Getting Started with CISL Facilities and Support

CESM Tutorial 11 August 2014

Rory Kelly
Consulting Services Group



CISL 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

- Computing Systems
 - Yellowstone
- Data Storage and Archival
 - Glade
 - HPSS
- Data Analysis and Visualization
 - Geyser and Caldera
- Allocations
- Additional Training Resources
- Contacting User support
- Questions



Yellowstone





Yellowstone IBM iDataPlex Cluster

Compute Nodes

- 4,518 Compute Nodes
- 16 cores, 2.6 GHz Intel Sandy Bridge per node
- 32 GB 1600 MHz DDR3 Memory per node
- 72,288 Total Cores, 1.44 TB Total Memory
- 6 login nodes

Interconnect

- Mellanox FDR Infiniband Network
- Fat-tree topology
- 13.6 GB/s bandwith per node, 2.5 μsec latency
- 31.7 TB/s bisection bandwidth

GLADE GPFS Filesystem

- 10.9 PB of useable storage
- 90 GB/s aggregate IO bandwidth
- Shared across compute and DAV resources



Accessing Yellowstone with Yubikey

- Use Secure Shell to log on with yubikey
 - o Terminal, Cygwin, PuTTY, etc.
- **Using your Yubikey token**
 - When you log in to yellowstone ssh -X <username>@yellowstone.ucar.edu your screen displays a response:
 - Token Response:
 - o 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 of pushing the button.
- More information of Yubikey:

http://www2.cisl.ucar.edu/docs/yubikeys



Shells

- We support four shells on yellowstone
 - tcsh
 - csh
 - bash
 - ksh
- You can change your default shell using the System Account Manager (SAM)

https://sam.ucar.edu

More information

http://www2.cisl.ucar.edu/resources/yellowstone/quick_start



Supported Compilers

- CISL supports the following compilers on yellowstone, geyser and caldera
 - Intel (C, C++, Fortran)
 - icc, icpc, ifort, mpiicc, mpiicpc, mpiifort
 - Portland Group (C, C++*, Fortran)
 - pgcc, pgCC, pgfortran, pgf90, mpipcc, mpipf90
 - Pathscale (C, C++*, Fortran)
 - pathcc, pathCC, pathf95, mpiecc, mpief90
 - GNU (C, C++, Fortran)
 - gcc, g++, gfortran, mpigcc
- More information

http://www2.cisl.ucar.edu/resources/yellowstone/code_dev/compiling



Commonly Used Software

- BLAS Basic Linear Algebra Subroutines
- HDF5 Hierarchical Data Format
- LAPACK and ScaLAPACK
- MKL Math Kernel Library of general-purpose math routines
- GSL GNU Scientific Library for C and C++ programmers
- NetCDF Network Common Data
- PnetCDF Parallel netCDF
- NCL NCAR Command Language
- CDO Climate Data Operators
- IDL Interactive Data Language
- R Statistical Computing Environment
- Python Scripting Language
- Matlab High Level Interactive Mathematical Environment



Using Modules

Modules help manage the user software, including compilers, libraries and dependencies between them.

Helpful module commands

- module av
 - lists available modules
- module list
 - show the modules currently loaded
- module load/unload <module-name>
 - load module module-name into the environment
- module swap <module 1> <module 2>
 - swap module 1 for module 2
- module help
 - display help on module commands
- module help <module-name>
 - display help specific to module-name



Using Modules

Helpful module commands (continued)

- module whatis <module-name>
 - short info on module-name
- module save <set-name>
 - save currently loaded module set as set-name
- module restore <set- name>
 - reload all modules in saved set set-name
- module purge
 - remove all loaded modules from environment
- module reset
 - reset module environment

