# sgi

Message Passing Toolkit (MPT) User Guide

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## **New Features in This Manual**

Information about the Array Services is now included in this manual. The MUNGE authentication service has been added to Array Services, and references to Secure Array Services have been removed. The MUNGE authentication service creates and validates credentials, and it scales for use in a high-performance cluster environment.

## **Record of Revision**

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| 001     | March 2004<br>Original Printing. This manual documents the Message Passing<br>Toolkit implementation of the Message Passing Interface (MPI). |
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## **About This Manual**

This publication describes the SGI<sup>®</sup> implementation of the Message Passing Interface (MPI) 2.09.

MPI consists of a library, which contains both normal and profiling entry points, and commands that support the MPI interface. MPI is a component of the SGI Message Passing Toolkit (MPT).

MPT is a software package that supports parallel programming on large systems and clusters of computer systems through a technique known as *message passing*. Systems running MPI applications must also be running Array Services software version 3.7 or later. This manual includes information about Array Services.

## **Related Publications and 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 MPI Standard, which is documented online at the following website:

http://www.mcs.anl.gov/mpi

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

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

- 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

• The comp.parallel.mpi newsgroup.

The MPInside Reference Guide describes the SGI MPInside MPI profiling tool.

## **Obtaining Publications**

You can obtain SGI documentation in the following ways:

• See the SGI Technical Publications Library at the following website:

http://docs.sgi.com

Manuals in various formats are available. This library contains the most recent and most comprehensive set of online books, release notes, man pages, and other information.

• You can also view man pages by typing man *title* on a command line.

## 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<br>user enters in interactive sessions. (Output is shown in<br>nonbold, fixed-space font.) |
| []         | Brackets enclose optional portions of a command or directive line.  |

...

Ellipses indicate that a preceding element can be repeated.

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## Introduction

Message Passing Toolkit (MPT) is a software package that supports interprocess data exchange for applications that use concurrent, cooperating processes on a single host or on multiple hosts. Data exchange is done through message passing, which is the use of library calls to request data delivery from one process to another or between groups of processes.

The MPT package contains the following components and the appropriate accompanying documentation:

- Message Passing Interface (MPI). MPI is a standard specification for a message passing interface, allowing portable message passing programs in Fortran and C languages. MPI is the dominant programming model on large scale HPC systems and clusters today. MPT supports version 2.2 of the MPI standard specification.
- The SHMEM<sup>™</sup> programming model. SHMEM 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. The SGI SHMEM programming model is the basis for the OpenSHMEM<sup>™</sup> programming model specification which is being developed by the Open Source Software Solutions multi-vendor working group.

SGI MPT is highly optimized for all SGI hardware platforms. The *SGI Performance Suite 1.x Start Here* lists all current SGI software and hardware manuals and can be found on the SGI Technical Publications Library at the following website:

#### http://docs.sgi.com

This chapter provides an overview of the MPI software that is included in the toolkit. It includes descriptions of the MPI standard compliance, the basic components of MPI, and the basic features of MPI. Subsequent chapters address the following topics:

- Chapter 2, "Installing and Configuring the Message Passing Toolkit (MPT)" on page 5
- Chapter 3, "Getting Started" on page 19
- Chapter 4, "Programming with SGI MPI" on page 31
- Chapter 5, "Debugging MPI Applications" on page 41
- Chapter 6, "PerfBoost" on page 45

- Chapter 7, "Berkeley Lab Checkpoint/Restart " on page 47
- Chapter 8, "Run-time Tuning" on page 49
- Chapter 9, "MPI Performance Profiling" on page 63
- Chapter 10, "Troubleshooting and Frequently Asked Questions" on page 73
- Chapter 11, "Array Services" on page 79

#### **MPI** Overview

MPI was created by the Message Passing Interface Forum (MPIF). MPIF is not sanctioned or supported by any official standards organization. Its goal was to develop a widely used standard for writing message passing programs.

SGI supports implementations of MPI that are released as part of the Message Passing Toolkit. The MPI standard is documented online at the following website:

http://www.mcs.anl.gov/mpi

#### **MPI 2.2 Standard Compliance**

The SGI MPI implementation complies with the MPI 2.2 standard.

#### **MPI** Components

The MPI library is provided as a dynamic shared object (DSO). A DSO is a file that ends in .so. The basic components that are necessary for using MPI are the libmpi.so library, the include files, and the mpirun command.

SGI includes profiling support in the libmpi.so library. Profiling support replaces all MPI\_Xxx prototypes and function names with PMPI\_Xxx entry points.

#### **SGI MPI Features**

The SGI MPI implementation offers a number of 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
- Multi-rail InfiniBand support, which takes full advantage of the multiple InfiniBand fabrics available on SGI<sup>®</sup> ICE<sup>™</sup> systems
- Use of hardware fetch operations (fetchops), where available, for fast synchronization and lower latency for short messages
- Optimized MPI-2 one-sided commands
- Interoperability with the SHMEM (LIBSMA) programming model
- High-performance communication support for partitioned systems

## Installing and Configuring the Message Passing Toolkit (MPT)

This chapter explains how to install the MPT software and how to configure your system to use it effectively. The information in this chapter also appears on your system in the MPT directory. To access the information online, change to the following directory:

/opt/sgi/mpt/mpt-*mpt\_rel*/doc/README.relnotes

For *mpt\_rel*, specify the MPT release number. For example, 2.09.

