

How to use the W&M High Performance Computing Cluster to run FEKO

by Shuangli Du
(February 18, 2020)

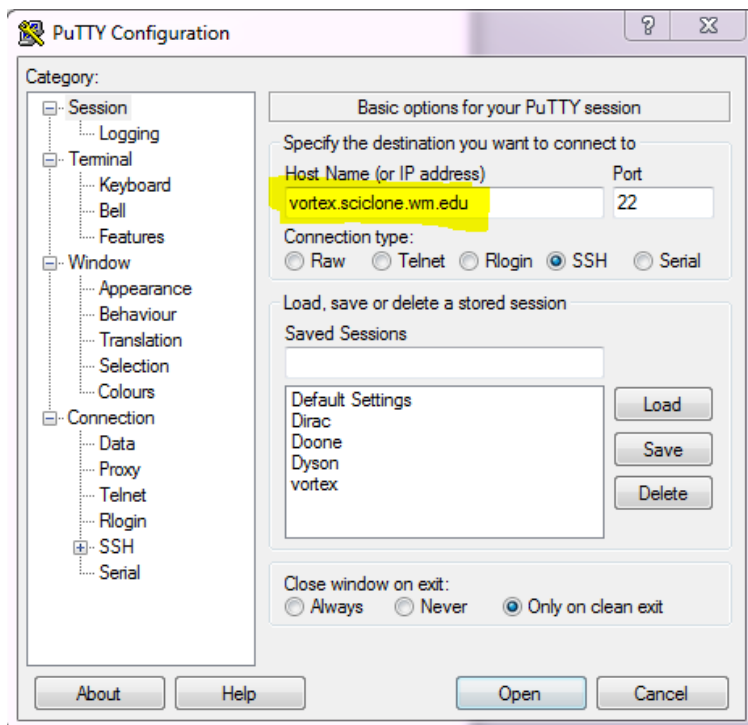
1. Apply for a WM HPC account

<https://www.wm.edu/offices/it/services/researchcomputing/acctreq/index.php>

2. Use SSH to log in

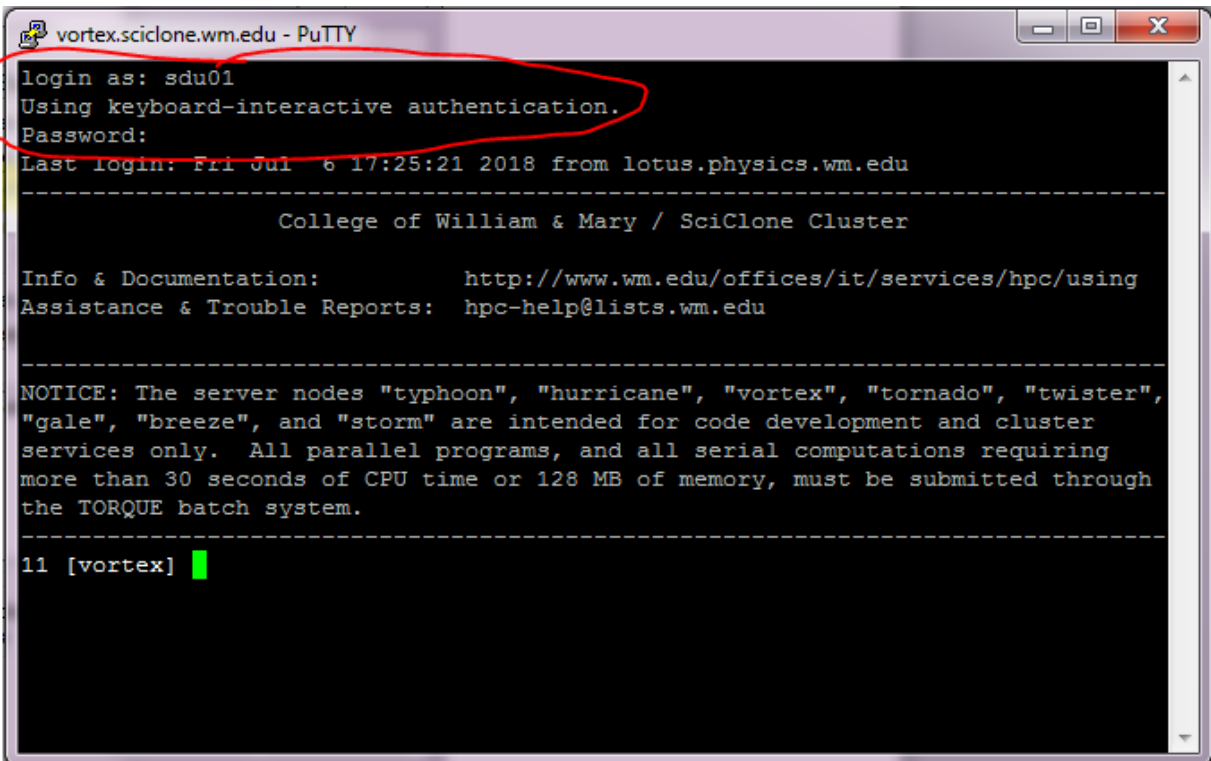
Tools: Putty, MOBAXterm

Here is an example using Putty:



Type the vortex.sciclone.wm.edu address into the PuTTY Host Name. Port 22 is for SSH, and also choose Connection type to be SSH. Then, press Open to login. These default settings can be saved.

If the computer is connecting with vortex for the first time, then you will be asked for authorization and you can just press “yes”.



```
vortex.sciclone.wm.edu - PuTTY
login as: sdu01
Using keyboard-interactive authentication.
Password:
Last login: Fri Jul 6 17:25:21 2018 from lotus.physics.wm.edu
-----
                College of William & Mary / SciClone Cluster

Info & Documentation:      http://www.wm.edu/offices/it/services/hpc/using
Assistance & Trouble Reports:  hpc-help@lists.wm.edu
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NOTICE: The server nodes "typhoon", "hurricane", "vortex", "tornado", "twister",
"gale", "breeze", and "storm" are intended for code development and cluster
services only. All parallel programs, and all serial computations requiring
more than 30 seconds of CPU time or 128 MB of memory, must be submitted through
the TORQUE batch system.
-----

11 [vortex] █
```

After you type your WM account ID and password (same as the one use for Banner and Blackboard), the information shown above will appear, and you are now connected to the WM HPC vortex front-end.

3. Change the module of your account (environment setting)

You only need to change your module setting once, if you only use FEKO.

