

**HIGH
PERFORMANCE
COMPUTING
WITH
PLYMOUTH
UNIVERSITY**

Using Ansys CFX on the HPC



***Author:
Peter Mills
HPC Administrator
University of Plymouth***

Using Ansys CFX on the HPC

Getting Started

The following is a guide to using Ansys CFX on the High Performance Computing Clusters.

Before we can consider running any code we need to get our files on to the cluster.

It is recommended that you use an ftp client such as Tunnelier.

The software and the user guide for Tunnelier is available from the HPC website - <http://www.plymouth.ac.uk/pages/view.asp?page=33934>

Understanding the file format in Ansys

To start a run in Ansys you need to have three files, these are

- The <filename>.sh is the bash script for running the job and contains run commands and other debugging information
- The timelimit.ccl defines the run time for the job if you open and edit this in note / wordpad you can change the time that the job will run for before it stops.
- The <filename>.def file is a definition file that is exported from Ansys CFX this contains all the run and settings data for your CFX model.

When your Ansys job is run, it will generate additional files, these are:-

- The <filename>.out file is the results from Ansys in text form
- The <filename>.res is the graphical results file that the user can view once the run is complete.

Note: The .out and .res are the output files generated by the job run.

These are the files that need to be copied back from the cluster to the local desktop to view their results.

- .res files will only be generated after the analysis has been successfully completed, if no .res appears then the run failed and by reading the .out you will be able to see why the run has failed.
- Once the user has download the .res and .out to the desktop they should be deleted from the cluster as they take up a lot of file space.

Example Files

Firstly, login to the cluster you will be taken to your home folder.

To start you off, you will find in your home directory a folder ansys_scripts

```

pmills@fotcluster2:~
[pmills@fotcluster2 ~]$ ls -la
total 236
drwx----- 35 pmills pmills  4096 Jan 25 13:55 .
drwxr-xr-x  6 root   root     0 Jan 25 13:53 ..
-rw-r--r--  1 root   root     16 Jan 20 14:39 ammentest
drwxr-xr-x  4 pmills pmills  4096 Jan 25 13:20 .ansys
-rw-rw-r--  1 pmills pmills  3840 Nov 11 2010 .ansys.gz
drwxr-xr-x  4 root   root     33 Jan 25 13:55 ansys_scripts
-rw-----  1 pmills pmills 11011 Jan 24 14:39 .bash_history
-rw-r--r--  1 pmills pmills   33 Jan 22 2009 .bash_logout
-rw-r--r--  1 pmills pmills  176 Jan 22 2009 .bash_profile
  
```

Now cd into the CFX folder, followed by the Default folder and you will see the files as shown below.

```

pmills@fotcluster2:~/ansys_scripts/CFX/Default
[pmills@fotcluster2 ansys_scripts]$ ls -la
total 4
drwxr-xr-x  4 root   root     33 Jan 25 13:55 .
drwx----- 35 pmills pmills 4096 Jan 25 13:55 ..
drwxr-xr-x  5 root   root     51 Jan 25 13:55 CFX
drwxr-xr-x  5 root   root     51 Jan 25 13:56 Mechanical
[pmills@fotcluster2 ansys_scripts]$ cd CFX
[pmills@fotcluster2 CFX]$ ls -la
total 0
drwxr-xr-x  5 root   root     51 Jan 25 13:55 .
drwxr-xr-x  4 root   root     33 Jan 25 13:55 ..
drwxr-xr-x  2 root   root    125 Jan 25 13:55 Default
drwxr-xr-x  2 root   root    131 Jan 25 13:55 Infiniband
drwxr-xr-x  2 root   root    125 Jan 25 13:55 Primare
[pmills@fotcluster2 CFX]$ cd Default
[pmills@fotcluster2 Default]$ ls -la
total 28424
drwxr-xr-x  2 root   root     125 Jan 25 13:55 .
drwxr-xr-x  5 root   root     51 Jan 25 13:55 ..
-rw-r--r--  1 root   root    1677 Jan 25 13:55 default.o4993
-rw-r--r--  1 root   root     905 Jan 25 13:55 default.sh
-rw-r--r--  1 root   root     138 Jan 25 13:55 timelimit.ccl
-rw-r--r--  1 root   root   983181 Jan 25 13:55 Venturi_001.out
-rw-r--r--  1 root   root 24371759 Jan 25 13:55 Venturi_001.res
-rw-r--r--  1 root   root  3728775 Jan 25 13:55 Venturi.def
[pmills@fotcluster2 Default]$
  
```

You should now see the files mentioned earlier in understanding the file formats in Ansys.

