sgi

Message Passing Toolkit (MPT) User Guide

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New Features in This Manual

This revision adds the following information:

- Updates to reflect support for the MPI 3.0 standard.
- Clarified information about how to configure SGI MPT on an SGI UV computer system
- Pointers for using SGI MPT in a kernel-based virtual machine (KVM).
- Information about how MPI programs run when Security-Enhanced Linux (SELinux) is enabled.
- Miscellaneous editorial corrections and additions.

In addition, information about SGI Unified Parallel C (UPC) has been removed.

Record of Revision

Version	Description
001	March 2004 Original Printing. This manual documents the Message Passing Toolkit implementation of the Message Passing Interface (MPI).
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003	June 2005 Supports the MPT 1.12 release.
004	June 2007 Supports the MPT 1.13 release.
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025 June 2014 Supports the SGI Performance Suite 1.8 release, the SGI MPT 2.10 release, and the SGI MPI 1.8 release.

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About This Guide

The SGI MPI software package facilitates parallel programming on large systems and on clusters of computer systems. SGI MPI supports both the Message Passing Interface (MPI) standard and the OpenSHMEM standard, as follows:

• The MPI standard supports C and Fortran programs with a library and supporting commands. MPI operates through a technique known as *message passing*, which is the use of library calls to request data delivery from one process to another or between groups of processes. MPI also supports parallel file I/O and remote memory access (RMA).

This publication describes SGI MPI 1.8, which supports the MPI 3.0 standard. SGI MPI includes significant features that make it the preferred implementation for use on SGI hardware. The following are some of these features:

- Data transfer optimizations for NUMAlink, where available, including single-copy data transfer.
- Multirail InfiniBand support, which takes full advantage of the multiple InfiniBand fabrics available on SGI[®] ICE[™] systems.
- Optimized MPI remote memory access (RMA) one-sided commands.
- Interoperability with the SHMEM (LIBSMA) programming model.
- High-performance communication support for partitioned systems.
- The OpenSHMEM standard describes a low-latency library that supports RMA on symmetric memory in parallel environments. The OpenSHMEM programming model is a partitioned global address space (PGAS) programming model that presents distributed processes with symmetric arrays that are accessible via PUT and GET operations from other processes.

This publication describes SGI SHMEM, which supports OpenSHMEM version 1.1. The SGI SHMEM programming model is the basis for the OpenSHMEM[™] programming model specification that is being developed by the Open Source Software Solutions multivendor working group.

SGI supports Security-Enhanced Linux (SELinux) on SGI UV computer systems that run the Red Hat Enterprise Linux (RHEL) operating system. If you want to use SGI MPI on an SGI UV system with SELinux Multi-Level Security (MLS) or Multi-Category Security (MCS), verify that your administrator has configured SELinux for SGI UV systems. For configuration information, see the following manual:

SGI UV System Software Installation and Configuration Guide

SGI's support for MPI and OpenSHMEM is built on top of the SGI Message Passing Toolkit (MPT). SGI MPT is a high-performance communications middleware software product that runs on SGI's shared memory and cluster supercomputers. On some of these machines, SGI MPT uses SGI Array Services to launch applications. SGI MPT is optimized for all SGI hardware platforms. This document describes SGI MPT 2.10.

Related SGI Publications

The release notes for the SGI Foundation Suite and the SGI Performance Suite list SGI publications that pertain to the specific software packages in those products. The release notes reside in a text file in the /docs directory on the product media. For example, SGI-MPI-1.x-readme.txt. After installation, the release notes and other product documentation reside in the /usr/share/doc/packages/product directory.

The MPInside Reference Guide describes SGI's MPInside MPI profiling tool.

All SGI software and hardware manuals and can be found in the SGI Technical Publications Library at the following website:

http://docs.sgi.com

Related Publications From Other Sources

Information about MPI is available from a variety of sources. Some of the following sources include pointers to other resources. For information about the MPI standard, see the following:

• The Message Passing Interface Forum's website, which is as follows:

http://www.mpi-forum.org/

 Using MPI — 2nd Edition: Portable Parallel Programming with the Message Passing Interface (Scientific and Engineering Computation), by Gropp, Lusk, and Skjellum. ISBN-13: 978-0262571326.

- The University of Tennessee technical report. See reference [24] from Using MPI: Portable Parallel Programming with the Message-Passing Interface, by Gropp, Lusk, and Skjellum. ISBN-13: 978–0262571043.
- Journal articles in the following publications:
 - International Journal of Supercomputer Applications, volume 8, number 3/4, 1994
 - International Journal of Supercomputer Applications, volume 12, number 1/4, pages 1 to 299, 1998

Conventions

The following conventions are used throughout this document:

Convention	Meaning
command	This fixed-space font denotes literal items such as commands, files, routines, path names, signals, messages, and programming language structures.
manpage(x)	Man page section identifiers appear in parentheses after man page names.
variable	Italic typeface denotes variable entries and words or concepts being defined.
user input	This bold, fixed-space font denotes literal items that the user enters in interactive sessions. (Output is shown in nonbold, fixed-space font.)
[]	Brackets enclose optional portions of a command or directive line.
	Ellipses indicate that a preceding element can be repeated.

Reader Comments

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Configuring the SGI Message Passing Toolkit (MPT) on an SGI UV Computer System

This chapter includes the following topics:

- "About Configuring SGI MPT" on page 1
- "Configuring SGI MPT on an SGI UV Computer (Single System Image)" on page 2
- "Configuring SGI MPT on an SGI UV Computer (Partitioned)" on page 8

Note: For information about how to configure SGI MPT on an SGI ICE X computer system, see the *SGI ICE X Installation and Configuration Guide*.

About Configuring SGI MPT

When you installed SGI Performance Suite, you also installed SGI MPT. Before you can run any SGI MPI programs, however, you need to configure the SGI MPT software. The procedures in this chapter explain how to configure SGI MPT.

SGI computers often host several released versions of SGI MPT. This environment provides users with the flexibility they need to develop and run MPI programs. The configuration instructions in this chapter explain how to accommodate these multiple versions if your site needs to have multiple versions installed.

The configuration procedure differs, depending on whether your SGI UV computer is partitioned or not, as follows:

• If you have an SGI UV system that is configured as a single system image (SSI), complete the following procedure:

"Configuring SGI MPT on an SGI UV Computer (Single System Image)" on page 2

• If you have an SGI UV system that is configured into two or more partitions, complete the following procedure:

"Configuring SGI MPT on an SGI UV Computer (Partitioned)" on page 8

Configuring SGI MPT on an SGI UV Computer (Single System Image)

The information in the following procedures explains how to configure SGI MPT on a large, single SGI UV SSI:

- "Verifying Prerequisites" on page 2
- "(Optional) Installing the SGI MPT Software Into a Nondefault Working Directory" on page 3
- "Adjusting File Resource Limits" on page 6
- "Completing the Configuration" on page 8

Verifying Prerequisites

The following procedure explains how to verify the SGI MPT software's installation prerequisites.

Procedure 1-1 To verify prerequisites

- 1. As the root user, log into the SGI UV computer.
- 2. (Conditional) Reboot the computer.

Perform this step if the SGI UV computer was not rebooted after SGI Performance Suite was installed.

If you do not know whether the computer has been rebooted, reboot at this time.

- 3. Verify that you have one of the following operating system software packages installed and configured:
 - Red Hat Enterprise Linux (RHEL) 6.5
 - SUSE Linux Enterprise Server (SLES) 11 SP3

You can type the following command to verify your operating system version:

cat /etc/issue

- 4. Type a series of cat(1) commands to verify that the following required products from the SGI Performance Suite 1.8 release are installed:
 - SGI Accelerate
 - SGI MPI

For example:

```
# cat /etc/sgi-accelerate-release
SGI Performance Suite 1.8, Build 710r19.sles11sp3-1404162103
# cat /etc/sgi-mpi-release
SGI MPI 1.8, Build 710r19.sles11sp3-1404162103
```

- 5. Proceed to one of the following:
 - "(Optional) Installing the SGI MPT Software Into a Nondefault Working Directory" on page 3, which explains how to configure SGI MPT in a way that lets you maintain more than one released version of the software on your SGI UV computer system.
 - "Adjusting File Resource Limits" on page 6, which assumes you want the SGI MPT software to remain in the default installation directory.

(Optional) Installing the SGI MPT Software Into a Nondefault Working Directory

Perform the procedures in this topic if you want to install SGI MPT into a custom, nondefault working directory. If you want to have more than one released version of SGI MPT available, make sure to perform the following procedures:

- "Using the cpio Utility to Install SGI MPT Into a Nondefault Working Directory" on page 3
- "Modifying the Module Files" on page 5

Using the cpio Utility to Install SGI MPT Into a Nondefault Working Directory

The default installation directory for SGI MPT is /opt/sgi/mpt/mpt-2.10. The procedure in this topic explains how to use the cpio utility to install SGI MPT into an alternate, nondefault directory. This procedure assumes that it is not important or desirable for the RPM database to track the versions of SGI MPT that are installed.

The following procedure explains how to install the SGI MPT software into an alternate directory.

Procedure 1-2 To use .cpio to install the SGI MPT RPM

1. Familiarize yourself with the current SGI MPT working directory structure, and create a directory for the SGI MPT software you want to configure at this time.

By default, the product installs into the /opt/sgi/mpt/mpt-2.10 directory.

If you already have a nondefault set of working directories, plan to continue to use that directory structure.

If you do not have a nondefault set of working directories, make a plan for that nondefault structure at this time. For example, use the mkdir(1) command to create the following directory:

mkdir -p /opt/sgimpi/mpt-2.10

The procedure in this topic, and the related topics, creates directory /opt/sgimpi as an example nondefault working directory, configures SGI MPI 2.10 in that directory, and uses that example directory in all the steps in the configuration procedure.

2. Type the following command, and verify that all SGI MPT packages are in the default installation directory at this time:

rpm -qa | grep sgi-mpt

Scan the rpm command output, and make sure that the following three SGI MPT packages appear:

```
sgi-mpt-shmem-2.10-sgi710r6.sles11sp3
sgi-mpt-2.10-sgi710r6.sles11sp3
sgi-mpt-fs-2.10-sgi710r6.sles11sp3
```

3. Use a series of rpm commands to remove the SGI MPT packages from the default installation directory.

Your goal is to remove only the following packages:

- sgi-mpt-shmem-release_number
- sgi-mpt-release_number
- sgi-mpt-fs-release_number

The rpm command you need to use has the following format:

rpm -e --nodeps package_name

For *package_name*, specify the name of the package in the default directory at this time.

For example:

```
# rpm -e --nodeps sgi-mpt-shmem-2.10-sgi710r6.sles11sp3
# rpm -e --nodeps sgi-mpt-2.10-sgi710r6.sles11sp3
# rpm -e --nodeps sgi-mpt-fs-2.10-sgi710r6.sles11sp3
```

4. Use the cd(1) command to change to the directory you created earlier in this procedure.

For example, type the following command:

cd /opt/sgimpi/mpt-2.10

5. For each installation package, type one rpm2cpio command, in the following format, to install the SGI MPT software:

rpm2cpio /full_path_to_RPM_file/sgi-mpt-mpt_release-*.rpm | cpio -idcmv

For *full_path_to_RPM_file*, specify the path that leads to the release packages, whether that be a mounted DVD or a network path.

For *mpt_release*, type the release version of SGI MPT. For example, 2.10.

For example:

- # rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-2.10-*.rpm | cpio -idcmv
- # rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-fs-2.10-*.rpm | cpio -idcmv
- # rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-shmem-2.10-*.rpm | cpio -idcmv

If you have other released versions of SGI MPT, you can repeat this step, modifying the commands for the other released versions as needed.

6. Proceed to the following:

"Modifying the Module Files" on page 5

Modifying the Module Files

The mpirun command assumes that the PATH environment variable and the LD_LIBRARY_PATH environment variable are configured for the default SGI MPT installation directory. The compilers, linkers, and loaders all use the values in these environment variables.

The following procedure explains how to reset the environment modules. For more information, see "Running MPI Jobs" on page 27.

Procedure 1-3 To reset environment modules

- 1. Open one of the following files from within a text editor:
 - On RHEL platforms, open the following file:

/location/usr/share/Modules/modulefiles/mpt/mpt_release

• On SLES platforms, open the following file:

/location/usr/share/modules/modulefiles/mpt/mpt_release

For *location*, specify the location of the module files. For example, /opt/sgimpi/mpt-2.10.

For *mpt_release*, specify the number of the SGI MPT release. For example, 2.10 RHEL platform example:

/opt/sgimpi/mpt-2.10/usr/share/Modules/modulefiles/mpt/2.10

2. Search for the following line:

set BASEPATH /opt/sgi/mpt/mpt-mpt_release

For *mpt_release*, specify the number of the SGI MPT release.

3. Edit the set BASEPATH line, prepending the new installation path.

For example:

setenv BASEPATH /opt/sgimpi/mpt-2.10/opt/sgi/mpt/mpt-2.10

4. Proceed to the following:

"Adjusting File Resource Limits" on page 6

Adjusting File Resource Limits

The following procedure explains how to increase resource limits on the number of open files and enforce new security policies.

Procedure 1-4 To adjust file resource limits

1. Type the following command to retrieve the number of cores on this computer:

```
# cat /proc/cpuinfo | grep processor | wc -1
```

In the preceding line, the last character is a lowercase L, not the number 1.

This $\operatorname{cat}(1)$ command returns the number of cores on the SGI UV computer system.

- 2. Use a text editor to open file /etc/security/limits.conf.
- 3. Add the following line to file /etc/security/limits.conf:

* hard nofile *limit*

For *limit*, specify an open file limit, for the number of MPI processes per host, based on the following guidelines:

Processes/host	limit
Fewer than 512	3000
Up to 1024	6000
Up to 2048	8192 (default)
4096 or more	21000

MPI jobs require a large number of file descriptors, and on larger systems, you might need to increase the system-wide limit on the number of open files. The default value for the file-limit resource is 8192. For example, the following line is suitable for 512 MPI processes per host:

- * hard nofile 3000
- 4. Add the following line to file /etc/security/limits.conf:
 - * hard memlock unlimited

The preceding line increases the resource limit for locked memory.

- 5. Save and close file /etc/security/limits.conf.
- 6. Use a text editor to open file /etc/pam.d/login, which is the Linux pluggable authentication module (PAM) configuration file.

7. Add the following line to file /etc/pam.d/login:

session required /lib/security/pam_limits.so

- 8. Save and close the file.
- 9. (Conditional) Update other authentication configuration files as needed.

Perform this step if your site allows other login methods, such as ssh, rlogin, and so on.

10. Proceed to the following:

"Completing the Configuration" on page 8

Completing the Configuration

The following procedure explains how to complete the SGI MPT configuration.

Procedure 1-5 To complete the SGI MPT configuration

- 1. Run a test SGI MPI program to make sure that the new software is working as expected.
- 2. (Conditional) Inform your user community of the location of the new SGI MPT release on this computer.

Perform this step if you moved the SGI MPT software to a nondefault location.

In this procedure's examples, the module files are located in the following directories:

• On RHEL platforms:

/opt/sgimpi/mpt-2.10/usr/share/Modules/modulefiles/mpt/mpt-2.10

• On SLES platforms:

/opt/sgimpi/mpt-2.10/usr/share/modules/modulefiles/mpt/mpt-2.10

Configuring SGI MPT on an SGI UV Computer (Partitioned)

You can configure SGI MPT on an SGI UV computer system that is divided into two or more partitions. Generally, you configure each partition individually, and then you configure the partitions into an array. If you have several partitions, you can use only some of them for the SGI MPT array; you do not have to configure all the partitions into an array.

The information in the following procedures explains how to configure SGI MPT on a partitoned SGI UV:

- "Verifying Prerequisites" on page 9
- "Configuring the OpenFabrics Enterprise Distribution (OFED) Software" on page 10
- "Adjusting File Resource Limits" on page 12
- "Creating a Directory and Removing the Current Software" on page 13
- "(Optional) Configuring the MUNGE Security Software" on page 15
- "Updating Other Partitions or Continuing the Configuration" on page 16
- "(Optional) Installing the SGI MPT Software Into an NFS-mounted Working Directory" on page 16
- "Configuring Array Services" on page 20
- "Enabling Cross-partition NUMAlink MPI Communication and Restarting Services" on page 23
- "Completing the Configuration" on page 24

Verifying Prerequisites

The following procedure explains how to verify the SGI MPT software's configuration prerequisites.

Procedure 1-6 To verify prerequisites

1. (Conditional) Make sure that an NFS share is available.

An NFS share is needed only if you plan to move the SGI MPT installation to a nondefault location on two or more partitions of an SGI UV computer.

- 2. As the root user, log into one of the partitions on the partitioned SGI UV computer.
- 3. (Conditional) Reboot the partition.

Perform this step if the SGI UV computer was not rebooted after SGI Performance Suite was installed.

If you do not know whether the computer has been rebooted, reboot at this time.

- 4. Verify that you have one of the following operating system software packages installed and configured:
 - Red Hat Enterprise Linux (RHEL) 6.5
 - SUSE Linux Enterprise Server (SLES) 11 SP3

You can type the following command to verify your operating system version:

cat /etc/issue

- 5. Type a series of cat(1) commands to verify that the following products from the SGI Performance Suite 1.8 release are installed:
 - SGI Accelerate
 - SGI MPI

For example:

```
# cat /etc/sgi-accelerate-release
SGI Performance Suite 1.8, Build 710r19.sles11sp3-1404162103
# cat /etc/sgi-mpi-release
SGI MPI 1.8, Build 710r19.sles11sp3-1404162103
```

6. Proceed to the following:

"Configuring the OpenFabrics Enterprise Distribution (OFED) Software" on page 10

Configuring the OpenFabrics Enterprise Distribution (OFED) Software

All SGI UV computers are equipped with NUMAlink technology. Some SGI UV computers are also equipped with InfiniBand hardware, which uses OFED software. The procedure in this topic explains how to test for the presence of InfiniBand hardware and how to specify the number of queue pairs (QPs) for the OFED software.

If you are installing a kernel-based virtual machine (KVM), be aware that neither SGI, nor RHEL, nor SLES support InfiniBand hardware within a KVM.

The following procedure explains how to adjust the log_num_qp parameter.

Procedure 1-7 To specify the log_num_qp parameter

1. Type the following command to determine whether this partition is equipped with InfiniBand hardware:

lspci | grep Mellanox

Note whether the command returns information similar to the following, which informs you of the presence of InfiniBand hardware:

03:00.0 Network controller: Mellanox Technologies MT27500 Family [ConnectX-3]

If the lspci command returns nothing, this partition is not connected to InfiniBand hardware. You do not need to perform the rest of this procedure. Proceed to:

"Adjusting File Resource Limits" on page 12

- 2. Type one of the following commands to determine whether the OFED software is installed on this partition:
 - On SLES 11 platforms, type the following:
 - # zypper info -t pattern ofed
 - On RHEL 6 platforms, type the following:
 - # yum grouplist "Infiniband Support"

The operating system packages include OFED by default.