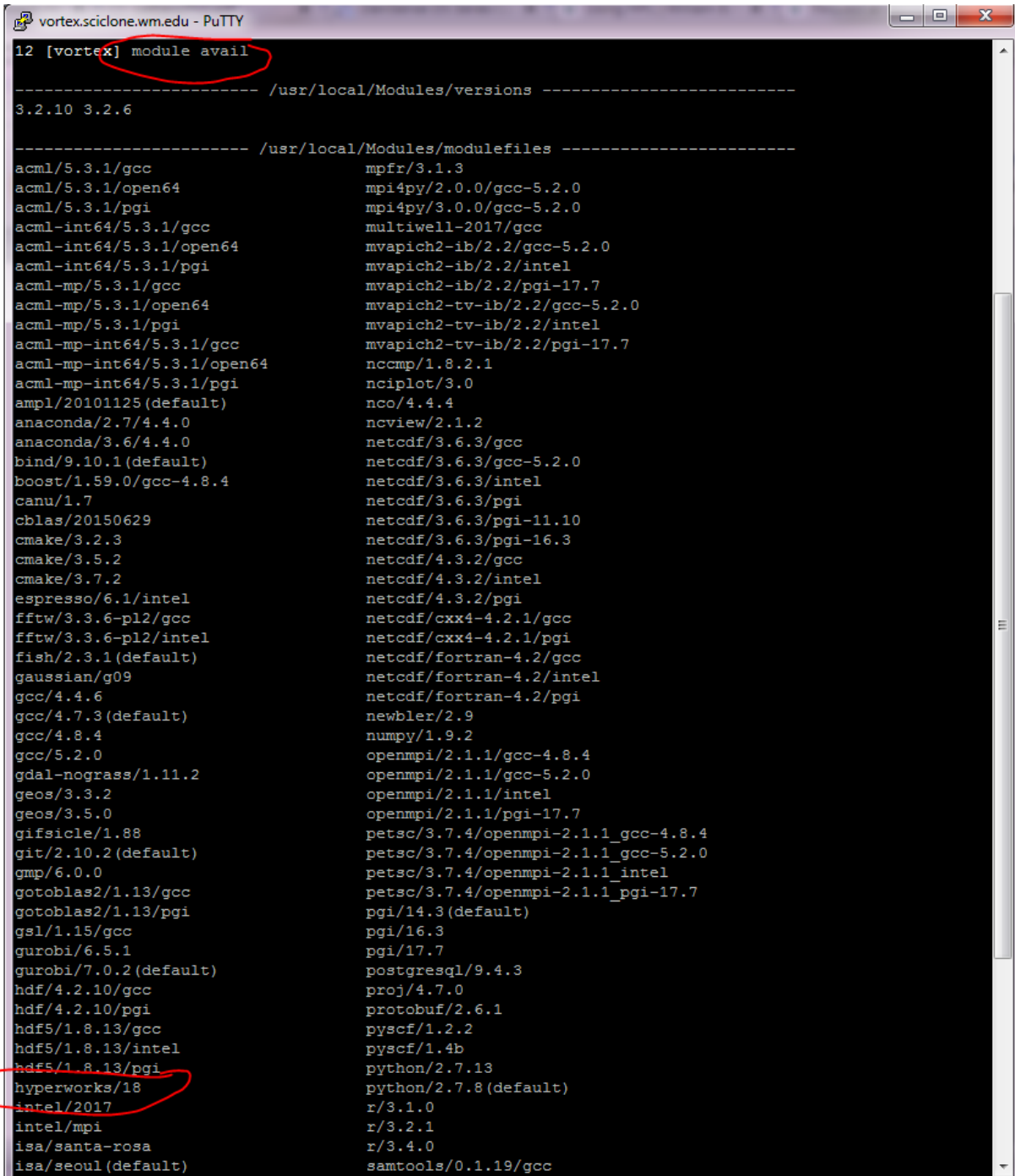
First, you should check whether your module list contains hyperwork/19 or not. If you did not change the setting previously, then it should not.

But you can type “module list” to show the modules that are activated now.

```
13 [vortex] module list
Currently Loaded Modulefiles:
 1) modules                3) torque/6.1.1.1      5) gcc/5.2.0
 2) maui/r156              4) isa/seoul           6) hyperworks/18
```

Here hyperworks/19 is on the list, because I already changed the module setting, if you cannot find hyperworks/19, then you should go through the following steps:

You can type “module avail” to check if the software that you want to use is on the list. We will use FEKO, so check to make sure that “hyperworks/19” is on the list.



```
vortex.sciclone.wm.edu - PuTTY
12 [vortex] module avail
----- /usr/local/Modules/versions -----
3.2.10 3.2.6
----- /usr/local/Modules/modulefiles -----
acml/5.3.1/gcc                mpfr/3.1.3
acml/5.3.1/open64            mpi4py/2.0.0/gcc-5.2.0
acml/5.3.1/pgi               mpi4py/3.0.0/gcc-5.2.0
acml-int64/5.3.1/gcc         multiwell-2017/gcc
acml-int64/5.3.1/open64     mvapich2-ib/2.2/gcc-5.2.0
acml-int64/5.3.1/pgi        mvapich2-ib/2.2/intel
acml-mp/5.3.1/gcc           mvapich2-ib/2.2/pgi-17.7
acml-mp/5.3.1/open64       mvapich2-tv-ib/2.2/gcc-5.2.0
acml-mp/5.3.1/pgi          mvapich2-tv-ib/2.2/intel
acml-mp-int64/5.3.1/gcc    mvapich2-tv-ib/2.2/pgi-17.7
acml-mp-int64/5.3.1/open64 nccmp/1.8.2.1
acml-mp-int64/5.3.1/pgi    nciplot/3.0
ampl/20101125(default)     nco/4.4.4
anaconda/2.7/4.4.0         ncview/2.1.2
anaconda/3.6/4.4.0         netcdf/3.6.3/gcc
bind/9.10.1(default)       netcdf/3.6.3/gcc-5.2.0
boost/1.59.0/gcc-4.8.4    netcdf/3.6.3/intel
canu/1.7                   netcdf/3.6.3/pgi
cblas/20150629             netcdf/3.6.3/pgi-11.10
cmake/3.2.3                netcdf/3.6.3/pgi-16.3
cmake/3.5.2                netcdf/4.3.2/gcc
cmake/3.7.2                netcdf/4.3.2/intel
espresso/6.1/intel         netcdf/4.3.2/pgi
fftw/3.3.6-pl2/gcc         netcdf/cxx4-4.2.1/gcc
fftw/3.3.6-pl2/intel      netcdf/cxx4-4.2.1/pgi
fish/2.3.1(default)       netcdf/fortran-4.2/gcc
gaussian/g09               netcdf/fortran-4.2/intel
gcc/4.4.6                  netcdf/fortran-4.2/pgi
gcc/4.7.3(default)        newbler/2.9
gcc/4.8.4                  numpy/1.9.2
gcc/5.2.0                  openmpi/2.1.1/gcc-4.8.4
gdal-noggrass/1.11.2      openmpi/2.1.1/gcc-5.2.0
geos/3.3.2                 openmpi/2.1.1/intel
geos/3.5.0                 openmpi/2.1.1/pgi-17.7
gifsicle/1.88              petsc/3.7.4/openmpi-2.1.1_gcc-4.8.4
git/2.10.2(default)       petsc/3.7.4/openmpi-2.1.1_gcc-5.2.0
gmp/6.0.0                  petsc/3.7.4/openmpi-2.1.1_intel
gotoblas2/1.13/gcc        petsc/3.7.4/openmpi-2.1.1_pgi-17.7
gotoblas2/1.13/pgi        pgi/14.3(default)
gsl/1.15/gcc               pgi/16.3
gurobi/6.5.1               pgi/17.7
gurobi/7.0.2(default)     postgresql/9.4.3
hdf/4.2.10/gcc            proj/4.7.0
hdf/4.2.10/pgi            protobuf/2.6.1
hdf5/1.8.13/gcc           pyscf/1.2.2
hdf5/1.8.13/intel         pyscf/1.4b
hdf5/1.8.13/pgi           python/2.7.13
hyperworks/19              python/2.7.8(default)
intel/2017                  r/3.1.0
intel/mpi                   r/3.2.1
isa/santa-rosa              r/3.4.0
isa/seoul(default)         samtools/0.1.19/gcc
```

Since “hyperworks/19” will conflict with the default compiler “intel/2017”, we need to delete “intel/2017” and then load “hyperworks/19”.

Before doing this operation, check your working platform with the command “echo \$PLATFORM”. Since we are working on vortex ,this should be “rhel6-opteron”.

```
17 [vortex] echo $PLATFORM
rhel6-opteron
```

Then type “ls -al” (ls = list, options -a all including .hidden .files, and -l long descriptions) to find the .cshrc file with the platform suffix, which is circled in red on the picture below:

```
18 [vortex] ls -al
total 172
drwx----- 14 sdu01 physg 4096 Jul  6 17:32 .
drwxr-xr-x 305 root  root 12288 Apr 11 2017 ..
drwxr-x---  3 sdu01 physg   26 Jul  6 15:41 .altair
drwxr-x---  5 sdu01 physg  106 Jul  6 17:35 .altair_licensing
drwxr-x---  3 sdu01 physg 4096 Jul  6 19:27 conductivity_patch
drwxr-x---  2 sdu01 physg   36 Jul  6 16:08 .config
-rw-r--r--  1 sdu01 physg 2990 Feb 23 2012 .cshrc
-rw-r--r--  1 sdu01 physg  401 Feb 11 2017 .cshrc.el7-phi
-rw-r--r--  1 sdu01 physg  529 Apr 19 14:57 .cshrc.el7-xeon
-rw-r--r--  1 sdu01 physg 1280 Jul  6 14:58 .cshrc.rhel6-opteron
-rw-r--r--  1 sdu01 physg 1214 Apr 19 15:53 .cshrc.rhel6-xeon
-rw-r--r--  1 sdu01 physg  894 Sep 23 2016 .cshrc.rhel7-xeon-hsep
-rw-r--r--  1 sdu01 physg 1239 Jul 24 2014 .cshrc.sles-opteron
-rw-r--r--  1 sdu01 physg 1467 Apr 19 16:00 .cshrc.storm
lrwxrwxrwx  1 sdu01 physg   22 Jul  2 16:10 data10 -> /sciclone/data10/sdu01
-rw-r--r--  1 sdu01 physg 82813 Apr 19 16:20 DC_five_defect_line_3D.cfx
drwxr-x---  3 sdu01 physg   36 Jul  6 15:23 .emacs.d
drwxr-xr-x  2 sdu01 physg  124 Jul  5 15:50 .fontconfig
```

