Compiling for the ARCHER hardware

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Modules

- The Cray Programming Environment uses the GNU “modules” framework to support multiple software versions and to create integrated software packages

  - As new versions of the supported software and associated man pages become available, they are installed and added to the Programming Environment as a new version, while earlier versions are retained to support legacy applications

  - System administrators will set the default version of an application, or you can choose another version by using modules system commands

  - Users can create their own modules, or administrators can install site specific modules available to many users.
Viewing the current module state

• Each login session has its own module state which can be modified by loading, swapping or unloading the available modules.

• This state affects the functioning of the compiler wrappers and in some cases runtime of applications.

• A standard, default set of modules is always loaded at login for all users.

• Current state can be viewed by running:

  `$> module list$`
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-crای_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 may be many hundreds of possible modules available to users.
  - Beyond the pre-loaded defaults there are many additional packages provided by Cray
  - Sites may choose to install their own versions.
- 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 individual 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

-------------------------------------------------------------------
Summary of Useful module commands

- Which modules are available?
  - module avail, module avail cce

- Which modules are currently loaded?
  - module list

- Load software
  - module load perftools

- Change programming environment
  - module swap PrgEnv-cray PrgEnv-gnu

- Change software version
  - module swap cce/8.0.2 cce/7.4.4

- Unload module
  - module unload cce

- Display module release notes
  - module help cce

- Show summary of module environment changes
  - module show cce
Compiling applications for the Cray XC
Compiler Driver Wrappers (1)

• 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
The scripts choose which compiler to use from the PrgEnv module loaded.

<table>
<thead>
<tr>
<th>PrgEnv</th>
<th>Description</th>
<th>Real Compilers</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrgEnv-cray</td>
<td>Cray Compilation Environment</td>
<td>crayftn, craycc, crayCC</td>
</tr>
<tr>
<td>PrgEnv-intel</td>
<td>Intel Composer Suite</td>
<td>ifort, icc, icpc</td>
</tr>
<tr>
<td>PrgEnv-gnu</td>
<td>GNU Compiler Collection</td>
<td>gfortran, gcc, g++</td>
</tr>
</tbody>
</table>

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.
- Check that the craype-ivybridge module is loaded
- The drivers automatically support an MPI build
  - No need to use specific wrappers such as mpiifort, mpicc or explicitly link to libraries
PLEASE NOTE: Cross Compiling Environment

• You are compiling on a Linux login node but generating an executable for a CLE compute node

• Do not use crayftn, craycc, ifort, icc, gcc, g++… unless you want a Linux executable for the login node
  • ALWAYS Use ftn, cc, or CC instead
  • Only use the direct compiler commands if the executable is supposed to run on the login nodes (utilities, setup, …)
Compiler Versions

• There are usually multiple versions of each compiler available to users.
  • The most recent version is usually the default and will be loaded when swapping PrgEnvs.
  • To change the version of the compiler in use, swap the Compiler Module. e.g. `module swap cce cce/8.1.6`

<table>
<thead>
<tr>
<th>PrgEnv</th>
<th>Compiler Module</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrgEnv-crty</td>
<td>cce</td>
</tr>
<tr>
<td>PrgEnv-intel</td>
<td>Intel</td>
</tr>
<tr>
<td>PrgEnv-gnu</td>
<td>gcc</td>
</tr>
<tr>
<td>PrgEnv-pgi</td>
<td>pgi</td>
</tr>
</tbody>
</table>
About the –I, –L and –l flags

- For libraries and include files covered by module files, you should NOT add anything to your Makefile
  - No additional MPI flags are needed (included by wrappers)
  - You do not need to add any -I, -l or –L flags for the Cray provided libraries

- If your Makefile needs an input for –L to work correctly, try using ‘.’

- If you really, really need a specific path, try checking ‘module show X’ for some environment variables
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
-----------------------------------------------
OpenMP

- OpenMP is supported by all of the PrgEnvs.

  - CCE (PrgEnv-cray) recognizes and interprets OpenMP directives by default. If you have OpenMP directives in your application but do not wish to use them, disable OpenMP recognition with –hnoomp.

