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

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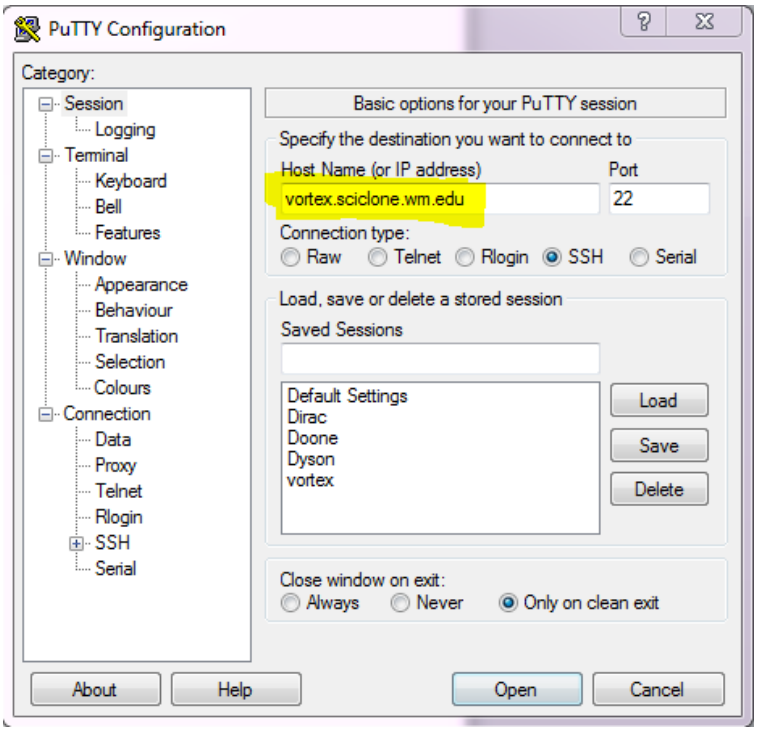
1. Apply for a WM HPC account