The .cshrc file is the module setting file: this suffix will determine the platform that we will be use. We use a text editor to change the module setting in this file.

Linux have a few built-in editors such as “vi”, “nano”, and “emacs”. Here we will use “nano” as an example.

Type “nano .cshrc.rhel6-opteron” and return

```
12 [vortex] nano .cshrc.rhel6-opteron
```

Then we will move into the nano editor window:

```
vortex.sciclone.wm.edu - PuTTY
GNU nano 2.0.9 File: .cshrc.rhel6-opteron
# Environment configuration for RHEL 6.x / Opteron environment.
#
# Revised:
# 02/23/2012 tom - To avoid conflicts in subshells, the ISA module is
# explicitly loaded here rather than letting it
# default.
# 03/13/1012 tom - Fix up the comments.
# 02/28/2013 tom - Add mvapich2-ib as the default MPI module.
# 05/22/2014 tom - Only available Xeon at the moment is
# sandy-bridge-ep.
# - Use MVAPICH2 1.9 as the default MPI.
#
# Personal module configuration:
# - Defaults to a 64-bit environment optimized for Intel Xeon
# Sandy Bridge-EP processors.
# - ISA module must be loaded before other modules.
# - Available ISA's include:
# seoul - Opteron 4334 (vortex: c18a, c18b)
# valencia - Opteron 4238 (vortex: s11b)
# santa-rosa - Opteron 2218 (typhoon: c9, c9a)
#
# module load isa/seoul
# module load hyperworks/18
#
# Select ONE of the following compiler modules, depending on your needs.
#
# For a high-performance x86/x64 compiler, use:
# module load intel/2017 mvapich2-ib/2.2/intel
#
# For applications which require a GCC compiler, we recommend:
#
# ^G Get Help ^C WriteOut ^R Read File ^Y Prev Page ^X Cut Text ^C Cur Pos
# ^X Exit ^J Justify ^W Where Is ^V Next Page ^U UnCut Text ^I To Spell
```

First, you should add a # before the line of module load intel/2017, to not use this line (# means comment line.)

Then type “module load hyperworks/19” at a line around other module lines.

Then press “Ctrl+O”, and then return to save the change. Use “Ctrl+X” to exit.

Or: use “Ctrl+X” to exit, press “y” to save changes, and press return to use the current name, or type a new name.

