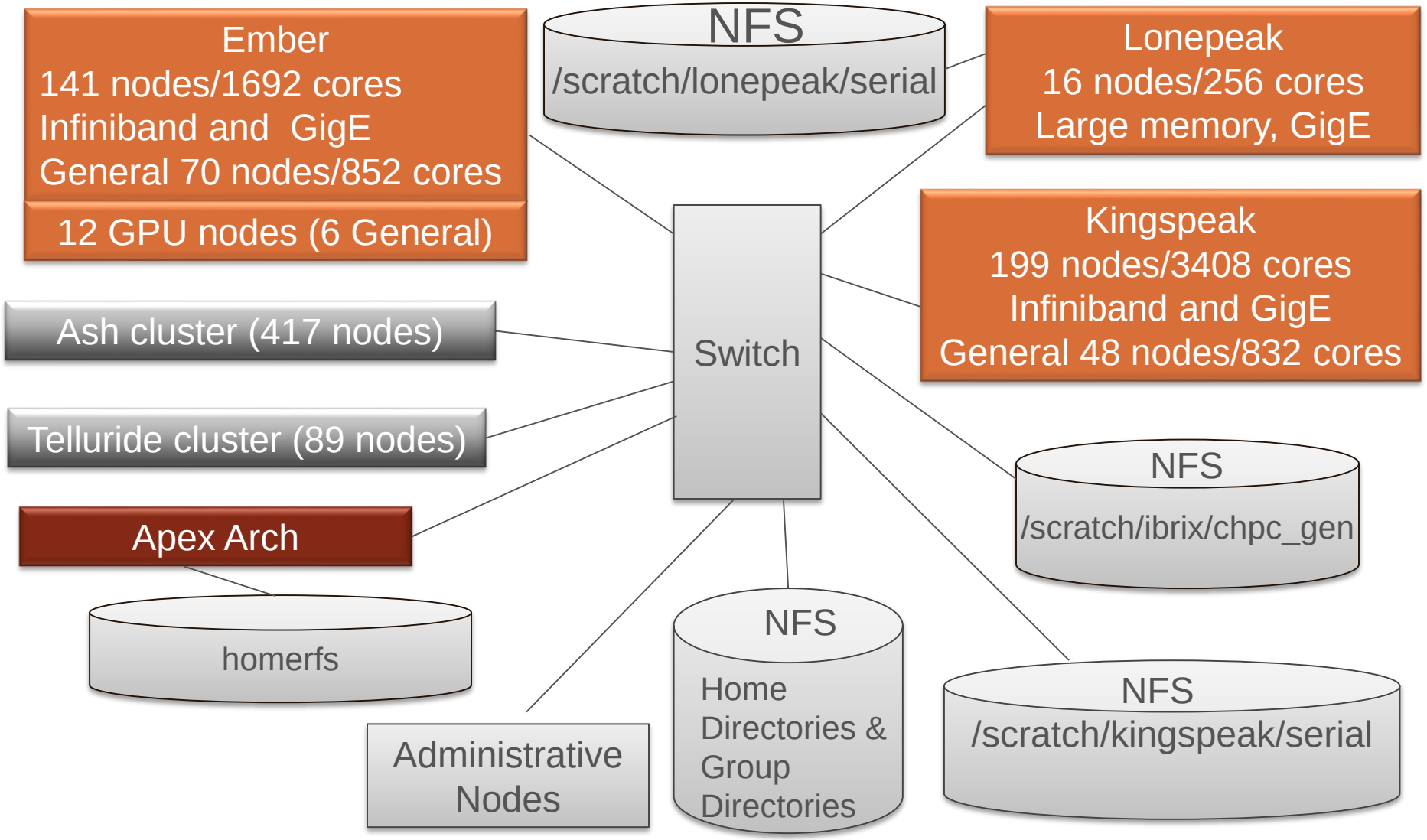
CHPC Resources & Best Practices

Anita Orendt
Assistant Director
Research Consulting & Faculty Engagement
anita.orendt@utah.edu

CHPC Mission

- The University of Utah's Center for High Performance Computing provides large-scale computer systems, storage, networking, and the expertise to optimize the use of these high-end computer technologies.
- CHPC supports faculty and research groups whose main focus requires computing, storage, and advanced networking as core instruments central to their research.


