Getting Started with CISL Facilities and Support

CESM Tutorial
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Si Liu

NCAR/CISL/OSD/USS

Consulting Services Group

CISL's Mission for User Support

CISL will provide a balanced set of services to enable researchers to utilize community resources securely, easily, and effectively.

CISL Strategic Plan

CISL also supports special colloquia, workshops and computational campaigns; giving users special privileges and access to facilities and services above normal service levels.

CISL Facilities Overview

Navigation and usage of the facilities require a basic familiarity with a number of the functional aspects of the facilities.

• Computing Systems
- o Bluefire (Mesa)
- o Lynx (Mesa)
- o Janus (CU)
- o Yellowstone (NWSC)

•Data Analysis and Visualization
- o Mirage and Storm
- o Geyser and Caldera (NWSC)

•Data Archival
- oHPSS
- oGLADE

•Allocations and Security

•User support

•Training

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Working with Bluefire

Computing System - Bluefire

- **IBM clustered Symmetric Multi-Processing (SMP) system**
  - Operating System: AIX (IBM-proprietary UNIX)
  - Batch system: Load Sharing Facility (LSF)
  - File system: General Parallel File System (GPFS)

- **127 32-way 4.7 GHz nodes**
  - 4,064 POWER6 processors
  - SMT enabled (64 SMT threads per node)
  - 76.4 TFLOPS

- **117 compute nodes (70.4 TFLOPS peak)**
  - 3,744 POWER6 processors (32 per node)
  - 69 compute nodes have 64 GB memory
  - 48 compute nodes have 128 GB memory

- **10 other nodes**
  - 2 interactive sessions/login nodes (256 GB memory)
  - 2 debugging and share queue nodes (256 GB memory)
  - 4 GPFS/VSD nodes
  - 2 service nodes

Compilers on Bluefire

- **Fortran 77 and Fortran 90/95 compilers:**
  - xlf, xlf_r, xlf90, xlf90_r
  - mpxlf, mpxlf_r, mpxlf90, mpxlf90_r
- **C and C++ compilers:**
  - xlc, xlc_r, xlC, xlC_r
  - mpcc, mpcc_r, mpCC, mpCC_r
- **The _r versions are thread safe**
  - We recommend them over the non _r versions.
- **Compile your source code**
  - xlc_r hello_world.c -o hello_world_c.exe
  - xlf90_r hello_world.f -o hello_world_f.exe
- **More information**
  http://www2.cisl.ucar.edu/docs/bluefire/compiling-and-optimization

Login to Bluefire with Yubikey

- **Security Shell(SSH)**
  - Cygwin, Putty, Terminal, etc.

- **Using your Yubikey token**
  - When you log in Bluefire,

    ssh your_logon@bluefire.ucar.edu

    your screen displays a response:

    Token_Response:

  - Enter your PIN number on the screen (do not hit enter), then touch the yubikey button. This will insert a new one-time password (OTP) and a return.
  - The yubikey is activated by the warmth of your finger not the pressure in pushing the button.

- **More information of Yubikey:**
  - https://www2.cisl.ucar.edu/docs/enabling-your-yubikey-token

A Job Script on Bluefire

#!/bin/csh
 # LSF batch script to run an MPI application

#BSUB -P 12345678 # project number (required)
#BSUB -W 1:00 # wall clock time (in minutes)
#BSUB -n 256 # number of MPI tasks
#BSUB -R "span[ptile=64]" # run 64 tasks per node
#BSUB -q workshop # queue setting: use 'workshop' queue this week
#BSUB -J myjob # job name
#BSUB -o myjob.%J.out # output filename
#BSUB –e myjob.%J.err # error filename

mpirun.lsf /usr/local/bin/launch ./MyProg.exe

For more examples, see the /usr/local/examples directory.

Submit, Delete, and Monitor Jobs on Bluefire

- **Job submission**
  - bsub < script

- **Monitor jobs**
  - bjobs
    - ➤ bjobs -u all
    - ➤ bjobs -q regular
  - bhist
    - ➤ bhist -n 0 jobid

- **Delete a job**
  - bkill jobid

Module Utility on Bluefire

Modify environment to find alternative compilers or software

- To show all available module files
  module av

- To see which modules are in force
  module list

- To load a new module (e.g. ImageMagick)
  module load ImageMagick-6.5.3-10

https://www2.cisl.ucar.edu/docs/bluefire/getting-started?tab=3

"Big 3": Get a Better Performance

- **Simultaneous Multi-Threading(SMT)**
  - a second, on-board "virtual" processor
  - 64 virtual cpus in each node

- **Multiple page size support**
  - 64-KB page size when running the 64-bit kernel
  - Large pages (16 MB) and "huge" pages (16 GB)

- **Processor binding**
  http://www2.cisl.ucar.edu/docs/bluefire/running-jobs?tab=3

Lynx

Computing System – Lynx

Single-cabinet Massively Parallel Processing Supercomputer

- Operating system: Cray Linux Environment
  - Compute Node Linux (CNL) – based on SuSE Linux SLES 10

- Batch System:
  - MOAB workload manager
  - Torque (aka OpenPBS) resource manager
  - Cray's ALPS (Application Level Placement Scheduler)

- File system: Luster file system

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Computing System – Lynx

- 76 compute nodes (8.026 TFLOPS peak)
  - o 12 processors per node, 912 compute processors
  - o Two hex-core AMD 2.2 GHz Opteron chips
  - o Each processor has 1.3 GB of memory and totaling 1.216 TB of memory in the system.