This chapter includes the following topics:

- "Verifying Prerequisites" on page 5
- "Installing and Configuring MPT" on page 6
- "(Conditional) Enabling MPT for Cluster Environments for Alternate-location Installations" on page 10
- "(Conditional) Resetting Environment Variables for Alternate-location Installations" on page 11
- "Configuring Array Services" on page 13
- "Restarting Services or Rebooting" on page 14
- "(Conditional) Adjusting File Descriptor Limits" on page 14
- "Adjusting the Resource Limit for Locked Memory" on page 16
- "(Conditional) Enabling Cross-partition NUMAlink MPI Communication" on page 17
- "Configuring OFED for MPT" on page 13

## **Verifying Prerequisites**

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

**Procedure 2-1** To verify prerequisites

1. Verify that you have 25 Mbytes of free disk space in the installation directory.

If you want to install the MPT software into the default installation directory, make sure there are 25 Mbytes of free space in /opt/sgi/mpt.

- 2. Verify that you have the following software installed and configured:
  - Red Hat Enterprise Linux (RHEL) 6.2, RHEL 6.3, or SUSE Linux Enterprise Server (SLES) 11 SP2.
  - OpenFabrics Enterprise Distribution (OFED) software. The operating system packages include OFED by default. To verify the OFED installation status, type one of the following commands:
    - On SLES 11 platforms, type the following:
      - # zypper info ---t pattern ofed
    - On RHEL 6 platforms, type the following:
      - # yum grouplist "Infiniband Support"
- 3. Proceed to the following:

"Installing and Configuring MPT" on page 6

## Installing and Configuring MPT

SGI distributes the MPT software as an RPM module. You can install the RPM itself, or you can use a .cpio file to install the RPM. In addition, you need to decide if you want to install the MPT software in the default location or if you want to install in a custom location.

Use one of the following procedures to install and configure the MPT software:

- "Installing the MPT RPM into the Default Location" on page 7
- "Installing the MPT RPM into an Alternate Location" on page 7
- "Using a .cpio File to Install the RPM into the Default Location or into an Alternate Location" on page 8

#### Installing the MPT RPM into the Default Location

The following procedure explains how to install the MPT RPM into its default location, which is /opt/sgi/mpt.

Procedure 2-2 To install the RPM into the default location

- 1. As the root user, log into the computer upon which you want to install the MPT software.
- 2. Type the following command:

# rpm -Uvh sgi-mpt-mpt\_rel-sgilrp\_rel.x86\_64.rpm

The variables in the preceding command are as follows:

- For *mpt\_rel*, type the release level of the MPT software that you want to install.
- For *lrp\_rel*, type the release level of the SGI Linux release product that includes the MPT software.

For example, to install the MPT 2.09 release, type the following command:

# rpm -Uvh sgi-mpt-2.09-sgi708.x86\_64.rpm

3. Proceed to:

"Configuring Array Services" on page 13

#### Installing the MPT RPM into an Alternate Location

You can install the MPT RPM in an alternate location. If you install the MPT RPM into an alternate directory, users need to reset certain environment variables after the installation. The installation procedure guides you to "(Conditional) Resetting Environment Variables for Alternate-location Installations" on page 11 in a later step.

The following procedure explains how to install the MPT RPM into an alternate location.

Procedure 2-3 To install the RPM into an alternate location

1. As the root user, log into the computer upon which you want to install MPT.

2. Type the following command:

```
# rpm -i --relocate /opt/sgi/mpt/mpt-mpt_rel=/path \
    --excludepath /usr sgi-mpt-mpt_rel-sgilrp_rel.x86_64.rpm
```

**Note:** The preceding command uses the  $\$  character to signify a line break. Type this command all on one line before you press Enter.

The variables in the preceding command are as follows:

- For mpt\_rel, type the release level of the MPT software that you want to install.
- For *path*, type the path to your alternate directory.
- For *lrp\_rel*, type the release level of the SGI Linux release product that includes the MPT software.

For example, to install the MPT 2.09 release into the /tmp directory, type the following command:

# rpm -i --relocate /opt/sgi/mpt/mpt-2.09=/tmp \
--excludepath /usr sgi-mpt-2.09-sgi708.x86\_64.rpm

- 3. Proceed to one of the following:
  - "(Conditional) Enabling MPT for Cluster Environments for Alternate-location Installations" on page 10
  - "Configuring Array Services" on page 13

#### Using a .cpio File to Install the RPM into the Default Location or into an Alternate Location

The procedure in this topic explains how to use a .cpio file to install the MPT software into the default location or into an NFS file system that is shared by a number of hosts. In this case, it is not important or desirable for the RPM database on only one of the machines to track the versions of MPT that are installed. You do not need root permission to install the MPT software if you use a .cpio file.

The following procedure explains how to use a .cpio file to install the MPT software.

Procedure 2-4 To use a .cpio file to install the MPT RPM

1. As the root user, log into the computer upon which you want to install MPT.

2. Use the cd command to change to the installation directory.

You can install the software in any directory to which you have write permission. The default installation directory is /opt/sgi/mpt.

If you install the MPT software into an alternate directory, you need to reset your environment variables later in the installation procedure. The installation procedure guides you to "(Conditional) Resetting Environment Variables for Alternate-location Installations" on page 11 in a later step.

3. Type the following command to install the MPT software:

rpm2cpio -sgi-mpt-mpt\_rel-\*.rpm | cpio -idcmv

For *mpt\_rel*, type the release version of MPT. For example, 2.09.