- 3. Use a text editor to open file /etc/modprobe.d/libmlx4.conf.
- 4. Add a line similar to the following to file /etc/modprobe.d/libmlx4.conf:

options mlx4_core log_num_qp=21

The default maximum number of queue pairs is 2^{18} (262144).

The log_num_qp parameter defines the log_2 of the number of queue pairs (QPs). This step specifies the maximum number of queue pairs (QPs) for SHMEM applications. If the log_num_qp parameter is set to a number that is too low, the system generates the following message:

MPT Warning: IB failed to create a QP

- 5. Save and close the file.
- 6. Proceed to the following:

"Adjusting File Resource Limits" on page 12

Adjusting File Resource Limits

The following procedure explains how to increase resource limits on the number of open files and how to enforce new security policies.

Procedure 1-8 To adjust file resource limits

1. Type the following command to retrieve the number of cores on this computer:

cat /proc/cpuinfo | grep processor | wc -1

In the preceding line, the last character is a lowercase L, not the number 1.

This cat(1) command returns the number of cores on the SGI UV computer system.

- 2. Use a text editor to open file /etc/security/limits.conf.
- 3. Add the following line to file /etc/security/limits.conf:

hard nofile *limit*

*

For *limit*, specify an open file limit, for the number of MPI processes per host, based on the following guidelines:

Processes/host	limit
Fewer than 512	3000
Up to 1024	6000
Up to 2048	8192 (default)
4096 or more	21000

MPI jobs require a large number of file descriptors, and on larger systems, you might need to increase the system-wide limit on the number of open files. The default value for the file-limit resource is 8192. For example, the following line is suitable for 512 MPI processes per host:

* hard nofile 3000

- 4. Add the following line to file /etc/security/limits.conf:
 - * hard memlock unlimited

The preceding line increases the resource limit for locked memory.

- 5. Save and close file /etc/security/limits.conf.
- 6. Use a text editor to open file /etc/pam.d/login, which is the Linux pluggable authentication module (PAM) configuration file.
- 7. Add the following line to file /etc/pam.d/login:

session required /lib/security/pam_limits.so

- 8. Save and close the file.
- 9. (Conditional) Update other authentication configuration files as needed.

Perform this step if your site allows other login methods, such as ssh, rlogin, and so on.

10. Proceed to the following:

"Creating a Directory and Removing the Current Software" on page 13

Creating a Directory and Removing the Current Software

The following procedure explains how to create an NFS-mounted directory and remove the SGI MPT software that currently resides on each partition.

Procedure 1-9 To create a directory

1. Familiarize yourself with the current SGI MPT working directory structure, and create a directory for the SGI MPT software you want to configure at this time.

By default, the product installs into the /opt/sgi/mpt/mpt-2.10 directory. Make a plan for the nondefault structure at this time. In a partitioned environment, you install SGI MPT into a central NFS-mounted location.

For example, use the mkdir(1) command to create the following alternate directory:

mkdir -p /nfsmount/sgimpi/mpt-2.10

This documentation uses directory /nfsmount/sgimpi/mpt-2.10 as an example nondefault working directory, configures SGI MPI 2.10 in that directory, and uses that example directory in the remaining steps of this configuration procedure.

2. Type the following command, and verify that all SGI MPT packages are in the default installation directory at this time:

rpm -qa | grep sgi-mpt

Scan the rpm command output, and make sure that the following three SGI MPT packages appear:

```
sgi-mpt-shmem-2.10-sgi710r6.sles11sp3
sgi-mpt-2.10-sgi710r6.sles11sp3
sgi-mpt-fs-2.10-sgi710r6.sles11sp3
```

3. Use a series of rpm commands to remove the SGI MPT packages from the default installation directory.

Your goal is to remove only the following packages:

- sgi-mpt-shmem-release_number
- sgi-mpt-release_number
- sgi-mpt-fs-release_number

The rpm command you need to use has the following format:

rpm -e --nodeps package_name

For *package_name*, specify the name of the package in the default directory at this time.

For example:

```
# rpm -e --nodeps sgi-mpt-shmem-2.10-sgi710r6.sles11sp3
# rpm -e --nodeps sgi-mpt-2.10-sgi710r6.sles11sp3
# rpm -e --nodeps sgi-mpt-fs-2.10-sgi710r6.sles11sp3
```

- 4. Proceed to one of the following:
 - "(Optional) Configuring the MUNGE Security Software" on page 15
 - "Updating Other Partitions or Continuing the Configuration" on page 16

(Optional) Configuring the MUNGE Security Software

Perform the procedure in this topic if you want to configure the MUNGE security software.

Array Services provides authentication services, but MUNGE provides additional authentication and security for Array Services operations. If you want to configure MUNGE, you need to configure it on each partition that you want to include in the array.

Procedure 1-10 To configure MUNGE

1. Verify that the partition is connected to a good time source, such as an NTP server.

MUNGE depends on time synchronization across all nodes in the array.

- 2. Type one of the following commands to start the MUNGE installation, and respond to the installation prompts:
 - On Red Hat Enterprise Linux platforms, type the following command:
 - # yum install munge
 - On SUSE Linux Enterprise Server platforms, type the following command:
 - # zypper install munge

For more information about how to install MUNGE, see the SGI MPI release notes.

- 3. Type the following command to restart MUNGE:
 - # service munge restart
- 4. Type the following command to verify the existance of a MUNGE key on the partition:
 - # md5sum /etc/munge/munge.key
- 5. (Conditional) Copy one partition's MUNGE key to all of the partitions.

Perform this step if this is the last partition that you need to configure.

Immediately after you install MUNGE, each partition should have a unique key. When you run the partitions as an array, however, each partition needs to have the same key. After you have MUNGE installed on all the partitions that you want to include in the array, select one partition, and copy that partition's MUNGE key to file /etc/munge/munge.key on each of the other partitions. 6. Proceed to the following:

"Updating Other Partitions or Continuing the Configuration" on page 16

Updating Other Partitions or Continuing the Configuration

At this point, at least one of the partitions on your SGI UV computer is configured correctly for SGI MPT.

The following procedure explains how to proceed.

Procedure 1-11 To assess progress

1. (Conditional) Configure additional partitions.

Make sure that you completed all the preceding procedures on all of the partitions that you want to include in the array before you continue with the procedures that follow.

If you want to include additional partitions in the array, repeat the following procedures on the additional partitions:

- "Verifying Prerequisites" on page 9
- "Configuring the OpenFabrics Enterprise Distribution (OFED) Software" on page 10
- "Adjusting File Resource Limits" on page 12
- "Creating a Directory and Removing the Current Software" on page 13
- "(Optional) Configuring the MUNGE Security Software" on page 15
- 2. Proceed to one of the following if all your partitions are ready to be configured into an array:
 - "(Optional) Installing the SGI MPT Software Into an NFS-mounted Working Directory" on page 16
 - "Configuring Array Services" on page 20

(Optional) Installing the SGI MPT Software Into an NFS-mounted Working Directory

The release notes explain how to install the SGI Performance Suite software and the SGI MPT software into the default installation directory, /opt/sgi/mpt/mpt-2.10.

The procedures in this topic explain how to create an alternate, NFS-mounted directory and install SGI MPT into that nondefault working directory.

Figure 1-1 on page 17 shows the SGI MPT environment that these procedures create on a partitioned SGI UV computer and on an NFS server.

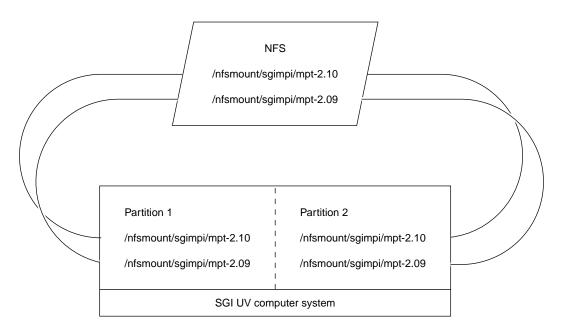


Figure 1-1 Directory Structure for NFS-mounted SGI MPT Software

In Figure 1-1 on page 17, note that the documentation does not describe how to mount SGI MPT 2.09 on an NFS share. The figure shows an example directory structure that could include both SGI MPT 2.10 and an earlier software revision.

Perform the following procedures if you want to have more than one released version of SGI MPT available:

- "Using the cpio Utility to Install SGI MPT Into a Nondefault Working Directory" on page 18
- "Modifying the Module Files" on page 19

Using the cpio Utility to Install SGI MPT Into a Nondefault Working Directory

The default installation directory for SGI MPT is /opt/sgi/mpt/mpt-2.10. The procedure in this topic explains how to use the cpio utility to install SGI MPT into an alternate, nondefault directory. This procedure assumes that it is not important or desirable for the RPM database to track the versions of SGI MPT that are installed.

The following procedure explains how to install the SGI MPT software into an alternate directory.

Procedure 1-12 To use .cpio to install the SGI MPT RPM

1. On one of the partitions, use the cd(1) command to change to the directory you created in the following procedure:

"Creating a Directory and Removing the Current Software" on page 13

For example, type the following command:

cd /nfsmount/sgimpi/mpt-2.10

2. For each installation package, type one rpm2cpio command, in the following format, to install the SGI MPT software:

rpm2cpio /full_path_to_RPM_file/sgi-mpt-mpt_release-*.rpm | cpio -idcmv

For *full_path_to_RPM_file*, specify the path that leads to the release packages. whether that be a mounted DVD or a network path.

For *mpt_release*, type the release version of SGI MPT.

For example:

```
# rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-2.10-*.rpm | cpio -idcmv
```

- # rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-fs-2.10-*.rpm | cpio -idcmv
- # rpm2cpio /mnt/mpi/sgi/x86_64/sgi-mpt-shmem-2.10-*.rpm | cpio -idcmv

If you have other released versions of SGI MPT, you can repeat this step, modifying the commands for the other released versions as needed.

3. Proceed to the following:

"Modifying the Module Files" on page 19

Modifying the Module Files

The mpirun command assumes that the PATH environment variable and the LD_LIBRARY_PATH environment variable are configured for the default SGI MPT installation directory. The compilers, linkers, and loaders all use the values in these environment variables.

The following procedure explains how to reset the environment modules. For more information, see "Running MPI Jobs" on page 27.

Procedure 1-13 To reset environment module files

- 1. Open one of the following files from within a text editor:
 - On RHEL platforms, open the following file:

location/usr/share/Modules/modulefiles/mpt/mpt_release

On SLES platforms, open the following file:

location/usr/share/modules/modulefiles/mpt/mpt_release

For *location*, specify the NFS-mounted location of the module files. For example, on a SLES platform with NFS-mounted packages, this could be /nfsmount/sgimpi/mpt-2.10.

For *mpt_release*, specify the number of the SGI MPT release you moved to the NFS mount. For example, 2.10.

2. Search for the following line:

set BASEPATH /opt/sgi/mpt/mpt-mpt_rel

For *mpt_release*, the file contains the release level of the SGI MPT software that you installed.

3. Edit the set BASEPATH line, prepending the new installation path.

For example:

setenv BASEPATH /nfsmount/sgimpi/mpt-2.10/opt/sgi/mpt/mpt-2.10

4. (Conditional) Modify the setenv BASEPATH line in the in the module file to reflect the locations of any other SGI MPT installations that you moved to nondefault location.

1: Configuring the SGI Message Passing Toolkit (MPT) on an SGI UV Computer System

Perform this step if you have more than one version of SGI MPT installed.

5. Proceed to the following:

"Configuring Array Services" on page 20

Configuring Array Services

SGI MPI depends on Array Services for several capabilities. During the configuration, your goal is to specify the partitions that you want to include in the array and to distribute the configuration files to each partition.

Table 1-1 on page 20 lists the documentation resources that contain additional configuration information.

 Table 1-1 Array Configuration Resources

Торіс	Documentation Resource
Advanced configuration information	"Additional Array Configuration Information" on page 93
Array Services overview	array_services(5)
Configuration file format	arrayd.conf (4) /usr/lib/array/arrayd.conf.template
Configuration file validator	ascheck(1)
Array Services configuration utility	arrayconfig(8)

The procedure in this topic uses the arrayconfig(8) command to specify SGI UV partitions for an array and to update the Array Services configuration files on each host.

Procedure 1-14 To configure Array Services for multiple partitions

1. (Optional) Synchronize and distribute secure shell (SSH) keys to each partition you want to include in the array.

If you have SSH keys configured, you can complete work on one partition and log into the next without typing passwords each time. When you configure Array Services, it might be convenient for you if SSH is configured in each partition.

2. Plan the authentication method you want the Array Services software to use.

Your choices are as follows:

• munge. Specify munge if you configured the MUNGE software in the following procedure:

"(Optional) Configuring the MUNGE Security Software" on page 15

- none. Disables all authentication.
- noremote. Disallows requests from remote systems.
- simple (default). Generates hostname/key pairs by using the OpenSSL rand command, 64-bit values (if available), or by using \$RANDOM Bash facilities.

For more information about the authentication levels, see arrayd.auth(5).

3. Log in as root to the partition to which you expect users to log in when they want to run SGI MPI jobs.

If you want to configure authentication simple, SGI requires that you run the arrayconfig(1M) command from the partition to which you expect users to run their SGI MPI jobs.

For all other authentication methods, SGI recommends that you run the arrayconfig(1M) command from the partition to which you expect users to run their SGI MPI jobs.

4. Use the arrayconfig(1M) command to specify the partitions that you want to include in the array.

The arrayconfig command configures the /etc/array/arrayd.conf and /etc/array/arrayd.auth files on each partition.

Type the arrayconfig(1M) command in the following format:

/usr/sbin/arrayconfig -a arrayname -A method -D -m hostname1 hostname2 ...

For *arrayname*, type a name for the array. For example, sgicluster. The default is default.

For *method*, type one of the following authentication methods: munge, none, noremote, or simple (default). For information about the authentication methods, see the arrayd.auth(4) man page.

For each *hostname*, specify the hostnames of the partitions upon which you installed the SGI Message Passing Toolkit (MPT) software. That is, for *hostname1*, *hostname2*, and so on, specify the hostnames of the partitions that you want to include in the array.

5. (Optional) Reset the default user account or the default array port.

By default, the Array Services installation and configuration process sets the following defaults in the /usr/lib/array/arrayd.conf configuration file:

• A default user account of arraysvcs.

Array Services requires that a user account exist on all hosts in the array for the purpose of running certain Array Services commands. If you create a different account, make sure to update the arrayd.conf file and set the user account permissions correctly on all hosts.

• A default port number of 5434.

The /etc/services file contains a line that defines the arrayd service and port number as follows:

sgi-arrayd 5434/tcp # SGI Array Services daemon

You can set any value for the port number, but all systems mentioned in the arrayd.conf file must use the same value.

6. Proceed to the following:

"Enabling Cross-partition NUMAlink MPI Communication and Restarting Services" on page 23

Note: If you have trouble with the Array Services configuration, examine the Array Services manual configuration procedure in the following topic:

Appendix B, "Configuring Array Services Manually"

Enabling Cross-partition NUMAlink MPI Communication and Restarting Services

When you configure a large SGI UV system into two or more NUMAlink-connected partitions, the partitions act as separate, clustered hosts. The hardware supports efficient and flexible global memory access for cross-partition communication on such systems, but to enable this access, you need to load special kernel modules. If you do not enable cross-partition NUMAlink MPI communication at this time, users might receive the following message when they run an application:

```
MPT ERROR from do_cross_gets/xpmem_get, rc = -1, errno = 22
```

Depending on your operating system, perform one of the following procedures to ensure that the kernel modules load every time the system boots:

- "Enabling Cross-partition Communication and Restarting Services (RHEL)" on page 23
- "Enabling Cross-partition Communication and Restarting Services (SLES)" on page 24

Enabling Cross-partition Communication and Restarting Services (RHEL)

The following procedure explains how to load the kernel modules on one partition that hosts a RHEL operating system.

Procedure 1-15 To load the kernel modules at boot

- As the root user, log into one of the partitions upon which you installed the SGI MPT software.
- 2. Type the following command:

echo "modprobe xpc" >> /etc/sysconfig/modules/sgi-propack.modules

- 3. Save and close the file.
- 4. Type one of the following command sequences:

reboot -f

Or

- # modprobe xpc
- # modprobe xpmem
- # /etc/init.d/procset restart
- # /etc/init.d/array restart

- 5. Repeat the preceding steps on the other partitions in the array.
- 6. Proceed to the following:

"Completing the Configuration" on page 24

Enabling Cross-partition Communication and Restarting Services (SLES)

The following procedure explains how to load the kernel modules on one partition that hosts a SLES operating system.

Procedure 1-16 To load the kernel modules at boot

- 1. As the root user, log into one of the partitions upon which you installed the SGI MPT software.
- 2. Use a text editor to open file /etc/sysconfig/kernel.
- 3. Within file /etc/sysconfig/kernel, search for the line that begins with MODULES_LOADED_ON_BOOT.
- 4. Add xpc to the list of modules that are loaded at boot time.
- 5. Save and close the file.
- 6. Type one of the following command sequences:

```
# reboot -f
Or
# modprobe xpc
# modprobe xpmem
# /etc/init.d/procset restart
```

- # /etc/init.d/array restart
- 7. Repeat the preceding steps on the other partitions in the array.
- 8. Proceed to the following:

"Completing the Configuration" on page 24

Completing the Configuration

The following procedure explains how to complete the SGI MPT configuration.

Procedure 1-17 To complete the SGI MPT configuration

- 1. Run a test SGI MPI program to make sure that the new software is working as expected.
- 2. (Conditional) Inform your user community of the location of the new SGI MPT release on this computer.

Perform this step if you moved the SGI MPT software to a nondefault location.

In this procedure's examples, the module files are located in the following directories:

• On RHEL platforms:

/nfsmount/sgimpi/mpt-2.10/usr/share/Modules/modulefiles/mpt/2.10

• On SLES platforms:

/nfsmount/sgimpi/mpt-2.10/usr/share/modules/modulefiles/mpt/2.10

Getting Started

This chapter provides procedures for building MPI applications. It provides examples of the use of the mpirun(1) command to launch MPI jobs. It also provides procedures for building and running SHMEM applications. It covers the following topics:

- "Compiling and Linking MPI Programs" on page 29
- "Running MPI Jobs with a Workload Manager" on page 32
- "Compiling and Running SHMEM Applications" on page 34
- "Using Huge Pages" on page 35

Running MPI Jobs

The following procedure explains how to run an MPI application when the SGI Message Passing Toolkit (MPT) software is installed in an alternate location.

