MPICH2 User's Guide*

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Contents

1	Introduction				
2	Mig	grating to MPICH2 from MPICH1			
	2.1	Defau	lt Runtime Environment	1	
	2.2	Startin	ng Parallel Jobs	2	
	2.3	Comm	nand-Line Arguments in Fortran	2	
3	Qui	ck Start			
4	4 Compiling and Linking			3	
	4.1	Specif	ying Compilers	4	
	4.2	.2 Shared Libraries		4	
	4.3	3 Special Issues for C++		4	
	4.4	Specia	d Issues for Fortran	5	
5	Rur	Running Programs with mpiexec			
5.1 Standard mpiexec		ard mpiexec	5		
	5.2	5.2 Extensions for All Process Management Environments		6	
	5.3 Extensions for the MPD Process Management Envir		sions for the MPD Process Management Environment .	6	
		5.3.1	Basic mpiexec arguments for MPD	6	
		5.3.2	Other Command-Line Arguments to mpiexec for MPD	7	
		5.3.3	Environment Variables Affecting mpiexec for MPD	11	
	5.4 Extensions for SMPD Process Management Environm		sions for SMPD Process Management Environment	12	
		5.4.1	mpiexec arguments for SMPD	12	
5.5 Extensions for the gforker Process Management E			sions for the gforker Process Management Environment	15	
		5.5.1	mpiexec arguments for gforker	15	

	5.6	Extensions for the hydra Process Management Environment .		
		5.6.1 mpiexec arguments for hydra	17	
	5.7 Restrictions of the remshell Process Management Environ			
	5.8 Using MPICH2 with SLURM and PBS			
		5.8.1 MPD in the PBS environment	19	
		5.8.2 OSC mpiexec	19	
6	naging the Process Management Environment	20		
	6.1	MPD	20	
7	Debugging			
	7.1	gdb via mpiexec	21	
	7.2	TotalView	24	
8	MPE			
	8.1	MPI Logging	26	
	8.2	User-defined logging	26	
	8.3	MPI Checking	27	
	8.4	MPE options	28	
9	Other Tools Provided with MPICH2			
10	10 MPICH2 under Windows			
	10.1	Directories	29	
	10.2	Compiling	29	
	10.3	Running	30	
\mathbf{A}	Frequently Asked Questions			

1

1 Introduction

This manual assumes that MPICH2 has already been installed. For instructions on how to install MPICH2, see the MPICH2 Installer's Guide, or the README in the top-level MPICH2 directory. This manual explains how to compile, link, and run MPI applications, and use certain tools that come with MPICH2. This is a preliminary version and some sections are not complete yet. However, there should be enough here to get you started with MPICH2.

2 Migrating to MPICH2 from MPICH1

If you have been using MPICH 1.2.x (1.2.7p1 is the latest version), you will find a number of things about MPICH2 that are different (and hopefully better in every case.) Your MPI application programs need not change, of course, but a number of things about how you run them will be different.

MPICH2 is an all-new implementation of the MPI Standard, designed to implement all of the MPI-2 additions to MPI (dynamic process management, one-sided operations, parallel I/O, and other extensions) and to apply the lessons learned in implementing MPICH1 to make MPICH2 more robust, efficient, and convenient to use. The MPICH2 Installer's Guide provides some information on changes between MPICH1 and MPICH2 to the process of configuring and installing MPICH. Changes to compiling, linking, and running MPI programs between MPICH1 and MPICH2 are described below.

2.1 Default Runtime Environment

In MPICH1, the default configuration used the now-old p4 portable programming environment. Processes were started via remote shell commands (rsh or ssh) and the information necessary for processes to find and connect with one another over sockets was collected and then distributed at startup time in a non-scalable fashion. Furthermore, the entanglement of process management functionality with the communication mechanism led to confusing behavior of the system when things went wrong.

MPICH2 provides a separation of process management and communication. The default runtime environment consists of a set of daemons, called mpd's, that establish communication among the machines to be used before application process startup, thus providing a clearer picture of what is wrong when communication cannot be established and providing a fast and scalable startup mechanism when parallel jobs are started. Section 6.1 describes the MPD process management system in more detail. Other process managers are also available.

2.2 Starting Parallel Jobs

MPICH1 provided the mpirun command to start MPICH1 jobs. The MPI-2 Forum recommended a standard, portable command, called mpiexec, for this purpose. MPICH2 implements mpiexec and all of its standard arguments, together with some extensions. See Section 5.1 for standard arguments to mpiexec and various subsections of Section 5 for extensions particular to various process management systems.

MPICH2 also provides an mpirun command for simple backward compatibility, but MPICH2's mpirun does not provide all the options of mpiexec or all of the options of MPICH1's mpirun.

2.3 Command-Line Arguments in Fortran

MPICH1 (more precisely MPICH1's mpirun) required access to command line arguments in all application programs, including Fortran ones, and MPICH1's configure devoted some effort to finding the libraries that contained the right versions of iargc and getarg and including those libraries with which the mpif77 script linked MPI programs. Since MPICH2 does not require access to command line arguments to applications, these functions are optional, and configure does nothing special with them. If you need them in your applications, you will have to ensure that they are available in the Fortran environment you are using.

3 Quick Start

To use MPICH2, you will have to know the directory where MPICH2 has been installed. (Either you installed it there yourself, or your systems administrator has installed it. One place to look in this case might be /usr/local.

If MPICH2 has not yet been installed, see the MPICH2 Installer's Guide.) We suggest that you put the bin subdirectory of that directory into your path. This will give you access to assorted MPICH2 commands to compile, link, and run your programs conveniently. Other commands in this directory manage parts of the run-time environment and execute tools.