For example:

```
% rpm2cpio -sgi-mpt-2.09-*.rpm | cpio -idcmv
opt/sgi/mpt/mpt-2.09/bin/mpirun
opt/sgi/mpt/mpt-2.09/include/mpi++.h
opt/sgi/mpt/mpt-2.09/include/mpi.h
...
opt/sgi/mpt/mpt-2.09/lib/libmpi++.so
opt/sgi/mpt/mpt-2.09/lib/libmpi.so
opt/sgi/mpt/mpt-2.09/lib/libmpi.so
...
```

4. List the files in the installation directory to confirm the installation.

For example:

```
% ls -R /tmp/opt/sgi/mpt/mpt-2.09
bin doc include lib man
/tmp/opt/sgi/mpt/mpt-2.09/bin:
mpirun
/tmp/opt/sgi/mpt/mpt-2.09/include:
MPI.mod mpi.h mpi_ext.h mpif.h mpio.h mpp
mpi++.h mpi.mod mpi_extf.h mpif_parameters.h mpiof.h
/tmp/opt/sgi/mpt/mpt-2.09/lib:
```

2: Installing and Configuring the Message Passing Toolkit (MPT)

- 5. Proceed to one of the following:
  - If you installed MPT in a nondefault location in a cluster environment, proceed to the following:

"(Conditional) Enabling MPT for Cluster Environments for Alternate-location Installations" on page 10

• If you installed MPT in a nondefault location, but not in a cluster environment, proceed to the following:

"(Conditional) Resetting Environment Variables for Alternate-location Installations" on page 11

• If you installed MPT in the default location, proceed to the following:

"Configuring Array Services" on page 13

## (Conditional) Enabling MPT for Cluster Environments for Alternate-location Installations

Perform this procedure if you installed MPT in an alternate location and you have MPT jobs that you need to run in a cluster environment.

The procedure in this topic explains how to copy all the MPT software modules to an NFS-mounted file system. This procedure enables the cluster nodes to access all the MPT software.

**Procedure 2-5** To enable MPT in cluster environments if MPT was installed in an alternate location

- 1. As the root user, log into the computer upon which you installed the MPT software.
- 2. Type the following command to create a tar file of the MPT software modules:
  - % tar cf /path/mpt.mpt\_rel.tar /opt/sgi/mpt/mpt-mpt\_rel

For *path*, type the path to your alternate directory.

For *mpt\_rel*, type the release level of the MPT software that you want to install.

3. Type the following command to copy the MPT software to the NFS file system:

% cp /path/mpt.mpt\_rel.tar /nfs\_dir

The variables in the preceding command are as follows:

- For *path*, type the path to your alternate directory.
- For *mpt\_rel*, type the release level of the MPT software.
- For *nfs\_dir*, type the NFS-mounted directory that the cluster-aware programs can access.
- 4. Use the cd(1) command to change to the NFS-mounted directory.

For example:

```
% cd /data/nfs
```

- 5. Type the following command to expand the file:
  - % tar xf mpt.mpt\_rel.tar

For *mpt\_rel*, type the release level of the MPT software.

6. Proceed to the following:

"(Conditional) Resetting Environment Variables for Alternate-location Installations" on page 11

## (Conditional) Resetting Environment Variables for Alternate-location Installations

Perform the procedure in this topic if you installed the MPT software into an alternate location.

The mpirun command assumes that the PATH and LD\_LIBRARY\_PATH environment variables are configured for the default MPT installation directory. The compilers, linkers, and loaders all use the values in these environment variables.

You can use the procedure in this topic to reset the environment variables either on the command line or in environment modules. For more information about environment modules, see "Running MPI Jobs" on page 19. Procedure 2-6 To reset environment variables — Method 1, using commands

- 1. Open the configuration file appropriate to your shell, and change the following variables:
  - For the tcsh shell, the commands are as follows:

```
setenv PATH /path/bin:${PATH}
setenv LD_LIBRARY_PATH /path/lib
```

For example:

setenv PATH /tmp/bin:\${PATH}
setenv LD\_LIBRARY\_PATH /tmp/lib

• For the bash shell, the commands are as follows:

export PATH=/path/bin:\${PATH}
export LD\_LIBRARY\_PATH=/path/lib

For example:

export PATH=/tmp/bin:\${PATH}
export LD\_LIBRARY\_PATH=/tmp/lib

For path, specify the full path to your alternate installation directory.

2. Proceed to the following:

"Configuring Array Services" on page 13

Procedure 2-7 To reset environment variables — Method 2, using environment modules

- 1. Examine the following example module files:
  - /opt/sgi/mpt/mpt-mpt\_rel/doc/mpivars.sh
  - /opt/sgi/mpt/mpt-mpt\_rel/doc/mpivars.csh
  - On RHEL platforms, see the following file:

/usr/share/Modules/modulefiles/mpt/mpt\_rel

• On SLES platforms, see the following file:

/usr/share/modules/modulefiles/mpt/mpt\_rel

For *mpt\_rel*, specify the release level of the MPT software that you installed.

- 2. Edit the module files and specify the variables needed.
- 3. Proceed to the following:

"Configuring Array Services" on page 13

## **Configuring Array Services**

Array Services must be configured and running on your SGI system or cluster before you start an MPI job.

Procedure 2-8 To enable Array Services

- 1. As the root user, log into one of the hosts.
- 2. Use one of the procedures in the following topic to configure Array Services:

"Configuring Array Services" on page 81

3. Proceed to the following:

"Configuring OFED for MPT" on page 13

## **Configuring OFED for MPT**

You can specify the maximum number of queue pairs (QPs) for SHMEM and UPC applications when run on large clusters over OFED fabric. 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

SHMEM and UPC codes use the InfiniBand RC protocol for communication between all pairs of processes in the parallel job, which requires a large number of QPs. The  $log_num_qp$  parameter defines the  $log_2$  of the number of QPs. The following procedure explains how to specify the  $log_num_qp$  parameter.

