Programming Environment

Cornell Center for Advanced Computing

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1. Orientation

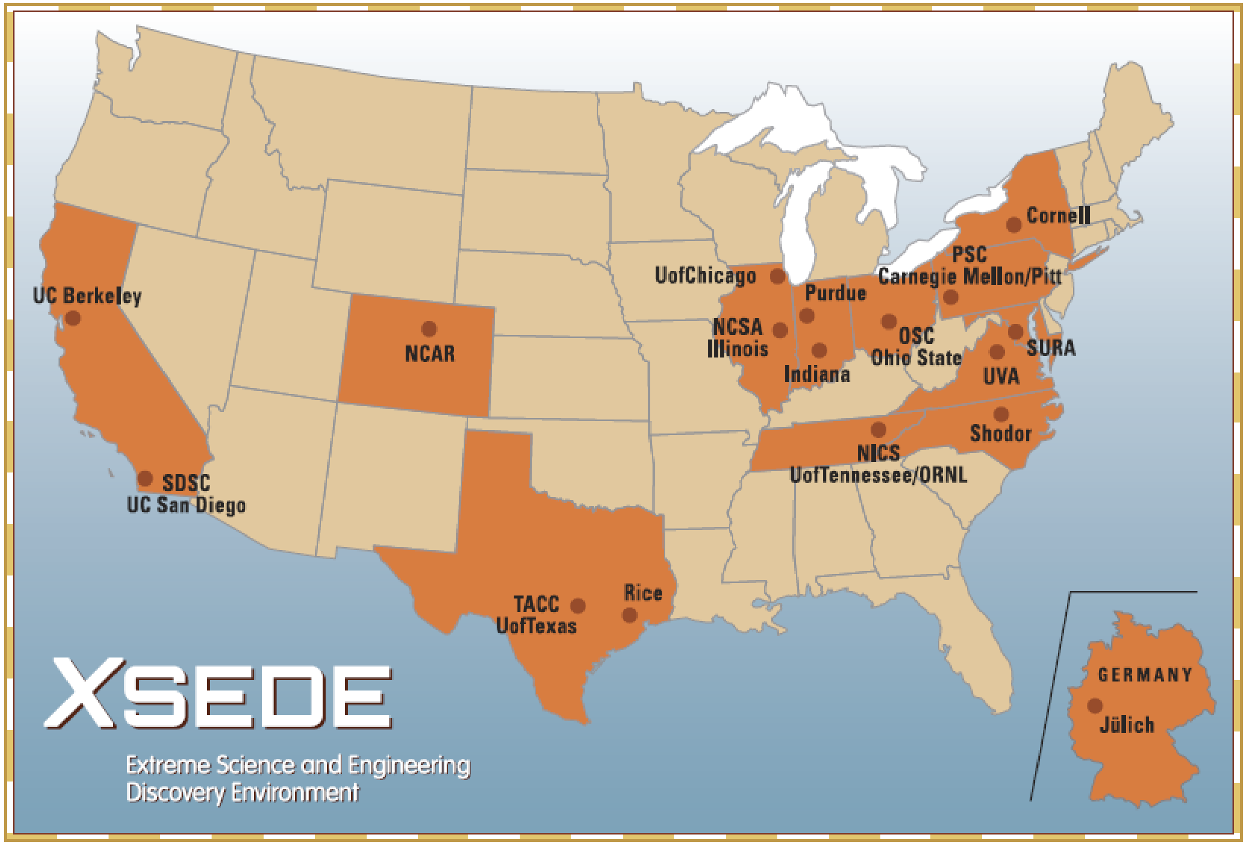
Orientation

- XSEDE – Extreme Science and Engineering Discovery Environment
  - Cyber infrastructure funded by NSF; a single virtual system
  - 9 supercomputers, 3 visualization systems, and 9 storage systems
  - 16 partner institutions

- TACC – Texas Advanced Computing Center
  - Ranger – Sun Constellation Linux Cluster, 90% dedicated to XSEDE
  - Longhorn – 256-Node Dell Visualization Cluster

- CAC – Cornell Center for Advanced Computing
  - HPC Systems – general use and private clusters
  - Red Cloud – on-demand research computing service

XSEDE


Cornell
PSC
Carnegie Mellon/Pitt
UofChicago
Purdue
UC Berkeley
NCSA
Illinois
OSC
Ohio State
SURA
NCAR
Indiana
UVA
Shodor
NICS
UofTennessee/ORNL
SDSC
UC San Diego
Rice
TACC
UofTexas
GERMANY
Jülich
XSEDE
Extreme Science and Engineering
Discovery Environment
110311

2. Allocations

XSEDE Allocations

Allocations provide computing, storage, and support services.