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

2. Use SSH to log in

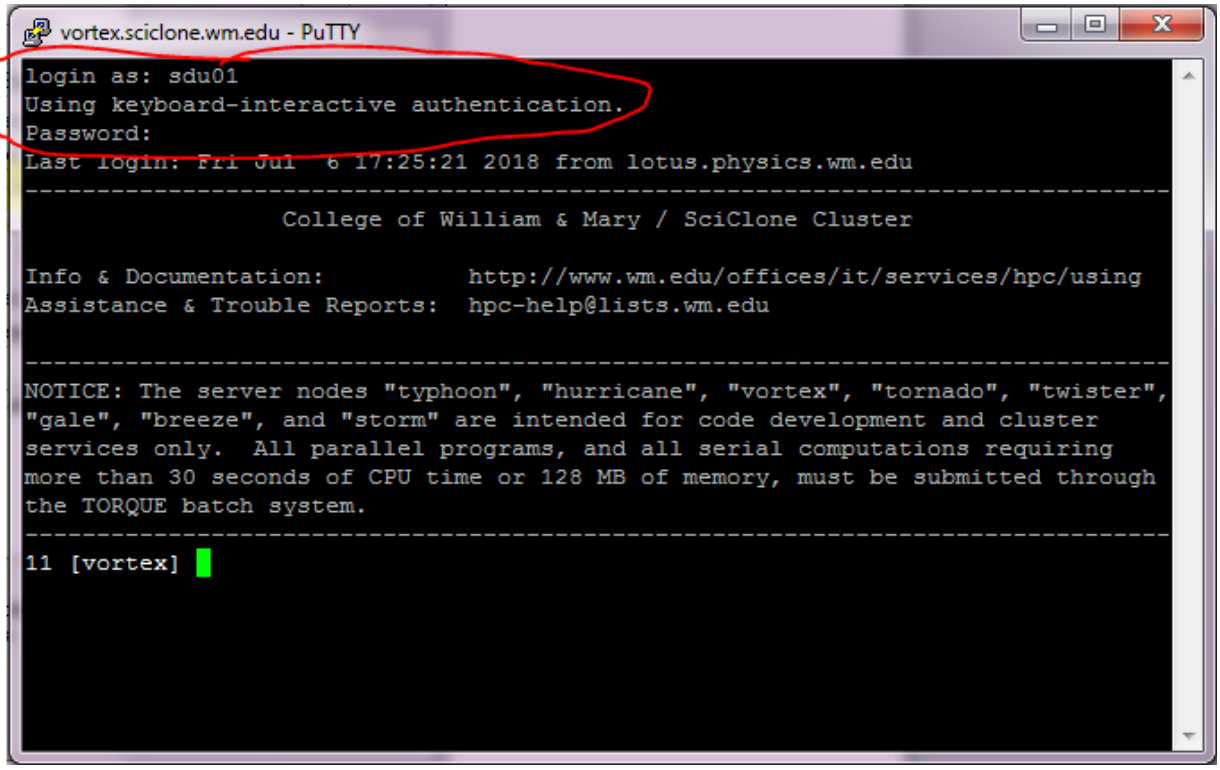
Tools: Putty, MOBAXterm

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”.