Procedure 2-1 To run jobs with SGI MPT installed in an alternate location

- 1. Determine the directory into which the SGI MPT software is installed.
- 2. Type one of the following commands to compile your program.

mpif90 -I /install_path/usr/include file.f -L lib_path/usr/lib

mpicc -I /install_path/usr/include file.c -L lib_path/usr/lib

The variables in the preceding command are as follows:

- For *install_path*, type the path to the directory in which the SGI MPT software is installed.
- For *file*, type the name of your C program file name.
- For *lib_path*, type the path to the library files.

For example:

% mpicc -I /tmp/usr/include simple1_mpi.c -L /tmp/usr/lib

3. (Conditional) Ensure that the program can find the SGI MPT library routines when it runs.

You can use either site-specific library modules, or you can specify the library path on the command line before you run the program.

If you use module files, set the library path in the mpt module file. Sample module files reside in the following locations:

- /opt/sgi/mpt/mpt-*mpt_rel*/doc
- /usr/share/modules/modulefiles/mpt/mpt_rel

If you want to specify the library path as a command, type the following command:

```
% setenv LD_LIBRARY_PATH /install_path/usr/lib
```

For *install_path*, type the path to the directory in which the SGI MPT software is installed.

Example 1. The following command assumes that the libraries reside in /tmp:

```
% setenv LD_LIBRARY_PATH /tmp/usr/lib
```

Example 2. The following command assumes that the libraries reside in /data/nfs/lib, which might be the case if you installed SGI MPT in an NFS-mounted file system:

```
% setenv LD_LIBRARY_PATH /data/nfs/lib
```

4. Type the following command to link the program:

```
% ldd a.out
libmpi.so => /tmp/usr/lib/libmpi.so (0x40014000)
libc.so.6 => /lib/libc.so.6 (0x402ac000)
libdl.so.2 => /lib/libdl.so.2 (0x4039a000)
/lib/ld-linux.so.2 => /lib/ld-linux.so.2 (0x4000000)
```

Line 1 in the preceding output shows the library path correctly as /tmp/usr/lib/libmpi.so. If you do not specify the correct library path, the SGI MPT software searches incorrectly for the libraries in the default location of /usr/lib/libmpi.so.

5. Use the mpirun(1) command to run the program.

For example, assume that you installed the SGI MPT software on an NFS-mounted file system (/data/nfs) in the alternate directory /tmp. Type the following command to run the program:

```
% /data/nfs/bin/mpirun -v -a myarray hostA,hostB -np 1 a.out
```

Compiling and Linking MPI Programs

The default locations for the include files, the .so files, the .a files, and the mpirun command are pulled in automatically.

To ensure that the mpt software module is loaded, type the following command:

% module load mpt

Once the SGI MPT RPM is installed as default, the commands to build an MPI-based application using the .so files are as follows:

• To compile using GNU compilers, choose one of the following commands:

% g++ -o myprog myprog.C -lmpi++ -lmpi % gcc -o myprog myprog.c -lmpi

• To compile programs with the Intel compiler, choose one of the following commands:

(Fortran - version 8)
(C - version 8)
(Fortan 90 wrapper compiler)
(MPI C wrapper compiler)
(MPI C++ wrapper compiler)

Note: Use the Intel compiler to compile Fortran 90 programs.

• To compile Fortran programs with the Intel compiler and enable compile-time checking of MPI subroutine calls, insert a USE MPI statement near the beginning of each subprogram to be checked. Also, use the following command:

% ifort -I/usr/include -o myprog myprog.f -lmpi (version 8)

Note: The preceding command assumes a default installation. If your site has more than one version of SGI MPT installed, or if your site installed MPT into a nondefault location, contact your system administrator to verify the location of the module files. For a nondefault installation location, replace /usr/include with the name of the relocated directory.

 The special case of using the Open64 compiler in combination with hybrid MPI/OpenMP applications requires separate compilation and link command lines. The Open64 version of the OpenMP library requires the use of the -openmp option on the command line for compiling, but it interferes with proper linking of MPI libraries. Use the following sequence:

% opencc -o myprog.o -openmp -c myprog.c % opencc -o myprog myprog.o -lopenmp -lmpi

Using mpirun to Launch an MPI Application

The mpirun(1) command starts an MPI application. For a complete specification of the command line syntax, see the mpirun(1) man page. This section summarizes the procedures for launching an MPI application.

Launching a Single Program on the Local Host

To run an application on the local host, enter the mpirun command with the -np argument. Your entry must include the number of processes to run and the name of the MPI executable file.

The following example starts three instances of the mtest application, which is passed an argument list (arguments are optional):

% mpirun -np 3 mtest 1000 "arg2"

Launching a Multiple Program, Multiple Data (MPMD) Application on the Local Host

You are not required to use a different host in each entry that you specify on the mpirun command. You can start a job that has multiple executable files on the same host. In the following example, one copy of prog1 and five copies of prog2 are run on the local host. Both executable files use shared memory.

% mpirun -np 1 prog1 : 5 prog2

Launching a Distributed Application

You can use the mpirun command to start a program that consists of any number of executable files and processes, and you can distribute the program to any number of hosts. A host is usually a single machine, but it can be any accessible computer running Array Services software. For available nodes on systems running Array Services software, see the /usr/lib/array/arrayd.conf file.

You can list multiple entries on the mpirun command line. Each entry contains an MPI executable file and a combination of hosts and process counts for running it. This gives you the ability to start different executable files on the same or different hosts as part of the same MPI application.

The examples in this section show various ways to start an application that consists of multiple MPI executable files on multiple hosts.

The following example runs ten instances of the a.out file on host_a:

% mpirun host_a -np 10 a.out

When specifying multiple hosts, you can omit the -np option and list the number of processes directly. The following example launches ten instances of fred on three hosts. fred has two input arguments.

% mpirun host_a, host_b, host_c 10 fred arg1 arg2

The following example launches an MPI application on different hosts with different numbers of processes and executable files:

% mpirun host_a 6 a.out : host_b 26 b.out

Using MPI Spawn Functions to Launch an Application

To use the MPI RMA process creation functions MPI_Comm_spawn or MPI_Comm_spawn_multiple, use the -up option on the mpirun command to specify the universe size. For example, the following command starts three instances of the mtest MPI application in a universe of size 10:

% mpirun -up 10 -np 3 mtest

By using one of the above MPI spawn functions, mtest can start up to seven more MPI processes.

When running MPI applications on partitioned SGI UV systems that use the MPI_Comm_spawn or MPI_Comm_spawn_multiple functions, you might need to explicitly specify the partitions on which additional MPI processes can be launched. For more information, see the mpirun(1) man page.

Running MPI Jobs with a Workload Manager

When an MPI job is run from a workload manager like PBS Professional, Torque, or Load Sharing Facility (LSF), it needs to start on the cluster nodes and CPUs that have been allocated to the job. For multi-node MPI jobs, the command that you use to start this type of job requires you to communicate the node and CPU selection information to the workload manager. SGI MPT includes one of these commands, mpiexec_mpt(1), and the PBS Professional workload manager includes another such command, mpiexec(1). The following topics describe how to start MPI jobs with specific workload managers:

- "PBS Professional" on page 32
- "Torque" on page 34
- "Simple Linux Utility for Resource Management (SLURM)" on page 34

PBS Professional

You can run MPI applications from job scripts that you submit through workload managers such as PBS Professional. The following procedures explain how to configure PBS job scripts to run MPI applications.

Procedure 2-2 To specify computing resources

1. Within a script, use the -l option on a #PBS directive line. These lines have the following format:

#PBS -1 select=processes:ncpus=threads[:other_options]

For processes, specify the total number of MPI processes in the job.

For *threads*, specify the number of OpenMP threads per process. For purely MPI jobs, specify 1.

For more information on resource allocation options, see the pbs_resources(7) man page from the PBS Professional software distribution.

Procedure 2-3 To run the MPI application

1. Use the mpiexec_mpt command included in SGI MPT.

The mpiexec_mpt command is a wrapper script that assembles the correct host list and corresponding mpirun command before it runs the assembled mpirun command. The format is as follows:

mpiexec_mpt [-n processes] ./a.out

For *processes*, specify the total number of MPI processes in the application. Use this syntax on both a single-host and clustered systems. For more information, see the mpiexec_mpt(1) man page.

Process and thread pinning onto CPUs is especially important on cache coherent non-uniform memory access (ccNUMA) systems like the SGI UV system series. Process pinning is performed automatically if PBS Professional is set up to run each application in a set of dedicated cpusets. In these cases, PBS Professional sets the PBS_CPUSET_DEDICATED environment variable to the value YES. This has the same effect as setting MPI_DSM_DISTRIBUTE=ON. Process and thread pinning are also performed in all cases where omplace(1) is used.

Example 2-1 Running an MPI application with 512 Processes

To run an application with 512 processes, include the following in the directive file:

```
#PBS -l select=512:ncpus=1
mpiexec_mpt ./a.out
```

Example 2-2 Running an MPI application with 512 Processes and Four OpenMP Threads per Process

To run an MPI application with 512 Processes and four OpenMP threads per process, include the following in the directive file:

```
#PBS -l select=512:ncpus=4
mpiexec_mpt omplace -nt 4 ./a.out
```

Some third-party debuggers support the mpiexec_mpt(1) command. The mpiexec_mpt(1) command includes a -tv option for use with TotalView and includes a -ddt option for use with DDT. For more information, see Chapter 4, "Debugging MPI Applications" on page 45.

PBS Professional includes an mpiexec(1) command that enables you to run SGI MPI applications. PBS Professional's command does not support the same set of extended options that the SGI mpiexec_mpt(1) supports.

Torque

When running Torque, SGI recommends the SGI MPT mpiexec_mpt(1) command to launch SGI MPT MPI jobs.

The basic syntax is as follows:

mpiexec_mpt -n P ./a.out

For *P*, specify is the total number of MPI processes in the application. This syntax applies whether running on a single host or a clustered system. See the mpiexec_mpt(1) man page for more details.

The mpiexec_mpt command has a -tv option for use by SGI MPT when running the TotalView Debugger with a workoad manager like Torque. For more information on using the mpiexec_mpt command -tv option, see "Using the TotalView Debugger with MPI Programs" on page 45.

Simple Linux Utility for Resource Management (SLURM)

SGI MPI is adapted for use with the SLURM workload manager. If you want to use SGI MPI with SLURM, use the SLURM pmi2 MPI plug-in. SGI MPI 1.8 requires SLURM 2.6 or later.

For general information about SLURM, see the following website:

http://slurm.schedmd.com

For more information about how to use MPI with SLURM, see the following website:

http://slurm.schedmd.com/mpi_guide.html

Compiling and Running SHMEM Applications

To compile SHMEM programs with a GNU compiler, choose one of the following commands:

% g++ compute.C -lsma -lmpi % gcc compute.c -lsma -lmpi To compile SHMEM programs with the Intel compiler, use the following commands:

% icc compute.C -lsma -lmpi % icc compute.c -lsma -lmpi % ifort compute.f -lsma -lmpi

You must use mpirun to launch SHMEM applications. The NPES variable has no effect on SHMEM programs. To request the desired number of processes to launch, you must set the -np option on mpirun.

The SHMEM programming model supports both single-host SHMEM applications and SHMEM applications that span multiple partitions. To launch a SHMEM application on more than one partition, use the multiple host mpirun syntax, as follows:

% mpirun hostA, hostB -np 16 ./shmem_app

For more information, see the intro_shmem(3) man page.

Using Huge Pages

You can use huge pages to optimize the performance of your MPI application. The MPI_HUGEPAGE_HEAP_SPACE environment variable (see the mpi(1) man page) defines the minimum amount of heap space each MPI process would allocate using huge pages. If set to a positive number, libmpi verifies that enough hugetlbfs overcommit resources are available at program start-up to satisfy that amount on all MPI processes. The heap uses all available hugetlbfs space, even beyond the specified minimum amount. A value of 0 disables this check and disables the allocation of heap variables on huge pages. Values can be followed by K, M, G, or T to denote scaling by 1024, 1024^2 , 1024^3 , or 1024^4 , respectively.

The following steps explain how to configure system settings for huge pages.

1. Type the following command to make sure that the current SGI MPT software release module is installed:

sys:~ # module load mpt

2. To configure the system settings for huge pages, as root user, perform the following:

sys:~ # mpt_hugepage_config -u
Updating system configuration

System config file:/proc/sys/vm/nr_overcommit_hugepagesHuge Pages Allowed:28974 pages (56 GB) 90% of memoryHuge Page Size:2048 KBHuge TLB FS Directory:/etc/mpt/hugepage_mpt

3. To view the current system configuration, perform the following command:

```
sys:~ # mpt_hugepage_config -v
Reading current system configuration
```

System config file:	<pre>/proc/sys/vm/nr_overcommit_hugepages</pre>
Huge Pages Allowed:	28974 pages (56 GB) 90% of memory
Huge Page Size:	2048 КВ
Huge TLB FS Directory:	<pre>/etc/mpt/hugepage_mpt (exists)</pre>

4. When running your SGI MPT program, set the MPI_HUGEPAGE_HEAP_SPACE environment variable to 1.

This activates the new libmpi huge page heap. Memory allocated by calls to the malloc function are allocated on huge pages. This makes single-copy MPI sends much more efficient when using the SGI UV global reference unit (GRU) for MPI messaging.

5. To clear the system configuration settings, as root user, type the following:

```
sys:~ # mpt_hugepage_config -e
Removing MPT huge page configuration
```

6. To verify that the SGI MPT huge page configuration has been cleared, retrieve the system configuration again, as follows:

uv44-sys:~ # mpt_hugepage_config -v Reading current system configuration

System config file:	/proc/sys/vm/nr_overcommit_hugepages
Huge Pages Allowed:	0 pages (0 KB) 0% of memory
Huge Page Size:	2048 KB
Huge TLB FS Directory:	<pre>/etc/mpt/hugepage_mpt (does not exist)</pre>

For more information about how to configure huge pages for MPI applications, see the mpt_hugepage_config(1) man page.

Programming with SGI MPI

Portability is one of the main advantages MPI has over vendor-specific message passing software. Nonetheless, the MPI Standard offers sufficient flexibility for general variations in vendor implementations. In addition, there are often vendor-specific programming recommendations for optimal use of the MPI library. The following topics explain how to develop or port MPI applications to SGI systems:

- "Job Termination and Error Handling" on page 37
- "Signals" on page 38
- "Buffering" on page 39
- "Multithreaded Programming" on page 40
- "Interoperability with the SHMEM programming model" on page 40
- "Miscellaneous Features of SGI MPI" on page 41
- "Programming Optimizations" on page 41
- "Additional Programming Model Considerations" on page 44

Job Termination and Error Handling

This section describes the behavior of the SGI MPI implementation upon normal job termination. Error handling and characteristics of abnormal job termination are also described.

MPI_Abort

In the SGI MPI implementation, a call to MPI_Abort causes the termination of the entire MPI job, regardless of the communicator argument used. The error code value is returned as the exit status of the mpirun command. A stack traceback is displayed that shows where the program called MPI_Abort.

Error Handling

The MPI Standard describes MPI error handling. Although almost all MPI functions return an error status, an error handler is invoked before returning from the function. If the function has an associated communicator, the error handler associated with that communicator is invoked. Otherwise, the error handler associated with MPI_COMM_WORLD is invoked.

The SGI MPI implementation provides the following predefined error handlers:

- MPI_ERRORS_ARE_FATAL. The handler, when called, causes the program to abort on all executing processes. This has the same effect as if MPI_Abort were called by the process that invoked the handler.
- MPI_ERRORS_RETURN. The handler has no effect.

By default, the MPI_ERRORS_ARE_FATAL error handler is associated with MPI_COMM_WORLD and any communicators derived from it. Hence, to handle the error statuses returned from MPI calls, it is necessary to associate either the MPI_ERRORS_RETURN handler or another user-defined handler with MPI_COMM_WORLD near the beginning of the application.

MPI_Finalize and Connect Processes

In the SGI implementation of MPI, all pending communications involving an MPI process must be complete before the process calls MPI_Finalize. If there are any pending send or recv requests that are unmatched or not completed, the application hangs in MPI_Finalize. For more details, see the MPI Standard.

If the application uses the MPI remote memory access (RMA) spawn functionality described in the MPI RMA standard, there are additional considerations. In the SGI implementation, all MPI processes are connected. The MPI RMA standard defines what is meant by connected processes. When the MPI RMA spawn functionality is used, MPI_Finalize is collective over all connected processes. Thus all MPI processes, both launched on the command line, or subsequently spawned, synchronize in MPI_Finalize.

Signals

In the SGI implementation, MPI processes are UNIX processes. As such, the general rule regarding signal handling applies as it would to ordinary UNIX processes.

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In addition, the SIGURG and SIGUSR1 signals can be propagated from the mpirun process to the other processes in the MPI job, whether they belong to the same process group on a single host, or are running across multiple hosts in a cluster. To make use of this feature, the MPI program must have a signal handler that catches SIGURG or SIGUSR1. When the SIGURG or SIGUSR1 signals are sent to the mpirun process ID, the mpirun process catches the signal and propagates it to all MPI processes.

Buffering

Most MPI implementations use buffering for overall performance reasons, and some programs depend on it. However, you should not assume that there is any message buffering between processes because the MPI Standard does not mandate a buffering strategy. Table 3-1 on page 39 illustrates a simple sequence of MPI operations that cannot work unless messages are buffered. If sent messages were not buffered, each process would hang in the initial call, waiting for an MPI_Recv call to take the message.

Because most MPI implementations do buffer messages to some degree, a program like this does not usually hang. The MPI_Send calls return after putting the messages into buffer space, and the MPI_Recv calls get the messages. Nevertheless, program logic like this is not valid according to the MPI Standard. Programs that require this sequence of MPI calls should employ one of the buffer MPI send calls, MPI_Bsend or MPI_Ibsend.

Table 3-1 Outline of Improper Dependence on Buffering

Process 1	Process 2
MPI_Send(2,)	MPI_Send(1,)
<pre>MPI_Recv(2,)</pre>	<pre>MPI_Recv(1,)</pre>

By default, the SGI implementation of MPI uses buffering under most circumstances. Short messages (64 or fewer bytes) are always buffered. Longer messages are also buffered, although under certain circumstances, buffering can be avoided. For performance reasons, it is sometimes desirable to avoid buffering. For further information on unbuffered message delivery, see "Programming Optimizations" on page 41.

