Getting Started with CISL Facilities and Support

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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 Analysis and Visualization
 - Geyser and Caldera
- o Data Archival
 - HPSS
 - GLADE
- Allocations and Security
- User support
- o **Training**

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

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



Caldera and Geyser Data Analysis and GPU Clusters

• 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

• 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

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

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



Accessing Yellowstone with Yubikey

• Use Secure Shell to log on with yubikey

• 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:

- 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



Systems Laboratory

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:

NCAR

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

Controlling Jobs With LSF

Job submission (bsub)

- o bsub < script</p>
- o bsub –U CESM_WS < script</p>
 - Submit a job against reservation CESM_WS

• Job Monitoring (bjobs and bhist)

- o **bjobs**
 - bjobs -u all
 - bjobs -q regular
- o **bhist**

bhist -n 0 jobid

Job Removal (bkill)

o bkill jobid

Computational & Information Systems Laboratory

Example LSF Job Script

#!/bin/csh

LSF batch script to run an MPI application

#BSUB -P SCSG0001 #BSUB -W 00:20 #BSUB -n 64 **#BSUB -J myjob** #BSUB -o myjob.%J.out #BSUB -e myjob.%J.err **#BSUB** -q regular

project code # wall-clock time (hrs:mins) # number of MPI tasks in job #BSUB -R "span[ptile=16]" # run 16 MPI tasks per node # job name # output file name %J is job ID # error file name %J is job ID # queue

#run the executable mpirun.lsf ./myjob.exe

For more info:

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



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

hsi "in cmdfile"

File of commands scripted in "cmdfile"

• Navigating HPSS while in HSI session

 \circ pwd , cd, ls, cdls

• More info

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

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

o [HSI]/home/user1-> cget file.01

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



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

User Support

• CISL Homepage:

o <u>http://www2.cisl.ucar.edu/</u>

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

CISL HELP

- o Call (303)497-2400
- Email to <u>cislhelp@ucar.edu</u>
- Submit an extraview ticket

