

A Brief Introduction to The Center for Advanced Computing

February 8, 2007

Hardware

- 376 Opteron nodes, over 890 cores
- Gigabit networking, Myrinet networking, Infiniband networking soon

Hardware: nyx

- nyx is the Opteron cluster; `nyx-login.engin.umich.edu` is the login host for this cluster
- Currently has 6TB NFS file system
- Running RedHat Enterprise Linux 4

Software

- openmpi – MPI libraries
- mcnp5 – Monte Carlo N-Particle Transport
- matlab – matrix math application
- fftw – Fast Fourier Transform Library (parallel and serial)
- fluent – fluid dynamics application
- gaussian – electro-chemical analysis application
- java – Sun's Java Language
- mathematica – symbolic math application
- nag – Numerical Algorithm Group's Fortran Compilers
- pgi – Portland Group Compilers
- R – matrix math application
- simpson – solid-state NMR simulation software
- and more...

Current List of Software

To get a current list of software on the cluster you are using, type `module avail`, you'll see something like:

```
----- /home/software/rhel4/Modules/3.2.1/modulefiles -----
R/2.2.1-gcc      gaussian/03-64bit  mcnp5/1.4          null              radmind/1.5.1
dot             hdf5/1.6.5-gcc    module-info        openmpi/1.0.1-gcc simpson/1.1.1-gcc
fftw/2.1.5-gcc  hdf5/1.6.5-pgi    modules            openmpi/1.0.2-gcc simpson/1.1.1-pgi
fftw/2.1.5-pgi  java/1.5.0_06     nag/7              openmpi/1.0.2-pgi torque
fluent/6.2      mathematica/5.2    netcdf/3.6.1-gcc  pdsh              use.own
gaussian/03-32bit matlab/7.1         netcdf/3.6.1-pgi  pgi/6.1(default)
```

- To select a software package, type:
`module load package/version`.
- To see what you have loaded, type: `module list`
- For help with the module command type: `module help`

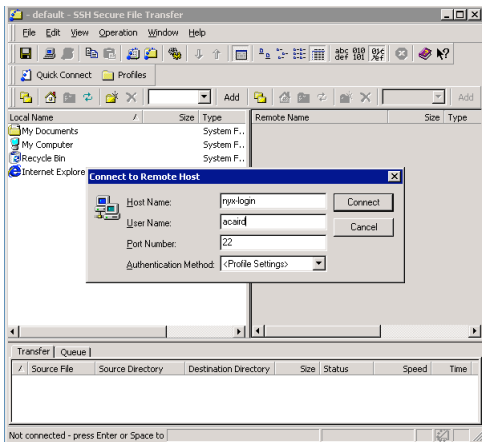
We load some basic utilities by default, so when you first log in you will see the Torque/PBS commands and the PGI compilers in your list of loaded modules.

Transferring Files

- Files are transferred to the file space on the clusters using either Secure Copy (`scp`) or Secure FTP (`sftp`).
- Your password for file transfers and logins is your UM Kerberos (Level-1) password and your login is your Uniqname.

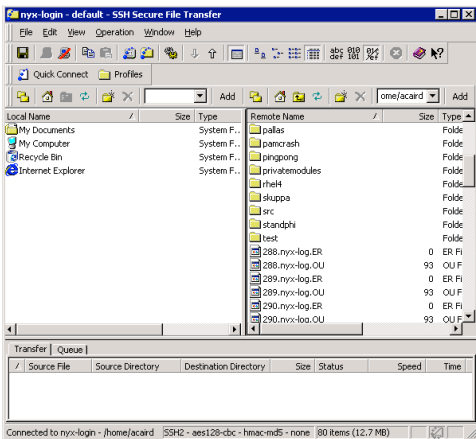
File Transfers: Windows

- SSH Secure Communications' Secure File Transfer
- click “Quick Connect”:



