



Molecular Science Computing Facility

Quick Reference Guide

<http://mscf.emsl.pnl.gov>

mscf-consulting@emsl.pnl.gov

Log on to NWMpp1

```
>> ssh mpp1.emsl.pnl.gov
```

Log on to Jupiter

```
>> ssh j01a01.jupiter.emsl.pnl.gov
or
>> ssh j01a03.jupiter.emsl.pnl.gov
```

Log on to NWEcs1

```
>> ssh x01n01.ecs1.emsl.pnl.gov
```

System Information

General details
>> sysinfo

Machine status
>> llstatus

Nodes available
>> window

Paths to include in UNIX Shell

```
/u/scripts
/u/tools
/u/apps
```

File Systems

NFS - permanent home directory; `/u/username`

AFS - `/afs/`, `/msrc` accessible from the login nodes

GPFS - cleaned periodically; `/gpfs/`, `/gpfs1` and `/gpfs2` on NWMpp1

Scratch - cleaned after job runs; `$TMPDIR`

The MSCF is part of the William R. Wiley Environmental Molecular Sciences Laboratory and is located at Pacific Northwest National Laboratory (PNNL), one of nine U.S. Department of Energy multiprogram national laboratories.

Allocation Information (QBank)

Account balance
>> qbalance

Transactions
>> qtxns -u *username*

Display default account
>> qlsuser

Job Commands

Submit job
>> llsubmit *jobscript*

Cancel job
>> llcancel *jobid*
or
>> canceljob *jobid*

Put [release] job on hold
>> llhold [-r] *jobid*

Status of all jobs
>> llq

Show queue of all jobs
>> showq



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Batch

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

General Flags

```
#@queue
#@class = batch
#@job_type = parallel
#@account_no = [accountname]
#@wall_clock_limit = <[[HH:]MM:]SS>
#@network.lapi = css0, shared, US
or #@network.mpi = css0, shared, US
```

Additional for NWMpp1

```
#@node = [min][,max]
```

Additional for NWEcs1 or Jupiter

Two of the following three:

```
#@node = [min][,max]
#@tasks_per_node = [# procs]
#@total_tasks = [# of tasks]
```

Execute Batch Job

To run a program, add the following lines to the *jobscript* file for a batch job. Submit by typing `llsubmit jobscript`. Type `poe -h` to see all `poe` options.

```
cat << EOFcat > poe.cmd
your_program
commands
quit
EOFcat
poe -cmdfile poe.cmd -newjob yes <poe options>
```

Interactive

Environment variables for interactive jobs. After setting these, run the job by typing `poe <your program> <poe options>`. Type `poe -h` to see all `poe` options.

General Variables

```
MP_ACCOUNT = [accountname]
MP_WCLIMIT = <[[HH:]MM:]SS>
MP_EUIDEVICE = css0
MP_EUILIB = US
MP_CSS_INTERRUPT = yes
MP_MSG_API = [LAPI | MPI]
```

Additional for NWMpp1

```
MP_NODES = [# of nodes]
```

```
MP_RMPOOL = 0
```

Additional for NWEcs1 or Jupiter

```
MP_NODES = [# of nodes]
```

```
MP_TASKS_PER_NODE = [# procs]
```

```
MP_ADAPTER_USE = shared
```

For assistance, call 509-376-1301 Mon-Fri 8:00 AM PST - 2:00 PM PST