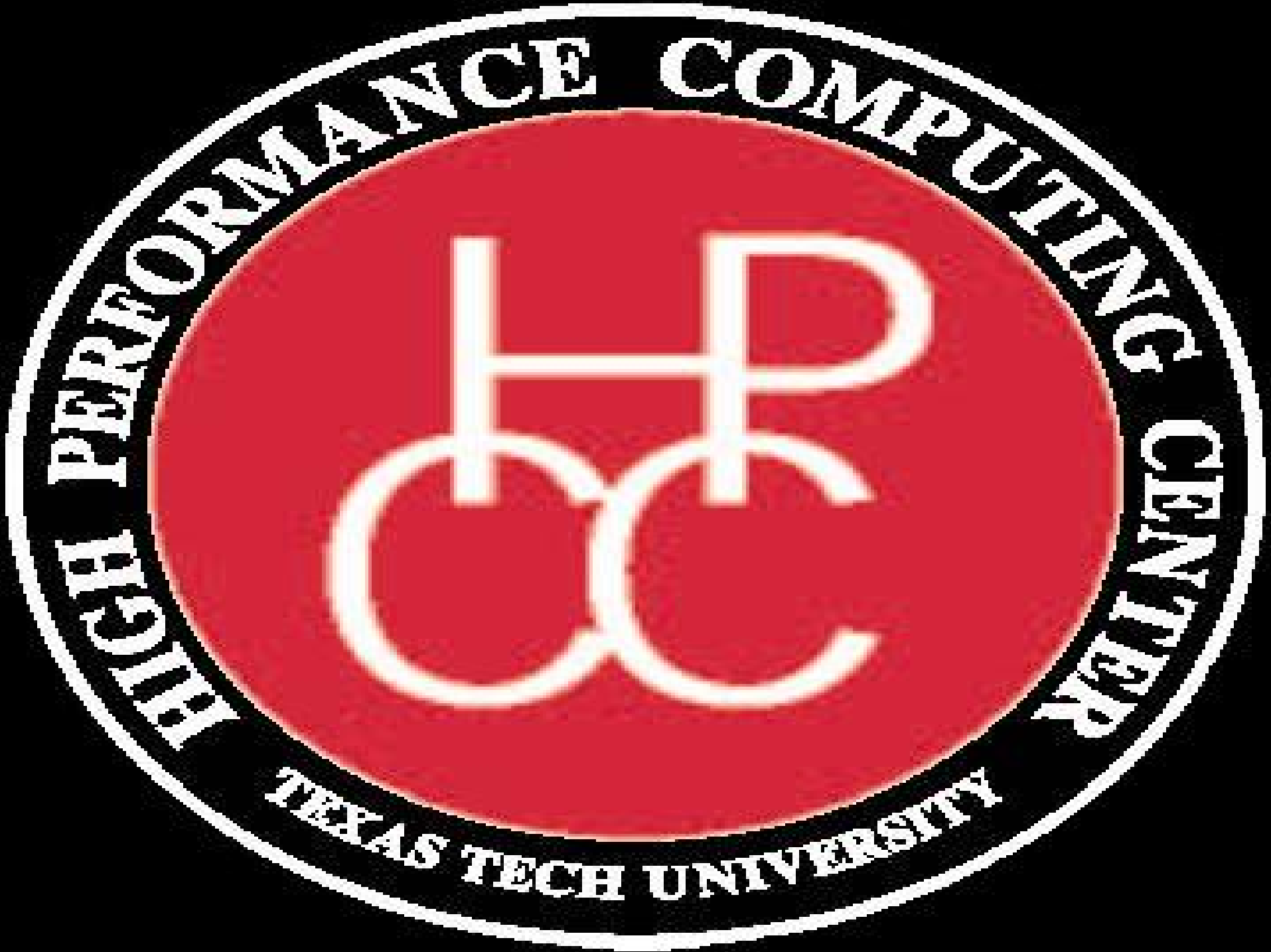

HIGH PERFORMANCE COMPUTING CENTER
TEXAS TECH UNIVERSITY

Resources at the HPCC

Pleione - Reese Center.

Pleione - 56-300 MHz processor SGI Origin 2000 with: 56 GB main memory/8 MB cache per processor, two-pipe Onyx-2 IR2 graphics system, 720 GB Fibrechannel disk storage, and 180 GB SCSI disk storage.