<table>
<thead>
<tr>
<th>PrgEnv</th>
<th>Enable OpenMP</th>
<th>Disable OpenMP</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrgEnv-cray</td>
<td>-homp (default)</td>
<td>-hnoomp</td>
</tr>
<tr>
<td>PrgEnv-intel</td>
<td>-openmp</td>
<td>(default)</td>
</tr>
<tr>
<td>PrgEnv-gnu</td>
<td>-fopenmp</td>
<td>(default)</td>
</tr>
</tbody>
</table>
Compiler man pages and documentation

• For more information on individual compilers

<table>
<thead>
<tr>
<th>PrgEnv</th>
<th>C</th>
<th>C++</th>
<th>Fortran</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrgEnv-cray</td>
<td>man craycc</td>
<td>man crayCC</td>
<td>man crayftn</td>
</tr>
<tr>
<td>PrgEnv-intel</td>
<td>man icc</td>
<td>man icpc</td>
<td>man ifort</td>
</tr>
<tr>
<td>PrgEnv-gnu</td>
<td>man gcc</td>
<td>man g++</td>
<td>man gfortran</td>
</tr>
<tr>
<td>Wrappers</td>
<td>man cc</td>
<td>man CC</td>
<td>man ftn</td>
</tr>
</tbody>
</table>

• To verify that you are using the correct version of a compiler, use:
  • -V option on a cc, CC, or ftn command with CCE and Intel
  • --version option on a cc, CC, or ftn command with GNU

• Cray Reference Manuals:
  • C and C++: [http://docs.cray.com/books/S-2179-81/](http://docs.cray.com/books/S-2179-81/)
  • Fortran: [http://docs.cray.com/books/S-3901-81/](http://docs.cray.com/books/S-3901-81/)
Dynamic compilation

- Default behaviour is to perform static linking
- Dynamic linking possible:
  - Use the -dynamic flag when invoking the compiler for linking.
  - Set the environment variable CRAYPE_LINK_TYPE=dynamic without any extra compilation/linking options.
- Will need to have libraries available on /work filesystem
OpenMP

- OpenMP is ON by default
  - This is the opposite default behavior that you get from GNU and Intel compilers
  - Optimizations controlled by -OthreadN (ftn) or -hthreadN (cc/CC), N=0-3 [default N=2]
  - To shut off use -O/-h thread0 or -xomp (ftn) or -hnoomp

- Autothreading is NOT on by default
  - -hautothread to turn on
  - Interacts with OpenMP directives

- If you do not want to use OpenMP and have OMP directives in the code, make sure to shut off OpenMP at compile time
CCE – GNU – Intel compilers

- More or less all optimizations and features provided by CCE are available in Intel and GNU compilers

- GNU compiler serves a wide range of users & needs
  - Default compiler with Linux, some people only test with GNU
  - GNU defaults are conservative (e.g. -O1)
    - -O3 includes vectorization and most inlining
  - Performance users set additional options
- Intel compiler is typically more aggressive in the optimizations
  - Intel defaults are more aggressive (e.g. -O2), to give better performance “out-of-the-box”
    - Includes vectorization; some loop transformations such as unrolling; inlining within source file
  - Options to scale back optimizations for better floating-point reproducibility, easier debugging, etc.
  - Additional options for optimizations less sure to benefit all applications
  - CCE is even more aggressive in the optimizations by default
    - Better inlining and vectorization
    - Aggressive floating-point optimizations
    - OpenMP enabled by default

- GNU users probably have to specify higher optimisation levels
## Cray, Intel and GNU compiler flags