Procedure 2-9 To specify the log\_num\_qp parameter

- 1. Log into one of the hosts upon which you installed the MPT software as the root user.
- 2. Use a text editor to open file /etc/modprobe.d/libmlx4.conf.

3. Add a line similar to the following to file /etc/modprobe.d/libmlx4.conf:

options mlx4\_core log\_num\_qp=21

By default, the maximum number of queue pairs is  $2^{17}$  (131072).

- 4. Save and close the file.
- 5. Repeat the preceding steps on other hosts.
- 6. Proceed to the following:

"Restarting Services or Rebooting" on page 14

## **Restarting Services or Rebooting**

The following procedure explains how to restart services. If you do not want to restart services, you can reboot your system.

Procedure 2-10 To restart services

- 1. Type the following commands:
  - # modprobe xpmem
  - # /etc/init.d/procset restart
    # /etc/init.d/arrayd restart
- 2. (Conditional) Log into other hosts and type the commands in the preceding step.

Perform this step if you want to run cluster-aware MPT programs.

Make sure to reboot or to restart services on all cluster hosts.

- 3. Proceed to one of the following:
  - "(Conditional) Adjusting File Descriptor Limits" on page 14
  - "Adjusting the Resource Limit for Locked Memory" on page 16

## (Conditional) Adjusting File Descriptor Limits

Perform the procedure in this chapter if you installed the MPT software on a large host with hundreds of processors.

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.

The following procedure explains how to increase the limit on the number of open files for all users.

Procedure 2-11 To increase the system limit on open files

- 1. As the root user, log in to the host upon which you installed the MPT software.
- 2. Use a text editor to open file /etc/pam.d/login.
- 3. Add the following line to file /etc/pam.d/login:

session required /lib/security/pam\_limits.so

- 4. Save and close the file.
- 5. Use a text editor to open file /etc/security/limits.conf.
- 6. 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          |
|----------------|----------------|
| 512            | 3000           |
| 1024           | 6000           |
| 8192           | 8192 (default) |
| 4096           | 21000          |

For example, the following line specifies 512 MPI processes per host:

\* hard nofile 3000

- 7. Save and close the file.
- 8. (Conditional) Update other files in the /etc/pam.d directory as needed.

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

Modify the other files in the <code>/etc/pam.d</code> directory to accommodate the increased file descriptor limits.

9. (Conditional) Repeat the preceding steps on other hosts.

Perform these steps if you installed the MPT software on more than one host.

10. Proceed to the following:

"Adjusting the Resource Limit for Locked Memory" on page 16

#### Adjusting the Resource Limit for Locked Memory

The following procedure increases the resource limit for locked memory.

Procedure 2-12 To increase the resource limit

- 1. As the root user, log into the host upon which you installed the MPT software.
- 2. Use a text editor to open file /etc/security/limits.conf.
- 3. Add the following line to file /etc/security/limits.conf:
  - \* hard memlock unlimited
- 4. (Conditional) Type the following commands to increase the resource limit for locked memory in the array services startup script:
  - # sed -i.bak 's/ulimit -n/ulimit -l unlimited ; ulimit -n/' \
     /etc/init.d/array
  - # /etc/init.d/array restart
- 5. (Conditional) Repeat the preceding steps on other hosts.

Perform these steps if you installed the MPT software on multiple hosts.

6. (Conditional) Proceed to the following procedure if you installed the MPT software on multiple hosts:

"(Conditional) Enabling Cross-partition NUMAlink MPI Communication" on page 17

### (Conditional) Enabling Cross-partition NUMAlink MPI Communication

Perform the procedure in this topic if you installed the MPT software on multiple software partitions on an SGI UV system.

Large SGI UV systems can be configured into two or more NUMAlink-connected *partitions*. These 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. SGI recommends that you complete the procedure in this topic as part of the installation. If you do not perform this procedure during installation, you might receive the following message during the run of your 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.

Procedure 2-13 To load the kernel modules at boot (SLES)

- 1. As the root user, log into one of the hosts upon which you installed the 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. To the list of modules that are load at boot time, add xpc.
- 5. Save and close the file.
- 6. Reinitialize the kernel modules.

To reinitialize the kernel modules, either reboot the system or type the following command:

- # modprobe xpc
- 7. Repeat the preceding steps on the other hosts.

Procedure 2-14 To load the kernel modules at boot (RHEL)

1. As the root user, log into one of the hosts upon which you installed the MPT software.

007-3773-022

2. Type the following command:

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

- 3. Save and close the file.
- 4. Reinitialize the kernel modules.

To reinitialize the kernel modules, either reboot the system or type the following command:

# modprobe xpc

5. Repeat the preceding steps on the other hosts.

## **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 21
- "Running MPI Jobs with a Workload Manager" on page 24
- "Compiling and Running SHMEM Applications" on page 27
- "Using Huge Pages" on page 27
- "Interoperation Between MPI, SHMEM, and UPC" on page 29

### **Running MPI Jobs**

The following procedure explains how to run an MPI application when the MPT software is installed in an alternate location.

