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Stampede
User Environment

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Overview

Effective users, good citizens

- Getting Started – Access to Stampede
- Getting Acquainted – A Tour of Stampede
- Getting Work Done – Using Stampede
- Getting Along – Good Citizenship

- Lab 1 – Test Drive (including tour of the MIC)
- Supplemental Material – end of slide deck

Disclaimers

- Audience: users new to supercomputing
- Tone: breadth rather than depth
- Moving target: much is pending or evolving

References: Not an Afterthought!

- User Guide(s), Usage Policies, etc. and associated links

  http://www.tacc.utexas.edu/user-services

  – Note "**Updates and Notices**" at top of Stampede User Guide
- man ("manual") pages and help systems
  – Try "`man`" and "`man -k`" before command name
    - Space bar to advance within man page, "q" key to exit
  – Try command name with `-h, --help, -help, help`
  – Try command name with no argument
- Web: tutorials, cheat sheets, forums
  – Include error messages in search strings
- XSEDE and TACC ticket systems

Getting Started

Access to Stampede and Other TACC Resources

Before you log in, you'll need…

- Portal Account
  - XSEDE users go to https://portal.xsede.org/
  - UT System users go to www.portal.tacc.utexas.edu
- Allocation (computing hours)
  - PI must request allocation through appropriate portal
  - PI may use portal to assign active users to an allocation
  - Allocation associated with "project name" (account code)
- Activation on TACC resources
  - Involves email handshake(s) with TACC user services
  - May take a few business days
  - Note that your TACC credentials (think ssh) may differ from XSEDE
  - TACC password resets can take 30+ minutes to propagate

Initial login with explicit ssh

- Start with a Linux-like terminal or equivalent* connected to internet
  - Linux command line
  - Mac terminal app
  - PuTTY, Secure Shell Client, GSI-SSH on XSEDE portal,…
- Connect to a login node with ssh or equivalent

```
% ssh stampede.tacc.utexas.edu
% ssh username@stampede.tacc.utexas.edu
% ssh -X stampede.tacc.utexas.edu
% ssh -Y stampede.tacc.utexas.edu
```

*many users will access Stampede through a special gateway designed and maintained for their research community; see e.g. xsede.org/gateways-overview

Shells and Startup Scripts

- OS is Linux
- bash is default shell, but TACC supports most major shells
  - bash, csh, tcsh, zsh, …
- Submit ticket to change default shell (chsh will not work)
- System-level startup files execute before account-level
- It's worth your trouble to understand startup files
  - e.g. .profile and .bashrc
  - Easy way to customize environment (e.g. prompt, aliases)
  - Caution: environment associated with shell (~ "window"), not acct
  - Caution: avoid using "echo" in startup scripts (will break scp et al!)

