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
- Supplemental Material

Disclaimers

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

Questions?

- Help with Linux/Unix in general
- Help with specific applications and programs
- Help with the environment at TACC in general (batch system, tape robot, Xeon PHI, ….)
- Advice with computing in general

Linux/Unix help

- 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
- Search for examples, templates, or cheat sheets online

Help with specific programs

- For programs managed by the "module" system (more details later):

```
module help petsc
module help fftw2
```

- See if there are webpages, user forums, etc.
- Maybe some experts at TACC knows more: submit a ticket

Help with the environment at TACC

- Read the user guides!
- User Guide(s), Usage Policies, etc. and associated links

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

  https://www.tacc.utexas.edu/user-services/user-guides/stampede-user-guide
- Or submit a ticket in the user portal

Help with computing in general

- Submit a ticket asking for advice.

  https://portal.tacc.utexas.edu/

  https://portal.xsede.org/web/xup/help-desk

- We love doing this stuff, so we're happy to talk to you and think about your application

- Possibility of extended support through XSEDE

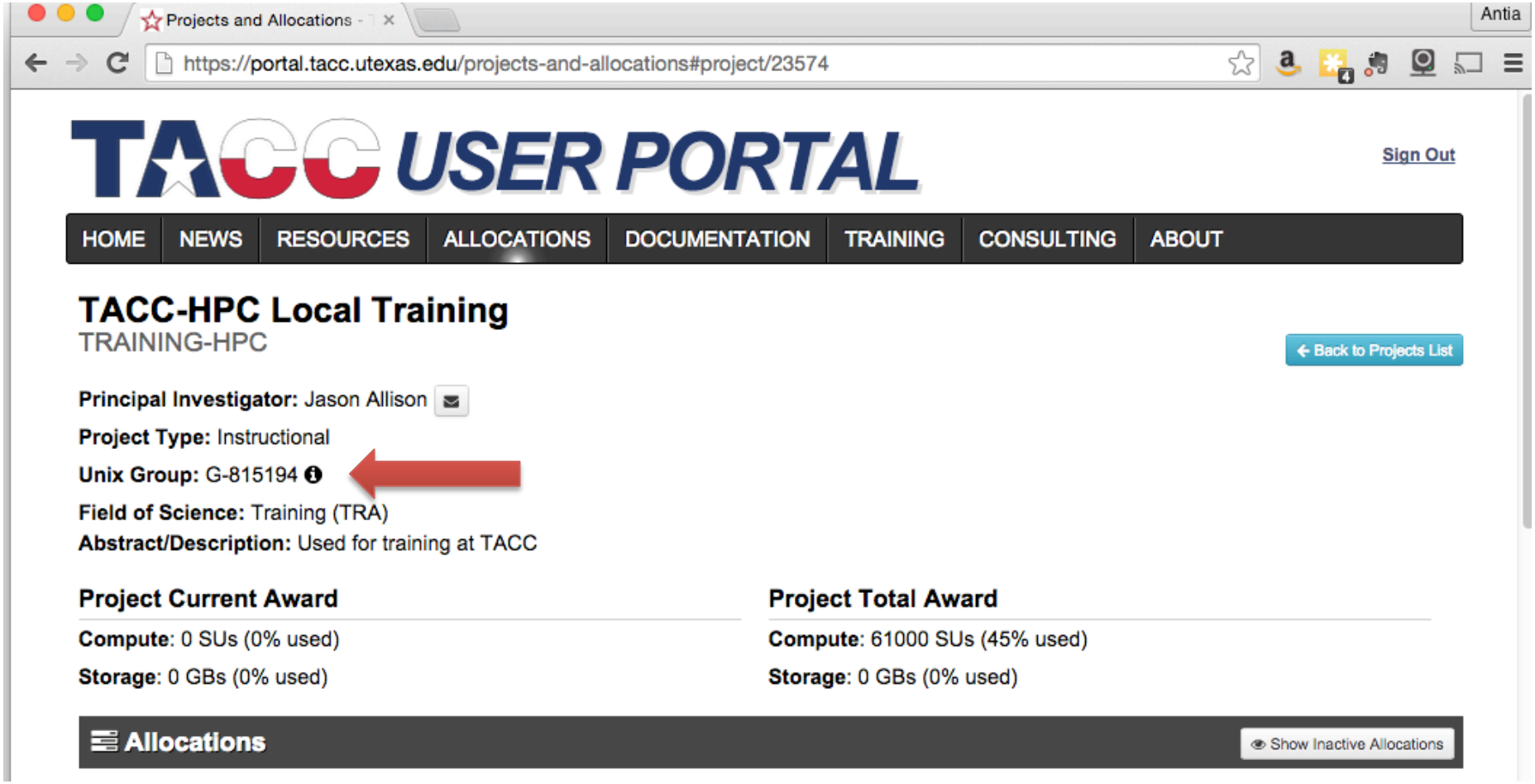
Getting Started

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

Your project



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

As you log in …

```