<table>
<thead>
<tr>
<th>Feature</th>
<th>Cray</th>
<th>Intel</th>
<th>GNU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Listing</td>
<td>-ra (fnt)</td>
<td>-opt-report3</td>
<td>-fdump-tree-all</td>
</tr>
<tr>
<td></td>
<td>-hlist=a (cc/CC)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Free format (ftn)</td>
<td>-f free</td>
<td>-free</td>
<td>-ffree-form</td>
</tr>
<tr>
<td>Vectorization</td>
<td>By default at -O1 and above</td>
<td>By default at -O2 and above</td>
<td>By default at -O3 or using -ffree-vectorize</td>
</tr>
<tr>
<td>Inter-Procedural Optimization</td>
<td>-hwp</td>
<td>-ipo</td>
<td>-flto (note: link-time optimization)</td>
</tr>
<tr>
<td>Floating-point optimizations</td>
<td>-hfpN, N=0...4</td>
<td>-fp-model [fast</td>
<td>fast=2</td>
</tr>
<tr>
<td>Suggested Optimization</td>
<td>(default)</td>
<td>-O2 -xAVX</td>
<td>-O2 -mavx -ffree-vectorize -ffast-math -funroll-loops</td>
</tr>
<tr>
<td>Aggressive Optimization</td>
<td>-O3 -hfp3</td>
<td>-fast</td>
<td>-Ofast -mavx -funroll-loops</td>
</tr>
<tr>
<td>OpenMP recognition</td>
<td>(default)</td>
<td>-fopenmp</td>
<td>-fopenmp</td>
</tr>
<tr>
<td>Variables size (ftn)</td>
<td>-s real64</td>
<td>-real-size 64</td>
<td>-freal-4-real-8</td>
</tr>
<tr>
<td></td>
<td>-s integer64</td>
<td>-integer-size 64</td>
<td>-finteger-4-integer-8</td>
</tr>
</tbody>
</table>
Requesting resources from PBS

Jobs provide a list of requirements as #PBS comments in the headers of the submission script, e.g.

```
#PBS -l walltime=12:00:00
```

These can be overridden or supplemented as submission by adding to the `qsub` command line, e.g.

```
> qsub -l walltime=11:59:59 run.pbs
```

Common options include:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-N &lt;name&gt;</td>
<td>A name for job,</td>
</tr>
<tr>
<td>-q &lt;queue&gt;</td>
<td>Submit job to a specific queues.</td>
</tr>
<tr>
<td>-o &lt;output file&gt;</td>
<td>A file to write the job’s stdout stream in to.</td>
</tr>
<tr>
<td>--error &lt;error file&gt;</td>
<td>A file to write the job’s stderr stream in to.</td>
</tr>
<tr>
<td>-j oe</td>
<td>Join stderr stream in to stdout stream as a single file</td>
</tr>
<tr>
<td>-l walltime=<a href="">HH:MM:SS</a></td>
<td>Maximum wall time job will occupy</td>
</tr>
<tr>
<td>-A &lt;code&gt;</td>
<td>Account to run job under (for controlling budgets)</td>
</tr>
</tbody>
</table>
Requesting parallel resources

Jobs must also request “chunks” of nodes:

This is done using the select option, e.g.

```
-l select=<numnodes>
```

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>select=&lt;numnodes&gt;</td>
<td>Requests &lt;numnodes&gt; nodes from the system.</td>
</tr>
<tr>
<td>select=bigmem=true</td>
<td>High memory nodes</td>
</tr>
</tbody>
</table>

```
qsub -l select=<numnodes> ./myjob.pbs
qsub -l select=<numnodes>:bigmem=true ./mybigjob.pbs
```
Launching Parallel applications

• Cray terminology
  • refer to compute resources in terms of Processing Elements
  • one MPI process corresponds to one PE
• aprun is the parallel job launcher
  • aprun launches parallel jobs on the compute nodes.
  • aprun man page contains several useful examples
• The most important parameters to set is -n:

<table>
<thead>
<tr>
<th>Description</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Number of PEs used by the application</td>
<td>-n</td>
</tr>
<tr>
<td>Number of PEs per compute node</td>
<td>-N</td>
</tr>
</tbody>
</table>

```plaintext
aprun -n 24 ./mympiprog.exe  # default -N 24
aprun -n 24 -N 12 ./mympiprog.exe  # uses 2 nodes
```
File Systems and Batch Jobs