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.

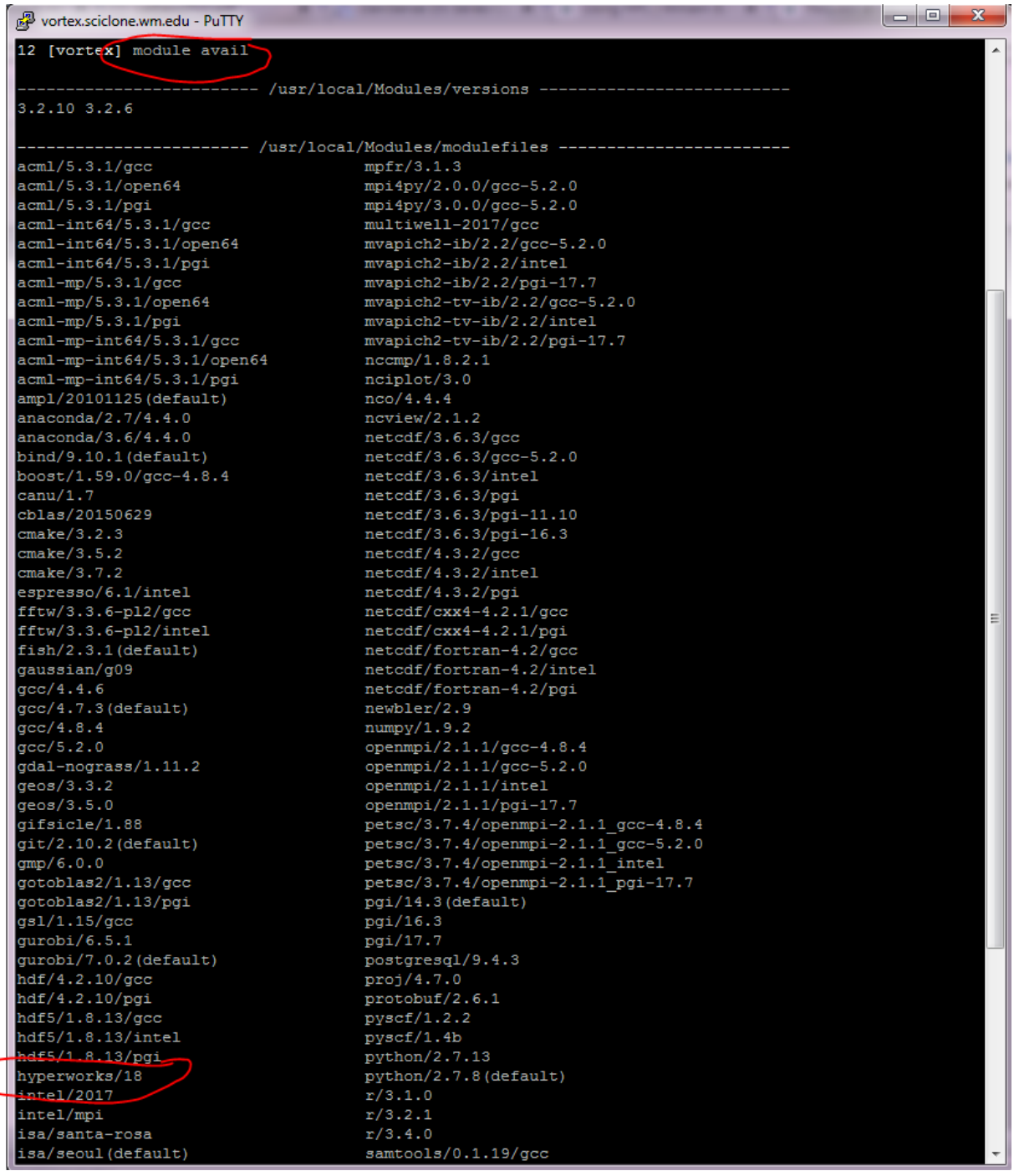
First, you should check whether your module list contains hyperwork/19 or not. If you did not change the setting previously, then it should not.

