Getting Started with CISL Facilities and Support

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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)
 - Lynx (Mesa)
 - o Janus (CU)
 - o Yellowstone (NWSC)
- Data Analysis and Visualization
 - o Mirage and Storm
 - o Geyser and Caldera (NWSC)

- Data ArchivalOHPSSOGLADE
- Allocations and Security
- User support
- Training



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)
 - o 76.4 TFLOPS
- 117 compute nodes (70.4 TFLOPS peak)
 - o 3,744 POWER6 processors (32 per node)
 - o 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:

- o xlc, xlc_r, xlC, xlC_r
- mpcc, mpcc_r, mpCC, mpCC_r

The _r versions are thread safe

o 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)
 - o Cygwin, Putty, Terminal, etc.
- Using your Yubikey token
 - o 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
 - o bsub < script</pre>
- Monitor jobs
 - o bjobs
 - ▶ bjobs -u all
 - bjobs -q regular
 - o bhist
 - bhist -n 0 jobid
- Delete a job
 - o 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
 - o 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
 - o Compute Node Linux (CNL) based on SuSE Linux SLES 10
- Batch System:
 - MOAB workload manager
 - o Torque (aka OpenPBS) resource manager
 - Cray's ALPS (Application Level Placement Scheduler)
- File system: Luster file system



Computing System – Lynx

- 76 compute nodes (8.026 TFLOPS peak)
 - o 12 processors per node, 912 compute processors
 - Two hex-core AMD 2.2 GHz Opteron chips
 - Each processor has 1.3 GB of memory and totaling 1.216
 TB of memory in the system.
- 10 I/O nodes
 - 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
 - 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
 - o Intel Compiler Suite
 - GNU Compiler Collection
- Load the corresponding PrgEnv-xxx module to change compilers

o ftn: Fortran programs

o cc: C programs

o CC: C++ programs

- More information
 - o <u>https://www2.cisl.ucar.edu/docs/lynx/compilers</u>



A job script on Lynx

```
#!/bin/bash
#PBS -q workshop
#PBS - I mppwidth=60 ###Number of Processors
#PBS - I 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
 - o qsub batch_script
- Check job status
 - o qstat -a
 - o showq
- Delete a job
 - o 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.



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)
 - o Open an HSI session
 - hsi to get in and establish session; end, exit, quit to get out
 - restricted shell-like environment
 - o hsi "in cmdfile"
 - File of commands scripted in "cmdfile"
- Navigating HPSS while in HSI session
 - o pwd, cd, ls, cdls
 - http://www2.cisl.ucar.edu/sites/default/files/HSI-command.pdf



Data Transfer

- Writing data cput command
 - o [HSI]/home/user1> cput file.01
 - o [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

0	/glade/home/username	10 TB
0	/glade/users/username	80 TB

o /glade/scratch/username204 TB

o /glade/proj* 555 TB



GLADE centralized file service

A centralized file service (Bluefire, Lynx, Mirage)

User home directory :

- /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
- 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'

- o ssh –X –I 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

- o Intel C, C++, F77, F90
- GNU C, C++, Fortran, Tools

Software tools

- o VAPOR, Paraview
- o NCL, NCO, NCARG, IDL
- o 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:
 - o http://www2.cisl.ucar.edu/
- CISL Consulting Services
 - o NCAR Mesa Lab Area 55, Floor 1B
- CISL HELP
 - o Call (303)497-2400
 - o Email to cislhelp@ucar.edu
 - o Submit an extraview ticket

