

MPI on Cirrus and ARCHER2

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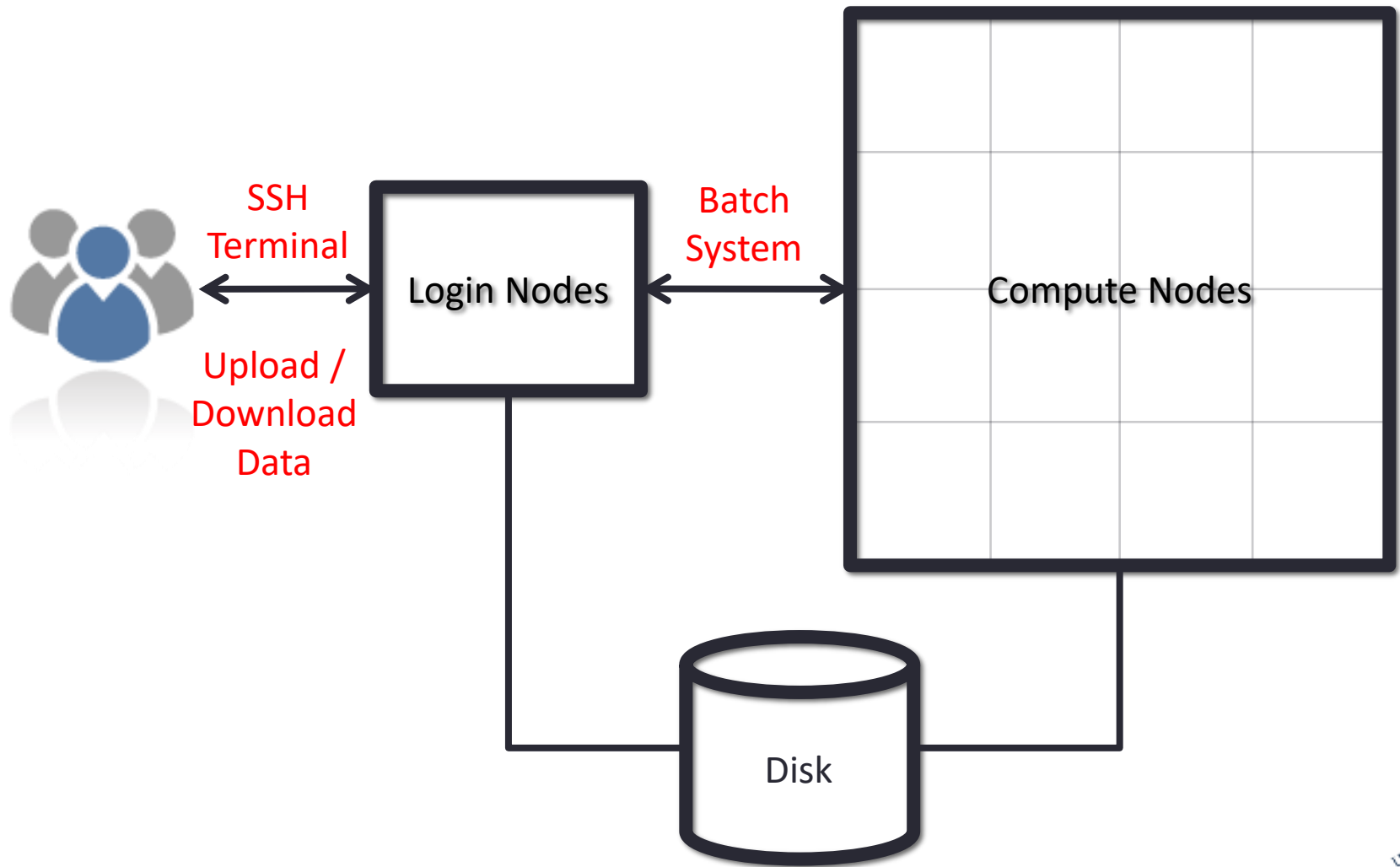
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Access

- ARCHER2: `ssh -X user@login.archer2.ac.uk`
- Cirrus: `ssh -X user@login.cirrus.ac.uk`
- You can access EPCC systems using ssh from anywhere
 - Linux: terminal + command line
 - Mac: Mac terminal + command line + enable an X server (e.g. xquartz) to display any graphics
 - Windows: need to install an ssh program such as MobaXterm
- This gives you access to a login node
 - a few login nodes, users assigned to different nodes depending on system load
 - login nodes shared by all users
 - the many hundreds of compute nodes are accessed exclusively via the SLURM batch system
 - on ARCHER2, MPI programs can only be run on the compute nodes
- Full instructions on access & login in separate document on course web pages

Typical HPC system layout



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 Intel Compilers
 - module load intel-20.4/compilers
- Load the Message-Passing Toolkit
 - module load mpt
- To automate, add these lines to your “.bash_profile” file

```
[user@cirrus] emacs -nw ~/.bash_profile
```

Compiling MPI Programs on Cirrus

- C programmers use: `mpicc -cc=icc`
- C++ programmers use: `mpicxx -cxx=icpc`
- Fortran programmers use: `mpif90 -fc=ifort`
- 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 SLURM: you submit a batch script that launches your program
- In **MPP-templates/** is a standard batch script: **cirrusmpi.job**
 - set up to run a program called “hello” on 4 processors
- To run on 4 processors: **sbatch cirrusmpi.job**
 - runs executable called “hello”
 - output will appear in a file called **hello-XXXX.out**
 - can follow job progress using **squeue** or **squeue -u <user>**
 - to see only your own jobs: **squeue --me**
 - full instructions included as comments in the template

