Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary

A Brief Introduction to The Center for Advanced Computing

February 8, 2007

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Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Hardware				

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

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Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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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

Resources ○○●○	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
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...

Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Current L	ist 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 be default, so when you first log in you will see the Torque/PBS commands and the PGI compilers in your list of loaded modules.

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Transfer	ring 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.

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Trar	nsfers: Windows	5		

- SSH Secure Communications' Secure File Transfer
- click "Quick Connect":

🚈 - default - SSH	Secure File Transfe	21		_ 🗆 ×
Eile Edit View	Operation Window	/ Help		
	a 🖻 🙇 🍋 🍕	J 1 🖬	≗ 2- 111 m abc 010 def 101	왕 🖸 🤣 🕅
Quick Connect	Profiles			
🔁 🖄 📾 🕫	🗳 🗙 📘	▼ Add [≧ @ @ ⊄ ₫>	Add
Local Name	7		Remote Name	Size Type
My Documents		System F.		
My Computer		System F		
Recycle Bin		System F		
CInternet Explore	Connect to Remote	Host		X
	Host Name:	nyx-login	Conn	ect
	User Name:	acaird	Can	
	_	22		
	Port Number:	144		
	Authenticatio	n Method: < Profile S	Settings>	
•		•	•	•
Transfer Queue				
✓ Source File	Source Directory	Destination Direct	tory Size Status	Speed Time
<u> </u>				
Not connected - press	Enter or Space to			

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Tran	sfers: Windows			

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

🚰 nyx-login - default - SSH	Secure File Tra	ansfer			- 🗆 ×
<u>Eile Edit View Operatio</u>	n <u>W</u> indow <u>H</u> e	lp .			
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	/ Size	Туре	Remote Name /	Size	Type 🔺
My Documents		System F	🔜 palas		Folde
Section 2017 My Computer		System F	pamcrash 📃		Folde
🔞 Recycle Bin		System F	pingpong		Folde
🔁 Internet Explorer		System F.,	privatemodules		Folde
			rhel4		Folde
			🚞 skuppa		Folde
			src .		Folde
			🔜 standphi		Folde
			test		Folde
			288.nyx-log.ER	0	ER Fi
			🔄 288.nyx-log.OU	93	OU F
			289.nyx-log.ER	0	ER Fi
			🔄 289.nyx-log.OU	93	OUF
			290.nyx-log.ER	0	ER Fi
4	1	E F	290.nvx-loa.OU	93	OUF
					<u> </u>
Transfer Queue					
/ Source File Source D	irectory De	stination Dire	tory Size Status	Speed	Time
<u> </u>					
Connected to nyx-login - /home;	lacaird SSH2 - a	es128-cbc - H	mac-md5 - none 80 items (12.7 f	4B) 🤣] /

• You can drag and drop files back and forth

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Trans	fers: 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

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Tran	nsfers: Mac			

• UM/RSG's Fugu

• Fill the in information as shown:

ocal Home History	Go To Reload Info	Edit New Folder Delete Disconnect Remote Home His
👚 acaird	: 1	
Name A	Size Date	
P NewInternet-final_report.pdf	507 KB Aug 27 2 🛓	
📁 News	136 B Oct 11 2	
🗊 no-tl	136 B Oct 30 1	
node-cost-sy-jan2005.pdf	252 KB Jan 13 2	Connect to: nyx-login.engin.umich.edu
Pictures	408 B Sep 3 20	() T
Public	136 B Dec 15 2	
sge-clu-plot.gplot	5 KB Oct 20 2	Username: acaird
Sites	170 B Dec 15 2	
🗊 src	306 B Oct 23 2	Port:
🖹 su	657 B Oct 20 2	Directory:
supportdb.pl	9 KB May 24 2	a state state a st
🗊 sw	238 B May 7 20	Advanced SFTP Options
sw2.gnuplot	4 KB Jun 18 2	
switch.gnuplot	4 KB Jun 18 2	
switchplot.gnuplot	4 KB Jun 16 2	
mtb.tar	100 KB Dec 17 2	Add to Favorites
test.gps	24 KB Jun 22 2	
tickets.ps	13 KB Jan 22 2 💡	Connect
Local		

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Trar	nsfers: Mac			

- Enter password when prompted
- You will see:

Cal Home History	Go To Reload	() Info	Edit	New Folder	Delete	Disconnect		Remote Home	Histor
👚 acaird	:	٢		🗊 acaird				•	٢
Name	Size Date		Nam	e			Size Date		
NewInternet-final_report.pdf	507 KB Aug 2		32	88.nyx-log	ER		0 Apr	19 20:39	
🗊 News	136 B Oct 1		m 2	88.nyx-log	.ou		93 B Apr	19 20:39	n
🗊 no-tl	136 B Oct 3	01	m 2	89.nyx-log	ER		0 Apr	19 20:44	
node-cost-sy-jan2005.pdf	252 KB Jan 1	3 2	m 2	89.nyx-log	.ou		93 B Apr	19 20:44	
Pictures	408 B Sep 3	20	m z	90.nvx-log	ER		0 Apr	19 20:51	0
Public	136 B Dec 1	5.2	The second	90.nvx-log	ou		93 B Apr	19 20:51	
sge-clu-plot.gplot	5 KB Oct 2	0 2	193	15.nyx-log	ER		0 Apr	21 12:30	
Sites	170 B Dec 1	5.2		15.nyx-log			93 B Apr		
src 🗊	306 B Oct 2	3 2		16.nyx-log				21 12:30	
🖹 su	657 B Oct 2	0 2		16.nyx-log			93 B Apr		
supportdb.pl	9 KB May 2	24.2		out			13 KB Mar	10 14:47	
🗊 sw	238 B May 1	20	Da	aa.f			364 B Mar	11 2005	
sw2.gnuplot	4 KB Jun 1	8 2	- Da	05			258 B Nov	8 12:57	
switch.gnuplot	4 KB Jun 1	8 2		uto			4 KB Mar	11 2005	
switchplot.gnuplot	4 KB Jun 1	6 2		ad			2 KB Oct		
mtb.tar	100 KB Dec 1	72		ad-nfs-iob.	ch		564 B Feb		
test.gps	24 KB Jun 2	2 2 U					4 KB Mar		
tickets.ps	13 KB Jan 2	2 2 7		wtest.q			597 8 Oct		Ť
Local						nyx-login.engi	n.umich.edu		

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• You can drag and drop files back and forth

Resources 0000	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary 0000
File Tra	nsfers: 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

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
File Tra	nsfers: Linux			

• Using scp:

```
% scp -r src nyx-login:
Password:
[...]
MP_memcpy.c
       6784
                             00.00
armci.c
       7590
                             00.00
       6432
                             00:00
gm.c
       gpshmem.c
                         2611
                             00.00
ib.c
       00:00
[...]
```

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• Using sftp:

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

• This works from the Mac Terminal, too.

Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Logging ir	1			

- Your login is your Uniquname
- 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

http://www.engin.umich.edu/caen/technotes/unixcommands/

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Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Logging in	1			

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Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Logging i	Logging in: Windows			

• Putty is a freely available SSH client for windows http:

//www.chiark.greenend.org.uk/~sgtatham/putty/

• To log in, enter the host as shown:

🔀 PuTTY Configuration 🛛 🛛 🛛					
Category:					
Session Logging	Basic options for your PuTTY sess				
⊟ Terminal Keyboard	Host Name (or IP address)	Port 22			
Bell Features Window	Protocol:	• SSH			
 Appearance Behaviour Transition Selection Colours Connection Proxy Telnet Riogin SSH Auth Tunnels Bugs 	Load, save or delete a stored session Saved Sessions				
	Default Settings lancaster login (Load Save Delete			
	Close window on exit: Always Never ⓒ Dnly on clea	an exit			
About	<u>O</u> pen	Cancel			

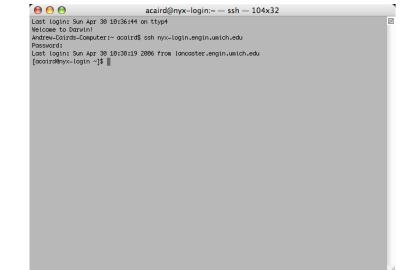
Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Logging i	n: Windows			

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



Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Logging i	n: Mac			

• Use the included SSH client from the Terminal program:



Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
Logging in	n: Linux			

• Use the included SSH client from and shell:



Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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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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Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Introduc	tion to the PBS	S Batch Svsten	า	

- 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

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Introduction to the PRS Batch System						
		000000				
Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary		