File Transfers: Windows

- agree to add key to local database (only happens once), click “OK” on “SSH Authentication Response”
- You will see:



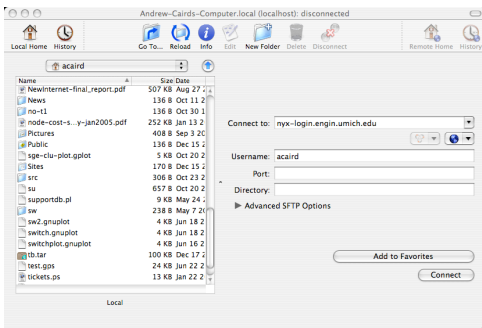
- You can drag and drop files back and forth

File Transfers: Windows

- There are other programs for Windows besides SSH's SCP program, any modern SCP/SFTP program will work
- SSH Secure Communications: <http://www.ssh.com>
- WinSCP: <http://winscp.net/eng/index.php>
- Putty: <http://www.chiark.greenend.org.uk/~sgtatham/putty/>
- Cygwin: <http://www.cygwin.com/>
- lots of others, see Google

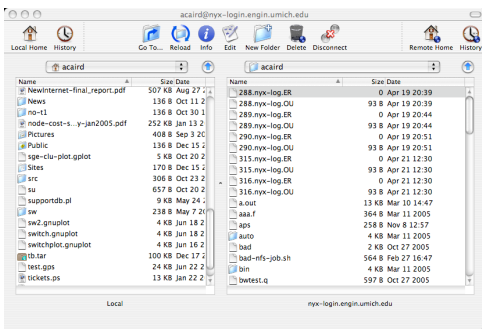
File Transfers: Mac

- UM/RSG's Fugu
- Fill the in information as shown:



File Transfers: Mac

- Enter password when prompted
- You will see:



- You can drag and drop files back and forth

File Transfers: Mac

- There are other programs besides Fugu
- Fugu: <http://rsug.itd.umich.edu/software/fugu/>
- Built-in scp/sftp from Terminal
- Rbrowser: <http://www.rbrowser.com/>
- Fetch: <http://fetchsoftworks.com/>
- lots of others, see Google

File Transfers: Linux

- Using scp:

```
% scp -r src nyx-login:
Password:
[...]
MP_memcpy.c          100% |*****| 6784      00:00
armci.c              100% |*****| 7590      00:00
gm.c                 100% |*****| 6432      00:00
gpshmem.c            100% |*****| 2611      00:00
ib.c                 100% |*****| 31924     00:00
[...]
```

- Using sftp:

```
% sftp nyx-login
Connecting to nyx-login...
Password:
sftp>
```

- This works from the Mac Terminal, too.

Logging in

- Your login is your Uniquename
- Your password is your ITD/ITCS Kerberos password (Level 1 password)
- Use `ssh` to connect to the clusters
- All access is command line — there is no graphical access to the clusters; any graphical pre- or post-processing should be done on your own computer
- For tutorials on using Linux, see:

- Introduction to Linux

<http://www.engin.umich.edu/caen/technotes/introunix/>

- Advanced Linux

<http://www.engin.umich.edu/caen/technotes/advancedunix/>

- Linux Commands

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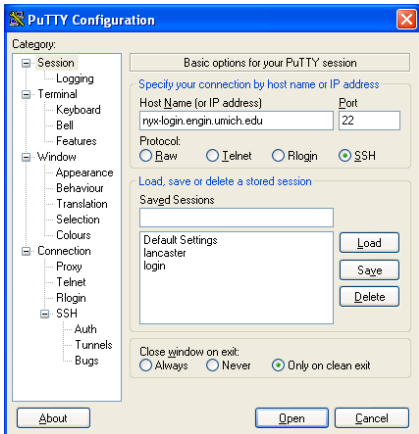
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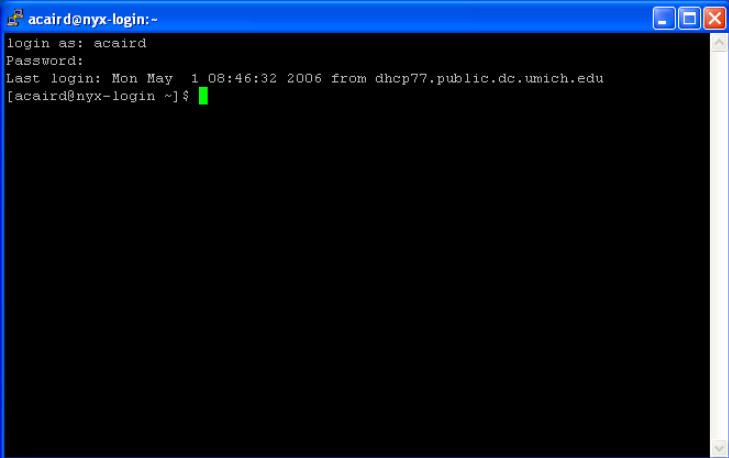
Logging in: Windows

- Putty is a freely available SSH client for windows
http:
[//www.chiark.greenend.org.uk/~sgtatham/putty/](http://www.chiark.greenend.org.uk/~sgtatham/putty/)
- To log in, enter the host as shown:



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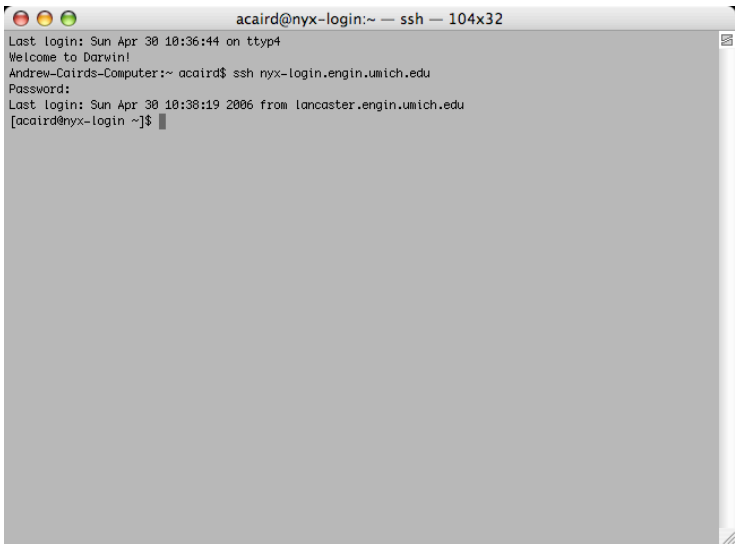
- Then enter your Uniqname and password and you'll get the shell prompt:

A terminal window titled 'acaird@nyx-login:~' with standard window controls (minimize, maximize, close) in the top right. The terminal text shows a successful login for user 'acaird'.

```
acaird@nyx-login:~  
login as: acaird  
Password:  
Last login: Mon May  1 08:46:32 2006 from dhcp77.public.dc.umich.edu  
[acaird@nyx-login ~]$ █
```

Logging in: Mac

- Use the included SSH client from the Terminal program:



The image shows a terminal window titled "acaired@nyx-login:~ — ssh — 104x32". The terminal output is as follows:

```
Last login: Sun Apr 30 10:36:44 on ttyp4
Welcome to Darwin!
Andrew-Cairds-Computer:~ acaired$ ssh nyx-login.engin.umich.edu
Password:
Last login: Sun Apr 30 10:38:19 2006 from lancaster.engin.umich.edu
[acaired@nyx-login ~]$
```

The terminal window includes standard macOS window controls (red, yellow, green buttons) and a scrollbar on the right side. At the bottom of the slide, there are navigation icons for a presentation slide, including arrows and symbols for back, forward, and search.