--------------------------------------------------------------------------------

---------------------- Project balances for user alamas -----------------------
| Name           Avail SUs     Expires | Name           Avail SUs     Expires |
| TACC-Team          -2293  2015-06-30 | A-ccsc            188581  2015-12-31 |
------------------------- Disk quotas for user alamas -------------------------
| Disk         Usage (GB)     Limit    %Used   File Usage       Limit   %Used |
| /home1             0.1       5.0     1.30          180      150000    0.12 |
| /work              0.2    1024.0     0.02         1895     3000000    0.06 |
--------------------------------------------------------------------------------

Tip 165   (See "module help tacc_tips" for features or how to disable)

   Do you want to use a hybrid code on 8 nodes using 2 MPI tasks and 8 OpenMP threads
   per node on Stampede? Be sure to use the "-N" option to specify the number of nodes
   that you want to use in addition to "-n".

   In this example, it will be "srun -N 8 -n 16..." or in your script "#SBATCH -N 8 \
   #SBATCH -n 16"

stampede3(1)$
```

Shells and Startup Scripts

- OS is Linux (Cent OS)
- 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 userid
  - 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
  - Blanks in filenames require some care
- Do NOT use MS Word (or so) to create job scripts and such. Also do not copy/paste from PDF files.

Getting Acquainted

A Tour of Stampede

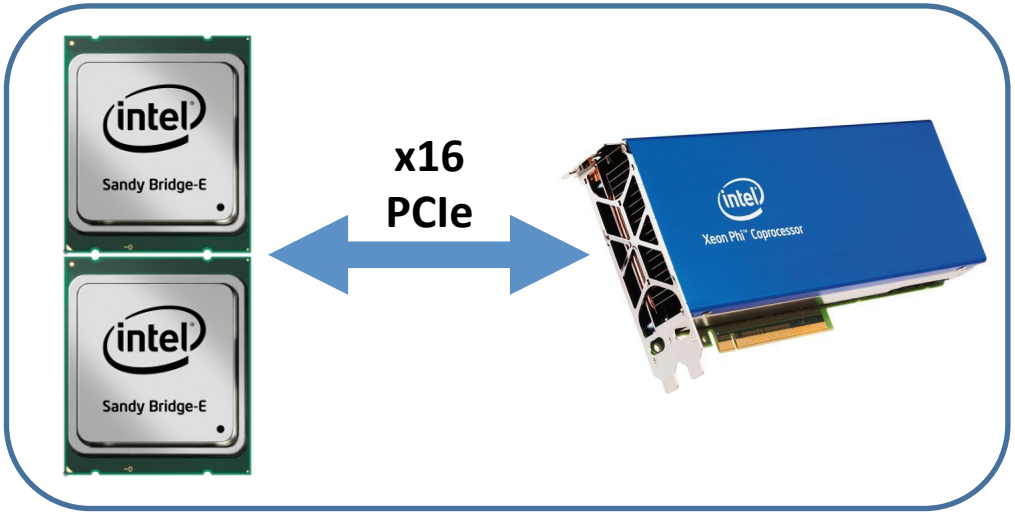
Typical Stampede Node (= blade)

