



TEXAS TECH UNIVERSITY™



HPCC New User Training

Getting Started

High Performance Computing Center

10/12/2011

OUTLINE



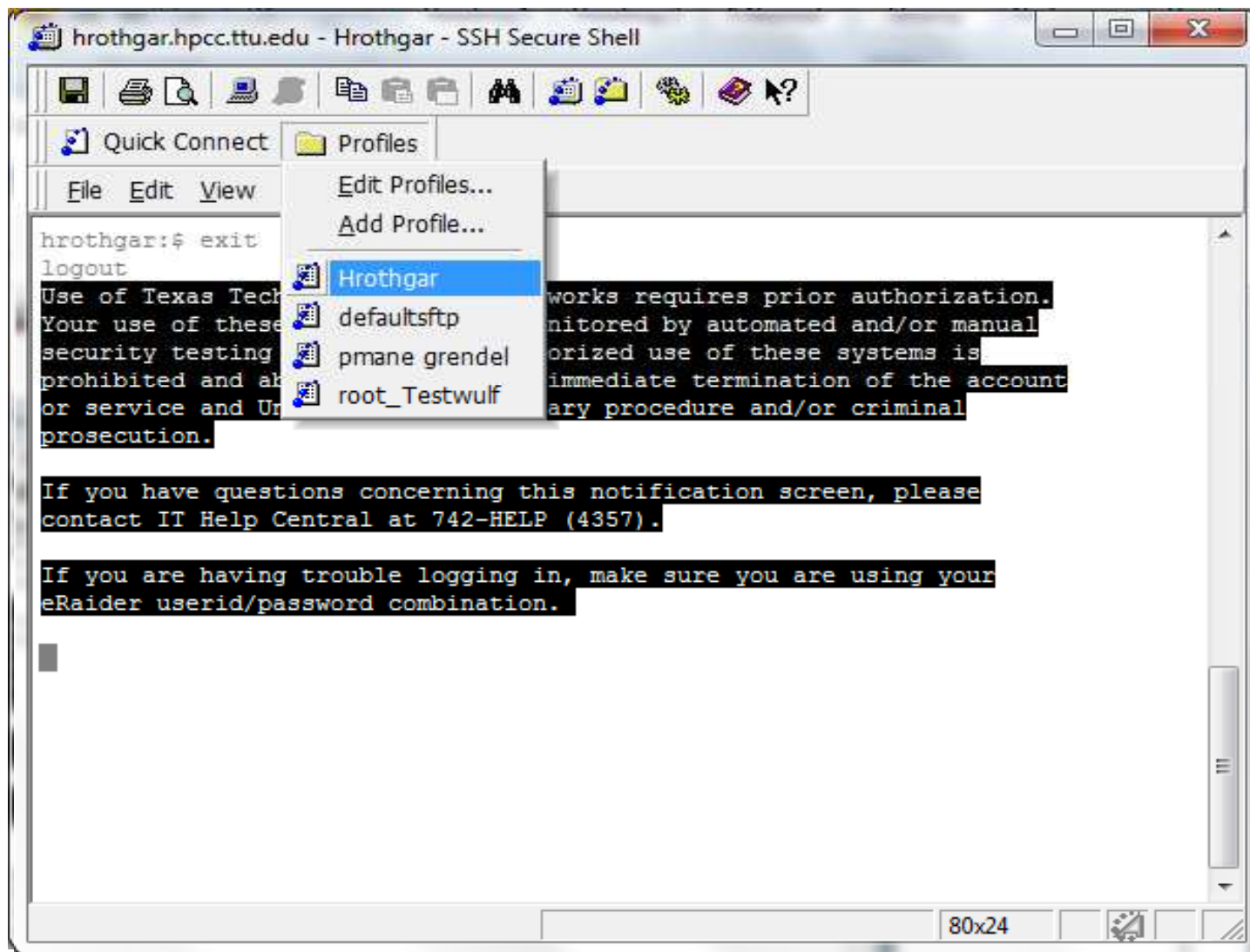
- Getting started
- Resources
- Linux commands
- Setting up environment
- Moving data
- File systems and quota
- X windows
- Using editors
- Compile, submit job and examine output
- Questions and contacts

Getting Started



- Request account:
<http://www.hpcc.ttu.edu/php/AccountRequest.php>
- E-raider authentication
- Log in to Hrothgar
 - *From Linux/Mac platform: `ssh <eraider>@hrothgar.hpcc.ttu.edu`*
 - *From Windows platform*
 - SSH Client: <http://charlotte.at.northwestern.edu/bef/SSHdist.html>
 - Putty : <http://www.chiark.greenend.org.uk/~sgtatham/putty/>
 - *User Guide: [Connect/Remote Login](#)*