Cirrus Filesystems

- Cannot run from the home file system
 - on logging in, working directory is */home/project/project/username/*
 - *project* is a code number, e.g. **m240c**
 - compute nodes can only see the */work/* file system, not */home/*
- Recommendation
 - do everything in */work/*
 - i.e. change directory to */work/project/project/username/*

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 SLURM batch system, job launcher is called `srun`

- Intel compilers: `module load intel-20.4/compilers`

- can 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-2.25/bin/mpicc
```

- to use Intel C compiler: `mpicc -cc=icc`

- to use Intel C++ compiler: `mpicxx -cxx=icpc`

- to use Intel Fortran compiler: `mpif90 -fc=ifort`

Compiling MPI Programs on ARCHER2

- 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
 - `clang`, `clang++` 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`”

ARCHER2 idiosyncrasies

- Not possible to run MPI programs directly on login nodes
- Can be a substantial delay in batch queues
 - have dedicated queues for some courses for more rapid turnaround
 - or use the short queue for development
- Cannot run from the home file system
 - on logging in, your working directory is /home/taXXX/taXXX/username/
 - compute nodes can only see the /work/ file system, not /home/
- Recommendation
 - do everything in /work/
 - i.e. change directory to /work/taXXX/taXXX/username/

Running on ARCHER2 back-end

- Run via a batch system
 - on ARCHER2 we use SLURM
 - submit a script that then launches your program
- In MPP-templates/ is a standard batch script: **archer2mpi.job**
 - set up to run a program called **hello** in the short queue
- Submit: **sbatch archer2mpi.job**
 - runs on 4 processes of a single ARCHER2 node (each node has 128 CPU-cores)
 - output will appear in a file called **hello-XXXXXX.out**
 - can follow job progress using command: **squeue -u \$USER**
 - full instructions included as comments in the template
- Batch script has instructions on how to use different queues

Running interactively

- Cannot run on ARCHER2 login node
 - must run on compute nodes via SLURM and sbatch
- However, can run “interactively”
 - sbatch command waits until resources are available
 - output appears on the screen in real time as your program runs
 - can be very useful for debugging (e.g. to detect deadlock)

```
srun --partition=standard --qos=short --reservation=shortqos \  
--time=00:01:00 --unbuffered --cpu-bind=cores --nodes=1 --tasks=4 ./hello
```

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 cc
 - see `hello.cc` and `Makefile_cc`

C++ interface is
now removed

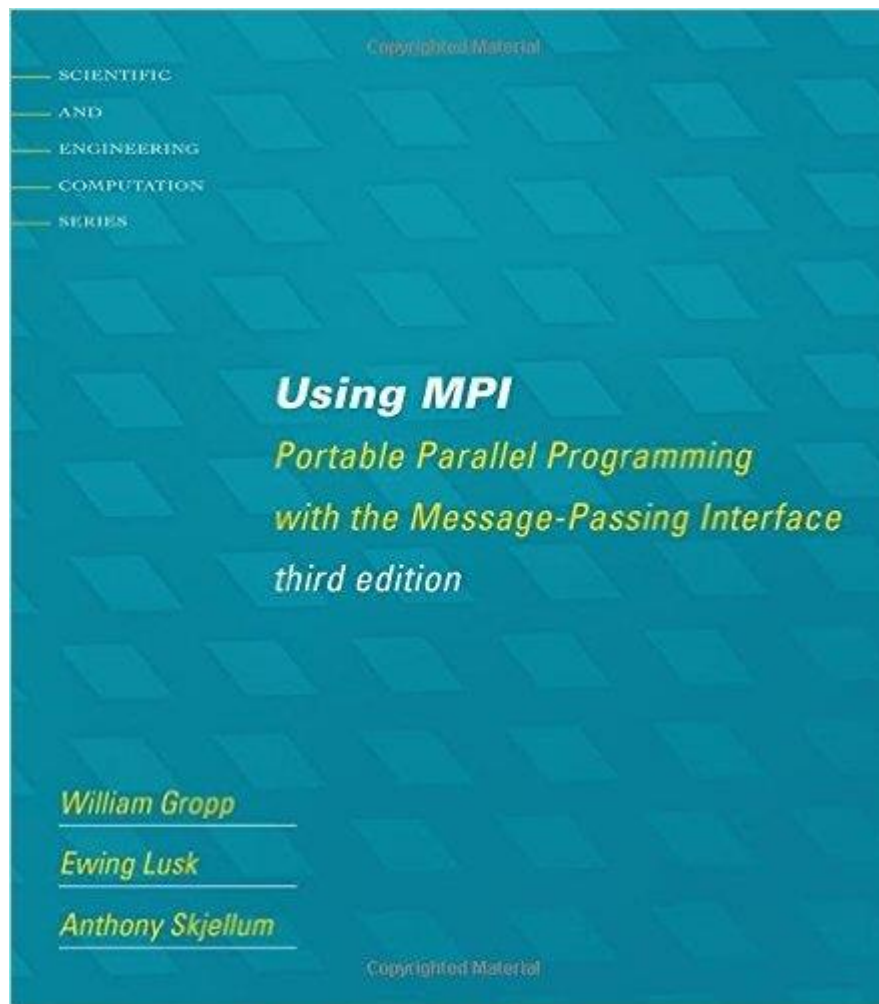
Must therefore
cross-call to C

Documentation

- ▶ MPI Standard available online
 - See: <http://www.mpi-forum.org/docs/>
 - currently version 4.0
- ▶ Available in printed form
 - <http://www.hlrs.de/mpi/mpi31/>
- ▶ Man pages available on Cirrus and ARCHER2
 - 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 HPC system
 - both interactively and in batch via SLURM and sbatch
 - 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