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MPI on ARCHER

Documentation

- See https://www.archer.ac.uk/documentation/user-guide/
  - Accessing the service
  - Resource Allocation and Job Execution

Access

- SSH access: **`ssh -X login.archer.ac.uk`**
  - flag **`-X`** ensures graphics are sent back to your workstation/laptop
- Using ssh
  - Trivial for Linux (open a terminal)
  - Mac (open a terminal)
    - local X server must be enabled to display any graphics
  - Windows
    - require an ssh-client, e.g. putty
      - http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html
      - select SSH -> X11 -> “Enable X11 forwarding”
    - require an X server, e.g. xming
      - http://sourceforge.net/projects/xming/

Setup

- Take a copy of `MPP-templates.tar`

```
wget http://archer.ac.uk/training/course-material/.../Exercises/MPP-templates.tar
```

  - replace "…" by YYY/MM/CourseName_Location

- unpack: `tar -xvf MPP-templates.tar`

Compilers on ARCHER

- ARCHER has 3 compilers available
  - Intel
  - GNU
  - Cray
- Cray compiler is the default when logging on
- Software on ARCHER is controlled using modules
  - the GNU “modules” framework to support multiple software versions and to create integrated software packages

Default modules example

```
adrianj@eslogin001:~> module list
Currently Loaded Modulefiles:
  1) modules/3.2.6.7
  2) nodestat/2.2-1.0500.41375.1.85.ari
  3) sdb/1.0-1.0500.43793.6.11.ari
  4) alps/5.0.3-2.0500.8095.1.1.ari
  5) MySQL/5.0.64-1.0000.7096.23.1
  6) lustre-cray_ari_s/2.3_3.0.58_0.6.6.1_1.0500.7272.12.1-
1.0500.44935.7.1
  7) udreg/2.3.2-1.0500.6756.2.10.ari
  8) ugni/5.0-1.0500.0.3.306.ari
  9) gni-headers/3.0-1.0500.7161.11.4.ari
 10) dmapp/6.0.1-1.0500.7263.9.31.ari
 11) xpmem/0.1-2.0500.41356.1.11.ari
 12) hss-llm/7.0.0
 13) Base-opts/1.0.2-1.0500.41324.1.5.ari
 14) craype-network-aries
 15) craype/1.06.05
 16) cce/8.2.0.181
...
```

Viewing available modules

- There are hundreds of possible modules available to users.
  - Beyond the pre-loaded defaults there are many additional packages provided by Cray
- Users can see all the modules that can be loaded using the command:
  - `module avail`
- Searches can be narrowed by passing the first few characters of the desired module, e.g.

```
adrianj@eslogin001 :~> module avail gc

------------------------------ /opt/modulefiles -------------------------
--
gcc/4.6.1          gcc/4.7.2          gcc/4.8.0
gcc/4.6.3          gcc/4.7.3          gcc/4.8.1(default)
```

Modifying the default environment

- Loading, swapping or unloading modules:
  - The default version of any inidividual modules can be loaded by name
    - e.g.: `module load perftools`
  - A specific version can be specified after the forward slash.
    - e.g.: `module load perftools/6.1.0`
  - Modules can be swapped out in place
    - e.g.: `module swap intel intel/13.1.1.163`
  - Or removed entirely
    - e.g.: `module unload perftools`
- Modules will automatically change values of variables like `PATH`, `MANPATH`, `LM_LICENSE_FILE`... etc
  - Modules also provide a simple mechanism for updating certain environment variables, such as `PATH`, `MANPATH`, and `LD_LIBRARY_PATH`
  - In general, you should make use of the modules system rather than embedding specific directory paths into your startup files, makefiles, and scripts

```
adrianj@eslogin008:~> module show fftw
-------------------------------------------------------------------
/opt/cray/modulefiles/fftw/3.3.0.4:

setenv           FFTW_VERSION 3.3.0.4
setenv           CRAY_FFTW_VERSION 3.3.0.4
setenv           FFTW_DIR /opt/fftw/3.3.0.4/sandybridge/lib
setenv           FFTW_INC /opt/fftw/3.3.0.4/sandybridge/include
prepend-path     PATH /opt/fftw/3.3.0.4/sandybridge/bin
prepend-path     MANPATH /opt/fftw/3.3.0.4/share/man
prepend-path     CRAY_LD_LIBRARY_PATH /opt/fftw/3.3.0.4/sandybridge/lib
setenv           PE_FFTW_REQUIRED_PRODUCTS PE_MPICH
prepend-path     PE_PKGCONFIG_PRODUCTS PE_FFTW
setenv           PE_FFTW_TARGET_interlagos interlagos
setenv           PE_FFTW_TARGET_sandybridge sandybridge
setenv           PE_FFTW_TARGET_x86_64 x86_64
setenv           PE_FFTW_VOLATILE_PKGCONFIG_PATH
/opt/fftw/3.3.0.4/@PE_FFTW_TARGET@/lib/pkgconfig
prepend-path     PE_PKGCONFIG_LIBS
fftw3f_mpi:fftw3f_threads:fftw3f:fftw3_mpi:fftw3_threads:fftw3
module-whatis    FFTW 3.3.0.4 - Fastest Fourier Transform in the West
-------------------------------------------------------------------
```