Procedure 3-1 To run jobs with MPT installed in an alternate location

- 1. Determine the directory into which the 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 -lmpi
```

mpicc -I /install\_path/usr/include file.c -L lib\_path/usr/lib -lmpi

The variables in the preceding command are as follows:

- For *install\_path*, type the path to the directory in which the 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 -lmpi

3. (Conditional) Ensure that the program can find the 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 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 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 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 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 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:

| <pre>% ifort -o myprog myprog.f -lmpi</pre> | (Fortran - version 8)           |
|---|---------------------------------|
| <pre>% icc -o myprog myprog.c -lmpi</pre>   | (C - version 8)                 |
| <pre>% mpif90 simple1_mpi.f</pre>           | (Fortan 90)                     |
| <pre>% mpicc -o myprog myprog.c</pre>       | (Open MPI C wrapper compiler)   |
| <pre>% mpicxx -o myprog myprog.C</pre>      | (Open 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 you installed MPT into a nondefault 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-2 Spawn Functions to Launch an Application

To use the MPI-2 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-2 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, Load Sharing Facility (LSF), or SGI<sup>®</sup> Simple Linux Utility for Resource Management (SLURM), 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. 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 24
- "Torque" on page 26
- "SLURM" on page 26

#### **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 3-2 To specify computing resources

Within a script, use the -1 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 3-3 To run the MPI application

Use the mpiexec\_mpt command included in the SGI Message Passing Toolkit (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(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 3-1 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 -n 512 ./a.out
```

**Example 3-2** 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 -1 select=512:ncpus=4
mpiexec_mpt -n 512 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 5, "Debugging MPI Applications" on page 41.

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 MPT mpiexec_mpt(1) command to launch MPT MPI jobs.   |
|        | The basic syntax is as follows:  |
|        | mpiexec_mpt -n P ./a.out   |
|        | For <i>P</i> , 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 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 41. |
| SLURM  |  |
|        | MPT can be used in conjunction with SGI <sup>®</sup> Simple Linux Utility for Resource<br>Management (SLURM) product. The SLURM product has been adapted for MPT. Just<br>use the sgimpi SLURM mpi plugin supplied in the product.                                 |
|        | Type the following commands to get started:  |
|        | <pre>% module load slurm % module load mpt % mpicc % srun -n16mpi=sgimpt a.out</pre>   |
|        | For information about how to install and configure SGI <sup>®</sup> SLURM, see the following:  |
|        | Simple Linux Utility for Resource Management Install Guide   |
|        | 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 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_hugepages |
|------------------------|--------------------------------------|
| Huge Pages Allowed:    | 28974 pages (56 GB) 90% of memory    |
| Huge Page Size:        | 2048 KB                              |
| Huge 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:/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 (exists)

4. When running your 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 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\_hugepagesHuge Pages Allowed:0 pages (0 KB) 0% of memoryHuge Page Size:2048 KBHuge TLB FS Directory:/etc/mpt/hugepage\_mpt (does not exist)

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

## Interoperation Between MPI, SHMEM, and UPC

The SGI UPC run-time environment depends on the SGI Message Passing Toolkit, which consists of the message passing interface (MPI) libraries and the SHMEM libraries. The MPI and SHMEM libraries provide job launch, parallel job control, memory mapping, and synchronization functions.

Just as with MPI or SHMEM jobs, you can use the mpirun(1) or mpiexec\_mpt(1) commands to launch UPC jobs. UPC thread numbers correspond to SHMEM PE numbers and MPI rank numbers for MPI\_COMM\_WORLD.

For more information, see the Unified Parallel C (UPC) User's Guide.

# 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 31
- "Signals" on page 32
- "Buffering" on page 33
- "Multithreaded Programming" on page 34
- "Interoperability with the SHMEM programming model" on page 34
- "Miscellaneous Features of SGI MPI" on page 35
- "Programming Optimizations" on page 35
- "Additional Programming Model Considerations" on page 38

## 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**

Section 7.2 of 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 section 7.5 of the MPI Standard.

If the application uses the MPI-2 spawn functionality described in Chapter 5 of the MPI-2 Standard, there are additional considerations. In the SGI implementation, all MPI processes are connected. Section 5.5.4 of the MPI-2 Standard defines what is meant by connected processes. When the MPI-2 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 4-1 on page 33 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 4-1 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 35.

## **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-2 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-2 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 37.

Note: Collectives are optimized across partitions by using the XPMEM driver which is explained in Chapter 8, "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 33, 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 51.

#### **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 the following:

Chapter 8, "Run-time Tuning" on page 49

#### Using Global Shared Memory

The MPT software includes the Global Shared Memory (GSM) Feature. This feature allows users to allocate globally accessible shared memory from within an MPI or SHMEM program. The GSM feature can be used to provide shared memory access across partitioned SGI UV systems and to provide additional memory placement options within a single-host configuration.

User-callable functions are provided to allocate a global shared memory segment, free that segment, and provide information about the segment. Once allocated, the application can use this new global shared memory segment via standard loads and stores, just as if it were a System V shared memory segment. For more information, see the GSM\_Intro or GSM\_Alloc man pages.

## 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-2 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 8, "Run-time Tuning" on page 49.

# **Debugging MPI Applications**

This chapter includes the following topics:

- "MPI Routine Argument Checking" on page 41
- "Using the TotalView Debugger with MPI Programs" on page 41
- "Using idb and gdb with MPI Programs" on page 42
- "Using the DDT Debugger with MPI Programs" on page 42

## **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 MPT mpiexec\_mpt(1) command has a -tv option for use by MPT with the TotalView Debugger. Note that the PBS Professional mpiexec(1) command does not support the -tv option.

