

MPI on Cirrus and ARCHER



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Access

- ARCHER: `ssh -XY user@login.archer.ac.uk`
- Cirrus: `ssh -XY user@cirrus-msc.epcc.ed.ac.uk`
 - you must use this dedicated MSc login node
- You can access systems using ssh from anywhere
 - Trivial for Linux
 - Mac: enable the X server (xquartz) to display any graphics
 - Windows: need to install ssh and an X-server, e.g. MobaXterm

Useful files and templates

- Take a copy of **MPP-templates.tar**
 - see the course web pages
- unpack: **tar -xvf MPP-templates.tar**
- Crib sheets for MPI programs available on course web pages

Setting up Cirrus environment

- Load the Message-Passing Toolkit
 - module load mpt
- Load the Intel Compilers
 - module load intel-compilers-18
- To automate, add these lines to your “.bash_profile” file

```
[user@cirrus] gedit ~/.bash_profile
```

Compiling MPI Programs on Cirrus

- C programmers use: `mpicc -cc=icc`
- C++ programmers use: `mpicxx -cxx=icpc`
- Fortran programmers use: `mpi f90`
- There is nothing magic about these MPI compilers!
 - simply wrappers which automatically include various libraries etc
 - compilation done by standard (e.g. Intel) compilers
 - icc, icpc and ifort
- You can use the supplied Makefiles for convenience
 - `make -f Makefile_c`
 - `make -f Makefile_cc`
 - `make -f Makefile_f90`
- Easiest to make a copy of one of these called “Makefile”
 - also need to change the line “MF=” in the Makefile itself

Running interactively on Cirrus

- Timings will not be reliable
 - shared with other users, many more processes than processors
 - but **very useful** during development and for debugging
- `mpirun -n 4 ./mpiprogram.exe`
 - runs your code on 4 processes
- NOTE
 - output might be buffered
 - if your program crashes, you may see no output at all
- It may help to explicitly flush prints to screen
 - `fflush(stdout);`
 - `FLUSH(6)`

Running batch jobs on Cirrus

- Run via a batch system
 - Cirrus uses Portable Batch System (PBS); submit script that launches your program
- In **MPP-templates/** is a standard batch script: **cirrusmpi.pbs**
 - make a copy of this file with a name that matches your executable, e.g.
 - `user@cirrus$ cp cirrusmpi.pbs hello.pbs`
- To run on 4 processors: **qsub hello.pbs**
 - use reserved queue during lab sessions, e.g. `qsub -q R12345 hello.pbs`
 - automatically runs executable called “hello”
 - output will appear in a file called **hello.pbs.oXXXXXX**
 - can follow job progress using `qstat` or `qstat -u $USER`
 - script also times your program using the Unix “time” command
 - full instructions included as comments in the template
 - no need to alter the script - just rename it as appropriate
 - e.g. to run a program “pingpong” make another copy called “pingpong.pbs”
- MSc students should alter charging: d171 -> d171-UUN
 - e.g. `#PBS -A d171-s1234567`

Cirrus idiosyncrasies

- By default, MPI wrappers are not in your path

```
user@cirrus$ mpicc
```

```
-bash: mpicc: command not found
```
- To access correct version: `module load mpt`
 - defaults to GNU compilers: gcc, g++ and gfortran
 - in PBS batch system, job launcher is called `mpiexec_mpt`
- Intel compilers: `module load intel-compilers-18`
 - add these to end of your `.bash_profile` file in home directory
 - to check you have the right version (similarly for mpif90):

```
user@cirrus$ which mpicc
```

```
/opt/hpe/hpc/mpt/mpt-2.16/bin/mpicc
```

- `mpif90` automatically picks up the Intel Fortran compiler
- to use Intel C [C++] compilers: `mpicc -cc=icc [-cc=icpc]`

Compiling MPI Programs on ARCHER

- C programmers use `cc`
- C++ programmers use `CC`
- Fortran programmers use `ftn`
- There is nothing magic about these MPI “compilers” !
 - simply wrappers which automatically include various libraries etc
 - compilation done by standard (Cray) compilers
 - `craycc`, `crayc++` and `crayftn`
- You can use the supplied Makefiles (C, C++, Fortran) for convenience
 - `make -f Makefile_c`
 - `make -f Makefile_cc`
 - `make -f Makefile_f90`
- Easiest to make a copy of your choice called “Makefile”
 - e.g. `cp Makefile_c Makefile`
 - also need to change the first line “MF=” in the Makefile itself
 - then you can just type “`make`”

ARCHER idiosyncrasies

- ▶ Not possible to run directly on front-end
- ▶ Can be a substantial delay in batch queues
 - we may have dedicated queues for the course for more rapid turnaround!
- ▶ Cannot run from the home file system
 - back-end nodes can only see the work file system
- ▶ Recommendation
 - do everything in `/work/`
 - i.e. change directory to `/work/y14/y14/username/`