Resources at the HPCC

- Antaeus – Reese Center
- Poseidon – North CS Building
- Weland - South Computing Center

- Linux clusters
- Uses PBS
- Very fast machines

Overview

- Which environment do I use?
- SSH
  - Setenv
  - Xhost
  - nedit&
  - PSCP (Windows) / SCP (Lunix)
  - Standard Unix commands
  - Compiling and running uniprocessor jobs

Overview (cont.)

- Linking to the IMSL library
- Compiler Optimizations
- Queue Submission

Which environment do I use?

Windows?

- **Using ssh/putty under Windows**
  To connect to Pleione, Antaeus, or Mathwulf using putty from a Windows PC, download putty.exe, which may make a shortcut on your desktop. To start putty.exe, click on the shortcut if you have one, or open a command window and type in putty. If the PC says "'PUTTY' is not recognized ..", make sure that the executable putty.exe is located in a directory that is in the system path, or start it from the directory containing the executable. A gray window should open. We will give sample connection instructions for pleione.hpcc.ttu.edu; Substitute antaeus.hpcc.ttu.edu or mathwulf.tosm.ttu.edu as required.
  We recommend the free programs putty/ p s c p / p s ftp for windows, open ssh for UNIX Linux/Mac OS X, and Nifty Telnet SSH for Mac OS 9. A good Windows commercial version is F-Secure SSH at http://www.f-secure.com/products/ssh.

- Unix/Linux?
  Bring up a terminal window and then type in ssh . (Next Slide)

SSH

This is the program you will use to log onto the network. This is used in lieu of telnet.

SSH, Secure Shell, is a program for logging into a remote machine and executing commands in a remote machine. It is intended to replace rlogin and rsh, and provide secure encrypted communications between two untrusted hosts over an insecure network. X11 connections and arbitrary TCP/IP.

How to SSH

At UNIX prompt, type ‘ssh name of server’

To log on to Pleione:

%ssh pleione.hpcc.ttu.edu
Login: <username>
Password: <your password>

SSH Cont.

To log on to Pleione:

```
%ssh  pleione.hpcc.ttu.edu
Login: <username>
Password: <your password>
```

SSH Cont.

To log on to Antaeus:

```
%ssh antaeus.hpcc.ttu.edu
Login: <username>
Password: <your password>
```

Setenv

For UNIX/LINUX or LINUX Emulators only:

setenv - change or add an environment variable

Why do we use setenv?

(ans.) In order to use certain graphical applications, i.e. the nedit& editor, to reroute graphical output to your terminal.

Ex:

% setenv DISPLAY yourmachine.ttu.edu:0.0

Note: Setenv would not be used on the Beowulf Clusters.

xhost

xhost - server access control program for X

Ex: xhost [[+-] machinename.ttu.edu]

% xhost + ehm77.ttu.edu

nedit&

Nedit& is a standard UNIX GUI (Graphical User Interface) style text editor for programs and plain-text files. It provides mouse based editing and a streamlined editing style.

To use nedit :

%nedit& <file name>

PSCP (Windows) / SCP (Lunix)

(Secure Copy) is used in copying files over the network securely. It uses ssh2 for data transfer, and uses the same authentication and provides the same security as ssh2. Unlike rcp, scp2 will ask for passwords or pass phrases if they are needed for authentication.

Ex for SCP:

% scp <filename> username@pleione.hpcc.ttu.edu:.

PSCP example

1. Go to Start Button, Run, type <cmd>, then DOS prompt will appear.
2. Type:

C:\ PSCP <filename> username@pleione.hpcc.ttu.edu:.

3. When prompted, type in your password.

Standard Unix commands

1. cat: Lists the contents of a file.
2. cd: change directory
3. chmod: change the permissions mode of a file or directory.
4. cp: copy files and directories.
5. find: search for files in a directory hierarchy.
6. ls: list directory contents.

Standard Unix commands

7. man: format and display the on-line manual pages.
8. mkdir: make directories.
9. mv: move (rename) files.
10. pwd prints the name of the current directory
11. rm: remove files or directories.
12. rmdir: remove empty directories.

vi editor

vi - a programmers text editor

You would use this to edit your programs on the Beowulf clusters or even on Pleione (if you do not want to use nedit&).

