Quick Start: Running MPI Programs on the ALCF Blue Gene/Q

ATPESC

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Sample files

- vesta:~rloy/public/atpesc2013

- Temporary fix: log in through
  - etherpad.mozilla.org/anl-training

Softenv

- "Keys" are read at login time to set enviroment variables like PATH.
  - Mira, Cetus, Vesta: ~/.soft
  - Tukey: ~/.soft.tukey
- To get started:

  # This key selects XL compilers to be used by mpi wrappers

  +mpiwrapper-xl

  @default

  # the end – do not put any keys after the @default
- After edits to .soft, type "resoft" or log out and back in again

Compiling

- Remember you need to cross-compile for the compute nodes
  - Check your Makefile for unintended references to e.g. /lib, /usr/lib, etc which are for front-end nodes (FENs).
- Invoking the compiler directly (bgxlc, gcc, etc) is tricky
  - correct compiler paths (/bgsys/drivers/ppcfloor vs /usr/bin)
  - must list all the system libraries correctly
- Much easier to use the wrappers
  - mpicc, mpixlc, mpicxx, mpixlcxx, mpif90, mpixlf90
  - Depending on your .soft keys you may get XL or Gnu
- Example: mpixlc –O3 –o hellompi hellompi.c

Job script

- Sample:

```
#!/bin/bash
# -p is mode (how many ranks per node)
# --np is number of ranks
runjob –p 16 –np 32 –block $COBALT_PARTNAME : hellompi
return 0
```

- Some args use ***single*** dash and some ***double*** dash (**man runjob**)
- Don't forget --block
- You can do multple runjobs in succession
  - Use normal shell redirection to separate output
- Use –envs to add environment variables
- Output to <jobid>.output,error,cobaltlog (use –O to change prefix)

Submitting your job

- qsub –A <project> -q <queue> -t <time> -n <nodes> --mode script ./jobscript.sh

  E.g.

  qsub –A ATPESC2013 –q Q.ATPESC2013 –t 10 –n 2 –mode script ./jobscript.sh

- ***Put this in a script so you have a record of what you did!***

- Make sure jobscript.sh is executable

- Set environment variable COBALT_PROJ to give a default for –A

- **man qsub** for more options

Managing job

- qstat – show what's in the queue
  - qstat | grep <username>
  - qstat <jobid>

- qdel <jobid>

- showres – show reservations currently set in the system

- **man qstat** for more options

Hands-on