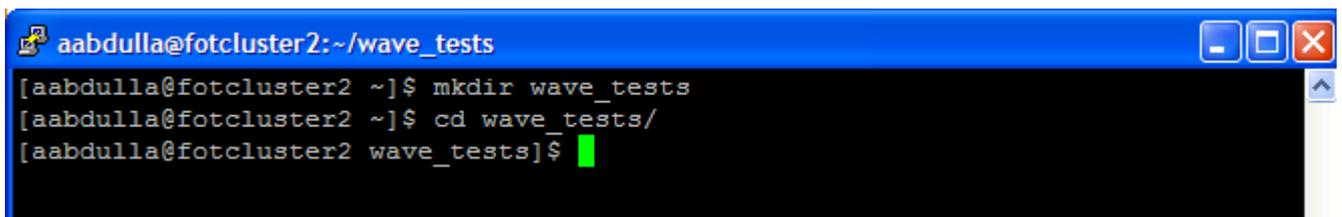
A copy of these files should be placed in what would be the working folder for the users Ansys runs. **Note** - The Venturi_001.out and the Venturi_001.res files are not required.

To copy the required files, firstly go back to the root of your home folder by using the command `cd ~`

Now create a new folder from which you will do your Ansys job runs.

Let's assume you wish to name the folder "`wave_tests`" the user should enter:

`mkdir wave_tests > now type cd wave_tests`



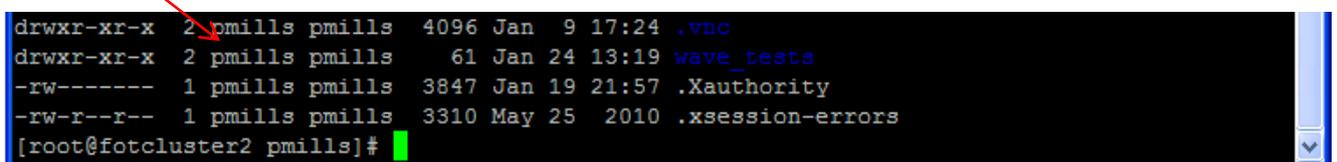
```
aabdulla@fotcluster2:~/wave_tests
[aabdulla@fotcluster2 ~]$ mkdir wave_tests
[aabdulla@fotcluster2 ~]$ cd wave_tests/
[aabdulla@fotcluster2 wave_tests]$
```

Finally to copy over the required sample files type the following –

```
cp /export/home/<username>/ansys_scripts/CFX/Default/default.sh
timelimit.ccl Venturi.def /export/home/<username>/wave_tests/
```

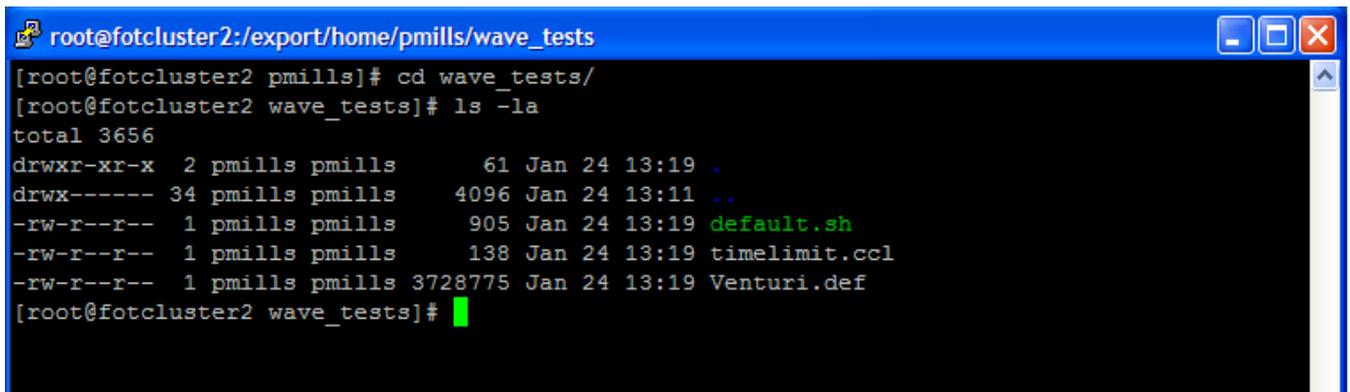
Before we can use these files we need to check the ownership of them.

