

# 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 an X server program, 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-17
- 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: `mpif90`
- 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
- May need to explicitly flush prints to screen
  - `FLUSH (6)`
  - `fflush(stdout) ;`

# 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: **d167 -> d167-UUN**
  - e.g. `#PBS -A d167-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 batch system, job launcher is called `mpiexec_mpt`
- Intel compilers: `module load intel-compilers-17`
  - 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

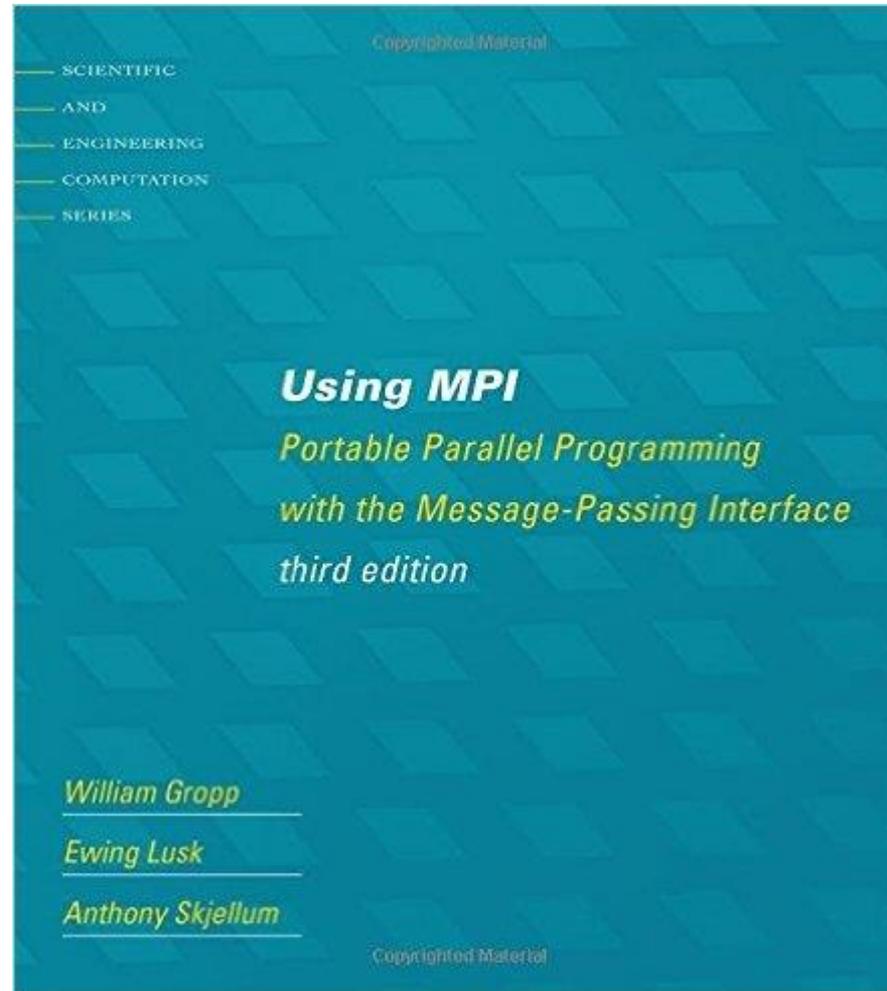
Must therefore  
cross-call to C

# 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 ness
  - 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