_TYPE}${SLURM_CPU_BIND_LIST}
```

6.2.10 Affinity/Multi-core Options with task/affinity and NUMA memory functions

These options are used when the task/affinity plug-in is enabled and the NUMA memory functions are available

`--mem_bind=[{quiet,verbose},]type`
Bind tasks to memory. Note that the resolution of CPU and memory binding may differ on some platforms. For example, CPU binding may be performed at the level of the cores within a processor while memory binding will be performed at the level of nodes, where the definition of "nodes" may differ from system to system. The use of a type other than "none" or "local" is not recommended. For greater control, try running a simple test code with the options "--cpu_bind=verbose,none --mem_bind=verbose,none" to determine the specific configuration.

`q[uiet],`
quietly bind before task runs (default)

`v[erbose],`
verbosely report binding before task runs

`no[ne]`
do not bind tasks to memory (default)

`rank`
bind by task rank (not recommended)

`local`
Use memory local to the processor in use

`map_mem:<list>`
bind by mapping a node's memory to tasks as specified where <list> is <cpuid1>,<cpuid2>,...<cpuidN>. CPU IDs are interpreted as decimal values unless they are preceded with "x", in which case they are interpreted as hexadecimal values (not recommended).

`mask_mem:<list>`
bind by setting memory masks on tasks as specified where <list> is <mask1>,<mask2>,...<maskN>. Memory masks are always interpreted as hexadecimal values but can be preceded with an optional "x" (not recommended).

To have SLURM always report on the selected memory binding for all SRUN commands executed in a shell, enable verbose mode separately from the command line with:

```
setenv SLURM_MEM_BIND verbose
```

SLURM_MEM_BIND will not propagate into the tasks environment (binding by default only affects the first SRUN). To propagate --mem_bind to successive SRUN commands, first do the following in each task:

```
setenv SLURM_MEM_BIND \
${SLURM_MEM_BIND_VERBOSE},${SLURM_MEM_BIND_TYPE}${SLURM_MEM_BIND_LIST}
```

See the ENVIRONMENT VARIABLES section for a more detailed description of the individual SLURM_CPU_BIND* and SLURM_MEM_BIND* variables.

`--network=type`
Specify the communication protocol to be used. The interpretation of type is system dependent.

6.2.11 Affinity/Multi-Core Options with UseCPUSETS parameter

The **UseCPUSETS** option modifies the Affinity/Multi-core operations to use the CPUsets facility in Linux instead of the **scheduler affinity** calls in the **task/affinity** plug-in. Job step initialization checks the **cpu_bind** and **mem_bind** parameters from SRUN, constructs a set of CPUs and memory, and creates a CPUset with these parameters. The name of the CPUset is **slurm** suffixed by **jobid** and **local task id**, e.g., **slurm47_1**. Each task on a given compute node is assigned to its own CPUset, which constrains the job to execute only on the CPUs and Memory nodes contained within the CPUset.

The following rules apply to the parameters in this mode:

1. If neither **cpu_bind** nor **mem_bind** are specified, no CPUset is created and the job runs with no restrictions.
2. **Mem_bind** is ignored if **cpu_bind** is not specified, as any CPU may be used by the task.

--cpu_bind options

None	no cpuset created, any processor may be used
Rank	CPUs assigned based on job **localid** + cpus/task
Map_cpu:<list>	CPUs are taken from the specified list according to **localid** of the task multiplied by the number of **CPUs** per task
Mask_cpu:<list>	CPU masks are taken from the list according to the **localid** order for the task. This allows specific CPU assignment under the control of the job requester.

--mem_bind options

None	Cpuset includes all parent's memory nodes
Rank	Not supported, same as **None**

Local	Memory nodes assigned based on CPUs allocated to cpuset
Map_mem:<list>	Not supported, same as **Local**
Mask_mem:<list>	Selects mask from the list in **localid** order for the task. This allows specific memory node assignment under the control of the job requester.

6.2.12 Help options

`--help`
Show this help message

`--usage`
Display brief usage message

6.2.13 Other options

`-V, --version`
output version information and exit

Unless the -a (--attach) or -A (--allocate) options are specified (see Allocate mode and Attaching to jobs below), SRUN will submit the job request to the SLURM job controller, then initiate all processes on the remote nodes. If the request cannot be met immediately, SRUN will block until the resources are free to run the job. If the -I (--immediate) option is specified, SRUN will terminate if resources are not immediately available.

When initiating remote processes, SRUN will propagate the current working directory, unless --chdir=path is specified, in which case path will become the working directory for the remote processes.

The -n, -c, and -N options control how CPUs and nodes will be allocated to the job. When specifying only the number of processes to run with -n, a default of one CPU per process is allocated. By specifying the number of CPUs required per task (-c), more than one CPU may be allocated per process. If the number of nodes is specified with -N, SRUN will attempt to allocate at least the number of nodes specified.

Combinations of the above three options may be used to change how processes are distributed across nodes and CPUs. For instance, by specifying both the number of processes and number of nodes on which to run, the number of processes per node is implied. However, if the number of CPUs per process is more important then number of processes (-n) and the number of CPUs per process (-c) should be specified.

SRUN will refuse to allocate more than one process per CPU unless --overcommit (-O) is also specified.

SRUN will attempt to meet the above specifications "at a minimum." That is, if 16 nodes are requested for 32 processes, and some nodes do not have 2 CPUs, the allocation of nodes will be increased in order to meet the demand for CPUs. In other words, a minimum of 16 nodes is being requested. However, if 16 nodes are requested for 15 processes, SRUN will consider this an error, as 15 processes cannot run across 16 nodes.

6.2.14 I/O Redirection

By default STDOUT and STDERR will be redirected from all tasks to the STDOUT and STDERR of SRUN, and STDIN will be redirected from the standard input of SRUN to all remote tasks. This behavior may be changed with the **--output**, **--error**, and **--input** (**-o**, **-e**, **-i**) options. Valid format specifications for these options are:

`all`
: STDOUT and STDERR are redirected from all tasks to SRUN. STDIN is broadcast to all remote tasks. (This is the default behavior.)

`none`
: STDOUT and STDERR are not received from any task. STDIN is not sent to any task (STDIN is closed).

`taskid`
: Redirects to SRUN (and hence to the attached terminal) STDOUT and STDERR from the single specified task whose relative ID is taskid, where the range for integer taskid starts at 0 (the first task) and runs through the total number of tasks in the current job step. This choice also redirects STDIN from SRUN (the terminal) to this single specified task.

`filename`
: SRUN will redirect STDOUT and/or STDERR to the named file from all tasks. STDIN will be redirected from the named file and broadcast to all tasks in the job. If the job is submitted in batch mode using the -b or --batch option, filename refers to a path on each of the nodes on which the job runs.

Note:
The file is read (-i) or written (-o or -e) only on the first node allocated to the job (not on each of the nodes).

Otherwise filename refers to a path on the host that runs SRUN. Depending on the cluster's file system layout, this may result in the output appearing in different places depending on whether the job is run in batch mode.

`format string`
: SRUN allows for a format string to be used to generate the named IO file described above. The following list of format specifiers may be used in the format string to generate a filename that will be unique to a given jobid, stepid, node, or task. In each case, the appropriate number of files are opened and associated with the corresponding tasks.

  `%J` jobid.stepid of the running job (e.g. "128.0").

  `%j` jobid of the running job.

  `%s` stepid of the running job.

  `%N` short hostname. This will create a separate IO file per node.

%n Node identifier relative to current job (e.g. "0" is the first node of the running job). This will create a separate IO file per node.

%t task identifier (rank) relative to current job. This will create a separate IO file per task.

A number placed between the percent character and format specifier may be used to zero-pad the result in the IO filename. This number is ignored if the format specifier corresponds to non-numeric data (%N for example).

Some examples of how the format string may be used for a four-task job step with a Job ID of 128 and step id of 0 are included below:

```
job%J.out   job128.0.out

job%4j.out   job0128.out

job%j-%2t.out job128-00.out, job128-01.out, ...
```

6.2.15 Allocate Mode

When the allocate option is specified (-A, --allocate) SRUN will not initiate any remote processes after acquiring resources. Instead, SRUN will spawn a subshell that has access to the acquired resources. Subsequent instances of SRUN from within this subshell will then run on these resources.

If the name of a script is specified on the command line with --allocate, the spawned shell will run the specified script. Resources allocated in this way will only be freed when the subshell terminates.

6.2.16 Attaching To a Running Job

Use of the **-a jobid** (or --**attach**) option allows SRUN to reattach to a running job, receive stdout and stderr from the job and forward signals to the job, just as if the current session of SRUN had started the job. (stdin, however, cannot be forwarded to the job.)

There are two ways to reattach to a running job. The default method is to attach to the current job in read-only. In this case, stdout and stderr are duplicated to the attaching SRUN, but signals are not forwarded to the remote processes (a single Ctrl-C will detach this read-only SRUN from the job). If the -j (--join) option is also specified, SRUN "joins" the running job, and is able to forward signals, connect stdin, and act, for the most part, much like the SRUN process that initiated the job.

Node and CPU selection options are not applicable when specifying --attach, and it is an error to use -n, -c, or -N in attach mode.

Note:
When attaching to a job script that was submitted in SLURM 'batch' mode (i.e., with the **batch** option), attaching to the job using **jobid** only will not attach the stdout and stderr from the script, as they will have been already mapped to files. In this case, it is necessary to attach to the **jobid.stepid** for the **SRUN** command contained in the script. The appropriate **jobid.stepid** can be determined by using the **squeue** command (see Section 6.4).

6.2.17 Environment Variables

Some **SRUN** options may be set via environment variables. These environment variables, along with their corresponding options, are listed below. (Note: command-line options will always override these settings.)

SLURM_CONF	The location of the SLURM configuration file.
SLURM_ACCOUNT	`-U, --account=account`
SLURM_CPU_BIND	`--cpu_bind=type`
SLURM_CPUS_PER_TASK	`-c, --ncpus-per-task=n`
SLURM_CORE_FORMAT	`--core=format`
SLURM_DEBUG	`-v, --verbose`
SLURMD_DEBUG	`-d, --slurmd-debug`
SLURM_DISTRIBUTION	`-m, --distribution=(block|cyclic|hostfile)`
SLURM_GEOMETRY	`-g, --geometry=X,Y,Z`
SLURM_LABELIO	`-l, --label`
SLURM_MEM_BIND	`--mem_bind=type`
SLURM_NETWORK	`--network=type`
SLURM_NNODES	`-N, --nodes=(n|min-max)`
SLURM_NO_ROTATE	`--no-rotate`
SLURM_NPROCS	`-n, --ntasks=n`
SLURM_OVERCOMMIT	`-o, --overcommit`
SLURM_PARTITION	`-p, --partition=partition`

SLURM_REMOTE_CWD	`-D, --chdir==dir`
SLURM_SRUN_COMM_IFHN	`--ctrl-comm-ifhn=addr`
SLURM_STDERRMODE	`-e, --error=mode`
SLURM_STDINMODE	`-i, --input=mode`
SLURM_STDOUTMODE	`-o, --output=mode`
SLURM_TASK_EPILOG	`--task-epilog=executable`
SLURM_TASK_PROLOG	`--task-prolog=executable`
SLURM_TIMELIMIT	`-t, --time=minutes`
SLURM_WAIT	`-W, --wait=seconds`
SLURM_DISABLE_STATUS	`-X, -disable-status`

Additionally, SRUN will set some environment variables in the environment of the executing tasks on the remote compute nodes. These environment variables are:

SLURM_CPU_BIND_VERBOSE
--cpu_bind verbosity (quiet, verbose).

SLURM_CPU_BIND_TYPE
--cpu_bind type (none, rank, map_cpu:, mask_cpu:)

SLURM_CPU_BIND_LIST
--cpu_bind map or mask list (<list of IDs or masks for this node>)

SLURM_CPUS_ON_NODE
Count of processors available to the job on this node

SLURM_CPUS_PER_TASK
-c, –ncpus-per-task=n (number of CPUs allocated per process)

SLURM_JOBID
Job id of the executing job

SLURM_LAUNCH_NODE_IPADDR
IP addresses of the node from which the task launch was initiated (from which the SRUN command was run)

SLURM_LOCALID
Node local task ID for the process within a job

SLURM_MEM_BIND_VERBOSE
--mem_bind verbosity (quiet, verbose).

SLURM_MEM_BIND_TYPE
--mem_bind type (none, rank, map_mem:, mask_mem:)

SLURM_MEM_BIND_LIST
--mem_bind map or mask list (<list of IDs or masks for this node>)

SLURM_NNODES
Total number of nodes in the job's resource allocation

SLURM_NODEID
The relative node ID of the current node

SLURM_NODELIST
List of nodes allocated to the job

SLURM_NPROCS
Total number of processes in the current job

SLURM_PROCID
The MPI rank (or relative process ID) of the current process

SLURM_TASKS_PER_NODE
Number of tasks to be initiated on each node. Values are comma separated and in the same order as SLURM_NODELIST. If two or more consecutive nodes are to have the same task count, that count is followed by "(x#)", where "#" is the repetition count. For example, "SLURM_TASKS_PER_NODE=2(x3),1" indicates that the first three nodes will each execute two tasks, and the fourth node will execute one task.

6.2.18 Signals and Escape Sequences

Signals sent to the SRUN command are automatically forwarded to the tasks it is controlling, with a few exceptions. The escape sequence <control-c> will report the state of all tasks associated with the SRUN command. If <control-c> is entered twice within one second, then the associated SIGINT signal will be sent to all tasks. If a third <control-c> is received, the job will be forcefully terminated without waiting for remote tasks to exit.

The escape sequence <control-z> is presently ignored. When implemented it will put the SRUN command into a mode in which various special actions may be invoked.

6.2.19 MPI Support

The **PMI** (Process Management Interface) is provided by MPIBull2 to launch processes on a cluster and provide services to the MPI interface. For example, a call to **pmi_get_appnum** returns the job id. This interface uses sockets to exchange messages.

In **MPIBull2**, this mechanism uses the MPD daemons running on each compute node. Daemons can exchange information and answer the **PMI** calls.

SLURM replaces the Process Management Interface with their own implementation and their own daemons. No MPD is needed and when a PMI request is sent (for example **pmi_get_appnum**), a SLURM extension must answer this request.

The following diagrams show the difference between the use of PMI with and without a resource manager that allows process management.

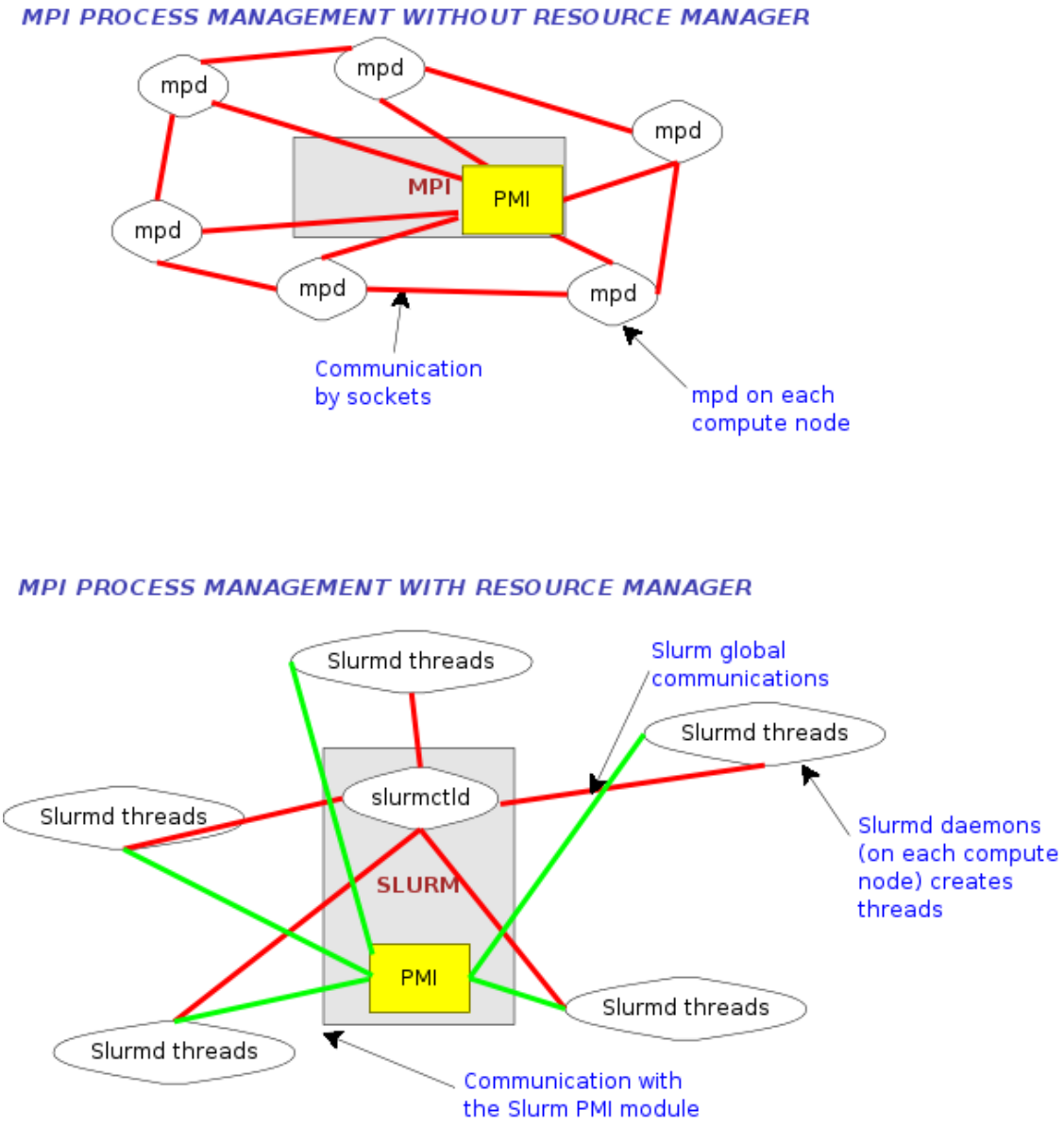


Figure 6-1. MPI Process Management With and Without Resource Manager

MPIBull2 jobs can be launched directly by the **srun** command. SLURM's *none* MPI plug-in must be used to establish communications between the launched tasks. This can be accomplished either using the SLURM configuration parameter *MpiDefault=none* in **slurm.conf** or srun's *--mpi=none* option. The program must also be linked with SLURM's implementation of the PMI library so that tasks can communicate host and port information at startup. (The system administrator can add this option to the mpicc and mpif*77* commands directly, so the user will not need to bother). **Do not use SLURM's MVAPICH plug-in for MPIBull2.**

```
$ mpicc -L<path_to_slurm_lib> -lpmi ...
$ srun -n20 --mpi=none a.out
```

Notes:

- Some MPIBull2 functions are not currently supported by the PMI library integrated with SLURM.
- Set the environment variable PMI_DEBUG to a numeric value of 1 or higher for the PMI library to print debugging information.

6.2.20 Multiple Program Configuration

Comments in the configuration file must have a "#" in column one. The configuration file contains the following fields separated by space:

`Task rank`
: One or more task ranks to use this configuration. Multiple values may be comma separated. Ranges may be indicated with two numbers separated with a '-' with the smaller number first (e.g. "0-4" and not "4-0"). To indicate all tasks, specify a rank of "*" (in which case, this option is not recommended).

`Executable`
: The name of the executable program. May be the fully-qualified pathname, if desired.

`Arguments`
: Program arguments. The expression "%t" will be replaced with the task's number. The expression "%o" will be replaced with the task's offset within this range (e.g. a configured task rank value of "1-5" would have offset values of "0-4"). Single quotes may be used to avoid having the enclosed values interpreted. This field is optional.

Example:

```
############################################################
# srun multiple program configuration file
#
# srun -n8 -l --multi-prog silly.conf
############################################################
4-6    hostname
1,7    echo task:%t
0,2-3   echo offset:%o

$ srun -n8 -l --multi-prog silly.conf
0: offset:0
1: task:1
2: offset:1
3: offset:2
4: linux15.llnl.gov
5: linux16.llnl.gov
6: linux17.llnl.gov
7: task:7
```

6.2.21 Examples

The following simple example demonstrates the execution of the command hostname over eight tasks. At least eight processors will be allocated to the job (the same as the task count). The output of each task will be preceded with its task number. (The machine "dev" in the example below has a total of two CPUs per node)

```
> srun -n8 -l hostname
0: dev0
1: dev0
2: dev1
3: dev1
4: dev2
5: dev2
6: dev3
7: dev3
```

The following example demonstrates how one might submit a script for later execution (batch mode). The script will be initiated when resources are available and no higher priority job is pending for the same partition. The script will execute on four nodes with one task per node implicitly.

```
> cat test.sh
#!/bin/sh
date
srun -l hostname

> srun -N4 -b test.sh
srun: jobid 42 submitted
```

The output of test.sh would be found in the default output file "slurm-42.out."

The SRUN -r option is used within a job script to run two job steps on disjoint nodes in the following example. The script is run using allocate mode, instead of batch mode in this case.

```
> cat test.sh
#!/bin/sh
echo $SLURM_NODELIST
srun -lN2 -r2 hostname
srun -lN2 hostname

> srun -A -N4 test.sh
dev[7-10]
0: dev9
1: dev10
0: dev7
1: dev8
```

The following script runs two job steps in parallel within an allocated set of nodes.

```
> cat test.sh
#!/bin/bash
srun -lN2 -n4 -r 2 sleep 60 &
srun -lN2 -r 0 sleep 60 &
sleep 1
squeue
squeue -s
wait

> srun -A -N4 test.sh
```

```
 JOBID PARTITION   NAME  USER ST  TIME NODES  NODELIST
 65641   batch test.sh grondo  R  0:01   4  dev[7-10]

STEPID   PARTITION    USER   TIME NODELIST
65641.0    batch   grondo   0:01 dev[7-8]
65641.1    batch   grondo   0:01 dev[9-10]
```

This example demonstrates how one executes a simple MPICH job. SRUN is used to build a list of machines (nodes) to be used by mpirun in its required format. A sample command line and the script to be executed follow.

```
> cat test.sh
#!/bin/sh
MACHINEFILE="nodes.$SLURM_JOBID"

# Generate Machinefile for mpich such that hosts are in the same
# order as if run via srun
#
srun -l /bin/hostname | sort -n | awk 'print $2}' > $MACHINEFILE

# Run using generated Machine file:
mpirun -np $SLURM_NPROCS -machinefile $MACHINEFILE mpi-app

rm $MACHINEFILE

> srun -AN2 -n4 test.sh
```

This simple example demonstrates the execution of different jobs on different nodes in the same SRUN. This can be done for any number of nodes or any number of jobs. The executables are placed on the nodes sited by the SLURM_NODEID environment variable, starting at 0 and going up to the number specified on the SRUN command line.

```
> cat test.sh
case $SLURM_NODEID in
 0) echo "I am running on "
  hostname ;;
 1) hostname
  echo "is where I am running" ;;
esac

> srun -N2 test.sh
dev0
is where I am running
I am running on
dev1
```

6.3 SBCAST

sbcast is used to copy a file to local disk on all nodes allocated to a job. This should be executed after a resource allocation has taken place and can be faster than using a single file system mounted on multiple nodes.

NAME

sbcast - transmit a file to the nodes allocated to a SLURM job.

SYNOPSIS

```
sbcast [-CfpsvV] SOURCE DEST
```

DESCRIPTION

sbcast is used to transmit a file to all nodes allocated to the **SLURM** job which is currently active. This command should only be executed within a **SLURM** batch job or within the shell spawned after the resources have been allocated to a SLURM. **SOURCE** is the name of the file on the current node. **DEST** should be the fully qualified pathname for the file copy to be created on each node. **DEST** should be on the local file system for these nodes.

Note: Parallel file systems may provide better performance than sbcast can provide.

OPTIONS

`-C, --compress`
Compress the file being transmitted.

`-f, --force`
If the destination file already exists, replace it.

`-F number, --fanout=number`
Specify the fanout of messages used for file transfer. Maximum value is currently eight.

`-p, --preserve`
Preserves modification times, access times, and modes from the original file.

`-s size, --size=size`
Specify the block size used for file broadcast. The size can have a suffix of k or m for kilobytes or megabytes respectively (defaults to bytes). This size is subject to rounding and range limits in order to maintain good performance. This value may need to be set on systems with very limited memory.

`-v, --verbose`
Provide detailed event logging whilst the program is executing.

`-V, --version`
Print version information and exit.

ENVIRONMENT VARIABLES

Some **sbcast** options may be set via environment variables. These environment variables, along with their corresponding options, are listed below.

Note: Command line options will always override these settings

SBCAST_COMPRESS `-C, --compress`

SBCAST_FANOUT `-F number, fB--fanout=number`

SBCAST_FORCE `-f, --force`

SBCAST_PRESERVE `-p, --preserve`

SBCAST_SIZE `-s size, --size=size`

EXAMPLE

Using a batch script, transmit local file **my.prog** to **/tmp/my.proc** on the local nodes and then execute it.