- Startup – for testing and preparing allocation request
  - Up to 200,000 core-hours, for 1 year
  - Submit Abstract, Awarded every 2 weeks
- Research – usually for funded research project
  - Unlimited core-hours, for 1 year
  - 10 page Request, Awarded quarterly
- Education – for classroom instruction and training sessions
  - Up to 200,000 core-hours, for 1 year
  - Submit CV and abstract, Awarded/2 weeks

https://portal.xsede.org/web/guest/allocations

Campus Champions

- The Campus Champions program supports campus representatives as a local source of knowledge on XSEDE resources.
- Contact your Campus Champion for
  - Trial allocation
  - Information on XSEDE and cyberinfrastructure resources

https://www.xsede.org/campus-champions

Contact Susan Mehringer at shm7@cornell.edu

4. Accessing Ranger

Login with SSH

- Putty for Windows
- Built-in as “ssh” for Linux or Mac

- You will be connected to login3.ranger.tacc.utexas.edu or login4
- **Do not** overwrite ~/.ssh/authorized_keys

Login now to ranger.tacc.utexas.edu:

```
% ssh username@ranger.tacc.utexas.edu
```

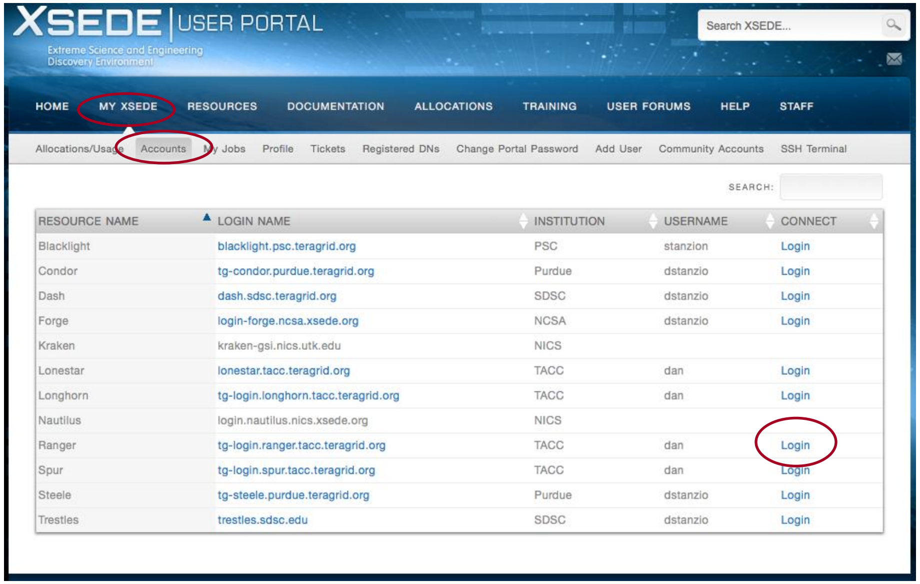
-or-

All Programs | ClassFiles | putty
use Host Name: ranger.tacc.utexas.edu

Login with SSO

- Log into the XSEDE User Portal
- Go to ‘My XSEDE’ tab
- Go to the ‘Accounts’ link
- Use the appropriate ‘login’ link

Login using the XSEDE portal



RESOURCE NAME	LOGIN NAME	INSTITUTION	USERNAME	CONNECT
Blacklight	blacklight.psc.teragrid.org	PSC	stanzion	Login
Condor	tg-condor.purdue.teragrid.org	Purdue	dstanzio	Login
Dash	dash.sdsc.teragrid.org	SDSC	dstanzio	Login
Forge	login-forge.ncsa.xsede.org	NCSA	dstanzio	Login
Kraken	kraken-gsi.nics.utk.edu	NICS		
Lonestar	lonestar.tacc.teragrid.org	TACC	dan	Login
Longhorn	tg-login.longhorn.tacc.teragrid.org	TACC	dan	Login
Nautilus	login.nautilus.nics.xsede.org	NICS		
Ranger	tg-login.ranger.tacc.teragrid.org	TACC	dan	Login
Spur	tg-login.spur.tacc.teragrid.org	TACC	dan	Login
Steele	tg-steele.purdue.teragrid.org	Purdue	dstanzio	Login
Trestles	trestles.sdsc.edu	SDSC	dstanzio	Login

Single Sign On (SSO)

- SSO is the default method; you’ll need to file a ticket to request a direct access password to the machine.
- SSO allows you to use just one username and password (your User Portal one) to log into every digital service on which you have an account.
- The easiest way to use SSO is via the XSEDE User Portal, but you can also use SSO via a desktop client or with an X.509 certificate.
- After you authenticate using SSO with your User Portal username and password, you will be recognized by all XSEDE services on which you have account, without having to enter your login information again for each resource.

VNC

- VNCServer
  - used to start a VNC (Virtual Network Computing) desktop.
  - a Perl script which simplifies the process of starting an Xvnc server.
  - can be run with no options at all. In this case it will choose the first available display number
- VNCServer copies a bitmap of the X-Windows screen across.
- Can be much less chatty than X-Windows.
- Good for remote graphics.
- VNCServer screen 4 uses TCP/IP port 5904.