One of the first commands you might run is mpich2version to find out the exact version and configuration of MPICH2 you are working with. Some of the material in this manual depends on just what version of MPICH2 you are using and how it was configured at installation time.

You should now be able to run an MPI program. Let us assume that the directory where MPICH2 has been installed is /home/you/mpich2-installed, and that you have added that directory to your path, using

```
setenv PATH /home/you/mpich2-installed/bin:$PATH
```

for tcsh and csh, or

```
export PATH=/home/you/mpich2-installed/bin:$PATH
```

for bash or sh. Then to run an MPI program, albeit only on one machine, you can do:

```
mpd &
cd /home/you/mpich2-installed/examples
mpiexec -n 3 cpi
mpdallexit
```

Details for these commands are provided below, but if you can successfully execute them here, then you have a correctly installed MPICH2 and have run an MPI program.

4 Compiling and Linking

A convenient way to compile and link your program is by using scripts that use the same compiler that MPICH2 was built with. These are mpicc, mpicxx, mpif77, and mpif90, for C, C++, Fortran 77, and Fortran 90 programs, respectively. If any of these commands are missing, it means that MPICH2 was configured without support for that particular language.

4.1 Specifying Compilers

You need not use the same compiler that MPICH2 was built with, but not all compilers are compatible. You can also specify the compiler for building MPICH2 itself, as reported by mpich2version, just by using the compiling and linking commands from the previous section. The environment variables MPICH_CC, MPICH_CXX, MPICH_F77, and MPICH_F90 may be used to specify alternate C, C++, Fortran 77, and Fortran 90 compilers, respectively.

4.2 Shared Libraries

Currently shared libraries are only tested on Linux and Mac OS X, and there are restrictions. See the *Installer's Guide* for how to build MPICH2 as a shared library. If shared libraries have been built, you will get them automatically when you link your program with any of the MPICH2 compilation scripts.

4.3 Special Issues for C++

Some users may get error messages such as

```
SEEK_SET is #defined but must not be for the C++ binding of MPI
```

The problem is that both stdio.h and the MPI C++ interface use SEEK_SET, SEEK_CUR, and SEEK_END. This is really a bug in the MPI-2 standard. You can try adding

```
#undef SEEK_SET
#undef SEEK_END
#undef SEEK_CUR
```

before mpi.h is included, or add the definition

```
-DMPICH_IGNORE_CXX_SEEK
```

to the command line (this will cause the MPI versions of SEEK_SET etc. to be skipped).

4.4 Special Issues for Fortran

MPICH2 provides two kinds of support for Fortran programs. For Fortran 77 programmers, the file mpif.h provides the definitions of the MPI constants such as MPI_COMM_WORLD. Fortran 90 programmers should use the MPI module instead; this provides all of the definitions as well as interface definitions for many of the MPI functions. However, this MPI module does not provide full Fortran 90 support; in particular, interfaces for the routines, such as MPI_Send, that take "choice" arguments are not provided.

5 Running Programs with mpiexec

If you have been using the original MPICH, or any of a number of other MPI implementations, then you have probably been using mpirun as a way to start your MPI programs. The MPI-2 Standard describes mpiexec as a suggested way to run MPI programs. MPICH2 implements the mpiexec standard, and also provides some extensions. MPICH2 provides mpirun for backward compatibility with existing scripts, but it does not support the same or as many options as mpiexec or all of the options of MPICH1's mpirun.

5.1 Standard mpiexec

Here we describe the standard mpiexec arguments from the MPI-2 Standard [1]. The simplest form of a command to start an MPI job is

```
mpiexec -n 32 a.out
```

to start the executable a.out with 32 processes (providing an MPI_COMM_WORLD of size 32 inside the MPI application). Other options are supported, for specifying hosts to run on, search paths for executables, working directories, and even a more general way of specifying a number of processes. Multiple sets of processes can be run with different exectuables and different values for their arguments, with ":" separating the sets of processes, as in:

mpiexec -n 1 -host loginnode master : -n 32 -host smp slave

The -configfile argument allows one to specify a file containing the specifications for process sets on separate lines in the file. This makes it unnecessary to have long command lines for mpiexec. (See pg. 353 of [2].)

It is also possible to start a one process MPI job (with a MPI_COMM_WORLD whose size is equal to 1), without using mpiexec. This process will become an MPI process when it calls MPI_Init, and it may then call other MPI functions. Currently, MPICH2 does not fully support calling the dynamic process routines from MPI-2 (e.g., MPI_Comm_spawn or MPI_Comm_accept) from processes that are not started with mpiexec.

5.2 Extensions for All Process Management Environments

Some mpiexec arguments are specific to particular communication subsystems ("devices") or process management environments ("process managers"). Our intention is to make all arguments as uniform as possible across devices and process managers. For the time being we will document these separately.

5.3 Extensions for the MPD Process Management Environment

MPICH2 provides a number of process management systems. The default is called MPD. MPD provides a number of extensions to the standard form of mpiexec.

5.3.1 Basic mpiexec arguments for MPD

The default configuration of MPICH2 chooses the MPD process manager and the "simple" implementation of the Process Management Interface. MPD provides a version of mpiexec that supports both the standard arguments described in Section 5.1 and other arguments described in this section. MPD also provides a number of commands for querying the MPD process management environment and interacting with jobs it has started.

Before running mpiexec, the runtime environment must be established. In the case of MPD, the daemons must be running. See Section 6.1 for how to run and manage the MPD daemons.

