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

ATPESC
July 28, 2013

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Sample files

- \texttt{vesta:~rloy/public/atpesc2013}

- Temporary fix: log in through
  - \url{etherpad.mozilla.org/anl-training}
**Softenv**

- "Keys" are read at login time to set environment 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 "resof" 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:

```bash
#!/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 multiple 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