Getting Started: using SSH Client



Resources



Hrothgar Cluster

- 7680 Cores for parallel job (12 Cores/Node, 640 Nodes)
- Intel(R) Xeon(R) @ 2.8 GHz
- 24 GB of memory per node
- DDR Infiniband for MPI communication & storage
- 644 TB of parallel Lustre file system (1.2 Petabytes in total)
- 86.2 Tflop peak performance.
- 1024 cores for serial job (8 Cores/Node, 128 nodes)
- Top 500 list: 147 in the world, 12 in Academic institutions in USA (June 2011)
- 432 cores (46 nodes) and 72 TB storage for community cluster

JANUS Windows Cluster

- 176 Cores. 22 nodes (8 Cores/Node)
- 16 GB of memory per node
- Visual Studio with Intel fortran
- 20 TB Storage

Linux Commands



ls (directory)	list your files	ls src
ls -a (file/dir)	hidden files	ls -a
ls -l (file/dir)	list size/detail	ls -l mpi.c
mkdir (dir)	create a directory	mkdir src
cd (directory)	change to directory	cd src;cd ../bin
cd (blank)	to your home dir	cd
rm (file)	delete a file	rm a.out
rm -r (dir)	delete a directory	rm -r src
vi (file)	terminal text editor	vi mpi.c
nedit (file)	Xwin text editor	nedit mpi.f
mv (file/dir)	move/rename	mv src src1
man command	display help info	man ls

Setting up Environment



- Softenv: set up environment variables (eg: PATH, LD_LIBRARY_PATH)

- *Important files: .soft, .bashrc, .profile*

Note: these files were set up at the time that user account was created. If they are messed up or damaged, use the following steps to restore.

```
cp /lustre/work/apps/examples/dot-soft .soft
cp /lustre/work/apps/examples/dot-bashrc .bashrc
ln -is .bashrc .profile
```

- *Check the content of .soft file: **more .soft***

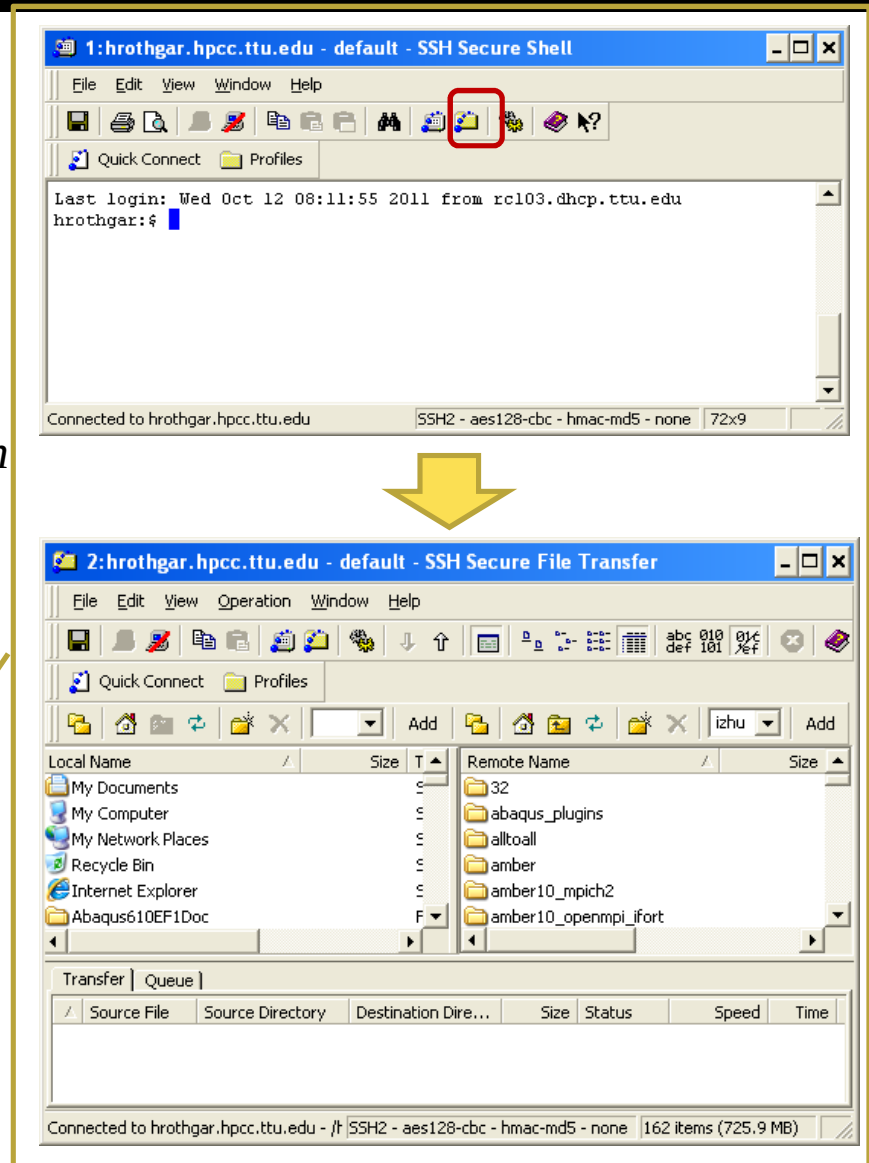
```
+sge
+intel
+openmpi
+gromacs
@default
```