We assume that the MPD ring is up and the installation's **bin** directory is in your path; that is, you can do:

mpdtrace

and it will output a list of nodes on which you can run MPI programs. Now you are ready to run a program with mpiexec. Let us assume that you have compiled and linked the program cpi (in the installdir/examples directory and that this directory is in your PATH. Or that is your current working directory and '.' ("dot") is in your PATH. The simplest thing to do is

```
mpiexec -n 5 cpi
```

to run cpi on five nodes. The process management system (such as MPD) will choose machines to run them on, and cpi will tell you where each is running.

You can use mpiexec to run non-MPI programs as well. This is sometimes useful in making sure all the machines are up and ready for use. Useful examples include

```
mpiexec -n 10 hostname
```

and

mpiexec -n 10 printenv

5.3.2 Other Command-Line Arguments to mpiexec for MPD

The MPI-2 standard specifies the syntax and semantics of the arguments -n, -path,-wdir, -host, -file, -configfile, and -soft. All of these are currently implemented for MPD's mpiexec. Each of these is what we call a "local" option, since its scope is the processes in the set of processes described between colons, or on separate lines of the file specified by -configfile. We add some extensions that are local in this way and some that are "global" in the sense that they apply to all the processes being started by the invocation of mpiexec.

The MPI-2 Standard provides a way to pass different arguments to different application processes, but does not provide a way to pass environment variables. MPICH2 provides an extension that supports environment variables. The local parameter <code>-env</code> does this for one set of processes. That is,

```
mpiexec -n 1 -env FOO BAR a.out : -n 2 -env BAZZ FAZZ b.out
```

makes BAR the value of environment variable FOO on the first process, running the executable a.out, and gives the environment variable BAZZ the value FAZZ on the second two processes, running the executable b.out. To set an environment variable without giving it a value, use '' as the value in the above command line.

The global parameter **-genv** can be used to pass the same environment variables to all processes. That is,

```
mpiexec -genv FOO BAR -n 2 a.out : -n 4 b.out
```

makes BAR the value of the environment variable F00 on all six processes. If -genv appears, it must appear in the first group. If both -genv and -env are used, the -env's add to the environment specified or added to by the -genv variables. If there is only one set of processes (no ":"), the -genv and -env are equivalent.

The local parameter -envall is an abbreviation for passing the entire environment in which mpiexec is executed. The global version of it is -genvall. This global version is implicitly present. To pass no environment variables, use -envnone and -genvnone. So, for example, to set only the environment variable FOO and no others, regardless of the current environment, you would use

```
mpiexec -genvnone -env FOO BAR -n 50 a.out
```

In the case of MPD, we currently make an exception for the PATH environment variable, which is always passed through. This exception was added to make it unnecessary to explicitly pass this variable in the default case.

A list of environment variable names whose values are to be copied from the current environment can be given with the -envlist (respectively, -genvlist) parameter; for example,

mpiexec -genvnone -envlist HOME, LD_LIBRARY_PATH -n 50 a.out

sets the HOME and LD_LIBRARY_PATH in the environment of the a.out processes to their values in the environment where mpiexec is being run. In this situation you can't have commas in the environment variable names, although of course they are permitted in values.

Some extension parameters have only global versions. They are

- -1 provides rank labels for lines of stdout and stderr. These are a bit obscure for processes that have been explicitly spawned, but are still useful.
- -usize sets the "universe size" that is retrieved by the MPI attribute MPI_UNIVERSE_SIZE on MPI_COMM_WORLD.
- -bnr is used when one wants to run executables that have been compiled and linked using the ch_p4mpd or myrinet device in MPICH1. The MPD process manager provides backward compatibility in this case.
- -machinefile can be used to specify information about each of a set of machines. This information may include the number of processes to run on each host when executing user programs. For example, assume that a machinefile named mf contains:

comment line
hosta
hostb:2
hostc ifhn=hostc-gige
hostd:4 ifhn=hostd-gige

In addition to specifying hosts and number of processes to run on each, this machinefile indicates that processes running on hostc and hostd should use the gige interface on hostc and hostd respectively for MPI communications. (ifhn stands for "interface host name" and should be set to an alternate host name for the machine that is used to designate an alternate communication interface.) This interface information causes the MPI implementation to choose the alternate host name when making connections. When the alternate hostname specifies a particular interface, MPICH communication will then travel over that interface.

You might use this machinefile in the following way:

Process rank 0 is to run on hosta, ranks 1 and 2 on hostb, rank 3 on hostc, and ranks 4-6 on hostd. Note that the file specifies information for up to 8 ranks and we only used 7. That is OK. But, if we had used "-n 9", an error would be raised. The file is not used as a pool of machines that are cycled through; the processes are mapped to the hosts in the order specified in the file.

A more complex command-line example might be:

Here, ranks 0-2 all run program p1 and are executed placing rank 0 on hosta and ranks 1-2 on hostb. Similarly, ranks 3-4 run p2 and are executed on hostc and hostd, respectively. Ranks 5-6 run on hostd and execute p3.

-s can be used to direct the stdin of mpiexec to specific processes in a parallel job. For example:

directs the stdin of mpiexec to all five processes.

directs it to just the process with rank 4, and

sends it to processes 1 and 3, while

sends stdin to processes 0, 1, 2, and 3.

The default, if -s is not specified, is to send mpiexec's stdin to process 0 only.

The redirection of -stdin through mpiexec to various MPI processes is intended primarily for interactive use. Because of the complexity of buffering large amounts of data at various processes that may not have read it yet, the redirection of large amounts of data to mpiexec's stdin is discouraged, and may cause unexpected results. That is,

```
mpiexec -s all -n 5 a.out < bigfile
```

should not be used if **bigfile** is more than a few lines long. Have one of the processes open the file and read it instead. The functions in MPI-IO may be useful for this purpose.