Connect with VNC

- Start VNC on Ranger
  - First ssh normally.
  - Type “vncserver” and look for screen number, for example. “4”.
- Connect with a client
  - RealVNC or TightVNC on Windows
  - On Linux, vinagre or vncviewer
  - Connect to “ranger.tacc.utexas.edu:4” or your port number
- Be sure to kill it when you are done
  - vncserver –kill 4

5. Login Environment

Account Info

Note your account number at bottom of splash screen.

```
--------------------- Project balances for user tg459571 ----------------------
| Name           Avail SUs     Expires |                                      |
| TG-TRA120006       5000   2013-01-04 |                                      |
------------------------ Disk quotas for user tg459571 ------------------------
| Disk         Usage (GB)     Limit    %Used   File Usage       Limit   %Used |
| /share              1.1       6.0    17.75        10535      100000   10.54 |
| /work               0.0     200.0     0.00            1     2000000    0.00 |
-------------------------------------------------------------------------------
```

Get the Lab Files

- TAR = Tape ARchive. Just concatenates files.
- tar <switches> <files>
  - z = compress or decompress
  - x = extract
  - c = create
  - v = verbose
  - t = list files
  - f = next argument is the file to read or write
- *~username* is the home directory of that user
- For example, to create a tar: *tar cvf myfiles.tar dir1 dir2 README*

Get the lab files:

```
% tar xvf ~tg459572/LABS/envi.tar
```

Change directory to the envi directory:

```
% cd envi
```

List the lab files:

```
% ls -la
```

Experiment

```
% echo $SHELL
% env     (show environment variables – persists)
% set     (show shell variables – current shell only)
% pwd
% ls –la
% df –h
% uname –a
% echo $WORK
% cd $HOME
% cat .login
% cat /usr/local/etc/login
% cat .login_user  (create, then edit this one to personalize)
% chsh –l
% man chsh (q to quit)
```

Startup Scripts & Modules

- Login shell is set with “`chsh –s <login shell>`”
  - Takes some time to propagate (~1 hour)
- “`chsh –l`” will list available login shells.
- Each shell reads a set of configuration scripts.
- Bourne-type shells (Bourne, Korn, and Bash Shells)

System-wide config scripts:

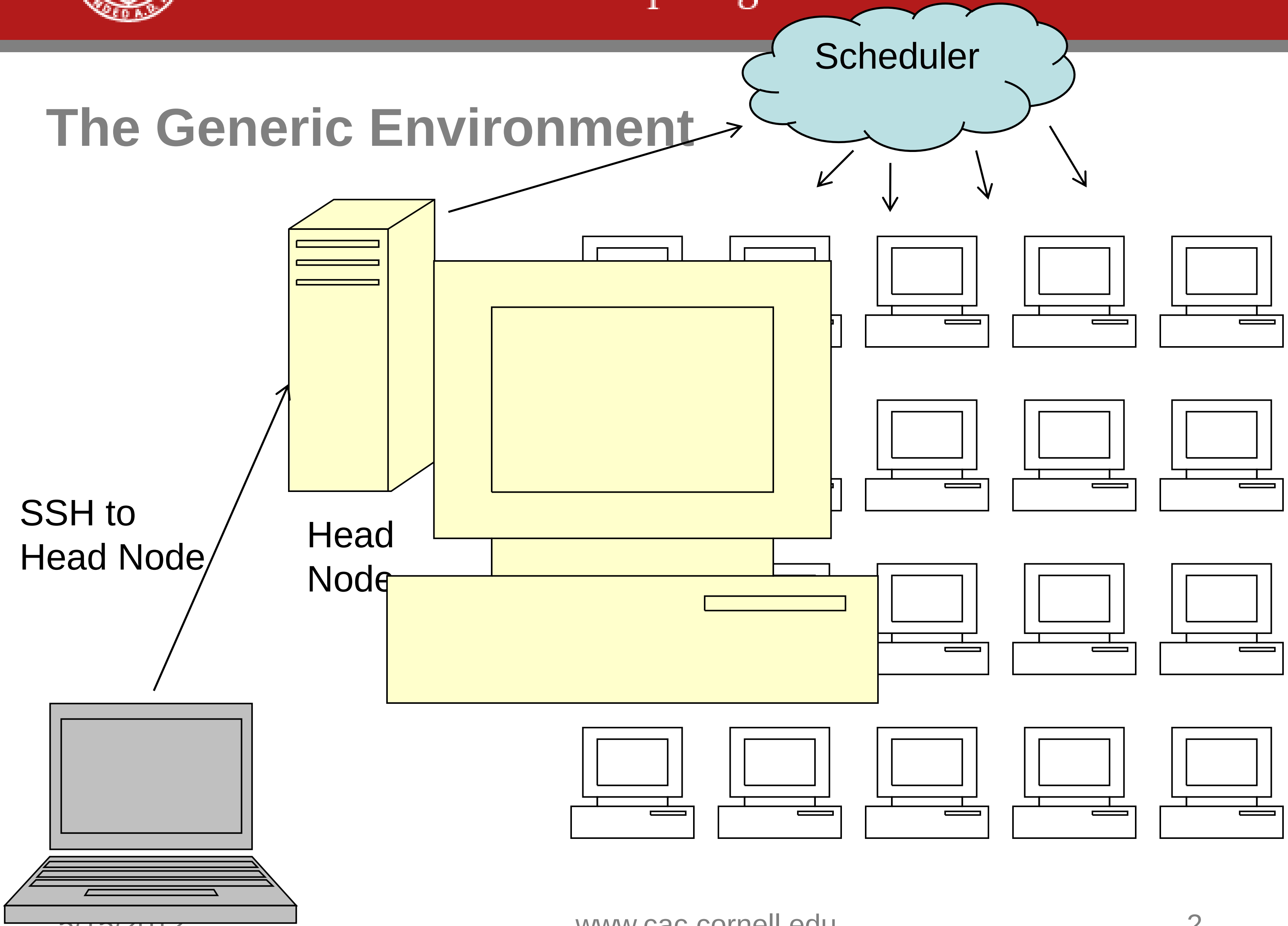
```
Bash: /etc/tacc/profile
       /etc/tacc/bashrc
      /etc/profile.d/<xxx>.sh
Tcsh: /etc/tacc/csh.cshrc
      /etc/tacc/csh.login
      /etc/profile.d/<xxx>.csh
```

