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

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• 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...

• **Step 1 -- TACC Portal Account**
  – [www.portal.tacc.utexas.edu](http://www.portal.tacc.utexas.edu)
  – Click on “Account Request”

• **Step 2 -- Portal Activation**
  – Click on the email confirmation
    • Check junk/spam mail if you don’t see the message

• **Step 3 – Allocation for specific machine(s)**
  – PI must request allocation
  – Allocation associated with a project name (used as account code in Stampede's scheduler)
  – PI assigns other activated users to the project
  – Unexpired Ranger SUs transfer to Stampede (3:1 exchange rate)
Initial Login

• 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, ksh, 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”

- 16 cores
- 32G RAM
- Two Xeon E5 8-core processors

Coprocessor (MIC)  
“Knights Corner”

- 61 lightweight cores
- 8G RAM
- Xeon Phi Coprocessor
- Each core has 4 hardware threads
- MIC runs lightweight Linux-like OS (BusyBox)

x16 PCIe
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

Internet

Login Node
  e.g. login1$
  sbatch job
  Queue

ssh

Compute Nodes
  e.g. c426-601

"Back end"

"Front end"
or "head node"

“Back end”
From any cpu host: the aliases \texttt{cdh}, \texttt{cdw} and \texttt{cds} change your working directory to your $\texttt{HOME}$, $\texttt{WORK}$ and $\texttt{SCRATCH}$ directories respectively.

From MIC coprocessor: file systems are visible, but cd aliases (e.g. \texttt{cdw}) and env variables (e.g. $\texttt{WORK}$) are not yet avail (cd to full explicit path).

### File System Specs

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

1. File System Specifications
2. Environmental Variable
3. User Size Limits
4. Characteristics

- Regular backups
- Not purged
- No backup
- Subject to purge after 10 days
- Essentially unlimited
- Files staged to and from tape
- Purged after job
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.
- Compression and optimization are rarely necessary.
- On Ranch, staging from tape takes time.
- Beware of cross-platform issues: filenames (spaces, capitalization).
- **See "Updates and Notices" at top of Stampede User Guide** for info regarding Ranger → Stampede file transfers.

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
% module load <module>
% module avail
% module unload <module>
% module swap <mod1> <mod2>
% module help <module>
% module spider
% module spider petsc

% ml
% ml <module>
% module reset

{lists options}
{add a module}
{lists available modules}
{remove a module}
{swap two modules}
{module-specific help}
{lists all modules}
{list all versions of petsc}
{abbrev for module list}
{abbrev for module load}
{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 gnu available
    • MPI with gnu requires additional Intel library
    • Other issues yet to be resolved; watch Stampede User Guide for more info
  – Expect additional specialized compilers as appropriate
    • 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 (`module load mkl`)
MPI Compilation

<table>
<thead>
<tr>
<th>Compiler</th>
<th>Language</th>
<th>Type Suffix</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>mpicc</td>
<td>c</td>
<td>.c</td>
<td>mpicc &lt;options&gt; prog.c</td>
</tr>
<tr>
<td>mpicxx</td>
<td>C++</td>
<td>.C, .cc, .cpp, .cxx</td>
<td>mpicxx &lt;options&gt; prog.cpp</td>
</tr>
<tr>
<td>mpif77</td>
<td>F77</td>
<td>.f, .for, .ftn</td>
<td>mpif77 &lt;options&gt; prog.f</td>
</tr>
<tr>
<td>mpif90</td>
<td>F90</td>
<td>.f90, .fpp</td>
<td>mpif90 &lt;options&gt; prog.f90</td>
</tr>
</tbody>
</table>

- 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 <optional 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 <options> --pty /bin/bash -l  # last char is lower case "el"
  ```
  ...where `<options>` resemble sbatch options, and include AT LEAST the following:
  ```
  -n 16          # cores
  -t 00:30:00    # max time requested
  -p development # queue (should be development or gpudev only)
  ```
  --will also need `-A <project_acct_name>` if 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`
  ```
  The arcane sequence `sinfo -o "$%20P %5a %.10l %16F"` is especially useful.
## General Use Stampede Queues*

<table>
<thead>
<tr>
<th>Queue</th>
<th>Max Runtime</th>
<th>Max Nodes (Cores)</th>
<th>Charge Rate</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>normal</td>
<td>24 hrs</td>
<td>250 (4000)</td>
<td>1</td>
<td>normal production</td>
</tr>
<tr>
<td>development</td>
<td>4 hrs</td>
<td>16 (256)</td>
<td>1</td>
<td>development nodes</td>
</tr>
<tr>
<td>largemem</td>
<td>24 hrs</td>
<td>4 (128)</td>
<td>2</td>
<td>large memory nodes</td>
</tr>
<tr>
<td>serial</td>
<td>12 hrs</td>
<td>1 (16)</td>
<td>1</td>
<td>serial or shared memory</td>
</tr>
<tr>
<td>large</td>
<td>24 hrs</td>
<td>1000 (16000)</td>
<td>1</td>
<td>large core counts</td>
</tr>
<tr>
<td>request</td>
<td>24 hrs</td>
<td>n/a</td>
<td>1</td>
<td>special requests</td>
</tr>
<tr>
<td>normal-mic</td>
<td>24 hrs</td>
<td>250 (4000)</td>
<td>1</td>
<td>early production mic nodes</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>gpu</td>
<td>24 hrs</td>
<td>32 (512)</td>
<td>1</td>
<td>GPU nodes</td>
</tr>
<tr>
<td>gpudev</td>
<td>4 hrs</td>
<td>4 (64)</td>
<td>1</td>
<td>GPU development nodes</td>
</tr>
<tr>
<td>vis</td>
<td>8 hrs</td>
<td>32 (512)</td>
<td>1</td>
<td>GPU nodes + VNC service</td>
</tr>
</tbody>
</table>

*Queue properties subject to change*
#!/bin/bash

# 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. Don’t use mpirun or srun.
Additional Software

• Stack is still under construction
• Computation: e.g. NumPy, SciPy, R,…
• Performance, Analysis, Debugging: e.g. 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