Multithreaded Programming

SGI MPI supports hybrid programming models, in which MPI is used to handle one level of parallelism in an application, while POSIX threads or OpenMP processes are used to handle another level. When mixing OpenMP with MPI, for performance reasons, it is better to consider invoking MPI functions only outside parallel regions, or only from within master regions. When used in this manner, it is not necessary to initialize MPI for thread safety. You can use MPI_Init to initialize MPI. However, to safely invoke MPI functions from any OpenMP process or when using Posix threads, MPI must be initialized with MPI_Init_thread.

When using MPI_Thread_init() with the threading level MPI_THREAD_MULTIPLE, link your program with -lmpi_mt instead of -lmpi. See the mpi(1) man page for more information about compiling and linking MPI programs.

Interoperability with the SHMEM programming model

You can mix SHMEM and MPI message passing in the same program. The application must be linked with both the SHMEM and MPI libraries. Start with an MPI program that calls MPI_Init and MPI_Finalize.

When you add SHMEM calls, the PE numbers are equal to the MPI rank numbers in MPI_COMM_WORLD. Do not call start_pes() in a mixed MPI and SHMEM program.

When running the application across a cluster, some MPI processes may not be able to communicate with certain other MPI processes when using SHMEM functions. You can use the shmem_pe_accessible and shmem_addr_accessible functions to determine whether a SHMEM call can be used to access data residing in another MPI process. Because the SHMEM model functions only with respect to MPI_COMM_WORLD, these functions cannot be used to exchange data between MPI processes that are connected via MPI intercommunicators returned from MPI remote memory access (RMA) spawn related functions.

SHMEM get and put functions are thread safe. SHMEM collective and synchronization functions are not thread safe unless different threads use different pSync and pWork arrays.

For more information about the SHMEM programming model, see the intro_shmem man page.

Miscellaneous Features of SGI MPI

This section describes other characteristics of the SGI MPI implementation that might be of interest to application developers.

stdin/stdout/stderr

In this implementation, stdin is enabled for only those MPI processes with rank 0 in the first MPI_COMM_WORLD. Such processes do not need to be located on the same host as mpirun. stdout and stderr results are enabled for all MPI processes in the job, whether started by mpirun or started by one of the MPI remote memory access (RMA) spawn functions.

MPI_Get_processor_name

The MPI_Get_processor_name function returns the Internet host name of the computer on which the MPI process that started this subroutine is running.

Programming Optimizations

The following topics describe how to use the optimized features of SGI's MPI implementation. You might need to modify your MPI application to use these recommendations.

Using MPI Point-to-Point Communication Routines

MPI provides for a number of different routines for point-to-point communication. The most efficient ones in terms of latency and bandwidth are the blocking and nonblocking send/receive functions, which are as follows:

- MPI_Send
- MPI_Isend
- MPI_Recv
- MPI_Irecv

Unless required for application semantics, avoid the synchronous send calls, which are as follows:

- MPI_Ssend
- MPI_Issend

Also avoid the buffered send calls, which double the amount of memory copying on the sender side. These calls are as follows:

- MPI_Bsend
- MPI_Ibsend

This implementation treats the ready send routines, MPI_Rsend and MPI_Irsend, as standard MPI_Send and MPI_Isend routines. Persistent requests do not offer any performance advantage over standard requests in this implementation.

Using MPI Collective Communication Routines

The MPI collective calls are frequently layered on top of the point-to-point primitive calls. For small process counts, this can be reasonably effective. However, for higher process counts of 32 processes or more, or for clusters, this approach can be less efficient. For this reason, a number of the MPI library collective operations have been optimized to use more complex algorithms.

Most collectives have been optimized for use with clusters. In these cases, steps are taken to reduce the number of messages using the relatively slower interconnect between hosts.

Some of the collective operations have been optimized for use with shared memory. On SGI UV systems, barriers and reductions have been optimized to use the SGI GRU hardware accelerator. The MPI_Alltoall routines also use special techniques to avoid message buffering when using shared memory. For more details, see "Avoiding Message Buffering — Single Copy Methods" on page 43.

Note: Collectives are optimized across partitions by using the XPMEM driver which is explained in Chapter 7, "Run-time Tuning". The collectives (except MPI_Barrier) try to use single-copy by default for large transfers unless MPI_DEFAULT_SINGLE_COPY_OFF is specified.

Using MPI_Pack/MPI_Unpack

While MPI_Pack and MPI_Unpack are useful for porting parallel virtual machine (PVM) codes to MPI, they essentially double the amount of data to be copied by both the sender and receiver. It is generally best to avoid the use of these functions by either restructuring your data or using derived data types. Note, however, that use of derived data types can lead to decreased performance in certain cases.

Avoiding Derived Data Types

Avoid derived data types when possible. In the SGI implementation, use of derived data types does not generally lead to performance gains. Use of derived data types might disable certain types of optimizations, for example, unbuffered or single copy data transfer.

Avoiding Wild Cards

The use of wild cards (MPI_ANY_SOURCE, MPI_ANY_TAG) involves searching multiple queues for messages. While this is not significant for small process counts, for large process counts, the cost increases quickly.

Avoiding Message Buffering — Single Copy Methods

One of the most significant optimizations for bandwidth-sensitive applications in the MPI library is single-copy optimization, avoiding the use of shared memory buffers. However, as discussed in "Buffering" on page 39, some incorrectly coded applications might hang because of buffering assumptions. For this reason, this optimization is not enabled by default for MPI_Send, but you can use the MPI_BUFFER_MAX environment variable to enable this optimization at run time. The following guidelines show how to increase the opportunity for use of the unbuffered pathway:

- The MPI data type on the send side must be a contiguous type.
- The sender and receiver MPI processes must reside on the same host. In the case of a partitioned system, the processes can reside on any of the partitions.
- The sender data must be globally accessible by the receiver. The SGI MPI implementation allows data allocated from the static region (common blocks), the private heap, and the stack region to be globally accessible. In addition, memory

allocated via the MPI_Alloc_mem function or the SHMEM symmetric heap accessed via the shpalloc or shmalloc functions is globally accessible.

Certain run-time environment variables must be set to enable the unbuffered, single copy method. For information about how to set the run-time environment, see "Avoiding Message Buffering – Enabling Single Copy" on page 55.

Managing Memory Placement

SGI UV series systems have a ccNUMA memory architecture. For single-process and small multiprocess applications, this architecture behaves similarly to flat memory architectures. For more highly parallel applications, memory placement becomes important. MPI takes placement into consideration when it lays out shared memory data structures and the individual MPI processes' address spaces. Generally, you should not try to manage memory placement explicitly. If you need to control the placement of the application at run time, however, see Chapter 7, "Run-time Tuning" on page 53.

Additional Programming Model Considerations

A number of additional programming options might be worth consideration when developing MPI applications for SGI systems. For example, the SHMEM programming model can provide a means to improve the performance of latency-sensitive sections of an application. Usually, this requires replacing MPI send/recv calls with shmem_put/shmem_get and shmem_barrier calls. The SHMEM programming model can deliver significantly lower latencies for short messages than traditional MPI calls. As an alternative to shmem_get/shmem_put/calls, you might consider the MPI remote memory accesss (RMA) MPI_Put/MPI_Get functions. These provide almost the same performance as the SHMEM calls, while providing a greater degree of portability.

Alternately, you might consider exploiting the shared memory architecture of SGI systems by handling one or more levels of parallelism with OpenMP, with the coarser grained levels of parallelism being handled by MPI. Also, there are special ccNUMA placement considerations to be aware of when running hybrid MPI/OpenMP applications. For further information, see Chapter 7, "Run-time Tuning" on page 53.

Debugging MPI Applications

This chapter includes the following topics:

- "MPI Routine Argument Checking" on page 45
- "Using the TotalView Debugger with MPI Programs" on page 45
- "Using idb and gdb with MPI Programs" on page 46
- "Using the DDT Debugger with MPI Programs" on page 46

MPI Routine Argument Checking

Debugging MPI applications can be more challenging than debugging sequential applications. By default, the SGI MPI implementation does not check the arguments to some performance-critical MPI routines, such as most of the point-to-point and collective communication routines. You can force MPI to always check the input arguments to MPI functions by setting the MPI_CHECK_ARGS environment variable. However, setting this variable might result in some degradation in application performance, so it is not recommended that it be set except when debugging.

Using the TotalView Debugger with MPI Programs

The syntax for running SGI MPI with the TotalView Debugger (TVD) from TotalView Technologies is as follows:

% totalview mpirun -a -np 4 a.out

Note that TVD is not expected to operate with MPI processes started via the MPI_Comm_spawn or MPI_Comm_spawn_multiple functions.

The SGI Message Passing Toolkit (MPT) mpiexec_mpt(1) command has a -tv option for use by SGI MPT with the TotalView Debugger. Note that the PBS Professional mpiexec(1) command does not support the -tv option.

To run an SGI MPT MPI job with TotalView without a workload manager (same as the above example), type the following:

% totalview mpirun -a -np 4 a.out

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To run an SGI MPT MPI job with the TotalView Debugger with a workoad manager, such as PBS Professional or Torque, type the following:

% mpiexec_mpt -tv -np 4 a.out

Using idb and gdb with MPI Programs

Because the idb and gdb debuggers are designed for sequential, non-parallel applications, they are generally not well suited for use in MPI program debugging and development. However, the use of the MPI_SLAVE_DEBUG_ATTACH environment variable makes these debuggers more usable.

If you set the MPI_SLAVE_DEBUG_ATTACH environment variable to a global rank number, the MPI process sleeps briefly in startup while you use idb or gdb to attach to the process. A message is printed to the screen, telling you how to use idb or gdb to attach to the process.

Similarly, if you want to debug the MPI daemon, setting MPI_DAEMON_DEBUG_ATTACH sleeps the daemon briefly while you attach to it.

Using the DDT Debugger with MPI Programs

Allinea Software's DDT product is a parallel debugger that supports SGI MPT. You can run DDT in either interactive (online) or batch (offline) mode. In batch mode, DDT can create a text or HTML report that tracks variable values and shows the location of any errors. DDT records the data for a program's variables across all processes, and DDT logs values in the HTML output files as sparkline charts.

For information about how to configure Allinea for use with MPI on SGI systems, use the instructions in the Allinea user guide that is posted to the following website:

http://content.allinea.com/downloads/userguide.pdf

Example 1. The following command starts DDT in interactive (online) mode:

ddt -np 4 a.out

Example 2. The following command generates a debugging report in HTML format:

ddt -offline my-log.html -np 4 a.out

Example 3. Assume that you want to trace variables x, y, and $my_arr(x,y)$ in parallel across all processes. The following command directs DDT to record the values of x, y, and $my_arr(x,y)$ each time it encounters line 147:

ddt -offline my-log.html -trace-at "my-file.f:147,x,y,my_arr(x,y)" -np 4 a.out

Example 4. You can specify batch (offline) DDT commands from within a queue submission script. Instead of specifying mpiexec_mpt -np 4 a.out, specify the following:

ddt -noqueue -offline my-log.html -trace-at "my-file.f:147,x,y,my_arr(x,y)" -np 4 a.out

Chapter 5

PerfBoost

SGI PerfBoost uses a wrapper library to run applications compiled against other MPI implementations under the SGI Message Passing Toolkit (MPT) product on SGI platforms. This chapter describes how to use PerfBoost software.

Note: The MPI C++ API is not supported with PerfBoost.

Using PerfBoost

To use PerfBoost with an SGI MPT MPI program, first load the perfboost environmental module (see Example 5-1 on page 49). Then insert the perfboost command in front of the executable name along with the choice of MPI implementation to emulate. Launch the application with the SGI MPT mpiexec_mpt(1) or mpirun(1) command. The following are MPI implementations and corresponding command line options:

MPI Implementation	Command Line Option
Platform MPI 7.1+	-pmpi
HP-MPI	-pmpi
Intel MPI	-impi
OpenMPI	-ompi
MPICH1	-mpich
MPICH2	-impi
MVAPICH2	-impi
Example 5-1 Using the SCI no.	rfboogt Software

Example 5-1 Using the SGI perfboost Software

The following are some examples that use perfboost:

% module load mpt
% module load perfboost

% mpirun -np 32 perfboost -impi a.out arg1

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% mpiexec_mpt perfboost -pmpi b.out arg1
% mpirun host1 32, host2 64 perfboost -impi c.out arg1 arg2

Environment Variables

The following environment variable is supported:

PERFBOOST_VERBOSE	Setting the PERFBOOST_VERBOSE environment variable enables a message when PerfBoost activates and also when the MPI application is completed through the MPI_Finalize() function. This message indicates that the PerfBoost library is active and also when the MPI application completes through the libperfboost wrapper library.
	Note: Some applications redirect stderr. In this case, the verbose messages might not appear in the application output.

The MPI environment variables that are documented in the MPI(1) man page are available to PerfBoost. MPI environment variables that are not used by SGI MPT are currently not supported.

MPI Supported Functions

SGI PerfBoost supports the commonly used elements of the C and Fortran MPI APIs. If a function is not supported, the job aborts and issues an error message. The message shows the name of the missing function. You can contact the SGI Customer Support Center at the following website to schedule a missing function to be added to PerfBoost:

https://support.sgi.com/caselist

Berkeley Lab Checkpoint/Restart

The SGI Message Passing Toolkit (MPT) supports the Berkeley Lab Checkpoint/Restart (BLCR) checkpoint/restart implementation. This implementation allows applications to periodically save a copy of their state. Applications can resume from that point if the application crashes or the job is aborted to free resources for higher priority jobs.

The following are the implementation's limitations:

- BLCR does not checkpoint the state of any data files that the application might be using.
- When using checkpoint/restart, MPI does not support certain features, including spawning and one-sided MPI.
- InfiniBand XRC queue pairs are not supported.
- Checkpoint files are often very large and require significant disk bandwidth to create in a timely manner.

For more information on BLCR, see https://ftg.lbl.gov/projects/CheckpointRestart.

BLCR Installation

To use checkpoint/restart with SGI MPT, BLCR must first be installed. This requires installing the blcr-, blcr-libs-, and blcr-kmp- RPMs. BLCR must then be enabled by root, as follows:

% chkconfig blcr on

BLCR uses a kernel module which must be built against the specific kernel that the operating system is running. In the case that the kernel module fails to load, it must be rebuilt and installed. Install the blcr-SRPM. In the blcr.spec file, set the kernel variable to the name of the current kernel, then rebuild and install the new set of RPMs.

Using BLCR with SGI MPT

To enable checkpoint/restart within SGI MPT, mpirun or mpiexec_mpt must be passed the -cpr option, for example:

% mpirun -cpr hostA, hostB -np 8 ./a.out

To checkpoint a job, use the mpt_checkpoint command on the same host where mpirun is running. mpt_checkpoint needs to be passed the PID of mpirun and a name with which you want to prefix all the checkpoint files. For example:

% mpt_checkpoint -p 12345 -f my_checkpoint

This will create a my_checkpoint.cps metadata file and a number of my_checkpoint.*.cpd files.

To restart the job, pass the name of the .cps file to mpirun, for example:

% mpirun -cpr hostC, hostD -np 8 mpt_restart my_checkpoint.cps

The job may be restarted on a different set of hosts but there must be the same number of hosts and each host must have the same number of ranks as the corresponding host in the original run of the job. Chapter 7

Run-time Tuning

This chapter discusses ways in which the user can tune the run-time environment to improve the performance of an MPI message passing application on SGI computers. None of these ways involve application code changes. This chapter covers the following topics:

- "Reducing Run-time Variability" on page 53
- "Tuning MPI Buffer Resources" on page 54
- "Avoiding Message Buffering Enabling Single Copy" on page 55
- "Memory Placement and Policies" on page 56
- "Tuning MPI/OpenMP Hybrid Codes" on page 58
- "Tuning for Running Applications Across Multiple Hosts" on page 59
- "Tuning for Running Applications over the InfiniBand Interconnect" on page 61
- "MPI on SGI UV Systems" on page 63
- "Suspending MPI Jobs" on page 65

Reducing Run-time Variability

One of the most common problems with optimizing message passing codes on large shared memory computers is achieving reproducible timings from run to run. To reduce run-time variability, you can take the following precautions:

- Do not oversubscribe the system. In other words, do not request more CPUs than are available and do not request more memory than is available. Oversubscribing causes the system to wait unnecessarily for resources to become available and leads to variations in the results and less than optimal performance.
- Avoid interference from other system activity. The Linux kernel uses more memory on node 0 than on other nodes (node 0 is called the kernel node in the following discussion). If your application uses almost all of the available memory per processor, the memory for processes assigned to the kernel node can unintentionally spill over to nonlocal memory. By keeping user applications off the kernel node, you can avoid this effect.

Additionally, by restricting system daemons to run on the kernel node, you can also deliver an additional percentage of each application CPU to the user.

- Avoid interference with other applications. You can use cpusets to address this problem also. You can use cpusets to effectively partition a large, distributed memory host in a fashion that minimizes interactions between jobs running concurrently on the system. See the *SGI Cpuset Software Guide* for information about cpusets.
- On a quiet, dedicated system, you can use dplace or the MPI_DSM_CPULIST shell variable to improve run-time performance repeatability. These approaches are not as suitable for shared, nondedicated systems.
- Use a workload manager; for example, Platform LSF from Platform Computing Corporation or PBS Professional from Altair Engineering, Inc. These workload managers use cpusets to avoid oversubscribing the system and possible interference between applications.

Tuning MPI Buffer Resources

By default, the SGI MPI implementation buffers messages that are longer than 64 bytes. The system buffers these longer messages in a series of 16 KB buffers. Messages that exceed 64 bytes are handled as follows:

• If the message is 128 k in length or shorter, the sender MPI process buffers the entire message.

In this case, the sender MPI process delivers a message header, also called a *control message*, to a mailbox. When an MPI call is made, the MPI receiver polls the mail box. If the receiver finds a matching receive request for the sender's control message, the receiver copies the data out of the buffers into the application buffer indicated in the receive request. The receiver then sends a message header back to the sender process, indicating that the buffers are available for reuse.

• If the message is longer than 128 k, the software breaks the message into chunks that are 128 k in length.

The smaller chunks allow the sender and receiver to overlap the copying of data in a pipelined fashion. Because there are a finite number of buffers, this can constrain overall application performance for certain communication patterns. You can use the MPI_BUFS_PER_PROC shell variable to adjust the number of buffers available for each process, and you can use the MPI statistics counters to determine if the demand for buffering is high.

Generally, you can avoid excessive numbers of retries for buffers if you increase the number of buffers. However, when you increase the number of buffers, you consume more memory, and you might increase the probability for cache pollution. *Cache pollution* is the excessive filling of the cache with message buffers. Cache pollution can degrade performance during the compute phase of a message passing application.

For information about statistics counters, see "MPI Internal Statistics" on page 75.

For information about buffering considerations when running an MPI job across multiple hosts, see "Tuning for Running Applications Across Multiple Hosts" on page 59.

For information about the programming implications of message buffering, see "Buffering" on page 39.