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.



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
```

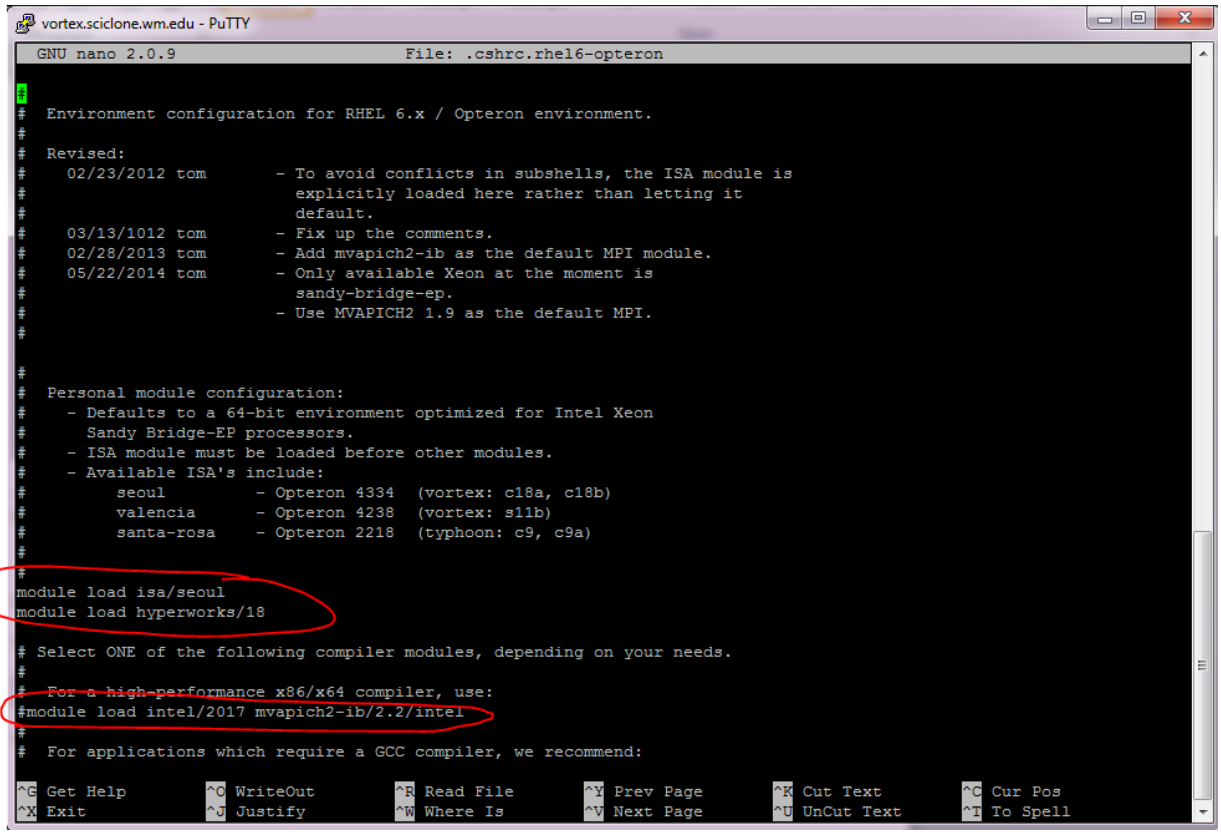
The .cshrc file is the module setting file: this suffix will determine the platform that we will be use. We use a text editor to change the module setting in this file.

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:



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.

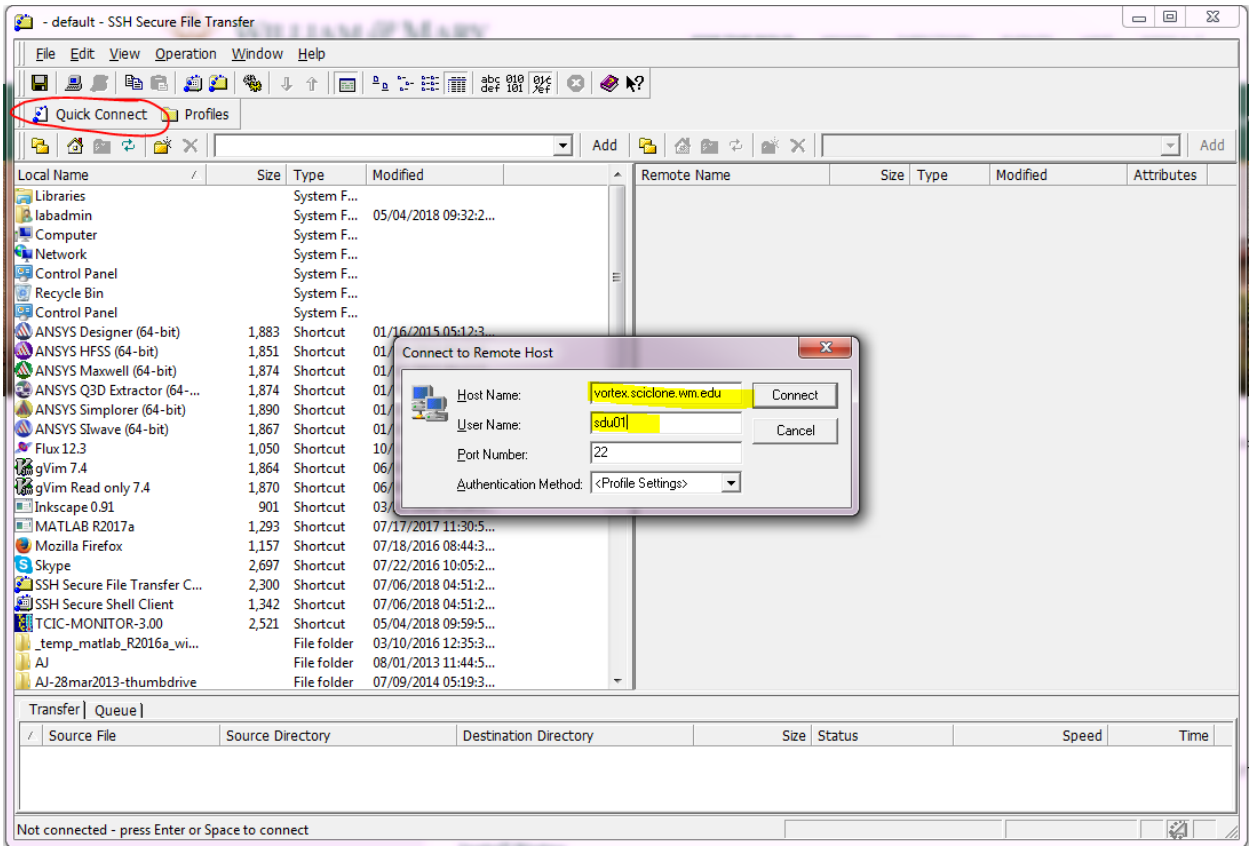
Now the module file has been changed.

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.

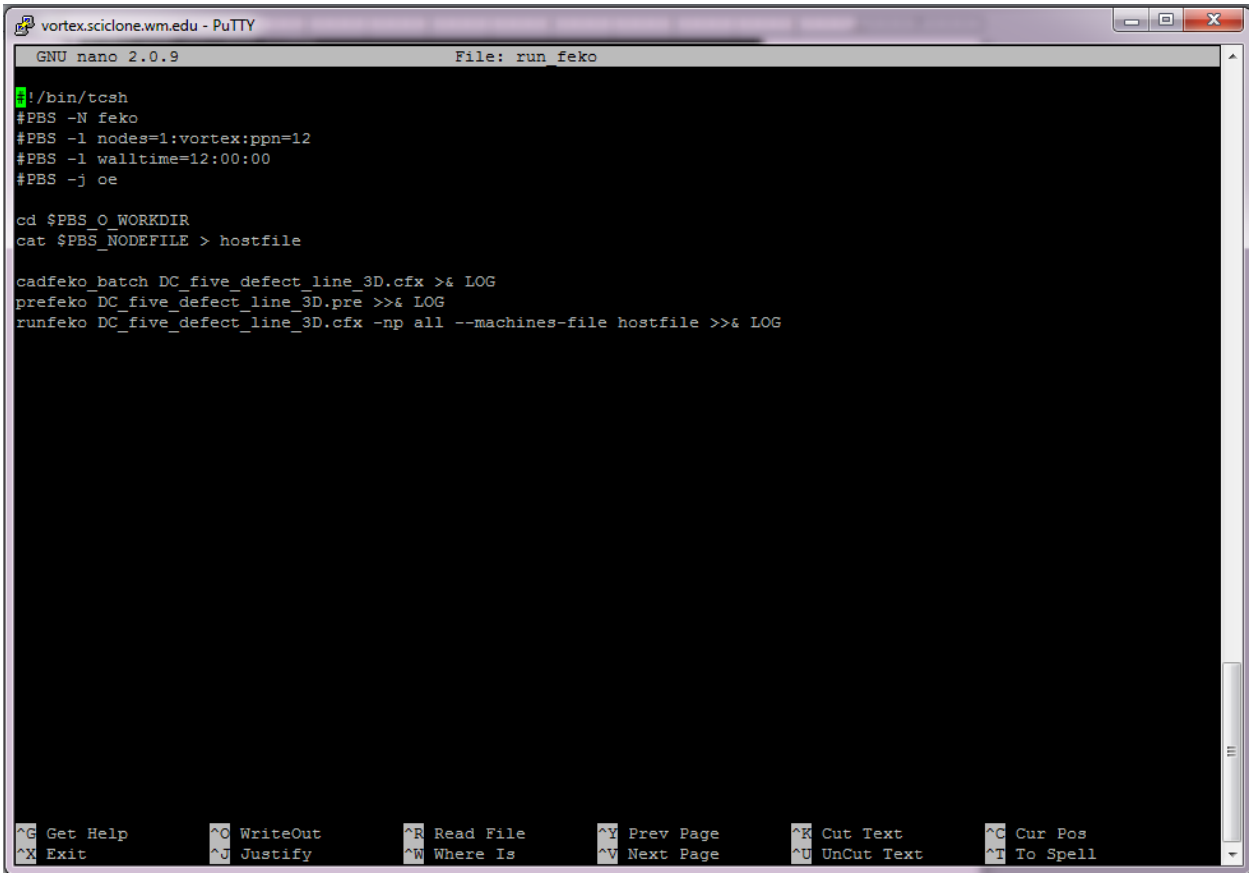
Do not keep working in the interaction batch for too long (i.e. few days), since this will keep other users from using these nodes. If you want to work on a long job, you should use the non-interaction batch by script. And also do not forget to exit before you turn off PuTTY, this might keep you logged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



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:
                                                                  Req'd       Req'd       Elap
Job ID                  Username    Queue    Jobname          SessID  NDS   TSK   Memory      Time    S   Time
----------------------- ----------- -------- ---------------- ------ ----- ------ --------- --------- - ---------
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.ol   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.