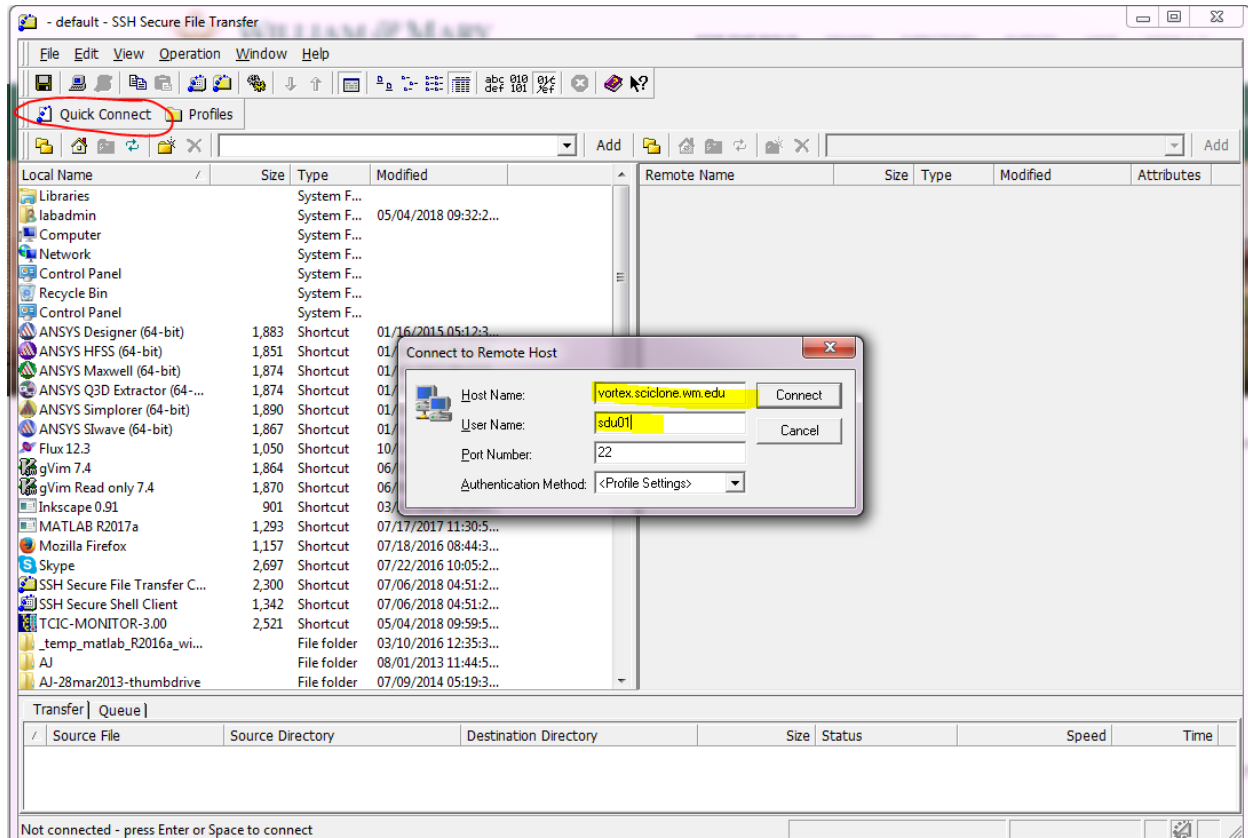
Now the module file has been changed.

Log out (you can just turn off PuTTY to end the session) and Log in again, and check the module list again, now you should find hyperworks/19 in the list.

4. Transfer the FEKO file into the HPC account folder.

You should download SSH secure Shell client and install the SSH secure file transfer.

And open it.



Press Quick Connect, and type the Host name and your user name, and then you will connect to the HPC with this file transfer.

On the left is your local (or [\\snapdragon](#)) file system.

Your files on the HPC server will be shown on the right hand side, and you can just drag the file from left to right to upload or right to left to download.

Only the .cfx file is needed to run jobs on the HPC.

5. Run FEKO file with Batch system.

Interaction Batch:

For small task, we can use interaction batch to run it.

```
15 [vortex] qsub -I -l walltime=30:00 -l nodes=1:vortex:ppn=12
qsub: waiting for job 4477591 to start
qsub: job 4477591 ready
```

Walltime is the maximum working time for this job (in hours). You can then ask for 1 node on vortex for 12 cores.

At present, I am not sure how to change the setting for more nodes and cores.

The number 4477591 is your job ID.

```
3 [vx05] exit
logout
qsub: job 4477591 completed
```

Type “exit” to log out the batch system.

