

MPICH2 User's Guide*

Version 1.3a2

Mathematics and Computer Science Division

Argonne National Laboratory

William Gropp
Ewing Lusk
David Ashton
Pavan Balaji
Darius Buntinas
Ralph Butler
Anthony Chan
David Goodell
Jayesh Krishna
Guillaume Mercier
Rob Ross
Rajeev Thakur
Brian Toonen

May 3, 2010

*This work was supported by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, SciDAC Program, Office of Science, U.S. Department of Energy, under Contract DE-AC02-06CH11357.

Contents

1	Introduction	1
2	Getting Started with MPICH2	1
2.1	Default Runtime Environment	1
2.2	Starting Parallel Jobs	1
2.3	Command-Line Arguments in Fortran	1
3	Quick Start	2
4	Compiling and Linking	3
4.1	Special Issues for C++	3
4.2	Special Issues for Fortran	3
5	Running Programs with mpiexec	4
5.1	Standard mpiexec	4
5.2	Extensions for All Process Management Environments	5
5.3	mpiexec Extensions for the Hydra Process Manager	5
5.4	mpiexec Extensions for the MPD Process Manager	5
5.4.1	Basic mpiexec arguments for MPD	5
5.4.2	Other Command-Line Arguments to mpiexec for MPD	6
5.4.3	Environment Variables Affecting mpiexec for MPD	10
5.5	Extensions for SMPD Process Management Environment	10
5.5.1	mpiexec arguments for SMPD	11
5.6	Extensions for the gforker Process Management Environment	13
5.6.1	mpiexec arguments for gforker	14
5.7	Restrictions of the remshell Process Management Environment	15

5.8	Using MPICH2 with SLURM and PBS	16
5.8.1	MPD in the PBS environment	16
5.8.2	OSC mpiexec	17
6	Managing the Process Management Environment	17
6.1	MPD	17
7	Debugging	18
7.1	gdb via mpiexec	18
7.2	TotalView	22
8	MPE	23
8.1	MPI Logging	23
8.2	User-defined logging	24
8.3	MPI Checking	25
8.4	MPE options	26
9	Other Tools Provided with MPICH2	27
10	MPICH2 under Windows	27
10.1	Directories	27
10.2	Compiling	27
10.3	Running	28
A	Frequently Asked Questions	29

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 Getting Started with MPICH2

MPICH2 is a high-performance and widely portable implementation of the MPI Standard, designed to implement all of MPI-1 and MPI-2 (including dynamic process management, one-sided operations, parallel I/O, and other extensions). The *MPICH2 Installer's Guide* provides some information on MPICH2 with respect to configuring and installing it. Details on compiling, linking, and running MPI programs are described below.

2.1 Default Runtime Environment

MPICH2 provides a separation of process management and communication. The default runtime environment in MPICH2 is called Hydra. Other process managers are also available.

2.2 Starting Parallel Jobs

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.

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:

```
cd /home/you/mpich2-installed/examples
mpiexec -n 3 ./cpi
```

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 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).

4.2 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`

The MPI-2 Standard describes `mpiexec` as a suggested way to run MPI programs. MPICH2 implements the `mpiexec` standard, and also provides some extensions.

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 -f machinefile -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 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 executables and different values for their arguments, with “:” separating the sets of processes, as in:

```
mpiexec -f machinefile -n 1 ./master : -n 32 ./slave
```

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 `mpiexec` Extensions for the Hydra Process Manager

MPICH2 provides a number of process management systems. Hydra is the default process manager in MPICH2. More details on Hydra and its extensions to `mpiexec` can be found at http://wiki.mcs.anl.gov/mpich2/index.php/Using_the_Hydra_Process_Manager

5.4 `mpiexec` Extensions for the MPD Process Manager

5.4.1 Basic `mpiexec` arguments for MPD

Before running MPD’s `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
```

5.4.2 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 `-env` 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 **FOO** 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

-l 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:

```
mpiexec -machinefile mf -n 7 p0
```

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:

```
mpiexec -l -machinefile mf -n 3 p1 : -n 2 p2 : -n 2 p3
```

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:

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

directs the `stdin` of `mpiexec` to all five processes.

```
mpiexec -s 4 -n 5 a.out
```

directs it to just the process with rank 4, and

```
mpiexec -s 1,3 -n 5 a.out
```

sends it to processes 1 and 3, while

```
mpiexec -s 0-3 -n 5 a.out
```

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 -l : -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.

5.4.3 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 ports 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.

5.5 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).

5.5.1 `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 = $m1 + m2 + \dots + mn$

`-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

-exitcodes
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 **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.

5.6 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.

5.6.1 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 <list>` 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 executables).
- `-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`.
- `-l` 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 arguments, 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_WORLD**s (e.g., ones that use **MPI_Comm_spawn** or **MPI_Comm_connect**).

MPIEXEC_PREFIX_STDERR Like **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.

5.7 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

There are multiple ways of using MPICH2 with SLURM or PBS. Hydra provides native support for both SLURM and PBS, and is likely the easiest way to use MPICH2 on these systems (see the Hydra documentation above for more details).

Alternatively, SLURM also provides compatibility with MPICH2's internal process management interface. To use this, you need to configure MPICH2 with SLURM support, and then use the `srun` job launching utility provided by SLURM.

For PBS, MPICH2 jobs can be launched in three ways: (i) use Hydra's `mpiexec` with the appropriate options corresponding to PBS, (ii) using MPD or (iii) 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 | uniq -C | 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 `-l` 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 let things progress normally.

The following script of a `-gdb` session gives an idea of how this works. Input keystrokes are sent to all processes unless specifically directed by the “`z`” command.

```
ksl2% mpiexec -gdb -n 10 cpi
```

```

0-9: (gdb) l
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: 12 int main(int argc, char *argv[])
0-9: 13 {
0-9: 14     int done = 0, n, myid, numprocs, i;
0-9: (gdb)
0-9: 15     double PI25DT = 3.141592653589793238462643;
0-9: 16     double mypi, pi, h, sum, x;
0-9: 17     double startwtime = 0.0, endwtime;
0-9: 18     int namelen;
0-9: 19     char processor_name[MPI_MAX_PROCESSOR_NAME];
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             myid, numprocs, processor_name);
0-9: 28     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 0x40000000000002541:
0-9:         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=0x60000fffffb4b8)
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=0x60000fffffb4b8)
0-9:   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)
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)
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
ksl2%

```

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:

```
totalview python -a 'which mpiexec' -tv su \
    <mpiexec args> <program> <program args>
```

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 `-tv su` 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`, `mpicxx`, `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 conflict and so the practice isn't supported.
- 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.

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.

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

```
int eventID_begin, eventID_end;
...
MPE_Log_get_state_eventIDs( &eventID_begin, &eventID_end );
...
MPE_Describe_state( eventID_begin, eventID_end,
                    "Multiplication", "red" );
...
MyAmult( Matrix m, Vector v )
{
    /* Log the start event of the red "Multiplication" state */
    MPE_Log_event( eventID_begin, 0, NULL );
    ... Amult code, including MPI calls ...
    /* Log the end event of the red "Multiplication" state */
    MPE_Log_event( eventID_end, 0, NULL );
}
```

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 `.lib` 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 5.5 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.