Screenshot with ownership showing the correct ownership of the folder.



```
drwxr-xr-x  2 pmills pmills  4096 Jan  9 17:24 .vnc
drwxr-xr-x  2 pmills pmills    61 Jan 24 13:19 wave_tests
-rw-----  1 pmills pmills  3847 Jan 19 21:57 .Xauthority
-rw-r--r--  1 pmills pmills  3310 May 25  2010 .xsession-errors
[root@fotcluster2 pmills]#
```

Also the files within the folder are also correct

A terminal window with a blue title bar containing the text 'root@fotcluster2:/export/home/pmills/wave_tests'. The terminal output shows the user navigating to the 'wave_tests' directory and listing files with 'ls -la'. The output lists three files: a directory '.', a directory '..', and three regular files: 'default.sh' (905 bytes), 'timelimit.ccl' (138 bytes), and 'Venturi.def' (3728775 bytes). The prompt returns to the root shell.

```
root@fotcluster2:/export/home/pmills/wave_tests
[root@fotcluster2 pmills]# cd wave_tests/
[root@fotcluster2 wave_tests]# ls -la
total 3656
drwxr-xr-x  2 pmills pmills    61 Jan 24 13:19 .
drwx----- 34 pmills pmills  4096 Jan 24 13:11 ..
-rw-r--r--  1 pmills pmills   905 Jan 24 13:19 default.sh
-rw-r--r--  1 pmills pmills   138 Jan 24 13:19 timelimit.ccl
-rw-r--r--  1 pmills pmills 3728775 Jan 24 13:19 Venturi.def
[root@fotcluster2 wave_tests]#
```

The files are now ready for use.

Setting up the files ready for job Submission

Once we have the three files in our home folder, we need to edit the script file (default.sh)

So that the file will run correctly and all the results will be outputted to the users home folder.

From within your home folder type - nano default.sh

When the file is displayed browse to the bottom of the file and you will see the following

```
#
# run the cfx job
#
parallel="-par -part $nodes -par-host-list $par_host_list"
cd /home/pmills/wave_tests
/opt/ansys_inc/v120/CFX/bin/cfx5solve -def Venturi.def -ccl timelimit.ccl
$parallel
```

Change the line

- cd /home/pmills/wave_tests

To the users name and the folder from which the script will be run.

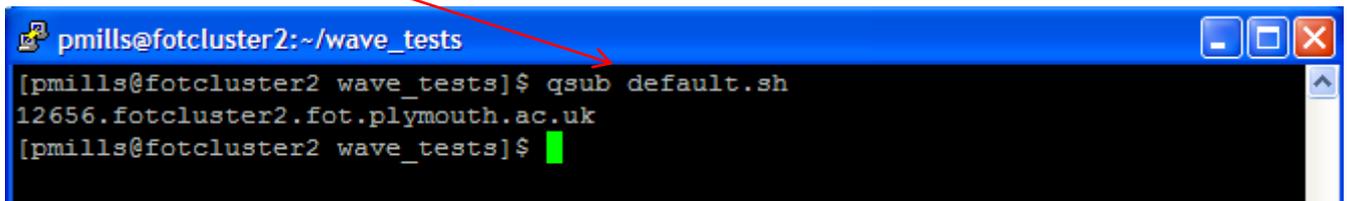
- cd /home/<username>/<folder name>
- Save the file, we are now ready to go.

Submitting an Ansys CFX job

When we submit the job, the scheduler on the cluster will decide which node/s the job will be run on.