A ":" can optionally be used between global args and normal argument sets, e.g.:

```
mpiexec -l -n 1 -host host1 pgm1 : -n 4 -host host2 pgm2 is equivalent to:
```

```
mpiexec -1 : -n 1 -host host1 pgm1 : -n 4 -host host2 pgm2
```

This option implies that the global arguments can occur on a separate line in the file specified by -configfile when it is used to replace a long command line.

5.3.3 Environment Variables Affecting mpiexec for MPD

A small number of environment variables affect the behavior of mpiexec.

- MPIEXEC_TIMEOUT The value of this environment variable is the maximum number of seconds this job will be permitted to run. When time is up, the job is aborted.
- MPIEXEC_PORT_RANGE If this environment variable is defined then the MPD system will restrict its usage of ports for connecting its various processes to ports in this range. If this variable is not assigned, but MPICH_PORT_RANGE is assigned, then it will use the range specified by MPICH_PORT_RANGE for its ports. Otherwise, it will use whatever paorts are assigned to it by the system. Port ranges are given as a pair of integers separated by a colon.
- MPIEXEC_BNR If this environment variable is defined (its value, if any, is currently insignificant), then MPD will act in backward-compatibility mode, supporting the BNR interface from the original MPICH (e.g. versions 1.2.0 1.2.7p1) instead of its native PMI interface, as a way for application processes to interact with the process management system.

MPD_CON_EXT Adds a string to the default Unix socket name used by mpiexec to find the local mpd. This allows one to run multiple mpd rings at the same time.

5.4 Extensions for SMPD Process Management Environment

SMPD is an alternate process manager that runs on both Unix and Windows. It can launch jobs across both platforms if the binary formats match (big/little endianness and size of C types—int, long, void*, etc).

5.4.1 mpiexec arguments for SMPD

mpiexec for smpd accepts the standard MPI-2 mpiexec options. Execute

mpiexec

or

mpiexec -help2

to print the usage options. Typical usage:

mpiexec -n 10 myapp.exe

All options to mpiexec:

-n x

-np x

launch x processes

-localonly x

-np x -localonly

launch x processes on the local machine

-machinefile filename

use a file to list the names of machines to launch on

-host hostname

launch on the specified host.

-hosts n host1 host2 ... hostn

-hosts n host1 m1 host2 m2 ... hostn mn

launch on the specified hosts. In the second version the number of processes = m1 + m2 + ... + mn

-dir drive:\my\working\directory

-wdir /my/working/directory

launch processes with the specified working directory. (-dir and -wdir are equivalent)

-env var val

set environment variable before launching the processes

-exit codes

print the process exit codes when each process exits.

-noprompt

prevent mpiexec from prompting for user credentials. Instead errors will be printed and mpiexec will exit.

-localroot

launch the root process directly from mpiexec if the host is local. (This allows the root process to create windows and be debugged.)

-port port

-p port

specify the port that smpd is listening on.

-phrase passphrase

specify the passphrase to authenticate connections to smpd with.

-smpdfile filename

specify the file where the ${\tt smpd}$ options are stored including the passphrase. (unix only option)

-path search_path

search path for executable,; separated

-timeout seconds

timeout for the job.

Windows specific options:

-map drive:\\host\share

map a drive on all the nodes this mapping will be removed when the processes exit

-logon

prompt for user account and password

-pwdfile filename

read the account and password from the file specified.

put the account on the first line and the password on the second

-nopopup_debug

disable the system popup dialog if the process crashes

-priority class[:level]

set the process startup priority class and optionally level. class =0,1,2,3,4= idle, below, normal, above, high level =0,1,2,3,4,5= idle, lowest, below, normal, above, highest the default is -priority 2:3

-register

encrypt a user name and password to the Windows registry.

-remove

delete the encrypted credentials from the Windows registry.

-validate [-host hostname]

validate the encrypted credentials for the current or specified host.

-delegate

use passwordless delegation to launch processes.

-impersonate

use passwordless authentication to launch processes.

-plaintext

don't encrypt the data on the wire.

5.5 Extensions for the gforker Process Management Environment

gforker is a process management system for starting processes on a single machine, so called because the MPI processes are simply forked from the mpiexec process. This process manager supports programs that use MPI_Comm_spawn and the other dynamic process routines, but does not support the use of the dynamic process routines from programs that are not started with mpiexec. The gforker process manager is primarily intended as a debugging aid as it simplifies development and testing of MPI programs on a single node or processor.

5.5.1 mpiexec arguments for gforker

In addition to the standard mpiexec command-line arguments, the gforker mpiexec supports the following options:

- -np <num> A synonym for the standard -n argument
- -env <name> <value> Set the environment variable <name> to <value> for the processes being run by mpiexec.
- -envnone Pass no environment variables (other than ones specified with other -env or -genv arguments) to the processes being run by mpiexec. By default, all environment variables are provided to each MPI process (rationale: principle of least surprise for the user)
- -envlist Pass the listed environment variables (names separated by commas), with their current values, to the processes being run by mpiexec.
- -genv <name> <value> The
- -genv options have the same meaning as their corresponding -env version, except they apply to all executables, not just the current executable (in the case that the colon syntax is used to specify multiple execuables).
- -genvnone Like -envnone, but for all executables
- -genvlist <list> Like -envlist, but for all executables
- -usize <n> Specify the value returned for the value of the attribute MPI_UNIVERSE_SIZE.