To run an 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 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 and SGI UPC. 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 6

# 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 6-1 on page 45). 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<br>Implementation                         | Command Line Option |  |
|---|---------------------|--|
| Platform MPI 7.1+                             | -pmpi               |  |
| HP-MPI  | -pmpi               |  |
| Intel MPI                                     | -impi               |  |
| OpenMPI                                       | -ompi               |  |
| MPICH1  | -mpich              |  |
| MPICH2  | -impi               |  |
| MVAPICH2                                      | -impi               |  |
| Example 6-1 Using the SCI performers Software |                     |  |

**Example 6-1** 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<br>enables a message when PerfBoost activates and also<br>when the MPI application is completed through the<br>MPI_Finalize() function. This message indicates<br>that the PerfBoost library is active and also when the<br>MPI application completes through the libperfboost<br>wrapper library. |
|-------------------|---|
|                   | <b>Note:</b> 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**

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 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 MPT**

To enable checkpoint/restart within 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.

# **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 49
- "Tuning MPI Buffer Resources" on page 50
- "Avoiding Message Buffering Enabling Single Copy" on page 51
- "Memory Placement and Policies" on page 52
- "Tuning MPI/OpenMP Hybrid Codes" on page 54
- "Tuning for Running Applications Across Multiple Hosts" on page 55
- "Tuning for Running Applications over the InfiniBand Interconnect" on page 57
- "MPI on SGI UV Systems" on page 59
- "Suspending MPI Jobs" on page 61

## **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 *Linux Resource Administration 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 71.

For information about buffering considerations when running an MPI job across multiple hosts, see "Tuning for Running Applications Across Multiple Hosts" on page 55.

For information about the programming implications of message buffering, see "Buffering" on page 33.

## 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-2 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-2 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.<br>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.<br>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 will get a physical CPU and memory on the node to which it was assigned. If this environment variable is used without specifying an MPI\_DSM\_CPULIST variable, it will cause MPI to assign MPI ranks starting at logical CPU 0 and incrementing until all ranks have been placed. Therefore, it is recommended that this variable be used only if running within a cpuset on a dedicated system.

### 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.

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 *Linux Resource Administration Guide*. For more information on using dplace, see the *Linux Application Tuning Guide*.

Example 8-1 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 8-1 on page 55, 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 MPT programs with PBS, see"Running MPI Jobs with a Workload Manager" on page 24.

## **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 23. 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 8-1 on page 56 specifies the order in which MPI probes for available interconnects.

| Interconnect | Default Order of Selection | Environment Variable to<br>Require Use |
|--------------|----------------------------|--|
| XPMEM        | 1                          | MPI_USE_XPMEM                          |
| InfiniBand   | 2                          | MPI_USE_IB                             |
| TCP/IP       | 3                          | MPI_USE_TCP                            |

 Table 8-1 Inquiry Order for Available Interconnects

The third column of Table 8-1 on page 56 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, MPT applications may not execute a fork() or system() call. The InfiniBand driver produces undefined results when an MPT process using InfiniBand forks.

### 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. 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, 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, 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 16384 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, 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<sup>®</sup> UV<sup>™</sup> 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 52), 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.

Chapter 9

# **MPI Performance Profiling**

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 63
- "Using the perfcatch Utility" on page 63
- "MPI\_PROFILING\_STATS Results File Example" on page 64
- "MPI Performance Profiling Environment Variables" on page 67
- "MPI Supported Profiled Functions"
- "Profiling MPI Applications" on page 69

## **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 64). 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 MPT      |
|-----------|-------------------|
| -v        | Supports MPI      |
| -vofed    | Supports OFED MPI |

Supports Intel MPI

To use perfcatch with an SGI Message Passing Toolkit MPI program, insert the perfcatch command in front of the executable name. Here are some examples:

mpirun -np 64 perfcatch a.out arg1
and

mpirun host1 32, host2 64 perfcatch a.out arg1

To use perfcatch with Intel MPI, add the -i options. An example is, 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

-i

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% Time in all profiled MPI routines, avg per rank 5.75004e-07 sec 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<br>rank | cnt/sec<br>0 |     | 1        |         |       |       |
|---------------|--------------|-----|----------|---------|-------|-------|
| send profile  |              |     |          |         |       |       |
| src<br>rank   | cnt/sec<br>0 | for | all<br>1 | destina | ation | ranks |
|               |              |     |          |         |       |       |
| ssend profile | 2            |     |          |         |       |       |
| src<br>rank   | cnt/sec<br>0 | -   | 1        |         |       |       |
|               |              |     |          |         |       |       |
| ibsend profil | Le           |     |          |         |       |       |
| src<br>rank   | cnt/sec<br>0 | for | all<br>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<br>immediately, that is, at the start of<br>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: Some functions may not be implemented in all language as indicated below.

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

| C Fortran | <pre>mpi_group_range_excl</pre> |
|-----------|---------------------------------|
| C Fortran | <pre>mpi_group_range_incl</pre> |
| C Fortran | mpi_group_union                 |
| C         | mpi_ibsend                      |
| C Fortran | mpi_init                        |
| C         | <pre>mpi_init_thread</pre>      |
| C Fortran | mpi_irecv                       |
| C Fortran | mpi_isend                       |
| C         | mpi_probe                       |
| C Fortran | mpi_recv                        |
| C Fortran | mpi_reduce                      |
| C Fortran | mpi_scatter                     |
| C Fortran | mpi_scatterv                    |
| C Fortran | mpi_send                        |
| C Fortran | mpi_sendrecv                    |
| C Fortran | mpi_ssend                       |
| C Fortran | mpi_test                        |
| C Fortran | mpi_testany                     |
| C Fortran | mpi_wait                        |
| C 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 70
- "MPI Internal Statistics" on page 71
- "Third Party Products" on page 71

### **Profiling Interface**

You can write your own profiling by using the MPI-1 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
               0
                   time 0.000000e+00
time 0.00000e+00
probe calls
             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
send calls
             0
                      time 0.000000e+00
ssend calls 0
                      time 0.000000e+00
isend calls
             22039 time 2.950286e+00
             0
wait calls
                      time 0.00000e+00
                                         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 8, "Run-time Tuning" on page 49.