More Info:

http://www2.cisl.ucar.edu/resources/software/modules



Controlling Jobs With LSF

- Job submission (bsub)
 - bsub < script
 - bsub -U CESM_WS < script
 - Submit a job against reservation CESM_WS
- Job Monitoring (bjobs and bhist)
 - o bjobs

bjobs -u all

bjobs -q regular

o bhist

bhist -n <#> jobid

- Job Removal (bkill)
 - o bkill jobid



Example LSF Job Script

```
#!/bin/csh
# LSF batch script to run an MPI application
#BSUB -P UESM0002
                           # project code
#BSUB -W 01:20
                           # wall-clock time (hrs:mins)
                           # number of MPI tasks in job
#BSUB -n 64
#BSUB -R "span[ptile=16]" # run 16 MPI tasks per node
#BSUB -J myjob
                           # job name
#BSUB -o myjob.%J.out
                           # output file name %J is job ID
#BSUB -e myjob.%J.err
                           # error file name %J is job ID
#BSUB -q regular
                           # queue
#run the executable
mpirun.lsf ./myjob.exe
```

For more info:

http://www2.cisl.ucar.edu/resources/yellowstone/using_resources/runningjobs



GLADE Shared File System

GLADE is a high performance GPFS file system shared across CISL HPC and DAV resources

File space	Quota	Back Up	Purge Period	Description
/glade/u/home/username	10 GB	Yes	None	Home directories
/glade/scratch/username	10 TB	No	90 days	Temporary space for short term use
/glade/p/work/username	512 GB	No	None	Work space for longer term storage
/glade/p/project_code	N/A	No	None	Shared space for project allocations



HPSS





HPSS Introduction

- High Performance Storage System (100+ PB of storage)
- Hierarchical Storage Interface (HSI) is the primary interface 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 is used for long term archiving of files, not for short term temporary storage.



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 start a session; end, exit, quit to stop session. restricted shell-like environment

o hsi "in cmdfile"

File of commands scripted in "cmdfile"

- Navigating HPSS while in HSI session
 - o On HPSS file system: pwd , cd, ls, , mkdir, cdls
 - o On GLADE file system: lpwd, pcd, lls, lmkdir, lcdls
- More info

http://www2.cisl.ucar.edu/docs/hpss/hsi



Data Transfer Individual Files

- 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
- Can also use wildcards for cget/cput
 - [HSI]/home/user1-> cget *.nc



Data Transfer Using HTAR for File Collections

- To ease transferring large numbers of files or whole file trees, use HTAR
 - htar -c -f ex_dir.tar ex_dir
- To list contents of an HTAR archive
 - htar -t -f ex_dir.tar
- Can add/retrieve files to an HTAR archive without downloading the whole archive
- More Info:
 - https://www2.cisl.ucar.edu/docs/hpss/htar



HPSS Help

- To get help with an HSI command that takes at least one argument, just type the command name without arguments
 - [HSI]/home/user1-> cput
- To get help with an HSI Command that takes no arguments, type the command followed by -?
 - [HSI]/home/user1-> ls -?



Data Analysis and Visualization Geyser and Caldera

Geyser

- 16 large memory nodes
- 40 cores, 2.4 GHz Intel Westmere EX per node
- 1 NVIDIA Quadro 6000 GPU per node
- 1 TB 1600 MHz DDR3 memory per node

Caldera

- 16 visualization / compute nodes
- 16 cores, 2.6 GHz Intel Sandy Bridge per node
- 2 NVIDIA Tesla M2070-Q GPUs per node
- 64 GB 1600 MHz DDR3 memory per node

Pronghorn

- 8 cores, 2.6 GHz Intel Sandy Bridge per node
- 2 Intel Xeon Phi 5110P coprocessors per node
- 64 GB DDR3-1600 memory per node



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

More info

 https://www2.cisl.ucar.edu/resources/ geyser_caldera/visualization



Allocations and Account Info

- For accounting info and allocations log on to the Systems Account Manager (SAM)
 - https://sam.ucar.edu
- Change shells
- Change default Unix group
- Change HPSS default project
- See active projects, charges, and balances
- https://www2.cisl.ucar.edu/docs/sam



Additional Training

- Consulting Group provides classes in topics of interest to yellowstone users
 - *Fortran, C, C++*
 - Python
 - NCL, IDL, Matlab
 - Parallel Computing with MPI and OpenMP
 - Visualization
 - Linux and UNIX Commands and System Use
- Classes are also archived for web viewing
- https://www2.cisl.ucar.edu/training



Contacting 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



Questions?