Avoiding Message Buffering – Enabling Single Copy

For message transfers between MPI processes within the same host or transfers between partitions, it is possible under certain conditions to avoid the need to buffer messages. Because many MPI applications are written assuming infinite buffering, the use of this unbuffered approach is not enabled by default for MPI_Send. This section describes how to activate this mechanism by default for MPI_Send.

For MPI_Isend, MPI_Sendrecv, and most collectives, this optimization is enabled by default for large message sizes. To disable this default single copy feature used for the collectives, use the MPI_DEFAULT_SINGLE_COPY_OFF environment variable.

Using the XPMEM Driver for Single Copy Optimization

MPI takes advantage of the XPMEM driver to support single copy message transfers between two processes within the same host or across partitions.

Enabling single copy transfers may result in better performance, since this technique improves MPI's bandwidth. However, single copy transfers may introduce additional synchronization points, which can reduce application performance in some cases.

The threshold for message lengths beyond which MPI attempts to use this single copy method is specified by the MPI_BUFFER_MAX shell variable. Its value should be set to the message length in bytes beyond which the single copy method should be tried. In general, a value of 2000 or higher is beneficial for many applications.

During job startup, MPI uses the XPMEM driver (via the xpmem kernel module) to map memory from one MPI process to another. The mapped areas include the static (BSS) region, the private heap, the stack region, and optionally the symmetric heap region of each process.

Memory mapping allows each process to directly access memory from the address space of another process. This technique allows MPI to support single copy transfers for contiguous data types from any of these mapped regions. For these transfers, whether between processes residing on the same host or across partitions, the data is copied using a bcopy process. A bcopy process is also used to transfer data between two different executable files on the same host or two different executable files across partitions. For data residing outside of a mapped region (a /dev/zero region, for example), MPI uses a buffering technique to transfer the data.

Memory mapping is enabled by default. To disable it, set the MPI_MEMMAP_OFF environment variable. Memory mapping must be enabled to allow single-copy transfers, MPI remote memory access (RMA) one-sided communication, support for the SHMEM model, and certain collective optimizations.

Memory Placement and Policies

The MPI library takes advantage of NUMA placement functions that are available. Usually, the default placement is adequate. Under certain circumstances, however, you might want to modify this default behavior. The easiest way to do this is by setting one or more MPI placement shell variables. Several of the most commonly used of these variables are described in the following sections. For a complete listing of memory placement related shell variables, see the MPI(1) man page.

MPI_DSM_CPULIST

The MPI_DSM_CPULIST shell variable allows you to manually select processors to use for an MPI application. At times, specifying a list of processors on which to run a job can be the best means to insure highly reproducible timings, particularly when running on a dedicated system.

This setting is treated as a comma and/or hyphen delineated ordered list that specifies a mapping of MPI processes to CPUs. If running across multiple hosts, the per host components of the CPU list are delineated by colons. Within hyphen delineated lists CPU striding may be specified by placing /# after the list where # is the stride distance.

Note: This feature should not be used with MPI applications that use either of the MPI remote memory access (RMA) spawn related functions.

Examples of settings are as follows:

Value	CPU Assignment
8,16,32	Place three MPI processes on CPUs 8, 16, and 32.
32,16,8	Place the MPI process rank zero on CPU 32, one on 16, and two on CPU 8.
8-15/2	Place the MPI processes 0 through 3 strided on CPUs 8, 10, 12, and 14
8-15,32-39	Place the MPI processes 0 through 7 on CPUs 8 to 15. Place the MPI processes 8 through 15 on CPUs 32 to 39.
39-32,8-15	Place the MPI processes 0 through 7 on CPUs 39 to 32. Place the MPI processes 8 through 15 on CPUs 8 to 15.
8-15:16-23	Place the MPI processes 0 through 7 on the first host on CPUs 8 through 15. Place MPI processes 8 through 15 on CPUs 16 to 23 on the second host.

Note that the process rank is the MPI_COMM_WORLD rank. The interpretation of the CPU values specified in the MPI_DSM_CPULIST depends on whether the MPI job is being run within a cpuset. If the job is run outside of a cpuset, the CPUs specify *cpunum* values beginning with 0 and up to the number of CPUs in the system minus one. When running within a cpuset, the default behavior is to interpret the CPU values as relative processor numbers within the cpuset.

The number of processors specified should equal the number of MPI processes that will be used to run the application. The number of colon delineated parts of the list must equal the number of hosts used for the MPI job. If an error occurs in processing the CPU list, the default placement policy is used.

MPI_DSM_DISTRIBUTE

Use the MPI_DSM_DISTRIBUTE shell variable to ensure that each MPI process gets a physical CPU and memory on the node to which it was assigned. MPI_DSM_DISTRIBUTE assigns MPI ranks, starting at logical CPU 0 and incrementing, until all ranks have been placed.

If you set both MPI_DSM_DISTRIBUTE and MPI_DSM_CPULIST, MPI_DSM_CPULIST overrides MPI_DSM_DISTRIBUTE.

MPI_DSM_VERBOSE

Setting the MPI_DSM_VERBOSE shell variable directs MPI to display a synopsis of the NUMA and host placement options being used at run time.

Using dplace for Memory Placement

The dplace tool offers another means of specifying the placement of MPI processes within a distributed memory host. The dplace tool and MPI interoperate to allow MPI to better manage placement of certain shared memory data structures when dplace is used to place the MPI job.

For instructions on how to use dplace with MPI, see the dplace(1) man page and the *Linux Application Tuning Guide*.

Tuning MPI/OpenMP Hybrid Codes

A hybrid MPI/OpenMP application is one in which each MPI process itself is a parallel threaded program. These programs often exploit the OpenMP parallelism at the loop level while also implementing a higher level parallel algorithm using MPI.

Many parallel applications perform better if the MPI processes and the threads within them are pinned to particular processors for the duration of their execution. For ccNUMA systems, this ensures that all local, non-shared memory is allocated on the same memory node as the processor referencing it. For all systems, it can ensure that some or all of the OpenMP threads stay on processors that share a bus or perhaps a processor cache, which can speed up thread synchronization.

The SGI Message Passing Toolkit (MPT) provides the omplace(1) command to help with the placement of OpenMP threads within an MPI program. The omplace

command causes the threads in a hybrid MPI/OpenMP job to be placed on unique CPUs within the containing cpuset. For example, the threads in a 2-process MPI program with 2 threads per process would be placed as follows:

rank 0 thread 0 on CPU 0
rank 0 thread 1 on CPU 1
rank 1 thread 0 on CPU 2
rank 1 thread 1 on CPU 3

The CPU placement is performed by dynamically generating a dplace(1) placement file and invoking dplace.

For detailed syntax and a number of examples, see the omplace(1) man page. For more information on dplace, see the dplace(1) man page. For information on using cpusets, see the *SGI Cpuset Software Guide*. For more information on using dplace, see the *Linux Application Tuning Guide*.

Example 7-1 How to Run a Hybrid MPI/OpenMP Application

Here is an example of how to run a hybrid MPI/OpenMP application with eight MPI processes that are two-way threaded on two hosts:

mpirun host1, host2 -np 4 omplace -nt 2 ./a.out

When using the PBS workload manager to schedule the a hybrid MPI/OpenMP job as shown in Example 7-1 on page 59, use the following resource allocation specification:

#PBS -l select=8:ncpus=2

And use the following mpiexec command with the above example:

mpiexec -n 8 omplace -nt 2 ./a.out

For more information about running SGI MPT programs with PBS, see"Running MPI Jobs with a Workload Manager" on page 32.

Tuning for Running Applications Across Multiple Hosts

When you are running an MPI application across a cluster of hosts, there are additional run-time environment settings and configurations that you can consider when trying to improve application performance. Systems can use the XPMEM interconnect to cluster hosts as partitioned systems, or use the InfiniBand interconnect or TCP/IP as the multihost interconnect.

When launched as a distributed application, MPI probes for these interconnects at job startup. For details of launching a distributed application, see "Launching a Distributed Application" on page 31. When a high performance interconnect is detected, MPI attempts to use this interconnect if it is available on every host being used by the MPI job. If the interconnect is not available for use on every host, the library attempts to use the next slower interconnect until this connectivity requirement is met. Table 7-1 on page 60 specifies the order in which MPI probes for available interconnects.

Interconnect	Default Order of Selection	Environment Variable Use
XPMEM	1	MPI_USE_XPMEM

2

3

4

 Table 7-1 Inquiry Order for Available Interconnects

InfiniBand

TCP/IP

InfiniBand Unreliable Datagram

The third column of Table 7-1 on page 60 also indicates the environment variable you can set to pick a particular interconnect other than the default.

In general, to insure the best performance of the application, you should allow MPI to pick the fastest available interconnect.

When using the TCP/IP interconnect, unless specified otherwise, MPI uses the default IP adapter for each host. To use a nondefault adapter, enter the adapter-specific host name on the mpirun command line.

When using the InfiniBand interconnect, SGI MPT applications may not execute a fork() or system() call. The InfiniBand driver produces undefined results when an SGI MPT process using InfiniBand forks.

to Require

MPI_USE_IB

MPI USE UD

MPI_USE_TCP

MPI_USE_IB

Requires the MPI library to use the InfiniBand driver as the interconnect when running across multiple hosts or running with multiple binaries. SGI MPT requires the OFED software stack when the InfiniBand interconnect is used. If InfiniBand is used, the MPI_COREDUMP environment variable is forced to INHIBIT, to comply with the InfiniBand driver restriction that no fork()s may occur after InfiniBand resources have been allocated. Default: Not set

MPI_IB_RAILS

When this is set to 1 and the MPI library uses the InfiniBand driver as the inter-host interconnect, SGI MPT will send its InfiniBand traffic over the first fabric that it detects. If this is set to 2, the library will try to make use of multiple available separate InfiniBand fabrics and split its traffic across them. If the separate InfiniBand fabrics do not have unique subnet IDs, then the rail-config utility is required. It must be run by the system administrator to enable the library to correctly use the separate fabrics. Default: 1 on all SGI UV systems.

MPI_IB_SINGLE_COPY_BUFFER_MAX

When MPI transfers data over InfiniBand, if the size of the cumulative data is greater than this value then MPI will attempt to send the data directly between the processes's buffers and not through intermediate buffers inside the MPI library. Default: 32767

For more information on these environment variables, see the ENVIRONMENT VARIABLES section of the mpi(1) man page.

Tuning for Running Applications over the InfiniBand Interconnect

When running an MPI application across a cluster of hosts using the InfiniBand interconnect, there are additional run-time environmental settings that you can consider to improve application performance, as follows:

MPI_NUM_QUICKS

Controls the number of other ranks that a rank can receive from over InfiniBand using a short message fast path. This is 8 by default and can be any value between 0 and 32.

MPI_NUM_MEMORY_REGIONS

For zero-copy sends over the InfiniBand interconnect, SGI MPT keeps a cache of application data buffers registered for these transfers. This environmental variable controls the size of the cache. It is 8 by default and can be any value between 0 and 32. If the application rarely reuses data buffers, it may make sense to set this value to 0 to avoid cache trashing.

MPI_CONNECTIONS_THRESHOLD

For very large MPI jobs, the time and resource cost to create a connection between every pair of ranks at job start time may be prodigious. When the number of ranks is at least this value, the MPI library will create InfiniBand connections lazily on a demand basis. The default is 1024 ranks.

MPI_IB_PAYLOAD

When the MPI library uses the InfiniBand fabric, it allocates some amount of memory for each message header that it uses for InfiniBand. If the size of data to be sent is not greater than this amount minus 64 bytes for the actual header, the data is inlined with the header. If the size is greater than this value, then the message is sent through remote direct memory access (RDMA) operations. The default is 8320 bytes.

MPI_IB_TIMEOUT

When an InfiniBand card sends a packet, it waits some amount of time for an ACK packet to be returned by the receiving InfiniBand card. If it does not receive one, it sends the packet again. This variable controls that wait period. The time spent is equal to $4 * 2 ^ MPI_IB_TIMEOUT$ microseconds. By default, the variable is set to 18.

MPI_IB_FAILOVER

When the MPI library uses InfiniBand and this variable is set, and an InfiniBand transmission error occurs, SGI MPT will try to restart the connection to the other rank. It will handle a number of errors of this type between any pair of ranks equal to the value of this variable. By default, the variable is set to 4.

MPI on SGI UV Systems

Note: This section does not apply to SGI UV 10 systems or SGI UV 20 systems.

The SGI[®] UV[™] series systems are scalable nonuniform memory access (NUMA) systems that support a single Linux image of thousands of processors distributed over many sockets and SGI UV Hub application-specific integrated circuits (ASICs). The UV Hub is the heart of the SGI UV system compute blade. Each "processor" is a hyperthread on a particular core within a particular socket. Each SGI UV Hub normally connects to two sockets. All communication between the sockets and the UV Hub uses Intel QuickPath Interconnect (QPI) channels. The SGI UV 1000 series Hub has four NUMAlink 5 ports that connect with the NUMAlink 5 interconnect fabric.

On SGI UV 2000 series systems, the UV Hub board assembly has a HUB ASIC with two identical hubs. Each hub supports one 8.0 GT/s QPI channel to a processor socket. The SGI UV 2000 series Hub has four NUMAlink 6 ports that connect with the NUMAlink 6 interconnect fabric.

The UV Hub acts as a crossbar between the processors, local SDRAM memory, and the network interface. The Hub ASIC enables any processor in the single-system image (SSI) to access the memory of all processors in the SSI. For more information on the SGI UV hub, SGI UV compute blades, QPI, and NUMAlink 5, or NUMAlink 6, see the *SGI Altix UV 1000 System User's Guide*, the *SGI Altix UV 100 System User's Guide* or *SGI UV 2000 System User's Guide*, respectively.

When MPI communicates between processes, two transfer methods are possible on an SGI UV system:

- By use of shared memory
- By use of the global reference unit (GRU), part of the SGI UV Hub ASIC

MPI chooses the method depending on internal heuristics, the type of MPI communication that is involved, and some user-tunable variables. When using the GRU to transfer data and messages, the MPI library uses the GRU resources it allocates via the GRU resource allocator, which divides up the available GRU resources. It fairly allocates buffer space and control blocks between the logical processors being used by the MPI job.

General Considerations

Running MPI jobs optimally on SGI UV systems is not very difficult. It is best to pin MPI processes to CPUs and isolate multiple MPI jobs onto different sets of sockets and Hubs, and this is usually achieved by configuring a workload manager to create a cpuset for every MPI job. MPI pins its processes to the sequential list of logical processors within the containing cpuset by default, but you can control and alter the pinning pattern using MPI_DSM_CPULIST (see "MPI_DSM_CPULIST" on page 56), omplace(1), and dplace(1).

Job Performance Types

The MPI library chooses buffer sizes and communication algorithms in an attempt to deliver the best performance automatically to a wide variety of MPI applications. However, applications have different performance profiles and bottlenecks, and so user tuning may be of help in improving performance. Here are some application performance types and ways that MPI performance may be improved for them:

Odd HyperThreads are idle.

Most high performance computing MPI programs run best using only one HyperThread per core. When an SGI UV system has multiple HyperThreads per core, logical CPUs are numbered such that odd HyperThreads are the high half of the logical CPU numbers. Therefore, the task of scheduling only on the even HyperThreads may be accomplished by scheduling MPI jobs as if only half the full number exist, leaving the high logical CPUs idle. You can use the cpumap(1) command to determine if cores have multiple HyperThreads on your SGI UV system. The output tells the number of physical and logical processors and if **Hyperthreading** is **ON** or **OFF** and how shared processors are paired (towards the bottom of the command's output).

If an MPI job uses only half of the available logical CPUs, set GRU_RESOURCE_FACTOR to 2 so that the MPI processes can utilize all the available GRU resources on a Hub rather than reserving some of them for the idle HyperThreads. For more information about GRU resource tuning, see the gru_resource(3) man page.

• MPI large message bandwidth is important.

Some programs transfer large messages via the MPI_Send function. To switch on the use of unbuffered, single copy transport in these cases you can set MPI_BUFFER_MAX to 0. See the MPI(1) man page for more details.

• MPI small or near messages are very frequent.

For small fabric hop counts, shared memory message delivery is faster than GRU messages. To deliver all messages within an SGI UV host via shared memory, set MPI_SHARED_NEIGHBORHOOD to "host". See the MPI(1) man page for more details.

Other ccNUMA Performance Issues

MPI application processes normally perform best if their local memory is allocated on the socket assigned to execute it. This cannot happen if memory on that socket is exhausted by the application or by other system consumption, for example, file buffer cache. Use the nodeinfo(1) command to view memory consumption on the nodes assigned to your job and use bcfree(1) to clear out excessive file buffer cache. PBS Professional workload manager installations can be configured to issue bcfree commands in the job prologue. For more information, see PBS Professional documentation and the bcfree(1) man page.

Suspending MPI Jobs

MPI software from SGI can internally use the XPMEM kernel module to provide direct access to data on remote partitions and to provide single copy operations to local data. Any pages used by these operations are prevented from paging by the XPMEM kernel module. If an administrator needs to temporarily suspend a MPI application to allow other applications to run, they can unpin these pages so they can be swapped out and made available for other applications.

Each process of a MPI application which is using the XPMEM kernel module will have a /proc/xpmem/pid file associated with it. The number of pages owned by this process which are prevented from paging by XPMEM can be displayed by concatenating the /proc/xpmem/pid file, for example:

```
# cat /proc/xpmem/5562
pages pinned by XPMEM: 17
To unpin the pages for use by other processes, the administrator must first suspend
all the processes in the application. The pages can then be unpinned by echoing any
value into the /proc/xpmem/pid file, for example:
```

echo 1 > /proc/xpmem/5562

The echo command will not return until that process's pages are unpinned.

When the MPI application is resumed, the XPMEM kernel module will prevent these pages from paging as they are referenced by the application.

MPI Performance Profiling

SGI includes profiling support in the libmpi.so library. Profiling support replaces all MPI_Xxx prototypes and function names with PMPI_Xxx entry points.

This chapter describes the perfcatch utility used to profile the performance of an MPI program and other tools that can be used for profiling MPI applications. It covers the following topics:

- "Overview of perfcatch Utility" on page 67
- "Using the perfcatch Utility" on page 67
- "MPI_PROFILING_STATS Results File Example" on page 68
- "MPI Performance Profiling Environment Variables" on page 71
- "MPI-supported, Profiled Functions"
- "Profiling MPI Applications" on page 73

Overview of perfcatch Utility

The perfcatch utility runs an MPI program with a wrapper profiling library that prints MPI call profiling information to a summary file upon MPI program completion. This MPI profiling result file is called MPI_PROFILING_STATS, by default (see "MPI_PROFILING_STATS Results File Example" on page 68). It is created in the current working directory of the MPI process with rank 0.