Running on ARCHER back-end

- Run via a batch system
 - on ARCHER we use the Portable Batch System (PBS)
 - submit a script that then launches your program
- In MPP-templates/ is a standard batch script: **archermpi.pbs**
 - make a copy of this file with a name that matches your executable, e.g.
 - `user@archer$ cp archermpi.pbs hello.pbs`
- Submit: **qsub -q RXXXXXX hello.pbs**
 - you will need to alter **NPROCS** (the argument to “**aprun**”) by hand
 - ... and **select** more than one node for more than 24 processes
 - output will appear in a file called **hello.pbs.oXXXXXX**
 - can follow job progress using **qstat** command
 - script also times your program using the Unix “time” command
 - full instructions included as comments in the template
- If there is no reserved queue
 - `qsub -q short hello.pbs`
 - short queue is for small jobs less than 20 minutes during working hours

C++ Interface

- MPI is not an OO interface
 - however, can be called from C++
- Originally had different function calls, e.g.
 - `MPI::Intracomm comm;`
 - `...`
 - `MPI::Init();`
 - `comm = MPI::COMM_WORLD;`
 - `rank = comm.Get_rank();`
 - `size = comm.Get_size();`
- Compiler is called `mpicxx`
 - see `hello.cc` and `Makefile_cc`

C++ interface is
now removed

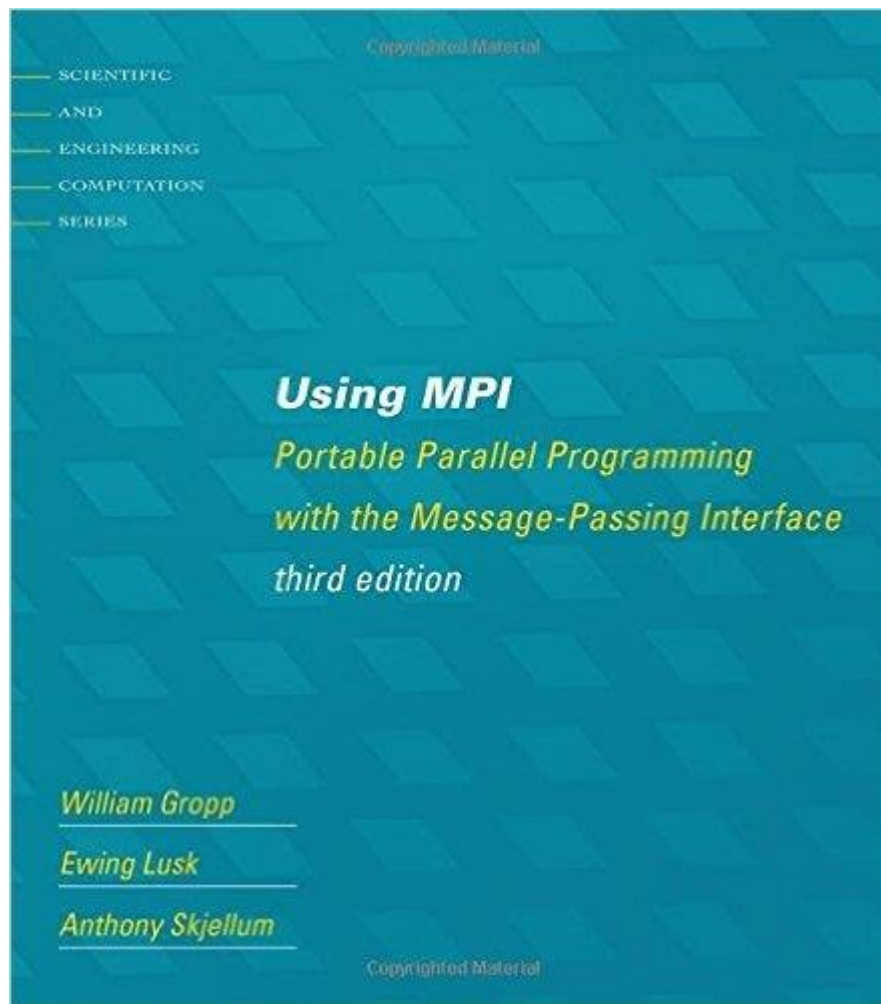
Must therefore
cross-call to C

Documentation

- ▶ MPI Standard available online
 - See: <http://www.mpi-forum.org/docs/>
 - currently version 3.1
- ▶ Available in printed form
 - <http://www.hlrs.de/mpi/mpi31/>
- ▶ Man pages available on Cirrus and ARCHER
 - must use the C style of naming: `man MPI_Routine_name`, e.g.:
 - `user@computer$ man MPI_Init`



MPI Books



Exercise: Hello World

The minimal MPI program

- See Exercise 1 on the exercise sheet
- Write an MPI program that prints a message to the screen
- Main purpose is to get you compiling and running parallel programs on cirrus
 - both on the login node and on compute nodes via PBS and qsub
 - also illustrates the SPMD model and use of basic MPI calls
- We supply some very basic template code
 - you need to add appropriate calls to compute rank and size