Ember
141 nodes/1692 cores
Infiniband and GigE
General 70 nodes/852 cores
12 GPU nodes (6 General)
NFS
/scratch/lonepeak/serial
Lonepeak
16 nodes/256 cores
Large memory, GigE
Kingspeak
199 nodes/3408 cores
Infiniband and GigE
General 48 nodes/832 cores
Ash cluster (417 nodes)
Switch
Telluride cluster (89 nodes)
NFS
/scratch/ibrix/chpc_gen
Apex Arch
homerfs
NFS
Home Directories & Group Directories
NFS
/scratch/kingspeak/serial
Administrative Nodes

Kingspeak

- Getting Started at CHPC
  https://www.chpc.utah.edu/docs/manuals/getting_started/
- Kingspeak User Guide
  https://wiki.chpc.utah.edu/display/DOCS/Kingspeak+User+Guide

- 32 Dual Socket-Eight Core Nodes (16 core/node) &
  12 Dual-Socket-Ten Core Nodes (20 core/node)
- Intel Xeon processors (Sandybridge/Ivybridge E5-2670)
- 2.6 (16 core) or 2.5 (20 core) Ghz speed with AVX support
- 64 Gbytes memory per node
- Mellanox FDR Infiniband interconnect
- OS RedHat Enterprise Linux 6

File Systems

- NFS mounted home directory
  - /uufs/chpc.utah.edu/common/home/***UNID***
  - 50GB quota
- Local scratch – local to the specific node
  - /scratch/local/
  - 337GB on 16 core; 803GB on 20 core nodes
- NFS mounted scratch – for this class only
  - /uufs/chpc.utah.edu/common/home/ci-water4-0/CS6965/
  - 80 TB

Accessing Clusters

- Login to the cluster interactive nodes with your unid and campus password
  - From linux/mac
    - open terminal
    - ssh unid@kingspeak.chpc.utah.edu
  - From windows – need to install ssh client on your PC
- Interactive nodes only used for short compiles, editing and very short test runs
- ***No more than 15 minutes and no jobs of any length that make heavy use of cpu or memory!***

SSH Client Choices for Windows

- PuTTY
  - http://www.chiark.greenend.org.uk/~sgtatham/putty/
- XShell4
  - http://www.netsarang.com/download/down_xsh.html

FastX – Tool for Remote X

- https://www.starnet.com/fastx
- Used to interact with remote linux systems graphically in much more efficient and effective way then simple X forwarding
- Graphical sessions can be detached from without being closing, allowing users to reattach to the session from the same or other systems
- Server on all interactive nodes as well as several dedicated fastx servers
- Clients for windows, mac and linux; can be installed on both university and personal desktops.

FastX

- For FastX – see “To Use” section of documentation at https://wiki.chpc.utah.edu/display/DOCS/FastX
- Download client from CHPC site at https://www.chpc.utah.edu/apps/profile/software.php
- Do install
- Start program
- Set host to kingspeak1.chpc.utah.edu OR kingspeak2.chpc.utah.edu

Security Policies

- No clear text passwords, use ssh and scp
- You may not share your account under any circumstances
- Don't leave your terminal unattended while logged into your account
- Do not introduce classified or sensitive work onto CHPC systems unless on Protected Environment

Security Policies

- Do not try to break passwords, tamper with files etc.
- Do not distribute or copy privileged data or software
- Report suspicions to CHPC (security@chpc.utah.edu)
- See http://www.chpc.utah.edu/docs/policies/security.html for more details

Login scripts

- CHPC provides login scripts ("dot" files) when creating account for both tcsh and bash shells
- These files set the environment so that compilers are found, batch system commands work – ***Do not remove or edit!***
- Shell set to tcsh – can change to bash at www.chpc.utah.edu (choose PROFILE, login, select edit profile)
- A few of you already had CHPC accounts – should refresh your .bashrc/.tcshrc files
  - wget http://www.chpc.utah.edu/docs/manuals/getting_started/code/chpc.tcshrc
  - mv chpc.tcshrc .tcshrc
  - And same with chpc.bashrc

Compiler Suites

- Gnu (4.4.7-3)
  - /usr/bin/
  - gcc, gfortran, g++
- Intel (composer_xe_2013_sp1.3.174)
  - /uufs/chpc.utah.edu/sys/pkg/intel/ics/bin
  - icc, ifort, icpc
- PGI (13.4)
  - /uufs/chpc.utah.edu/sys/pkg/pgi/std_rh6
  - pgcc, pgf90, pgCC

MPI options – MVAPICH2

- Defaults to mvapich2 Version 1.9 built with gcc for Infiniband
  - /uufs/kingspeak.peaks/sys/pkg/mvapich2/std
    - source /uufs/kingspeak.peaks/sys/pkg/mvapich2/std/etc/mvapich2.csh
- Also builds for intel and PGI
  - /uufs/kingspeak.peaks/sys/pkg/mvapich2/std_intel
    - source /uufs/kingspeak.peaks/sys/pkg/mvapich2/std_intel/etc/mvapich2.csh
  - /uufs/kingspeak.peaks/sys/pkg/mvapich2/std_pgi
    - source /uufs/kingspeak.peaks/sys/pkg/mvapich2/std_intel/etc/mvapich2.csh
- Also OpenMPI