```
> cat my.job
#!/bin/bash
sbcast my.prog /tmp/my.prog
srun /tmp/my.prog


> srun --nodes=8 --batch my.job
srun: jobid 12345 submitted
```

6.4 SQUEUE (List Jobs)

SQUEUE displays (by default) the queue of running and waiting jobs (or "*job steps*"), including the **JobId** (used for **SCANCEL**), and the nodes assigned to each running job. However, **SQUEUE** reports can be customized to cover any of 24 different job properties, sorted by the most important properties. It also displays the job ID and job name for every job currently managed by the SLURM control daemon (**SLURMCTLD**). The status and resource information for each job (such as time used so far, or a list of committed nodes) are presented in a table whose content and format details can be controlled with the **SQUEUE** options.

NAME

SQUEUE - view information about jobs located in the SLURM scheduling queue.

SYNOPSIS

```
squeue  [OPTIONS...]
```

DESCRIPTION

SQUEUE is used to view job and job step information for jobs managed by SLURM.

OPTIONS

`-a, --all`
Display information about jobs and job steps in all partitions. This causes information to be displayed about partitions that are configured as hidden and partitions that are unavailable to user's group.

`--help`
Print a help message describing all SQUEUE options.

`--hide`
Do not display information about jobs and job steps in all partitions. By default, information about partitions that are configured as hidden or are not available to the user's group will not be displayed (i.e. this is the default behavior).

`--usage`
Print a brief help message listing the SQUEUE options.

`-h, --noheader`
Do not print a header on the output.

`-i <seconds>, --iterate=<seconds>`
Repeatedly gather and report the requested information at the interval specified (in seconds). By default, prints a time stamp with the header.

`-j, --jobs`
Specify the jobs to view. This flag indicates that a comma-separated list of jobs to view follows without an equal sign (see examples). Defaults to all jobs.

`-l, --long`
Report more of the available information for the selected jobs or job steps, subject to any constraints specified.

`-n <node_name>, --node=<node_name>`
Report only on jobs allocated to the specified node. This may either be the NodeName or NodeHostname, as defined in slurm.conf in the event that they differ. A node_name of localhost is mapped to the current host name.

`-o <output_format>, --format=<output_format>`
Specify the information to be displayed.

```
The default format for jobs is:
   Default  "%.7i %.9P %.8j %.8u %.2t %.9M %.6D %R"
If –l or --long is specified, the default job format is:
   -l, --long  "%.7i %.9P %.8j %.8u %.8T %.9M %.9l %.6D %R"
Format strings used internally by  SQUEUE when running with
various options are:
   -s, --steps "%10i %.8j %.9P %.8u %.9M %N"
```

The field specifications available include:

%a	Account associated with the job
%b	Time at which the job began execution
%c	Minimum number of CPUs (processors) per node requested by the job. This reports the value of the SRUN --mincpus option with a default value of zero.
%C	Number of CPUs (processors) requested to the job or job step. This reports the value of the SRUN --ntasks option with a default value of zero.
%d	Minimum size of temporary disk space (in MB) requested by the job
%D	Number of nodes allocated to the job or the minimum number of nodes required by a pending job. The actual number of nodes allocated to a pending job may exceed this number if the job specified a node range count or the cluster contains nodes with varying processor counts.
%e	Time at which the job ended or is expected to end (based upon its time limit)
%E	Job dependency. This job will not begin execution until the dependent job completes. A value of zero implies this job has no dependencies.
%f	Features required by the job
%g	Group name
%G	Group ID

%h	The nodes allocated to the job can be shared with other jobs
%i	Job or job step id
%j	Job or job step name
%l	Time limit of the job in days-hours:minutes:seconds. The value may be "NOT_SET" if not yet established or "UNLIMITED" for no limit.
%m	Minimum size of memory (in MB) requested by the job
%M	Time used by the job or job step in days-hours:minutes:seconds. The days and hours are printed only as needed. For job steps, this field shows the elapsed time since execution began and thus will be inaccurate for job steps that have been suspended.
%n	List of node names explicitly requested by the job
%N	List of nodes allocated to the job or job step. In the case of a COMPLETING job, the list of nodes will comprise only those nodes that have not yet been returned to service. This may result in the node count being greater than the number of listed nodes.
%o	Minimum number of nodes requested by the job
%O	Are contiguous nodes requested by the job
%p	Priority of the job (converted to a floating point number between 0.0 and 1.0).
%P	Partition of the job or job step
%r	The reason why a job is waiting for execution. See the JOB REASON CODES section below for more information.
%R	For running or completed jobs: the list of allocated nodes. For pending jobs: the reason why a job is waiting for execution is printed within parenthesis. See the JOB REASON CODES section below for more information.
%s	Node selection plug-in specific data. Possible data includes: Geometry requirement of resource allocation (X,Y,Z dimensions), Connection type, Permit rotation of geometry (yes or no), etc.
%S	Start time of the job or job step
%t	Job state, compact form: PD (pending), R (running), CA (cancelled), CG (completing), CD (completed), F (failed), TO (timeout), and NF (node failure). See the JOB STATE CODES section below for more information.

%T Job state, extended form: PENDING, RUNNING, SUSPENDED, CANCELLED, COMPLETING, COMPLETED, FAILED, TIMEOUT, and NODE_FAIL. See the JOB STATE CODES section below for more information.

%u User name

%U User ID

%x List of node names explicitly excluded by the job

%.<*> right justification of the field

%<Number><*> size of field

-v
Display all job information.

-p <part_list>, --partition=<part_list>
Specify the partitions of the jobs or steps to view. Accepts a comma-separated list of partition names.

-s, --steps
Specify the job steps to view. This flag indicates that a comma-separated list of job steps to view follows without an equal sign (see examples). The job step format is "job_id.step_id". The default is all job steps.

-S <sort_list>, --sort=<sort_list>
Specification of the order in which records should be reported. This uses the same field specification as the <output_format>. Multiple sorts may be performed by listing multiple sort fields separated by commas. The field specifications may be preceded by "+" or "-" for ascending (default) and descending order respectively. For example, a sort value of "P,U" will sort the records by partition name then by user id. The default value of sort for jobs is "P,t,-p" (increasing partition name then within a given partition by increasing node state and then decreasing priority). The default value of sort for job steps is "P,i" (increasing partition name, then within a given partition by increasing step id).

-t <state_list>, --states=<state_list>
Specify the states of jobs to view. Accepts a comma-separated list of state names or "all". If "all" is specified then jobs of all states will be reported. If no state is specified then pending, running, and completing jobs are reported. Valid states (in both extended and compact form) include: PENDING (PD), RUNNING (R), SUSPENDED (S), COMPLETING (CG), COMPLETED (CD), CANCELLED (CA), FAILED (F), TIMEOUT (TO), and NODE_FAIL (NF). Note that the <state_list> supplied is case insensitive ("pd" and "PD" work the same). See the JOB STATE CODES section below for more information.

-u <user_list>, --user=<user_list>
Specifies a comma separated list of users whose jobs or job steps are to be reported. The list can consist of user names or user id numbers.

`-v, --verbose`
Report details of SQUEUE'S actions.

`-V , --version`
Print version information and exit.

JOB REASON CODES

The following codes identify the reason why a job is waiting for execution. A job may be waiting for more than one reason, in which case only one of those reasons is displayed.

Dependency	This job is waiting for a dependent job to complete.
None	No reason is set for this job.
PartitionDown	The partition required by this job is in a DOWN state.
PartitionNodeLimit	The number of nodes required by this job is outside of its partitions current limits.
PartitionTimeLimit	The job's time limit exceeds its partition's current time limit.
Priority	One or more higher priority jobs exist for this partition.
Resources	The job is waiting for resources to become available.

JOB STATE CODES

Jobs typically pass through several states in the course of their execution. The typical states are PENDING, RUNNING, SUSPENDED, COMPLETING, and COMPLETED. An explanation of each state follows.

`CA`	`CANCELLED`	Job was explicitly cancelled by the user or system administrator. The job may or may not have been initiated.
`CD`	`COMPLETED`	Job has terminated all processes on all nodes.
`CG`	`COMPLETING`	Job is in the process of completing. Some processes on some nodes may still be active.
`F`	`FAILED`	Job terminated with non-zero exit code or other failure condition.
`NF`	`NODE_FAIL`	Job terminated due to failure of one or more allocated nodes.
`PD`	`PENDING`	Job is awaiting resource allocation.
`R`	`RUNNING`	Job currently has an allocation.
`S`	`SUSPENDED`	Job has an allocation, but execution has been suspended.

TO TIMEOUT	Job terminated upon reaching its time limit.

ENVIRONMENT VARIABLES

Some **SQUEUE** options may be set via environment variables. These environment variables, along with their corresponding options, are listed below. (Note: Command-line options will always override these settings.)

SLURM_CONF	The location of the SLURM configuration file.
SQUEUE_ALL	`-a, --all`
SQUEUE_FORMAT	`-o <output_format>, --format=<output_format>`
SQUEUE_PARTITION	`-p <part_list>, --partition=<part_list>`
SQUEUE_SORT	`-S <sort_list>, --sort=<sort_list>`
SQUEUE_STATES	`-t <state_list>, --states=<state_list>`
SQUEUE_USERS	`-u <user_list>, --users=<user_list>`

Examples

Print the jobs scheduled in the debug partition and in the COMPLETED state in the format with six right justified digits for the job id followed by the priority with an arbitrary field size:

```
# squeue -p debug -t COMPLETED -o "%.6i %p"
 JOBID PRIORITY
 65543 99993
 65544 99992
 65545 99991
```

Print the job steps in the debug partition sorted by user:

```
# squeue -s -p debug -S u
  STEPID       NAME  PARTITION     USER  TIME_USED  NODELIST(REASON)
 65552.1      test1      debug    alice       0:23  dev[1-4]
 65562.2    big_run      debug      bob       0:18  dev22
 65550.1     param1      debug  candice    1:43:21  dev[6-12]
```

Print information only about jobs 12345, 12346, and 12348:

```
# squeue --jobs 12345,12346,12348
 JOBID PARTITION  NAME  USER  ST TIME_USED NODES  NODELIST(REASON)
 12345     debug  job1  dave   R      0:21     4  dev[9-12]
 12346     debug  job2  dave   PD     0:00     8  (Resources)
 12348     debug  job3  ed     PD     0:00     4  (Priority)
```

Print information only about job step 65552.1:

```
# squeue --steps 65552.1
  STEPID   NAME   PARTITION    USER   TIME_USED   NODELIST(REASON)
 65552.1  test2       debug   alice       12:49   dev[1-4]
```

6.5 SINFO (Report Partition and Node Information)

SINFO displays a summary of status information on SLURM-managed partitions and nodes (*not* jobs). Customizable SINFO reports can cover the node count, state, and name list for a whole partition, or the CPUs, memory, disk space, or current status for individual nodes as specified. These reports can assist in planning job submittals and avoiding hardware problems. The SINFO output is a table whose content and format can be controlled using the SINFO options.

NAME

SINFO - view information about SLURM nodes and partitions.

SYNOPSIS

```
sinfo [OPTIONS...]
```

DESCRIPTION

SINFO is used to view partition and node information for a system running SLURM.

OPTIONS

`-a, --all`
Display information about all partitions. This causes information to be displayed about partitions that are configured as hidden and partitions that are unavailable to user's group.

`--help`
Print a message describing all SINFO options.

`--hide`
Do not display information about hidden partitions. By default, partitions that are configured as hidden or are not available to the user's group will not be displayed (i.e. this is the default behavior).

`--usage`
Print a brief message listing the SINFO options.

`-d, --dead`
If set, only report state information for non-responding (dead) nodes.

`-e, --exact`
If set, do not group node information on multiple nodes unless their configurations to be reported are identical. Otherwise CPU count, memory size, and disk space for nodes will be listed with the minimum value followed by a "+" for nodes with the same partition and state (e.g., "250+").

`-h, --noheader`
Do not print a header on the output.

`-i <seconds>, --iterate=<seconds>`
Print the state on a periodic basis. Sleep for the indicated number of seconds between reports. By default, prints a time stamp with the header.

`-l, --long`
Print more detailed information. This is ignored if the `--`format option is specified.

`-n <nodes>, --nodes=<nodes>`
Print information only about the specified node(s). Multiple nodes may be comma separated or expressed using a node range expression. For example, "linux[00-07]" would indicate eight nodes, "linux00" through "linux07."

`-N, --Node`
Print information in a node-oriented format. The default is to print information in a partition-oriented format. This is ignored if the -format option is specified.

`-o <output_format>, --format=<output_format>`
Specify the information to be displayed using an SINFO format string. Format strings transparently used by SINFO when running with various options are:

```
Default          "%9P %5a %.10l %.5D %6t %N"

--summarize      "%9P %5a %.10l %15F %N"

--long           "%9P %5a %.10l %.8s %4r %5h %10g %.5D %11T
%N"

--Node           "%#N %.5D %9P %6t"

