

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

ATPESC
July 28, 2013

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Sample files

- `vesta:~rloy/public/atpesc2013`



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 "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 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 64 --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