- *Add the application variables you want to use:*
 - find the softenv entry for the application: *soft-list.sh*
 - Add the application: *echo +matlab >> .soft*
 - Activate: *resoft*

Moving Data



- Linux platform:
 - *Scp*
 - Local to remote: `scp filename eraider@hrothgar.hpcc.ttu.edu`
 - Remote to local: `scp eraider@hrothgar.hpcc.ttu.edu: <path to file> .`
 - *Sftp*
 - eg: `sftp eraider@hrothgar.hpcc.ttu.edu`
`put filename`
`get filename`
- Windows platform
 - *SSH Client*
 - *Winscp*
- User guide: [How to transfer data](#)



File Systems and Quota



- \$HOME (/home/eraider)
 - *150 GB per user*
 - *Back-up*
- \$WORK (/lustre/work/eraider)
 - *700GB per user*
 - *No back-up*
- \$SCRATCH (/lustre/scratch/eraider)
 - *560 TB shared, no quota limitation*
 - *Purged periodically*

Out of quota:
Account locked!

X Windows



- Linux/Mac platform

- `ssh -y <eraider>@hrothgar.hpcc.ttu.edu`
- `xterm`

- Windows platform

- *Install X-win32 (Contact hpccsupport@ttu.edu for the installation file and serial number)*
- *Start X-win32 locally (Start -> X-Win32 5.3 -> X-Win32)*
- *Log in to Hrothgar*
 - `cp /lustre/work/apps/examples/SetDisplay.sh .` (first time)
 - `. SetDisplay.sh` (every time)
- *Test*
 - `echo $DISPLAY` (W.X.Y.Z:0.0)
 - `nedit`

- [X-win32 user guide](#)

Using Editors



- GUI editors: refer to X-window usage
 - *nedit* (*nedit newfile.txt, nedit oldfile.txt*)
 - *gedit* (*gedit newfile.txt, gedit oldfile.txt*)
 - *emacs*
- Terminal editors
 - *vi* (*vi filename.exe*)
 - *emacs -nw*
- User guide : [Using Editors](#)



■ Hello World example (serial)

- *Source code*
cp /lustre/work/apps/examples/serial/hello.c .
- *Compile*
icc hello.c (Intel compiler)
gcc hello.c (GNU compiler)
- *Default executable: a.out*
- *Give the executable a meaningful name*
icc -o hello hello.c

```
#include<stdio.h>
#include<math.h>
void main()
{
    printf("Hello world");
}
```

Compiling -- parallel



■ Hello World example (parallel)

- *Source code*
cp /lustre/work/apps/examples/mpi/helloworld.c .
- *Compile*
mpicc -o hello helloworld.c (OpenMPI compiler)

```
#include <stdio.h>
#include <mpi.h>

int main (argc, argv)
    int argc;
    char *argv[];
{
    int rank, size;

    MPI_Init (&argc, &argv);    /* starts MPI */
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);    /* get current process id */
    MPI_Comm_size (MPI_COMM_WORLD, &size);    /* get number of processes */
    printf( "Hello world from process %d of %d\n", rank, size );
    MPI_Finalize();
    return 0;
}
```



■ Scheduler: SGE

- *Public queues (available to all users)*
 - normal: 48 hours, for parallel jobs
 - serial: 120 hours, for serial jobs
 - matlab: 120 hours, two simultaneous jobs per user, for Matlab jobs only
- *Community cluster queues (access restricted)*
 - ancellcc
 - greencc
 - hasecc
 - kangcc

Submit jobs



- Serial example
 - *cp /lustre/work/apps/examples/serial/SimpleScript.sh .*
 - *qsub SimpleScript.sh*

```
#!/bin/bash
#$ -V
#$ -cwd
#$ -S /bin/bash
#$ -N serial-job
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q serial
#$ -P hrothgar

./a.out
```

Submit jobs



■ Parallel example

- *cp /lustre/work/apps/examples/mpi/mpi.sh .*
- *qsub mpi.sh*

```
#!/bin/bash
#$ -V
#$ -cwd
#$ -S /bin/bash
#$ -N mpi
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q normal
#$ -pe fill 12
#$ -P hrothgar

cmd="$MCMD -np $NSLOTS -$MFIL
$SGE_CWD_PATH/machinefile.$JOB_ID $SGE_CWD_PATH/a.out"
echo cmd=$cmd
$cmd
```

Monitor jobs



- Check job status
 - Command: *qstatus*
 - *job-ID, prior, name, user, state, submit/start at, queue*
 - “r”: running
 - “qw”: waiting in the queue
 - “E”: error
- Job output
 - Standard: *\$JOB_NAME.o\$JOB_ID*
 - Error: *\$JOB_NAME.e\$JOB_ID*
- User guide: *Submit and Check status of jobs*

Contact info



- <http://www.hpcc.ttu.edu>
- <http://www.hpcc.ttu.edu/php/NewUser.php>
- hpccsupport@ttu.edu
- ESB-141

Questions?