### **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 smaller, 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 even more problematic 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 users encounter when starting to use SGI MPI, as well as 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 73
- "My code runs correctly until it reaches MPI\_Finalize() and then it hangs." on page 75
- "My hybrid code (using OpenMP) stalls on the mpirun command." on page 75
- "I keep getting error messages about MPI\_REQUEST\_MAX being too small." on page 75
- "I am not seeing stdout and/or stderr output from my MPI application." on page 76
- "How can I get the MPT software to install on my machine?" on page 76
- "Where can I find more information about the SHMEM programming model? " on page 76
- "The  ${\tt ps}(1)$  command says my memory use (SIZE) is higher than expected. " on page 76
- "What does MPI: could not run executable mean?" on page 77
- "How do I combine MPI with insert favorite tool here?" on page 77
- "Why do I see "stack traceback" information when my MPI job aborts?" on page 78

# 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 21.

### 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 MPT software to install on my machine?

MPT RPMs are included in the SGI Performance Suite releases. In addition, you can obtain MPT RPMs from the SGI Support website at

http://support.sgi.com
under "Downloads".

## 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 79
- "Retrieving the Array Services Release Notes" on page 80
- "Installing Array Services" on page 81
- "Configuring Array Services" on page 81
- "Managing Local Processes" on page 87
- "Using Array Services Commands" on page 88
- "Array Services Commands" on page 90
- "Obtaining Information about the Array" on page 92
- "Additional Array Configuration Information" on page 95
- "Configuring Array Commands" on page 101

## **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 and UPC 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<sup>®</sup> MPI uses Array Services to launch parallel applications. For information on MPI, see the *Message Passing Toolkit (MPT) User's Guide*.

SGI includes MUNGE software in the SGI MPI and in the SGI UPC software distributions. 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 11-1 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.

### Installing Array Services

The SGI MPI system installation process installs and pre-configures the Array Services software on each host. This installation supports single-host Message Passing Interface (MPI) jobs. Typically, you perform a system reboot after you install the SGI MPI software, so you do not need to perform any additional steps to install Array Services.

The following procedure explains how to install and configure Array Services on single-host, running system.

Procedure 11-2 To install Array Services on a running system

1. Type the following command to stop the Array Services daemon:

% /etc/init.d/array stop

- 2. Upgrade the SGI MPI software.
- 3. Type the following command to restart the Array Services daemon:
  - % /etc/init.d/array start

# **Configuring Array Services**

If you want to run MPI jobs, make sure to configure Array Services first. SGI MPI depends on Array Services for several capabilities. During the configuration, your goal is to specify the hosts that you want to include in the array and to distribute the configuration files to each host.

Lists the documentation resources that contain additional configuration information.

| Торіс                                   | Documentation Resource  |  |
|---|---|--|
| Advanced configuration information      | "Additional Array Configuration Information" on page<br>95    |  |
| Array Services overview                 | array_services(5)   |  |
| Array Services daemon<br>overview       | arrayd(1m)  |  |
| Configuration file format               | arrayd.conf <b>(4)</b><br>/usr/lib/array/arrayd.conf.template |  |
| Configuration file validator            | ascheck(1)  |  |
| Array Services<br>configuration utility | arrayconfig(1m)<br>arrayconfig_tempo(8)                       |  |

### Table 11-1 Array Configuration Resources

You can configure Array Services manually or in a automated way. Use one of the following procedures to configure Array Services:

- "Method 1 Configuring Array Services on Multiple Hosts (Automatic Method)" on page 82
- "Method 2 Configuring Array Services on Multiple Hosts (Manual Method)" on page 84

### Method 1 — Configuring Array Services on Multiple Hosts (Automatic Method)

The procedure in this topic uses the arrayconfig(8) command to specify hosts for an array and to update the Array Services configuration files on each host. If you want to configure an array on an SGI ICE or SGI ICE X system, use this procedure as a guide along with the information in the arrayconfig\_tempo(8) man page.

The following procedure shows an automated way to configure Array Services to run on multiple hosts.

Procedure 11-3 To configure Array Services for multiple hosts (automated method)

1. (Optional) Install the MUNGE package from the SGI MPI software distribution on all hosts that you want to include in the array.

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 or SGI UPC release notes.

2. 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.

3. Use the arrayconfig(1M) command to specify the hosts 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 host.

In the following example command format -a specifies the array name, -A specifies an authentication method, -D copies the files to the other hosts, and -m specifies the names of the other hosts:

# /usr/sbin/arrayconfig -a arrayname -A method -D -m host1 host2 ...

For *arrayname*, type a name for the array.

For *method*, type one of the following authentication methods: NONE, SIMPLE, or MUNGE. For information about the authentication methods, see the arrayd.auth(4) man page.

For *host1*, specify the hostname of the computer upon which you installed the MPT software. If you installed the MPT software on multiple hosts, specify the hostnames of the other computers that you want to include in the array for *host2*, *host3*, and so on.

4. (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 daemona

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

5. Type the following command to restart Array Services:

/etc/init.d/array restart

### Method 2 — Configuring Array Services on Multiple Hosts (Manual Method)

The following procedure explains a manual procedure that configures Array Services to run on multiple hosts, such as clustered or SSI systems.

Procedure 11-4 To configure Array Services for multiple hosts (manual method)

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 or SGI UPC 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 daemona

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.

## 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 (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 11-2 on page 88 summarizes information about local process management.