--long –Node     "%#N %.5D %9P %11T %.4c %.6m %.8d %.6w %8f
%R"

--list-reasons "%35R %N"

--long --list-reasons "%50R %6t %N"
```

In the above format strings the use of "#" represents the maximum length of a node list to be printed.

The field specifications available include:

%a State/availability of a partition

%A Number of nodes by state in the format "allocated/idle". Do not use this with a node state option ("%t" or "%T") or the different node states will be placed on separate lines.

%c Number of CPUs per node

%C Number of CPUs per partition in the format "allocated/idle/total"

%d Size of temporary disk space per node in megabytes

%D Number of nodes

%f Features associated with the nodes

%F Number of nodes by state in the format "allocated/idle/other/total". Do not use this with a node state option ("%t" or "%T") or the different node states will be placed on separate lines.

%g Groups which may use the nodes

%h Jobs may share nodes, "yes", "no", or "force"

%l Maximum time for any job in the format "days-hours:minutes:seconds"

%m Size of memory per node in megabytes

%N List of node names

%P Partition name

%r Only user root may initiate jobs, "yes" or "no"

%R The reason why a node is unavailable (down, drained, or draining states)

%s Maximum job size in nodes

%t State of nodes, compact form

%T State of nodes, extended form

%w Scheduling weight of the nodes

%.<*> right justification of the field

%<Number><*> size of field

-r, --responding
If set, only report state information for responding nodes.

-R, --list-reasons
List reasons nodes are down or drained. When nodes are in these states SLURM supports the optional inclusion of a "reason" string by an administrator. This option will display the first 35 characters of the reason field and list of nodes with that reason that are, by default, down, drained, or draining. This option may be used with other node-filtering options (e.g. -r, -d, -t, -n), however, combinations of these options that result in a list of nodes that are not down or drained will not produce any output. When used with -l the output additionally includes the current node state.

-s, --summarize
List only a partition state summary with no node state details. This is ignored if the --format option is specified.

`-S <sort_list>, --sort=<sort_list>`
Specification of the order in which records should be reported. This uses the same field specification as the <output_format>. Multiple sorts may be performed by listing multiple sort fields separated by commas. The field specifications may be preceded by "+" or "-" for ascending (default) and descending order respectively. The partition field specification, "P", may be preceded by a "#" to report partitions in the same order that they appear in the SLURM configuration file, **slurm.conf**. For example, a sort value of "+P, -m" requests that records be printed in order of increasing partition name and within a partition by decreasing memory size. The default value of sort is "#P, -t" (partitions ordered as configured then decreasing node state). If the --Node option is selected, the default sort value is "N" (increasing node name).

`-t <states> , --states=<states>`
List nodes which have the given state(s). Multiple states may be comma separated and the comparison is case insensitive. Possible values include (case insensitive): ALLOC, ALLOCATED, COMP, COMPLETING, DOWN, DRAIN, DRAINED, DRNG, DRAINING, IDLE, UNK, and UNKNOWN. By default nodes in the specified state are reported whether they are responding or not. The --dead and --responding options may be used to filter nodes by the responding flag.

`-p <partition>, --partition=<partition>`
Print information only about the specified partition.

`-v, --verbose`
Provide detailed event logging through program execution.

`-V, --version`
Print version information and exit.

Output Field Descriptions

AVAIL
Partition state: up or down.

CPUS
Count of CPUs (processors) on these nodes.

CPUS (A/I)
Count of allocated CPUs and idle CPUs per nodes.

GROUPS
Resource allocations in this partition are restricted to the named groups. "all" indicates that all groups may use this partition.

JOB_SIZE
Minimum and maximum node count that can be allocated to any user job. A single number indicates the minimum and maximum node count are the same. infinite is used to identify partitions without a maximum node count.

TIMELIMIT

Maximum time limit for any user job in days-hours:minutes:seconds. “infinite” is used to identify partitions without a job time limit.

MEMORY
Size of actual memory in megabytes on these nodes.

NODELIST
Names of nodes associated with this configuration/partition.

NODES
Count of nodes with this particular configuration.

NODES(A/I)
Count of nodes with this particular configuration by node state in the form "available/idle".

NODES(A/I/O/T)
Count of nodes with this particular configuration by node state in the form "available/idle/other/total".

PARTITION
Name of a partition. Note that the suffix "*" identifies the default partition.

ROOT
Is the ability to allocate resources in this partition restricted to user root, yes or no.

SHARE
Defines whether jobs can share allocated resources. “no” indicates resources are never shared. “force” indicates resources are always available to be shared. “yes” indicates resources may be shared or not per job’s resource allocation.

STATE
State of the nodes. Possible states include: down, unknown, idle, allocated, drained, draining, completing and their abbreviated forms: down, unk, idle, alloc, drain, drng, and comp respectively. Note that the suffix "*" identifies nodes that are presently not responding.

TMP_DISK
Size of temporary disk space in megabytes on these nodes.

Node State Codes

Node state codes are shortened as required for the field size. If the node state code is followed by "*", this indicates the node is presently not responding and will not be allocated any new work. If the node remains non-responsive, it will be placed in the DOWN state (except in the case of DRAINED, DRAINING, or COMPLETING nodes).

ALLOCATED
The node has been allocated to one or more jobs.

ALLOCATED+

The node is allocated to one or more active jobs plus one or more jobs are in the process of COMPLETING.

COMPLETING
All jobs associated with this node are in the process of COMPLETING. This node state will be removed when all of the job's processes have terminated and the SLURM epilog program (if any) has terminated. See the Epilog parameter description in the slurm.conf man page for more information.

DOWN
The node is unavailable for use. SLURM can automatically place nodes in this state if some failure occurs. System administrators may also explicitly place nodes in this state. If a node resumes normal operation, SLURM can automatically return it to service. See the **ReturnToService** and **SlurmdTimeout** parameter descriptions in the **slurm.conf** man page for more information.

DRAINED
The node is unavailable for use per system administrator request. See the update node command in the **scontrol** man page or the **slurm.conf** man page for more information.

DRAINING
The node is currently executing a job, but it will not be allocated to additional jobs. The node state will be changed to state DRAINED when the last job on it completes. Nodes enter this state per system administrator request. See the update node command in the scontrol man page or the slurm.conf man page for more information.

IDLE
The node is not allocated to any jobs and is available for use.

UNKNOWN
The SLURM controller has just started and the node's state has not yet been determined.

Environment Variables

Some **SINFO** options may be set via environment variables. These environment variables, along with their corresponding options, are listed below. (Note: Command-line options will always override these settings.)

SLURM_CONF	The location of the SLURM configuration file.
SINFO_ALL	`-a, --all`
SINFO_FORMAT	`-o <output_format>, --format=<output_format>`
SINFO_PARTITION	`-p <partition>, --partition=<partition>`
SINFO_SORT	`-S <sort>, --sort=<sort>`

Examples

Report basic node and partition configurations:

```
> sinfo
PARTITION AVAIL TIMELIMIT NODES STATE  NODELIST
batch     up     infinite     2 alloc  adev[8-9]
batch     up     infinite     6 idle   adev[10-15]
debug*    up        30:00     8 idle   adev[0-7]
```

Report partition summary information:

```
> sinfo -s
PARTITION AVAIL TIMELIMIT NODES(A/I/O/T) NODELIST
batch     up     infinite 2/6/0/8        adev[8-15]
debug*    up        30:00 0/8/0/8        adev[0-7]
```

Report more complete information about the partition debug:

```
> sinfo --long --partition=debug
PARTITION AVAIL TIMELIMIT JOB_SIZE ROOT SHARE GROUPS NODES STATE NODELIST
debug*    up        30:00       8 no   no    all        8 idle  dev[0-7]
```

Report only those nodes that are in state DRAINED:

```
> sinfo --states=drained
PARTITION AVAIL NODES TIMELIMIT STATE  NODELIST
debug*    up        2     30:00 drain  adev[6-7]
```

Report node-oriented information with details and exact matches:

```
> sinfo -Nel
NODELIST  NODES PARTITION STATE  CPUS MEMORY TMP_DISK WEIGHT FEATURES REASON
adev[0-1]     2 debug*    idle      2   3448    38536     16 (null)   (null)
adev[2,4-7]   5 debug*    idle      2   3384    38536     16 (null)   (null)
adev3         1 debug*    idle      2   3394    38536     16 (null)   (null)
adev[8-9]     2 batch     allocated 2    246    82306     16 (null)   (null)
adev[10-15]   6 batch     idle      2    246    82306     16 (null)   (null)
```

Report only down, drained and draining nodes and their reason field:

```
> sinfo -R
REASON                               NODELIST
Memory errors                        dev[0,5]
Not Responding                       dev8
```

Report partition information that includes the number of allocated and idle CPUs.

```
> sinfo -o "%9P %5a %.5D  %.10A %.12C %N"
PARTITION AVAIL NODES  NODES(A/I)  CPUS(A/I/T) NODELIST
global*   up       28        1/26    8/208/224 linux[10-37]
bench     up       11        1/10      8/80/88 linux[10-20]
batch     up       10        0/10      0/80/80 linux[21-30]
```

6.6 SCANCEL (Signal/Cancel Jobs)

SCANCEL cancels a running or waiting job, or sends a specified signal to all processes on all nodes associated with a job (only job owners or their administrators can cancel jobs). SCANCEL may also be used to cancel a single job step instead of the whole job.

NAME

SCANCEL - Used to signal jobs or job steps that are under the control of SLURM.

SYNOPSIS

```
scancel [OPTIONS...] [job_id[.step_id]] [job_id[.step_id]...]
```

DESCRIPTION

SCANCEL is used to signal or cancel jobs or job steps. An arbitrary number of jobs or job steps may be signaled using job specification filters or a space-separated list of specific job and/or job step IDs. A job or job step can only be signaled by the owner of that job or user root. If an attempt is made by an unauthorized user to signal a job or job step, an error message will be printed and the job will not be signaled.

Options

`--help`
Print a help message describing all SCANCEL options.

`--usage`
Print a brief help message listing the SCANCEL options.

`-b, --batch`
Signal only the batch job shell.

`-i, --interactive`
Interactive mode. Confirm each job_id.step_id before performing the cancel operation.

`-n, --name=job_name`
The name of the jobs to be signaled.

`-p, --partition=partition_name`
The name of the partition from which jobs are to be signaled.

`-q, --quiet`
Do not report an error if the specified job is already completed. This option is incompatible with the `--verbose` option.

`-s, --signal=signal_name`
The name or number of the signal to be sent. Default value is "KILL".

`-t, --state=job_state_name`
The state of the jobs to be signaled. job_state_name may have a value of either "PENDING", "RUNNING" or "SUSPENDED".

`-u, --user=user_name`
The name of the user whose jobs are to be signaled.

`-v, --verbose`
Print additional logging. Using -v multiple times increases logging detail. This option is incompatible with the `--quiet` option.

`-V, --Version`
Print the version number of the command.

Arguments

`job_id`
The SLURM job ID of the job to have one or more of its steps signaled.

`step_id`
The step ID of the job step to be signaled. If none is provided and the `--batch` option is not used, then all jobs steps associated with the provided job_id will be signaled.

Environment Variables

Some SCANCEL options may be set via environment variables. These environment variables, along with their corresponding options, are listed below. **Note:** Command-line options will always override these settings.

SLURM_CONF	The location of the SLURM configuration file.
SCANCEL_BATCH	`-b, --batch`
SCANCEL_INTERACTIVE	`-i, --interactive`
SCANCEL_NAME	`-n, --name=job_name`
SCANCEL_PARTITION	`-p, --partition=partition_name`
SCANCEL_STATE	`-t, --state=job_state_name`
SCANCEL_USER	`-u, --user=user_name`
SCANCEL_VERBOSE	`-v, --verbose`

Notes:

- If multiple filters are supplied (e.g. `--partition` and `--name`) only the jobs satisfying all of the filtering options will be signaled.
- If a signal value of "KILL" (the default value) is to be sent to an entire job, this will result in the job's termination and its resource allocation being released.
- Canceling a job step will not result in a job being terminated. The job must be cancelled to release a resource allocation.

Examples

Send SIGTERM to steps 1 and 3 of job 1234:

```
scancel --signal=TERM 1234.1 1234.3
```

Cancel job 1234 along with all of its steps:

```
scancel 1234
```

Cancel all pending jobs belonging to user "bob" in partition "debug":

```
scancel --state=PENDING --user=bob --partition=debug
```

6.7 SACCT (Accounting Data)

NAME

SACCT - displays accounting data for all jobs and job steps in the SLURM job accounting log.

SYNOPSIS