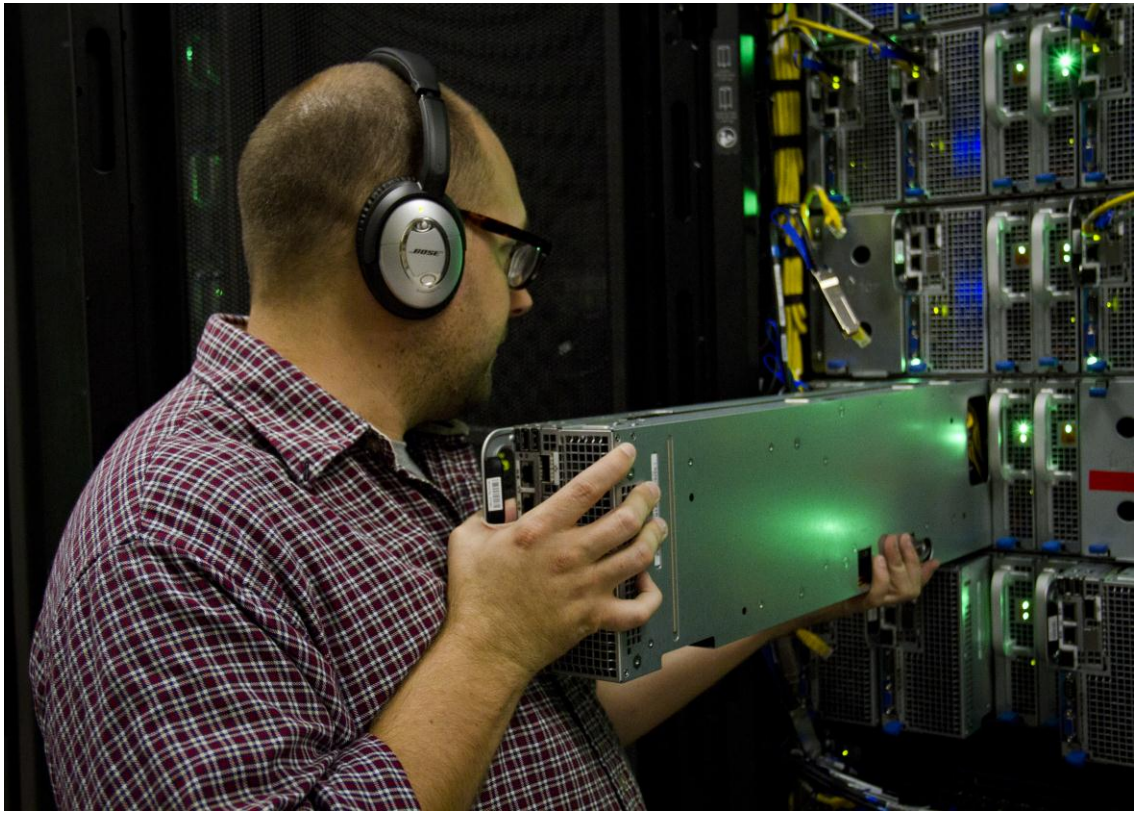
Text Editors

- Pick a favorite; become proficient
  - nano – simple
  - vi (vim) – terse
  - emacs – powerful
- Appreciate cross-platform issues
  - Win to Linux – dos2unix utility
  - Linux to Win – Wordpad rather than Notepad
  - Linux filenames are case sensitive
  - Linux doesn't handle blanks in filenames well

Getting Acquainted

A Tour of Stampede

Typical Stampede Node (= blade)

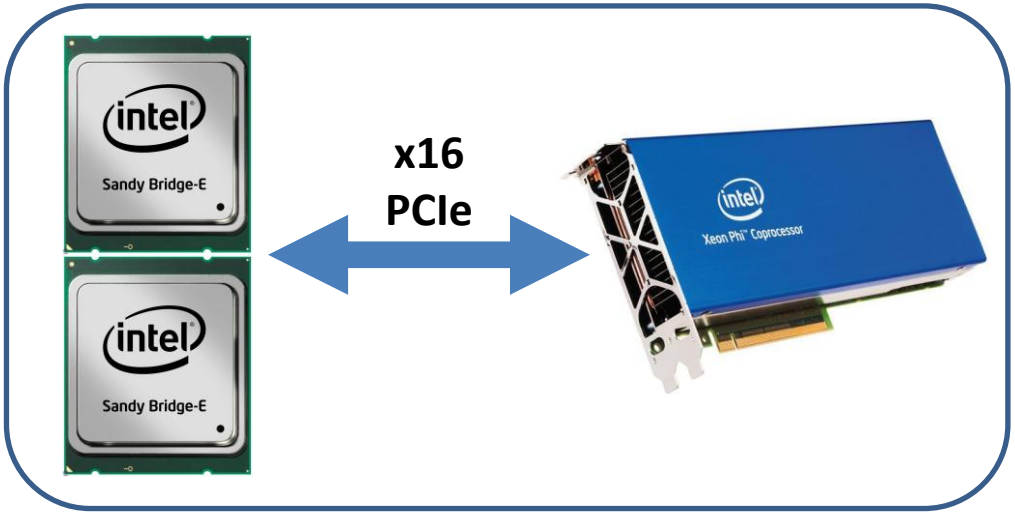


Dell PowerEdge 8220
("DCS Zeus")
Compute Node

Typical Stampede Node (= blade)

CPU (Host)
"Sandy Bridge"

Coprocessor (MIC)
"Knights Corner"