Using the perfcatch Utility

The syntax of the perfcatch utility is, as follows:

perfcatch [-v | -vofed | -i] cmd args

The perfcatch utility accepts the following options:

No option Supports the SGI Message Passing Toolkit (MPT) -v Supports MPI

-vofedSupports OFED MPI-iSupports Intel MPI

To use perfcatch with an SGI Message Passing Toolkit MPI program, insert the perfcatch command in front of the executable name, as the following examples show:

- mpirun -np 64 perfcatch a.out arg1
- mpirun host1 32, host2 64 perfcatch a.out arg1

To use perfcatch with Intel MPI, add the -i option, as follows:

mpiexec -np 64 perfcatch -i a.out arg1

For more information, see the perfcatch(1) man page.

MPI_PROFILING_STATS Results File Example

The MPI profiling result file has a summary statistics section followed by a rank-by-rank profiling information section. The summary statistics section reports some overall statistics, including the percent time each rank spent in MPI functions, and the MPI process that spent the least and the most time in MPI functions. Similar reports are made about system time usage.

The rank-by-rank profiling information section lists every profiled MPI function called by a particular MPI process. The number of calls and the total time consumed by these calls is reported. Some functions report additional information such as average data counts and communication peer lists.

An example MPI_PROFILING_STATS results file is, as follows:

_____ PERFCATCHER version 22 (C) Copyright SGI. This library may only be used on SGI hardware platforms. See LICENSE file for details. _____ MPI program profiling information Job profile recorded Wed Jan 17 13:05:24 2007 Program command line: /home/estes01/michel/sastest/mpi_hello_linux Total MPI processes 2 0.0054768 sec Total MPI job time, avg per rank Profiled job time, avg per rank 0.0054768 sec Percent job time profiled, avg per rank 100% 0.001 sec Total user time, avg per rank Percent user time, avg per rank 18.2588% Total system time, avg per rank 0.0045 sec Percent system time, avg per rank 82.1648% 5.75004e-07 sec Time in all profiled MPI routines, avg per rank Percent time in profiled MPI routines, avg per rank 0.0104989% Rank-by-Rank Summary Statistics _____ Rank-by-Rank: Percent in Profiled MPI routines Rank:Percent 0:0.0112245% 1:0.00968502% Least: Rank 1 0.00968502% Most: Rank 0 0.0112245% Load Imbalance: 0.000771% Rank-by-Rank: User Time Rank:Percent 0:17.2683% 1:19.3699% Least: Rank 0 17.2683% Most: Rank 1 19.3699% Rank-by-Rank: System Time Rank:Percent

```
1:77.4796%
     0:86.3416%
 Least: Rank 1 77.4796%
Most: Rank 0 86.3416%
Notes
____
Wtime resolution is
                            5e-08 sec
Rank-by-Rank MPI Profiling Results
-----
Activity on process rank 0
        Single-copy checking was not enabled.
              calls: 1 time: 6.50005e-07 s 6.50005e-07 s/call
comm_rank
Activity on process rank 1
        Single-copy checking was not enabled.
              calls: 1 time: 5.00004e-07 s 5.00004e-07 s/call
comm_rank
-----
recv profile
         cnt/sec for all remote ranks
local
    ANY_SOURCE 0
                     1
rank
_____
recv wait for data profile
         cnt/sec for all remote ranks
        0
local
              1
rank
-----
recv wait for data profile
```

local rank	cnt/sec 0		1			
send profile						
src rank	cnt/sec 0	for	all 1	destina	ation	ranks
ssend profile	2					
src rank	cnt/sec 0	-	1			
ibsend profil	Le					
src rank	cnt/sec 0	for	all 1	destina	ation	ranks

MPI Performance Profiling Environment Variables

The MPI performance-profiling environment variables are as follows:

Variable	Description
MPI_PROFILE_AT_INIT	Activates MPI profiling immediately, that is, at the start of MPI program execution.
MPI_PROFILING_STATS_FILE	Specifies the file where MPI profiling results are written. If not

specified, the file
MPI_PROFILING_STATS is written.

MPI-supported, Profiled Functions

The MPI-supported, profiled functions are as follows:

Note: As indicated in the following list, some functions might not be implemented in all languages.

Languages	Function
C and Fortran	mpi_allgather
C and Fortran	mpi_allgatherv
C and Fortran	mpi_allreduce
C and Fortran	mpi_alltoall
C and Fortran	mpi_alltoallv
C and Fortran	mpi_alltoallw
C and Fortran	mpi_barrier
C and Fortran	mpi_bcast
C and Fortran	mpi_comm_create
C and Fortran	mpi_comm_free
C and Fortran	mpi_comm_group
C and Fortran	mpi_comm_rank
C and Fortran	mpi_finalize
C and Fortran	mpi_gather
C and Fortran	mpi_gatherv
С	mpi_get_count
C and Fortran	<pre>mpi_group_difference</pre>
C and Fortran	mpi_group_excl
C and Fortran	<pre>mpi_group_free</pre>
C and Fortran	<pre>mpi_group_incl</pre>

C and Fortran	mpi_group_intersection
C and Fortran	<pre>mpi_group_range_excl</pre>
C and Fortran	<pre>mpi_group_range_incl</pre>
C and Fortran	mpi_group_union
C	mpi_ibsend
C and Fortran	mpi_init
C	<pre>mpi_init_thread</pre>
C and Fortran	mpi_irecv
C and Fortran	mpi_isend
C	mpi_probe
C and Fortran	mpi_recv
C and Fortran	mpi_reduce
C and Fortran	mpi_scatter
C and Fortran	mpi_scatterv
C and Fortran	mpi_send
C and Fortran	mpi_sendrecv
C and Fortran	mpi_ssend
C and Fortran	mpi_test
C and Fortran	mpi_testany
C and Fortran	mpi_wait
C and Fortran	mpi_wait

Profiling MPI Applications

This section describes the use of profiling tools to obtain performance information. Compared to the performance analysis of sequential applications, characterizing the performance of parallel applications can be challenging. Often it is most effective to first focus on improving the performance of MPI applications at the single process level.

It may also be important to understand the message traffic generated by an application. A number of tools can be used to analyze this aspect of a message passing application's performance, including Performance Co-Pilot and various

third-party products. In this section, you can learn how to use these various tools with MPI applications. It covers the following topics:

- "Profiling Interface" on page 74
- "MPI Internal Statistics" on page 75
- "Third-party Products" on page 75

Profiling Interface

You can write your own profiling by using the MPI standard PMPI_* calls. In addition, either within your own profiling library or within the application itself you can use the MPI_Wtime function call to time specific calls or sections of your code.

The following example is actual output for a single rank of a program that was run on 128 processors, using a user-created profiling library that performs call counts and timings of common MPI calls. Notice that for this rank most of the MPI time is being spent in MPI_Waitall and MPI_Allreduce.

```
Total job time 2.203333e+02 sec
Total MPI processes 128
Wtime resolution is 8.000000e-07 sec
activity on process rank 0
comm_rank calls 1 time 8.800002e-06
get_count calls 0 time 0.000000e+00
ibsend calls 0 time 0.000000e+00
probe calls
               0
                   time 0.000000e+00
time 0.00000e+00
             0
recv calls
                                                                      wait time 0.00000e+00
                                         avg datacnt 0 waits 0
irecv calls 22039 time 9.76185e-01
                                         datacnt 23474032 avg datacnt 1065
             0
send calls
                      time 0.000000e+00
ssend calls 0
                      time 0.000000e+00
isend calls
              22039 time 2.950286e+00
             0
                      time 0.00000e+00
wait calls
                                         avg datacnt 0
waitall calls 11045 time 7.73805e+01
                                         # of Regs 44078 avg data cnt 137944
barrier calls 680 time 5.133110e+00
alltoall calls 0
                      time 0.0e+00
                                         avg datacnt 0
alltoallv calls 0
                      time 0.000000e+00
                      time 0.000000e+00
reduce calls 0
allreduce calls 4658 time 2.072872e+01
bcast calls 680 time 6.915840e-02
```

```
gather calls0time 0.000000e+00gatherv calls0time 0.000000e+00scatter calls0time 0.000000e+00scatterv calls0time 0.000000e+00activity on process rank 1...
```

MPI Internal Statistics

MPI keeps track of certain resource utilization statistics. These can be used to determine potential performance problems caused by lack of MPI message buffers and other MPI internal resources.

To turn on the displaying of MPI internal statistics, use the MPI_STATS environment variable or the -stats option on the mpirun command. MPI internal statistics are always being gathered, so displaying them does not cause significant additional overhead. In addition, one can sample the MPI statistics counters from within an application, allowing for finer grain measurements. If the MPI_STATS_FILE variable is set, when the program completes, the internal statistics will be written to the file specified by this variable. For information about these MPI extensions, see the mpi_stats man page.

These statistics can be very useful in optimizing codes in the following ways:

- To determine if there are enough internal buffers and if processes are waiting (retries) to acquire them
- To determine if single copy optimization is being used for point-to-point or collective calls

For additional information on how to use the MPI statistics counters to help tune the run-time environment for an MPI application, see Chapter 7, "Run-time Tuning" on page 53.

Third-party Products

Two third-party tools that you can use with the SGI MPI implementation are Vampir from Pallas (www.pallas.com) and Jumpshot, which is part of the MPICH distribution. Both of these tools are effective for small, short-duration MPI jobs. However, the trace files these tools generate can be enormous for longer running or

highly parallel jobs. This causes a program to run more slowly, but the larger problems is that the tools to analyze the data are often overwhelmed by the amount of data.

Troubleshooting and Frequently Asked Questions

This chapter provides answers to some common problems that users encounter when thay start to use SGI MPI and provides answers to other frequently asked questions. It covers the following topics:

- "What are some things I can try to figure out why mpirun is failing? " on page 77
- "My code runs correctly until it reaches MPI_Finalize() and then it hangs." on page 79
- "My hybrid code (using OpenMP) stalls on the mpirun command." on page 79
- "I keep getting error messages about MPI_REQUEST_MAX being too small." on page 79
- "I am not seeing stdout and/or stderr output from my MPI application." on page $80\,$
- "How can I get the SGI Message Passing Toolkit (MPT) software to install on my machine?" on page 80
- "Where can I find more information about the SHMEM programming model? " on page $80\,$
- "The $\mathtt{ps}(1)$ command says my memory use (SIZE) is higher than expected. " on page 80
- "What does MPI: could not run executable mean?" on page 81
- "How do I combine MPI with insert favorite tool here?" on page 81
- "Why do I see "stack traceback" information when my MPI job aborts?" on page 82

What are some things I can try to figure out why mpirun is failing?

Here are some things to investigate:

• Look in /var/log/messages for any suspicious errors or warnings. For example, if your application tries to pull in a library that it cannot find, a message should appear here. Only the root user can view this file.

- Be sure that you did not misspell the name of your application.
- To find dynamic link errors, try to run your program without mpirun. You will get the "mpirun must be used to launch all MPI applications" message, along with any dynamic link errors that might not be displayed when the program is started with mpirun.

As a last resort, setting the environment variable LD_DEBUG to all will display a set of messages for each symbol that rld resolves. This produces a lot of output, but should help you find the cause of the link error.

- Be sure that you are setting your remote directory properly. By default, mpirun attempts to place your processes on all machines into the directory that has the same name as \$PWD. This should be the common case, but sometimes different functionality is required. For more information, see the section on \$MPI_DIR and/or the -dir option in the mpirun man page.
- If you are using a relative pathname for your application, be sure that it appears in \$PATH. In particular, mpirun will not look in '.' for your application unless '.' appears in \$PATH.
- Run /usr/sbin/ascheck to verify that your array is configured correctly.
- Use the mpirun -verbose option to verify that you are running the version of MPI that you think you are running.
- Be very careful when setting MPI environment variables from within your .cshrc or .login files, because these will override any settings that you might later set from within your shell (due to the fact that MPI creates the equivalent of a fresh login session for every job). The safe way to set things up is to test for the existence of \$MPI_ENVIRONMENT in your scripts and set the other MPI environment variables only if it is undefined.
- If you are running under a Kerberos environment, you may experience unpredictable results because currently, mpirun is unable to pass tokens. For example, in some cases, if you use telnet to connect to a host and then try to run mpirun on that host, it fails. But if you instead use rsh to connect to the host, mpirun succeeds. (This might be because telnet is kerberized but rsh is not.) At any rate, if you are running under such conditions, you will definitely want to talk to the local administrators about the proper way to launch MPI jobs.
- Look in /tmp/.arraysvcs on all machines you are using. In some cases, you might find an errlog file that may be helpful.

- You can increase the verbosity of the Array Services daemon (arrayd) using the -v option to generate more debugging information. For more information, see the arrayd(8) man page.
- Check error messages in /var/run/arraysvcs.

My code runs correctly until it reaches MPI_Finalize() and then it hangs.

This is almost always caused by send or recv requests that are either unmatched or not completed. An unmatched request is any blocking send for which a corresponding recv is never posted. An incomplete request is any nonblocking send or recv request that was never freed by a call to MPI_Test(), MPI_Wait(), or MPI_Request_free().

Common examples are applications that call MPI_Isend() and then use internal means to determine when it is safe to reuse the send buffer. These applications never call MPI_Wait(). You can fix such codes easily by inserting a call to MPI_Request_free() immediately after all such isend operations, or by adding a call to MPI_Wait() at a later place in the code, prior to the point at which the send buffer must be reused.

My hybrid code (using OpenMP) stalls on the mpirun command.

If your application was compiled with the Open64 compiler, make sure you follow the instructions about using the Open64 compiler in combination with MPI/OpenMP applications described in "Compiling and Linking MPI Programs" on page 29.

I keep getting error messages about MPI_REQUEST_MAX being too small.

There are two types of cases in which the MPI library reports an error concerning MPI_REQUEST_MAX. The error reported by the MPI library distinguishes these.

MPI has run out of unexpected request entries; the current allocation level is: XXXXXX

The program is sending so many unexpected large messages (greater than 64 bytes) to a process that internal limits in the MPI library have been exceeded. The options here are to increase the number of allowable requests via the MPI_REQUEST_MAX shell variable, or to modify the application.

MPI has run out of request entries; the current allocation level is: MPI_REQUEST_MAX = XXXXX

You might have an application problem. You almost certainly are calling MPI_Isend() or MPI_Irecv() and not completing or freeing your request objects. You need to use MPI_Request_free(), as described in the previous section.

I am not seeing stdout and/or stderr output from my MPI application.

All stdout and stderr is line-buffered, which means that mpirun does not print any partial lines of output. This sometimes causes problems for codes that prompt the user for input parameters but do not end their prompts with a newline character. The only solution for this is to append a newline character to each prompt.

You can set the MPI_UNBUFFERED_STDIO environment variable to disable line-buffering. For more information, see the MPI(1) and mpirun(1) man pages.

How can I get the SGI Message Passing Toolkit (MPT) software to install on my machine?

SGI MPT RPMs are included in the SGI Performance Suite releases. In addition, you can obtain SGI MPT RPMs from the following SGI Support website, under the **Downloads** link:

http://support.sgi.com

Where can I find more information about the SHMEM programming model?

See the intro_shmem(3) man page.

The ps(1) command says my memory use (SIZE) is higher than expected.

At MPI job start-up, MPI calls the SHMEM library to cross-map all user static memory on all MPI processes to provide optimization opportunities. The result is large virtual

memory usage. The ps(1) command's SIZE statistic is telling you the amount of virtual address space being used, not the amount of memory being consumed. Even if all of the pages that you could reference were faulted in, most of the virtual address regions point to multiply-mapped (shared) data regions, and even in that case, actual per-process memory usage would be far lower than that indicated by SIZE.

What does MPI: could not run executable mean?

This message means that something happened while mpirun was trying to launch your application, which caused it to fail before all of the MPI processes were able to handshake with it.

The mpirun command directs arrayd to launch a master process on each host and listens on a socket for those masters to connect back to it. Since the masters are children of arrayd, arrayd traps SIGCHLD and passes that signal back to mpirun whenever one of the masters terminates. If mpirun receives a signal before it has established connections with every host in the job, it knows that something has gone wrong.

How do I combine MPI with insert favorite tool here?

In general, the rule to follow is to run mpirun on your tool and then the tool on your application. Do not try to run the tool on mpirun. Also, because of the way that mpirun sets up stdio, seeing the output from your tool might require a bit of effort. The most ideal case is when the tool directly supports an option to redirect its output to a file. In general, this is the recommended way to mix tools with mpirun. Of course, not all tools (for example, dplace) support such an option. However, it is usually possible to make it work by wrapping a shell script around the tool and having the script do the redirection, as in the following example:

```
> cat myscript
    #!/bin/sh
    setenv MPI_DSM_OFF
    dplace -verbose a.out 2> outfile
    > mpirun -np 4 myscript
    hello world from process 0
    hello world from process 1
    hello world from process 2
    hello world from process 3
```

```
> cat outfile
there are now 1 threads
Setting up policies and initial thread.
Migration is off.
Data placement policy is PlacementDefault.
Creating data PM.
Data pagesize is 16k.
Setting data PM.
Creating stack PM.
Stack pagesize is 16k.
Stack placement policy is PlacementDefault.
Setting stack PM.
there are now 2 threads
there are now 3 threads
there are now 4 threads
there are now 5 threads
```

Why do I see "stack traceback" information when my MPI job aborts?

More information can be found in the MPI(1) man page in descriptions of the MPI_COREDUMP and MPI_COREDUMP_DEBUGGER environment variables.

Array Services

This chapter includes the following topics:

- "About Array Services" on page 83
- "Retrieving the Array Services Release Notes" on page 84
- "Managing Local Processes" on page 85
- "Using Array Services Commands" on page 86
- "Array Services Commands" on page 87
- "Obtaining Information About the Array" on page 90
- "Additional Array Configuration Information" on page 93
- "Configuring Array Commands" on page 99

About Array Services

The SGI Array Services software enables parallel applications to run on multiple hosts in a cluster, or *array*. Array Services provides cluster job launch capabilities for SGI Message Passing Toolkit jobs.

The array can consist of the following:

- Multiple single system images (SSIs) on an SGI UV system
- Multiple compute nodes plus a service node on an SGI ICE or SGI ICE X system
- Multiple physical machines

An array system is bound together with a high-speed network and the Array Services software. Array users can access the system with familiar commands for job control, login and password management, and remote execution. Array Services facilitates global session management, array configuration management, batch processing, message passing, system administration, and performance visualization.

The Array Services software package includes the following:

• An array daemon that runs on each node. The daemon groups logically related processes together across multiple nodes. The process groups create a global process namespace across the array, facilitate accounting, and facilitate administration.

The daemon maintains information about node configuration, process IDs, and process groups. Array daemons on the nodes cooperate with each other.