User-customizable config script:

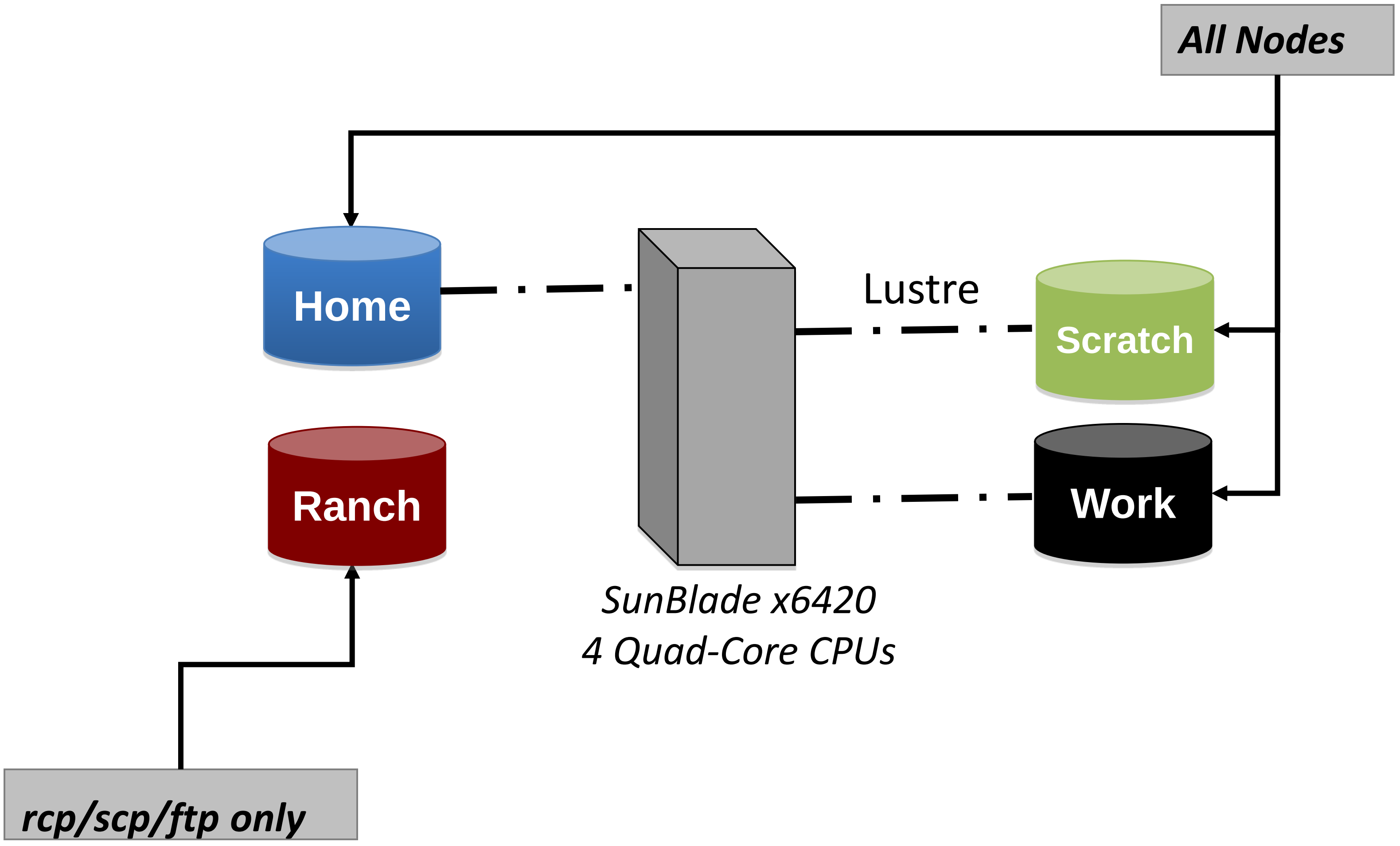
```
Bash: ~/.bashrc, ~/.profile
Tcsh: ~/.cshrc,  ~/.login
```

3. Ranger Overview

The Generic Environment



Available File Systems (Ranger)