Logging in: Linux

- Use the included SSH client from and shell:

Tools

- All of the standard GNU/Linux tools are also available: make, autoconf, awk, sed, Perl, Python,
- We support emacs, vi{m}, and nano (a pico-like editor) on the clusters. etc.
- Only use notepad on Windows!
- If made on windows fix with dos2unix filename

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Introduction to the PBS Batch System

- All access to the compute nodes (everything other than the login node) is via the batch system
- We use a system called Torque, it is derived from PBS
- The batch system controls access to queues
- The scheduling system decides if and where jobs can run
- There are two general queues: `long` and `short`
- There are many private queues for people who own or rent nodes
- If you don't know use the `route` queue

Introduction to the PBS Batch System

The steps to using the batch system are:

- 1 Create a batch file: this is a short (5-15 lines) text file with some batch commands and the commands to run your program
- 2 Submit the file to the batch system
- 3 Check on the status of your job
- 4 Delete your job if you want to cancel it

Creating a PBS Batch File

A simple single cpu example

```
#!/bin/sh
#PBS -N 1-cpu
#PBS -l nodes=1,walltime=1:00:00
#PBS -m abe
#PBS -M brockp@umich.edu
#PBS -q route
#PBS -joe
#PBS -V
cd ~/input1dir/
mcnp5.mpi i=input o=output r=restart
```

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Creating a PBS Batch File

A more complicated example:

```
#!/bin/sh
#PBS -N mcnp-8x2
#PBS -l nodes=8:ppn=2,walltime=8:00:00
#PBS -q route
#PBS -M brockp@umich.edu
#PBS -m ae
#PBS -j oe
#PBS -V
cd ${HOME}/input2/
echo "I ran on: "
cat $PBS_NODEFILE
mpirun -np 16 mcnp5.mpi i=input2 o=output2 r=restart2
```

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Submitting, Checking, and Deleting Batch Jobs

- After you create your PBS script, you need to submit it:

```
$ qsub mcnp.q  
542.nyx-login.engin.umich.edu
```

- After you submit your script, you can check on the status of your job:

```
$ qstat -au brockp  
nyx-login.engin.umich.edu:  
Job ID          Username Queue   Jobname   SessID NDS   TSK Memory Time   S Time  
-----  
542.nyx-login.engin. brockp  short   mcnp-8x2   18922    8  --   --   08:00 R 00:00  
  
$ checkjob 542  
[... lots of output ...]
```

- If you want to delete your job:

```
$ qdel 542
```

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```

```
$ checkjob 542  
[... lots of output ...]
```

- If you want to delete your job:

```
$ qdel 542
```

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```

```
$ checkjob 542
[... lots of output ...]
```

- If you want to delete your job:

```
$ qdel 542
```

PBS Email

PBS will send an email at the start and end of your job if you use the `-m` and `-M` options in your PBS script. The email after a job completes successfully looks like:

```
Date: Sun, 30 Apr 2006 12:50:17 -0400
From: adm <adm@nyx-login.engin.umich.edu>
To: "Palen, Brock E" <brockp@umich.edu>
Subject: PBS JOB 542.nyx-login.engin.umich.edu
-----
```

```
PBS Job Id: 542.nyx-login.engin.umich.edu
Job Name:   mcnp-8x2
Execution terminated
Exit_status=0
resources_used.cput=13:17:26
resources_used.mem=1220672kb
resources_used.vmem=11146704kb
resources_used.walltime=00:49:57
```

- Total Consumed CPU time: 47846 Sec.
- Total Real Time: 2997
- 16x Faster than 1 CPU
- BUT: Only 98%

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Understanding the Scheduler

The scheduler determines what jobs can run, when they can run, and where. There are many factors that go into the scheduler's decision.

