

**File Transfer**

Few small files, use scp or sftp

Larger files & better use of bandwidth use bbcp or GridFTP protocol

For GridFTP Clients,

*globus-url-copy <source\_url> <destination\_url>*

URL definitions;

*gsiftp://<hostname>/<full path>*

Kraken's URL is *gridftp.kraken.nics.xsede.org*

**Job Scheduling**

For each user, only 5 jobs are eligible to be scheduled.

Larger size jobs have higher priority and smaller size jobs do run effectively as backfill. The queue type is assigned based on core size. Jobs larger than 49,537 are placed in the Capability queue- this queue is only enabled after weekly Preventive Maintenance (PM). Please contact us if you would to run Capability.



Kraken Cray XT5

112,896 compute cores

Node configuration

Two 2.6 GHz six-core AMD Opterons

16 GB memory

Access

Via One Time Passcode (OTP), ssh

*kraken.nics.tennessee.edu*

Via GSISSH

*kraken-gsi.nics.tennessee.edu*

**Job submission**

PBS script that can be submitted to the queue via *qsub*

```
#!/bin/bash
#PBS -S /bin/bash
#PBS -A my_allocation
#PBS -l size=192,walltime=01:35:00
cd /lustre/scratch/$USER
aprun -n $PBS_NNODES ./a.out
```

The aprun command can have the following options

- n Total number of MPI processes (default: 1)
- N Number of MPI processes per node (1 to 12)
- S Number of MPI processes per socket (1 to 6)
- d Specifies number of cores per MPI process (for use with OpenMP, 1 to 12)

Compute nodes only see Lustre space, make sure all needed data exists there  
Module commands can be placed in a PBS script.

**File Systems**

NFS Home space (quota enforced).

\$HOME points to /nics/[a-d]/home/\$USER

Lustre scratch (no quota, 30 day purge policy).

\$CUE\_SCRATCH points to /lustre/scratch/\$USER

To find out what files could be purged,

*lfs find \$CUE\_SCRATCH -atime +30 | xargs ls -l --time=atime --sort=time*

HPSS storage (OTP access only).

*hsi*

Will start an interactive session.

*hsi {put | get} local\_file : hpss\_file*

Where *local\_file* is the location and name of the local file and *hpss\_file* is the location and name of the file on HPSS. Order of arguments do not change.

*htar*

Combines tar and hsi commands.

*htar -cvf temp.tar .*

This will tar the current directory (into temp.tar) and place it in your HPSS space.

**Modules**

*module avail*

Lists all available installed packages/software.

*module list*

Lists all currently loaded modules in your environment.

*module avail {package}*

This will list all currently installed versions of the specified package. Notice (default), if you want a different version, you will have to *module load {package/version#}*.

*module load {package/version}*

This will load package.

*module unload {package}*

Removes package from environment.

*module swap {A} {B}*

Swaps loaded {A} package with {B} package.

*module show {package}*

This shows the modified paths of the compiler/software, in case you would like to see libraries or the executables.

**Compiling**

*module avail PrgEnv*

Lists all installed compilers.

To compile a program that runs on the compute nodes, use the powerful Cray compiler wrappers. These wrappers automatically gather information from the currently loaded modules and programming environment, to simplify the linking process.

	Cray wrapper	GNU	Intel	PGI
C	cc	gcc	icc	pgcc
C++	CC	g++	icpc	pgCC
Fortran	ftn	gfortran	ifort	pgf90 pgf77