- An array configuration database. The database describes the array configuration and provides reference information for array daemons and user programs. Each node hosts a copy of the array configuration database.
- Commands, libraries, and utilities such as ainfo(1), arshell(1), and others.

The Message Passing Interface (MPI) of SGI MPI uses Array Services to launch parallel applications.

SGI includes MUNGE software in the SGI MPI software distribution. This optional, open-source product provides secure Array Services functionality. MUNGE allows a process to authenticate the UID and GID of another local or remote process within a group of hosts that have common users and groups. MUNGE authentication, which also includes the Array Services data exchanged in the array, is encrypted. For more information about MUNGE, see the MUNGE website, which is at the following location:

http://munge.googlecode.com/

The Array Services package requires that the process sets service be installed and running. This package is provided in the sgi-procset RPM. You can type the following commands to verify that the process sets service is installed and running:

rpm -q sgi-procset
/etc/init.d/procset status

Retrieving the Array Services Release Notes

The following procedure explains how to find the array services release note information.

Procedure 10-1 To retrieve Array Services release note information

1. Type the following command to retrieve the location of the Array Services release notes:

```
# rpm -qi sgi-arraysvcs
/usr/share/doc/sgi-arraysvcs-3.7/README.relnotes
```

2. Use a text editor or other command to display the file that the rpm(8) command returns.

Managing Local Processes

Each UNIX process has a *process identifier* (PID), a number that identifies that process within the node where it runs. It is important to realize that a PID is local to the node; so it is possible to have processes in different nodes using the same PID numbers.

Within a node, processes can be logically grouped in *process groups*. A process group is composed of a parent process together with all the processes that it creates. Each process group has a *process group identifier* (PGID). Like a PID, a PGID is defined locally to that node, and there is no guarantee of uniqueness across the array.

Monitoring Local Processes and System Usage

You query the status of processes using the system command ps. To generate a full list of all processes on a local system, use a command such as the following:

ps -elfj

You can monitor the activity of processes using the command top for an ASCII display in a terminal window.

Scheduling and Killing Local Processes

You can schedule commands to run at specific times using the at command. You can kill or stop processes using the kill command. To destroy the process with PID 13032, use a command such as the following:

kill -KILL 13032

Summary of Local Process Management Commands

Table 10-1 on page 86 summarizes information about local process management.

Table 10-1 Information Sources: Local Process Management

Торіс	Man Page
Process ID and process group	intro(2)
Listing and monitoring processes	ps(1), top(1)
Running programs at low priority	nice(1), batch(1)
Running programs at a scheduled time	at(1)
Terminating a process	kill(1)

Using Array Services Commands

When an application starts processes on more than one node, the PID and PGID are no longer adequate to manage the application. The Array Services commands enable you to view the entire array and to control the processes on multinode programs.

You can type Array Services commands from any workstation connected to an array system. You do not have to be logged in to an array node. Table 10-2 on page 86 shows the commands that are common to Array Services operations.

Table 10-2 Common Array Services Commands

Торіс	Man Page
Array Services Overview	array_services(5)
ainfo command	ainfo(1)
array command	array(1) or arrayd.conf(4)
arshell command	arshell(1)
newsess command	newsess(1)

About Array Sessions

Array Services is composed of a daemon-a background process that is started at boot time in every node-and a set of commands such as ainfo(1). The commands call on the daemon process in each node to get the information they need.

One concept that is basic to Array Services is the *array session*, which is a term for all the processes of one application, wherever they may execute. Normally, your login shell, with the programs you start from it, constitutes an array session. A batch job is an array session, and you can create a new shell with a new array session identity.

About Names of Arrays and Nodes

Each node is a server, and as such each node has a hostname. An array system as a whole has a name, too. In most installations there is only a single array, and you never need to specify which array you mean. However, it is possible to have multiple arrays available on a network, and you can direct Array Services commands to a specific array.

About Authentication Keys

It is possible for the array administrator to establish an authentication code, which is a 64-bit number, for all or some of the nodes in an array. There can be a single authentication code number for each node. Your system administrator can tell you if this is necessary.

When authentication keys are implemented, you need to specify the authentication key as the argument to the -s option on the command line of each Array Services command. The code applies to any command entered at that node or addressed to that node.

Array Services Commands

The Array Services package includes an array daemon, an array configuration database, and several commands. Some utilities enable you to retrieve information about the array. Other utilities let the administrator query and manipulate distributed array applications. The Array Services commands are as follows:

Command	Purpose
ainfo command	Queries the array configuration database. Retrieves information about processes.
array command	Runs a specified command on one or more nodes. Commands are predefined by the administrator in the configuration database.
arshell command	Starts a command remotely on a different node.
	The arshell command is like rsh in that it runs a command on another machine under the userid of the invoking user. Use of authentication codes makes Array Services somewhat more secure than rsh.

The ainfo(1), array(1), and arshell(1) commands accept a common set of options plus some command-specific options. Table 10-3 on page 88 summarizes the common options. The default values of some options are set by environment variables.

Option	Used In	Description
-a array	ainfo, array	Specify a particular array when more than one is accessible.
-D	ainfo, array, arshell	Send commands to other nodes directly, rather than through arrayd daemon.
– F	ainfo, array, arshell	Forward commands to other nodes through the arrayd daemon.
-Kl number	ainfo, array	Authentication key for the local node. This is a 64-bit number.
-Kr number	ainfo, array	Authentication key for the remote node. This is a 64-bit number.
-1 . This letter is a lowercase letter "L", for "local".	ainfo, array	Execute in context of the destination node, not necessarily the current node.

 Table 10-3 Array Services Command Option Summary

Option	Used In	Description
-l port	ainfo, array, arshell	Nonstandard port number of array daemon.
-s hostname	ainfo, array	Specify a destination node.

Specifying a Single Node

The -1 and -s options work together. The -1 option restricts the scope of a command to the node where the command is executed. This option is a lowercase letter "L", for "local". By default, that is the node where the command is entered. When -1 is not used, the scope of a query command is all nodes of the array. The -s option directs the command to be executed on a specified node of the array. These options work together in query commands as follows:

- To query all nodes as seen by the local node, use neither option.
- To query only the local node, use only -1.
- To query all nodes as seen by a specified node, use only -s.
- To query only a particular node, use both -s and -1.

Common Environment Variables

The Array Services commands depend on environment variables to define default values for the less-common command options. These variables are summarized in Table 10-4.

Variable Name	Use	Default When Undefined
ARRAYD_FORWARD	When defined with a string starting with the letter y , all commands default to forwarding through the array daemon (option $-F$).	Commands default to direct communication (option –D).
ARRAYD_PORT	The port (socket) number monitored by the array daemon on the destination node.	The standard number of 5434, or the number given with option –p.
ARRAYD_LOCALKEY	Authentication key for the local node (option $-K1$).	No authentication unless the -Kl option is used.
ARRAYD_REMOTEKEY	Authentication key for the destination node (option -Kr).	No authentication unless -Kr option is used.
ARRAYD	The destination node, when not specified by the $-s$ option.	The local node, or the node given with -s.

 Table 10-4 Array Services Environment Variables

Obtaining Information About the Array

Any user of an array system can use Array Services commands to check the hardware components and the software workload of the array. The commands needed are ainfo and array.

Learning Array Names

If your network includes more than one array system, you can use ainfo arrays at one array node to list all the array names that are configured, as in the following example.

```
homegrown% ainfo arrays
Arrays known to array services daemon
ARRAY DevArray
IDENT 0x3381
ARRAY BigDevArray
IDENT 0x7456
ARRAY test
```

IDENT 0x655e

Array names are configured into the array database by the administrator. Different arrays might know different sets of other array names.

Learning Node Names

You can use ainfo machines to learn the names and some features of all nodes in the current array, as in the following example.

homegrown 175% **ainfo -b machines** machine homegrown homegrown 5434 192.48.165.36 0 machine disarray disarray 5434 192.48.165.62 0 machine datarray datarray 5434 192.48.165.64 0 machine tokyo tokyo 5434 150.166.39.39 0

In this example, the -b option of ainfo is used to get a concise display.

Learning Node Features

You can use ainfo nodeinfo to request detailed information about one or all nodes in the array. To get information about the local node, use ainfo -l nodeinfo. However, to get information about only a particular other node, for example node tokyo, use -l and -s, as in the following example:

```
homegrown 181% ainfo -s tokyo -l nodeinfo
Node information for server on machine "tokyo"
MACHINE tokyo
   VERSION 1.2
   8 PROCESSOR BOARDS
       BOARD: TYPE 15 SPEED 190
          CPU:
               TYPE 9 REVISION 2.4
           FPU:
               TYPE 9
                        REVISION 0.0
   16 IP INTERFACES HOSTNAME tokyo HOSTID 0xc01a5035
       DEVICE et0
                  NETWORK
                               150.166.39.0 ADDRESS 150.166.39.39 UP
       DEVICE atm0 NETWORK 255.255.255.255 ADDRESS
                                                        0.0.0.0 UP
       DEVICE atm1 NETWORK 255.255.255.255 ADDRESS
                                                            0.0.0.0 UP
. . .
   0 GRAPHICS INTERFACES
```

MEMORY

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10: Array Services

512 MB MAIN MEMORY INTERLEAVE 4

The preceding example has been edited for brevity.

If the -1 option is omitted, the destination node will return information about every node that it knows.

Learning User Names and Workload

The system commands who(1), top(1), and uptime(1) are commonly used to get information about users and workload on one server. The array(1) command offers array-wide equivalents to these commands.

Learning User Names

To get the names of all users logged in to the whole array, use array who. To learn the names of users logged in to a particular node, for example tokyo, use -1 and -s, as in the following example:

homegrown	n 180% array	-s tokyo -l who
joecd	tokyo	frummage.eng.sgi -tcsh
joecd	tokyo	frummage.eng.sgi -tcsh
benf	tokyo	einstein.ued.sgi. /bin/tcsh
yohn	tokyo	rayleigh.eng.sg vi +153 fs/procfs/prd
•••		

The preceding example has been edited for brevity and security.

Learning Workload

Two variants of the array command return workload information. The array-wide equivalent of uptime is array uptime, as follows:

```
homegrown 181% array uptime
homegrown: up 1 day, 7:40, 26 users, load average: 7.21, 6.35, 4.72
disarray: up 2:53, 0 user, load average: 0.00, 0.00, 0.00
datarray: up 5:34, 1 user, load average: 0.00, 0.00, 0.00
tokyo: up 7 days, 9:11, 17 users, load average: 0.15, 0.31, 0.29
homegrown 182% array -1 -s tokyo uptime
tokyo: up 7 days, 9:11, 17 users, load average: 0.12, 0.30, 0.28
```

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The command array top lists the processes that are currently using the most CPU time. The output identifies each process by its internal array session handle (ASH) value. The following is example output:

homegrown 183% arr a	ay top				
ASH	Host	PID	User	%CPU	Command
0x1111ffff0000000	homegrown	5	root	1.20	vfs_sync
0x1111ffff000001e9	homegrown	1327	arraysvcs	1.19	atop
0x1111ffff000001e9	tokyo	19816	arraysvcs	0.73	atop
0x1111ffff000001e9	disarray	1106	arraysvcs	0.47	atop
0x1111ffff000001e9	datarray	1423	arraysvcs	0.42	atop
0x1111ffff0000000	homegrown	20	root	0.41	ShareII
0x1111ffff00000c0	homegrown	29683	kchang	0.37	ld
0x1111ffff000001e	homegrown	1324	root	0.17	arrayd
0x1111ffff0000000	homegrown	229	root	0.14	routed
0x1111ffff0000000	homegrown	19	root	0.09	pdflush
0x1111ffff000001e9	disarray	1105	arraysvcs	0.02	atopm

The -1 and -s options can be used to select data about a single node, as usual.

Additional Array Configuration Information

The system administrator has to initialize the array configuration database, a file that is used by the Array Services daemon in executing almost every ainfo and array command.

Security Considerations for Standard Array Services

The array services daemon, arrayd(1M), runs as root. As with other system services, if it is configured carelessly it is possible for arbitrary and possibly unauthorized user to disrupt or even damage a running system.

By default, most array commands are executed using the user, group, and project ID of either the user that issued the original command, or arraysvcs. When adding new array commands to arrayd.conf, or modifying existing ones, always use the most restrictive IDs possible in order to minimize trouble if a hostile or careless user were to run that command. Avoid adding commands that run with more powerful IDs, such as user root or group sys, than the user. If such commands are necessary,

analyze them carefully to ensure that an arbitrary user would not be granted any more privileges than expected, much the same as one would analyze a setuid program.

In the default array services configuration, the arrayd daemon allows all the local requests to access arrayd but not the remote requests. In order to let the remote requests access the arrayd, the AUTHENTICATION parameter needs to be set to NONE in the /usr/lib/array/arrayd.auth file. By default it is set to NOREMOTE. When the AUTHENTICATION parameter is set to NONE, the arrayd daemon assumes that a remote user will accurately identify itself when making a request. In other words, if a request claims to be coming from user abc, the arrayd daemon assumes that it is in fact from user abc and not somebody spoofing abc. This should be adequate for systems that are behind a network firewall or otherwise protected from hostile attack, and in which all the users inside the firewall are presumed to be non-hostile. On systems for which this is not the case, because they are attached to a public network or because individual machines cannot be trusted, the Array Services AUTHENTICATION parameter should be set to NOREMOTE. When AUTHENTICATION is set to NONE, all requests from remote systems are authenticated using a mechanism that involves private keys that are known only to the super-users on the local and remote systems. Requests originating on systems that do not have these private keys are rejected. For more details, see the section on authentication information in the arrayd.conf(4) man page.

The arrayd daemon does not support mapping user, group or project names between two different namespaces; all members of an array are assumed to share the same namespace for users, groups, and projects. Thus, if systems A and B are members of the same array, username abc on system A is assumed to be the same user as username abc on system B. This is most significant in the case of username root. Authentication should be used if necessary to prevent access to an array by machines using a different namespace.

About the Uses of the Configuration Files

The configuration files are read by the Array Services daemon when it starts. Typically, the daemon starts in each node during the system startup. You can also run the daemon from a command line in order to check the syntax of the configuration files.

The configuration files contain the following data, all of which is needed by ainfo and array:

- The names of array systems, including the current array but also any other arrays on which a user could run an Array Services command. ainfo reports this information.
- The names and types of the nodes in each named array, especially the hostnames that would be used in an Array Services command. ainfo reports this information.
- The authentication keys, if any, that must be used with Array Services commands. The -Kl and -Kr command options use this information. For more information, see "Array Services Commands" on page 87.
- The commands that are valid with the array command.

About Configuration File Format and Contents

A configuration file is a readable text file. The file contains entries of the following four types, which are detailed in later topics.

Array definition	Describes this array and other known arrays, including array names and the node names and types.
Command definition	Specifies the usage and operation of a command that can be invoked through the array command.
Authentication	Specifies authentication numbers that must be used to access the array.
Local option	Options that modify the operation of the other entries or arrayd.

Blank lines, white space, and comment lines beginning with a pound character (#) can be used freely for readability. Entries can be in any order in any of the files read by arrayd.

Besides punctuation, entries are formed with a keyword-based syntax. Keyword recognition is not case-sensitive; however keywords are shown in uppercase in this text and in the man page. The entries are primarily formed from keywords, numbers, and quoted strings, as detailed in the man page arrayd.conf(4).

Loading Configuration Data

The Array Services daemon, arrayd, can take one or more filenames as arguments. It reads them all, and treats them like logical continuations. In effect, it concatenates them. If no filenames are specified, it reads /usr/lib/array/arrayd.conf and /usr/lib/array/arrayd.auth. A different set of files, and any other arrayd command-line options, can be written into the file /etc/config/arrayd.options, which is read by the startup script that launches arrayd at boot time.

Since configuration data can be stored in two or more files, you can combine different strategies, for example:

- One file can have different access permissions than another. Typically, /usr/lib/array/arrayd.conf is world-readable and contains the available array commands, while /usr/lib/array/arrayd.auth is readable only by root and contains authentication codes.
- One node can have different configuration data than another. For example, certain commands might be defined only in certain nodes; or only the nodes used for interactive logins might know the names of all other nodes.
- You can use NFS-mounted configuration files. You could put a small configuration file on each machine to define the array and authentication keys, but you could have a larger file defining array commands that is NFS-mounted from one node.

After you modify the configuration files, you can make arrayd reload them by killing the daemon and restarting it in each machine. The script /etc/init.d/array supports this operation:

To kill daemon, execute this command:

/etc/init.d/array stop

To kill and restart the daemon in one operation; perform the following command:

/etc/init.d/array restart

The Array Services daemon in any node knows only the information in the configuration files available in that node. This can be an advantage, in that you can limit the use of particular nodes; but it does require that you take pains to keep common information synchronized. "Designing New Array Commands" on page 104 summarizes an automated way to do this.

About Substitution Syntax

The arrayd.conf(4) man page explains the syntax rules for forming entries in the configuration files. An important feature of this syntax is the use of several kinds of text substitution, by which variable text is substituted into entries when they are executed.

Most of the supported substitutions are used in command entries. These substitutions are performed dynamically, each time the array command invokes a subcommand. At that time, substitutions insert values that are unique to the invocation of that subcommand. For example, the value <code>%USER</code> inserts the user ID of the user who is invoking the array command. Such a substitution has no meaning except during execution of a command.

Substitutions in other configuration entries are performed only once, at the time the configuration file is read by arrayd. Only environment variable substitution makes sense in these entries. The environment variable values that are substituted are the values inherited by arrayd from the script that invokes it, which is /etc/init.d/array.

Testing Configuration Changes

The configuration files contain many sections and options. The Array Services command ascheck performs a basic sanity check of all configuration files in the array.

After making a change, you can test an individual configuration file for correct syntax by executing arrayd as a command with the -c and -f options. For example, suppose you have just added a new command definition to /usr/lib/array/arrayd.local. You can check its syntax with the following command:

arrayd -c -f /usr/lib/array/arrayd.local

When testing new commands for correct operation, you need to see the warning and error messages produced by arrayd and processes that it may spawn. The stderr messages from a daemon are not normally visible. You can make them visible by the following procedure:

1. On one node, kill the daemon, as follows:

/etc/init.d/array stop

2. In one shell window on that node, start arrayd with the options -n -v, as follows:

/usr/sbin/arrayd -n -v

Instead of moving into the background, it remains attached to the shell terminal.

Note: Although arrayd becomes functional in this mode, it does not refer to /etc/config/arrayd.options, so you need to specify explicitly all command-line options, such as the names of nonstandard configuration files.