Compilers on ARCHER

- All applications that will run in parallel on the Cray XC should be compiled with the standard language wrappers.

  The compiler drivers for each language are:
  - `cc` – wrapper around the C compiler
  - `CC` – wrapper around the C++ compiler
  - `ftn` – wrapper around the Fortran compiler

- These scripts will choose the required compiler version, target architecture options, scientific libraries and their include files automatically from the module environment.

- Use them exactly like you would the original compiler, e.g. To compile `prog1.f90` run

```
ftn -c prog1.f90
```

Compilers on ARCHER

- The scripts choose which compiler to use from the `PrgEnv` module loaded

PrgEnv	Description	Real Compilers
PrgEnv-cray	Cray Compilation Environment	crayftn, craycc, crayCC
PrgEnv-intel	Intel Composer Suite	ifort, icc, icpc
PrgEnv-gnu	GNU Compiler Collection	gfortran, gcc, g++

- Use module swap to change `PrgEnv`, e.g.
  - `module swap PrgEnv-cray PrgEnv-intel`
- `PrgEnv-cray` is loaded by default at login. This may differ on other Cray systems.
  - use `module list` to check what is currently loaded
- The Cray MPI module is loaded by default (`cray-mpich`).
  - To support SHMEM load the `cray-shmem` module.
- The drivers automatically support an MPI build
  - No need to use specific wrappers such as mpiifort, mpicc

Compiling MPI Programs ARCHER

- Fortran programmers use ftn
- C programmers use cc (CC for C++)
- There is nothing magic about these compilers!
  - simply wrappers which automatically include various libraries etc
  - compilation done by standard compilers
    - ifort and icc
    - gfortran and gcc
    - craycc and crayftn
- 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

- All jobs on ARCHER must be run through the batch system
  - This controls resource allocation and usage
  - Ensures fair access, charges usage against budgets, etc…
- General batch jobs are run for you
  - No access to the running job, cannot see what is happening until the job finishes.
- It is possible to do interactive runs so you can run the MPI program yourself (although you still don't get access to the compute nodes)
  - To submit a interactive job reserving 8 nodes (192 cores) for 1 hour you would use the following qsub command:

```
qsub -IVl select=8,walltime=1:0:0 -A [project code]
```

  - When you submit this job your terminal will display something like:

```
qsub: waiting for job 492383.sdb to start
```

Running on ARCHER

- Run via a batch system
  - ARCHER uses PBS (Portable Batch System)
  - 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@eslogin003$ cp mpibatch.pbs hello.pbs`**
- For 4 processors:

```
qsub -q resnum -l select=1:mpiprocs=4 hello.pbs
```

  - automatically runs executable called “hello”
  - resnum should be replaced with the id of the reservation we are using
  - output will appear in a file called **`hello.pbs.oXXXXX`**
  - can follow job progress using **`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”

Filesystems on ARCHER

- ARCHER has 3 file systems:
  - home – NFS, not accessible on compute nodes
    - For source code and critical files
    - Backed up
    - > 200 TB total
  - /work – Lustre, accessible on all nodes
    - High-performance parallel filesystem
    - Not backed-up
    - > 4PB total
  - RDF – GPFS, not accessible on compute nodes
    - Long term data storage