```
sacct options
```

DESCRIPTION

Accounting information for jobs invoked with SLURM is logged in the job accounting log file.

The **SACCT** command displays job accounting data stored in the job accounting log file in a variety of forms for your analysis. The SACCT command displays information about jobs, job steps, status, and exit codes by default. The output can be tailored with the use of the **--fields=** option to specify the fields to be shown.

For the root user, the SACCT command displays job accounting data for all users, although there are options to filter the output to report only the jobs from a specified user or group.

For the non-root user, the SACCT command limits the display of job accounting data to jobs that were launched with their own user identifier (UID) by default. Data for other users can be displayed with the `--`**all**, `--`**user**, or `--`**uid** options.

Note:

Much of the data reported by SACCT has been generated by the **wait3()** and **getrusage()** system calls. Some systems gather and report incomplete information for these calls; SACCT reports values of 0 for this missing data. See the **getrusage** man page for your system to obtain information about which data are actually available on your system.

Options

`-a , --all`

Displays the job accounting data for all jobs in the job accounting log file. This is the default behavior when the SACCT command is executed by the root user.

`-b , --brief`

Displays a brief listing, which includes the following data:

- jobid
- status
- exitcode

This option has no effect when the `--`-dump option is also specified.

`-d , --dump`

Displays (dumps) the raw data records.

This option overrides the --brief and --fields= options.

The section titled "INTERPRETING THE --dump OPTION OUTPUT" describes the data output when this option is used.

`-S , --stat`

Queries the status of a job as the job is running displaying the following data:

- jobid
- vsize
- rss
- pages
- cputime
- ntasks
- status

The --jobs=job(.step) option must also be included. If no (.step) is given, the job.0 step will be received.

`-e time_spec , --expire=time_spec`

Removes job data from SLURM's current accounting log file (or the file specified with --file) for jobs that completed more than time_spec ago and appends them to the expired log file.

If time_spec is an integer value only, it is interpreted as minutes. If time_spec is an integer followed by "h", it is interpreted as a number of hours. If time_spec is an integer followed by "d", it is interpreted as number of days. For example, "--expire=14d" purges the job accounting log of all jobs that completed more than 14 days ago.

The expired log file is a file with the same name as the accounting log file, with ".expired" appended to the file name. For example, if the accounting log file is /var/log/slurmacct.log, the expired log file will be /var/log/slurmacct.log.expired.

`-F field_list , --fields=field_list`

Displays the job accounting data specified by the field_list operand, which is a comma-separated list of fields. Space characters are not allowed in the field_list.

See the --help-fields option for a list of the available fields. See the section titled "Job Accounting Fields" for a description of each field.

The job accounting data is displayed in the order specified by the field_list operand. Thus, the following two commands display the same data but in different order:

```
# sacct --fields=jobid,status
Jobid     Status
3         COMPLETED
3.0       COMPLETED

# sacct --fields=status,jobid
Status           Jobid
COMPLETED        3
COMPLETED        3.0
```

The default value for the field_list operand is "jobid,partition,process,ncpus,status,exitcode".
This option has no effect when the --dump option is also specified.

`-f file, --file=file`
Causes the SACCT command to read job accounting data from the named file instead of the current SLURM job accounting log file.

`-O , --formatted_dump`
Dumps accounting records in an easy-to-read format.
This option is provided for debugging.

`-g gid, --gid=gid`
Displays the statistics only for the jobs started with GID gid.

`-g group, --group=group`
Displays the statistics only for the jobs started by users in the group group.

`-h , --help`
Displays a general help message.

`--help-fields`
Displays a list of fields that can be specified with the --fields option.
The available fields are the following:

account	blockid	cpu	cputime	elapsed	end
exitcode	gid	group	idrss	inblock	isrss
ixrss	job	jobid	jobname	majflt	minflt
msgrcv	msgsnd	ncpus	nivcsw	nodes	nprocs
nsignals	nswap	ntasks	nvcsw	outblocks	pages
partition	rss	start	status	submit	systemcpu
uid	user	usercpu	vsize		

These fields are described in the section titled "**Job Accounting Fields:**"

`-j job(.step) , --jobs=job(.step)`
Displays information about the specified job(.step) or list of job(.step)s.
The job(.step) parameter is a comma-separated list of jobs.
Space characters are not permitted in this list.
The default is to display information on all jobs.

`-l, --long`
Displays a long listing, which includes the following data:

- jobid
- jobname
- partition
- vsize
- rss
- pages
- cputime

- ntasks
- ncpus
- elapsed
- status
- exitcode

`--noheader`

Prevents the display of the heading over the output. The default action is to display a header.

This option has no effect when used with the `--dump` option.

`-p partition_list , --partition=partition_list`

Displays information about jobs and job steps specified by the partition_list operand, which is a comma-separated list of partitions. Space characters are not allowed in the partition_list.

The default is to display information on jobs and job steps on all partitions.

`-s state_list , --state=state_list`

Selects jobs based on their current state, which can be designated with the following state designators:

- r running
- s suspended
- ca cancelled
- cd completed
- pd pending
- f failed
- to timed out
- nf node_fail

The state_list operand is a comma-separated list of these state designators. Space characters are not allowed in the state_list.

`-t , --total`

Displays only the cumulative statistics for each job.

Intermediate steps are displayed by default.

`-u uid, --uid=uid`

Displays the statistics only for the jobs started by the user whose UID is uid.

`-u user, --user=user`

Displays the statistics only for the jobs started by user user.

`--usage`

Displays a help message.

`-v , --verbose`

Reports the state of certain variables during processing.

This option is primarily used for debugging.

Job Accounting Fields

The following describes each job accounting field:

- account — user-supplied account number of the job
- cpu — sum of the system time (systemcpu) and user time (usercpu) in seconds
- cputime — minimum CPU time of any process followed by its task id along with the average of all processes running in the step
- elapsed — job's elapsed time (format : [DD-[hh:]]mm:ss) as defined by the following:
  DD days
  hh hours
  mm minutes
  ss seconds
- end — termination time of the job (format : MM/DD-hh:mm:ss) as defined by the following:
  MM month
  DD days
  hh hours
  mm minutes
  ss seconds
- exitcode — The first non-zero error code returned by any job step.
- gid — The group identifier of the user who ran the job.
- group — The group name of the user who ran the job.
- idrss — Maximum unshared data size (in KB) of any process.
- inblocks — Total block input operations for all processes.
- isrss — Maximum unshared stack space size (in KB) of any process.
- ixrss — Maximum shared memory (in KB) of any process.
- job — The SLURM job identifier of the job.
- jobid — The number of the job or job step. It is in the form: job.jobstep.
- jobname — The name of the job or job step.
- majflt — Maximum number of major page faults for any process.
- minflt — Maximum number of minor page faults (page reclaims) for any process.
- msgrcv — Total number of messages received for all processes.
- msgsnd — Total number of messages sent for all processes.
- ncpus — Total number of CPUs allocated to the job.
- nivcsw — Total number of involuntary context switches for all processes.
- nodes — List of nodes allocated to the job.
- nprocs — Total number of tasks in job. Identical to ntasks.
- nsignals — Total number of signals received for all processes.
- nswap — Maximum number of swap operations of any process.

- ntasks Total number of tasks in job.
- nvcsw Total number of voluntary context switches for all processes.
- outblocks Total block output operations for all processes.
- pages Maximum page faults of any process followed by its task id along with the average of all processes running in the step.
- partition Identifies the partition on which the job ran.
- rss Maximum resident set size of any process followed by its task id along with the average of all processes running in the step.
- start Initiation time of the job in the same format as end.
- status Displays the job status, or state. Output can be RUNNING, SUSPENDED, COMPLETED, CANCELLED, FAILED, TIMEOUT, or NODE_FAIL.
  If the job has been CANCELLED, the status will include the user ID of the user who cancelled the job.
- submit The time and date stamp (in Universal Time Coordinated, UTC) the job was submitted. The format of the output is identical to that of the end field.
- systemcpu The amount of system CPU time. The format of the output is identical to that of the elapsed field.
- uid The user identifier of the user who ran the job.
- uid.gid The user and group identifiers of the user who ran the job. (This field is used in record headers, and simply concatenates the uid and gid fields.)
- user The user name of the user who ran the job.
- usercpu The amount of user CPU time. The format of the output is identical to that of the elapsed field.
- vsize Maximum Virtual Memory size of any process followed by its task id along with the average of all processes running in the step.

6.7.1 Interpreting the Dump Option

The --**dump** option of the SACCT command displays data in a horizontal list of fields depending on the record type; there are three record types: **JOB_START**, **JOB_STEP**, and **JOB_TERMINATED**. There is a subsection that describes the output for each record type.

When the data output is a job accounting field, as described in the section titled "Job Accounting Fields", only the name of the job accounting field is listed. Otherwise, additional information is provided.

Note:

The output for the JOB_STEP and JOB_TERMINATED record types presents a pair of fields for the following data: Total CPU time, Total User CPU time, and Total System CPU time. The first field of each pair is the time in seconds expressed as an integer. The second field of each pair is the fractional number of seconds multiplied by one million. Thus, a pair of

fields output as "1 024315" means that the time is 1.024315 seconds. The least significant digits in the second field are truncated in formatted displays.

Output for the JOB_START Record Type

The following describes the horizontal fields output by the SACCT --dump option for the JOB_START record type.

Field#	Field
1	job
2	partition
3	The job's start time; this value is the number of non-leap seconds since the Epoch (00:00:00 UTC, January 1, 1970)
4	submitted
5	blockid
6	(Reserved)
7	JOB_START (literal string)
8	Job Record Version (1)
9	The number of fields in the record (17)
10	uid
11	gid
12	The job name
13	Batch Flag (0=no batch)
14	Relative SLURM priority
15	ncpus
16	nodes
17	account

Output for the JOB_STEP Record Type

The following describes the horizontal fields output by the SACCT --dump option for the JOB_STEP record type.

Field#	Field
1	job
2	partition
3	The job's start time; this value is the number of non-leap seconds since the Epoch (00:00:00 UTC, January 1, 1970)
4	submitted
5	blockid
6	(Reserved)
7	JOB_STEP (literal string)
8	Job Record Version (1)
9	The number of fields in the record (55)
10	jobid
11	end

12 Completion Status; the mnemonics, which may appear in uppercase or lowercase, are:
- CA Cancelled
- CD Completed successfully
- F Failed
- NF Job terminated from node failure
- R Running
- S Suspended
- TO Timed out

13 exitcode
14 ntasks
15 ncpus
16 Elapsed time in seconds expressed as an integer.
17 Integer portion of the Total CPU time in seconds for all processes.
18 Fractional portion of the Total CPU time for all processes expressed in microseconds.
19 Integer portion of the Total User CPU time in seconds for all processes.
20 Fractional portion of the Total User CPU time for all processes expressed in microseconds.
21 Integer portion of the Total System CPU time in seconds for all processes.
22 Fractional portion of the Total System CPU time for all processes expressed in microsecs.
23 rss
24 ixrss
25 idrss
26 isrss
27 minflt
28 majflt
29 nswap
30 inblocks
31 outblocks
32 msgsnd
33 msgrcv
34 nsignals
35 nvcsw
36 nivcsw
37 max_vsize
38 max_rss
39 max_vsize_node
40 max_vsize_task
41 ave_vsize
42 max_rss_node
43 max_rss_task
44 ave_rss
45 max_pages
46 max_pages_node
47 max_pages_task
48 ave_pages
49 min_cpu
50 min_cpu_node
51 min_cpu_task

52 ave_cpu
53 stepname
54 nodes
55 account

Output for the JOB_TERMINATED Record Type

The following describes the horizontal fields output by the SACCT --dump option for the JOB_TERMINATED (literal string) record type.

Field#	Field
1	job
2	partition
3	the jobs start time; this value is the number of non-leap seconds since the Epoch (00:00:00 UTC, January 1, 1970)
4	submitted
5	blockid
6	(Reserved)
7	JOB_TERMINATED (literal string)
8	Job Record Version (1).
9	The number of fields in the record (56). Although thirty-eight fields are displayed by the SACCT command for the JOB_TERMINATED record, only fields 1 through 12 are recorded in the actual data file; the SACCT command aggregates the remainder.
10	the total time elapsed in seconds for the job.
11	end
12	completion Status; the mnemonics, which may appear in uppercase or lowercase, are: CA Cancelled CD Completed successfully F Failed NF Job terminated from node failure R Running TO Timed out
13	exitcode
14	ntasks
15	ncpus
16	Elapsed time in seconds expressed as an integer.
17	Integer portion of the Total CPU time in seconds for all processes.
18	Fractional portion of the Total CPU time for all processes expressed in microseconds.
19	Integer portion of the Total User CPU time in seconds for all processes.
20	Fractional portion of the Total User CPU time for all processes expressed in microseconds.
21	Integer portion of the Total System CPU time in seconds for all processes.
22	Fractional portion of the Total System CPU time for all processes expressed in microseconds.
23	rss
24	ixrss
25	idrss

26 isrss
27 minflt
28 majflt
29 nswap
30 inblocks
31 outblocks
32 msgsnd
33 msgrcv
34 nsignals
35 nvcsw
36 nivcsw
37 max_vsize
38 max_rss
39 max_vsize_node
40 max_vsize_task
41 ave_vsize
42 max_rss_node
43 max_rss_task
44 ave_rss
45 max_pages
46 max_pages_node
47 max_pages_task
48 ave_pages
49 min_cpu
50 min_cpu_node
51 min_cpu_task
52 ave_cpu
53 --
54 nodes
55 account
56 requid

6.7.2 Examples

The following example illustrates the default invocation of the SACCT command:

```
# sacct
Jobid    Jobname     Partition  Ncpus  Status      Exitcode
2        script01    srun           1  RUNNING     0
3        script02    srun           1  RUNNING     0
4        endscript   srun           1  RUNNING     0
4.0                  srun           1  COMPLETED   0
```

The following example shows the same job accounting information with the brief option.