- 10 I/O nodes
  - o A single dual-core AMD 2.6 GHz Opteron chip and 8 GB of memory
  - o 2 login nodes, 4 nodes reserved for system functions
  - o 4 nodes are for external Lustre file system and GPFS file system testing

Compilers on Lynx

- **Available compilers**
  - PGI Programming Environment
  - EKOPATH ("PathScale") Compiler Suite
  - Intel Compiler Suite
  - GNU Compiler Collection

- **Load the corresponding PrgEnv-xxx module to change compilers**
  - ftn: Fortran programs
  - cc: C programs
  - CC: C++ programs

- **More information**
  - https://www2.cisl.ucar.edu/docs/lynx/compilers

A job script on Lynx

```
#!/bin/bash
#PBS -q workshop
#PBS -l mppwidth=60          ###Number of Processors
#PBS -l walltime=01:30:00
#PBS –N example
#PBS -e testrun.$PBS_JOBID.err
#PBS -o testrun.$PBS_JOBID.out

cd $PBS_O_WORKDIR
aprun -n 60 ./My_Prog.exe
```

Submit, Delete, and Monitor Jobs on Lynx

- **Submit a job**
  - qsub batch_script

- **Check job status**
  - qstat –a
  - showq

- **Delete a job**
  - qdel jobid

HPSS

HPSS Introduction

- High Performance Storage System (12+ PB of data)

- Hierarchical Storage Interface (HSI) is the primary interface supporting for data transfer to/from HPSS along with metadata access and data management.

- HPSS Tape Archiver (HTAR) is used to package files on your file system to a single archive file and then send it to HPSS.

- HPSS files have NO expiration date. They remain in the archive until they are explicitly deleted. Once deleted, they cannot be recovered.

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Hierarchical Storage Interface (HSI)

- **POSIX like interface**

- **Different ways to invoke HSI**
  - Command line invocation
    - **hsi** cmd
    - **hsi** cget hpssfile (from your default dir on HPSS)
    - **hsi** cput myfile (to your default dir on HPSS)
  - Open an HSI session
    - hsi to get in and establish session; end, exit, quit to get out
    - restricted shell-like environment
  - hsi "in cmdfile"
    - File of commands scripted in "cmdfile"

- **Navigating HPSS while in HSI session**
  - pwd , cd, ls, cdls
  - http://www2.cisl.ucar.edu/sites/default/files/HSI-command.pdf

Data Transfer

- **Writing data – cput command**

  - *[HSI]/home/user1>* *cput file.01*
  - *[HSI]/home/user1>* *cput file.01 : new.hpss.file*

- **Reading data – cget command**

  - *[HSI]/home/user1->* *cget file.01*
  - *[HSI]/home/user1->* *cget file.01 : hpss.file*

GLADE centralized file service

- **The Globally Accessible Data Environment**

- **High performance shared file system technology**

- **Shared work spaces across CISL's HPC resources**

- **Multiple different spaces**
  - /glade/home/username   10 TB
  - /glade/users/username   80 TB
  - /glade/scratch/username   204 TB
  - /glade/proj*   555 TB

GLADE centralized file service

A centralized file service (Bluefire, Lynx, Mirage)

- **User home directory :**
  - o   /glade/home/username
  - o   10 GB quota per user
  - o   Backup

- **Scratch (temporary computational space):**
  - o   /glade/scratch/username
  - o   2 TB quota per user
  - o   NO Backup

Data Analysis and Visualization

- **Data Analysis and Visualization**
  - High-end servers available 7 x 24 for interactive data analysis, data-post processing and visualization

- **Data Sharing**
  - Shared data access within the lab
  - Access to the NCAR Archival Systems and NCAR Data Sets

- **Remote Visualization**
  - Access to visual computing platforms from the convenience of your office using tcp/ip based remote image delivery service

- **Visualization Consulting**
  - Consult with CISL staff on your visualization problems

Working on Mirage/Storm

- **Log on to 'mirage'**
  - ssh –X –l username mirage[0-2].ucar.edu
  - One-time password using CryptoCard or Yubikey
  - Use 'free' or 'top' to see if there is currently enough resources

- **Development environments**
  - Intel C, C++, F77, F90
  - GNU C, C++, Fortran, Tools

- **Software tools**
  - VAPOR, Paraview
  - NCL, NCO, NCARG, IDL
  - Matlab, R
  - ImageMagick

Yellowstone Environment

- **Petascale computing resource**

  NCAR-Wyoming Supercomputing Center in Cheyenne, Wyoming

- **Production computing operations is expected to begin in summer/fall 2012.**
  - Computing resources: 30 times the workload throughput of NCAR's current Bluefire supercomputer
  - New centralized file system and data storage system (GLADE): 15 times the sustained I/O bandwidth and 12 times the capacity of CISL's current GLADE system
  - Combined data analysis and visualization (DAV) systems (Geyser and Caldera): 20 times increase in CISL's dedicated DAV resources
  - High Performance Storage System (HPSS): expanded more

Future Reference

- Bluefire User Guide
  http://www2.cisl.ucar.edu/docs/bluefire-user-guide
- Lynx User Guide
  http://www2.cisl.ucar.edu/docs/lynx-user-guide
- Mirage/Storm User Guide
  http://www2.cisl.ucar.edu/docs/mirage-storm
- Glade File System
  http://www2.cisl.ucar.edu/resources/glade
- HPSS User Guide
  http://www2.cisl.ucar.edu/docs/hpss

User Support

- **CISL Homepage:**
  - http://www2.cisl.ucar.edu/

- **CISL Consulting Services**
  - NCAR Mesa Lab Area 55, Floor 1B

- **CISL HELP**
  - Call (303)497-2400
  - Email to cislhelp@ucar.edu
  - Submit an extraview ticket