

# HPE Performance Software — Message Passing Interface User Guide

#### Abstract:

The HPE Performance Software — Message Passing Interface (HPE Performance MPI) software supports the MPI standard. HPE Performance MPI facilitates parallel programming on large systems and on computer system clusters.

Part Number: 007-3773-032 Published: August 2017 Edition: Revision 32 ©1996, 1998-2017, Hewlett Packard Enterprise Development LP

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# **Record of Revision**

Version	Description
001	March 2004 Original Printing. This manual documents the Message Passing Toolkit implementation of the Message Passing Interface (MPI).
002	November 2004 Supports the MPT 1.11 release.
003	June 2005 Supports the MPT 1.12 release.
004	June 2007 Supports the MPT 1.13 release.
005	October 2007 Supports the MPT 1.17 release.
006	January 2008 Supports the MPT 1.18 release.
007	May 2008 Supports the MPT 1.19 release.
008	July 2008 Supports the MPT 1.20 release.
009	October 2008 Supports the MPT 1.21 release.
010	January 2009 Supports the MPT 1.22 release.
011	April 2009 Supports the MPT 1.23 release.
012	October 2009 Supports the MPT 1.25 release.

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013	April 2010 Supports the MPT 2.0 release.
014	July 2010 Supports the MPT 2.01 release.
015	October 2010 Supports the MPT 2.02 release.
016	February 2011 Supports the MPT 2.03 release.
017	March 2011 Supports additional changes for the MPT 2.03 release.
018	August 2011 Supports changes for the MPT 2.04 release.
019	November 2011 Supports changes for the MPT 2.05 release.
020	May 2012 Supports changes for the MPT 2.06 release.
021	November 2012 Supports changes for the MPT 2.07 release.
022	May 2013 Supports changes for the Performance Suite 1.6 release and the MPT 2.0.9 release.
023	November 2013 Supports the SGI Performance Suite 1.7 release, the MPT 2.09 release, and the MPI 1.7 release.
024	February 2014 Supports the SGI Performance Suite 1.7 release, the MPT 2.09 release, and the MPI 1.7 release. Clarifies SLURM support.

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025 June 2014 Supports the SGI Performance Suite 1.8 release, the SGI MPT 2.10 release, and the SGI MPI 1.8 release. This is the last revision of this documentation with the title Message Passing Toolkit (MPT) User Guide. 026 May 2015 Supports the SGI Performance Suite 1.10 release, the SGI MPT 2.12 release, and the SGI MPI 1.10 release. This documentation is now called the SGI MPI and SGI SHMEM User Guide. 027 November 2015 Supports the SGI Performance Suite 1.11 release, the SGI MPT 2.13 release, and the SGI MPI 1.11 release. 028 May 2016 Supports the SGI Performance Suite 1.12 release, the SGI MPT 2.14 release, and the SGI MPI 1.12 release. 029 May 2016 Supports the SGI Performance Suite 1.12 release, the SGI MPT 2.14 release, and the SGI MPI 1.12 release and adds third-party compatibility information. 030 November 2016 Supports the SGI Performance Suite 1.13 release, the SGI MPT 2.15 release, and the SGI MPI 1.13 release and adds third-party compatibility information. 031 June 2017 Supports the HPE Performance Software - Message Passing Interface 1.0 release, the HPE MPT 2.16 release, and the SGI MPI 1.14 release. 032 August 2017 Supports the HPE Performance Software - Message Passing

Interface 1.0 release and the MPT 2.16 release.

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## **About This Guide**

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

The HPE Performance Software — Message Passing Interface (HPE Performance MPI) software supports the MPI standard. HPE Performance MPI facilitates parallel programming. This publication describes HPE Performance MPI 1.0, which supports the MPI 3.1 standard.

HPE Performance MPI supports the OpenSHMEM standard. The OpenSHMEM standard describes a low-latency library that supports RMA on symmetric memory in parallel environments. The OpenSHMEM programming model is a partitioned global address space (PGAS) programming model that presents distributed processes with symmetric arrays that are accessible via PUT and GET operations from other processes. This publication describes software that supports OpenSHMEM version 1.3. The HPE SHMEM programming model is the basis for the OpenSHMEM™ programming model specification that is being developed by the Open Source Software Solutions multivendor working group.

The following significant features make HPE Performance MPI the preferred implementation:

- Data transfer optimizations for NUMAlink, where available, including single-copy data transfer.
- Multirail InfiniBand support, which takes full advantage of the multiple InfiniBand fabrics available on HPE SGI 8600 and SGI ICE systems.
- Optimized MPI remote memory access (RMA) one-sided commands.
- Support for multiple application binary interfaces (ABIs), including MPICH and OpenMPI.

HPE's support for MPI and OpenSHMEM is built on top of the Message Passing Toolkit (MPT). MPT is a high-performance communications middleware software product. On some platforms, MPT uses Array Services to launch applications. MPT is optimized for large-scale, high-performance cluster computing.

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# **Compatibility Information**

The following table describes compatibility between HPE Performance MPI and other products.

Technology	Notes	
Red Hat Enterprise Linux (RHEL) operating system	RHEL 6.X and RHEL 7.X	
SLES operating system	SLES 12 SPX and SLES 11 SPX	
CentOS operating system	CentOS 6.X and 7.X	
Fortran 2008	Supports Fortran 2008.	
Computing platforms	Platforms:	
	<ul> <li>HPE SGI 8600 cluster systems</li> <li>HPE Apollo 2000, 6000, and 6500 cluster systems</li> <li>HPE Apollo 20 and 40 cluster systems</li> <li>HPE Proliant systems</li> <li>HPE Integrity MC 990 X systems</li> <li>SGI ICE cluster systems</li> <li>SGI Rackable cluster systems</li> <li>SGI UV systems</li> </ul>	
Multi-rail InfiniBand (IB)		
Multi-rail Intel Omni-Path Architecture (OPA)	No support for MPI spawn	
TCP/IP communication		
Mellanox Fabric Collective Accelerator (FCA) 3.x / HCOLL		
NVIDIA GPUDirect remote direct memory access (RDMA) over IB NVIDIA GPUDirect RDMA	Requires Mellanox Open Fabrics Enterprise Distribution (OFED). No support for MPI RMA passive windows.	

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Technology	Notes	
Checkpoint-restart (CPR), supported through Berkeley Lab checkpoint restart (BLCR).	Supports jobs running over shared memory, InfiniBand, and TCP/IP. No support for CPR when using the following:	
	<ul> <li>OpenSHMEM</li> <li>MPI remote memory access (RMA) passive windows</li> <li>MPI Spawn</li> <li>Process managment interface (PMI), which is commonly used by the simple Linux utility for resource management (SLURM)</li> </ul>	
Third-party debugging and profiling tools:	Contact HPE for information about additional debugging	
<ul><li>Allinea DDT</li><li>RogueWave TotalView</li><li>Tuning and Analysis Utilities (TAU)</li><li>Vampir</li></ul>	and profiling tools.	
Process management interfaces (PMIs), specifically PMIx and PMI2.	Supported when running under SLURM.	
Third-party workload managers:		
<ul> <li>Altair PBS Professional</li> <li>SLURM</li> <li>UNIVA Grid Engine</li> <li>IBM LSF</li> <li>Moab / TORQUE</li> </ul>		

**Note:** This documentation uses the term *cluster* to refer to cluster computers, cluster systems, or cluster nodes in HPE Apollo systems, HPE SGI 8600 systems, SGI ICE systems, and SGI Rackable systems. The term *cluster* does not pertain to HPE Integrity MC 990 X systems or to SGI UV computer systems because they are large-memory, single system image (SSI) systems.

If you use an HPE Integrity MC 990 X system, you can assume that all references to SGI UV systems also apply to HPE Integrity MC 990 X systems.

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#### HPE Performance Software Suite Publications and General MPI Information

The HPE Performance Software Suite Publications are as follows:

- The HPE Performance Software Message Passing Interface User Guide describes how to use the HPE Performance Software Message Passing Interface software.
- The HPE Performance Software Message Passing Interface MPInside Reference Guide describes the MPI profiling tool called MPInside.
- The HPE Performance Software Message Passing Interface Cpuset Software Guide describes how to use cpusets.
- MPInside(3)

This man page lists all the MPInside environment variables that HPE supports.

• MPInside-exp(3)

This man page lists MPInside environment variables that HPE supports on an experimental basis. Use of these environment variables can generate unexpected results. The HPE Performance MPI documentation uses some of these experimental variables in examples and procedures.

- The HPE Performance Software Message Passing Interface release notes contain information about the specific software packages included in each product. The release notes are available in the following locations:
  - The HPE Performance MPI release notes are posted to the following SGI website:

https://support1-sgi.custhelp.com/app/answers/detail/a\_id/6093

**Note:** To access documentation through the SGI customer portal, first log in, and then navigate to the link. You can log in at the following website:

https://support.sgi.com/login

- On the product media. The release notes reside in a text file in the /docs directory on the product media.
- On the system. After installation, the release notes and other product documentation reside in the

/opt/hpe/hpc/mpt/mpt-version\_number/doc/README.relnotes directory.

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For example, you can use the following rpm(8) command to retrieve the location of the Array Services release notes:

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

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

For information about the MPI standard, see the following:

- The Message Passing Interface Forum's website, which is as follows: http://www.mpi-forum.org/
- Using MPI 2nd Edition: Portable Parallel Programming with the Message Passing Interface (Scientific and Engineering Computation), by Gropp, Lusk, and Skjellum. ISBN-13: 978-0262571326.
- The University of Tennessee technical report. See reference [24] from *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, by Gropp, Lusk, and Skjellum. ISBN-13: 978–0262571043.
- Journal articles in the following publications:
  - International Journal of Supercomputer Applications, volume 8, number 3/4, 1994
  - International Journal of Supercomputer Applications, volume 12, number 1/4, pages 1 to 299, 1998

#### **HPE Websites**

The following HPE websites might interest you:

- Hewlett Packard Enterprise Information Library: www.hpe.com/info/EIL
- Single Point of Connectivity Knowledge (SPOCK) Storage compatibility matrix: www.hpe.com/storage/spock
- Storage white papers and analyst reports: www.hpe.com/storage/whitepapers

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# **Configuring the Message Passing Toolkit (MPT)**

This chapter includes the following topics:

- "About Configuring MPT" on page 1
- "Configuring MPT on an SGI UV Computer System" on page 5

## **About Configuring MPT**

When you installed the HPE Performance Suite — Message Passing Interface (HPE Performance MPI) software, you also installed MPT. Before you can run any HPE Performance MPI programs, however, you need to configure the MPT software. The procedures in this chapter explain how to configure MPT.

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

The configuration procedure differs, depending on your platform, as follows:

 On a cluster computing system, the MPT installation and configuration procedure includes image-management steps.

For information about how to configure MPT on an HPE SGI 8600 system, an SGI ICE system, an HPE Apollo 20 series system, an HPE Apollo 40 series system, or an SGI Rackable cluster system, see the following:

HPE SGI Management Suite Installation and Configuration Guide

For information about how to install and configure MPT and Array Services on an HPE Apollo 6500 series, an HPE Apollo 6000 series, an HPE Apollo 2000 series, see the following:

"Installing the Array Services Software on HPE Apollo Cluster Systems" on page 2

On an HPE Integrity MC990 X system or on a SGI UV system, see the following:
 "Configuring MPT on an SGI UV Computer System" on page 5

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## Installing the Array Services Software on HPE Apollo Cluster Systems

You need to install and configure Array Services software on the cluster before any HPE Performance MPI programs can run. The HPE factory installs Array Services on many HPE cluster systems. If you administer one of the following cluster systems, however, you need to install the Array Services software manually:

- HPE Apollo 6500
- HPE Apollo 6000
- HPE Apollo 2000

The arrayconfig(1M) command creates the following files on the compute service node to which you are logged in:

- /etc/array/arrayd.conf
- /etc/array/arrayd.auth

**Note:** If SLURM is installed on the cluster, you do not need to install Array Services. Clusters with SLURM do not use the Array Services software.

The following topics explain how to install and configure Array Services:

- "Installing and Configuring Array Services on HPE Apollo Cluster Systems" on page 2
- "Array Services Security Options" on page 4
- "Array Services Configuration Examples" on page 5

#### Installing and Configuring Array Services on HPE Apollo Cluster Systems

The following procedure explains how to install Array Services on HPE Apollo systems.

**Procedure 1-1** To install Array Services

- 1. Log into the head node.
- 2. Write the list of cluster nodes to a temporary file:
  - \$ cmu\_show\_nodes > nodes.txt

3. (Conditional) Edit the node list to include only the compute nodes that you want to include in the array.

Complete this step if you do not want to include all the cluster nodes in the array.

4. Copy the list of cluster nodes to a directory of your choosing on one of the compute nodes.

For example:

```
$ scp nodes.txt first compute node:/somewhere
```

The preceding command copies the nodes.txt file to the somewhere directory on first compute node.

5. Use the ssh(1) command to log into the compute node to which you wrote the node list.

For example:

```
$ ssh first_compute_node
```

6. Change to the directory in which the node list resides.

For example:

```
$ cd somewhere
```

7. Use the arrayconfig(8) command to configure the nodes into an array.

The command format is as follows:

```
/usr/sbin/arrayconfig -a arrayname -f -m -A method node node ...
```

The command parameters are as follows:

- For arrayname, specify a name for the array. The default is default.
- For *method*, specify munge, none, or simple. For information about the security levels, see the following:

"Array Services Security Options" on page 4

• For *node*, specify the nodes to include. For example /tmp/nodelist or a list of individual node names.

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For example, the following command configures the nodes into an array and uses the -D parameter to distribute the arrayd.conf file:

\$ arrayconfig -fmD -a default -A simple 'cat nodes.txt'

#### **Array Services Security Options**

The following list explains the Array Services security options.

simple (default) Generates hostname/key pairs by using either the

 $Open SSL, \ {\tt rand} \ command, \ 64-bit \ values \ (if \ available)$ 

or by using \$RANDOM Bash facilities.

munge Configures additional security provided by MUNGE.

The installation process installs MUNGE by default.

none You can configure none in one of the following ways:

 none on all nodes, including the login node. The login node can be a compute node that is designated for user logins and/or other services.

When you specify none, Array Services disables all authentication.

OR

 none on the the compute nodes and noremote on the login node. A security setting of noremote prevents remote logins to the array.

When you specify noremote on the compute services nodes and specify none on the compute nodes, users must run their jobs directly from the compute services nodes. In this case, users cannot submit HPE Performance MPI jobs remotely.

"Manually Configuring Array Services on Multiple Hosts" on page 128 explains how to configure noremote on the login node.

#### **Array Services Configuration Examples**

Example 1. To specify that array myarray use MUNGE security and include all HPE Apollo compute nodes, type the following command:

# /usr/sbin/arrayconfig -a myarray -f -m -A munge /tmp/nodelist

Example 2. To specify that array yourarray use no security, include one compute service node, and include all HPE Apollo compute nodes, type the following command:

# /usr/sbin/arrayconfig -a yourarray -f -m -A none n1 /tmp/nodelist

## Configuring MPT on an SGI UV Computer System

The information in the following procedures explains how to configure MPT on an SGI UV system:

- "Verifying Prerequisites" on page 5
- "(Optional) Installing the MPT Software Into a Nondefault Working Directory" on page 6
- "Adjusting File Resource Limits" on page 9
- "Completing the Configuration" on page 10

#### **Verifying Prerequisites**

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

**Procedure 1-2** To verify prerequisites

- 1. As the root user, log into the SGI UV computer.
- 2. Verify that you have one of the following operating system software packages installed and configured:

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- Red Hat Enterprise Linux (RHEL) 7 or 6
- SLES 12 or 11

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

```
# cat /etc/*release
```

Type the following command to verify that the HPE Performance MPI 1.0 release is installed:

```
# cat /etc/sgi-mpi-release
HPE Performance Software - Message Passing Interface 1.0
SGI MPI 1.14, Build xxxxxx.sles12sp2-xxxxxxxxxx
```

- 4. Proceed to one of the following:
  - "(Optional) Installing the MPT Software Into a Nondefault Working Directory" on page 6, which explains how to configure MPT in a way that lets you maintain more than one released version of the software on your SGI UV computer system.
  - "Adjusting File Resource Limits" on page 9, which assumes you want the MPT software to remain in the default installation directory.

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

Perform the procedure in this topic if you want to install MPT into a custom, nondefault working directory. You might want to perform the procedure in this topic if, for example, you have a nondefault filesystem or if you want to use HPE Performance MPI on one of the following platforms:

- HPE Apollo 6500 system
- HPE Apollo 6000 system
- HPE Apollo 2000 system

The RPM utility enables you to create, install, and manage relocatable packages. You can install a matched set of MPT RPMs in either the default location or an alternate location. The default location for installing the MPT RPM is /opt/hpe/hpc/mpt-2.rel\_level. To install the MPT RPM in an alternate

location, use the --relocate parameter to the rpm command. The --relocate parameter specifies an alternate base directory for the MPT software installation.

Either /opt/hpe/hpc/mpt/mpt-2.rel\_level or both /opt/hpe/hpc/mpt/mpt-2.rel\_level and

/usr/share/modules/modulefiles/mpt can be relocated. The post installation script reconfigures the module file for the new location as long as the *oldpath* argument in the rpm(8) command precisely matches the description in the RPM info. The general format for the rpm command is as follows:

rpm --relocate oldpath=newpath

• For *oldpath*, specify the MPT software's current location.

If you install the MPT software in an alternate location, the rpm command's *oldpath* argument must precisely match the relocation listed in the RPM for the environment module automatic modification feature to be correct.

• For *newpath*, specify the location to which you want to install the MPT software.

Procedure 1-3 To install the MPT software in an alternate location

1. Plan how to avoid problems related to uninstalled RPM dependencies.

The following are two approaches:

• Option 1: If you install from a system that does not run MPT jobs, it might be appropriate to use the --nodeps parameter on the rpm(8) command line. This parameter directs the rpm(8) command to ignore dependencies.

•

Option 2: If you install from a system or cluster nodes upon which MPT jobs need to run, type the following package manager commands on each cluster node or cluster node image to locally install the needed prerequisites on all the cluster nodes:

- On SLES platforms, type the following command:
  - # zypper install cpuset-utils arraysvcs xpmem libbitmask
- On RHEL platforms, type the following command:
  - # yum install cpuset-utils arraysvcs xpmem libbitmask
- 2. Use the rpm command to specify an alternate location for the MPT software bundle.

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Example 1. The following example shows how to install MPT in /usr/local/hpe/mpt-pt.16 rather than in /opt, which is the default:

```
# rpm -i --relocate /opt/hpe/hpc/mpt/mpt-2.16=/usr/local/hpe/mpt/mpt-2.16 \
sgi-mpt-*.x86.rpm
```

Example 2: The following RHEL example shows how to install the modules, in addition to the total MPT software bundle, to /usr/local/hpe/mpt/mpt-2.16 and /usr/local/mod/mpt-2.16:

```
# rpm -i --relocate /opt/hpe/hpc/mpt/mpt-2.16=/usr/local/hpe/mpt/mpt-2.16 \
--relocate /usr/share/Modules/modulefiles/mpt=/usr/local/mod/mpt-2.16 \
sgi-mpt-*.x86_64.rpm
```

In the preceding RHEL example, note that the Modules directory in the argument to the second --relocate parameter begins with an uppercase letter.