- -1 Label standard out and standard error (stdout and stderr) with the rank of the process
- -maxtime <n> Set a timelimit of <n> seconds.
- -exitinfo Provide more information on the reason each process exited if there is an abnormal exit

In addition to the commandline argments, the gforker mpiexec provides a number of environment variables that can be used to control the behavior of mpiexec:

- MPIEXEC_TIMEOUT Maximum running time in seconds. mpiexec will terminate MPI programs that take longer than the value specified by MPIEXEC TIMEOUT.
- MPIEXEC UNIVERSE SIZE Set the universe size
- MPIEXEC_PORT_RANGE Set the range of ports that mpiexec will use in communicating with the processes that it starts. The format of this is <low>:<high>. For example, to specify any port between 10000 and 10100, use 10000:10100.
- MPICH_PORT_RANGE Has the same meaning as MPIEXEC_PORT_RANGE and is used if MPIEXEC_PORT_RANGE is not set.
- MPIEXEC_PREFIX_DEFAULT If this environment variable is set, output to standard output is prefixed by the rank in MPI_COMM_WORLD of the process and output to standard error is prefixed by the rank and the text (err); both are followed by an angle bracket (>). If this variable is not set, there is no prefix.
- MPIEXEC_PREFIX_STDOUT Set the prefix used for lines sent to standard output. A %d is replaced with the rank in MPI_COMM_WORLD; a %w is replaced with an indication of which MPI_COMM_WORLD in MPI jobs that involve multiple MPI_COMM_WORLDs (e.g., ones that use MPI_Comm_spawn or MPI_Comm_connect).
- $\label{eq:mpiexec_prefix_stderr} \mbox{MPIEXEC_PREFIX_STDOUT, but for standard error.}$

MPIEXEC_STDOUTBUF Sets the buffering mode for standard output. Valid values are NONE (no buffering), LINE (buffering by lines), and BLOCK (buffering by blocks of characters; the size of the block is implementation defined). The default is NONE.

MPIEXEC_STDERRBUF Like MPIEXEC_STDOUTBUF, but for standard error.

5.6 Extensions for the hydra Process Management Environment

hydra is a process management system for starting processes using the native launcher daemons present on the system such as ssh, slurm, pbs. This process manager does not support programs that use MPI_Comm_spawn and the other dynamic process routines.

5.6.1 mpiexec arguments for hydra

In addition to the standard mpiexec command-line arguments, the hydra mpiexec supports the following options:

- -np <num> A synonym for the standard -n argument
- -env <name> <value> Set the environment variable <name> to <value> for the processes being run by mpiexec.
- -envnone Pass no environment variables (other than ones specified with other -env or -genv arguments) to the processes being run by mpiexec.
 By default, all environment variables are provided to each MPI process (rationale: principle of least surprise for the user)
- -envlist -envlist > Pass the listed environment variables (names separated by commas), with their current values, to the processes being run by mpiexec.
- -genv <name> <value> The
- -genv options have the same meaning as their corresponding -env version, except they apply to all executables, not just the current executable (in the case that the colon syntax is used to specify multiple execuables).
- -genvnone Like -envnone, but for all executables

-genvlist <list> Like -envlist, but for all executables

In addition to the commandline argments, the hydra mpiexec provides a number of environment variables that can be used to control the behavior of mpiexec:

MPIEXEC_TIMEOUT Maximum running time in seconds. mpiexec will terminate MPI programs that take longer than the value specified by MPIEXEC_TIMEOUT.

MPIEXEC_PORT_RANGE Set the range of ports that mpiexec will use in communicating with the processes that it starts. The format of this is <low>:<high>. For example, to specify any port between 10000 and 10100, use 10000:10100.

MPICH_PORT_RANGE Has the same meaning as MPIEXEC_PORT_RANGE and is used if MPIEXEC_PORT_RANGE is not set.

HYDRA_HOST_FILE Specifies the host file to use to launch processes.

HYDRA_USE_LOCALHOST Forces hydra to spawn all processes on the local host.

5.7 Restrictions of the remshell Process Management Environment

The remshell "process manager" provides a very simple version of mpiexec that makes use of the secure shell command (ssh) to start processes on a collection of machines. As this is intended primarily as an illustration of how to build a version of mpiexec that works with other process managers, it does not implement all of the features of the other mpiexec programs described in this document. In particular, it ignores the command line options that control the environment variables given to the MPI programs. It does support the same output labeling features provided by the gforker version of mpiexec. However, this version of mpiexec can be used much like the mpirun for the ch_p4 device in MPICH-1 to run programs on a collection of machines that allow remote shells. A file by the name of machines should contain the names of machines on which processes can be run, one machine name per line. There must be enough machines listed to satisfy the requested number of processes; you can list the same machine name multiple times if necessary.

For more complex needs or for faster startup, we recommend the use of the mpd process manager.

5.8 Using MPICH2 with SLURM and PBS

MPICH2 can be used in both SLURM and PBS environments. If configured with SLURM, use the srun job launching utility provided by SLURM. For PBS, MPICH2 jobs can be launched in two ways: (i) using MPD or (ii) using the OSC mpiexec.

5.8.1 MPD in the PBS environment

PBS specifies the machines allocated to a particular job in the file \$PBS_NODEFILE. But the format used by PBS is different from that of MPD. Specifically, PBS lists each node on a single line; if a node (n0) has two processors, it is listed twice. MPD on the other hand uses an identifier (ncpus) to describe how many processors a node has. So, if n0 has two processors, it is listed as n0:2.

