EMSL: Molecular Science Computing
Quick Reference Guide

WEB: http://www.emsl.pnl.gov/capabilities/computing/

External users log on to Chinook
$ ssh <UserID>@chinook.emsl.pnl.gov
First: enter PASSCODE from secureID
Second: enter Kerberos password

Internal users log on to Chinook
$ ssh <UserID>@chinook.emsl.pnl.gov
(enter Kerberos password)

Note:
Machines use Secure Shell Protocol 2.
You may have to use ssh2 or ssh -2

System Information
Machine status
$ sinfo

Nodes available
$ showbf -c normal

Job Commands
Submit job
$ msub *jobscript.msub*

Show all jobs in queue
$ showq

Status of all your jobs
$ showq | grep <UserID>

Cancel job
$ canceljob *jobid*

Estimate Job start
$ showstart *jobid*

Allocation Information (Gold)
Account balance and account name
$ gbalance -h -u <UserID>

Using modules to set up your environment
List loaded modules
$ module list

Available modules
$ module avail

Removing modules
$module unload <*module*>

Adding new modules
$ module load <*module*>

Swapping modules
{DO NOT USE module swap}

Removing all modules
$ module purge

Available modules
Default environment: pnnl_env
Note: Environment set default Integer*4

Integer*8 environment: pnnl_env/i8
Use: module purge
Use: module load pnnl_env/1.2.i8

Application specific modules are available and get loaded in the submit_apps scripts

Mounted File Systems
Backed-up home directory; /home/UserID

NWfs - archive file system; external access using: sftp nwfs.emsl.pnl.gov

Global File System - cleaned periodically; /dtemp/UserID

Scratch - cleaned after job runs; /scratch **Version 3: April, 2009**

The EMSL is the Environmental Molecular Sciences Laboratory and is located at Pacific Northwest National Laboratory (PNNL), one of the U.S. Department of Energy multiprogram national laboratories.

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E-mail Address: mscf-consulting@emsl.pnl.gov

Batch
Control flags for batch job script file, jobscript. See our website for sample scripts.

```
#!/bin/csh
#MSUB -A <your Gold account>
#MSUB -l "walltime=04:30:00"          # (HH:MM:SS)
#MSUB -l "nodes=<number-of-nodes>:ppn=8"      # (8 cores/node)
#MSUB -m ae                           # e-mail on "abort" or at the "end"
#MSUB -o <your output file>.%j
#MSUB -e <your error file>.%j
#MSUB -N <job name>
#MSUB -M <your email address>
```

To run a program, add the following lines to the jobscript file for a batch job.

crun -nodes <*# of nodes*> -cores <*# of cores*> <*your program*> <*your args*>

To copy a file or binary to /scratch on all the nodes (using one CPU per node):
bcastf /dtemp/<UserID>/<your *file*> /scratch/<your *file*>
rank0scrcp /scratch/<your *file*> /dtemp/<UserID>/<your *file*>

Execute Batch Job
Submit your job to the queue by typing: msub *jobscript.msub*

Interactive Job
Start your interactive job/session (X-windows required) by typing:
isub -A <*your Gold account*> -N <*# of nodes*> -W <*time limit HH:MM*> -s <*shell*>
To run a program in the interactive X terminal, type:
crun -nodes <*# of nodes*> -cores <*# of cores*> <*your program*> <*your args*>

Intel Compiler
Default compiler is Intel compiler:
ifort - fortran77 and fortran 90 compiler
icc - C and C++ compiler

Intel MKL BLAS & LAPACK
Note: variables MLIB_LIB and MLIB_LDFLAGS are set by the module environment

For Integer*4 and Integer*8 compiled code, include on the link line: ${MLIB_LDFLAGS}
This environmental variable includes both the -L and -l arguments for MKL

Useful Intel compiler flags
-i8 : integer*8 ; -i4 : integer*4
-O2 : default optimization level
-xW : better suited for Chinook
-FR : free format fortran
-Vaxlib : link in portability library
Do NOT use -ftz or -fpe flags

Linking MPI with Intel compiler
Automatic: use mpif90 or mpicc
For Details include -show: mpif90 -show or mpicc -show
Note: If these do not work, contact MSC Consultants [use e-mail address below]

For assistance, email mscf-consulting@emsl.pnl.gov