- 3. From another shell window on the same or other nodes, issue ainfo and array commands to test the new configuration data. Diagnostic output appears in the arrayd shell window.
- 4. Terminate arrayd and use the following command to restart it as a daemon:
 - # /usr/sbin/arrayd -v

During steps 1, 2, and 4, the test node might not respond to ainfo and array commands, so warn users that the array is in test mode.

Specifying Arrayname and Machine Names

The following lines are a simple example of an array definition within an arrayd.conf file:

array simple machine congo machine niger machine nile

The array name simple is the value the user must specify in the -a option. For more information, see "Array Services Commands" on page 87.

One array name should be specified in a DESTINATION ARRAY local option as the default array and reported by ainfo dflt. Local options are listed under "Configuring Local Options" on page 103.

Specifying IP Addresses and Ports

The simple machine subentries shown in the example are based on the assumption that the hostname is the same as the machine's name to domain name services (DNS).

If a machine's IP address cannot be obtained from the given hostname, provide a hostname subentry to specify either a fully qualified domain name (FQDN) or an IP address, as follows:

```
array simple

machine congo

hostname congo.engr.hitech.com

port 8820

machine niger

hostname niger.engr.hitech.com

machine nile

hostname "198.206.32.85"
```

The preceding example shows how to use the port subentry to specify that arrayd in a particular machine uses a different socket number than the default of 5434.

Specifying Additional Attributes

If you want the ainfo command to display certain strings, you can insert these values as subentries to the array entry. The following are some examples of attributes:

```
array simple
    array_attribute config_date="04/03/96"
    machine a_node
    machine_attribute aka="congo"
    hostname congo.engr.hitech.com
```

Tip: You can write code that fetches any array name, machine name, or attribute string from any node in the array.

Configuring Array Commands

The user can invoke arbitrary system commands on single nodes using the arshell command. The user can also launch MPI programs that automatically distribute over multiple nodes. However, the only way to launch coordinated system programs on all nodes at once is to use the array command. This command does not accept any system command; it only permits execution of commands that the administrator has configured into the Array Services database.

You can define any set of commands that your users need. You have complete control over how any single array node executes a command. For example, the definition can be different in different nodes. A command can simply invoke a standard system command, or, since you can define a command as invoking a script, you can make a command arbitrarily complex.

Operation of Array Commands

When a user invokes the array command, the subcommand and its arguments are processed by the destination node specified by -s. Unless the -l option was given, that daemon also distributes the subcommand and its arguments to all other array nodes that it knows about. Remember that the destination node might be configured with only a subset of nodes. At each node, arrayd searches the configuration database for a COMMAND entry with the same name as the array subcommand.

In the following example, the subcommand uptime is processed by arrayd in node tokyo:

array -s tokyo uptime

When arrayd finds the subcommand valid, it distributes it to every node that is configured in the default array at node tokyo.

The COMMAND entry for uptime is distributed in this form. You can read it in the file /usr/lib/array/arrayd.conf.

The INVOKE subentry tells arrayd how to execute this command. In this case, it executes a shell script /usr/lib/array/auptime, passing it one argument, the name of the local node. This command is executed at every node, with %LOCAL replaced by that node's name.

Summary of Command Definition Syntax

Look at the basic set of commands distributed with Array Services. This command set resides in /usr/lib/array/arrayd.conf. Each COMMAND entry is defined using the subentries shown in Table 10-5, which the arrayd.conf(4) man page also describes.

Table 10-5 Subentries of	a COMMAND Definition
--------------------------	----------------------

Keyword	Meaning of Following Values
COMMAND	The name of the command as the user gives it to array.
INVOKE	A system command to be executed on every node. The argument values can be literals, or arguments given by the user, or other substitution values.
MERGE	A system command to be executed only on the distributing node, to gather the streams of output from all nodes and combine them into a single stream.
USER	The user ID under which the INVOKE and MERGE commands run. Usually given as USER %USER, so as to run as the user who invoked array.
GROUP	The group name under which the INVOKE and MERGE commands run. Usually given as GROUP %GROUP, so as to run in the group of the user who invoked array. For more information, see the groups(1) man page.
PROJECT	The project under which the INVOKE and MERGE commands run. Usually given as PROJECT %PROJECT, so as to run in the project of the user who invoked array. For more information, see the projects(5) man page.
OPTIONS	A variety of options to modify this command. For more information, see Table 10-7.

The system commands called by INVOKE and MERGE must be specified as full pathnames because arrayd has no defined execution path. As with a shell script, these system commands are often composed from a few literal values and many substitution strings. The substitutions that are supported, all of which are documented in detail in the arrayd.conf(4) man page, are summarized in Table 10-6.

Substitution	Replacement Value
<pre>%1%9; %ARG(n); %ALLARGS; %OPTARG(n)</pre>	Argument tokens from the user's subcommand. <i>*OPTARG</i> does not produce an error message if the specified argument is omitted.
%USER, %GROUP, %PROJECT	The effective user ID, effective group ID, and project of the user who invoked array.
%REALUSER, %REALGROUP	The real user ID and real group ID of the user who invoked array.
%ASH	The internal array session handle (ASH) number under which the INVOKE or MERGE command is to run.
%PID(ash)	List of PID values for a specified ASH. %PID(%ASH) is a common use.
%ARRAY	The array name, either default or as given in the $-a$ option.
%LOCAL	The hostname of the executing node.
%ORIGIN	The full domain name of the node where the array command ran and the output is to be viewed.
%OUTFILE	List of names of temporary files, each containing the output from one node's INVOKE command. Valid only in the MERGE subentry.

Table 10-6 Substitutions Used in a <code>COMMAND</code> Definition

The ${\tt OPTIONS}$ subentry permits a number of important modifications of the command execution. Table 10-7 summarizes these.

 Table 10-7 Options of the COMMAND Definition

Keyword	Effect on Command
LOCAL	Do not distribute to other nodes. Effectively forces the -l option.
NEWSESSION	Execute the INVOKE command under a newly created ASH. %ASH in the INVOKE line is the new ASH. The MERGE command runs under the original ASH, and %ASH substitutes as the old ASH in that line.

Keyword	Effect on Command
SETRUID	Set both the real and effective user ID from the USER subentry. Typically, USER only sets the effective UID.
SETRGID	Set both the real and effective group ID from the GROUP subentry. Typically, GROUP sets only the effective GID.
QUIET	Discard the output of INVOKE, unless a MERGE subentry is given. If a MERGE subentry is given, pass INVOKE output to MERGE as usual, and discard the MERGE output.
NOWAIT	Discard the output and return as soon as the processes are invoked. Do not wait for completion. A MERGE subentry is ineffective.

Configuring Local Options

The ${\tt LOCAL}$ entry specifies options to ${\tt arrayd}$ itself. The most important options are summarized in Table 10-8.

Table 10-8 Subentries of the <code>LOCAL</code> Entry

Subentry	Purpose
DIR	Pathname for the arrayd working directory, which is the initial, current working directory of INVOKE and MERGE commands. The default is /usr/lib/array.
DESTINATION ARRAY	Name of the default array, used when the user omits the –a option. When only one ARRAY entry is given, it is the default destination.
USER, GROUP, PROJECT	Default values for COMMAND execution when USER, GROUP, or PROJECT are omitted from the COMMAND definition.
HOSTNAME	Value returned in this node by %LOCAL. Default is the hostname.
PORT	Socket to be used by arrayd.

If you do not supply LOCAL USER, GROUP, and PROJECT values, the default values for USER and GROUP are arraysvcs.

The HOSTNAME entry is needed whenever the hostname command does not return a node name as specified in the ARRAY MACHINE entry. In order to supply a LOCAL HOSTNAME entry unique to each node, each node needs an individualized copy of at least one configuration file.

Designing New Array Commands

A basic set of commands is distributed in the file

/usr/lib/array/arrayd.conf.template. You should examine this file carefully before defining commands of your own. You can define new commands which then become available to the users of the array system.

Typically, a new command will be defined with an INVOKE subentry that names a script written in sh, csh, or Perl syntax. You use the substitution values to set up arguments to the script. You use the USER, GROUP, PROJECT, and OPTIONS subentries to establish the execution conditions of the script.

Within the invoked script, you can write any amount of logic to verify and validate the arguments and to execute any sequence of commands. For an example of a script in Perl, see /usr/lib/array/aps, which is invoked by the array ps command.

Note: Perl is a particularly interesting choice for array commands, since Perl has native support for socket I/O. In principle at least, you could build a distributed application in Perl in which multiple instances are launched by array and coordinate and exchange data using sockets. Performance would not rival the highly tuned MPI libraries, but development would be simpler.

The administrator has need for distributed applications as well, since the configuration files are distributed over the array. Here is an example of a distributed command to reinitialize the Array Services database on all nodes at once. The script to be executed at each node, called /usr/lib/array/arrayd-reinit would read as follows:

```
#!/bin/sh
# Script to reinitialize arrayd with a new configuration file
# Usage: arrayd-reinit <hostname:new-config-file>
sleep 10  # Let old arrayd finish distributing
rcp $1 /usr/lib/array/
/etc/init.d/array restart
```

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exit O

The script uses rcp to copy a specified file, presumably a configuration file such as arrayd.conf, into /usr/lib/array. This fails if %USER is not privileged. Then the script restarts arrayd to reread configuration files.

The command definition is as follows:

```
command reinit
invoke /usr/lib/array/arrayd-reinit %ORIGIN:%1
user %USER
group %GROUP
options nowait # Exit before restart occurs!
```

The INVOKE subentry calls the restart script shown above. The NOWAIT option prevents the daemon's waiting for the script to finish because the script kills the daemon.

Guidelines for Using SGI MPT on a Virtual Machine Within an SGI UV Computer System

This appendix section includes the following topics:

- "About SGI MPT on a Virtual Machine" on page 107
- "Installing Software Within the Virtual Machine (VM)" on page 108
- "Adjusting SGI UV Virtual Machine System Settings" on page 108
- "Running SGI MPI Programs From Within a Virtual Machine (VM)" on page 110

About SGI MPT on a Virtual Machine

You can configure a virtual machine (VM) on an SGI UV system. The VM creates a general-purpose computer, and MPT can run on that computer. When you use SGI MPT from within a VM, however, you can expect differences in the computing environment and differences with regard to your application's behavior.

For information about how to configure a VM on an SGI system, see the documentation for Red Hat Enterprise Linux (RHEL) or for SUSE Linux Enterprise Server (SLES).

If you are an administrator, use the information in the following topics to configure the VM environment appropriately:

- "Installing Software Within the Virtual Machine (VM)" on page 108
- "Adjusting SGI UV Virtual Machine System Settings" on page 108

If you are an application developer, use the information in the following topic to understand how your program might behave differently when running from within a VM:

• "Running SGI MPI Programs From Within a Virtual Machine (VM)" on page 110

Installing Software Within the Virtual Machine (VM)

The following procedure explains the software that you need to install in the VM in order for MPI programs to run on the VM.

Procedure A-1 To install the software for MPI programs

1. Install and configure the operating system (RHEL or SLES) and the SGI Foundation Software on the SGI UV computer.

For installation information, see the SGI UV System Software Installation and Configuration Guide.

2. Install and configure the VM according to your operating system vendor's instructions.

Note that RHEL and SLES do not support InfiniBand technology from within a VM. Other OFED providers support InfiniBand technology from within a VM through single-root I/O virtualization (SR-IOV), but SGI does not support SR-IOV or other alternatives to the distribution-supplied OFED.

3. (Optional) Install the SGI Foundation Software into the VM.

For installation information, see the SGI UV System Software Installation and Configuration Guide.

4. Install the SGI Performance Suite software into the VM.

For installation information, see the SGI Performance Suite release notes.

5. Install SGI MPT into the VM.

For installation information, see Chapter 2, "Getting Started" on page 27.

Adjusting SGI UV Virtual Machine System Settings

For best performance, SGI recommends to change certain operating system settings after the software installation is complete.

The following procedure explains how to adjust the number of files that can be open at a given time.

Procedure A-2 To adjust system settings

1. Log into the SGI UV system as the root user.

2. Type cpumap command to retrieve the number of cores on the SGI UV computer.

For example:

# cpumap							
This is an SGI UV							
model name	: Genuine Intel(R)	CPU @ 2	.60GHz				
Architecture	: x86_64						
cpu MHz	: 2600.072						
cache size	: 20480 KB (Last L	B (Last Level)					
Total Number of Socke	ets	: 16					
Total Number of Cores		: 128	(8 per	socket	t)		
Hyperthreading		: ON					
Total Number of Physical Processors		: 128					
Total Number of Logical Processors		: 256	(2 per	Phys I	Processor)		
UV Information							
HUB Version:		UVHub	3.0				
Number of Hubs:		16					
Number of connected Hubs:		16					
Number of connected	NUMAlink ports:	128					

The Total Number of Cores line reveals that there are 128 cores, 8 per socket.

3. Display the contents of the /etc/sysctl-conf file.

For example, type the following command:

less /etc/sysctl.conf
...
fs.file-max = 8204481
...

4. (Conditional) Use a text editor to open file sysctl.conf and increase the value of the fs.file-max parameter in the /etc/sysctl.conf file.

Perform this step if the number of cores on your computer is greater than 512 and the fs.file-max parameter is set to less than 10,000,000.

For optimum performance within a VM, set the fs.file-max parameter that is at least 10000000 on SGI UV systems with 512 cores or more.

Running SGI MPI Programs From Within a Virtual Machine (VM)

The following list explains some of the differences between running an MPI or SHMEM program on native SGI hardware versus running an MPI or SHMEM program from within a VM hosted by an SGI UV system:

• Hardware-dependent features might not exist on a VM.

When you run an MPI program on a VM, the environment detects the virtual nature of the platform and ignores any SGI hardware-specific features. The following hardware features are not available to an application that runs in a VM: NUMAlink, Superpages, the SGI UV timer, the HUB ASIC, hardware performance counters, and global reference units (GRUs). In addition, processor-specific performance diagnostics are limited.

If your application uses hardware technologies that are not specific to SGI systems, you can expect that the VM can honor those non-specific technologies.

Topology characteristics might be different.

An application that relies on the topology of an SGI system needs to be run on a VM that was configured with topology that mimics the SGI computer system. MPI programs do not automatically use special topology characteristics effectively. If the application requires special heuristics for locality and placement, you need to configure that into the VM.

• XPMEM libraries are beneficial in very large VMs.

SGI has tested XPMEM on VMs. XPMEM loads, and your application can call XPMEM routines successfully. However, XPMEM is useful only on systems with very large memory.

• No InfiniBand support.

The RHEL and SLES operating systems do not support InfiniBand technology in VMs. Consult your system administrator to find out if single-root I/O virtualization (SR-IOV) is configured on the VM.

Configuring Array Services Manually

This appendix contains the following topics:

- "About Configuring Array Services Manually" on page 111
- "Configuring Array Services on Multiple Partitions or Hosts" on page 111

About Configuring Array Services Manually

The SGI MPT configuration procedures explain how to configure Array Services in an automated way on SGI UV partitioned systems and on SGI ICE X systems. The information in this appendix section explains how to configure Array Services in a manual way, which allows you to make customizations if necessary.

Configuring Array Services on Multiple Partitions or Hosts

The following procedure explains how to configure Array Services to run on multiple hosts, such as exist on an SGI UV partitioned system or an SGI ICE X system.

Procedure B-1 To configure Array Services for multiple hosts

1. Log in as root on one of the hosts you want to include in the array.

You must be logged in as an administrator to perform this procedure.

For example, on an SGI ICE X system, log into one of the service nodes. You can include service nodes and compute nodes in the array.

2. (Optional) Install the MUNGE package from the SGI MPI software distribution.

The optional MUNGE software package enables additional security for Array Services operations.

During MUNGE installation, make sure of the following:

• The MUNGE key that is used is the same across all the nodes in the array.

The MUNGE key resides in /etc/munge/munge.key.

• You configure a good time clock source, such as an NTP server. MUNGE depends on time synchronization across all nodes in the array.

To install MUNGE, use one of the following commands:

- On Red Hat Enterprise Linux platforms: yum install munge
- On SUSE Linux Enterprise Server platforms: zypper install munge

For more information about how to install MUNGE, see the SGI MPI release notes.

- 3. Open file /usr/lib/array/arrayd.conf with a text editor.
- 4. Edit the /usr/lib/array/arrayd.conf file to list the machines in your cluster.

This file enables you to configure many characteristics of an array services environment. The required specifications are as follows:

- The array name.
- The hostnames of the array participants.
- A default destination array.

For more information about the additional characteristics that you can specify in the arrayd.conf file, see the arrayd.conf(4) man page.

For an example arrayd.conf file, see file /usr/lib/array/arrayd.conf.template.

Example 1. The following lines specify an array name (sgicluster) and two hostnames. Specify each hostname on its own line. array and machine are keywords in the file.

```
array sgicluster
machine host1
machine host2
```

Example 2. The following line sets a default array name.

destination array sgicluster

- 5. Save and close file /usr/lib/array/arrayd.conf.
- 6. Use a text editor to open file /usr/lib/array/arrayd.auth.

- 7. Search for the string AUTHENTICATION NOREMOTE, and insert a # character in column 1 to comment out the line.
- 8. Enable the security level under which you want Array Services to operate.

This step specifies the authentication mechanism to use when Array Services messages pass between the Array Services daemons. Possible security levels are NONE, SIMPLE, or MUNGE, as follows:

- If no authentication is required, remove the # character from column 1 of the AUTHENTICATION NONE line.
- To enable simple authentication, ensure that there is no # in column 1 of the AUTHENTICATION SIMPLE line. This is the default.
- To enable authentication through MUNGE, remove the # character from column 1 of the AUTHENTICATION MUNGE line.

Make sure that MUNGE has been installed, as prescribed earlier in this procedure.

For information about the authentication methods, see the arrayd.auth(4) man page.

- 9. Save and close file /usr/lib/array/arrayd.auth.
- 10. (Optional) Reset the default user account or the default array port.

By default, the Array Services installation and configuration process sets the following defaults in the /usr/lib/array/arrayd.conf configuration file:

• A default user account of arraysvcs.

Array Services requires that a user account exist on all hosts in the array for the purpose of running certain Array Services commands. If you create a different account, make sure to update the arrayd.conf file and set the user account permissions correctly on all hosts.

• A default port number of 5434.

The /etc/services file contains a line that defines the arrayd service and port number as follows:

sgi-arrayd 5434/tcp # SGI Array Services daemon

You can set any value for the port number, but all systems mentioned in the arrayd.conf file must use the same value.

11. Type the following comand to restart Array Services:

/etc/init.d/array restart

12. Repeat the preceding steps on the other hosts or copy the /usr/lib/array/arrayd.conf and /usr/lib/array/arrayd.auth files to the other hosts.

The Array Services feature requires that the configuration files on each participant host include the list of host participants and the authentication method. The files can contain additional, host-specific information.

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