- Limits

- Maximum number of jobs eligible for scheduling: 4
- Maximum number of CPUs in use by one person: depends on queue
- Maximum number of jobs in the queue at one time: no limit

- Priority

- Who you are: user and group level priorities
- How long you've waited: the longer you wait, the higher your priority
- Your recent usage (fairshare): People with less usage over the past month will have a higher priority than those with a lot of usage

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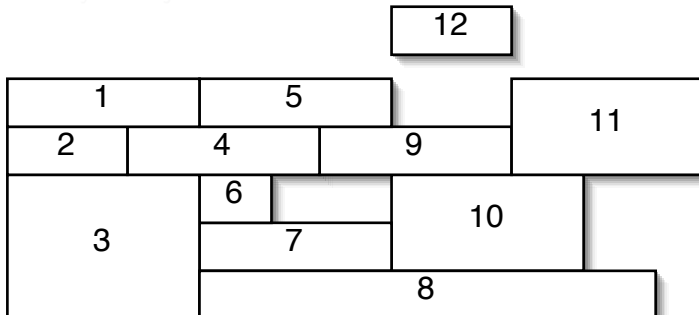
Understanding the Scheduler

- Reservations

- Advance reservations: holds nodes for users or groups
- Job reservations: scheduler will reserve nodes for the next several jobs in each queue

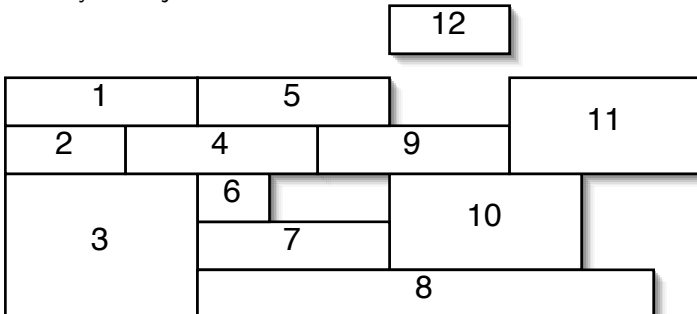
- Backfill

- If the reservations leave holes in the schedule, they may be filled by short jobs that otherwise would have waited.



Understanding the Scheduler

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 - Job reservations: scheduler will reserve nodes for the next several jobs in each queue
- Backfill
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Understanding the Scheduler

There are several commands that can give you insight into the scheduler's decisions.

- `showq` — shows the state of the queue at that moment in time, showing the running jobs in order of soonest to finish to longest to finish; the idle jobs in order of priority; and the blocked jobs in the order they were submitted
- `diagnose -p` — shows the factors that go into computing the priority for all of the idle jobs
- `checkjob jobnumber` — for idle jobs this will show why the job can't start
- `showstart jobnumber` — this makes a (poor) estimate of when the job will start

Summary

- Resources

- Lots of CPUs
- A reasonable amount of software
- Watch or subscribe to <http://cac.engin.umich.edu> for updates

- Access

- All access is via the SSH family of commands: `ssh`, `sftp`, `scp`
- There are lots of clients for these commands for the different platforms
- There is no graphical access, everything is via the command line

Summary

- Job Submission
 - Every job needs a PBS script file
 - Two most important commands: `qsub` and `qstat -au username`
- Job Scheduling
 - Scheduling depends on a lot of factors, it is best to submit jobs and let the scheduler optimize for their start.

Summary

- News: <http://cac.engin.umich.edu>
 - RSS feed
 - New of changes, outages, other pertinent piece of information
- Contact: cac-support@umich.edu
 - Questions or concerns should be sent here (not to an individual) since this is read by six people. The odds of a quick reply are best this way.
 - We aren't parallel programmers, but we'll do what we can to help.

Example

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Open a shell....

- 1 `cp -r ~brockp/mcnp_example /`
- 2 `cat mcnp.q`
- 3 `module load mcnp5`
- 4 `qsub mcnp.q`
- 5 `qstat -u $USER`

Example

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- 1 `cp -r ~/brockp/mcnp_example /`
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