```
# sacct --brief
Jobid   Status      Exitcode
2       RUNNING     0
3       RUNNING     0
4       RUNNING     0
4.0     COMPLETED   0

# sacct --total
Jobid   Jobname     Partition  Ncpus   Status   Exitcode
```

```
3       sja_init    andy           1   COMPLETED    0
4       sjaload     andy           2   COMPLETED    0
5       sja_scr1    andy           1   COMPLETED    0
6       sja_scr2    andy          18   COMPLETED    2
7       sja_scr3    andy          18   COMPLETED    0
8       sja_scr5    andy           2   COMPLETED    0
9       sja_scr7    andy          90   COMPLETED    1
10      endscript   andy         186   COMPLETED    0
```

The following example demonstrates the ability to customize the output of the SACCT command. The fields are displayed in the order designated on the command line.

```
# sacct --fields=jobid,ncpus,ntasks,nsignals,status
Jobid  Ncpus  Ntasks  Nsignals        Status
3         2      1          0       COMPLETED
3.0       2      1          0       COMPLETED
4         2      2          0       COMPLETED
4.0       2      2          0       COMPLETED
5         2      1          0       COMPLETED
5.0       2      1          0       COMPLETED
```

6.8 Global Accounting API

Note:

The Global Accounting API only applies to clusters which use **SLURM** and the Load Sharing Facility (**LSF**) batch manager from **Platform Computing** together.

Both the **LSF** and **SLURM** products can produce an accounting file. The Global Accounting API offers the capability of merging the data from these two accounting files and presenting it as a single record to the program using this API.

Perform the following steps to call the Global Accounting API:

After SLURM has been installed (assumes **/usr** folder), build the Global Accounting API library by going to the **/usr/lib/slurm/bullacct** folder and executing the following command:

```
make –f makefile-lib
```

This will build the library **libcombine_acct.a**. This **makefile-lib** assumes that the SLURM product is installed in the **/usr** folder, and **LSF** is installed in **/app/slurm/lsf/6.2.** If this is not the case, the **SLURM_BASE** and **LSF_BASE** variables in the **makefile-lib** file must be modified to point to the correct location.

After the library is built, add the library **/usr/lib/slurm/bullacct/libcombine_acct.a** to the link option when building an application that will use this **API**.

In the user application program, add the following:

```
//  for new accounting record
//  assumes Slurm is installed under the opt/slurm folder

#include "/usr/lib/slurm/bullacct/combine_acct.h"

//  define file pointer for LSF and Slurm log file
FILE *lsb_acct_fg = NULL;    // file pointer for LSF accounting log file
FILE *slurm_acct_fg = NULL;  // file pointer for Slurm log file
int status, jobId;
struct CombineAcct newAcct;  // define variable for the new records

//  call cacct_init routine to open lsf and slurm log file,
//  and initialize the newAcct structure
status = cacct_init(&lsb_acct_fg, &slurm_acct_fg, &newAcct);

//  if the status returns 0 imply no error,
//    all log files are opened successfully.
//  then call get_combine_acct_info rountine to get the
//    combine accounting record.

//  the calling sequence is
//    int get_combine_acct_info(File *lsb_acct_fg,
//                              File *slurm_acct_fg,
//                              int   jobId,
//                              CombineAcct *newAcct);
//  where:
//  lsb_acct_fg is the pointer to the LSF accounting log file
//  slurm_acct_fg is the pointer to the Slurm accounting log file
//  jobid is the job Id from the LSF accounting log file
```

```
  //  newAcct is the address of the variable to hold the new record
  //  information.

  //  This routine will use the input LSF job ID to locate the LSF accounting
  //  information in the LSF log file, then get the SLURM_JOBID and locate the
  //  SLURM accounting information in the SLURM log file.
  //  This routine will return a zero to indicate that both records are found
  //  and processed successfully, otherwise one or both records are in error
  //  and the content in the newAcct variable is undefined.
  //  For example:

  //  to get the combine acct information for a specified jobid(2010)

    jobId = 2010;
    status = get_combine_acct_info(lsb_acct_fg,
                                   slurm_acct_fg,
                                   jobId,
                                   &newAcct);

  //  to display the record call display_combine_acct_record routine.

  display_combine_acct_record(&newAcct);

  //  when finished accessing the record, the user must close the log files and
  //  the free memory used in the newAcct variable by calling cacct_wrapup
  //  routine.
  //  For example:
  //
    if (lsb_acct_fg != NULL)              // if open successfully before
      cacct_wrapup(&lsb_acct_fg, &slurm_acct_fg, &newAcct);

  //  if an extra combine account variable is needed , the user can define
  //  the new variable and call init_cacct_rec to initialize the record
  //  and call free_cacct_ptrs to free the memory used in the new variable.
  //  For example:

  //  to define variable for the new record
      struct CombineAcct otherAcct;

  //  before using the variable otherAcct do:
     init_cacct_rec(&otherAcct);

  //  when done do the following to free the memory used by the otherAcct
  //  variable.
      free_cacct_ptrs(&otherAcct);
```

The new record contains the combined accounting information as follows:

```
/* combine LSF and SLURM acct log information */
struct CombineAcct {

         /* part one is the LSF information */

    char   evenType[50];
    char   versionNumber[50];
    time_t eventTime;
    int    jobId;
    int    userId;
    long   options;
    int    numProcessors;
    time_t submitTime;
    time_t beginTime;
    time_t termTime;
    time_t startTime;
    char   userName[MAX_LSB_NAME_LEN];
    char   queue[MAX_LSB_NAME_LEN];
    char   *resReq;
```

```
    char   *dependCond;
    char   *preExecCmd;             /* the command string to be pre_executed */
    char   fromHost[MAXHOSTNAMELEN];
    char   cwd[MAXFILENAMELEN];
    char   inFile[MAXFILENAMELEN];
    char   outFile[MAXFILENAMELEN];
    char   errFile[MAXFILENAMELEN];
    char   jobFile[MAXFILENAMELEN];
    int    numAskedHosts;
    char   **askedHosts;
    int    numExecHosts;
    char   **execHosts;
    int    jStatus;                  /* job status */
    double hostFactor;
    char   jobName[MAXLINELEN];
    char   command[MAXLINELEN];
    struct lsfRusage LSFrusage;
    char   *mailUser;                /* user option mail string */
    char   *projectName;             /* the project name for this job, used
                                        for accounting purposes */
    int    exitStatus;               /* job status */
    int    maxNumProcessors;
    char   *loginShell;              /* login shell specified by user */
    char   *timeEvent;
    int    idx;                      /* array idx, must be 0 in JOB_NEW */
    int    maxRMem;
    int    maxRswap;
    char   inFileSpool[MAXFILENAMELEN];  /* spool input file */
    char   commandSpool[MAXFILENAMELEN]; /* spool command file */
    char   *rsvId;
    char   *sla;              /* The service class under which the job runs. */
    int    exceptMask;
    char   *additionalInfo;
    int    exitInfo;
    char   *warningAction;             /* warning action, SIGNAL | CHKPNT |
                                          command, NULL if unspecified */
    int    warningTimePeriod;          /* warning time period in seconds,
                                          -1 if unspecified */
    char   *chargedSAAP;
    char   *licenseProject;            /* License Project */
    int    slurmJobId;                 /* job id from slurm */

     /* part two is the SLURM info minus the duplicated infomation from LSF */

    long   priority;                   /* priority */
    char   partition[64];              /* partition node */
    int    gid;                        /* group ID */
    int    blockId;                    /* Block ID */
    int    numTasks;                   /* nproc */
    double aveVsize;                   /* ave vsize */
    int    maxRss;                     /* max rss */
    int    maxRssTaskId;               /* max rss task  */
    double aveRss;                     /* ave rss */
    int    maxPages;                   /* max pages */
    int    maxpagestaskId;             /* max pages task */
    double avePages;                   /* ave pages */
    int    minCpu;                     /* min cpu */
    int    minCpuTaskId;               /* min cpu task */
    char   stepName[NAME_SIZE];        /* step process name */
    char   stepNodes[STEP_NODE_BUF_SIZE];  /* step node list */
    int    maxVsizeNode;               /* max vsize node */
    int    maxRssNodeId;               /* max rss node */
    int    maxPagesNodeId;             /* max pages node */
    int    minCpuTimeNodeId;           /* min cpu node */
    char   *account;                   /* account number */

};
```

Chapter 7. Launching an Application

7.1 Batch Managers for BAS4 for Xeon

Different batch managers are supported for **BAS4 for Xeon** to run batch jobs. These include **PBS Professional** Batch Manager from **Altair Engineering**, or the **Load Sharing Facility** Batch Manger from **Platform Computing**.

7.1.1 Batch Management with PBS Professional

For more information on the options for using **PBS Professional** see the PBS Professional 9.0 *Administrator's Guide* and *User's Guide* available on the **PBS Pro CD-ROM**

Important
PBS Professional does not work with **SLURM** and should only be installed on clusters which do not use **SLURM**. If SLURM has been installed see your System Administrator or chapter 7 in the **BAS4 for Xeon** *Administrator's Guide*.

7.1.2 Using PBS Professional

Pre -requisites

1. The User **ssh** keys should have been dispatched so that the User can access the Compute Nodes. See the **BAS4 for Xeon** *Administrator's Guide* for details on how to do this.

2. To use **PBS Professional** with **MPIBull2,** the home directory of the user should include the **mpd.conf** file, and this should include the user's password details. Only the user should have read and write rights for the **mpd.conf** file.

Submitting a script

Run the command below to see the job submission script, named **test.pbs**, in this example:

```
cat test.pbs
```

The script will appear, similar to that below, and can be edited if necessary.

```
#!/bin/bash
#PBS -l select=2:ncpus=3:mpiprocs=3
#PBS -l place=scatter
source /opt/mpi/mpibull2-1.2.1-4.t/share/setenv_mpibull2.sh
mpirun -n 6 hostname
```

Launching a job

Use the **qsub** command to launch a job with this script, as below: .

```
qsub test.pbs
```

The output will be in the format:

```
466.zeus0
```

This indicates that the number of the job is **466** on machine **zeus0.**

Displaying the results for a job

Use the command **qstat** to see the details of the jobs submitted.

```
qstat -an
```

```
zeus0:
                                                                  Req'd  Req'd   Elap
Job ID    Username    Queue  Jobname   SessID NDS TSK Memory Time  S Time

--------------- -------- -------- ---------- ------ --- --- ------ ------

466.zeus0  <user_name> workq  test.pbs  11449   2   6    --    --  R 00:00

           zeus8/0*3+zeus9/0*3
```

Here it is possible to see that, as specified in the script, the job is running on 3 CPUs on two nodes, named **zeus8** and **zeus9.**

Tracing a job

Run the command **tracejob** to see the progress for a specific job (466), for example:

```
tracejob 466
```

This will give output, similar to that below, showing all the job execution steps that have been carried out.

```
        Job: 466.zeus0

10/30/2007 12:43:46  L    Considering job to run
10/30/2007 12:43:46  S    enqueuing into workq, state 1 hop 1
10/30/2007 12:43:46  S    Job Queued at request of user@zeus0, owner =
<user_name>@zeus0, job name = test.pbs, queue = workq
10/30/2007 12:43:46  S    Job Run at request of Scheduler@zeus0 on hosts
(zeus8:ncpus=3:mpiprocs=3)+(zeus9:ncpus=3:mpiprocs=3)
10/30/2007 12:43:46  S    Job Modified at request of Scheduler@zeus0
10/30/2007 12:43:46  L    Job run
10/30/2007 12:43:48  S    Obit received momhop:1 serverhop:1 state:4
substate:42
10/30/2007 12:43:48  S    Exit_status=0 resources_used.cpupercent=0
resources_used.cput=00:00:01 resources_used.mem=2764kb
resources_used.ncpus=6   resources_used.vmem=30612kb
resources_used.walltime=00:00:02
10/30/2007 12:43:48  S    dequeuing from workq, state 5
```

Exiting a job

Use the command below to see look at the error log, if a job exits before it has completed:

```
cat test.pbs.e466
```

Ifthe **mpirun -n 6 hostname** command in the job script completes successfully, run the command below.