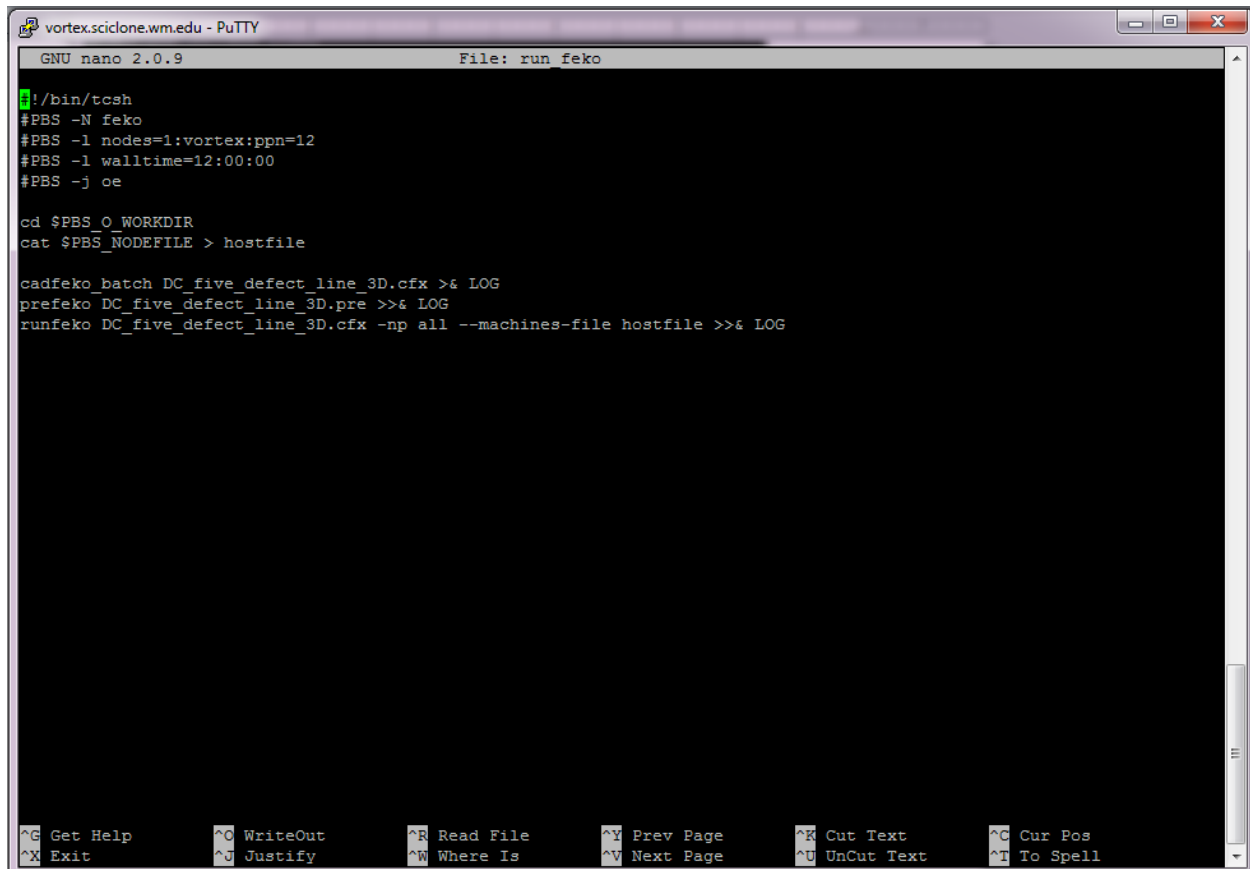
Do not keep working in the interaction batch for too long (i.e. few days), since this will keep other users from using these nodes. If you want to work on a long job, you should use the non-interaction batch by script. And also do not forget to exit before you turn off PuTTY, this might keep you logged into the batch system.

Non-interaction Batch:

Type “ls” and check whether you have a file called “run_feko”

This is the example of a feko running script. If you don’t have it, you can get it at \\SNAPDRAGON\Common\Shuangli\SuperComputer\run_feko_file and put it into your HPC account. This uses a generic name “input.cfx” as the file to run. Typically we use the folder structure to name jobs, and then change the file name to “input.cfx” to use the same run_feko file. You can also leave the file name and change it in 3 locations in the run_feko file.

Type “nano run_feko” to check the feko file.



```
GNU nano 2.0.9 File: run_feko
#!/bin/tcsh
#PBS -N feko
#PBS -l nodes=1:vortex:ppn=12
#PBS -l walltime=12:00:00
#PBS -j oe

cd $PBS_O_WORKDIR
cat $PBS_NODEFILE > hostfile

cadfeko_batch DC_five_defect_line_3D.cfx >& LOG
prefeko DC_five_defect_line_3D.pre >>& LOG
runfeko DC_five_defect_line_3D.cfx -np all --machines-file hostfile >>& LOG

^G Get Help      ^O WriteOut     ^R Read File    ^Y Prev Page    ^K Cut Text     ^C Cur Pos
^X Exit          ^J Justify     ^W Where Is    ^V Next Page    ^U UnCut Text  ^T To Spell
```

Change the file names of last three lines to your feko program name. At this point, the feko running script has been set.

