MPI on Cirrus and ARCHER

Access

- CP-Lab machines directly accessible in lab room 1028
- external access:

  gateway: `ssh -Y user@ph-cplab.ph.ed.ac.uk`

  then: `ssh -Y cplabXXX` (pick your favourite machine)

  – gateway machine has very limited software available
- ARCHER: `ssh -Y user@login.archer.ac.uk`
- Cirrus: `ssh -Y 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 an X server program, eg xming (which is free!)

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 Learn under “problems sheets”

Compiling MPI Programs on Cirrus

- Fortran programmers use mpif90
- C programmers use mpicc
- 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 and ifort

- You can use the supplied Makefiles for convenience
  - make –f Makefile_c
  - 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 ./mpiprog.exe
  - runs your code on 4 processes

- NOTE
  - output might be buffered
  - if your program crashes, you may see no output at all
- May need to explicitly flush prints to screen
  - FLUSH(6)
  - fflush(stdout);

Running batch jobs on Cirrus

- Run via a batch system
  - on Cirrus we use the Portable Batch System (PBS)
  - submit a script that then 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`
  - automatically runs executable called “hello”
  - output will appear in a file called `hello.pbs.oXXXXX`
  - 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
    - eg to run a program “pingpong” make another copy called “pingpong.pbs”

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`
  - in batch system, job launcher is called `mpiexec_mpt`
- Intel compilers: `module load intel-compilers-16`
  - 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/sgi/mpt/mpt-2.14/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

- Fortran programmers use ftn
- C programmers use cc
- There is nothing magic about these MPI compilers!
  - simply wrappers which automatically include various libraries etc
  - compilation done by standard (Cray) compilers
    - crayftn and craycc

- You can use the supplied Makefiles for convenience
  - make –f Makefile_c
  - 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

ARCHER idiosyncracies

- Not possible to run directly on front-end

- Can be a substantial delay in batch queues
  - we may sometimes have dedicated queues for the course
  - instant turnaround!

- Cannot run from the home file system
  - back-end nodes can only see the work file system

- Recommendation
  - do everything in /work/
  - change directory to /work/d122/d122/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: mpibatch.pbs
  - make a copy of this file with a name that matches your executable, eg
  - `user@archer$ cp archermpi.pbs hello.pbs`
- Submit: `qsub -q short hello.pbs`
  - short queue is for jobs less than 20 minutes
  - 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.oXXXXX`
  - 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

C++ Interface

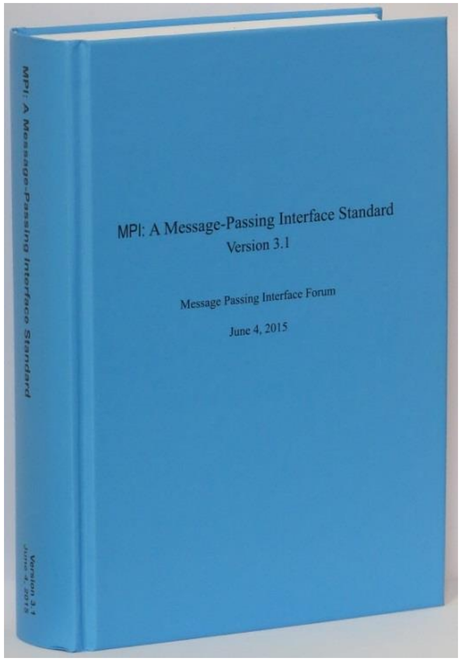
- MPI is not an OO interface
  - however, can be called from C++
- Function calls are different, eg:
  - `MPI::Intracomm comm;`
  - `...`
  - `MPI::Init();`
  - `comm = MPI::COMM_WORLD;`
  - `rank = comm.Get_rank();`
  - `size = comm.Get_size();`
- Compiler is called mpicxx
  - see hello.cc and Makefile_cc

