

MPI on morar and ARCHER

- ▶ morar available directly from CP-Lab machines

- ▶ external access to morar:

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

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

- ▶ external access to ARCHER:

`ssh -X user@login.archer.ac.uk`

- ▶ You can access systems using ssh from anywhere

- Trivial for Linux

- Mac

- manually enable the X server to display any graphics

- Windows

- need to install an X server program, eg xming (which is free!)

- ▶ Take a copy of `MPP-templates.tar`
 - stored at learn.ed.ac.uk
- ▶ **unpack:** `tar xvf MPP-templates.tar`

- ▶ 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 (Portland Group) compilers
 - pgf90 and pgcc
- ▶ 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

- ▶ Timings will not be reliable
 - shared with other users, many more processes than processors
 - but **very useful** during development and for debugging
- ▶ `mpiexec -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);`

- ▶ Run via a batch system
 - on morar we use Sun Grid Engine (SGE)
 - submit a script that then launches your program

- ▶ In MPP-templates/ is a standard batch script: `mpibatch.sge`
 - make a copy of this file with a name that matches your executable, eg
 - `user@cplab$ cp mpibatch.sge hello.sge`

- ▶ To run on 4 processors: `qsub -pe mpi 4 hello.sge`
 - automatically runs executable called “hello”
 - output will appear in a file called `hello.sge.oXXXXXX`
 - can follow job progress using `qmon` GUI or `qstat` or `qstat -u "*"`
 - 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.sge”

- ▶ **Do not** use the default version of MPI
 - very old and out-of-date
- ▶ **Access correct version:** `module load mpich2-pgi`
 - add this to end of your `.bash_profile` file in home directory
 - to check (similarly for mpif90)

```
user@cplab$ which mpicc
/opt/mpich2-pgi/bin/mpicc
```

- ▶ **Output files**
 - will probably see a file called `hello.sge.eXXXXX`
 - contains a spurious error message – ignore it!

- ▶ 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

- ▶ 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/y14/y14/guestXX/`

- ▶ 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 mpibatch.pbs hello.pbs`
- ▶ Submit: `qsub -q <reserved queue ID> hello.pbs`
 - we have a reserved queue **RXXXXXX** for the courses
 - 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

- ▶ 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

▶ MPI Standard available online

- See: <http://www.mpi-forum.org/docs/>

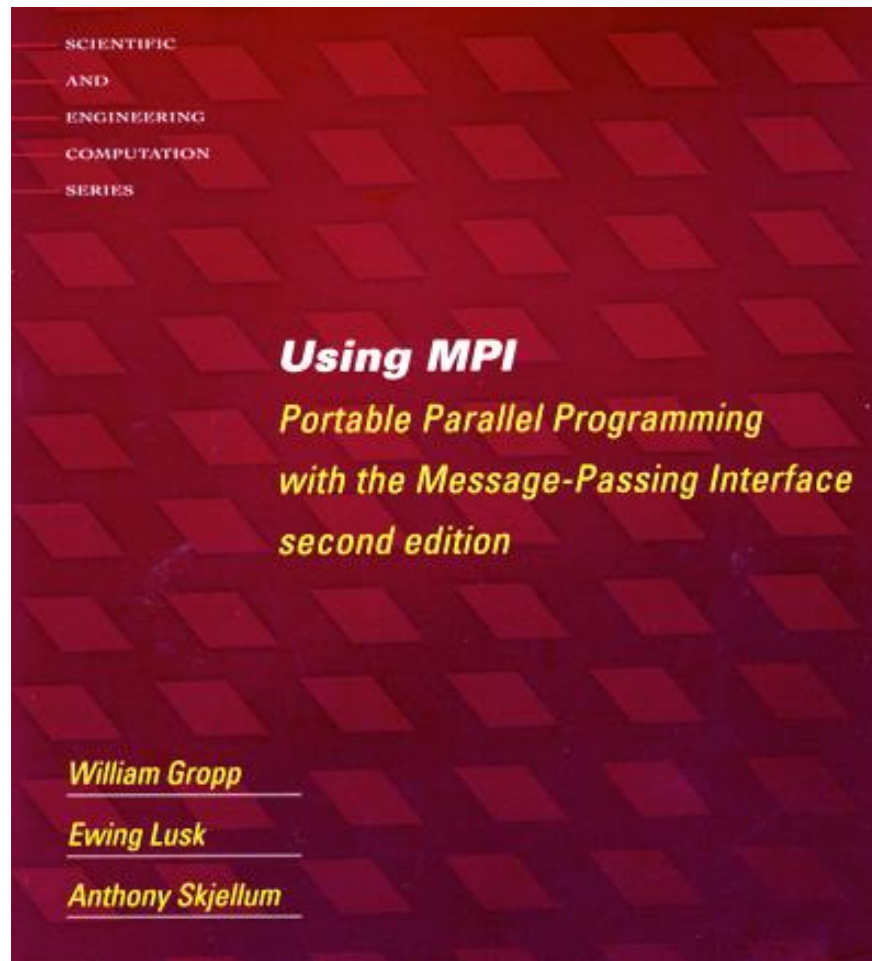
▶ Available in printed form

- <http://www.hlrs.de/mpi/mpi22/>



▶ Man pages available on CP-Lab and ARCHER

- must use the C style of naming: `man MPI_Routine_name`, eg:
- `user@cplab$ man MPI_Init`



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 nesc
 - 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