```
cat essai.pbs.o466
```

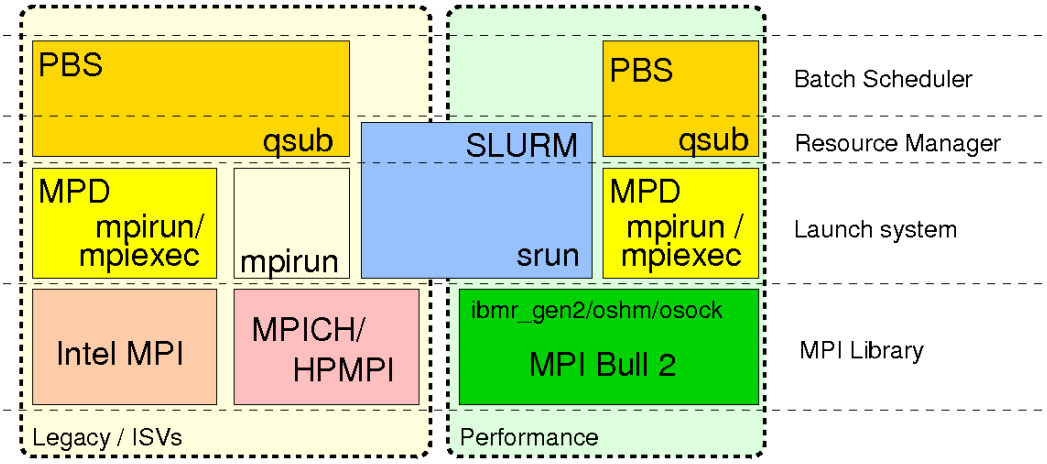
The output will list the nodes used, for example:

```
zeus8
zeus8
zeus8
zeus9
zeus9
zeus9
```

7.2 Launching an Application with a Batch Manager

The launching tool for an application depends on the MPI library used by the application.

Below is a global view of the different possibilities available:



See *section 2.2* in this manual for more information about using MPI.

7.3 Launching an Application without a Batch Manager

Platform	Application		Launching tool
Clusters with no Resource Manager	Serial		none
	Parallel	OpenMP	none
		MPIBull2	mpiexec/mpirun (MPD)
Clusters with SLURM	Serial		srun
	Parallel	OpenMP on one node	srun –A srun –c <no. of CPUs>
		MPI	srun
		Hybrid (MPI + OpenMP)	srun –c <no. of CPUs per MPI task>

Table 7-1. Launching without a Batch Manager for different clusters

Chapter 8. Application Debugging Tools

8.1 Overview

There are two types of debuggers; symbolic ones and non-symbolic ones.

A symbolic debugger gives access to a program's source code. This means that:

- The lines of the source file can be accessed.
- The program variables can be accessed by name.

Whereas a non-symbolic debugger enables access only to the lines of the machine code program and top physical addresses.

The following tools are described:

- 8.2 *GDB*
- 8.3 *IDB*
- 8.4 *TotaLView*
- 8.5 *DDT*
- 8.6 *MALLOC_CHECK_ - Debugging Memory Problems in C programs*
- 8.7 *Dmalloc Library*
- 8.8 *Electric Fence*

8.2 GDB

GDB stands for Gnu DeBugger. It is a powerful Open-source debugger, which can be used either through a command line interface, or a graphical interface such as **XXGDB** or **DDD** (Data Display Debugger). It is also possible to use an **emacs/xemacs** interface.

GDB supports parallel applications and threads.

GDB is published under the GNU license.

8.3 IDB

IDB is a debugger delivered with Intel compilers. It can be used with C/C++ and F90 programs.

8.4 TotalView

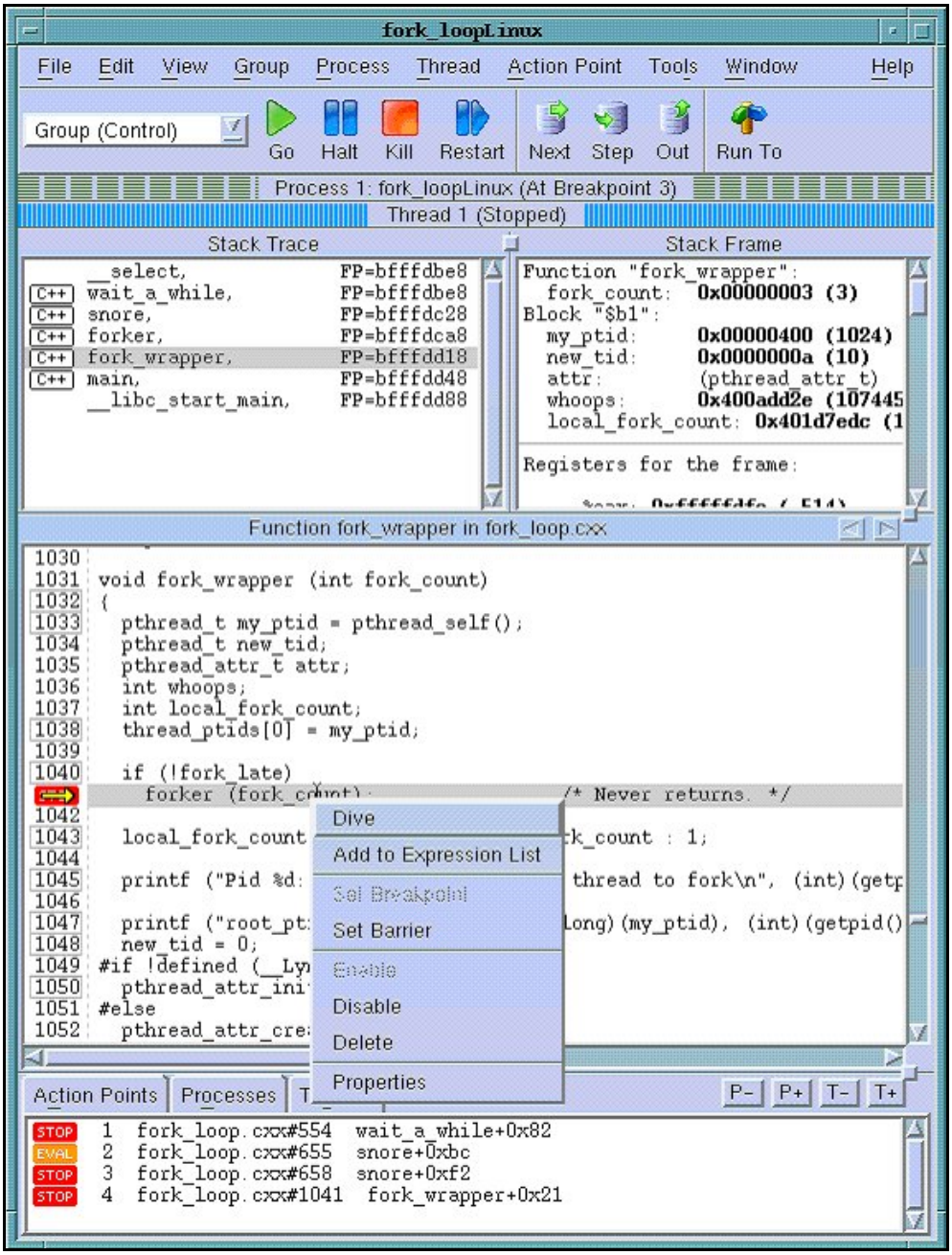


Figure 8-1 Totalview graphical interface – image taken from www.etnus.fr

TotalView™ is a proprietary software application from **Etnus** and is not included with the **BAS4 for Xeon** distribution. Totalview™ is used in the same way as standard symbolic debuggers for C, C++ and Fortran (*77*, 90 and HPF) programs. It can also debug **MPI** or **OpenMPI** applications. **TotalView™** has the advantage of being a debugger which supports multi-processes and multi-threading. It can take control of the various processes or threads of the program and make it possible for the user to visualize the evolution of the execution in the same window or in different windows. The processes may be local or remote.
It works just as well with mono-processor, SMP, clustered, distributed and MPP systems.

TotalView™ accepts new processes and threads exactly as generated by the application and regardless of the processor used for the execution. It is also possible to connect to a process started up outside **TotalView™**. Data tables can be filtered, displayed, and viewed in order to monitor the behavior of the program. Finally, you can descend *("call the components and details of...")* into the objects and structures of the program.

The program which needs debugging must be compiled with the **'- g'** option, and then breakpoints should be added to the program to control its execution.

TotalView™ is an Xwindows application. Context-sensitive help provides you with basic information. You may download **TotalView™** in the directory **/opt/totalview**.

Before running **TotalView™**, update your environment using the following command:

```
source /opt/totalview/totalview-vars.sh
```

Then enter:

```
totalview&
```

For additional information, and for copies of the documentation for **Totalview™**, please refer to http://www.etnus.com/.

8.5 DDT

DDT™ is a proprietary debugging tool from **Allinea** and is not included with the **BAS4 for Xeon** distribution.

Its source code browser shows at a glance the state of the processes within a parallel job, and simplifies the task of debugging large numbers of simultaneous processes. **DDT** has a range of features designed to debug effectively - from deadlock and memory leak tools, to data comparison and group wise process control, and it interoperates with all known **MPIBull2** implementations

For multi-threaded or **OpenMP** development **DDT** allows threads to be controlled individually and collectively, with advanced capabilities to examine data across threads.

The Parallel Stack Viewer allows the program state of all processes and threads to be seen at a glance making parallel programs easier to manage.

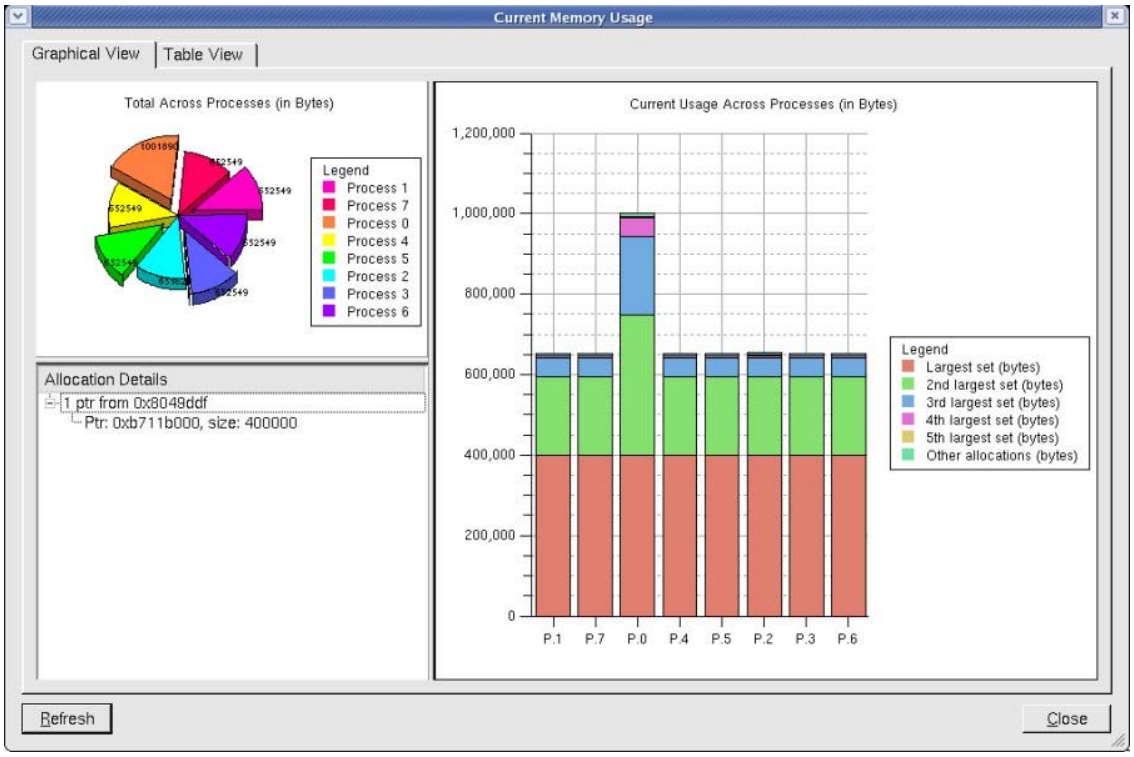


Figure 8-2. The Graphical User Interface for DDT

DDT can find memory leaks, and detect common memory usage errors before your program crashes.

A programmable STL Wizard enables **C++** Standard Template Library variables and the abstract data they represent -including lists, maps, sets, multimaps, and strings – to be viewed easily.

Developers of scientific code have full access to modules, allocated data, strings and derived types for **Fortran 77, 90,** and **95**.

MPI message queues can be examined in order to identify deadlocks in parallel code and data may be viewed in 3D with the multi-dimensional array viewer.

It is possible to run **DDT** with the **PBS-Professional** Batch Manager.

For more information refer to http://allinea.com/

8.6 MALLOC_CHECK_ - Debugging Memory Problems in C programs

When developing an application, the developer should ensure that all the buffers allocated during the run-time of the application are freed afterwards. However, even if he is vigilant, it is not unusual for memory leaks to be introduced into the code.

A simple way to detect these memory leaks is to use the environment variable **MALLOC_CHECK __**. This variable ensures that allocation routines check that each allocated buffer is freed correctly. The routines then become more 'tolerant' and allow byte overflows on both sides of blocks or for the block to be released again.
According to the value of **MALLOC_CHECK __**, when a release or allocation error appears the application behaves as follows:

- If **MALLOC_CHECK __** is set to 1, an error message is written when exiting normally.
- If **MALLOC_CHECK __** is set to 2, an error message is written when exiting normally and the process aborts. A core file is created. You should check that it is possible to create a core file by using the command *ulimit –c*. If not, enter the command *ulimit -c unlimited*.
- For any other value of **MALLOC_CHECK __**, the error is ignored and no message appears.

Example.c program:

```
#include <stdio.h>
#include <stdlib.h>
#define SIZE 256

int main(void){

  char *buffer;

  buffer = (char *)calloc(256*sizeof(char));
  if(!buffer){
    perror(``malloc failed'');
    exit(-1);
  }

  strcpy(buffer, ``fills the buffer'');
  free(buffer);
  fprintf(stdout, ``Buffer freed for the first time'');
  free(buffer);
  fprintf(stdout,``Buffer freed for the second time'');
  return(0);

}
```

A program which is executed with the environmental variable **MALLOC_CHECK __** set to 1 gives the following result:

$ export MALLOC_CHECK__=1

$./example

```
Buffer freed for the first time
Segmentation fault
```

$ ulimit –c 0

```
# The limit for the core file size must be changed to allow files
bigger than 0 bytes to be generated
```

$ ulimit –c unlimited `# Allows an unlimited core file to be generated`

A program which is executed with the environmental variable **MALLOC_CHECK __** set to 2 gives the following result:

$ export MALLOC_CHECK__=2

$ ./example

```
Buffer freed for the first time

Segmentation fault (core dumped)
```

Example Program Analysis using the GDB Debugger

The core file should be analyzed to identify where the problem is (the program should be compiled with the option - G):

```
$ gdb example -c core
GNU gdb 6.3-debian
Copyright 2004 Free Software Foundation, Inc.
GDB is free software, covered by the GNU General Public License,
 and you are welcome to change it and/or distribute copies of it
 under certain conditions.
Type "show copying" to see the conditions. There is absolutely no
 warranty for GDB. Type "show warranty" for details.
This GDB was configured as "i386-linux"...Using host libthread_db
 library "/lib/libthread_db.so.1".

Core was generated by `./example'.
Program terminated with signal 11, Segmentation fault.
Reading symbols from /lib/libc.so.6...done.
Loaded symbols for /lib/libc.so.6
Reading symbols from /lib/ld-linux.so.2...done.
Loaded symbols for /lib/ld-linux.so.2
#0  0x40097354 in mallopt () from /lib/libc.so.6
(gdb) bt
#0  0x40097354 in mallopt () from /lib/libc.so.6
#1  0x4009615f in free () from /lib/libc.so.6
#2  0x0804852f in main () at exemple.c:18
(gdb)
```

The **bt** command is used to display the current memory stack. In this example the last line indicates the problem came from line 18 in the main function of the **example.c** file. Looking at the **example.c** program on page 7.4 we can see that line 18 corresponds to the second call to the free function which created the memory overflow.

8.7 Dmalloc Library

Dmalloc is an open source library and is included in the **BAS4 for Xeon** distribution to help with application development and to ensure that memory leaks are detected quickly. This tool is complementary to the use of MALLOC_CHECK __ and is used to find memory leaks in C programs.

The debug memory allocation or dmalloc library is a memory management routine which provides powerful debugging facilities which are configurable at runtime. These facilities include such things as memory-leak tracking, fence-post write detection, file/line number reporting, and general logging of statistics. Thus it makes it possible to obtain precise information about a memory allocation problem. Small changes must be made to the code to run it. It also provides support for the debugging of threaded programs.

This **dmalloc** library substitutes the primitive calls **malloc**, **calloc**, **realloc** and **free** with the primitives which are available in the **dmalloc** library.

The **dmalloc** User's Guide and further information is available from the site http://www.dmalloc.com

8.8 Electric Fence

Electric Fence is an open source **malloc** debugger for Linux and Unix. It stops your program on the exact instruction that overruns or under-runs a **malloc()** buffer.

Electric Fence is installed only on the management node.

Electric Fence helps you detect two common programming bugs:

- Software that overruns the boundaries of a **malloc()** memory allocation.
- Software that touches a memory allocation that has been released by **free().**

You can use the following example, replacing **`icc --version`** by the command line of your program.

```
[test@host ]$LD_PRELOAD=/usr/local/tools/ElectricFence-2.2.2/lib/libefence.so.0.0
icc --version

Electric Fence 2.2.0 Copyright (C) 1987-1999 Bruce Perens <bruce@perens.com>

……..
```

For more details about Electric Fence please refer to http://perens.com/FreeSoftware/ .

Appendix A. Application Troubleshooting

A list of frequently asked questions (FAQs) with solutions and advice follows:

- **Problems when compiling and executing**
  - I get the message: "`error while loading shared libraries`" when a program executes.
  - My parallel program cannot find the program on the other machines.
  - How do I optimize compilation with the **Intel Fortran compiler**?
  - How do I optimize compilation with the **Intel C / C++ compiler**?
  - Can I run applications compiled under previous OS releases?
  - I get lots of "`unaligned access`" error messages.
- **OpenMP**
  - To run a program parallelized with OpenMP, how do I **define the number of threads** (processors) used?

I get the message: "`error while loading shared libraries`" when a program executes.

Add the path for this library to the LD_LIBRARY_PATH environment variable.

My parallel program cannot find the program on the other machines.

You must have the binaries on all machines running the benchmarks and respect the tree structure of the machine from which the benchmark is started, or use NFS.

How do I optimize compilation and debugging with the Intel Fortran compiler?

For optimization, add the following compilation options:

-implicitnone	Forces the declaration of variables: If a variable is used without being declared, this triggers errors on compilation.
-mp	Respects IEEE standard double precision.
-unroll2	To unroll a loop: This favors vectorization and the instructions pipeline.
-ip, -ipo	Optimizes calls to a subprogram (parameter management).
-auto	Allocates the variables dynamically to the stack rather than in static storage in the memory.
-zero	Implicitly initializes variables to 0.
-ftz	flush-to-zero.
-i-dynamic	Avoids loading static libraries and therefore reduces the size of the executable.
-parallel	Parallelizes certain sequences (supplied by the par_report option).
-par_report3	Provides information about how successful the compilation has been (e.g. parallelized loops).
-openmp	Takes into account OpenMP directives.

For debugging, add the following compilation options:

-g	debugging
-fpp	pre-processing

How do I optimize compilation and debugging with the Intel C / C++ compiler?

Add the following compilation options:

-O3	Highest code optimization possible.
-mp	Respects IEEE standard double precision.
-ip, -ipo	Optimizes calls to a subprogram (parameter management).
-unroll	(to unroll a loop): This favors vectorization and the instructions pipeline.

I get lots of "unaligned access" error messages.

These are not errors, but warnings. The application made an unaligned access and the processor had to get help from the kernel to access the data. This message can be ignored but be aware that too many unaligned accesses can be a source of performance loss. To hide these messages, run:

```
prctl --unaligned=silent
```

To help debugging the program, run:

```
prctl --unaligned=signal
```

I have a problem with memory allocations when I use Ethernet MPICH.

Error message displayed during execution:

```
p3_1858: (18446744073792.328125) xx_shmalloc: returning NULL;
requested 65584 bytes
p3_1858: (18446744073792.328125) p4_shmalloc returning NULL; request =
65584 bytes
You can increase the amount of memory by setting the environment
variable
P4_GLOBMEMSIZE (in bytes)
```

The memory that the communication requires cannot be allocated correctly. To do this, run the following command:

```
export P4_GLOBMEMSIZE=100000000
```

To run a program parallelized with OpenMP, how do I define the number of threads (processors) used?

Run the commands:

```
export  OMP_NUM_THREADS=2 to run the program on 2 processors
export  OMP_NUM_THREADS=4 to run the program on 4 processors
```

Glossary and Acronyms

A

ANL
Argonne National Laboratory (MPICH2)

API
Application Programmer Interface

B

BIOS
Basic Input Output System

B-SPS
Bull Scalable Port Switch

C

CLI
Command Line Interface

G

GCC
GNU C Compiler

GDB
Gnu Debugger

GNU
GNU's Not Unix

GPL
General Public License

GUI
Graphical User Interface

GUID
Globally Unique Identifier

H

HDD
Hard Disk Drive

HBA
Host Bus Adapter

HPC
High Performance Computing

HSC
Hot Swap Controller

I

ICC
Intel C Compiler

IDE
Integrated Device Electronics

IFORT
Intel Fortran Compiler

IPMI
Intelligent Platform Management Interface

K

KDM
Kernel Data Mover

KSIS
Utility for Image Building and Deployment

L

LSF
Load Sharing Facility

LUN
Logical Unit Number

M

MPD
MPI Process Daemons

MPI
Message Passing Interface

N

NFS
Network File System

NPTL
Native POSIX Thread Library

NTFS
New Technology File System (Microsoft)

NVRAM
Non Volatile Random Access Memory

O

OEM
Original Equipment Manufacturer

OPK
OEM Preinstall Kit (Microsoft)

P

PAPI
Performance Application Programming Interface

PCI
Peripheral Component Interconnect (Intel)

PDU
Power Distribution Unit

PM
Process Manager

PMI
Process Management Interface

PMU
Performance Monitoring Unit

PVFS
Parallel Virtual File System

R

RPM
RPM Package Manager

S

SCI
Scalable Coherent Interconnect

SDR
Sensor Data Record

SDP
Sockets Direct Protocol

SEL
System Event Log

SCSI
Small Computer System Interface

SM
System Management

SMP
Symmetric Multi Processing. The processing of programs by multiple processors that share a common operating system and memory.

SNMP
The protocol governing network management and the monitoring of network devices and their functions.

SOL
Serial Over LAN

SSH
Secure Shell

U

UA
User's Application

V

VGA
Video Graphic Adapter

X

XHPC
Xeon High Performance Computing

XIB
Xeon InfiniBand

Index

N

P

R

S

T

V

Technical publication remarks form

Title:	BAS4 for Xeon User's Guide

Reference:	86 A2 91ET 02

Date:	December 2007

ERRORS IN PUBLICATION

SUGGESTIONS FOR IMPROVEMENT TO PUBLICATION

Your comments will be promptly investigated by qualified technical personnel and action will be taken as required.
If you require a written reply, please include your complete mailing address below.

NAME: _____ DATE: _____

COMPANY: _____

ADDRESS: _____

_____

Please give this technical publication remarks form to your BULL representative or mail to:

Bull - Documentation Dept.
1 Rue de Provence
BP 208
38432 ECHIROLLES CEDEX
FRANCE
info@frec.bull.fr

Technical publications ordering form

To order additional publications, please fill in a copy of this form and send it via mail to:

BULL CEDOC
357 AVENUE PATTON
B.P.20845
49008 ANGERS CEDEX 01
FRANCE

Phone: +33 (0) 2 41 73 72 66
FAX: +33 (0) 2 41 73 70 66
E-Mail: srv.Duplicopy@bull.net

Reference	Designation	Qty
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
_ _ _ _ _ _ _ _ _ [_ _]		
[_ _] : The latest revision will be provided if no revision number is given.		

NAME: ____________________ DATE: __________

COMPANY: ____________________

ADDRESS: ____________________

____

PHONE: ____________________ FAX: __________

E-MAIL: ____________________

For Bull Subsidiaries:
Identification: ____________________

For Bull Affiliated Customers:
Customer Code: ____________________

For Bull Internal Customers:
Budgetary Section: ____________________

For Others: Please ask your Bull representative.

BULL CEDOC
357 AVENUE PATTON
B.P.20845
49008 ANGERS CEDEX 01
FRANCE

REFERENCE
86 A2 91ET 02