Example 3. The following SLES example shows how to install the modules, in addition to the total MPT software bundle, to /usr/local/hpe/mpt/mpt-2.16 and /usr/local/mod/mpt-2.16:

```
# rpm -i --relocate /opt/hpe/hpc/mpt/mpt-2.16=/usr/local/hpe/mpt/mpt-2.16 \
--relocate /usr/share/modules/modulefiles/mpt=/usr/local/mod/mpt-2.16 \
sgi-mpt-*.x86_64.rpm
```

In the preceding SLES example, note that the modules directory in the argument to the second --relocate parameter begins with a lowercase letter.

Example 4:

The following example rpm command output shows the available relocations:

```
# rpm -qpi sgi-mpt-2.16-sgi*.x86_64.rpm
... Relocations: /opt/hpe/hpc/mpt/mpt-2.16 /usr/share/modules/modulefiles/mpt
```

**Note:** In the preceding output, the example shows only the significant message at the end of the output string.

#### 3. Proceed to the following:

"Adjusting File Resource Limits" on page 9

For more information about using the rpm command, see the rpm man page.

#### **Adjusting File Resource Limits**

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

#### Procedure 1-4 To adjust file resource limits

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

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

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

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

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

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

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

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

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

The preceding line increases the resource limit for locked memory.

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

```
session required /lib/security/pam_limits.so
```

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

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

10. Proceed to the following:

"Completing the Configuration" on page 10

#### **Completing the Configuration**

The following procedure explains how to complete the MPT configuration.

Procedure 1-5 To complete the MPT configuration

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

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

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

• On RHEL platforms:

```
/opt/mpt/mpt-2.16/usr/share/Modules/modulefiles/mpt/mpt-2.16
```

• On SLES platforms:

```
/opt/mpt-2.16/usr/share/modules/modulefiles/mpt/mpt-2.16
```

# **Getting Started**

This chapter includes the following topics:

- "About Running MPI Applications" on page 11
- "Loading the MPI Software Module and Specifying the Library Path" on page 11
- "Compiling and Linking the MPI Program" on page 13
- "Launching the MPI Application" on page 15
- "Compiling and Running OpenSHMEM Applications" on page 21
- "Building MPI Fortran Modules" on page 23
- "Using Huge Pages" on page 25
- "Using HPE Performance MPI in an SELinux Environment (RHEL Platforms Only)" on page 27

# **About Running MPI Applications**

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.

The process of running MPI applications consists of the following procedures:

- "Loading the MPI Software Module and Specifying the Library Path" on page 11
- "Compiling and Linking the MPI Program" on page 13
- "Launching the MPI Application" on page 15

# Loading the MPI Software Module and Specifying the Library Path

You need to ensure that programs can find the MPT library routines when the programs run.

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

The following procedure explains how to specify the path to the MPI libmpi.so library.

#### **Procedure 2-1** To determine the library path

1. (Optional) Set the library path in the mpt module file.

Complete this step if your site uses module files.

Sample module files reside in the following locations:

- /opt/hpe/hpc/mpt/mpt-mpt\_rel/doc
- /usr/share/modules/modulefiles/mpt/mpt\_rel

To load the MPT module, type the following command:

```
% module load mpt
```

2. Determine the directory into which the MPT software is installed.

```
% ldd a.out
libmpi.so => /tmp/usr/lib/libmpi.so (0x40014000)
libmpi.so => /(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 (0x40000000)
```

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.

3. Type the following command to set the library path:

```
% setenv LD LIBRARY PATH /library_path/usr/lib
```

For *library\_path*, type the path to the directory in which the MPT software is installed.

Example 1. The following command uses information from the previous step to set the library path to /tmp/usr/lib:

```
% 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
```

## Compiling and Linking the MPI Program

You can use one of the MPI wrapper compiler commands to run your program, or you can call the compiler directly. The following topics explain these two alternatives:

- "Compiling With the Wrapper Compilers" on page 13
- "Compiling With the GNU or Intel Compilers" on page 14

#### **Compiling With the Wrapper Compilers**

The MPI wrapper compilers automatically incorporate the compiling and linking functions into the compiler command. If possible, use one of the following wrapper compiler commands to run your program:

- mpif08 -I /install\_path/usr/include file.f -L lib\_path/usr/lib
- mpif90 -I /install\_path/usr/include file.f -L lib\_path/usr/lib
- mpicxx -I /install\_path/usr/include file.c -L lib\_path/usr/lib
- mpicc -I /install\_path/usr/include file.c -L lib\_path/usr/lib

The variables in the preceding commands 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 or Fortran program file name.
- For *lib\_path*, type the path to the library files.

For example:

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```
% mpicc -I /tmp/usr/include simple1 mpi.c -L /tmp/usr/lib
```

#### Compiling With the GNU or Intel Compilers

This topic explains how to run an MPI program if you need to call the GNU or Intel compilers directly. When 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 compilers, choose one of the following commands:

```
% icc -o myprog myprog.c -lmpi # C - version 8
% mpif08 simple1_mpi.f # Fortran 2008 wrapper compiler
% mpif90 simple1_mpi.f # Fortran 90 wrapper compiler
% ifort -o myprog myprog.f -lmpi # Fortran - version 8
% mpicc -o myprog myprog.c # MPI C wrapper compiler
% mpicxx -o myprog myprog.C # MPI C++ wrapper compiler
```

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

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

```
% ifort -I/usr/include -o myprog myprog.f -lmpi # version 8
```

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

• The special case of using the Open64 compiler in combination with hybrid MPI/OpenMP applications requires separate compilation and link command lines. The Open64 version of the OpenMP library requires the use of the -openmp

option on the command line for compiling, but it interferes with proper linking of MPI libraries. Use the following sequence:

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

## Launching the MPI Application

You can use either a workload manager or the mpirun command to launch an MPI application.

The following topics explain these alternatives:

- "Using a Workload Manager to Launch an MPI Application" on page 15
- "Using the mpirun Command to Launch an MPI Application" on page 17
- "Using MPI Spawn Functions to Launch an MPI Application" on page 19

#### Using a Workload Manager to Launch an MPI Application

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

- "PBS Professional" on page 15
- "Torque" on page 16
- "Simple Linux Utility for Resource Management (SLURM)" on page 17

#### **PBS Professional**

You can run MPI applications from job scripts that you submit through workload managers such as the PBS Professional workload manager.

Process and thread pinning onto CPUs is especially important on cache-coherent non-uniform memory access (ccNUMA) systems such as 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 if omplace(1) is used.

Example 1. To run an MPI application with 512 processes, include the following in the directive file:

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

Example 2. To run an MPI application with 512 Processes and four OpenMP threads per process, include the following in the directive file:

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

Some third-party debuggers support the <code>mpiexec\_mpt(1)</code> command. The <code>mpiexec\_mpt(1)</code> command includes a <code>-tv</code> option for use with TotalView and includes a <code>-ddt</code> option for use with DDT. For more information, see Chapter 4, "Debugging MPI Applications" on page 39.

PBS Professional includes an mpiexec(1) command that enables you to run HPE Performance Software — Message Passing Interface (HPE Performance MPI) applications. PBS Professional's command does not support the same set of extended options that the mpiexec mpt(1) supports.

For more information about the PBS Professional workload manager, see the following website:

http://www.pbsworks.com/SupportGT.aspx?d=PBS-Professional,-Documentation

#### **Torque**

When running Torque, HPE recommends that you use the following mpiexec\_mpt(1) command to launch MPT jobs:

```
mpiexec mpt [-n P] ./a.out
```

The *P* argument is optional. By default, the program runs with the original number of processes specified on the job initialization in Torque. To use *P*, specify is the total number of MPI processes in the application. This syntax applies whether running on a single host or a clustered system.

For more information, see the <code>mpiexec\_mpt(1)</code> man page. The <code>mpiexec\_mpt</code> command has a <code>-tv</code> option for use by MPT when running the TotalView Debugger with a workoad manager like Torque. For more information about using the <code>mpiexec\_mpt</code> command <code>-tv</code> option, see "Using the TotalView Debugger with MPI Programs" on page 39.

#### Simple Linux Utility for Resource Management (SLURM)

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

For general information about SLURM, see the following website:

http://slurm.schedmd.com

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

http://slurm.schedmd.com/mpi\_guide.html

#### Using the mpirun Command to Launch an MPI Application

The mpirun(1) command starts an MPI application. Use the mpirun(1) command when you are not using a resource manager, such as PBS Professional.

For a complete specification of the command line syntax, see the mpirun(1) man page.

The following topics explain how to use the mpirun command to launch a variety of applications:

- "Launching a Single Program on the Local Host" on page 17
- "Launching a Multiple Program, Multiple Data (MPMD) Application on the Local Host" on page 18
- "Launching a Distributed Application" on page 18

#### 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.

Example 1. The following command 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.

Example 1. The following command runs one copy of prog1 and five copies of prog2 on the local host, and both executable files use shared memory:

```
% mpirun -np 1 prog1 : -np 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 the Array Services software. For a list of the available nodes on systems running Array Services software, type the following command:

```
% ainfo machines
```

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 show various ways to start an application that consists of multiple MPI executable files on multiple hosts.

Example 1. The following command runs ten instances of the a.out file on host a:

```
% mpirun host a -np 10 a.out
```

Example 2. The following command launches ten instances of fred on each of three hosts. fred has two input arguments.

```
% mpirun host_a, host_b, host_c -np 10 fred arg1 arg2
```

Example 3. The following command launches ten instances of fred, with different numbers of instances on each processor:

```
% mpirun host a -np 2, host b -np 3, host c -np 5 fred arg1 arg2
```

Example 4. The following command launches an MPI application on different hosts with different numbers of processes and executable files:

```
% mpirun host_a 6 a.out : host_b -np 26 b.out
```

#### Using MPI Spawn Functions to Launch an MPI Application

The following two functions enable the MPI spawn feature:

- MPI Comm spawn
- MPI Comm spawn multiple

For information about how to use the spawn functions, see the following:

- "Specifying the Universe Size Automatically" on page 19
- "Specifying the Universe Size Directly" on page 20
- "Specifying the Universe Size on the mpirun Command" on page 20
- "Specifying Host Information" on page 20

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

#### Specifying the Universe Size Automatically

You can specify the universe size automatically when you specify the <code>-spawn</code> parameter on the <code>mpiexec\_mpt</code> command and use the following MPI process creation functions:

- MPI Comm spawn
- MPI Comm spawn multiple

For example, assume that when you submitted a job, you specified 10 processes. The following command starts three instances of the mtest MPI application, so the application can spawn seven more:

```
% mpiexec mpt -spawn -np 3 mtest
```

#### Specifying the Universe Size Directly

You can specify the universe size directly by setting one of the following shell variables:

• MPI UNIVERSE SIZE

Set MPI\_UNIVERSE\_SIZE to the maximum number of processes possible in the universe.

• MPI UNIVERSE

Set MPI\_UNIVERSE to control both the universe size and the possible set of hosts that processes can run on.

This variable specifies hosts upon which processes can be launched. The syntax for this variable is a list of hp\_specs without a specified application or argument list. For example:

```
- "host_a, host_b"
- "host_a 8, host_b 16"
- "host_a, host_b 12"
- "host a, host b -np 16"
```

If MPI\_UNIVERSE is not specified, MPI spawn requests place new processes on the local host.

#### Specifying the Universe Size on the mpirun Command

If you use the mpirun command, you can use the -up parameter to specify the universe size.

#### **Specifying Host Information**

You can pass host information to MPI\_Comm\_spawn or MPI\_Comm\_spawn\_multiple in MPI\_info objects. When you use this method, you can specify hosts that are outside of the list of hosts specified to MPI\_UNIVERSE. The following are the supported MPI\_info keys and the values associated with the keys:

Info Key	Value String
hostfile	The name of the file that contains the lists of hosts upon which to spawn MPI processes. Use a space character or a tab character to separate multiple host names.
MPI_SGI_NODELIST	The list of hosts upon which to spawn MPI processes. Use a space character or a tab character to separate multiple host names.

The following examples call MPI\_Comm\_spawn using the MPI\_SGI\_NODELIST and hostlist MPI info objects to specify the hosts on which to launch MPI processes.

#### Example 1:

```
MPI_Info info;
MPI_Info_create(&info);
MPI_Info_set(info, "MPI_SGI_NODELIST", "host_b host_b");
MPI_Comm_spawn("b.out", MPI_ARGV_NULL, 2, info,...);

Example 2:

char * list = "host_b host_b";
int fd = open("list.txt", O_WRONLY);
write(fd, list, strlen(list) + 1);
MPI_Info_set(info, "hostfile", "list.txt");
MPI_Comm_spawn("b.out", MPI_ARGV_NULL, 2, info,...);

% export MPI_UNIVERSE="host_a 4"
% export MPI_UNIVERSE_SIZE=20
% mpiexec_mpt -np 3 coupler
```

The preceding lines run two b.out processes on host\_b. If the coupler program launches any spawn processes that do not specify the desired hosts in their info argument then they are placed within the defined MPI\_UNIVERSE. At any single point in time, the sum of the number of starting processes, processes launched into the hosts in MPI\_UNIVERSE, and hosts launched onto specified hosts cannot be greater than MPI\_UNIVERSE\_SIZE.

## **Compiling and Running OpenSHMEM Applications**

The following procedure explains how to compile and run OpenSHMEM programs in general terms.

#### Procedure 2-2 Compiling and Running OpenSHMEM applications

1. Use one of the OpenSHMEM wrapper compiler commands to run your program or call the compiler directly.

To use the wrapper compiler, use one of the following commands:

- oshcc
- oshCC
- oshfort

To compile the OpenSHMEM program directly, use GNU compiler or Intel compiler commands.

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

```
- g++ compute.C -lsma -lmpi
- gcc compute.c -lsma -lmpi
```

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

```
icc compute.C -lsma -lmpiicc compute.c -lsma -lmpiifort compute.f -lsma -lmpi
```

2. Use the mpirun command or the mpiexec\_mpt command to launch the OpenSHMEM application.

When you are not using a resource manager, such as PBS Professional or SLURM, set the -np option on the command to request the desired number of processes to launch. The NPES variable has no effect on OpenSHMEM programs.

The OpenSHMEM programming model supports single-host OpenSHMEM applications.

For more information, see the intro\_shmem(3) man page.

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## **Building MPI Fortran Modules**

The /opt/hpe/hpc/mpt/mpt-2.16/fortran\_module\_generator directory contains all the source code needed to build your own Fortran modules. This topic explains how to use environment variables and the make(1) command to generate the modules.

The following procedure explains how to build MPI Fortran modules.

#### Procedure 2-3 To build MPI Fortran modules

1. Set the environment variables you need for the compiler and (optionally) for any additional flags you need.

The environment variables are as follows:

Variable	Content
FC	This environment variable is required.
	Set this variable to the compiler command used to generate the modules.
FCFLAGS	This environment variable is optional.
	If you do not set this environment variable, Intel compiler support is assumed, and the system tags buffers with <code>!DEC\$</code> ATTRIBUTES NO_ARG_CHECK.
	If you set this environment variable, set it to one of the following values:
	<ul> <li>USE_GCC_FORTRAN, which tags buffers with the following:</li> </ul>
	!GCC\$ NO_ARG_CHECK
	<ul> <li>USE_PGI_FORTRAN, which tags buffers with the foillowing:</li> </ul>
	!DIR\$ IGNORE_TKR
	• USE_TS29113_FORTRAN, which tags buffers with the following:
	TYPE(*), DIMENSION()

Set FCFLAGS to this value if your compiler supports TS 29113.

Example 1. If you have an Intel compiler that supports TS 29113, specify the following environment variables:

```
FC=ifort FCFLAGS="-DUSE TS29113 FORTRAN" make
```

Example 2. If you have a GNU Fortran compiler, specify the following environment variables:

```
FC=gfortran FCFLAGS="-DUSE_GCC_FORTRAN" make
```

Example 3. If you have a GNU Fortran compiler that supports TS 29113, specify the following environment variables:

```
FC=gfortran FCFLAGS="-DUSE TS29113 FORTRAN" make
```

2. Choose an installation path, and run the following command:

```
DESTDIR=install_path make install
```

For *install\_path*, specify the path to the generated \*.mod files.

For example:

```
% make install DESTDIR=/opt/hpe/hpc/mpt/mpt-2.16/include/custom_dir
```

- 3. Set the MPI\_CUSTOM\_FORTRAN\_MODULES\_PATH environment variable to the directory path you set with the make(1) command.
- 4. Set the MPIF90\_F90 environment variable and the MPIF08\_F08 environment variable to the compiler that you used to generate the Fortran modules.
- 5. Set the LD\_LIBRARY\_PATH environment variable to include MPI\_CUSTOM\_FORTRAN\_MODULES\_PATH.

Make sure that MPI\_CUSTOM\_FORTRAN\_MODULES\_PATH is ordered before MPT's LD LIBRARY PATH. This ordering avoids loading the default libmpi fo8.

That is, if you use the following common idiom, make sure that the following idiom is processed after the MPT module is loaded:

```
LD_LIBRARY_PATH=$MPI_CUSTOM_FORTRAN_MODULES_PATH:$LD_LIBRARY_PATH
```

The HPE Performance MPI compiler helpers automatically detect the path to the HPE Performance MPI Fortran modules you built. Note that the compiler helpers

need to know which compiler you are using. If you do not use mpif90 or mpif08, you can simply use the following compiler options:

- For Fortran 2008, use -I\$MPI\_CUSTOM\_FORTRAN\_MODULES\_PATH -LMPI\_CUSTOM\_FORTRAN\_MODULES\_PATH -lmpi f08
- For Fortran 2003, use -I\$MPI\_CUSTOM\_FORTRAN\_MODULES\_PATH
- 6. (Optional) Update the following environment variables in the module files for your compilers and for your users:
  - MPI CUSTOM FORTRAN MODULES PATH
  - MPIF90 F90
  - MPIF08 F08
  - LD LIBRARY PATH

## **Using Huge Pages**

Huge pages optimize MPI application performance. The

MPI\_HUGEPAGE\_HEAP\_SPACE environment variable defines the minimum amount of heap space each MPI process can 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<sup>2</sup>, 1024<sup>3</sup>, or 1024<sup>4</sup>, respectively.

For information about the  $\texttt{MPI\_HUGEPAGE\_HEAP\_SPACE}$  environment variable, see the mpi(1) man page.