Ex:

%vi program.c

Basic vi commands

1. To begin editing, type “a or i”
2. To delete one character, hit esc then type “x”
3. To delete a line, hit esc then type “dd”
4. If the arrow keys do not work, to move in the environment, hit esc then use ‘h’ for left, ‘j’ for down, ‘k’ for up, and ‘l’ for right.

Basic vi commands (cont)

5. To save your work, hit esc, colon ‘:’ then hit ‘w’ <return>.
6. To save your work and quit, hit esc, colon ‘:’ then hit ‘wq’ <return>.
7. To quit without saving your work, hit esc, colon ‘:’ then hit ‘q’ <return>.

For more info see the man pages on Pleione

Ex: %man vi

or invest in ‘Introduction to UNIX’ at the ATLC for $2.50.

Compiling and running uniprocessor jobs (Beowulf)

C

- Compile
  $ cc filename.c
- Run
  $ ./a.out

Fortran

- Compile
  $ g77 filename.f
  or
  $ lf95 filename.f
- Run
  $ ./a.out

Compiling and running uniprocessor jobs (Pleione)

C

- Compile
  %cc filename.c
- Run
  % ./a.out

Fortran

- Compile
  % f90 filename.f
- Run
  % ./a.out

Examples

For example code with scripts showing how to run and compile, you may utilize the following directory :

- On Pleione

/scratch/MA5345/

Compiler Optimizations

-O[n] Specifies the basic level of optimization desired. n can be one of the following:

0 Turns off all optimizations. This is the default.

1 Turns on local optimizations that can be done quickly.

Compiler Optimizations

2 Turns on extensive optimization. The optimizations at this level are generally conservative, in the sense that they are virtually always beneficial, provide improvements commensurate to the compile time spent to achieve them, and avoid changes which affect such things as floating point accuracy.

Compiler Optimizations

3 Turns on aggressive optimization. The optimizations at this level are distinguished from -O2 by their aggressiveness, generally seeking highest-quality generated code even if it requires extensive compile time. They may include optimizations that are generally beneficial but may hurt performance.

-Ofast [= ipxx]

Selects optimizations that maximize performance for the given SGI target platform, ipxx.

The Queue

- The Beowulf clusters use PBS:

PBS stands for Portable Batch System. It is a networked subsystem for submitting, monitoring, and controlling a work load of batch jobs on one or more systems.

- Pleione (SGI) uses LSF:

LSF stands for Load Sharing Facility. It is used to submit, monitor, and control a work load of batch jobs on one or more nodes.

Queue Submission on Beowulf

qsub - To create a job is to submit an executable script to a batch server. The batch server will be the default server unless the -q option is specified. See discussion of PBS_DEFAULT under Environment Variables below. Typically, the script is a shell script which will be executed by a command shell such as sh or csh.

Queue Submission on Beowulf

```
#!/bin/ sh
#PBS -N testpar
#PBS -r n
#PBS -e testpar.err
#PBS -o testpar.log
#PBS -m ae
#PBS -q long
#PBS -l nodes=4
NPROCSP=4
SSH_NO_PASSWD=1
#
cd $PBS_O_WORKDIR
#PBS_NODEFILE= machinefile
NPROCS=`wc -l < ${PBS_NODEFILE}`
if [ `expr ${NPROCS}` -ge `expr ${NPROCSP}` ];
then
NPROCS=${NPROCSP}
fi
echo "This job has available $NPROCS nodes:"
cat $PBS_NODEFILE
#./mains
$PBS_O_WORKDIR/mpirun -v -machinefile $PBS_NODEFILE -np $NPROCS time ./a.out
```

Queue Submission on Beowulf

If you copy the previous script into a file called batchsub, the following command would then submit the job to the queue :

```
# qsub batchsub
```

Other Queue Commands

- qdel – deletes a submission from the queue

  Example :
  # qdel job_identifier
- qstat – shows status of submitted jobs

  Example :
  # qstat

Queue Submission on Pleione

Submit a job for batched execution on host(s) that satisfy the resource requirements of the job and can provide a fast turnaround time. If the load of all the candidate hosts is too high, or some specific conditions configured in LSF are not satisfied, the job will be executed later when system resources become available and the conditions are satisfied. This allows the system to restrict the number of jobs that are executed simultaneously so as to keep system overhead low, and to adjust the number of started jobs based on the current system load. Jobs are started and suspended according to the current system load.