File System on Ranger

Environmental Variable	User Access Limits	Lifetime
$HOME	6 GB quota	Project
$WORK	350 GB quota	Project
$SCRATCH	~400 TB	10 Days

```
%lfs quota -u <username> $HOME
%lfs quota –u <username> $WORK
%lfs quota –u <username> $SCRATCH
%cd      change directory to $HOME
%pwd
%cdw     change directory to $WORK
%pwd
%cds     change directory to $SCRATCH
%pwd
```

TACC HPC/DATA Systems

System	Ranger	Lonestar	Longhorn
Purpose	HPC	HPC	Data Analysis
Nodes	3,936	1,888	256
CPUS/node x cores/CPUS	4 x 4	2 x 6	2 x 4 + 2GPUs
Total cores	62,976	22,656	2,048
CPUS	AMD Barcelona 2.3GHz	Intel Westmere 3.3GHz	Intel Nehalem +NVIDIA 2.5 GHz +Quadro Plex S4s
Memory	2GB/core	2GB/core	6GB/core (240 nodes) 18GB/core (16 nodes)
Interconnect	SDR IB	QDR IB	QDR IB
Disk	1.7PB Lustre (IB)	1PB Lustre (IB)	0.2PB Lustre (10GigE)

Storage Systems

High Speed Disk-- Corral

- 1 PB Data Direct Disk
- 800TB Lustre File System
- 200TB Data Collections
- InfiniBand interconnect
- Access: as /corral file system on ranger, lonestar and longhorn; ssh/scp; requires allocation

DDN S2A 9900 Disk

Tape Storage -- Ranch

- 10PB capacity
- 70 TB cache
- 10Gb Ethernet interconnect
- Access: scp/bbcp to ranch.tacc.utexas.edu; or rsh/ssh

STK SL8500 Tape Lib

6. Software

Software

Software section in User Guide

Software list available on Ranger

Software list available on XSEDE

The ***module*** utility is used to provide a consistent, uniform method to access software.

MODULE Command (Ranger-only)

- Affects $PATH, $MANPATH, $LIBPATH
- Load specific versions of libraries/executables
- Works in your batch file
- Define environment variables:
  - TACC_MKL_LIB, TACC_MKL_INC, TACC_GOTOBLAS_LIB
- Order matters! First choose compiler, then application software.

Module

This utility is used to set up your PATH and other environment variables:

% module help	{lists options}
% module list	{lists loaded modules}
% module avail	{lists available modules}
% module load pgi	{add a module}
% module load intel	{try to load intel}
% module swap pgi intel	{swap two modules}
% module load boost	{add a module}
% module unload boost	{remove a module}
% module help <mod1>	{module-specific help}
% module spider	{lists all modules}
% module spider petsc	{list all version of petsc}

More Module Notes:

- Create your own initial default setup

```
% module purge; module load TACC
% module load git boost petsc
% module setdefault
```

- Family
  TACC supports two Families: Compilers and MPI implementations.
  You can only have one member of the family.
- Only one compiler, one MPI stack.
- Env. Var: TACC_FAMILY_COMPILER: intel, pgi, gcc
- Env. Var: TACC_FAMILY_MPI: mvapich, mvapich2, openmpi
- Can be used in Makefiles, and Scripts.

Two Time Commands

- Used to see how long your program runs and estimate if it’s having gross difficulties
- /usr/bin/time generally gives more information

```
login3% cd $HOME/envi/intro
login3% make
g++ hello.c -o hello
login3% time ./hello
Hello world!
0.000u 0.004s 0:00.01 0.0%      0+0k 0+0io 0pf+0w

login3% /usr/bin/time ./hello
Hello world!
0.00user 0.00system 0:00.00elapsed 133%CPU (0avgtext+0avgdata
3120maxresident)k
0inputs+0outputs (0major+238minor)pagefaults 0swaps
```

7. Editing Files

vi (short for “visual”)

- “vi filename” will open it or create it if it doesn’t exist.
- Command mode: keystrokes are commands
- Input mode: keystrokes are text you are adding to the file
- Last line mode: start with : end with <return>
- Examples:

– i	Insert characters before current position (use ESC to exit)
– dd	Delete current line
– R	Overwrite existing text (until ESC)
– u	Undo last operation
– :wq	Writes a file to disk and exit editor
– :q!	Quit without saving

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 (search with regular expressions, etc..)

emacs

- emacs is actually a lisp interpreter with extensions to use it as a text editor

- Can perform the same operations as in vi

- Uses series of multiple keystroke combinations to execute commands

- “Hard to learn, easy to use”

Use Your Computer’s Editor

Copying the file to your computer might be quicker than learning a new editor. Use a simple file transfer client:

Start menu
All Programs
Class Files
SSH Secure Shell
Secure File Transfer Client ← Right click, “Pin to Start Menu”