16 cores
32G RAM

Two Xeon E5
8-core processors

61 lightweight cores
8G RAM

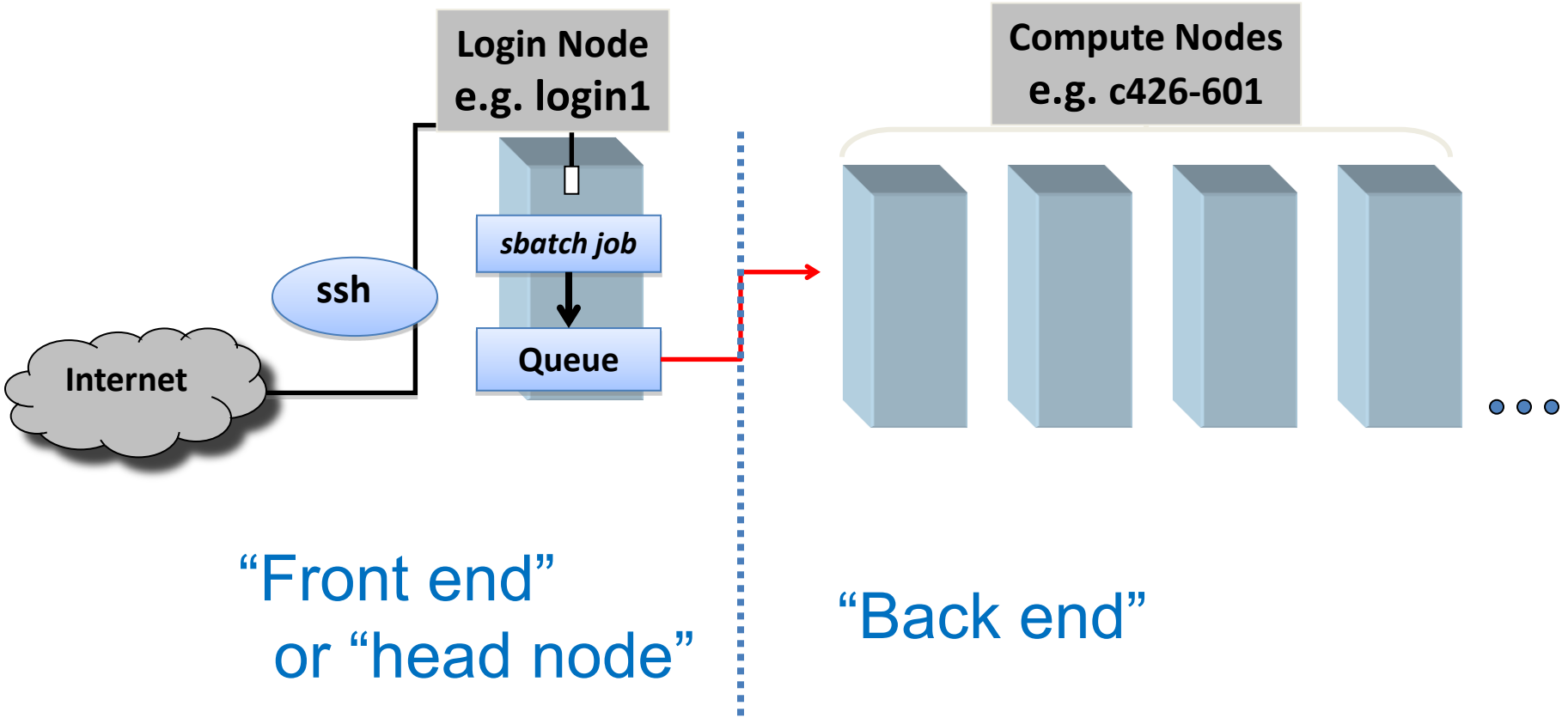
Xeon Phi Coprocessor
Each core has 4 hardware threads

MIC runs lightweight
Linux-like OS (BusyBox)

Stampede Basic Specs

- ~6400 nodes (= blades) in 160 racks
- Typical node
  - 16 cores on host, 32G RAM
  - 61 cores on MIC coprocessor, 8G RAM
- Specialized nodes
  - 16 large-memory nodes (32 Xeon cores, 1T RAM) with Fermi-class GPUs for visualization (no CUDA, no MIC)
  - 128 GPU nodes, each with NVIDIA Kepler2 and a MIC
  - Login nodes don't have MIC coprocessors

Nodes Have Personalities and Purposes



File System Specs

Environmental Variable	User Size Limits	Characteristics
$HOME	5.0 GB	Regular backups
$WORK	400 GB	Not purged No backup
$SCRATCH	(~8.5PB total)	Subject to purge after 10 days
$ARCHIVER:$ARCHIVE (Ranch home directory)	Essentially unlimited	Files staged to and from tape
/tmp (local to node)	~80 GB per node	Purged after job

- From any cpu host: the aliases **`cdh`**, **`cdw`** and **`cds`** change your working directory to your $HOME, $WORK and $SCRATCH directories respectively.
- From MIC coprocessor: file systems are visible, but cd aliases (e.g. cdw) and env variables (e.g. $WORK) are not yet avail (cd to full explicit path).