Batch System Information

- Used to access compute nodes
- Two components
  - Torque (OpenPBS) -- Resource Manager
  - Moab (Maui) – Scheduler – enforces policies and sets job priorities

Batch commands

- qsub <script> -- *submit job*
- qstat -- *lists all jobs in queue*
- qdel $jobid -- *deletes job*
- pbsnodes –a -- *lists all nodes in cluster*

- showq -- *lists all jobs in queue*
- showstat $jobid -- *shows estimated start time*
- checkjob $jobid -- *give more detailed info about job*

Batch Policies

- https://wiki.chpc.utah.edu/pages/viewpage.action?pageId=281706582
- https://wiki.chpc.utah.edu/display/policy/2.1.4+Kingspeak+Job+Scheduling+Policy
- Walltime limit – 72 hours
- Accounts
  - **CS6965** for general allocation
  - **owner-guest** for guest jobs on owner nodes on kingspeak

Sample Batch Script

```
#PBS -S /bin/tcsh
#PBS -l nodes=2:ppn=16,walltime=1:00:00
#PBS -A CS6965
#PBS -N myjob

# Create scratch directory
mkdir -p /uufs/chpc.utah.edu/common/home/ci-water4-0/CS6965/$USER/$PBS_JOBID
# Change to working directory
cd /uufs/chpc.utah.edu/common/home/ci-water4-0/CS6965/$USER/$PBS_JOBID
# Copy data files to scratch directory
cp $HOME/work_dir/files /uufs/chpc.utah.edu/common/home/ci-water4-
   0/CS6965/$USER/$PBS_JOBID #Execute Job

source /uufs/kingspeak.peaks/sys/pkg/mvapich2/1.9i/etc/mvapich2.sh

mpiexec -np 40 -machinefile $PBS_NODEFILE ./mycode
# Copy files back home and cleanup

cp * $HOME/work_dir && rm -rf /uufs/chpc.utah.edu/common/home/ci-water4-
   0/CS6965/$USER/$PBS_JOBID
```

Getting Help

- CHPC website and wiki
  - www.chpc.utah.edu and wiki.chpc.utah.edu
    - Getting started guide, cluster usage guides, software manual pages, CHPC policies
- Jira Ticketing System
  - Email: issues@chpc.utah.edu
- Help Desk: 405 INSCC, 581-6440 (9-5 M-F)
- We use chpc-hpc-users@lists.utah.edu for sending messages to users (such as downtimes, outages) – also Twitter (@CHPCOutages and @CHPCUpdates)

CHPC Fall Presentation Series

All Presentations in INSCC Auditorium (Room 110) unless noted

September 9, 2014 1-2 pm **Overview of CHPC**
September 11, 2014, 2-3pm **Protected Environment at CHPC**
****BMI Green Conference Room (421 Wakara Way, room 2002W)
September 16, 2014, 1-3pm **Introductory Linux for HPC Part 1**
September 18, 2014, 1-3pm **Introductory Linux for HPC Part 2**
September 23, 2014, 1-2pm **XSEDE Resource Support at CHPC**
September 25, 2014, 1-2pm **Introduction to Scientific Visualization**
September 25, 2014, 2-3pm **NLP and AI Services at CHPC**
**BMI Classroom (421 Wakara Way Room 1470)
September 30, 2014, 1-2pm **Chemistry Packages at CHPC**

October 2, 2014, 1-3pm **Hands-on Introduction to Python, Part 1**
October 7, 2014, 1-3pm **Hands-on Introduction to Python, Part 2**
October 9, 2014, 1-3pm **Hands-on Introduction to Numpy & Scipy**
October 21, 2014, 1-2pm **Introduction to Parallel Computing**
October 23, 2014, 1-2pm **Introduction to Programming with MPI**
October 30, 2014, 1-2pm **Introduction to Programming with OpenMP**
November 4, 2014, 1-2pm **Hybrid MPI-OpenMP Programming**
November 6, 2014, 1-2pm **Introduction to I/O at CHPC**
November 11, 2014, 1-2pm **Introduction to Debugging**
November 13, 2014, 1-2pm **Introduction to Profiling**
November 18, 2014, 1-2pm **Introduction to GPU Programming**

http://www.chpc.utah.edu/docs/presentations/