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

Procedure 2-4 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. Log in as the root user, and type the following command to configure the system settings for huge pages:

```
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. Type the following command to retrieve the current system configuration:

```
sys:~ # mpt hugepage config -v
Reading current 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
                                                  (exists)
```

4. When running your MPT program, make sure the MPI HUGEPAGE HEAP SPACE environment variable is set to 1.

This activates the new libmpi huge page heap. Memory allocated by calls to the malloc function are allocated on huge pages.

5. Log in as the root user, and type the following command to clear the system configuration settings:

```
sys:~ # mpt hugepage config -e
Removing MPT huge page configuration
```

6. To verify that the MPT huge page configuration has been cleared, type the following command to retrieve the system configuration again:

```
uv44-sys:~ # mpt hugepage config -v
Reading current system configuration
System config file:
                          /proc/sys/vm/nr overcommit hugepages
Huge Pages Allowed:
                         0 pages (0 KB) 0% of memory
Huge Page Size:
                          2048 KB
Huge TLB FS Directory:
                          /etc/mpt/hugepage mpt (does not exist)
```

26 007-3773-032 For more information about how to configure huge pages for MPI applications, see the mpt hugepage config(1) man page.

## Using HPE Performance MPI in an SELinux Environment (RHEL Platforms Only)

HPE supports Security-Enhanced Linux (SELinux) for single-host runs on SGI computer systems that run the Red Hat Enterprise Linux (RHEL) operating system. The following guidelines pertain to using SELinux:

- Configure SELinux. For configuration information, see the following manual:
   SGI UV System Software Installation and Configuration Guide
- Set the MPI USE ARRAY environment variable as follows:

```
MPI_USE_ARRAY=false
```

When set to false, Array Services is disabled. For more information about this environment variable, see the MPI(1) man page.

For more information about how to run HPE Performance MPI with security software, contact your technical support representative.

## **Using HPE Performance MPI With NVIDIA GPUs**

HPE Performance MPI supports the use of data buffers in graphics processing unit (GPU) memory as the source or target of data movement by MPI or OpenSHMEM functions. To enable this feature, set MPI USE CUDA=true.

If your program sends GPU data to other hosts over Mellanox InfiniBand connections, HPE Performance MPI supports the GPUDirect RDMA feature.

For more information, see the documentation from NVIDIA and Mellanox about GPUDirect RDMA.

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# Programming With the HPE Performance Software — Message Passing Interface (HPE Performance MPI)

This chapter includes the following topics:

- "About Programming With HPE Performance MPI" on page 29
- "Job Termination and Error Handling" on page 29
- "Signals" on page 31
- "Buffering" on page 31
- "Multithreaded Programming" on page 32
- "Interoperability with the OpenSHMEM programming model" on page 33
- "Miscellaneous HPE Performance MPI Features" on page 33
- "Programming Optimizations" on page 34
- "Additional Programming Model Considerations" on page 37

## **About Programming With HPE Performance 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. This chapter's topics explain how to develop or port MPI applications to SGI systems.

## **Job Termination and Error Handling**

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

This section includes the following topics:

- "MPI Abort" on page 30
- "Error Handling" on page 30
- "MPI Finalize and Connect Processes" on page 31

#### MPI\_Abort

In the HPE Performance MPI implementation, a call to MPI\_Abort has the following effect:

- The MPI job terminates, regardless of the communicator argument used.
- The error code value is returned as the exit status of the mpirun command.
- A stack traceback is displayed that shows where the program called MPI Abort.

#### **Error Handling**

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

The HPE Performance MPI implementation provides the following predefined error handlers:

- MPI\_ERRORS\_ARE\_FATAL. 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. This 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.

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#### MPI Finalize and Connect Processes

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

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

## **Signals**

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

In addition, certain 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. These signals are as follows:

- SIGURG
- SIGUSR1
- SIGINT
- SIGTERM

To use this feature, the MPI program must have a signal handler that catches the signal. When the signal is sent to the mpirun process ID, the mpirun process catches the signal and propagates it to all MPI processes.

## **Buffering**

Most MPI implementations use buffering for overall performance reasons, and some programs depend on it. However, you should not assume that there is any message buffering between processes because the MPI Standard does not mandate a buffering

strategy. Table 3-1 on page 32 illustrates a simple sequence of MPI operations that cannot work unless messages are buffered. If sent messages are not buffered, each process hangs in the initial call, waiting for an MPI Recy call to take the message.

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

Table 3-1 Outline of Improper Dependence on Buffering

Process 1	Process 2
MPI_Send(2,)	MPI_Send(1,)
MPI_Recv(2,)	MPI_Recv(1,)

By default, the HPE 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 34.

## **Multithreaded Programming**

HPE Performance MPI supports a hybrid programming model, in which MPI handles one level of parallelism in an application and 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 as follows:

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- If you use the compiler wrappers for MPI or SHMEM, use the -mt option on the command line.
- If you want to call the compilers directly, use the <code>-lmpi\_mt</code> parameter instead of the <code>-lmpi</code> parameter on the compiler command line.

For more information about compiling and linking MPI programs, see the mpi(1) man page.

## Interoperability with the OpenSHMEM programming model

You can mix OpenSHMEM and MPI message passing in the same program. The application must be linked with both the OpenSHMEM and MPI libraries.

Start with an MPI program that calls MPI\_Init (or MPI\_Init\_thread()) and MPI\_Finalize. Next, add OpenSHMEM calls, and be aware that the PE numbers are equal to the MPI rank numbers in MPI COMM WORLD.

If your program uses both OpenSHMEM and MPI, make sure your program includes calls to the <code>shmem\_init()</code> and <code>shmem\_finalize()</code> library routines. This practice is similar to how you include calls to <code>MPI\_Init()</code> (or <code>MPI\_Init\_thread())</code> and <code>MPI Finalize</code>.

When running the application across a cluster using OpenSHMEM and OpenSHMEM functions, some processes might not be able to communicate with other processes. You can use the <code>shmem\_pe\_accessible</code> and <code>shmem\_addr\_accessible</code> functions to determine whether an OpenSHMEM call can be used to access data residing in another process. Because the OpenSHMEM model functions only with respect to <code>MPI\_COMM\_WORLD</code>, these functions cannot be used to exchange data between MPI processes that are connected via MPI intercommunicators returned from MPI spawn-related functions.

For more information about the OpenSHMEM programming model, see the intro shmem(3) man page.

#### Miscellaneous HPE Performance MPI Features

The following other characteristics of the HPE Performance MPI implementation might interest you:

• stdin/stdout/stderr.

In this implementation, stdin is enabled for only the process that is rank 0 in the first MPI\_COMM\_WORLD. Such processes do not need to be located on the same host as mpirun. The stdout and stderr results are enabled for all MPI processes in the job, whether started by mpirun or started by one of the MPI spawn functions.

• MPI Get processor name

The MPI\_Get\_processor\_name function returns the Internet host name of the computer upon which the MPI process that started this subroutine is running.

## **Programming Optimizations**

You might need to modify your MPI application to use the HPE Performance MPI optimization features.

The following topics describe how to use the optimized features of HPE's MPI implementation:

- "Using MPI Point-to-Point Communication Routines" on page 34
- "Using MPI Collective Communication Routines" on page 35
- "Using MPI Pack/MPI Unpack" on page 35
- "Avoiding Derived Data Types" on page 36
- "About Wild Cards" on page 36
- "Avoiding Message Buffering Single Copy Methods" on page 36
- "Managing Memory Placement" on page 37

#### **Using MPI Point-to-Point Communication Routines**

MPI provides 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.

HPE's MPI 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. The MPI\_Alltoall routines also use special techniques to avoid message buffering when using shared memory. For more information, see "Avoiding Message Buffering — Single Copy Methods" on page 36.

#### 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. Generally, either restructure your data or use derived data

types to avoid using these functions. 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 HPE implementation, using derived data types does not generally lead to performance gains. Using derived data types might disable certain types of optimizations, for example, unbuffered or single copy data transfer.

#### **About 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.

MPT can make certain optimizations if the application does not make calls to variations of MPI\_Recv() with MPI\_ANY\_SOURCE. When MPI\_WILDCARDS=false is in effect, MPT assumes that the application does not contain receive calls with rank wild cards. This assumption enables MPT to make some bandwidth optimizations in its Intel Omni-Path Architecture code. MPT supports the MPI\_WILDCARDS environment variable only on systems that include the Intel Omni-Path Architecture. For information about more environment variables that MPT supports on the Intel Onmi-Path Architecture, see the following:

"Tuning for Running Applications Over the Intel Omni-Path Interconnect" on page 61

#### Avoiding Message Buffering — Single Copy Methods

One of the most significant optimizations for bandwidth-sensitive applications in the MPI library is single-copy optimization, which avoids using shared memory buffers. However, as discussed in "Buffering" on page 31, 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.

• The sender data must be globally accessible by the receiver. The HPE Performance 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 52.

#### **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. To control the placement of the application at run time, however, see Chapter 7, "Run-time Tuning" on page 49.

## **Additional Programming Model Considerations**

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

Alternately, you might consider exploiting the shared memory architecture of SGI systems by handling one or more levels of parallelism with OpenMP, with the coarser grained levels of parallelism being handled by MPI. Also, there are special ccNUMA placement considerations to be aware of when running hybrid MPI/OpenMP applications. For further information, see Chapter 7, "Run-time Tuning" on page 49.

## **Debugging MPI Applications**

This chapter includes the following topics:

- "MPI Routine Argument Checking" on page 39
- "Using the TotalView Debugger with MPI Programs" on page 39
- "Using idb and gdb with MPI Programs" on page 40
- "Using the DDT Debugger with MPI Programs" on page 40
- "Using Valgrind With MPI Programs" on page 41

## **MPI Routine Argument Checking**

Debugging MPI applications can be more challenging than debugging sequential applications. By default, the HPE Performance Software — Message Passing Interface (HPE Performance 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 HPE Performance 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 Message Passing Toolkit (MPT) <code>mpiexec\_mpt(1)</code> command has a <code>-tv</code> option for use by MPT with the TotalView Debugger. Note that the PBS Professional <code>mpiexec(1)</code> command does not support the <code>-tv</code> option. TotalView does not operate with MPI processes started via the <code>MPI\_Comm\_spawn</code> or <code>MPI\_Comm\_spawn</code> multiple functions.

Example 1. To run an MPT MPI job with TotalView without a workload manager, type the following:

% totalview mpirun -a -np 4 a.out

Example 2. 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 MPT. You can run DDT in either interactive (online) or batch (offline) mode. In batch mode, DDT can create a text or HTML report that tracks variable values and shows the location of any errors. DDT records the data for a program's variables across all processes, and DDT logs values in the HTML output files as sparkline charts.

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

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

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

```
# ddt -np 4 a.out
```

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

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

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

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

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

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

## **Using Valgrind With MPI Programs**

Valgrind is a tool that can profile your program and can automatically detect memory management and threading bugs.

Valgrind is not compatible with the memory mapping functionality in MPT. When MPT detects that Valgrind is in use, MPT automatically enables the MPI\_MEMMAP\_OFF environment variable, which disables MPT's own memory mapping.

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## Using perfboost

This chapter includes the following topics:

- "About perfboost" on page 43
- "Using perfboost" on page 43
- "MPI Supported Functions" on page 44

## About perfboost

The performance boosting tool, perfboost, uses a wrapper library to run applications compiled against other Message Passing Interface (MPI) implementations under the Message Passing Toolkit (MPT) product on HPE hardware platforms. This chapter describes how to use perfboost.

Note: perfboost does not support the MPI C++ API.

## Using perfboost

The following procedure explains how to use perfboost with an HPE Performance Software — Message Passing Interface (HPE Performance MPI) program.

Procedure 5-1 To use perfboost

1. Load the perfboost environment module.

The module include the PERFBOOST VERBOSE environment variable.

If you set the PERFBOOST\_VERBOSE environment variable, it enables a message when PerfBoost activates and also when the MPI application is completed through the MPI\_Finalize() function. This message indicates that the perfboost library is active and also indicates when the MPI application completes through the libperfboost wrapper library.

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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 MPT are currently not supported.

**Note:** Some applications redirect stderr. In this case, the verbose messages might not appear in the application output.

2. Type a command that inserts the perfboost command in front of the executable name along with the choice of MPI implementation to emulate.

In other words, run the executable file with the MPT  $mpiexec\_mpt(1)$  or the mpirun(1) command.

The following are MPI implementations and corresponding command line options:

Implementation	<b>Command Line Option</b>
Platform MPI 7.1+	-pmpi
Intel MPI	-impi
OpenMPI	-ompi
MPICH1	-mpich
MPICH2, version 2 and later	-impi
MVAPICH2, version 2 and later	-impi

The following are some examples that use perfboost:

```
% module load mpt
% module load perfboost

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

## **MPI Supported Functions**

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 customer support center at the following website to schedule a missing function to be added to perfboost:

https://support.sgi.com/caselist

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## **Berkeley Lab Checkpoint/Restart (BLCR)**

This chapter includes the following topics:

- "About BLCR" on page 47
- "BLCR Installation" on page 47
- "Using BLCR with MPT" on page 48

#### **About BLCR**

The Message Passing Toolkit (MPT) supports BLCR checkpoint/restart. This checkpoint/restart implementation allows applications to periodically save a copy of their state. Applications can resume from that point if the application crashes or if 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, the Message Passing Interface (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 the following:

http://crd.lbl.gov/departments/computer-science/CLaSS/research/BLCR/

#### **BLCR Installation**

To use checkpoint/restart with MPT, BLCR must first be installed.

Procedure 6-1 To install BCLR

1. Log in as the root user.

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2. Install the blcr-, blcr-libs-, and blcr-kmp- RPMs.

BLCR uses a kernel module that must be built against the specific kernel that the operating system is running. If the kernel module fails to load, you need to rebuild and reinstall. Install the blcr- source RPM. 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.

3. Type the following command to enable BLCR:

```
# chkconfig blcr on
```

## **Using BLCR with MPT**

To enable checkpoint/restart within MPT, you need to pass the -cpr option to mpirun or mpiexec\_mpt. For example:

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

To checkpoint a job, run the mpt\_checkpoint command on the same host upon which mpirun is running. Make sure to pass the mpt\_checkpoint command the PID of mpirun and the name with which you want to prefix all the checkpoint files. For example:

```
% mpt checkpoint -p 12345 -f my checkpoint
```

The preceding example command creates 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
```

You can restart the job on a different set of hosts, but the number of hosts must be the same. In addition, 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 includes the following topics:

- "About Run-time Tuning" on page 49
- "Reducing Run-time Variability" on page 50
- "Tuning MPI Buffer Resources" on page 51
- "Avoiding Message Buffering Enabling Single Copy" on page 52
- "Memory Placement and Policies" on page 53
- "Tuning MPI/OpenMP Hybrid Codes" on page 55
- "Tuning Running Applications Across Multiple Hosts" on page 57
- "Tuning for Running Applications over the InfiniBand Interconnect" on page 59
- "MPI on SGI UV Systems" on page 62
- "Measuring Parallelization and Parallelizing Your Code" on page 64
- "Suspending MPI Jobs" on page 67

## **About Run-time Tuning**

This chapter describes the ways in which a user can tune the run-time environment to improve the performance of a Message Passing Interface (MPI) message passing application on SGI hardware platforms. None of these ways involve application code changes.

The run-time tuning topics are as follows:

- "Reducing Run-time Variability" on page 50
- "Tuning MPI Buffer Resources" on page 51
- "Avoiding Message Buffering Enabling Single Copy" on page 52
- "Memory Placement and Policies" on page 53
- "Tuning MPI/OpenMP Hybrid Codes" on page 55

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- "Tuning Running Applications Across Multiple Hosts" on page 57
- "Tuning for Running Applications over the InfiniBand Interconnect" on page 59
- "Tuning for Running Applications Over the Intel Omni-Path Interconnect" on page 61
- "MPI on SGI UV Systems" on page 62
- "Suspending MPI Jobs" on page 67

## **Reducing Run-time Variability**

One of the most common problems with optimizing message passing codes on large, shared-memory computers is to achieve 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, leads to variations in the results, and leads to 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 also known as the kernel node.
  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 of the kernel node, you can
  avoid this effect.
  - By restricting system daemons to run on the kernel node, you can also deliver an additional percentage of each application CPU to the user program.
- Avoid interference with other applications. If necessary, use cpusets to address this
  problem. The cpuset software enables you to partition a large, distributed memory
  host in a fashion that minimizes interactions between jobs running concurrently on
  the system. For more information about cpusets, see the following:
  - HPE Performance Software Message Passing Interface Cpuset Software Guide
- On a quiet, dedicated system, you can use the dplace(1) tool or the MPI\_DSM\_CPULIST environment variable to improve run-time performance repeatability. These approaches are not suited to shared, nondedicated systems.

 Use a workload manager such as Platform LSF from IBM or PBS Professional from Altair Engineering, Inc. These workload managers use cpusets to avoid oversubscribing the system and to avoid possible interference between applications.

# **Tuning MPI Buffer Resources**

By default, the HPE Performance Software — Message Passing Interface (HPE Performance 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 76.

For information about buffering considerations when running an MPI job across multiple hosts, see "Tuning Running Applications Across Multiple Hosts" on page 57.

For information about the programming implications of message buffering, see "Buffering" on page 31.

# **Avoiding Message Buffering – Enabling Single Copy**

It is possible to avoid the need to buffer messages for message transfers between MPI processes within the same host or message transfers that use devices that support remote direct memory access (RDMA), such as InfiniBand.

The following topics provide more information about buffering:

- "Buffering and MPI Send" on page 52
- "Using the XPMEM Driver for Single Copy Optimization" on page 52

### Buffering and MPI Send

Many MPI applications are written to assume infinite buffering, so message buffering is not enabled 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 uses the XPMEM driver to support single-copy message transfers between two processes within the same host.

Enabling single-copy transfers can increase performance because this technique improves MPI's bandwidth. On the other hand, single-copy transfers can introduce additional synchronization points, which can reduce application performance.

The MPI\_BUFFER\_MAX environment variable specifies the threshold for message lengths. Its value should be set to the message length, in bytes, beyond which you want MPI to use the single-copy method. 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 between processes residing on the same host, MPI uses the bcopy process to copy the data. The bcopy process also transfers data between two different executable files on the same host. For data residing outside of a mapped region (a /dev/zero region, for example), MPI uses a buffering technique to transfer the data.

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

# **Memory Placement and Policies**

The MPI library takes advantage of NUMA placement functions that are available. Usually, the default placement is adequate. However, you can set one or more environment variables to modify the default behavior.

For a complete list of the environment variables that control memory placement, see the MPI(1) man page.

The following topics contain information on environment variables and tools that enable you to tune memory placement:

- "MPI\_DSM\_CPULIST" on page 53
- "MPI DSM DISTRIBUTE" on page 55
- "MPI DSM VERBOSE" on page 55
- "Using dplace" on page 55

#### MPI DSM CPULIST

The MPI\_DSM\_CPULIST environment variable allows you to select the 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.

The setting is an ordered list that uses commas (,) and hyphens (-) to specify a mapping of MPI processes to CPUs. If running across multiple hosts, separate the per-host components of the CPU list with a colon (:). Wen using a hyphen-delineated list, you can specify CPU striding by specifying /stride\_distance after the list.

#### For example:

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

Note that the process rank is the MPI\_COMM\_WORLD rank. The interpretation of the CPU values specified in the MPI\_DSM\_CPULIST depends on whether the MPI job is being run within a cpuset, as follows:

- 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.
- If the job is run 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 are 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

The MPI\_DSM\_DISTRIBUTE environment variable ensures that each MPI process gets a physical CPU and memory on the node to which it was assigned.

MPI DSM DISTRIBUTE assigns MPI ranks, as follows:

- On systems that do not include InfiniBand interconnect, MPI\_DSM\_DISTRIBUTE
  assigns MPI ranks starting at logical CPU 0 and incrementing until all ranks have
  been placed.
- On systems that include InfiniBand interconnect, if the job spans hosts, MPI\_DSM\_DISTRIBUTE assigns MPI ranks starting with the CPU that is closest to the first InfiniBand host channel adapter (HCA).

If you set both MPI\_DSM\_DISTRIBUTE and MPI\_DSM\_CPULIST, MPI\_DSM\_CPULIST overrides MPI DSM DISTRIBUTE.

#### MPI DSM VERBOSE

Setting the MPI\_DSM\_VERBOSE environment variable directs MPI to display a synopsis of the NUMA and host placement options being used at run time.

#### Using dplace

The dplace tool offers another way to specify the placement of MPI processes within a distributed memory host. The dplace tool and MPI interoperate, and allow MPI to better manage placement of certain shared memory data structures.

For information about dplace with MPI, see the following:

- "dplace Command" on page 106
- The dplace(1) man page.
- 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 that uses MPI.

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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 pinning ensures that all local, non-shared memory is allocated on the same memory node as the processor referencing the memory. For all systems, pinning can ensure that some or all of the OpenMP threads stay on processors that share a bus or perhaps a processor cache, which can speed up thread synchronization.

The Message Passing Toolkit (MPT) provides the omplace(1) command to help with the placement of OpenMP threads within an MPI program. The omplace(1) 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 more information, see the following:

- "NUMA Tools" on page 105
- The omplace(1) man page.
- The dplace(1) man page.
- The Linux Application Tuning Guide for SGI X86-64 Based Systems.
- The HPE Performance Software Message Passing Interface Cpuset Software Guide.

#### **Example 7-1** Running a Hybrid MPI/OpenMP Application

The following command line runs 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 hybrid MPI/OpenMP job, use the following resource allocation specification:

```
#PBS -l select=8:ncpus=2
```

• In addition, use the following mpiexec mpt command:

```
mpiexec_mpt -n 8 omplace -nt 2 ./a.out
```

For more information about running MPT programs with PBS, see the following:

"Using a Workload Manager to Launch an MPI Application" on page 15

# **Tuning Running Applications Across Multiple Hosts**

When you run an MPI application across a cluster of hosts, you can use the environment variables in this topic to improve application performance across these hosts.

Table 7-1 on page 57 shows the interconnect types and the run-time environment settings and configurations that you can use to improve performance.

Table 7-1 Available Interconnects and the Inquiry Order for Available Interconnects

Interconnect Type	Default Order of Selection	Environment Variable Required
XPMEM	1	MPI_USE_XPMEM
Intel Omni-Path Architecture	2	MPI_USE_OPA
InfiniBand	3	MPI_USE_IB
InfiniBand Unreliable Datagram	4	MPI_USE_UD
TCP/IP	5	MPI_USE_TCP

Table 7-1 on page 57 shows the different types of interconnects that systems can employ as the multihost interconnect. When launched as a distributed application, MPI probes for these interconnects at job startup. For information about how to launch a distributed application, see "Using the mpirun Command to Launch an MPI Application" on page 17.

When MPI detects a high-performance interconnect, MPI attempts to use this interconnect, if it is available, on every host being used by the MPI job. If the interconnect is not available for use on every host, the library attempts to use the next slower interconnect until this connectivity requirement is met. Table 7-1 on page 57 specifies the order in which MPI probes for available interconnects.

The third column of Table 7-1 on page 57 indicates the environment variable you can set to pick a particular interconnect other than the default. In general, to insure the best application performance, 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.

The following environment variables enable you to tune your application for multiple hosts:

#### Variable Purpose

MPI IB RAILS

When set to 1 and the MPI library uses the InfiniBand driver as the inter-host interconnect, MPT sends InfiniBand traffic over the first fabric that it detects. Default on all SGI UV systems.

When set to 1+, MPT sends all traffic across the first fabric, but if it encounters communication problems, it starts to use both fabrics.

When set to 2, the library tries to use multiple, available, separate, InfiniBand fabrics and splits the traffic across them.

MPI\_IB\_SINGLE\_COPY\_BUFFER\_MAX

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

The default is 32767.

MPI\_USE\_IB

When set, the MPI library uses 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() actions occur after InfiniBand resources have been allocated.

The default is false.

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 you run an MPI application across a cluster of hosts using the InfiniBand interconnect, there are run-time environment variables that you can set to to improve application performance. The following are these variables:

#### Variable Purpose

MPI HCOLL IB OFFLOAD

Enables or disables the Mellanox fabric collectives accelerator (FCA) offload. If FCA offload is configured on your cluster, set MPI HCOLL IB OFFLOAD=true.

Make sure that the Mellanox HCOLL libraries are specified in your library path. You can do this by either loading the hpcx software module, if available, or by making sure that the location of libhcoll.so is in your LD LIBRARY PATH environment variable.

The default is  ${\tt MPI\_COLL\_HCOLL=false}.$ 

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 can be prodigious. When the number of ranks is set to at least this value, the MPI library creates InfiniBand connections on a demand basis. The default is 1025 ranks.

MPI\_IB\_FAILOVER

When the MPI library uses InfiniBand fabric and this variable is set, if an InfiniBand transmission error occurs, MPT tries to restart the connection to the other rank a certain number of times. The

MPI\_IB\_FAILOVER variable specifies the number of times MPT tries to restart the connection. MPT can handle a number of errors of this type between any pair of ranks equal to the value of this variable. The default is 32 times.

MPI\_IB\_PAYLOAD

When the MPI library uses InfiniBand fabric, it allocates 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 16512 bytes.

MPI IB RNR TIMER

When a packet arrives at an InfiniBand host channel adaptor (HCA) and there are no remaining receive buffers for it, the receiving HCA sends a negative acknowledgement (NAK) to the requestor. The requesting HCA tries again after some period of time, and this variable controls the delay time.

If you set a value higher than the default, performance can degrade in some circumstances. The higher value, however, is likely to improve fabric health significantly during high congestion. For precise translations of this value to delay times, see Table 45 of the official InfiniBand specification. The default is 14.

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 the wait period. The time spent is equal to  $4.096 \times 2^n$ , where n is specified by the MPI\_IB\_TIMEOUT variable. By default, the variable is set to 18, and the time spent is expressed in microseconds.

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 environment variable controls the size of the cache. If the application rarely reuses data buffers, it may make sense to set this value to 0 to

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avoid cache trashing. By default, this variable is set to 1024 (1K). The possible range is from 0 to 8192 (8K).

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.

## Tuning for Running Applications Over the Intel Omni-Path Interconnect

When you run an MPI application across a cluster of hosts using the Intel Omni-Path interconnect, there are run-time environment variables that you can set to to improve application performance. The following are these variables:

#### Variable Purpose

MPI OPA PAYLOAD

When the MPI library uses Intel Omni-Path fabric, it allocates memory for each message header that it uses for transfer. If the size of the 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, the message is sent through remote direct memory access (RDMA) operations. The default is 16512 bytes.

MPI\_OPA\_SINGLE\_COPY\_BUFFER\_MAX

If MPI transfers data over Intel Omni-Path fabric and if the size of the cumulative data is greater than this value, then MPI attempts to send the data directly between the processes's buffers and not through intermediate buffers inside the MPI library. The default is 32767.

MPI\_WILDCARDS

If MPT can assume that an application does not make receive calls with rank wild cards, then MPT can perform some automatic optimizations. For more information, see the following:

#### "About Wild Cards" on page 36

## MPI on SGI UV Systems

The  $SGI^{\otimes}$   $UV^{\text{\tiny IM}}$  series systems are scalable, nonuniform memory access (NUMA) systems that support a single Linux image of thousands of processors distributed over many sockets and many SGI UV hub application-specific integrated circuits (ASICs). The SGI 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. Typically, each SGI UV hub connects to two sockets. All communication between the sockets and the SGI UV hub uses Intel QuickPath Interconnect (QPI) channels. The following information pertains to specific SGI UV systems:

- On SGI UV 3000 systems and SGI UV 300 systems, the SGI UV hub board assembly has an SGI UV hub ASIC with two identical hubs. Each hub supports one 9.6 GT/s QPI channel to a processor socket. On SGI UV 3000 systems and the SGI UV 300 systems, the hub has eight NUMAlink 7 ports that connect with the NUMAlink 7 interconnect fabric.
- On SGI UV 2000 systems, the SGI UV hub board assembly has an SGI UV 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 eight NUMAlink 6 ports that connect with the NUMAlink 6 interconnect fabric.
- The SGI UV 1000 system's hub has four NUMAlink 5 ports that connect with the NUMAlink 5 interconnect fabric.

The SGI 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.

When MPI communicates between processes on an SGI UV system, it uses the shared memory transfer method.

For more information about the SGI UV hub, SGI UV compute blades, QPI, and NUMAlink 5, or NUMAlink 6, see your hardware documentation.

The following topics contain more information about using MPI on SGI UV systems:

- "General Considerations" on page 63
- "Performance Problems and Corrective Actions" on page 63

• "Other ccNUMA Performance Considerations" on page 64

#### **General Considerations**

To run an MPI job optimally on an SGI UV system, it is best to pin MPI processes to CPUs and isolate multiple MPI jobs onto different sets of sockets and hubs. To accomplish this, you can configure 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 the following:

- MPI\_DSM\_CPULIST. For more information, see "MPI\_DSM\_CPULIST" on page 53.
- omplace(1)
- dplace(1)

### **Performance Problems and Corrective Actions**

The MPI library chooses buffer sizes and communication algorithms in an attempt to deliver the best performance to a wide variety of MPI applications automatically. The following list of performance problems can be remedied:

· 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 can be accomplished by scheduling MPI jobs as if only half the full number exist, leaving the high logical CPUs idle. You can use the <code>cpumap(1)</code> command to determine if cores have multiple HyperThreads on your SGI UV system. The output shows the following:

- The number of physical and logical processors.
- Whether HyperThreading is on or off.
- The way in which shared processors are paired. This information appears towards the bottom of the command's output.
- MPI large message bandwidth is inappropriate.

Some programs transfer large messages via the MPI\_Send function. To use unbuffered, single-copy transport in these cases, set MPI\_BUFFER\_MAX=0. For more information, see MPI(1).

MPI small or near messages are very frequent.

For small fabric hop counts, use shared memory message delivery. To deliver all messages within an SGI UV host via shared memory, set MPI SHARED NEIGHBORHOOD=HOST. For more information, see MPI(1).

#### Other ccNUMA Performance Considerations

MPI application processes typically perform better if their local memory is allocated on the socket assigned to execute the process. This cannot happen if memory on that socket is exhausted, either by the application itself or by other system consumption (for example, by file buffer cache).

You can use the nodeinfo(1) command to view memory consumption on the nodes assigned to your job, and you can use the bcfree(1)bcfree command to clear out excessive file buffer cache. PBS Professional workload manager installations can be configured to issue bcfree(1) commands in the job prologue.

For more information, see the PBS Professional documentation and bcfree(1).

# Measuring Parallelization and Parallelizing Your Code

When tuning for performance, first assess the amount of code that is parallelized in your program. Use the following formula to calculate the amount of code that is parallelized:

```
p=N(T(1)-T(N)) / T(1)(N-1)
```

In this equation, T(1) is the time the code runs on a single CPU and T(N) is the time it runs on N CPUs. Speedup is defined as T(1)/T(N).

If speedup/N is less than 50% (that is, N>(2-p)/(1-p)), stop using more CPUs and tune for better scalability.

You can use one of the following to display CPU activity:

• The top(1) command.

- The vmstat(8) command.
- The open source Performance Co-Pilot tools. For example, pmval(1) (pmval kernel.percpu.cpu.user) or the visualization command pmchart(1).

Next, focus on using one of the following parallelization methodologies:

- "Using SGI MPI" on page 65
- "Using OpenMP" on page 65
- "Identifying OpenMP Nested Parallelism" on page 66
- "Using Compiler Options" on page 66
- "Identifying Opportunities for Loop Parallelism in Existing Code" on page 67

#### **Using SGI MPI**

The SGI Performance Suite includes the SGI Message Passing Toolkit (SGI MPT). SGI MPT includes both the SGI Message Passing Interface (SGI MPI) and SGI SHMEM. SGI MPI is optimized and more scalable for SGI UV series systems than the generic MPI libraries. SGI MPI takes advantage of the SGI UV architecture and SGI nonuniform memory access (NUMA) features.

Use the -lmpi compiler option to use MPI. For a list of environment variables that are supported, see the mpi(1) man page.

The MPIO\_DIRECT\_READ and MPIO\_DIRECT\_WRITE environment variables are supported under Linux for local XFS filesystems in SGI MPT version 1.6.1 and beyond.

MPI provides the MPI-2 standard MPI I/O functions that provide file read and write capabilities. A number of environment variables are available to tune MPI I/O performance. The mpi io(3) man page describes these environment variables.

For information about performance tuning for MPI applications, see the following:

• HPE Performance Software - Message Passing Interface MPInside Reference Guide

#### **Using OpenMP**

OpenMP is a shared memory multiprocessing API, which standardizes existing practice. It is scalable for fine or coarse grain parallelism with an emphasis on performance. It exploits the strengths of shared memory and is directive-based. The

OpenMP implementation also contains library calls and environment variables. OpenMP is included with the C, C++, and Fortran compilers.

To use OpenMP directives, specify the ifort -openmp or icc -openmp compiler options. These options use the OpenMP front-end that is built into the Intel compilers. The latest Intel compiler OpenMP run-time library name is libiomp5.so. The latest Intel compiler also supports the GNU OpenMP library as an either/or option, in other words, do not mix-and-match the GNU library with the Intel version.

For more information, see the OpenMP standard at the following website:

http://www.openmp.org/wp/openmp-specifications

### **Identifying OpenMP Nested Parallelism**

The following Open MP nested parallelism output shows two primary threads and four secondary threads, called master/nested:

```
% cat place_nested
```

firsttask cpu=0

```
thread name=a.out oncpu=0 cpu=4 noplace=1 exact onetime thread name=a.out oncpu=0 cpu=1-3 exact thread name=a.out oncpu=4 cpu=5-7 exact

% dplace -p place_nested a.out

Master thread 0 running on cpu 0

Master thread 1 running on cpu 4

Nested thread 0 of master 0 gets task 0 on cpu 0 Nested thread 1 of master 0 gets task 1 on cpu 1

Nested thread 2 of master 0 gets task 2 on cpu 2 Nested thread 3 of master 0 gets task 3 on cpu 3

Nested thread 0 of master 1 gets task 0 on cpu 4 Nested thread 1 of master 1 gets task 1 on cpu 5
```

Nested thread 2 of master 1 gets task 2 on cpu 6 Nested thread 3 of master 1 gets task 3 on cpu 7

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

#### **Using Compiler Options**

You can use compiler options to invoke automatic parallelization. Use the <code>-parallel</code> or <code>-par\_report</code> options to the <code>ifort</code> or <code>icc</code> compiler commands. These options show which loops were parallelized and the reasons why some loops were not parallelized. If a source file contains many loops, it might be necessary to add the <code>-override\_limits</code> flag to enable automatic parallelization. The code generated by the <code>-parallel</code> option is based on the OpenMP API. The standard OpenMP environment variables and Intel extensions apply.

There are some limitations to automatic parallelization:

- For Fortran codes, only DO loops are analyzed
- For C/C++ codes, only for loops using explicit array notation or those using pointer increment notation are analyzed. In addition, for loops using pointer arithmetic notation are not analyzed, nor does it analyze while or do while loops. The compiler also does not check for blocks of code that can be run in parallel.

### Identifying Opportunities for Loop Parallelism in Existing Code

Another parallelization optimization technique is to identify loops that have a potential for parallelism, such as the following:

- Loops without data dependencies; a *data dependency conflict* occurs when a loop has results from one loop pass that are needed in future passes of the same loop.
- Loops with data dependencies because of temporary variables, reductions, nested loops, or function calls or subroutines.

Loops that do not have a potential for parallelism are those with premature exits, too few iterations, or those where the programming effort to avoid data dependencies is too great.

# **Suspending MPI Jobs**

Internally, the HPE Performance MPI software uses the XPMEM kernel module tprovide single-copy operations to local data. The XPMEM kernel module prevents any pages used by these operations from paging. If an administrator needs to temporarily suspend an 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 an MPI application that is using the XPMEM kernel module has a <code>/proc/xpmem/pid</code> file associated with it. File <code>/proc/xpmem/pid</code> includes the number of pages owned by this process that are prevented from paging by XPMEM. You can display the content of this file. For example:

```
# cat /proc/xpmem/5562
pages pinned by XPMEM: 17
```

The following procedure explains how to unpin the pages for use by other processes.

#### Procedure 7-1 To unpin pages

- 1. Log in as the system administrator.
- 2. Suspend all the processes in the application.
- 3. Use the echo(1) command to unpin the pages.

You can echoing any value into the /proc/xpmem/pid file.

For *pid*, specify the process ID.

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

For example:

# echo 1 > /proc/xpmem/5562

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

# HPE Performance Software — Message Passing Interface (HPE Performance MPI) Performance Profiling

This chapter includes the following topics:

- "About HPE Performance MPI Performance Profiling" on page 69
- "Using perfcatch(1)" on page 70
- "Writing Your Own Profiling Interface" on page 75
- "Using Third-party Profilers" on page 76
- "MPI Internal Statistics" on page 76

# About HPE Performance MPI Performance Profiling

Performance profiling occurs when you run your MPI program or SHMEM program with a tool that can aggregate run time statistics. Profiling tools gather statistics that show the amount of time that your program spends in MPI, the number of messages sent, or the number of bytes sent. MPT includes profiling support in the libmpi.so library. When you use a profiling tool, the tool automatically replaces all MPI\_XXX prototypes and function names with PMPI XXX entry points.

This chapter 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 HPE's MPInside and various third-party products.

The following topics contain more information about profiling:

• HPE Performance Software - Message Passing Interface MPInside Reference Guide. This manual explains how to use the MPInside profiling tool.

- "Using perfcatch(1)" on page 70
- "Writing Your Own Profiling Interface" on page 75
- "Using Third-party Profilers" on page 76
- "MPI Internal Statistics" on page 76

## Using perfcatch(1)

You can use the perfcatch utility to profile the performance of an MPI program or SHMEM program. The perfcatch utility runs the MPI program with the wrapper library, libmpi.so, and writes MPI call profiling information information to MPI PROFILING STATS.

The following topics contain more information about perfcatch(1):

- "The perfcatch(1) Command" on page 70
- "MPI PROFILING STATS Results File Example" on page 71
- "Environment Variables Used With perfcatch(1)" on page 74

#### The perfcatch(1) Command

The following format shows how to use the perfcatch command:

```
mpiexec mpt [ mpi_params ] perfcatch [ -i ] cmd [ args ]
```

By default, perfcatch assumes an MPT program. The perfcatch utility accepts the following options:

mpi params Optional. Specifies the MPI parameters needed to launch the program.

-i Specifies to use Intel MPI.

cmd Specifies the name of the executable program. For example, a.out.

args Optional. Specifies additional command line arguments.

To use perfeatch with an HPE Performance MPI program, insert the perfeatch command in front of the executable file name, as the following examples show:

- mpiexec\_mpt -np 64 perfcatch a.out arg1
- mpiexec mpt host1 32, host2 64 perfcatch a.out arg1

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

```
mpiexec -np 64 perfcatch -i a.out arg1
```

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

### MPI PROFILING STATS Results File Example

The perfcatch(1) utility's output file is called MPI\_PROFILING\_STATS. Upon program completion, the MPI\_PROFILING\_STATS file resides in the current working directory of the MPI process with rank 0.

This output file includes a summary statistics section followed by a rank-by-rank profiling information section. The summary statistics section reports some overall statistics. These statistics include 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.

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

The following is an example MPI PROFILING STATS results file:

007-3773-032

\_\_\_\_\_\_ PERFCATCHER version 22 (C) Copyright Hewlett Packard Enterprise Development LP. This library may only be used on HPE 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 Total MPI job time, avg per rank 0.0054768 sec Profiled job time, avg per rank 0.0054768 sec Percent job time profiled, avg per rank 100% Total user time, avg per rank 0.001 sec 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%

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Rank-by-Rank: System Time Rank:Percent

```
0:86.3416%
                  1:77.4796%
 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
rank
_____
recv wait for data profile
          cnt/sec for all remote ranks
local
rank
-----
recv wait for data profile
```

```
cnt/sec for all remote ranks
local
rank
-----
send profile
          cnt/sec for all destination ranks
 src
rank
ssend profile
          cnt/sec for all destination ranks
 src
rank
ibsend profile
          cnt/sec for all destination ranks
 src
rank
```

# **Environment Variables Used With perfcatch**(1)

The MPI performance-profiling environment variables are as follows:

Variable	Description
MPI_PROFILE_AT_INIT	Activates MPI profiling immediately, that is, at the start of MPI program execution. To use this environment variable, set it to any value. For example, set MPI_PROFILE_AT_INIT to 1.

MPI PROFILING STATS FILE

Specifies the perfeatch output file. This is the file to which MPI profiling results are written. By default, the profiler writes to MPI PROFILING STATS.

# Writing Your Own Profiling Interface

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

The following example output is 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 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
get_count calls 0
                  time 0.000000e+00
ibsend calls 0
                  time 0.000000e+00
probe calls
                 time 0.000000e+00
time 0.00000e+00
            0
recv calls
            0
                                   avg datacnt 0 waits 0
                                                             wait time 0.00000e+00
irecv calls 22039 time 9.76185e-01
                                    datacnt 23474032 avg datacnt 1065
send calls
            0
                  time 0.000000e+00
            0 time 0.000000e+00
ssend calls
isend calls 22039 time 2.950286e+00
wait calls
            0 time 0.00000e+00
                                    avg datacnt 0
waitall calls 11045 time 7.73805e+01
                                    # of Reqs 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
reduce calls 0 time 0.000000e+00
allreduce calls 4658 time 2.072872e+01
bcast calls 680 time 6.915840e-02
gather calls 0 time 0.000000e+00
```

```
gatherv calls 0 time 0.000000e+00 scatter calls 0 time 0.000000e+00 scatterv calls 0 time 0.000000e+00 activity on process rank 1
```

# **Using Third-party Profilers**

You can use third-party profiling tools with HPE Performance MPI. The following are examples of tools to consider:

- The TAU Performance System profiler from the University of Oregon. This software is a portable profiling and tracing toolkit for performance analysis of parallel programs written in Fortran, C, C++, UPC, Java, and Python.
- The Allinea MAP profiler. The Allinea MAP profiler is part of the Allinea Forge toolkit

#### **MPI Internal Statistics**

MPI keeps track of certain resource utilization statistics. You can use these statistics to determine potential performance problems caused by a lack of MPI message buffers or other MPI internal resources.

To display 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 finely grained measurements.

If the MPI\_STATS\_FILE environment variable is set, when the program completes, the system writes internal statistics to the file specified by this variable.

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

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

For additional information on how to use the MPI statistics counters to help tune the run-time environment for an MPI application, see Chapter 7, "Run-time Tuning" on page 49.

# **Troubleshooting and Frequently Asked Questions**

This chapter includes the following topics:

- "About Troubleshooting" on page 79
- "Why Is the mpiexec\_mpt(1) Command Failing?" on page 80
- "Why Does My Code Run Correctly Until It Reaches MPI\_Finalize() and Then Hang?" on page 82
- "Why Does My Hybrid Code (Using OpenMP) Stall on the mpirun Command?" on page 83
- "Why Do I Keep Receiving Warning Messages About the MPI\_REQUEST\_MAX Value Being Too Small?" on page 83
- "Why Is It That I Do I Not See Any stdout And/Or stderr Output From My MPI Application?" on page 83
- "How Do I Install the MPT Software On My Machine?" on page 84
- "Where Can I Find More Information About the OpenSHMEM Programming Model?" on page 84
- "Why Does the ps(1) command Say That My Memory Use (SIZE) Is Higher Than Expected?" on page 84
- "What Does The MPI: could not run executable Message Mean?" on page 84
- "How Do I Combine MPI With insert favorite tool here?" on page 85
- "Why Do I See "stack traceback" Information When My MPI Job Aborts?" on page 86

# **About Troubleshooting**

This chapter provides answers to the following questions that users might ask when they start to use HPE Performance Software — Message Passing Interface (HPE Performance MPI):

- "Why Is the mpiexec mpt(1) Command Failing?" on page 80
- "Why Does My Code Run Correctly Until It Reaches MPI\_Finalize() and Then Hang?" on page 82
- "Why Does My Hybrid Code (Using OpenMP) Stall on the mpirun Command?" on page 83
- "Why Do I Keep Receiving Warning Messages About the MPI\_REQUEST\_MAX Value Being Too Small?" on page 83
- "Why Is It That I Do I Not See Any stdout And/Or stderr Output From My MPI Application?" on page 83
- "How Do I Install the MPT Software On My Machine?" on page 84
- "Where Can I Find More Information About the OpenSHMEM Programming Model? " on page 84
- "Why Does the ps(1) command Say That My Memory Use (SIZE) Is Higher Than Expected?" on page 84
- "What Does The MPI: could not run executable Message Mean?" on page 84
- "How Do I Combine MPI With insert favorite tool here?" on page 85
- "Why Do I See "stack traceback" Information When My MPI Job Aborts?" on page 86

# Why Is the mpiexec mpt(1) Command Failing?

If the mpiexec mpt(1) command fails, investigate the following:

- Look in /var/log/messages for any suspicious errors or warnings. For example, if your application tries to load 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 the following:

Run your program without mpiexec\_mpt(1). When you do not use
 mpiexec\_mpt, the output includes dynamic link errors that might not
 otherwise be displayed. In addition, the output includes the following message:

```
mpiexec_mpt must be used to launch all MPI applications
```

- Run your program with mpiexec\_mpt(1). Set the LD\_DEBUG environment variable to all, which generates output that includes a set of messages for each symbol that rld resolves. This variable produces a lot of output, but it can help you find the cause of the link error.
- Verify that you set your remote directory properly. By default, mpiexec\_mpt(1) 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 mpiexec\_mpt(1) man page's sections on \$MPI DIR and/or the -dir option.
- If you use a relative pathname for your application, verify that it appears in the \$PATH environment variable. In particular, the mpiexec\_mpt(1) command does not look in the working directory (".") for your application unless "." appears in SPATH
- Run the following command to verify that your array is configured correctly:

```
/usr/sbin/ascheck
```

- Run the mpiexec\_mpt -verbose command to verify that you are running the version of MPI that you think you are running.
- Be very careful when you set MPI environment variables from within your .cshrc or .login files because these files override any settings that you might later set from within your shell. The reason for this is 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 in a Kerberos environment, you can experience unpredictable results because <code>mpiexec\_mpt(1)</code> cannot pass tokens. For example, in some cases, if you use <code>telnet(1)</code> to connect to a host and then try to run <code>mpiexec\_mpt</code> on that host, it fails. However, if you instead use <code>rsh(1)</code> to connect to the host, <code>mpiexec\_mpt</code> succeeds. This might be because <code>telnet</code> is kerberized, but <code>rsh</code> is not. If you are running under such conditions, talk to your local administrator about the proper way to launch MPI jobs.

Look in the following directory on all the machines you are using:

```
/tmp/.arraysvcs
```

In some cases, you might find a helpful errlog file.

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

# Why Does My Code Run Correctly Until It Reaches MPI\_Finalize() and Then Hang?

A code hang is almost always caused by a send request or a recv request that is either unmatched or not completed. These request types are as follows:

- An *unmatched request* is any blocking send request for which a corresponding recv request 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(). To fix such codes, update your code in one of the following ways:

- Insert a call to MPI\_Request\_free() immediately after all such isend operations.
- Add a call to MPI\_Wait() at a later place in the code, prior to the point at which
  the send buffer must be reused.
- Set MPI\_REQUEST\_DEBUG=true, which causes MPT to check for this condition at MPI\_Finalize() time.

# Why Does My Hybrid Code (Using OpenMP) Stall 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 the following topic:

"Compiling and Linking the MPI Program" on page 13

# Why Do I Keep Receiving Warning Messages About the MPI\_REQUEST\_MAX Value Being Too Small?

The MPI library generates the following warning message when the MPI REQUEST MAX value is not set appropriately:

MPT Warning: MPT has run out of preallocated request entries. This may slow performance or fragment memory. Please increase MPI REQUEST MAX.

The following are the conditions under which the MPI library generates the preceding message:

- The program uses a very large number of simultaneous transfer requests, much larger than the number of requests for which MPT preallocates. To fix this, use the MPI REQUEST MAX shell variable to increase the number of preallocated requests.
- The application calls MPI\_Isend() or MPI\_Irecv() and does not complete or free the requested objects. To fix this, use MPI\_Request\_free(), as described in the following:

"Why Does My Code Run Correctly Until It Reaches MPI\_Finalize() and Then Hang?" on page 82

# Why Is It That I Do I Not See Any stdout And/Or stderr Output From My MPI Application?

All stdout output and stderr output is line-buffered, which means that the mpirun(1) command 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

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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 Do I Install the MPT Software On My Machine?

The MPT RPMs are included in the HPE Performance Software releases. In addition, you can obtain MPT RPMs from the customer portal at the following URL:

https://support.sgi.com

# Where Can I Find More Information About the OpenSHMEM Programming Model?

See the intro shmem(3) man page.

# Why Does the ps(1) command Say That My Memory Use (SIZE) Is Higher Than Expected?

At job start-up, the MPI and OpenSHMEM libraries cross-map all user static and heap memory of the processes on the local host 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 used, not the amount of memory 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 The MPI: could not run executable Message Mean?

This message means that something happened while mpiexec\_mpt(1) was trying to launch your application, which caused it to fail before all of the MPI processes were able to handshake with it.

The mpiexec\_mpt command directs arrayd to launch a shepherd process on each host and listens on a socket for those shepherds to connect back to it. Because the shepherds are children of arrayd, arrayd traps SIGCHLD and passes that signal back to mpiexec\_mpt whenever one of the shepherds terminates. If mpiexec\_mpt receives a signal before it establishes connections with every host in the job, it knows that something has gone wrong.

#### How Do I Combine MPI With insert favorite tool here?

Different MPI implementations use different methods of launching their worker processes. Some tools expect a method that is different from MPT's default. If you set the shell variable MPI\_SHEPHERD=true, then MPT attempts to use a launch method that is similar to some other MPI implementations. Use of this option can disable some less-common features, such as spawning and checkpoint-restart support.

In general, the rule to follow is to run the mpiexec\_mpt command on your tool and then run the tool on your application. Do not try to run the tool on mpiexec mpt.

Also, because of the way that mpiexec\_mpt sets up stdio, viewing 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 mpiexec\_mpt. Many tools, for example, dplace(1), do not support such an option. However, you might be able to wrap a shell script around the tool and have the script do the redirection, as in the following example:

```
> cat myscript
#!/bin/sh
# NOTE: The example shown is for illustrative purposes only and #
# has not been evaluated for use in a production environment.
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 4 threads
there are now 5 threads
```



**Caution:** The preceding script example is for illustrative purposes only and has not been evaluated for use in a production environment.

# Why Do I See "stack traceback" Information When My MPI Job Aborts?

For information, see the MPI\_COREDUMP environment variable description and the MPI\_COREDUMP\_DEBUGGER environment variable description on the MPI(1) man page.

# **Array Services**

This chapter includes the following topics:

- "About Array Services" on page 87
- "Installing and Configuring Array Services" on page 89
- "Array Services Commands and Arguments" on page 89
- "Array Services Environment Variables" on page 91
- "Obtaining Information About the Array" on page 92

# **About Array Services**

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

The array can consist of the following:

- Multiple server nodes on a cluster computing 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, authentication, 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.

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

The Message Passing Interface (MPI) of the HPE Performance Software — Message Passing Interface (HPE Performance MPI) software uses Array Services to launch parallel applications.

The HPE Performance MPI software distribution includes the MUNGE software. 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 at the following location:

http://dun.github.io/munge/

The Array Services package requires that the process sets service be installed and running. This package is provided in the sgi-procset RPM. Use one of the following command sets to verify that the process sets service is installed and running:

• On RHEL 7.X or SLES 12 SPX systems, type the following commands:

```
# rpm -q sgi-procset
# systemctl status procset
```

• On RHEL 6.X or SLES 11 SPX systems, type the following commands:

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

The following topics contain end-user information about Array Services:

- "Installing and Configuring Array Services" on page 89
- "Array Services Commands and Arguments" on page 89
- "Array Services Environment Variables" on page 91
- "Obtaining Information About the Array" on page 92

**Note:** For Array Services information that pertains to system administration, see the following:

Appendix B, "Array Services System Administration Information"

# **Installing and Configuring Array Services**

The system administrator needs to install and configure the Array Services software before end users can use Array Services or run HPE Performance Software — Message Passing Interface (HPE Performance MPI) programs.

See one of the following for automated installation information:

• On an HPE SGI 8600 system, an HPE Apollo 40 system, an HPE Apollo 20 system, an SGI ICE system, or an SGI Rackable cluster system, see the following manual:

HPE SGI Management Suite Installation and Configuration Guide

• On an HPE Apollo 6500 system, HPE Apollo 6000 system, or an HPE Apollo 2000 system, see the following:

"Installing the Array Services Software on HPE Apollo Cluster Systems" on page 2

For information about the manual installation procedure, see the following:

Appendix B, "Array Services System Administration Information" on page 127

# **Array Services Commands and Arguments**

When an application starts multiple processes on multiple nodes, a Linux process identifier (PID) and a process group identifier (PGID) are no longer adequate to manage the application. The Array Services commands enable you to view the entire array and to control processes on multiple nodes. 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.

To retrieve overview information about Array Services online, see the following man(1) page:

array services(5)

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The following topics contain more information about Array Services commands:

- "Array Services Commands" on page 90
- "Additional Information for the ainfo(1) Command and array(1) Command" on page 91

#### **Array Services Commands**

The following are the Array Services commands:

• ainfo(1)

Retrieves information about the different arrays at your site and about the nodes included in each array. At most sites, there is only one array, but you can have multiple arrays at your site. The command output includes the hostnames for each node in each array at your site.

• array(1)

Runs a system command on one or more nodes and returns output to stdout. As arguments, array(1) accepts several options and the one system command that you want to run on the array. There is a default set of system commands, but your system administrator determines the list of commands available to you at your site.

arshell(1)

Runs a system command remotely on a different node. As arguments, arshell(1) accepts several options and the one system command that you want to run on the remote 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) online man(1) pages explain the arguments that each command accepts. For specific information about each command's arguments, see the individual command man(1) pages.

### Additional Information for the ainfo(1) Command and array(1) Command

The ainfo(1) command and array(1) command support several common command line arguments. For comprehensive information about these commands, see the ainfo(1) and array(1) online man(1) pages.

The following information supplements the information on the man(1) pages:

• Your array administrator might have established an authentication code, which is a 64-bit number, for all or some of the nodes in an array.

The ainfo(1) and array(1) commands accept the -Kl number and -Kr number options. For number, specify the 64-bit authentication key number for the local node or the remote node that you want to target with the command. The code applies to any command entered at that node or addressed to that node.

Your system administrator can tell you if it is necessary to specify an authentication code.

Note that in the case of -Kl *number*, the option letter is a lowercase letter "L", for "local".

- The -l and -s options work together. The -l option restricts the scope of a command to the node upon which the command is run. This option is a lowercase letter "L", for "local". By default, that is the node where the command is entered. When -l is not used, the command queries all nodes of the array. The -s option runs the command on a specified node of the array. These options work together as follows:
  - To query all nodes as seen by the local node, use neither option.
  - To guery 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.

# **Array Services Environment Variables**

The Array Services commands depend on environment variables to define default values for the less-common command options. Table 10-1 summarizes these variables.

**Table 10-1** Array Services Environment Variables

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

# **Obtaining Information About the Array**

You can use Array Services commands and system commands to retrieve information about the array. For example, you can use the  $\mathtt{ainfo}(1)$  command and the  $\mathtt{array}(1)$  command to check the hardware components and the software workload on the array. In addition, you can use system commands, such as  $\mathtt{who}(1)$ ,  $\mathtt{top}(1)$ , and  $\mathtt{uptime}(1)$ , to retrieve information about users and workload on a node. To obtain array-wide information, use these commands with the  $\mathtt{array}(1)$  command.

The following topics include examples that show how to retrieve information about the array:

- "Retrieving Array Names" on page 93
- "Retrieving Node Names" on page 93
- "Retrieving User Names" on page 93
- "Retrieving Workload Information" on page 94

### **Retrieving Array Names**

The following command shows how to retrieve the names of all arrays configured at your site:

```
homegrown% ainfo arrays
Arrays known to array services daemon
ARRAY DevArray
   IDENT 0x3381
ARRAY BigDevArray
   IDENT 0x7456
ARRAY test
   IDENT 0x655e
```

Your system adminstrator configures the arrays at your site. Different arrays might know different sets of other array names.