File Transfers

- We recommend starting with scp or rsync; other protocols possible.
- Avoid using recursive (-r) flag with large transfers; bundle files with tar utility.
- Avoid simultaneous transfers and tar jobs on login nodes.
- Compression and optimization are rarely necessary.
- On Ranch, staging from tape takes time.
- Beware of cross-platform issues: filenames (spaces, capitalization).

http://www.tacc.utexas.edu/user-services/user-guides/ranch-user-guide

Getting Work Done

Using Stampede

Lmod: TACC's Module System

- "Sets the table" by loading software tools you need
- Prevents errors by managing dependencies
- Why this is so important
  - Multiple compilers
  - Multiple MPI stacks (each dependent on compilers)
  - Varied user apps, libraries, tools (often dependent on compiler and MPI stack)
- Modules can affect MIC operations, but Lmod not currently available on MICs themselves

Key Module Commands

```
% module help                          {lists options}
% module load <module>                 {add a module}
% module avail                         {lists available modules}
% module unload <module>               {remove a module}
% module swap <mod1> <mod2>            {swap two modules}
% module help <module>                 {module-specific help}
% module spider                        {lists all modules}
% module spider petsc                  {list all versions of petsc}

% ml                                   {abbrev for module list}
% ml <module>                          {abbrev for module load}
% module reset                         {return to system defaults}
```

(Personal) Default Modules

- Save/restore personal default module environment:

```
$ module reset  # return to sys default
$ module load ddt
$ module load fftw3
$ module save   # now loaded at login or restore
```

- Save/restore named collections of modules:

```
$ module save chemtools
    ...
$ module restore chemtools
```

  - Execute "`module help`" for more info

- This is a great way to achieve reliability and repeatability

Compilers

- Intel 13 is the compiler of choice for Stampede
  - The only compiler that supports Xeon Phi coprocessor
  - Currently three versions of gcc suite are also available
    - MPI with gcc requires additional Intel library
    - Other issues yet to be resolved; watch Stampede User Guide for more info
  - We also support other specialized compilers
    - E.g. cuda support (nvcc): `module load cuda`
- Compilers available from login nodes and compute node hosts
  - Compilers not visible from MIC coprocessors…
  - …but you can compile for the MIC from a Sandy Bridge host
- Numerous math libraries available, but MKL's MIC support makes it especially important (www.intel.com/software/products/mkl)

MPI Compilation

Command	Language	Type Suffix	Example
mpicc	c	.c	`mpicc <options> prog.c`
mpicxx	C++	.C, .cc, .cpp, .cxx	`mpicxx <options> prog.cpp`
mpif77	F77	.f, .for, .ftn	`mpif77 <options> prog.f`
mpif90	F90	.f90, .fpp	`mpif90 <options> prog.f90`

- mvapich2 and impi (Intel) currently supported.
- The mpiXXX commands are shell scripts.
- They call the underlying C/C++/Fortran compiler.

Your Ticket to Compute Nodes

- Four ways to get to the back end (compute nodes):
  - SLURM batch job: **`sbatch <batchfilename>`**
  - SLURM interactive session: **`srun <flags>`**
  - Run special app that connects to back end: e.g. **`ddt`**
  - ssh to node on which you already have a job running

    -- once on compute node, **`ssh mic0`** gets you to its mic
- If you don't use sbatch, srun, or equivalent, you're running on the front end (login nodes) – don't do this!
  - Don't launch exe (e.g. **`./a.out`**) on the command line
  - One of the easiest ways to get your account suspended

Key SLURM and Related Commands

- To launch a batch job

  `sbatch <batchfilename>`

- To launch a one-node, sixteen core interactive session in the development queue

```
$ srun --pty -n 16 -t 00:30:00 -p development -A 20130418HPC /bin/bash -l

  # last char is lower case "el" (launches bash as login shell)
  # -A flag is optional unless you have multiple projects
```

- To view all jobs in the queues: `squeue | more` or `showq | more`
- To view status of your own jobs:

  `squeue –u <userid>` or `showq -u <userid>`
- To delete a job: `scancel <jobid>`
- To view status of queues: `sinfo -o "%20P %5a"`
  - Ignore queue limits reported by this command; they are not the ones in force.