Queue Submission on Pleione

- #BSUB –q short -n 4
- cpuset -q batch -A mpirun -miser 4 ./a.out > output

Queue Submission on Pleione

If you copy the previous script into a file called batchsub, the following command would then submit the job to the queue :

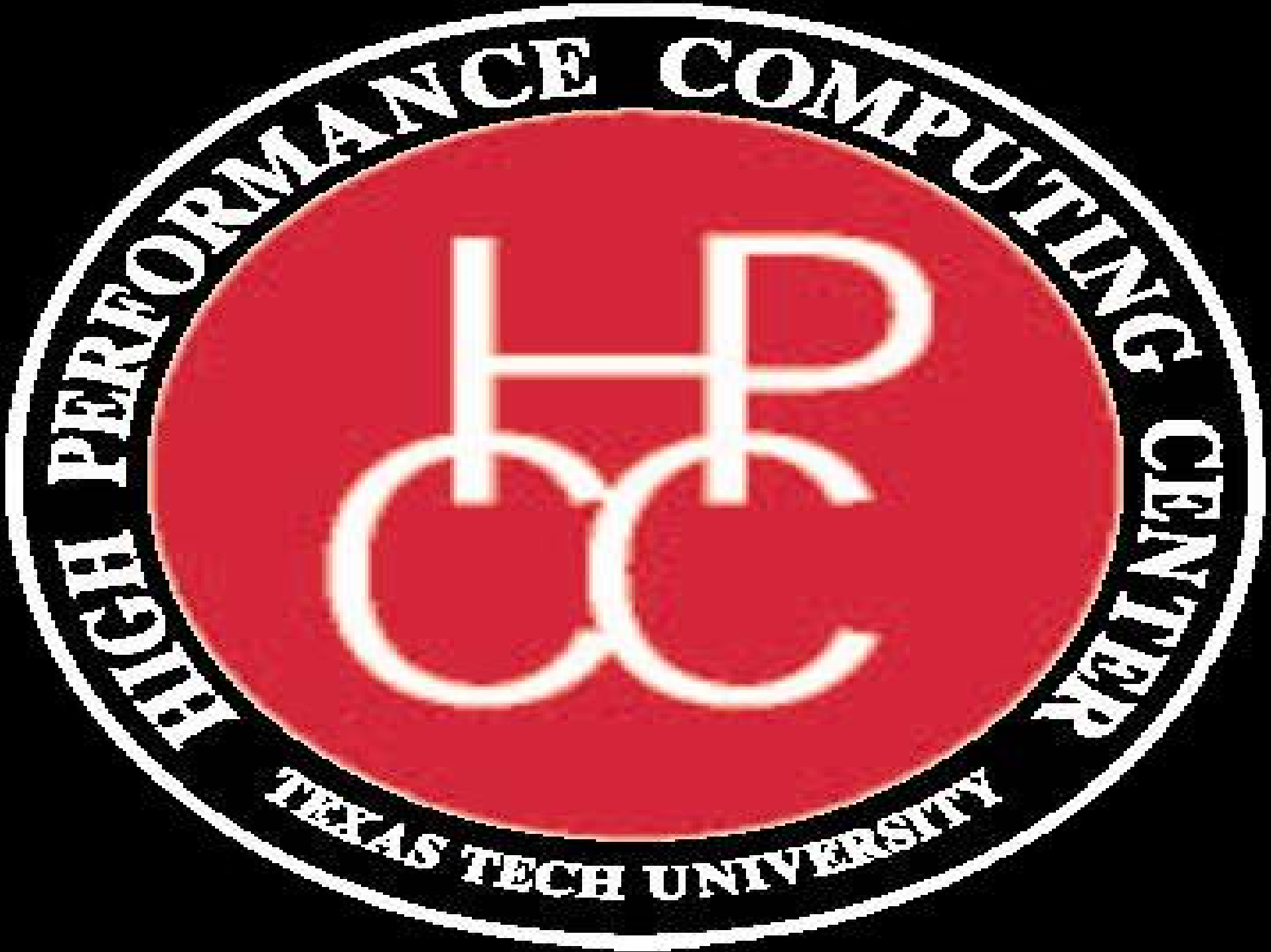
```
% bsub < batchsub
```

Other Queue Commands

- bkill – deletes a submission from the queue

  Example :
  # bkill job_identifier
- bjobs – shows status of submitted jobs

  Example :
  # bjobs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