One way to convert the node file to the MPD format is as follows:

sort $PBS_NODEFILE \mid uniq -C \mid awk '{ printf("%s:%s", $2, $1); }' > mpd.nodes$

Once the PBS node file is converted, MPD can be normally started within the PBS job script using mpdboot and torn down using mpdallexit.

```
mpdboot -f mpd.hosts -n [NUM_NODES_REQUESTED]
mpiexec -n [NUM_PROCESSES] ./my_test_program
mpdallexit
```

5.8.2 OSC mpiexec

Pete Wyckoff from the Ohio Supercomputer Center provides a alternate utility called OSC mpiexec to launch MPICH2 jobs on PBS systems without using MPD. More information about this can be found here: http://www.osc.edu/~pw/mpiexec

6 Managing the Process Management Environment

Some of the process managers supply user commands that can be used to interact with the process manager and to control jobs. In this section we describe user commands that may be useful.

6.1 MPD

mpd starts an mpd daemon.

mpdboot starts a set of mpd's on a list of machines.

mpdtrace lists all the MPD daemons that are running. The -1 option lists full hostnames and the port where the mpd is listening.

mpdlistjobs lists the jobs that the mpd's are running. Jobs are identified by the name of the mpd where they were submitted and a number.

mpdkilljob kills a job specified by the name returned by mpdlistjobs

mpdsigjob delivers a signal to the named job. Signals are specified by name or number.

You can use keystrokes to provide signals in the usual way, where mpiexec stands in for the entire parallel application. That is, if mpiexec is being run in a Unix shell in the foreground, you can use ^C (control-C) to send a SIGINT to the processes, or ^Z (control-Z) to suspend all of them. A suspended job can be continued in the usual way.

Precise argument formats can be obtained by passing any MPD command the --help or -h argument. More details can be found in the README in the mpich2 top-level directory or the README file in the MPD directory mpich2/src/pm/mpd.

7 Debugging

Debugging parallel programs is notoriously difficult. Here we describe a number of approaches, some of which depend on the exact version of MPICH2 you are using.

7.1 gdb via mpiexec

If you are using the MPD process manager, you can use the -gdb argument to mpiexec to execute a program with each process running under the control of the gdb sequential debugger. The -gdb option helps control the multiple instances of gdb by sending stdin either to all processes or to a selected process and by labeling and merging output. The current implementation has some minor limitations. For example, we do not support setting your own prompt. This is because we capture the gdb output and examine it before processing it, e.g. merging identical lines. Also, we set a breakpoint at the beginning of main to get all processes synchronized at the beginning. Thus, the user will have a duplicate, unusable breakpoint if he sets one at the very first executable line of main. Otherwise, to the extent possible, we try to simply pass user input through to gdb and lets things progress normally.

The following script of a <code>-gdb</code> session gives an idea of how this works. Input keystrokes are sent to all processes unless specifially directed by the "z" command.

```
ksl2% mpiexec -gdb -n 10 cpi
     (gdb) 1
0-9: 5 double f(double);
0-9: 6
0-9: 7 double f(double a)
0-9: 8 {
0-9: 9
            return (4.0 / (1.0 + a*a));
0-9: 10
0-9:
      11
0-9:
                int main(int argc,char *argv[])
      12
0-9: 13
                {
0-9: 14
                    int done = 0, n, myid, numprocs, i;
0-9:
      (gdb)
                    double PI25DT = 3.141592653589793238462643;
0-9:
      15
0-9:
     16
                    double mypi, pi, h, sum, x;
0-9:
      17
                    double startwtime = 0.0, endwtime;
0-9:
      18
                    int namelen;
                    char processor_name[MPI_MAX_PROCESSOR_NAME];
0-9:
     19
0-9: 20
0-9: 21
                    MPI_Init(&argc,&argv);
0-9: 22
                    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
0-9: 23
                    MPI_Comm_rank(MPI_COMM_WORLD,&myid);
0-9: 24
                    MPI_Get_processor_name(processor_name,&namelen);
```

```
0-9: (gdb)
0-9: 25
0-9: 26
                   fprintf(stdout, "Process %d of %d is on %s\n",
0-9: 27
0-9: 28
                           myid, numprocs, processor_name);
                   fflush(stdout);
0-9: 29
0-9: 30
                  n = 10000;
                                    /* default # of rectangles */
0-9: 31
                  if (myid == 0)
0-9: 32
                       startwtime = MPI_Wtime();
0-9: 33
0-9: 34
                   MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
0-9: (gdb) b 30
0-9: Breakpoint 2 at 0x4000000000002541:
                     file /home/lusk/mpich2/examples/cpi.c, line 30.
0-9: (gdb) r
0-9: Continuing.
0: Process 0 of 10 is on ksl2
1: Process 1 of 10 is on ksl2
2: Process 2 of 10 is on ksl2
3: Process 3 of 10 is on ksl2
4: Process 4 of 10 is on ksl2
5: Process 5 of 10 is on ksl2
6: Process 6 of 10 is on ksl2
7: Process 7 of 10 is on ksl2
8: Process 8 of 10 is on ksl2
9: Process 9 of 10 is on ksl2
0-9:
0-9: Breakpoint 2, main (argc=1, argv=0x60000ffffffffb4b8)
0-9: at /home/lusk/mpich2/examples/cpi.c:30
0-9: 30
                  n = 10000;
                                * default # of rectangles */
0-9: (gdb) n
0-9: 31
                  if (myid == 0)
0-9: (gdb) n
0: 32
               startwtime = MPI_Wtime();
1-9: 34
                   MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
0-9: (gdb) z 0
0: (gdb) n
0: 34
           MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
0: (gdb) z
0-9: (gdb) where
0-9: #0 main (argc=1, argv=0x60000fffffffb4b8)
         at /home/lusk/mpich2/examples/cpi.c:34
0-9: (gdb) n
0-9: 36
                  h = 1.0 / (double) n;
0-9: (gdb)
```

```
0-9: 37
                  sum = 0.0;
0-9: (gdb)
0-9: 39
                  for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
0-9: 41
                       x = h * ((double)i - 0.5);
0-9: (gdb)
0-9: 42
                       sum += f(x);
0-9: (gdb)
0-9: 39
                  for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
0-9: 41
                       x = h * ((double)i - 0.5);
0-9: (gdb)
0-9: 42
                       sum += f(x);
0-9: (gdb)
0-9: 39
                  for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
                      x = h * ((double)i - 0.5);
0-9: 41
0-9: (gdb)
0-9: 42
                      sum += f(x);
0-9: (gdb)
0-9: 39
                 for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
0-9: 41
                      x = h * ((double)i - 0.5);
0-9: (gdb)
0-9: 42
                      sum += f(x);
0-9: (gdb)
0-9: 39
                  for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
0-9: 41
                      x = h * ((double)i - 0.5);
0-9: (gdb)
0-9: 42
                      sum += f(x);
0-9: (gdb)
0-9: 39
                  for (i = myid + 1; i <= n; i += numprocs)
0-9: (gdb)
0-9: 41
                      x = h * ((double)i - 0.5);
0-9: (gdb)
0-9: 42
                      sum += f(x);
0-9: (gdb) p sum
0: $1 = 19.999875951497799
1: $1 = 19.999867551672725
2: $1 = 19.999858751863549
3: $1 = 19.999849552071328
4: $1 = 19.999839952297158
5: $1 = 19.999829952542203
6: $1 = 19.999819552807658
```

```
7: $1 = 19.999808753094769
8: $1 = 19.999797553404832
9: $1 = 19.999785953739192
0-9: (gdb) c
0-9: Continuing.
0: pi is approximately 3.1415926544231256, Error is 0.0000000008333325
1-9:
1-9: Program exited normally.
1-9: (gdb) 0: wall clock time = 44.909412
0:
0: Program exited normally.
0: (gdb) q
0-9: MPIGDB ENDING
ks12%
```