- After login, you are placed in the /home filesystem
  - e.g. /home/y14/y14/guest01/
- Login nodes can see /home and /work filesystems
- Compute nodes can only see /work
- You must launch all parallel jobs from /work
  - cd /work/y14/y14/guest01/nobelprizejobs/
  - qsub nobelprize.pbs
- Very common mistake
  - jobs submitted from /home/ will almost certainly fail at runtime
Example batch script

#!/bin/bash --login

# PBS job options (name, compute nodes, job time)
#PBS -N Example_MPI_Job
#PBS -l select=64
#PBS -l walltime=00:20:00

# Replace [project code] below with your project code (e.g. t01)
#PBS -A [project code]

# Make sure any symbolic links are resolved to absolute path
export PBS_O_WORKDIR=$(readlink -f $PBS_O_WORKDIR)

# Change to the directory that the job was submitted from
# (remember this should be on the /work filesystem)
cd $PBS_O_WORKDIR

# Launch the parallel job
# Using 1536 MPI processes and 24 MPI processes per node
aprun -n 1536 ./my_mpi_executable.x arg1 arg2
PBS configuration

- Users usually submit to a single (default) queue
  - unless there is a special reserved queue, e.g. during a course
  - PBS decides when to run your job based on requested resources
  - assumes you will run for all the time requested on all the nodes
  - maximum runtime: 24 hours
  - maximum job size: entire machine

- Limits
  - maximum number of jobs in the system: 16 (max 8 running)
  - after this jobs are rejected
  - jobs rejected at submission if
    - budget code does not have enough time
    - you specify a budget you do not have access to
  - jobs may queue indefinitely
    - if a valid budget has insufficient resources when PBS attempts to run the job
Special Queues

• Low priority – run only when resources are lightly used
  • `qsub -q low submit.pbs`
  • maximum 3 hours and 512 nodes; user not charged

• Long jobs
  • `qsub -q long submit.pbs`
  • maximum of 48 hours and 256 nodes

• Short / debug queue – enabled 10:00 – 17:00 Mon - Fri
  • `qsub -q short submit.pbs`
  • maximum of 20 minutes and 8 nodes
Postprocessing / Serial nodes

- 2 nodes each with 40 Intel cores and 1 TB of memory
  - different architecture from compute nodes
  - not supported by Cray programming environment
  - general purpose: not as tightly controlled as the compute nodes

- Compiling
  - compile post-processing jobs directly calling gcc, gfortran, icc or ifort

- Running
  - qsub -l select=serial=true:ncpus=1 submit.pbs
Project Management
ARCHER SAFE

• All users have a web account on the SAFE: www.archer.ac.uk/safe/

• Single point of contact for
  • managing machine account(s) for users (e.g. password request)
  • managing projects for Principal Investigators
Job charging

- Jobs must be charged to a “budget” or CPU account
  - standard budget is the project name, e.g. #PBS –A y14
  - individual projects may set up sub-budgets, e.g. y14-dev
  - this is all controlled by the Principal Investigator via the SAFE
- Allocation done in units of “kAU”s
  - 1 kilo Allocation Unit = 1000 Gflop-hours (on Linpack benchmark)
  - On ARCHER, 1 kAU = 56 pence (for EPSRC/NERC users)
    - 1 core-hour = 0.015 kAU; 1 node-hour = 0.36 kAU
    - charged for a full node regardless of how many cores you use
    - charged for how long your job actually runs
      - regardless of what you requested or whether job completed successfully
What now?

- You can attempt the ARCHER driving test
  - www.archer.ac.uk/training/course-material/online/driving_test.php

- On successful completion, eligible users can apply for
  - account on ARCHER
  - 1,200 kAUs of time (80,000 core-hours) over 12 months

- Further information
  - This online material: www.archer.ac.uk/training/course-material/online/.
  - Documentation: http://www.archer.ac.uk/documentation/.
  - Helpdesk: support@archer.ac.uk
  - Training: http://www.archer.ac.uk/training/.