MPICH2 User's Guide*

Version 1.4

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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 <code>/usr/local</code>. If MPICH2 has not yet been installed, see the <code>MPICH2 Installer's Guide</code>.) We suggest that you put the <code>bin</code> 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 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

-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.

5.5 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).

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.

5.6 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.

5.7 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

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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 two ways: (i) use Hydra's mpiexec with the appropriate options corresponding to PBS, or (ii) using the OSC mpiexec.

5.7.1 OSC mpiexec

Pete Wyckoff from the Ohio Supercomputer Center provides a alternate utility called OSC mpiexec to launch MPICH2 jobs on PBS systems. More information about this can be found here: http://www.osc.edu/~pw/mpiexec

6 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.

6.1 TotalView

MPICH2 supports use of the TotalView debugger from Etnus. If MPICH2 has been configured to enable debugging with TotalView then one can debug an MPI program using

```
totalview -a mpiexec -a -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.

If you have 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.

7 Checkpointing

MPICH2 supports checkpoint/rollback fault tolerance when used with the Hydra process manager. Currently only the BLCR checkpointing library is supported. BLCR needs to be installed separately. Below we describe how to enable the feature in MPICH2 and how to use it. This information can also be found on the MPICH Wiki: http://wiki.mcs.anl.gov/mpich2/index.php/Checkpointing

7.1 Configuring for checkpointing

First, you need to have BLCR version 0.8.2 installed on your machine. If it's installed in the default system location, add the following two options to your configure command:

```
--enable-checkpointing --with-hydra-ckpointlib=blcr
```

If BLCR is not installed in the default system location, you'll need to tell MPICH2's configure where to find it. You might also need to set the LD_LIBRARY_PATH environment variable so that BLCR's shared libraries can be found. In this case add the following options to your configure command:

```
--enable-checkpointing --with-hydra-ckpointlib=blcr
--with-blcr=BLCR_INSTALL_DIR LD_LIBRARY_PATH=BLCR_INSTALL_DIR/lib
```

where BLCR_INSTALL_DIR is the directory where BLCR has been installed (whatever was specified in --prefix when BLCR was configured). Note, checkpointing is only supported with the Hydra process manager. Hyrda

will used by default, unless you choose something else with the --with-pm= configure option.

After it's configured, compile as usual (e.g., make; make install).

7.2 Taking checkpoints

To use checkpointing, include the -ckpointlib option for mpiexec to specify the checkpointing library to use and -ckpoint-prefix to specify the directory where the checkpoint images should be written:

```
shell$ mpiexec -ckpointlib blcr \
    -ckpoint-prefix /home/buntinas/ckpts/app.ckpoint \
    -f hosts -n 4 ./app
```

While the application is running, the user can request for a checkpoint at any time by sending a SIGUSR1 signal to mpiexec. You can also automatically checkpoint the application at regular intervals using the mpiexec option -ckpoint-interval to specify the number of seconds between checkpoints:

The checkpoint/restart parameters can also be controlled with the environment variables <code>HYDRA_CKPOINTLIB</code>, <code>HYDRA_CKPOINT_PREFIX</code> and <code>HYDRA_CKPOINT_INTERVAL</code>.

Each checkpoint generates one file per node. Note that checkpoints for all processes on a node will be stored in the same file. Each time a new checkpoint is taken an additional set of files are created. The files are numbered by the checkpoint number. This allows the application to be restarted from checkpoints other than the most recent. The checkpoint number can be specified with the <code>-ckpoint-num</code> parameter. To restart a process:

```
shell$ mpiexec -ckpointlib blcr \
    -ckpoint-prefix /home/buntinas/ckpts/app.ckpoint \
    -ckpoint-num 5 -f hosts -n 4
```

Note that by default, the process will be restarted from the first checkpoint, so in most cases, the checkpoint number should be specified. 8 MPE 14

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()

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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.

- 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.

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.

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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!
                    3 of
                                     4 is alive
 Process
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 5.4 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.