Start Secure File Transfer Client

Use Quick Connect, specify hostname ranger.tacc.utexas.edu

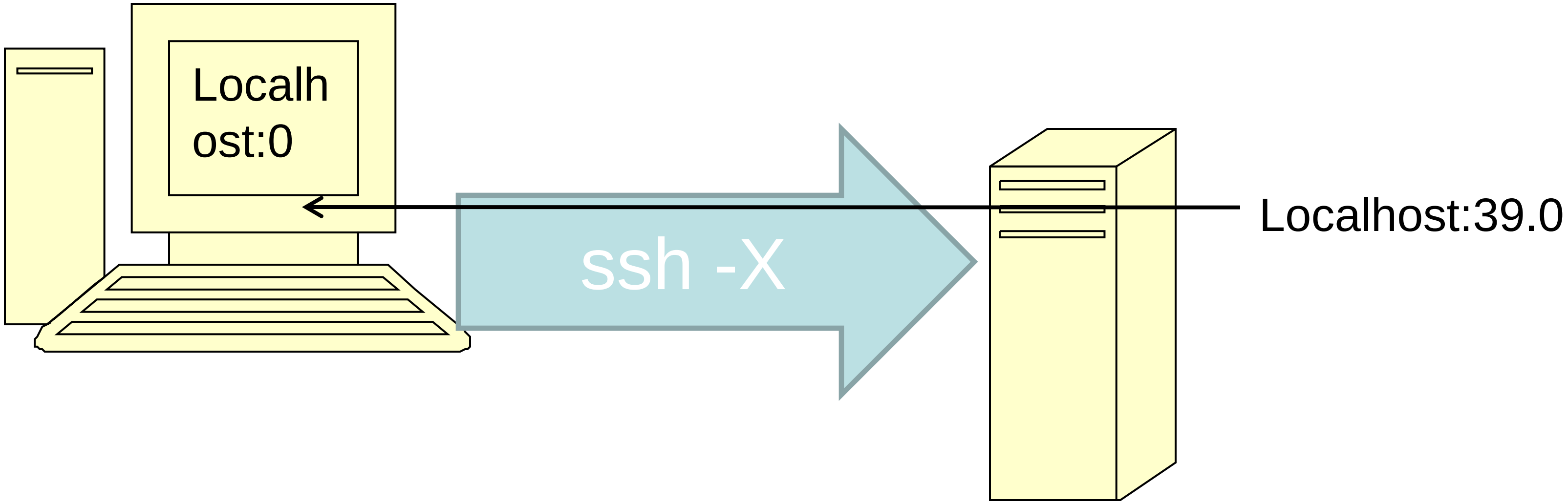
In the left pane, navigate to the desktop.

Drag files between panes to copy.

Again with X-Windows

- Start X-Windows server on local machine.

```
>echo $DISPLAY localhost:39.0
>emacs README&
```