You can attach to a running job with

```
mpiexec -gdba <jobid>
```

where <jobid> comes from mpdlistjobs.

7.2 TotalView

MPICH2 supports use of the TotalView debugger from Etnus, through the MPD process manager only. If MPICH2 has been configured to enable debugging with TotalView (See the section on configuration of the MPD process manager in the *Installer's Guide*) then one can debug an MPI program started with MPD by adding -tv to the global mpiexec arguments, as in

```
mpiexec -tv -n 3 cpi
```

You will get a popup window from TotalView asking whether you want to start the job in a stopped state. If so, when the TotalView window appears, you may see assembly code in the source window. Click on main in the stack window (upper left) to see the source of the main function. TotalView will show that the program (all processes) are stopped in the call to MPI_Init.

When debugging with TotalView using the above startup sequence, MPICH2 jobs cannot be restarted without exiting TotalView. In MPICH2 version 1.0.6 or later, TotalView can be invoked on an MPICH2 job as follows:

and the MPICH2 job will be fully restartable within TotalView.

If you have MPICH2 version 1.0.6 or later and TotalView 8.1.0 or later, you can use a TotalView feature called indirect launch with MPICH2. Invoke TotalView as:

totalview <program> -a <program args>

Then select the Process/Startup Parameters command. Choose the Parallel tab in the resulting dialog box and choose MPICH2 as the parallel system. Then set the number of tasks using the Tasks field and enter other needed mpiexec arguments into the Additional Starter Arguments field.

If you want to be able to attach to a running MPICH2 job using TotalView, you must use the -tvsu option to mpiexec when starting the job. Using this option will add a barrier inside MPI_Init and hence may affect startup performance slightly. It will have no effect on the running of the job once all tasks have returned from MPI_Init. In order to debug a running MPICH2 job, you must attach TotalView to the instance of Python that is running the mpiexec script. If you have just one task running on the node where you invoked mpiexec, and no other Python scripts running, there will be three instances of Python running on the node. One of these is the parent of the MPICH2 task on that node, and one is the parent of that Python process. Neither of those is the instance of Python you want to attach to—they are both running the MPD script. The third instance of Python has no children and is not the child of a Python process. That is the one that is running mpiexec and is the one you want to attach to.

8 MPE

MPICH2 comes with the same MPE (Multi-Processing Environment) tools that are included with MPICH1. These include several trace libraries for recording the execution of MPI programs and the Jumpshot and SLOG tools for performance visualization, and a MPI collective and datatype checking library. The MPE tools are built and installed by default and should be available without requiring any additional steps. The easiest way to use

MPE profiling libraries is through the -mpe= switch provided by MPICH2's compiler wrappers, mpicc, mpicx, mpif77, and mpif90.

8.1 MPI Logging

MPE provides automatic MPI logging. For instance, to view MPI communication pattern of a program, fpilog.f, one can simply link the source file as follows:

```
mpif90 -mpe=mpilog -o fpilog fpilog.f
```

The -mpe=mpilog option will link with appropriate MPE profiling libraries. Then running the program through mpiexec will result a logfile, Unknown.clog2, in the working directory. The final step is to convert and view the logfile through Jumpshot:

jumpshot Unknown.clog2

8.2 User-defined logging

In addition to using the predefined MPE logging to log MPI calls, MPE logging calls can be inserted into user's MPI program to define and log states. These states are called User-Defined states. States may be nested, allowing one to define a state describing a user routine that contains several MPI calls, and display both the user-defined state and the MPI operations contained within it.