C++ interface is now deprecated

Advised to cross-call to C

Documentation

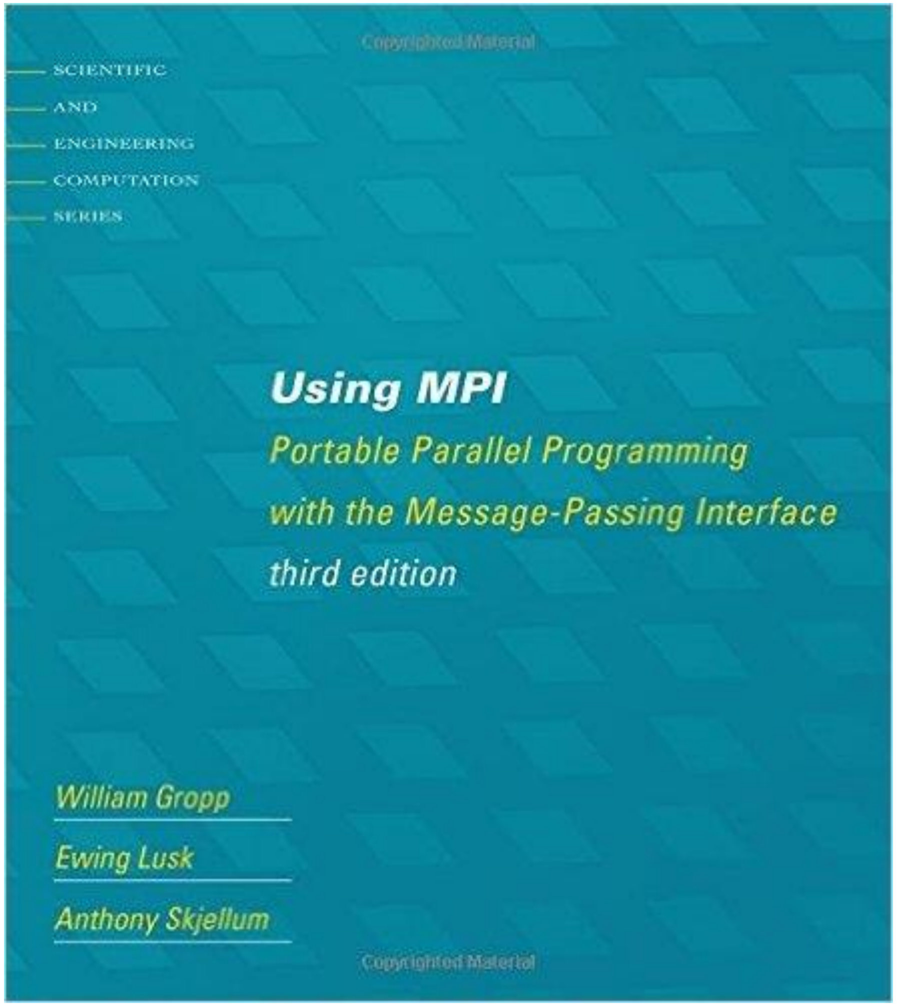
- MPI Standard available online
  - See: http://www.mpi-forum.org/docs/
  - currently version 3.1


MPI: A Message-Passing Interface Standard
Version 3.1
Message Passing Interface Forum
June 4, 2015
MPI: A Message-Passing Interface Standard
Version 3.1
June 4, 2015

- Available in printed form
  - http://www.hlrs.de/mpi/mpi31/

- Man pages available on CP-Lab and ARCHER
  - must use the C style of naming: man MPI_Routine_name, eg:
  - `user@computer$ man MPI_Init`

MPI Books



SCIENTIFIC
AND
ENGINEERING
COMPUTATION
SERIES

Using MPI

Portable Parallel Programming with the Message-Passing Interface

third edition

William Gropp

Ewing Lusk

Anthony Skjellum

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 ness
  - also illustrates the SPMD model and use of basic MPI calls
- We supply some very basic template code
  - see pages 4 and 5 of the notes as well