The steps to using the batch system are:

 Create a batch file: this is a short (5-15 lines) text file with some batch commands and the commands to run your program

- Submit the file to the batch system
- One Check on the status of your job
- Oelete your job if you want to cancel it

Resources 0000	Mechanics: Access 000000000000	Mechanics: Usage	The Scheduler	Summary 0000
Creating a	a PBS Batch	File		

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```
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
```

Resources 0000	Mechanics: Access	Mechanics: Usage	The Scheduler 000	Summary 0000
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Creating a PBS Batch File				

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Resources 0000	Mechanics: Access	Mechanics: Usage ○00●000	The Scheduler	Summary 0000
Creating a	PBS Batch Fi	le		

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Resources 0000	Mechanics: Access	Mechanics: Usage ○00●000	The Scheduler	Summary 0000
Creating a	PBS Batch Fi	le		

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Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Creating a	PBS Batch Fi	le		

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```

Resources 0000	Mechanics: Access	Mechanics: Usage ○000●00	The Scheduler 000	Summary 0000		
Creating a PBS Batch File						
A mor #!/bi	e complicated exam	iple:				

#PBS -N mcnp-8x2

#PBS -1 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=restar

Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Creating a	PBS Batch Fi	le		

A more complicated example:

#!/bin/sh

#PBS -N mcnp-8x2

#PBS -1 nodes=8:ppn=2,walltime=8:00:00

#PBS -q route #PBS -M brockp@umich e

#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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Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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Creating a	PBS Batch Fil	le		

A more complicated example:

- #!/bin/sh
- **#PBS** -N mcnp-8x2
- #PBS -1 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

Resources 0000	Mechanics: Access	Mechanics: Usage ○000●00	The Scheduler	Summary 0000
Creating a	a PBS Batch	File		

#!/bin/sh

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#PBS −V

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mpirun -np 16 mcnp5.mpi i=input2 o=output2 r=restart2

Resources 0000	Mechanics: Access	Mechanics: Usage ○○○○●○○	The Scheduler	Summary 0000
Creating a	a PBS Batch	File		

- #!/bin/sh
- **#PBS** -N mcnp-8x2
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- **#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

Resources 0000	Mechanics: Access	Mechanics: Usage ○000●00	The Scheduler	Summary 0000
Creating a	a PBS Batch	File		

#!/bin/sh **#PBS** -N mcnp-8x2 #PBS -1 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

Resources 0000	Mechanics: Access	Mechanics: Usage ○000●00	The Scheduler	Summary 0000
Creating a	a PBS Batch	File		

#!/bin/sh **#PBS** -N mcnp-8x2 #PBS -1 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



• 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:

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

• If you want to delete your job:

\$ qdel 542

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• 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 TD Username Queue Jobname SessID NDS TSK Memory Time S Time ----- -542.nvx-login.engin. brockp short mcnp-8x2 18922 8 ----- 08:00 R 00:00 \$ checkjob 542 [... lots of output ...]

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If you want to delete your job:

\$ qdel 542



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	aail			

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

спап

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

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Understar	nding the Sche	duler		

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

- Limits
 - Maximum number 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

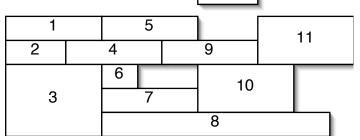
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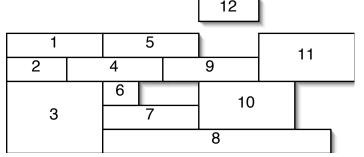
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- Reservations
 - Advance reservations: holds nodes for users or groups
 - Job reservations: scheduler will reserve nodes for the next several jobs in each queue
- Backfill
 - If the reservations leave holes in the schedule, they may be filled by short jobs that otherwise would have waited.



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Understa	nding the Sche	eduler		

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

Resources	Mechanics: Access	Mechanics: Usage	The Scheduler	Summary
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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

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary ○●○○
Summarv				

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

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary 0000
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.

Resources 0000	Mechanics: Access	Mechanics: Usage 0000000	The Scheduler	Summary ○○○●
Example				

Example

- o cp -r ~brockp/mcnp_example /
- 2 cat mcnp.q
- In module load mcnp5
- 🕘 qsub mcnp.q
- 🗿 qstat -u \$USER

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