### **Retrieving Node Names**

The following command uses the -b option of ainfo(1) command to retrieve a brief version of the information about all the nodes in the current array:

```
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
```

#### **Retrieving User Names**

Example 1. The following array who command retrieves the names of all users logged in to the array:

```
mynode% array who

frederik corfu rummage.eng.sgi -tcsh

stefaan sf yoga.eng.sgi -tcsh

timo tokyo frost.ued.sgi /bin/tcsh

wim boston sig.eng.sgi vi +153 fs/procfs/prd

ruben paris mountain.eng.sgi -tcsh

...
```

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Example 2. The following command retrieves the names of users logged in to the node named tokyo. This command uses the -1 and -s options.

```
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
...
```

The preceding examples have been edited for brevity and security.

# **Retrieving Workload Information**

Example 1. The following command shows how to use the uptime(1) command to retrieve information for the entire array:

```
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
```

Example 2. The following command shows how to use the uptime(1) command to retrieve information about a single node:

```
homegrown 182% array -l -s tokyo uptime
tokyo: up 7 days, 9:11, 17 users, load average: 0.12, 0.30, 0.28
```

Example 3. The following command shows how to use the top(1) command to lists the processes that are currently using the most CPU time:

#### 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
0x1111ffff00000000	homegrown	20	root	0.41	ShareII
0x1111ffff00000c0	homegrown	29683	kchang	0.37	ld

0x1111ffff000001e	homegrown	1324	root	0.17	arrayd
0x1111ffff00000000	homegrown	229	root	0.14	routed
0x1111ffff00000000	homegrown	19	root	0.09	pdflush
0x1111ffff000001e9	disarray	1105	arraysvcs	0.02	atopm

The output identifies each process by its internal array session handle (ASH) value. As an alternative, you could use the -1 and -s options to select data about a single node.

# Using the Message Passing Toolkit (MPT) Plugin for Nagios

This chapter includes the following topics:

- "About the MPT Plugin for Nagios" on page 97
- "Installing the MPT Nagios Plugin on the Admin Node" on page 98
- "(Optional) Installing the MPT Nagios Plugin on an HPE SGI 8600 Rack Leader Controller or SGI ICE Rack Leader Controller" on page 101
- "Viewing MPT Messages From Within Nagios and Clearing the Messages" on page 102
- "(Optional) Modifying the Notification Email" on page 104

# **About the MPT Plugin for Nagios**

Nagios is a web-based system monitoring tool that HPE automatically installs on cluster computing systems. Nagios enables you to monitor the cluster infrastructure. When you install the optional MPT plugin for Nagios, the MPT system log messages that typically appear in /var/log/messages also appear in the Nagios graphical user interface (GUI). The plugin scans the system log for messages that MPT has logged, and in the Nagios GUI, the plugin displays the number of error messages and warning messages that the plugin encountered in the scan.

The following topics provide more information about the MPT plugin for Nagios:

- "Installing the MPT Nagios Plugin on the Admin Node" on page 98
- "(Optional) Installing the MPT Nagios Plugin on an HPE SGI 8600 Rack Leader Controller or SGI ICE Rack Leader Controller" on page 101
- "Viewing MPT Messages From Within Nagios and Clearing the Messages" on page 102
- "(Optional) Modifying the Notification Email" on page 104

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# Installing the MPT Nagios Plugin on the Admin Node

The following procedure explains how to install the MPT Nagios plugin on the admin node.

Procedure 11-1 To install the MPT Nagios plugin on the admin node

- 1. Locate the HPE Performance Software installation DVD, and insert the DVD into the DVD reader on the admin node.
- 2. Log into the admin node as the root user.
- 3. Change to the RPM repository directory.
- 4. Type one of the following commands to install the plugin:
  - On RHEL 7 systems or RHEL 6 systems, type the following command:

```
# yum install checkmpt-plugin
```

On SLES 12 systems or SLES 11 systems, type the following commands:

```
# zypper in checkmpt-plugin
```

The preceding commands install the following files:

```
/opt/hpe/hpc/mpt/checkmpt-plugin/README
/opt/sgi/nagios/libexec/check_mpt
```

Use a text editor to open file /opt/hpe/hpc/mpt/checkmpt-plugin/README, and leave the file open in a window on your desktop.

This file contains a shorthand version of these installation instructions. Some steps in this installation procedure require you to insert specific lines into specific files, and it is easiest to copy the lines out of the README file and modify them as this procedure explains.

6. Type the following command to edit file sudoers:

```
# visudo
```

7. Copy the following lines from the README file to the end of the sudoers file, and replace <nagiosuser> and <PLUGINSDIR> with values that are valid at your site:

```
# check_mpt plugin for Nagios (needs access to syslogs)
<nagiosuser> ALL=NOPASSWD: <PLUGINSDIR>/check_mpt
```

```
# end check mpt
```

Replace the variables in the preceding lines as follows:

- Replace <nagiosuser> with the Nagios username assigned when Nagios was installed. By default, this username is nagios.
- Replace <PLUGINSDIR> with the directory in which the Nagios plugin resides. By default, this is /opt/sgi/nagios/libexec.
- 8. Save and close the sudoers file.
- 9. Use a text editor to open file commands.cfg.

By default, this file resides in the following directory:

```
/opt/sgi/nagios/etc/objects
```

10. Copy the following lines from the README file to the end of the commands.cfg file:

You do not need to assign values to \$ARG1\$ or \$ARG2\$. A later step in this procedure populates these arguments with values.

- 11. Save and close the commands.cfg file.
- 12. Use a text editor to open file localhost.cfg.

By default, this file resides in the following directory:

```
/opt/sgi/nagios/etc/objects
```

13. Copy the following lines from the README file to the end of the localhost.cfg file:

```
service_description check_mpt
check_command check_mpt!10!5
max_check_attempts 2
normal_check_interval 2
retry_check_interval 1
}
# end of check_mpt
```

The key lines in the preceding module have the following effects:

Line	Comment
use local-service	Use the generic Nagios template.
host_name localhost	Run on localhost or similar.
service_description check_mpt	Declare the service name.
check_command check_mpt!10!5	Is CRITICAL if >10 warnings / >5 errors.
max_check_attempts 2	If OK, try check again.
normal_check_interval 2	Run check every 2 minutes.
retry_check_interval 1	Retry every 1 minute.

- 14. Save and close file localhost.cfg.
- 15. Type the following command to verify the changes you made and to make sure that there are no conflicts:

```
nagios_dir/bin/nagios -v nagios_dir/etc/nagios.cfg
```

For *nagios\_dir*, specify the Nagios home directory. By default, this directory is /opt/sgi/nagios.

16. Restart Nagios on the node.

This command differs, depending on your platform, as follows:

• To restart Nagios on RHEL 7 and SLES 12 platforms, type the following command:

```
# systemctl restart Nagios
```

 To restart Nagios on RHEL 6 and SLES 11 platforms, type the following command:

```
# service nagios restart
```

You need to restart Nagios after you change any of the Nagios .cfg files.

17. On the admin node, use a shell command to set the following environment variable:

```
MPI SYSLOG COPY=1
```

For example:

```
# set MPI SYSLOG COPY=1
```

Make sure to set this value in your shell before you run any HPE Performance Software — Message Passing Interface (HPE Performance MPI) or SHMEM applications.

18. (Optional) Leave the DVD in the admin node's DVD reader, and proceed to the following:

"(Optional) Installing the MPT Nagios Plugin on an HPE SGI 8600 Rack Leader Controller or SGI ICE Rack Leader Controller" on page 101

# (Optional) Installing the MPT Nagios Plugin on an HPE SGI 8600 Rack Leader Controller or SGI ICE Rack Leader Controller

In addition to the admin node, you can also install the plugin on one or more rack leader controllers (RLCs). The installation procedure is very similar to the procedure that explains how to install the plugin on the admin node. After you install the plugin on an RLC, you can start Nagios on that RLC to monitor the following:

- · The messages on that RLC
- The messages related to that RLC's compute nodes

The following procedure explains how to install the plugin on an RLC.

Procedure 11-2 To install the MPT plugin on an RLC

1. From the admin node, use the ssh command to log into one of the RLCs as the root user.

- 2. Use the information in the following steps to install the plugin on the RLC:
  - Procedure 11-1, step 4 on page 98 through
  - Procedure 11-1, step 17 on page 101

# Viewing MPT Messages From Within Nagios and Clearing the Messages

The following procedure explains how to retrieve MPT messages and clear MPT messages.

Procedure 11-3 To retrieve and clear MPT messages

1. Log into one of the cluster nodes.

If you log into the admin node and start Nagios from the admin node, Nagios displays information for the whole cluster.

If you log into one of the RLCs and start Nagios from one of the RLCs, Nagios displays information for that RLC and its subordinate nodes.

2. Start Nagios.

Type one of the following URLs into your browser:

• To start Nagios on the admin node, type the following:

```
http://admin_name/nagios/rlc_name
```

For admin\_name, type the hostname or IP address of the admin node.

• To start Nagios on one of the RLCs, type the following:

```
http://admin_name/nagios/rlc_name
```

For admin\_name, type the hostname or IP address of the admin node.

For *rlc\_name*, type the hostname or IP address of the RLC. For example, rllead.

3. Type in the Nagios user's username and password.

By default, the username is nagiosadmin. By default, the password is sgisgi.

4. Look for MPT information in the Nagios interface.

By default, the plugin scans the messages in the  $\var/\log\mbox{messages}$  and reports messages to Nagios, as follows:

- If you installed the plugin on the admin node, the plugin sends messages to Nagios for the admin node.
- If you installed the plugin on one or more RLCs, the plugin sends messages to Nagios for the RLC and the RLC compute nodes. You need to start Nagios on the RLC to observe the messages related to that RLC.

If you click an MPT message from within the Nagios interface, you retrieve more information about the message.

- 5. Use administrator commands to remedy the error conditions, if needed.
- 6. On the admin node, run the check\_mpt command to clear the messages that Nagios reported.

If you installed the plugin on the RLCs, run the check mpt on RLCs, too.

The MPT plugin works by scanning <code>/var/log/messages</code>, from beginning to end. To stop the plugin from repeatedly scanning the log file, a file offset is preserved. After you run the <code>check\_mpt</code> command, the changes appear in Nagios after the next scan.

The following examples show how to use options to the <code>check\_mpt</code> command to direct the plugin to scan the system log according to your site preferences.

Example 1. To direct the plugin to scan for only newly logged messages, use the -C option. The -C option clears all current message counts and requests that Nagios continue its scan for new messages. Also, the -C parameter changes the Nagios CRITICAL and WARNING status back to OK after you correct the reported error condition. To use this option, type the following command:

```
# check mpt -C
```

Example 2. The -X parameter directs the plugin to start a new scan of /var/log/messages, clears the MPT message counts, and resets the offsets to 0. You can run check\_mpt with the -X parameter after each log rotation. This command is as follows:

# check\_mpt -X

The check\_mpt command accepts additional parameters. For more information on these parameters, type the following command to retrieve a usage statement:

```
# check mpt -h
```

# (Optional) Modifying the Notification Email

In addition to the notifications that Nagios reports in the Nagios GUI, Nagios also sends email notifications of alert conditions. If you modify the Nagios email configuration file, the Nagios email can include hostname information, which can let you identify the node upon which the error condition occurred more easily.

The commands.cfg file contains the following:

If you change \$HOSTALIAS\$ to hostname, the Nagios emails include the hostname of the node upon which the error condition occurred. For example, the following file shows this enhancement:

For more information about Nagios and the Nagios email reporting feature, see your Nagios documentation.

# **High Performance Computing Tools**

The following topics contain information about the high performance computing tools you can use with MPI programs:

- "NUMA Tools" on page 105
- "Flexible File I/O (FFIO)" on page 113

### **NUMA Tools**

For information about the NUMA Tools, see the following:

- "About the NUMA Tools" on page 105
- "dplace Command" on page 106
- "omplace Command" on page 112
- The cpuset information in the HPE Performance Software Message Passing Interface Cpuset Software Guide
- taskset(1) command information in the Linux Application Tuning Guide

#### **About the NUMA Tools**

The NUMA Tools enable data placement to specific memory locations, which minimizes communication overhead within an application.

The dplace(1) tool and and the cpuset tools are built upon the cpusets API. You can use these tools avoid poor data locality in your application caused by process or thread drift from CPU to CPU. The omplace(1) tool works like the dplace(1) tool and is designed for use with OpenMP applications. The differences among these tools are as follows:

- The taskset(1) command restricts execution to the listed set of CPUs when you specify the -c or --cpu-list option. The process is free to move among the CPUs that you specify.
- The dplace(1) tool differs from taskset(1) in that dplace(1) binds processes to specified CPUs in round-robin fashion. After a process is pinned, it does not

migrate, so you can use this for increasing the performance and reproducibility of parallel codes.

 Cpusets are named subsets of system cpus/memories and are used extensively in batch environments. For more information about cpusets, see the HPE Performance Software - Message Passing Interface Cpuset Software Guide.

# dplace Command

You can use the dplace(1) command to improve the performance of processes running on your SGI nonuniform memory access (NUMA) machine.

By default, memory is allocated to a process on the node on which the process is executing. If a process moves from node to node while it is running, a higher percentage of memory references are made to remote nodes. Because remote accesses typically have higher access times, performance can degrade. CPU instruction pipelines also have to be reloaded.

The dplace(1) command specifies scheduling and memory placement policies for the process. You can use the dplace command to bind a related set of processes to specific CPUs or nodes to prevent process migrations. In some cases, this improves performance because a higher percentage of memory accesses are made to local nodes.

Processes always execute within a cpuset. The cpuset specifies the CPUs on which a process can run. By default, processes usually execute in a cpuset that contains all the CPUs in the system. For information about cpusets, see the *HPE Performance Software - Message Passing Interface Cpuset Software Guide*.

The dplace(1) command creates a placement container that includes all the CPUs, or a subset of CPUs, of a cpuset. The dplace process is placed in this container and, by default, is bound to the first CPU of the cpuset associated with the container. Then dplace invokes exec to run the command.

The command runs within this placement container and remains bound to the first CPU of the container. As the command forks child processes, the child processes inherit the container and are bound to the next available CPU of the container.

If you do not specify a placement file, dplace binds processes sequentially in a round-robin fashion to CPUs of the placement container. For example, if the current cpuset consists of physical CPUs 2, 3, 8, and 9, the first process launched by dplace is bound to CPU 2. The first child process forked by this process is bound to CPU 3. The next process, regardless of whether it is forked by a parent or a child, is bound to

CPU 8, and so on. If more processes are forked than there are CPUs in the cpuset, binding starts over with the first CPU in the cpuset.

For more information about dplace(1), see the dplace(1) man page. The dplace(1) man page also includes examples of how to use the command.

#### **Example 12-1** Using the dplace(1) command with MPI Programs

The following command improves the placement of MPI programs on NUMA systems and verifies placement of certain data structures of a long-running MPI program:

```
% mpirun -np 64 /usr/bin/dplace -s1 -c 0-63 ./a.out
```

The -s1 parameter causes dplace(1) to start placing processes with the second process, p1. The first process, p0, is not placed because it is associated with the job launch, not with the job itself. The -c 0-63 parameter causes dplace(1) to use processors 0-63.

You can then use the dlook(1) command to verify placement of the data structures in another window on one of the slave thread PIDs. For more information about the dlook command, see the dlook(1) man page.

#### **Example 12-2** Using the dplace(1) command with OpenMP Programs

The following command runs an OpenMP program on logical CPUs 4 through 7 within the current cpuset:

```
% efc -o prog -openmp -O3 program.f
% setenv OMP_NUM_THREADS 4
% dplace -c4-7 ./prog
```

**Example 12-3** Using the dplace(1) command with OpenMP Programs

The dplace(1) command has a static load balancing feature, so you do not have to supply a CPU list. To place prog1 on logical CPUs 0 through 3 and prog2 on logical CPUs 4 through 7, type the following:

```
% setenv OMP_NUM_THREADS 4
% dplace ./prog1 &
% dplace ./prog2 &
```

You can use the dplace -q command to display the static load information.

**Example 12-4** Using the dplace(1) command with Linux commands

The following examples assume that you run the dplace commands from a shell that runs in a cpuset consisting of physical CPUs 8 through 15.

Command	Run Location
dplace -c2 date	Runs the date command on physical CPU 10.
dplace make linux	Runs gcc and related processes on physical CPUs 8 through 15.
dplace -c0-4,6 make linux	Runs gcc and related processes on physical CPUs 8 through 12 or 14.
taskset 4,5,6,7 dplace app	The taskset command restricts execution to physical CPUs 12 through 15. The dplace command sequentially binds processes to CPUs 12 through 15.

**Example 12-5** Using the dplace command and a debugger for verification

To use the dplace command accurately, you should know how your placed tasks are being created in terms of the fork, exec, and pthread\_create calls. Determine whether each of these worker calls are an MPI rank task or are groups of pthreads created by rank tasks. Here is an example of two MPI ranks, each creating three threads:

```
cat <<EOF > placefile
firsttask cpu=0
exec name=mpiapp cpu=1
fork name=mpiapp cpu=4-8:4 exact
thread name=mpiapp oncpu=4 cpu=5-7 exact thread name=mpiapp oncpu=8
cpu=9-11 exact EOF

# mpirun is placed on cpu 0 in this example
# the root mpiapp is placed on cpu 1 in this example
# or, if your version of dplace supports the "cpurel=" option:
# firsttask cpu=0
# fork name=mpiapp cpu=4-8:4 exact
# thread name=mpiapp oncpu=4 cpurel=1-3 exact
```

```
# create 2 rank tasks, each will pthread_create 3 more
# ranks will be on 4 and 8
# thread children on 5,6,7 9,10,11
dplace -p placefile mpirun -np 2 ~cpw/bin/mpiapp -P 3 -1
```

exit

You can use the debugger to determine if it is working. It should show two MPI rank applications, each with three pthreads, as follows:

```
>> pthreads | grep mpiapp
px *(task struct *)e00002343c528000
                                              17769
                                                      17763 0
                                      17769
                                                                     mpiapp
      member task: e000013817540000
                                      17795
                                              17769
                                                      17763 0
                                                                   5 mpiapp
      member task: e000013473aa8000
                                      17796
                                              17769
                                                      17763 0
                                                                   6 mpiapp
     member task: e000013817c68000
                                      17798
                                              17769
                                                      17763 0
                                                                     mpiapp
px *(task_struct *)e0000234704f0000
                                      17770
                                              17770
                                                      17763 0
                                                                     mpiapp
     member task: e000023466ed8000
                                              17770
                                      17794
                                                      17763 0
                                                                   9 mpiapp
      member task: e00002384cce0000
                                      17797
                                              17770
                                                      17763 0
                                                                     mpiapp
      member task: e00002342c448000
                                      17799
                                              17770
                                                      17763 0
                                                                     mpiapp
```

You can also use the debugger to see a root application, the parent of the two MPI rank applications, as follows:

```
>> ps | grep mpiapp

0xe00000340b300000 1139 17763 17729 1 0xc800000 - mpiapp

0xe000002343c528000 1139 17769 17763 0 0xc800040 - mpiapp

0xe0000234704f0000 1139 17770 17763 0 0xc800040 8 mpiapp
```

#### These are placed as specified:

```
>> oncpus e00002343c528000 e000013817540000 e000013473aa8000
>> e000013817c68000 e0
000234704f0000 e000023466ed8000 e00002384cce0000 e00002342c448000
task: 0xe00002343c528000 mpiapp cpus_allowed: 4
task: 0xe000013817540000 mpiapp cpus_allowed: 5
task: 0xe000013473aa8000 mpiapp cpus_allowed: 6
task: 0xe000013817c68000 mpiapp cpus_allowed: 7
task: 0xe0000234704f0000 mpiapp cpus_allowed: 8
task: 0xe000023466ed8000 mpiapp cpus_allowed: 9
task: 0xe00002384cce0000 mpiapp cpus_allowed: 10
```

task: 0xe00002342c448000 mpiapp cpus allowed: 11

**Example 12-6** Using the dplace(1) command for compute thread placement troubleshooting

Sometimes compute threads do not end up on unique processors when using commands such a dplace(1) or profile.pl.

