Introduction to High Performance Computing

Blue Waters User Guide

- Blue Waters Cray XE6 system specifications:
  - In total of 22,640 compute nodes
  - Each compute node has 2 AMD Bulldozer CPU sockets of 16 cores each, so in total, a Blue Waters compute node consists of 32 cores sharing one address space
  - Each compute node has 64 GB of memory
- Each account has a user name traxxx
- Each student should use only their account, and only for the course
- Passwords can not be changed
- To login to Blue Waters: `ssh traxxx@bwbay.ncsa.illinois.edu`
- You submit a job script using `qsub` command
- To load Cray PETSc do: `module load cray-petsc`
- To use Intel software stack instead of Cray: `module swap PrgEnv-cray PrgEnv-gnu`
- Once you login to the system for the first time, copy the Problem Set #4 directory to your home directory as follows: `cp -iR /projects/eot/bagx/ps4 ./`
- To compile the code do: `make all`
- Modify the sample job script (`job.pbs`) in the ps4 directory to execute your code, then do: `qsub job.pbs` to submit your job script to the scheduler
- Wait till your job gets executed, it may take time, and as soon as it finishes, the executable outputs will be piped into two test files of name <`job_id`>`.out` and <`job_id`>`.err`
- DO NOT run your executable directly; just submit it and the scheduler will take care of it
- To monitor when your job is scheduled and when it is executing, do: `qstat -u traxxx`
- For more information, please refer to: `https://bluewaters.ncsa.illinois.edu/getting-started`