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

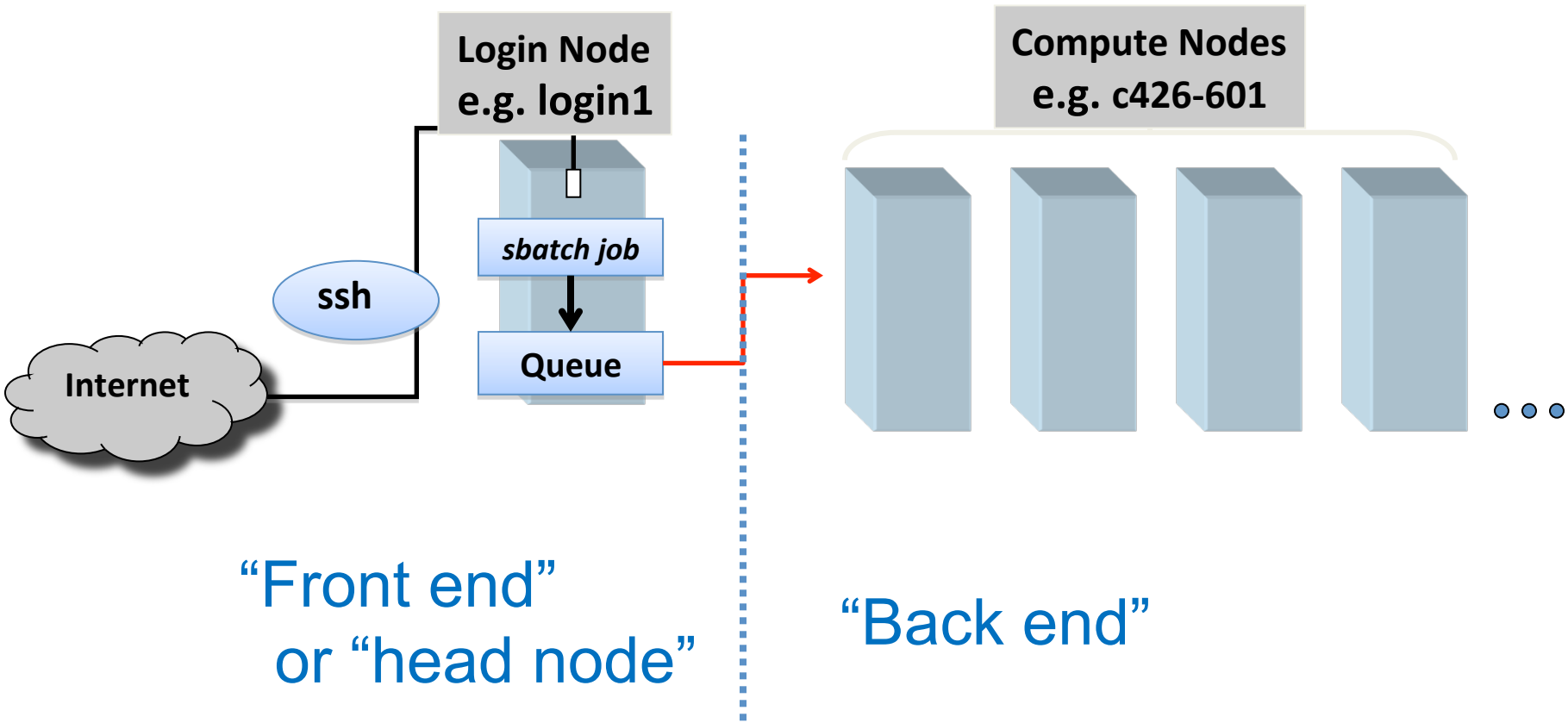
Xeon Phi Coprocessor
Each core has 4 hardware threads

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



What does this mean?

- Do not run parallel programs on the login nodes
  - Either it's simply not possible
  - Or you'll annoy the system administrators (and they may lock your account)
- Instead: submit a batch job. We'll get to that.

