# Getting Started with CISL Facilities and Support

CESM Tutorial
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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
  - 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 on Yubikey:

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

# Supported Shells

- We support four shells on yellowstone
    - tcsh
    - csh
    - bash
    - ksh

- Change default shell in SAM (System Account Manager)
    - https://sam.ucar.edu

- More information

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

# Supported Compilers

CISL supports multiple compilers on yellowstone

- Intel (C, C++, Fortran)
    - icc, icpc, ifort, mpiicc, mpiicpc, mpiifort
- Portland Group (C, C++, Fortran)
    - pgcc, pgCC, pgfortran, pgf90, mpipcc, mpipf90
- GNU (C, C++, Fortran)
    - gcc, g++, gfortran, mpigcc
- Pathscale (C, C++, Fortran)
    - pathcc, pathCC, pathf95, mpiecc, mpief90

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 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

# Job Control With LSF

- Job submission (bsub)
  - `bsub < script`
  - `bsub –U CESM_WS < script`
    - Submit a job against reservation CESM_WS
- Job Monitoring (bjobs and bhist)
  - `bjobs`
  - `bjobs -u all`
  - `bjobs -q regular`
  - `bhist`
  - `bhist –n <#> jobid`
- Job Removal (bkill)
  - `bkill jobid`

# Example LSF Job Script

```csh
#!/bin/csh
# LSF batch script to run an MPI application
#
#BSUB -P UESM0002                  # project code
#BSUB -W 01:20                     # wall-clock time (hrs:mins)
#BSUB -n 64                        # number of MPI tasks in job
#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
```
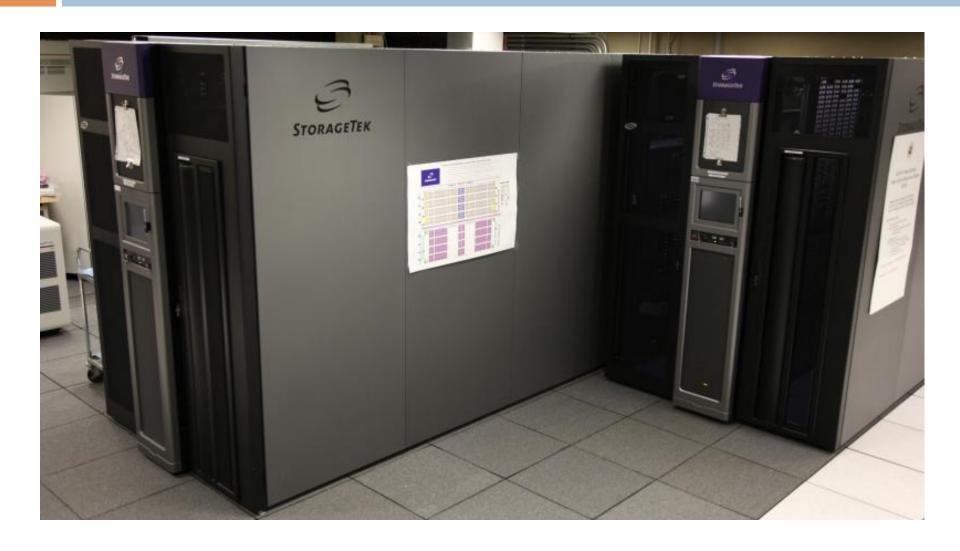
For more info:
http://www2.cisl.ucar.edu/resources/yellowstone/using_resources/runningjobs

# GLADE Shared File System

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

| File space | Quota | Back Up | Purge Period | Description |
|---|---|---|---|---|
| /glade/u/home/username | 10 GB | Yes | None | Home directories |
| /glade/scratch/username | 10 TB | No | 60 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
  - hsi "in cmdfile"
    - File of commands scripted in "cmdfile"
- Navigating HPSS while in HSI session
  - On HPSS file system:  pwd , cd, ls, , mkdir, cdls
  - 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: HTAR for File Collections

- Use HTAR for large numbers of files or file trees
  - `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/from 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
  - 16 large memory nodes
  - 40 cores, 2.4 GHz Intel Westmere EX per node
  - 1 NVIDIA Quadro K5000 GPU per node
  - 1 TB 1600 MHz DDR3 memory per node

- Caldera
  - 30 visualization / compute nodes
  - 16 cores, 2.6 GHz Intel Sandy Bridge per node
  - 2 NVIDIA Tesla K20X GPUs per node (some nodes)
  - 64 GB 1600 MHz DDR3 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 your laptop
- 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

More Info

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?