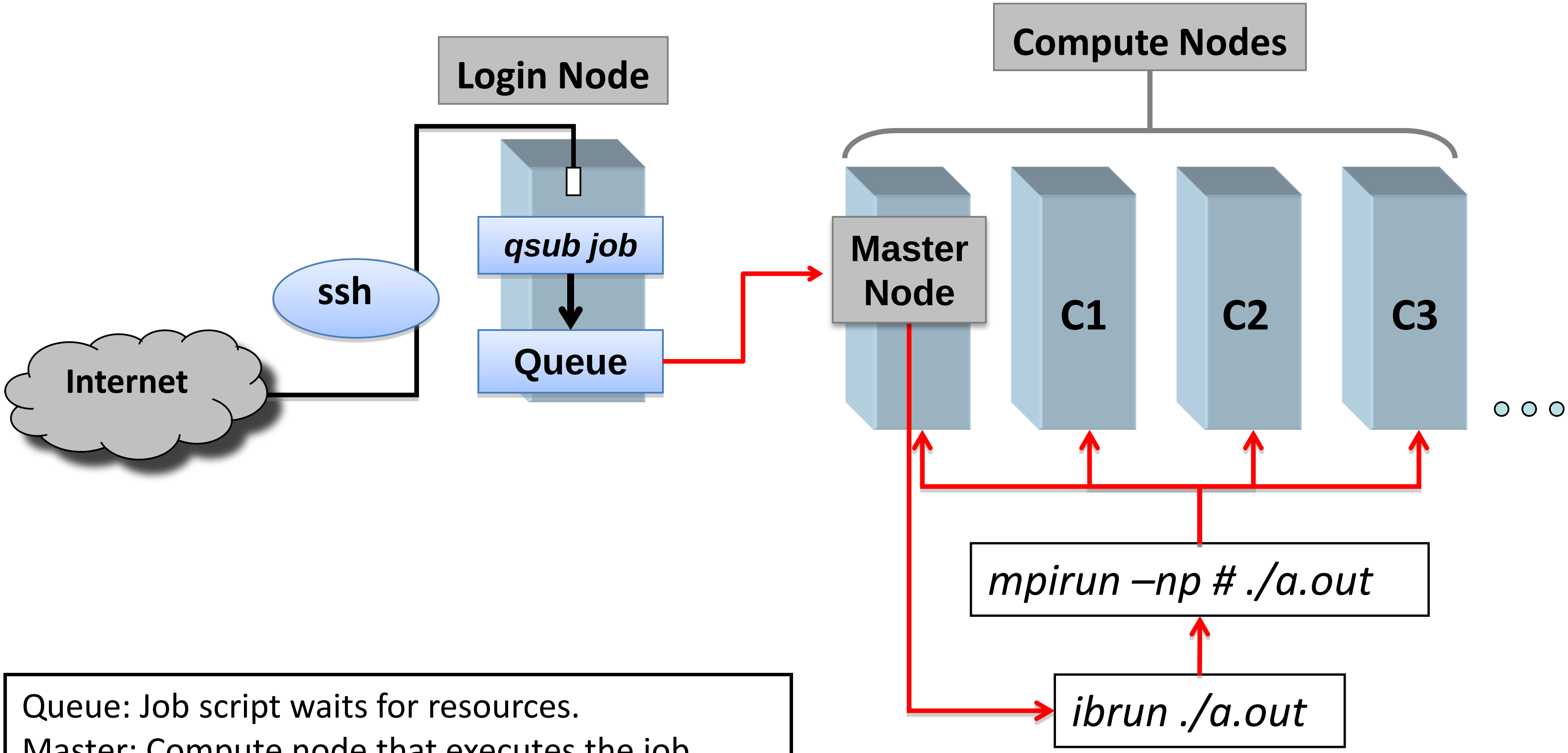
```
>jobs
>kill %1
```

Login with X-Windows

- Start Exceed->Exceed on Windows Startup menu (Already started on Mac and Linux)
- ssh –X on Linux, Mac. For Windows, select in Putty Connection->SSH->X11, and check “X11 Forwarding”
- Type in username and password.
- echo $DISPLAY
- emacs README&   # This runs emacs in the background.
- At the command prompt, type “jobs” to see that you have a job running in the background.
- Try Emacs for a while, then kill it with
- kill %1

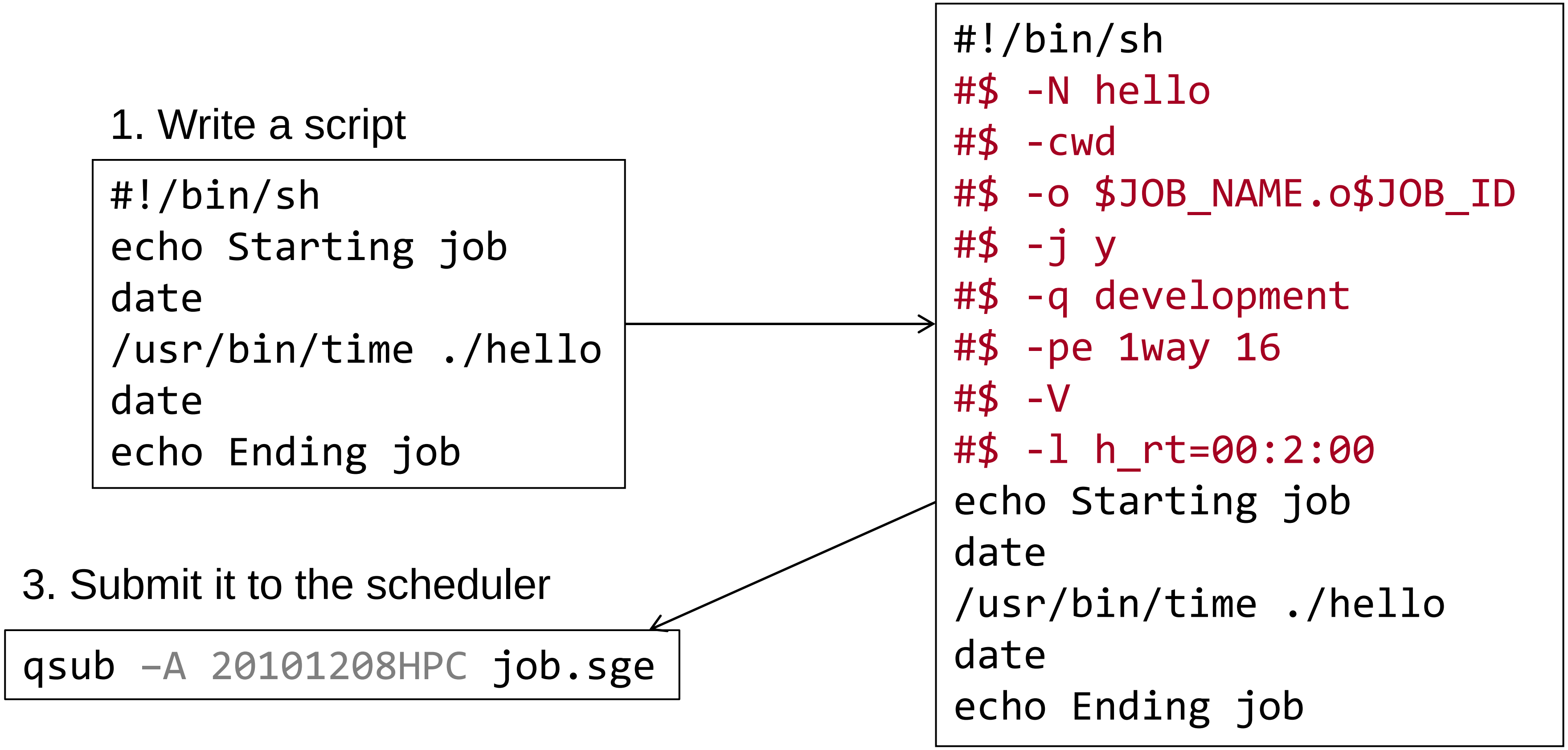
8. Batch Job Submission with Sun Grid Engine (SGE)

Batch Submission Process



Queue: Job script waits for resources.
Master: Compute node that executes the job script, launches all MPI processes.