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, rsync, or globus-online
  - other protocols possible
- Avoid using recursive (-r) flag with large transfers
  - bundle files with tar utility
- Avoid simultaneous transfers and (large) tar jobs on login nodes
- Compression and optimization are rarely necessary
- On Ranch, staging from tape takes time
  http://www.tacc.utexas.edu/user-services/user-guides/ranch-user-guide
- Beware of cross-platform issues

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 several versions of gcc suite are also available
  - We also support other specialized compilers
    - e.g. cuda support (nvcc): `module load cuda`
- Compilers available from login nodes and some 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>`**

    -- Also try **`idev`** `(recommended methods)`
  - Run special application 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

idev

https://portal.tacc.utexas.edu/software/idevs.edu/software/idev

```
$idev
Defaults file    : ~/.idevrc
Default  project : A-ccsc
Default  time    : 30 min.
Default  queue   : development
System           : Stampede
 FYI: You have 3 INACTIVE reservations.
      Idev is not asking to use them because they are INACTIVE.
      If you want to wait on them use the -r option.
-----------------------------------------------------------------
              Welcome to the Stampede Supercomputer
-----------------------------------------------------------------

--> Verifying valid submit host (login3)...OK
--> Verifying valid jobname...OK
--> Enforcing max jobs per user...OK
--> Verifying availability of your home dir (/home1/03302/alamas)...OK
--> Verifying availability of your work dir (/work/03302/alamas)...OK
--> Verifying availability of your scratch dir (/scratch/03302/alamas)...OK
--> Verifying valid ssh keys...OK
--> Verifying access to desired queue (development)...OK
--> Verifying job request is within current queue limits...OK
--> Checking available allocation (A-ccsc)...OK
Submitted batch job 4963946
```

idev

```
 After your idev job begins to run, a command prompt will appear,
 and you can begin your interactive development session.
 We will report the job status every 4 seconds: (PD=pending, R=running).

job status:  R
--> Job is now running on masternode= c557-501...OK
--> Sleeping for 7 seconds...OK
--> Checking to make sure your job has initialized an env for you....OK
--> Creating interactive terminal session (login) on master node c557-501.
TACC Stampede System
LosF 0.40.0 (Top Notch)
Provisioned on 23-Sep-2012 at 15:37

Sc557-501(1)$
```

Compute node!

Not all compute nodes are created equal. Nodes in the development queue have a full set of compiler tools. Other queues are more limited.

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 | less` or `showq | less`
- 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)	Max Jobs	Charge Rate	Purpose
normal	48 hrs	256 (4k)	50	1	normal production
development	2 hrs	16 (256)	1	1	development nodes
largemem	48 hrs	4 (128)	4	2	large memory nodes
serial	12 hrs	1 (16)	8	1	serial or shared memory
large	24 hrs	1024 (16k)	50	1	large core counts
normal-mic	48 hrs	256 (4k)	50	1	early production mic nodes
normal-2mic	24 hrs	128 (2k)	50	1	nodes with 2 mics
gpu	24 hrs	32 (512)	50	1	GPU nodes
gpudev	4 hrs	4 (64)	5	1	GPU development nodes
vis	8 hrs	32 (512)	50	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=alamas@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 always 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; make; make install`
- Submit a ticket asking TACC to install something

Check my own environment

```
$ module load sanitytool
$ sanitycheck  -v
        sanitycheck Version:  1.0.1 @git@ 2014-05-09 20:00
          1: SSH Permission Test:
          Passed
          2: SSH Key Test:
          Passed
          3: Report Standard Variables, and check file system availability:
          Passed
          ……

          9: Check scheduler commands
          Passed
        ------------------
        All tests passed
        ------------------
```

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
  - Compilers are also visible on some 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.
- Modest postprocessing (gnuplot and such)

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.viemu.com/vi-vim-cheat-sheet.gif
  - http://www.cse.scu.edu/~yfang/coen11/vi-CheatSheet.pdf
- emacs command cheat sheet
  - http://www.ic.unicamp.br/~helio/disciplinas/MC102/Emacs_Reference_Card.pdf
  - http://www.mcs.sdsmt.edu/lpyeatt/courses/EmacsCheatSheet.pdf