The typical way to insert user-defined states is as follows:

• Get handles from MPE logging library: MPE_Log_get_state_eventIDs() has to be used to get unique event IDs (MPE logging handles). ¹ This is important if you are writing a library that uses the MPE logging routines from the MPE system. Hardwiring the eventIDs is considered a bad idea since it may cause eventID confict and so the practice isn't supported.

¹Older MPE libraries provide MPE_Log_get_event_number() which is still being supported but has been deprecated. Users are strongly urged to use MPE_Log_get_state_eventIDs() instead.

• Set the logged state's characteristics: MPE_Describe_state() sets the name and color of the states.

• Log the events of the logged states: MPE_Log_event() are called twice to log the user-defined states.

Below is a simple example that uses the 3 steps outlined above.

The logfile generated by this code will have the MPI routines nested within the routine MyAmult().

Besides user-defined states, MPE2 also provides support for user-defined events which can be defined through use of MPE_Log_get_solo_eventID() and MPE_Describe_event(). For more details, e.g. see cpilog.c.

8.3 MPI Checking

To validate all the MPI collective calls in a program by linking the source file as follows:

```
mpif90 -mpe=mpicheck -o wrong_reals wrong_reals.f
```

Running the program will result with the following output:

```
> mpiexec -n 4 wrong_reals
Starting MPI Collective and Datatype Checking!
Process
                    3 of
                                     4 is alive
Backtrace of the callstack at rank 3:
       At [0]: wrong_reals(CollChk_err_han+0xb9)[0x8055a09]
       At [1]: wrong_reals(CollChk_dtype_scatter+0xbf)[0x8057bff]
       At [2]: wrong_reals(CollChk_dtype_bcast+0x3d)[0x8057ccd]
       At [3]: wrong_reals(MPI_Bcast+0x6c)[0x80554bc]
       At [4]: wrong_reals(mpi_bcast_+0x35)[0x80529b5]
       At [5]: wrong_reals(MAIN__+0x17b)[0x805264f]
       At [6]: wrong_reals(main+0x27)[0x80dd187]
        At [7]: /lib/libc.so.6(__libc_start_main+0xdc)[0x9a34e4]
       At [8]: wrong_reals[0x8052451]
[cli_3]: aborting job:
Fatal error in MPI_Comm_call_errhandler:
```

Collective Checking: BCAST (Rank 3) --> Inconsistent datatype signatures detected between rank 3 and rank 0.

The error message here shows that the MPI_Bcast has been used with inconsistent datatype in the program wrong_reals.f.

8.4 MPE options

Other MPE profiling options that are available through MPICH2 compiler wrappers are

-mpe=mpilog : Automatic MPI and MPE user-defined states logging.

This links against -llmpe -lmpe.

-mpe=mpitrace : Trace MPI program with printf.

This links against -ltmpe.

-mpe=mpianim : Animate MPI program in real-time.

This links against -lampe -lmpe.

-mpe=mpicheck : Check MPI Program with the Collective & Datatype

Checking library. This links against -lmpe_collchk.

-mpe=graphics : Use MPE graphics routines with X11 library.

This links against -lmpe <X11 libraries>.

-mpe=log : MPE user-defined states logging.

This links against -lmpe.

-mpe=nolog : Nullify MPE user-defined states logging.

This links against -lmpe_null.

-mpe=help : Print the help page.

For more details of how to use MPE profiling tools, see mpich2/src/mpe2/README.

9 Other Tools Provided with MPICH2

MPICH2 also includes a test suite for MPI-1 and MPI-2 functionality; this suite may be found in the mpich2/test/mpi source directory and can be run with the command make testing. This test suite should work with any MPI implementation, not just MPICH2.

10 MPICH2 under Windows

10.1 Directories

The default installation of MPICH2 is in C:\Program Files\MPICH2. Under the installation directory are three sub-directories: include, bin, and lib. The include and lib directories contain the header files and libraries necessary to compile MPI applications. The bin directory contains the process manager, smpd.exe, and the MPI job launcher, mpiexec.exe. The dlls that implement MPICH2 are copied to the Windows system32 directory.

10.2 Compiling

The libraries in the lib directory were compiled with MS Visual C++ .NET 2003 and Intel Fortran 8.1. These compilers and any others that can link

with the MS .1ib files can be used to create user applications. gcc and g77 for cygwin can be used with the libmpich*.a libraries.

For MS Developer Studio users: Create a project and add

C:\Program Files\MPICH2\include

to the include path and

C:\Program Files\MPICH2\lib

to the library path. Add mpi.lib and cxx.lib to the link command. Add cxxd.lib to the Debug target link instead of cxx.lib.

Intel Fortran 8 users should add fmpich2.lib to the link command.

Cygwin users should use libmpich2.a libfmpich2g.a.

10.3 Running

MPI jobs are run from a command prompt using mpiexec.exe. See Section 5.4 on mpiexec for smpd for a description of the options to mpiexec.

A Frequently Asked Questions

The frequently asked questions are maintained online here: http://wiki.mcs.anl.gov/mpich2/index.php/Frequently_Asked_Questions

References

- [1] Message Passing Interface Forum. MPI2: A Message Passing Interface standard. *International Journal of High Performance Computing Applications*, 12(1–2):1–299, 1998.
- [2] Marc Snir, Steve W. Otto, Steven Huss-Lederman, David W. Walker, and Jack Dongarra. *MPI—The Complete Reference: Volume 1, The MPI Core*, 2nd edition. MIT Press, Cambridge, MA, 1998.