General Use Stampede Queues*

Queue	Max Runtime	Max Nodes (Cores)	Charge Rate	Purpose
normal	24 hrs	250 (4000)	1	normal production
development	4 hrs	16 (256)	1	development nodes
largemem	24 hrs	4 (128)	2	large memory nodes
serial	12 hrs	1 (16)	1	serial or shared memory
large	24 hrs	1000 (16000)	1	large core counts
normal-mic	24 hrs	250 (4000)	1	early production mic nodes
gpu	24 hrs	32 (512)	1	GPU nodes
gpudev	4 hrs	4 (64)	1	GPU development nodes
vis	8 hrs	32 (512)	1	GPU nodes + VNC service

*Queue properties subject to change

SLURM: Basic MPI Job Script

```
#!/bin/bash                 # Don't miss this line!

#----------------------------------------------------
# Generic SLURM script -- MPI
#----------------------------------------------------

#SBATCH -J myjob           # Job name
#SBATCH -o myjob.%j.out    # stdout; %j expands to jobid
#SBATCH -e myjob.%j.err    # stderr; skip to combine stdout and stderr
#SBATCH -p development     # queue
#SBATCH -N 2               # Number of nodes, not cores (16 cores/node)
#SBATCH -n 32              # Total number of MPI tasks (if omitted, n=N)
#SBATCH -t 00:30:00        # max time

#SBATCH --mail-user=djames@tacc.utexas.edu
#SBATCH --mail-type=ALL

#SBATCH -A TG-01234        # necessary if you have multiple project accounts

module load fftw3          # You can also load modules before launching job
module list

ibrun ./main.exe           # Use ibrun for MPI codes. Don't use mpirun or srun.
```

Additional Software

- Stack is still under construction
- Computation: e.g. R, Octave, PETSc, …
- Python module gives you NumPy, SciPy, MatPlotLib, …
- Analysis and Debugging: e.g. tau, papi, perfexpert, ddt, …
- Parameter Studies: pylauncher and launcher
- High performance file i/o: hdf5, parallel hdf5, netcdf
- Build and install your own tools
  - We strongly recommend installing in $WORK
  - Download tar archive, not pre-packaged installer
  - Standard trick: `./configure --prefix=$WORK/myapps`

Getting Along

Good Citizenship

The Keys to Good Citizenship

Remember you are sharing resources

(login nodes, file systems, bandwidth)

Use components for intended purposes

Login nodes: appropriate use

- Building software
  - But Stampede compilers are also visible on compute nodes
- Managing files
  - Editing, transfers, tar/untar
- Submitting, monitoring, managing batch jobs
  - sbatch, showq, squeue, squeue -u username, scancel…
- Launching interactive sessions
  - srun, ddt, etc.

Login nodes: inappropriate use

- Don’t do science on the front end
  - Access compute nodes with sbatch, srun, or equiv
  - Don’t launch exe directly
- Avoid simultaneous instances of demanding processes
  - Parallel builds (e.g. `make -j`), tar/untar, transfers

File System Citizenship

- Avoid running jobs from $HOME
- Run demanding jobs from $SCRATCH
- Avoid frequent i/o when possible
- Minimize simultaneous i/o from many processes
- Learn to recognize/avoid other stressors
  - e.g. under-the-table stat (du, default ls) on big dirs
- Know when it's time to learn/use parallel i/o

Lab 1

Test Drive

Overview of Lab

- Part 0 – Grab the Lab Files
- Part 1 – Run an MPI Batch Job (sbatch)
- Part 2 – An Interactive Session (srun)
- Part 3 – Run MIC App from the Host
- Part 4 – Visit the MIC

- Secure Shell Client terminal program available on TACC laptops
- Slides contain supplemental info on editors

Supplemental Material

nano

- All operations/commands are preceded by the Control key:
  - ^G Get Help
  - ^O WriteOut
  - ^X Exit
  - ….
- If you have modified the file and try to exit (^X) without writing those changes (^O) you will be warned.
- Makes text editing simple, but it has less powerful options than vi and emacs (search with regular expressions, etc..)

vi/vim & emacs

- vi/vim command cheat sheet
  - http://www.tuxfiles.org/linuxhelp/vimcheat.html
- emacs command cheat sheet
  - http://emacswiki.org/emacs/ReferenceCards