Filesystems on ARCHER

- 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/y07/y07/username/
  - Copy and compile code there, submit jobs from there

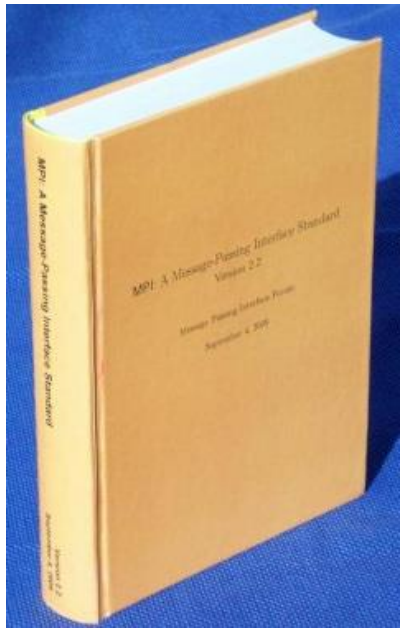
C++ Interface

- 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

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



- Available in printed form
  - http://www.hlrs.de/mpi/mpi22/

- Man pages
  - must use the C style of naming: man MPI_Routine_name, eg:
  - **`user@eslogin003$ man MPI_Init`**

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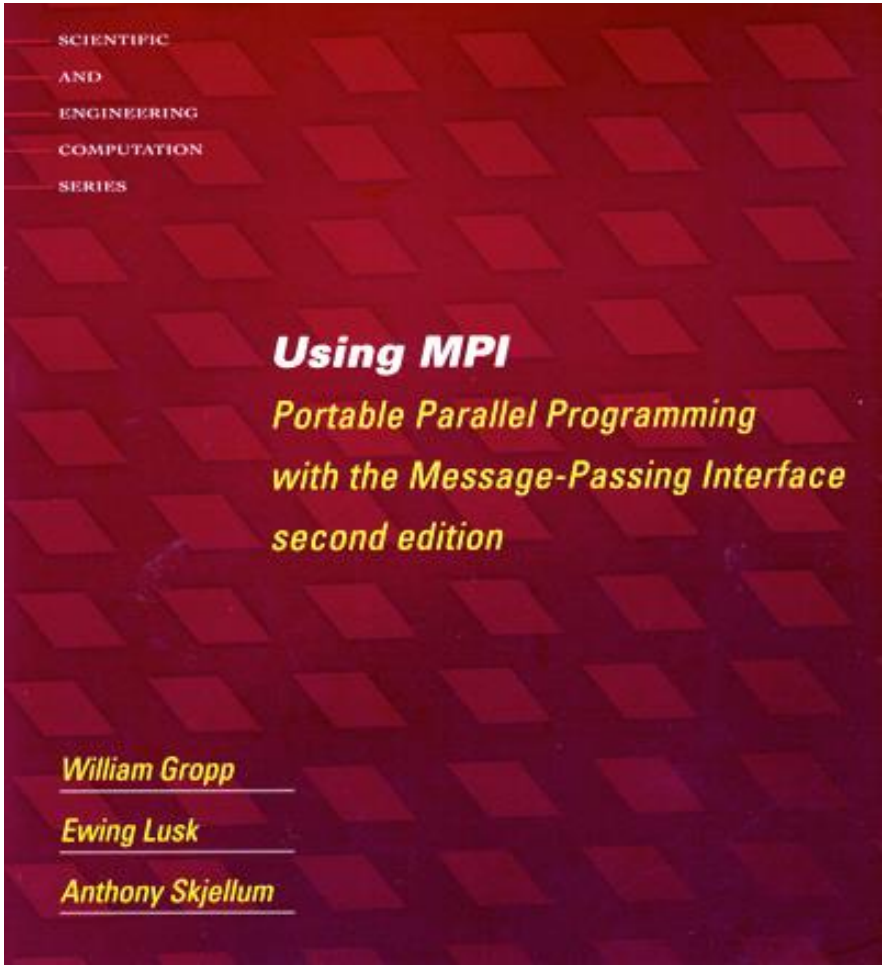
MPI Books



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 anselm
  - 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