Here are some details on this script:

-N means job name, so this job is named feko. This name is shown in the queue list.

-l is the parameters setting, like nodes, core and wall time.

-j is the input output setting: oe means output and error information will be written together.

\$PBS_O_WORKDIR means your current working directory. So put this run_feko file with your .cfx file in the same folder.

Use “Ctrl+O” to save, and “Ctrl+X” to exit.

Next, you can type “qsub run_feko” to run the script. This submits a job into the Queue.

```
21 [vortex] qsub run_feko
4477768
```

The following numbers are your job ID.

You can type “qsu” to check the current job condition:

```
22 [vortex] qsu
vortex.sciclone.wm.edu:
Job ID      Username   Queue    Jobname      SessID  NDS   TSK   Req'd   Req'd   S   Elap
-----
4477216     sdu01     ql       feko         39204   1     12    --      24:00:00 R  03:31:42
```

[The job shown here is a job I ran earlier.]

You can also type “less LOG” to check the LOG file while the job is running, and to check the current job status. You can use “tail LOG” to view the last few lines, or “cat LOG” to see the whole thing. The LOG is only generated once the job starts running (second to last column status -> R), not just in queue (Q).

After the job is done, you can download the output files from the Secure file transfer shell (reload, then drag right to left) to your computer and then you can check the post feko from your computer.

```
23 [vortex] ls
conductivity_patch      DC_five_defect_line_3D.cfx      DC_five_defect_line_3D.out      LOG          scr20
#.cshrc.rhel6-opteron# DC_five_defect_line_3D_Currents1.o1 DC_five_defect_line_3D.pre      lscr        scr30
data10                  DC_five_defect_line_3D_Currents1.os DC_five_defect_line_3D.str      pscr        test
DC_five_defect_line_3D.bof DC_five_defect_line_3D.fek      feko.o4477768                  run_feko
DC_five_defect_line_3D.cfm DC_five_defect_line_3D_NearField1.hfe hostfile                          scr10
```

A short list of useful commands:

HPC specific command:

1. qsub #filename#: submit your job into the batch system
2. qsu: list all status of your job
3. qstat ###jobid### : see status of that job
4. qdel ###jobid### : delete job from queue or stop running
5. qstat : see status of all jobs on the cluster
6. qstat -u #username# : check all existing jobs from that user (eg. qstat -u sdu01 will list all of my jobs)
7. showstart ###jobid###: show the estimated earliest start time for this job.
8. freenodes: show the number of free nodes in each cluster

Linux commands:

9. ls : lists the files located in the present working directory
 - a. -a option to show all, including hidden files
 - b. -l gives extra info for each file
10. pwd : tells you the folder you are in. "present working directory"
11. cd : change directory.
 - a. "cd subfoldername" to go down
 - b. "cd .."to go up one level
 - c. "cd" to go to your home folder
12. rm : remove file or empty folder (eg. rm feko/temp will delete "temp" file or empty "temp" folder under feko direction). This command cannot remove folder with file in it.
13. rm -rf : remove folder and all file in that folder, so take care before you do that.
14. mv #original# #newdir# : move file or folder "original" into "newdir" direction.
15. mv #original# #newname#: rename file or folder "original" to "newname".
16. cp #original# #newdir# : copy file or folder "original" into new direction.
17. cp #original# #newname#: copy file or folder "original" at current folder and name it "newname"
18. mkdir #foldername#: make direction (make a folder called "foldername")
19. nano #filename# : use word editor "nano" to open "filename" file.
20. cat #file#: show all the text in that file to the screen.
21. more #file#: show all the text page by page till end of that file. (use q to quit)
22. less #file#: show all the text page by page (able to scroll back). (use q to quit)
23. tail #file#: show last few line of that file
24. tail -f #file#: show last few line of that file and update display in real time.
25. man #commandname#: gives the syntax, options, and usage for a command.