In this example, assume that the dplace -s1 -c0-15 command bound 16 processes to run on 0-15 CPUs. However, output from the top(1) command shows only 13 CPUs running with CPUs 13, 14, and 15 still idle, and CPUs 0, 1 and 2 are shared with 6 processes.

263 processes: 225	1 5.		<b>J</b> .	-			4410
CPU states: cpu total	1265.6%	_		0.0%	-		idle 291.2%
cpu00	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu01	90.1%	0.0%	0.0%	0.0%	9.7%	0.0%	0.0%
cpu02	99.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu03	99.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu04	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu05	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu06	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu07	88.4%	0.0%	10.6%	0.0%	0.8%	0.0%	0.0%
cpu08	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu09	99.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu10	99.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
cpu11	88.1%	0.0%	11.2%	0.0%	0.6%	0.0%	0.0%
cpu12	99.7%	0.0%	0.2%	0.0%	0.0%	0.0%	0.0%

cpu13 0.0% 0.0% 2.5% 0.0% 0.0% 0.0% 97.4%

cpu14 0.8% 0.0% 1.6% 0.0% 0.0% 0.0% 97.5%

cpu15 0.0% 0.0% 2.4% 0.0% 0.0% 0.0% 97.5%

Mem: 60134432k av, 15746912k used, 44387520k free, 0k shrd,

672k buff

351024k active, 13594288k inactive

Swap: 2559968k av, 0k used, 2559968k free

2652128k cached

PID USER	PRI	NI	SIZE	RSS	SHARE	STAT	%CPU	%MEM	TIME	CPU	COMMAND
7653 ccao	25	0	115G	586M	114G	R	99.9	0.9	0:08	3	mocassin
7656 ccao	25	0	115G 5	586M	114G F	2	99.9	0.9	0:08	6 n	nocassin
7654 ccao	25	0	115G	586M	114G	R	99.8	0.9	0:08	4	mocassin
7655 ccao	25	0	115G	586M	114G	R	99.8	0.9	0:08	5	mocassin
7658 ccao	25	0	115G	586M	114G	R	99.8	0.9	0:08	8	mocassin
7659 ccao	25	0	115G	586M	114G	R	99.8	0.9	0:08	9	mocassin
7660 ccao	25	0	115G	586M	114G	R	99.8	0.9	0:08	10	mocassin
7662 ccao	25	0	115G	586M	114G	R	99.7	0.9	0:08	12	mocassin
7657 ccao	25	0	115G	586M	114G	R	88.5	0.9	0:07	7	mocassin
7661 ccao	25	0	115G	586M	114G	R	88.3	0.9	0:07	11	mocassin
7649 ccao	25	0	115G	586M	114G	R	55.2	0.9	0:04	2	mocassin
7651 ccao	25	0	115G	586M	114G	R	54.1	0.9	0:03	1	mocassin
7650 ccao	25	0	115G	586M	114G	R	50.0	0.9	0:04	0	mocassin
7647 ccao	25	0	115G	586M	114G	R	49.8	0.9	0:03	0	mocassin

```
7652 ccao 25 0 115G 586M 114G R 44.7 0.9 0:04 2 mocassin
7648 ccao 25 0 115G 586M 114G R 35.9 0.9 0:03 1 mocassin
```

Even if an application starts some threads executing for a very short time, the threads still have taken a token in the CPU list. Then, when the compute threads are finally started, the list is exhausted and restarts from the beginning. Consequently, some threads end up sharing the same CPU. To bypass this, try to eliminate the ghost thread creation, as follows:

• Check for a call to the system function. This is often responsible for the placement failure due to unexpected thread creation. If all the compute processes have the same name, you can do this by issuing a command such as the following:

```
% dplace -c0-15 -n compute-process-name ...
```

• You can also run dplace -e -c0-32 on 16 CPUs to understand the pattern of the thread creation. If this pattern is the same from one run to the other (unfortunately race between thread creation often occurs), you can find the right flag to dplace. For example, if you want to run on CPUs 0-3, with dplace -e -C0-16 and you see that threads are always placed on CPU 0, 1, 5, and 6, then one of the following commands should place your threads correctly:

```
dplace -e -c0,1,x,x,x,2,3 or dplace -x24 -c0-3 # x24 = 11000, place the 2 first and skip 3 before placing
```

#### omplace Command

The omplace(1) command controls the placement of MPI processes and OpenMP threads. This command is a wrapper script for dplace(1). Use omplace(1), rather than dplace(1), if your application uses MPI, OpenMP, pthreads, or hybrid MPI/OpenMP and MPI/pthreads codes. The omplace(1) command generates the proper dplace(1) placement file syntax automatically. It also supports some unique options, such as block-strided CPU lists.

The omplace(1) command causes the successive threads in a hybrid MPI/OpenMP job to be placed on unique CPUs. The CPUs are assigned in order from the effective CPU list within the containing cpuset. The CPU placement is performed by

dynamically generating a placement file and invoking dplace(1) with the MPI job launch.

For example, to run two MPI processes with four threads per process, and to display the generated placement file, type a command similar to the following:

```
# mpirun -np 2 omplace -nt 4 -vv ./a.out
```

The preceding command places the threads as follows:

```
rank 0 thread 0 on CPU 0 rank 0 thread 1 on CPU 1 rank 0 thread 2 on CPU 2 rank 0 thread 3 on CPU 3 rank 1 thread 0 on CPU 4 rank 1 thread 1 on CPU 5 rank 1 thread 2 on CPU 6 rank 1 thread 3 on CPU 7
```

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

# Flexible File I/O (FFIO)

The following topics explain how to use FFIO:

- "About FFIO" on page 113
- "Environment Variables" on page 114
- "FFIO Examples" on page 116
- "Multithreading Considerations" on page 118
- "Application Examples " on page 119
- "Event Tracing " on page 120
- "System Information and Issues " on page 121

#### **About FFIO**

Flexible File I/O (FFIO) can improve the file I/O performance of existing applications without having to resort to source code changes. The current executable remains

unchanged. Knowledge of source code is not required, but some knowledge of how the source and the application software work can help you better interpret and optimize FFIO results. To take advantage of FFIO, all you need to do is to set some environment variables before running your application.

The FFIO subsystem allows you to define one or more additional I/O buffer caches for specific files to augment the Linux kernel I/O buffer cache. The FFIO subsystem then manages this buffer cache for you. In order to accomplish this, FFIO intercepts standard I/O calls such as open, read, and write, and replaces them with FFIO equivalent routines. These routines route I/O requests through the FFIO subsystem, which uses the user-defined FFIO buffer cache.

FFIO can bypass the Linux kernel I/O buffer cache by communicating with the disk subsystem via direct I/O. This bypass gives you precise control over cache I/O characteristics and allows for more efficient I/O requests. For example, doing direct I/O in large chunks (for example, 16 megabytes) allows the FFIO cache to amortize disk access. All file buffering occurs in user space when FFIO is used with direct I/O enabled. This differs from the Linux buffer cache mechanism, which requires a context switch in order to buffer data in kernel memory. Avoiding this kind of overhead helps FFIO to scale efficiently.

Another important distinction is that FFIO allows you to create an I/O buffer cache dedicated to a specific application. The Linux kernel, on the other hand, has to manage all the jobs on the entire system with a single I/O buffer cache. As a result, FFIO typically outperforms the Linux kernel buffer cache when it comes to I/O intensive throughput.

#### **Environment Variables**

To use FFIO, set one of the following environment variables: LD\_PRELOAD or FF IO OPTS.

In order to enable FFIO to trap standard I/O calls, set the LD\_PRELOAD environment variable, as follows:

# export LD PRELOAD="/usr/lib64/libFFIO.so"

The LD\_PRELOAD software is a Linux feature that instructs the linker to preload the indicated shared libraries. In this case, libffio.so is preloaded and provides the routines that replace the standard I/O calls. An application that is not dynamically

linked with the glibc library cannot work with FFIO because the standard I/O calls cannot be intercepted. To disable FFIO, type the following:

```
# unset LD PRELOAD
```

The FFIO buffer cache is managed by the FF\_IO\_OPTS environment variable. The syntax for setting this variable can be quite complex. A simple format for defining this variable is as follows:

export FF\_IO\_OPTS 'string(eie.direct.mbytes:size:num:lead:share:stride:0)'

You can use the following parameters with the FF IO OPTS environment variable:

string	Matches the names of files that can use the buffer cache.
size	Number of 4k blocks in each page of the I/O buffer cache.
num	Number of pages in the I/O buffer cache.
lead	The maximum number of read-ahead pages.
share	A value of 1 means a shared cache, 0 means private.
stride	Note that the number after the stride parameter is always 0.

0.01

Example 1. Assume that you want a shared buffer cache of 128 pages. Each page is to be 16 megabytes (that is, 4096\*4k). The cache has a lead of six pages and uses a stride of one. The command is as follows:

```
% setenv FF IO OPTS 'test*(eie.direct.mbytes:4096:128:6:1:1:0)'
```

Each time the application opens a file, the FFIO code checks the file name to see if it matches the string supplied by FF\_IO\_OPTS. The file's path name is not considered when checking for a match against the string. For example, file names of /tmp/test16 and /var/tmp/testit both match.

Example 2. This more complicated usage of FF\_IO\_OPTS builds upon the previous example. Multiple types of file names can share the same cache, as the following example shows:

```
% setenv FF IO OPTS 'output* test*(eie.direct.mbytes:4096:128:6:1:1:0)'
```

Example 3. You can specify multiple caches with FF\_IO\_OPTS. In the example that follows, files of the form output\* and test\* share a 128 page cache of 16 megabyte

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pages. The file special42 has a 256-page private cache of 32 megabyte pages. The command, which uses the backslash (\) continuation character, is as follows:

```
% setenv FF_IO_OPTS 'output* test*(eie.direct.mbytes:4096:128:6:1:1:0) \
special42(eie.direct.mbytes:8192:256:6:0:1:0)'
```

Additional parameters can be added to FF\_IO\_OPTS to create feedback that is sent to standard output. For examples of this diagnostic output, see the following:

"FFIO Examples" on page 116

# **FFIO Examples**

This topic includes some simple FFIO examples. Assume that LD\_PRELOAD is set for the correct library, and FF IO OPTS is defined as follows:

```
% setenv FF_IO_OPTS 'test*(eie.direct.mbytes:4096:128:6:1:1:0)'
```

It can be difficult to tell what FFIO might or might not be doing even with a simple program. The examples in this topic use a small C program called fio that reads 4-megabyte chunks from a file for 100 iterations. When the program runs, it produces the following output:

```
% ./fio -n 100 /build/testit
Reading 4194304 bytes 100 times to /build/testit
Total time = 7.383761
Throughput = 56.804439 MB/sec
```

Example 1. You can direct a simple FFIO operations summary to standard output by making the following simple addition to FF IO OPTS:

```
% setenv FF IO OPTS 'test*(eie.direct.mbytes:4096:128:6:1:1:0, event.summary.mbytes.notrace )'
```

This new setting for FF\_IO\_OPTS generates the following summary on standard output when the program runs:

function	times	wall	all	mbytes	mbytes	min	max	avg
	called	time	hidden	requested	delivered	request	request	request
open	1	0.00						
read	2	0.61		32	32	16	16	16
reada	29	0.01	0	464	464	16	16	16
fcntl								
reca	all							
read	da 29	8.11						
othe	er 5	0.00						
flush	1	0.00						
close	1	0.00						

Two synchronous reads of 16 megabytes each were issued, for a total of 32 megabytes. In addition, there were 29 asynchronous reads (reada) issued, for a total of 464 megabytes.

Example 2. You can generate additional diagnostic information by specifying the .diag modifier. The following is an example of the diagnostic output generated when the .diag modifier is used:

```
% setenv FF IO OPTS 'test*(eie.direct.diag.mbytes:4096:128:6:1:1:0 )'
% ./fio -n 100 /build/testit
Reading 4194304 bytes 100 times to /build/testit
Total time = 7.383761
Throughput = 56.804439 MB/sec
eie close EIE final stats for file /build/testit
eie close Used shared eie cache 1
eie_close 128 mem pages of 4096 blocks (4096 sectors), max_lead = 6 pages
eie close advance reads used/started : 23/29 79.31%
                                                          (1.78 seconds wasted)
eie close write hits/total :
                                           0/0
                                                   0.00%
eie close read hits/total
                                 :
                                         98/100 98.00%
eie close mbytes transferred parent --> eie --> child
                                                          sync
                                                                     async
eie close
                                     0
                                                   0
                                                           0
                                                                        Ω
                                                          2
                                                                       29 (0,0)
eie close
                                     400
                                                496
eie_close
                              parent <-- eie <-- child
eie_close EIE stats for Shared cache 1
eie close 128 mem pages of 4096 blocks
```

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```
eie close advance reads used/started :
                                        23/29
                                                 79.31%
                                                         (0.00 seconds wasted)
eie close write hits/total :
                                         0/0
                                                  0.00%
eie close read hits/total
                                        98/100
                                                 98.00%
eie close mbytes transferred parent --> eie --> child
                                                         sync
                                                                    async
eie close
                                      0
                                                          0
                                                                      0
eie close
                                    400
                                               496
                                                                      29 (0,0)
```

The preceding output lists information for both the file and the cache. In the mbytes transferred information, the lines in **bold** are for write and read operations, respectively. Only for very simple I/O patterns can the difference between (parent --> eie) and (eie --> child) read statistics be explained by the number of read aheads. For random reads of a large file over a long period of time, this is not the case. All write operations count as async.

You can generate additional diagnostic information by specifying the .diag modifier and the .event.summary modifier. The two modifiers operate independently from one another. The following specification uses both modifiers:

```
% setenv FF_IO_OPTS 'test*(eie.diag.direct.mbytes:4096:128:6:1:1:0, event.summary.mbytes.notrace )'
```

# **Multithreading Considerations**

FFIO works with applications that use MPI for parallel processing. An MPI job assigns each thread a number or rank. The master thread has rank 0, while the remaining slave threads have ranks from 1 to *N*-l where *N* is the total number of threads in the MPI job. It is important to consider that the threads comprising an MPI job do not necessarily have access to each others' address space. As a result, there is no way for the different MPI threads to share the same FFIO cache. By default, each thread defines a separate FFIO cache based on the parameters defined by FF IO OPTS.

Having each MPI thread define a separate FFIO cache, based on a single environment variable (FF\_IO\_OPTS), can waste a lot of memory. Fortunately, FFIO provides a mechanism that allows you to specify a different FFIO cache for each MPI thread via the following environment variables:

```
setenv FF_IO_OPTS_RANKO 'result*(eie.direct.mbytes:4096:512:6:1:1:0)'
setenv FF_IO_OPTS_RANK1 'output*(eie.direct.mbytes:1024:128:6:1:1:0)'
setenv FF_IO_OPTS_RANK2 'input*(eie.direct.mbytes:2048:64:6:1:1:0)'
.
.
setenv FF_IO_OPTS_RANKN-1 ... (N = number of threads).
```

Each rank environment variable is set using the exact same syntax as FF\_IO\_OPTS and each defines a distinct cache for the corresponding MPI rank. If the cache is designated as shared, all files within the same ranking thread can use the same cache. FFIO works with SGI MPI, HP MPI, and LAM MPI. In order to work with MPI applications, FFIO needs to determine the rank of callers by invoking the mpi\_comm\_rank\_() MPI library routine. Therefore, FFIO needs to determine the location of the MPI library used by the application. To accomplished this, set one, and only one, of the following environment variables:

- setenv SGI MPI /usr/lib
- setenv LAM MPI
- setenv HP MPI

**Note:** LAM MPI and HP MPI are usually distributed via a third party application. The precise paths to the LAM and the HP MPI libraries are application dependent. See the application installation guide to find the correct path.

To use the rank functionality, both the MPI and FF\_IO\_OPTS\_RANKO environment variables must be set. If either variable is not set, then the MPI threads all use FF\_IO\_OPTS. If both the MPI and the FF\_IO\_OPTS\_RANKO variables are defined but, for example, FF\_IO\_OPTS\_RANK2 is undefined, all rank 2 files generate a no match with FFIO. This means that none of the rank 2 files are cached by FFIO. In this case, the software does not default to FF\_IO\_OPTS.

Fortran and C/C++ applications that use the pthreads interface create threads that share the same address space. These threads can all make use of the single FFIO cache defined by FF IO OPTS.

#### **Application Examples**

FFIO has been deployed successfully with several high-performance computing applications, such as Nastran and Abaqus. In a recent customer benchmark, an eight-way Abaqus throughput job ran approximately twice as fast when FFIO was used. The FFIO cache used 16-megabyte pages (that is, page\_size = 4096) and the cache size was 8.0 gigabytes. As a rule of thumb, it was determined that setting the FFIO cache size to roughly 10-15% of the disk space required by Abaqus yielded

```
reasonable I/O performance. For this benchmark, the FF_IO_OPTS environment variable was defined as follows:
```

For the MPI version of Abaqus, different caches were specified for each MPI rank, as follows:

# **Event Tracing**

If you specify the .trace option as part of the event parameter, you can enable the event tracing feature in FFIO.

For example:

```
% setenv FF IO OPTS 'test*(eie.direct.mbytes:4096:128:6:1:1:0, event.summary.mbytes.trace )'
```

This option generates files of the form ffio.events.pid for each process that is part of the application. By default, event files are placed in /tmp. To chang this destination, set the FFIO\_TMPDIR environment variable. These files contain time-stamped events for files using the FFIO cache and can be used to trace I/O activity such as I/O sizes and offsets.

# **System Information and Issues**

The FFIO subsystem supports applications written in C, C++, and Fortran. C and C++ applications can be built with either the Intel or gcc compiler. Only Fortran codes built with the Intel compiler work with FFIO.

The following restrictions on FFIO must also be observed:

- The FFIO implementation of pread/pwrite is not correct. The file offset advances.
- Do not use FFIO for I/O on a socket.
- Do not link your application with the librt asynchronous I/O library.
- FFIO does not intercept calls that operate on files in /proc, /etc, and /dev.
- FFIO does not intercept calls that operate on stdin, stdout, and stderr.
- FFIO is not intended for generic I/O applications such as vi, cp, or mv, and so on.

# Guidelines for Using the Message Passing Toolkit (MPT) on a Virtual Machine Within an SGI UV Computer System

This appendix section includes the following topics:

- "About MPT on a Virtual Machine" on page 123
- "Installing Software Within the Virtual Machine (VM)" on page 124
- "Adjusting SGI UV Virtual Machine System Settings" on page 124
- "Running HPE Performance Software Message Passing Interface (HPE Performance MPI) Programs From Within a Virtual Machine (VM)" on page 126

#### **About MPT on a Virtual Machine**

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

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

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

- "Installing Software Within the Virtual Machine (VM)" on page 124
- "Adjusting SGI UV Virtual Machine System Settings" on page 124

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

 "Running HPE Performance Software — Message Passing Interface (HPE Performance MPI) Programs From Within a Virtual Machine (VM)" on page 126

# Installing Software Within the Virtual Machine (VM)

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

#### **Procedure A-1** To install the software for MPI programs

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

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

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

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

3. (Optional) Install the HPE System Foundation Software into the VM.

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

4. Install the HPE Performance Software into the VM.

For installation information, see the HPE Performance Software release notes.

5. Install MPT into the VM.

For installation information, see Chapter 2, "Getting Started" on page 11.

# **Adjusting SGI UV Virtual Machine System Settings**

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

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

#### Procedure A-2 To adjust system settings

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

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

For example:

```
# cpumap
This is an SGI UV
model name
                : Genuine Intel(R) CPU @ 2.60GHz
Architecture
               : x86_64
cpu MHz
                : 2600.072
cache size : 20480 KB (Last Level)
Total Number of Sockets
                                : 16
Total Number of Cores
                                       (8 per socket)
                                : 128
Hyperthreading
                                : ON
Total Number of Physical Processors
                                : 128
Total Number of Logical Processors
                                : 256
                                      (2 per Phys Processor)
UV Information
 HUB Version:
                                 UVHub 3.0
Number of Hubs:
                                 16
Number of connected Hubs:
                                 16
Number of connected NUMAlink ports:
                                 128
______
```

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

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

For example, type the following command:

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

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

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

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

# Running HPE Performance Software — Message Passing Interface (HPE Performance MPI) Programs From Within a Virtual Machine (VM)

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

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

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

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

Topology characteristics might be different.

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

XPMEM libraries are beneficial in very large VMs.

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

No InfiniBand support.

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

# **Array Services System Administration Information**

This appendix contains the following topics:

- "About Installing and Configuring Array Services Manually" on page 127
- "Installing the Array Services Software on HPE Apollo Cluster Systems" on page 2
- "Manually Configuring Array Services on Multiple Hosts" on page 128
- "Changing the Security Access Level in the AUTHENTICATION parameter" on page 131
- "Configuring Nodes Into Arrays" on page 132
- "About the Array Configuration Files" on page 134
- "Designing Array Services Commands" on page 136
- "Testing Configuration Changes After Creating New Array Services Commands" on page 144

# **About Installing and Configuring Array Services Manually**

The topics in this appendix section contain information for system administrators who support the Array Services software on a cluster computing system. These topics explain how to install Array Services manually and how to configure Array Services to suit your site's needs.

The topics in this appendix section are as follows:

- "Manually Configuring Array Services on Multiple Hosts" on page 128
- "Changing the Security Access Level in the AUTHENTICATION parameter" on page 131
- "Configuring Nodes Into Arrays" on page 132
- "About the Array Configuration Files" on page 134
- "Designing Array Services Commands" on page 136

 "Testing Configuration Changes After Creating New Array Services Commands" on page 144

### **Manually Configuring Array Services on Multiple Hosts**

You can configure Array Services in an automated way or manually. The following list shows where you can find the standard, automated procedures:

- For cluster systems, use the information in the following:
  - HPE SGI Management Suite Installation and Configuration Guide
  - "Installing the Array Services Software on HPE Apollo Cluster Systems" on page 2
- For SGI UV computer systems, use the information in the following:

Chapter 1, "Configuring the Message Passing Toolkit (MPT)" on page 1

The information in this appendix section explains how to configure Array Services in a manual way, which allows you to make customizations at installation time, if necessary.

The following procedure explains how to configure Array Services to run on multiple hosts.

**Procedure B-1** To configure Array Services for multiple hosts

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

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

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

2. (Optional) Install the MUNGE package from the HPE Performance Software — Message Passing Interface (HPE Performance 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 HPE Performance MPI release notes.

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

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 /etc/array/arrayd.conf.

- 6. Use a text editor to open file /etc/array/arrayd.auth.
- 7. (Optional) Change the authentication method from the default of NOREMOTE to a method of your choosing.

By default, the Array Services software does not allow remote access to the array. You can change this authentication method. For information about the various authentication methods, see the following:

"Changing the Security Access Level in the AUTHENTICATION parameter" on page 131

To change the access method, complete the following steps:

- Search for the string AUTHENTICATION NOREMOTE, and insert a # character in column 1 to comment out the line.
- 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.

- Save and close file /etc/array/arrayd.auth.
- 8. (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 /etc/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 # Array Services daemon
```

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

- 9. Type one of the following commands to restart Array Services:
  - On RHEL 7.*X* or SLES 12 SP*X* systems, type the following command:

```
systemctl restart array
```

• On RHEL 6.*X* or SLES 11 SP*X* systems, type the following command:

```
/etc/init.d/array restart
```

 Repeat the preceding steps on the other hosts or copy the /etc/array/arrayd.conf and /etc/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.

# Changing the Security Access Level in the AUTHENTICATION parameter

The AUTHENTICATION parameter in the /etc/array/arrayd.auth file specifies access to the array. The AUTHENTICATION parameter can have one of the following settings:

• NOREMOTE (default).

When set to NOREMOTE, the arrayd daemon allows only local access to the array. That is, the arrayd daemon does not allow remote requests to access the array.

Use NOREMOTE if the array is attached to a public network or if individual machines cannot be trusted.

#### NONE.

When set to NONE, the arrayd daemon assumes that remote users identify themselves accurately and honestly when making requests. 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.

All requests from remote systems are authenticated using a mechanism that involves private keys that are known only to the superusers on the local and remote systems. Requests originating on systems that do not have these private keys are rejected. For more information, see the section on authentication information in the arrayd.conf(4) man page.

This setting should be adequate for systems that are behind a network firewall or otherwise protected from hostile attack. In this situation, all the users inside the firewall are presumed to be non-hostile.

Do not set AUTHENTICATION to NONE if the array is attached to a public network or if individual machines cannot be trusted.

- SIMPLE. Generates hostname/key pairs by using the OpenSSL rand command, 64-bit values (if available), or by using \$RANDOM Bash facilities. For more information, see arrayd.auth(5).
- MUNGE.

When set to MUNGE, uses the MUNGE credential encoder. For more information, see munge(1).

The Array Services daemon, arrayd, runs as root and does not support mapping of 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 to prevent access to an array by machines using a different namespace.

# **Configuring Nodes Into Arrays**

The following topics contain examples that show how to specify the nodes in an array in the arrayd.conf(5) file:

"Specifying an Array Name and Machine Names" on page 133

- "Specifying IP Addresses and Ports" on page 133
- "Specifying Additional Attributes" on page 134

#### Specifying an Array Name and Machine Names

Often, the hostname of each node is the same as the node's name to the site domain name services (DNS). The following example defines an array where this is the case:

```
array simple
machine congo
machine niger
machine nile
```

To access this array, the user needs to specify the the array name, simple, as the argument to the -a option on the array command and the ainfo command.

One array name should be specified in a DESTINATION ARRAY local option as the default array and reported by ainfo dflt. Local options are listed under "Configuring Local Options" on page 141.

# **Specifying IP Addresses and Ports**

At your site, 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 uses the port subentry to specify that arrayd in a particular machine use a different socket number than the default of 5434.

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#### **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:

```
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.

# **About the Array Configuration Files**

The Array Services configuration files are as follows:

- /etc/array/arrayd.conf
- /etc/array/arrayd.auth
- /etc/sysconfig/array

The configuration files contain array information, node information, authentication key information, and valid commands. The Array Services daemon reads each configuration file when it starts. Typically, the daemon starts on each node at boot time and then runs as a background process. The Array Services commands call the daemon process on each node to obtain information. You can also run the daemon from a command line. For example, you might want to run the daemon from a command line to check the syntax of a configuration file.

The following topics contain more configuration file information:

- "About Configuration File Formats and Contents" on page 134
- "About Loading Configuration Data" on page 135

#### **About Configuration File Formats and Contents**

A configuration file is a readable text file that contains the following types of entries:

- Array definition information, which describes this array and other known arrays, including array names and the node names and types.
- Command definitions, which specifies the usage and operation of a command that can be invoked through the array command.
- Authentication information, which specifies the authentication key numbers used to access the array. Not all arrays use authentication keys.
- Local options, which are options that modify the operation of the other entries or arrayd.

Within the configuration files, you can use blank lines, white space, and comment lines that begin with a pound character (#) for readability. Entries can be in any order in any of the Array Services configuration files.

Besides punctuation, entries have a keyword-based syntax. Keyword recognition is not case sensitive, but keywords appear in uppercase in this documentation and in the man(1) page. As the arrayd.conf(4) man page describes, the entries are formed from keywords, numbers, and quoted strings.

#### **About Loading Configuration Data**

When run as a command, the Array Services daemon, arrayd, accepts one or more file names as arguments. It reads them all and treats them like logical continuations. In effect, it concatenates them. If you do not specify any file names, it reads the following configuration files:

- /etc/array/arrayd.conf
- /etc/array/arrayd.auth
- /etc/sysconfig/array

This file can contain a list of files and arrayd command-line options. The start-up script that launches arrayd at boot time reads this file.

Because configuration data can reside in two or more files, you can combine different strategies. For example:

 One file can have different access permissions than another. Typically, /etc/array/arrayd.conf is world-readable and contains the available array commands, while /etc/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 on 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 and restarting the daemon on each machine, as follows:

- To kill the daemon, use one of the following commands:
  - On RHEL 7 or SLES 12 systems, type the following:

```
systemctl stop array
```

- On RHEL 6 or SLES 11 systems, type the following:

```
/etc/init.d/array stop
```

- To kill and restart the daemon in one operation, use one of the following commands:
  - On RHEL 7 or SLES 12 systems, type the following:

```
systemctl restart array
```

On RHEL 6 or SLES 11 systems, type the following:

```
/etc/init.d/array restart
```

The Array Services daemon on any node can access only the information in the configuration files on that node. One advantage to this design is that you can limit the use of particular nodes. At the same time, though, you need insure that common information is synchronized. "Designing New Array Commands" on page 142 summarizes a way to do this.

# **Designing Array Services Commands**

By default, most Array Services commands run using the user, group, and project ID of either the user that issued the original command or arraysvcs. When you add new array commands to arrayd.conf, or when you modify existing array commands, always use the most restrictive IDs possible. This practice minimizes

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.

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 configuration file.

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

#### **About Substitution Syntax**

The arrayd.conf(4) man page explains the syntax rules for 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 run.

Most of the supported substitutions are used in command entries. These substitutions are performed dynamically each time the array command invokes a subcommand. At that time, substitutions insert values that are unique to the invocation of that subcommand. For example, the value <code>%USER</code> inserts the user ID of the user who is invoking the array command. Such a substitution has meaning only when the command runs.

Substitutions in other configuration entries are performed only once, at the time arrayd reads the configuration file. 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 as follows:

• On RHEL 7 or SLES 12 systems, the script is as follows:

/usr/lib/systemd/system/array.service

• On RHEL 6 or SLES 11 systems, the script is as follows:

/etc/init.d/array

#### **About Array Command Operations**

When a user runs an array command, it has the following format:

```
array [options] subcommand
```

The specified *subcommand* operates on nodes as follows:

- If the user does not specify any options, the *subcommand* runs on the whole array.
- If the user specifies the -1 option, the *subcommand* runs on the local node.
- If the user specifies the -s *node* option, the command runs on all nodes that *node* knows about.

Remember that the destination node can be configured with only a subset of nodes. At each node, arrayd searches the configuration file for a COMMAND entry with the same name as the subcommand.

• If the user specifies both -1 and -s *node*, the subcommand runs on the specified *node*.

For example, in the following command, arrayd processes the uptime subcommand on node tokyo:

```
array -s tokyo uptime
```

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

In the /etc/array/arrayd.conf on tokyo, the COMMAND entry for uptime is as follows:

```
command uptime
  invoke /usr/lib/array/auptime %LOCAL
```

The INVOKE subentry tells arrayd how to run this command. In this case, it run a shell script, /usr/lib/array/auptime, and passes one argument, the name of the local node. This command runs on every node, with %LOCAL replaced by that node's name.

#### **Command Definition Syntax Summary**

The basic set of commands distributed with Array Services resides in /etc/array/arrayd.conf. Each COMMAND entry is defined using the subentries shown in Table B-1, which the arrayd.conf(4) man page also describes.

Table B-1 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 run on every node. Specify the full path to the system command. The argument values can be literals, user-supplied arguments, or other substitution values.
MERGE	A system command to be run only on the distributing node. Specify the full path to the system command. Its purpose is 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. Typically specified as USER %USER, so as to run as the user who invoked array.
GROUP	The group name under which the INVOKE and MERGE commands run. Typically specified as GROUP %GROUP, so as to run in the group of the user who invoked array. For more information, see the groups(1) man page.
PROJECT	The project under which the INVOKE and MERGE commands run. Typically specified as PROJECT %PROJECT, so as to run in the project of the user who invoked array. For more information, see the projects(5) man page.
OPTIONS	A variety of options to modify this command. For more information, see Table B-3.

As with a shell script, system commands are often composed from a few literal values and many substitution strings. Table B-2 shows the substitutions that are supported, all of which are documented in detail in the <code>arrayd.conf(4)</code> man page:

Table B-2 Substitutions Used in a COMMAND Definition

Substitution	Replacement Value
%1%9; %ARG(n); %ALLARGS; %OPTARG(n)	Argument tokens from the user's subcommand. %OPTARG does not produce an error message if the specified argument is omitted.
%USER, %GROUP, %PROJECT	The effective user ID, effective group ID, and project of the user who invoked array.
%REALUSER, %REALGROUP	The real user ID and real group ID of the user who invoked array.
%ASH	The internal array session handle (ASH) number under which the INVOKE or MERGE command is to run.  The term <i>array session</i> includes all the processes for one application, regardless of where the processes run. Typically, an array session includes the user's login shell and the programs the user started from the login shell. A batch job is an array session.
%PID( <i>ash</i> )	List of process identifier (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 where the output is to be viewed.
%OUTFILE	List of names of temporary files, each containing the output from one node's INVOKE command. Valid only in the MERGE subentry.

The  ${\tt OPTIONS}$  subentry permits a number of important modifications of the command execution. Table B-3 summarizes these.

Table B-3 Options of the COMMAND Definition

Keyword	Effect on Command
LOCAL	Does not distribute to other nodes. Effectively forces the $\mbox{-}\mbox{1}$ option.
NEWSESSION	Runs the INVOKE command under a newly created ASH. The %ASH in the INVOKE line is the new ASH. The MERGE command runs under the original ASH, and %ASH substitutes as the old ASH in that line.
SETRUID	Sets both the real and the effective user ID from the USER subentry. Typically, USER sets only the effective UID.
SETRGID	Sets both the real and effective group ID from the GROUP subentry. Typically, GROUP sets only the effective GID.
QUIET	Discards the output of INVOKE, unless a MERGE subentry is present. If a MERGE subentry is present, passes INVOKE output to MERGE as usual, and discards the MERGE output.
NOWAIT	Discards the output and returns as soon as the processes are invoked. Does not wait for completion. A MERGE subentry is ineffective.

# **Configuring Local Options**

The  ${\tt LOCAL}$  entry specifies options to arrayd itself. Table B-4 summarizes the most important options.

Table B-4 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 specified, it is the default destination.

Subentry	Purpose
USER, GROUP, PROJECT	Default values for COMMAND execution when USER, GROUP, or PROJECT are omitted from the COMMAND definition.
HOSTNAME	Value returned in this node by $\mbox{\ensuremath{\$LOCAL}}.$ 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(1) 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**

The /usr/lib/array/arrayd.conf.template file contains a basic set of commands. Examine this file carefully before defining commands of your own. Any new commands that you design become available to the users of the array system. You can develop new administrative commands, too.

Typically, a new command is defined with an INVOKE subentry that names a script written in sh, csh, or Perl syntax. You can 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 run any command sequence. 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 because 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 following example shows an administrator command called reinit, which reinitializes the Array Services configuration file on all nodes at once:

• The shell script in file /usr/lib/array/arrayd-reinit reinitializes each Array Services configuration file, on each node, simultaneously. The script is designed for RHEL 7 systems and SLES 12 systems and is as follows:

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

• The following is the command definition:

The INVOKE subentry calls the script shown previously. The NOWAIT option prevents the daemon from waiting for the script to finish. The script stops the daemon.



**Caution:** The preceding example is for illustrative purposes only and has not been evaluated for use in a production environment.

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# Testing Configuration Changes After Creating New Array Services Commands

The configuration files contain many sections and options. You can use the ascheck command to perform a basic sanity check of all configuration files in the array.

After making a change, you can run the arrayd command with the -c and -f options to test an individual configuration file for correct syntax. For example, assume that you added a new command definition to /etc/array/arrayd.local. You can type the following command to check its syntax:

```
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 the arrayd command and by the processes that the arrayd command can spawn. Typically, the stderr messages from a daemon are not visible.

#### **Procedure B-2** To test configuration changes

- Notify the array's users that you are able to start an array configuration update.
   Users might experience a lack of response to ainfo and array commands.
- 2. Log into one of the nodes as the root user, and type one of the following commands:
  - On RHEL 7.X or SLES 12 SPX systems, type the following command:
    - # systemctl stop array
  - On RHEL 6.X or SLES 11 SPX systems, type the following command:
    - # /etc/init.d/array stop
- 3. In one shell window on that node, type the following arrayd command:
  - # /usr/sbin/arrayd -n -v

The preceding command prevents the arrayd command from moving into the background. The command remains attached to the shell terminal.

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

- 4. From another shell window on the same node (or on another node), issue ainfo and array commands to test the new configuration data.
  - Observe that diagnostic output appears in the arrayd shell window.
- 5. From the shell window in which you typed the /usr/sbin/arrayd -n -v command, type CTRL-c to terminate the arrayd daemon.
- 6. Type one of the following commands to start the arrayd daemon:
  - On RHEL 7.X or SLES 12 SPX systems, type the following command:
    - # systemctl start array
  - On RHEL 6.*X* or SLES 11 SP*X* systems, type the following command:
    - # /etc/init.d/array start

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