Table 11-2 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 11-3 on page 88 shows the commands that are common to Array Services operations.

 Table 11-3 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.<br>Commands are predefined by the administrator in the<br>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 11-4 on page 90 summarizes the common options. The default values of some options are set by environment variables.

 Table 11-4 Array Services Command Option Summary

| Option   | Used In                  | Description   |
|----------|--------------------------|---|
| -a array | ainfo, array             | Specify a particular array when more than one is accessible.              |
| -D       | ainfo, array,<br>arshell | Send commands to other nodes directly, rather than through arrayd daemon. |
| -F       | ainfo, array,<br>arshell | Forward commands to other nodes through the arrayd daemon.                |

| Option                                       | Used In                  | Description   |
|--|--------------------------|---|
| -Kl number                                   | ainfo, array             | Authentication key (a 64-bit number) for the local node.                      |
| -Kr number                                   | ainfo, array             | Authentication key (a 64-bit number) for the remote node.                     |
| -1 (lowercase<br>letter "L", for<br>"Local") | ainfo, array             | Execute in context of the destination node, not necessarily the current node. |
| -l port                                      | ainfo, array,<br>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 (letter ell for "local") option restricts the scope of a command to the node where the command is executed. 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 (server, or node name) 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 11-5.

| 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<br>monitored by the array daemon<br>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<br>-Kl option is used.                  |
| ARRAYD_REMOTEKEY | Authentication key for the destination node (option -Kr).   | No authentication unless<br>-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 11-5 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
```

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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. (The example has been edited for brevity.)

```
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

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11: Array Services

```
MEMORY
512 MB MAIN MEMORY
INTERLEAVE 4
```

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. (The example has been edited for brevity and security.)

```
homegrown 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
...
```

#### 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
```

007-3773-022

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% array 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 (for example, those that are attached to a public network, or when individual machines otherwise 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. Normally it is started 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 data 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 (reported by ainfo).

- The names and types of the nodes in each named array, especially the hostnames that would be used in an Array Services command (reported by ainfo).
- The authentication keys, if any, that must be used with Array Services commands (required as -Kl and -Kr command options, see "Array Services Commands" on page 90).
- 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. (An automated way to do this is summarized under "Designing New Array Commands" on page 106.)

### **About Substitution Syntax**

The man page arrayd.conf(4) details 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 <code>array</code> 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 (detailed in the section that follow this one). 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 restart it as a daemon (without -n).

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 (see "Array Services Commands" on page 90).

One array name should be specified in a DESTINATION ARRAY local option as the default array (reported by ainfo dflt). Local options are listed under "Configuring Local Options" on page 105.

#### 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 (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 (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 (/usr/lib/array/arrayd.conf). Each COMMAND entry is defined using the subentries shown in Table 11-6. (These are described in great detail in the man page arrayd.conf(4).)

### Table 11-6 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.<br>Usually given as USER %USER, so as to run as the user who invoked<br>array.   |
| GROUP   | The group name under which the INVOKE and MERGE commands<br>run. Usually given as GROUP %GROUP, so as to run in the group of<br>the user who invoked array (see the groups(1) man page).      |
| PROJECT | The project under which the INVOKE and MERGE commands run.<br>Usually given as PROJECT %PROJECT, so as to run in the project of<br>the user who invoked array (see the projects(5) man page). |
| OPTIONS | A variety of options to modify this command; see Table 11-8.  |

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 (which are documented in detail in the arrayd.conf(4) man page) are summarized in Table 11-7.

| Substitution   | Replacement Value   |
|--|---|
| %1%9;<br>%ARG( <i>n</i> );<br>%ALLARGS;<br>%OPTARG( <i>n</i> ) | Argument tokens from the user's subcommand. %OPTARG does<br>not produce an error message if the specified argument is<br>omitted.     |
| %USER,<br>%GROUP,<br>%PROJECT                                  | The effective user ID, effective group ID, and project of the user who invoked array.   |
| %REALUSER,<br>%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<br>one node's INVOKE command (valid only in the MERGE<br>subentry). |

 Table 11-7 Substitutions Used in a COMMAND Definition

The OPTIONS subentry permits a number of important modifications of the command execution; these are summarized in Table 11-8.

| Keyword    | Effect on Command   |
|------------|---|
| LOCAL      | Do not distribute to other nodes (effectively forces the -1 option).  |
| NEWSESSION | Execute the INVOKE command under a newly created ASH.<br>%ASH in the INVOKE line is the new ASH. The MERGE<br>command runs under the original ASH, and %ASH substitutes as<br>the old ASH in that line. |
| SETRUID    | Set both the real and effective user ID from the USER subentry (normally USER only sets the effective UID).   |
| SETRGID    | Set both the real and effective group ID from the GROUP subentry (normally 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<br>invoked; do not wait for completion (a MERGE subentry is<br>ineffective).   |
|            |   |

### Table 11-8 Options of the COMMAND Definition

## **Configuring Local Options**

The LOCAL entry specifies options to arrayd itself. The most important options are summarized in Table 11-9.

Table 11-9 Subentries of the LOCAL 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.                 |

| Subentry                | Purpose  |
|-------------------------|--|
| USER, GROUP,<br>PROJECT | Default values for COMMAND execution when USER,<br>GROUP, or PROJECT are omitted from the COMMAND<br>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
exit 0
```

The script uses rcp to copy a specified file (presumably a configuration file such as arrayd.conf) into /usr/lib/array (this will fail if %USER is not privileged). Then the script restarts arrayd (see /etc/init.d/array) to reread configuration files.

The command definition would be 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, since the script will kill the daemon.

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