Submit a Job



2. Add batch instructions

```
#!/bin/sh
#$ -N hello
#$ -cwd
#$ -o $JOB_NAME.o$JOB_ID
#$ -j y
#$ -q development
#$ -pe 1way 16
#$ -V
#$ -l h_rt=00:2:00
echo Starting job
date
/usr/bin/time ./hello
date
echo Ending job
```

1. Write a script

```
#!/bin/sh
echo Starting job
date
/usr/bin/time ./hello
date
echo Ending job
```

3. Submit it to the scheduler

```
qsub –A 20101208HPC job.sge
```

Queue Examples

```
login3% qconf -sql
clean
development
large
long
normal
request
reservation
Serial
stci
sysdebug
systest
vis
```

Slots = number of cores, 16 per node
pe = wayness, how many cores per node
Job is killed if over time limit.

```
login3% qconf -sq development
qname                     development
qtype                     BATCH INTERACTIVE
pe_list                   16way 15way 14way 12way 8way 4way 2way 1way
slots                     16
tmpdir                    /tmp
…
```

Why 15way?

Submit a Job Example

```
cd $HOME/envi/intro
ls -la
cat Makefile                    # Review the makefile
make                            # Compile hello.c
ls –la                          # Take a look at what compiled
./hello                         # Run compiled program
less job.sge                    # View the script (q)
qsub –A TG-TRA120006 job.sge            # Submit the job
showq –u                        # Look at your job(s)
```

States

- Unscheduled – Likely not good
- DepWait – You can ask that one job run after another finishes.
- w(aiting) – Queued, waiting for resources to run.
- r(unning) – As far as SGE is concerned, it’s going.
- h(old)
- s(uspended)
- E(rror)
- d(eletion)

SGE: Basic MPI Job Script

#!/bin/bash	Shell
#$ -pe 16way 32	Wayness and total core number
#$ -N hello	Job name
#$ -o $JOB_ID.out	stdout file name (%J = jobID)
#$ -e $JOB_ID.err	stderr file name
#$ -q normal	Submission queue
#$ -A A-ccsc	Your Project Name
#$ -l h_rt=00:15:00	Max Run Time (15 minutes)
ibrun ./hello	Execution command

Parallel Environment

- Each node has 16 cores and is used by one person at a time

- #$ -pe 1way 16 Run one task on a node with 16 cores
- #$ -q serial
- ./hello

- #$ -pe 8way 64 Run 8 tasks/node on 4 nodes
- #$ -q normal
- export MY_NSLOTS=31 Launch 31 tasks
- Ibrun ./a.out Run with mpi wrapper

SGE: Memory Limits

- Default parallel job submission allocates all 16 compute cores per node.
- If you need more memory per MPI task, you can request fewer cores per node by using one of the ‘Nway’ environments below.
- Even if you only launch 1 task/node, you will still be charged for all 16!

Parallel environment	Description
16way	16 tasks/node, 1.9GB/task
8way	8 tasks/node, 3.8GB/task
4way	4 tasks/node, 7.6GB/task
2way	2 tasks/node, 15.2 GB/task
1way	1 task/node, 30.4 GB/task

SGE Batch

```
% cd $HOME/envi/batch
% ls -la
% mpif90 –O3  mpihello.f90 –o mpihello
            OR
% mpicc  –O3  mpihello.c –o mpihello
% cat job                    (edit account?)
% qsub job
% watch showq -u -l          (Ctrl-C to quit watching)
% vi job                     (add “sleep 60”)
% qsub job                   (observe the returned jobid)
% qdel jobid
```

10. Miscellaneous

Precision

The precision program computes prints *sin(π)*. The *π* constant uses “E” (double precision) format in one case and “D” (single) in the other.

```
% cd $HOME/envi/precision
% cat precision.f
% module load intel
% ifort –FR precision.f
 (or)
% ifort precision.f90
% ./a.out
```

(The ifc compiler regards “.f” files as F77 fixed format programs. The –FR option specifies that the file is free format.)

Makefiles

% cd $HOME/envi/using_makefiles	
% cat Makefile	Read over the Makefile
% make	Compile the program, generate a.out
% make	Reports “up to date”, i.e. not recompiled
% touch suba.f	Simulate changing a file
% make	suba.f (and only suba.f) is recompiled

Questions?

- CAC
  help@cac.cornell.edu
- XSEDE
  - portal.xsede.org -> Help
  - portal.xsede.org -> My XSEDE -> Tickets
  - portal.xsede.org -> Documentation -> Knowledge Base