To submit a job to the cluster we need to submit the script file using the following format

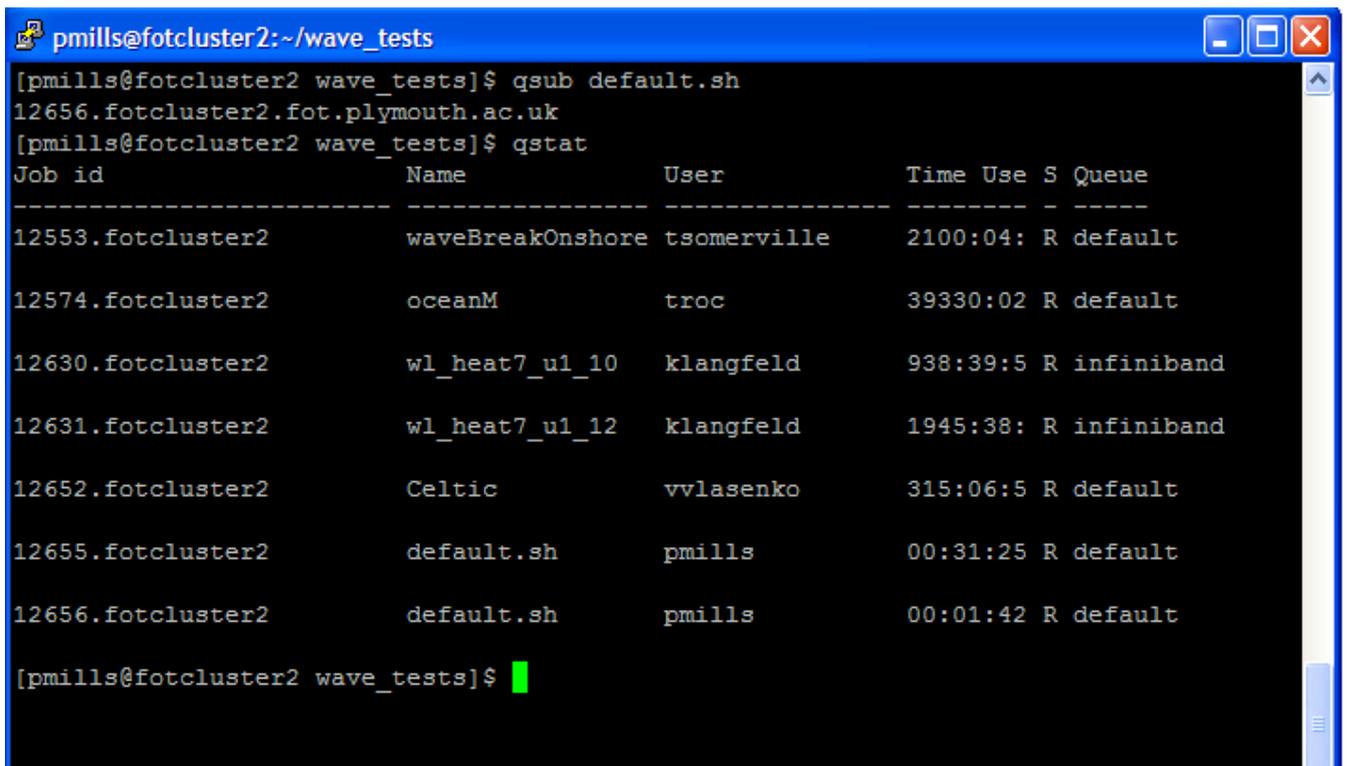
- `qsub <filename>`.
eg. `qsub default.sh`



A terminal window titled 'pmills@fotcluster2:~/wave_tests'. The prompt is '[pmills@fotcluster2 wave_tests]\$'. The user enters 'qsub default.sh'. The output is '12656.fotcluster2.fot.plymouth.ac.uk'. The prompt returns to '[pmills@fotcluster2 wave_tests]\$' with a green cursor. A red arrow points from the text 'eg. qsub default.sh' to the command in the terminal.

```
pmills@fotcluster2:~/wave_tests
[pmills@fotcluster2 wave_tests]$ qsub default.sh
12656.fotcluster2.fot.plymouth.ac.uk
[pmills@fotcluster2 wave_tests]$
```

To check the progress of our job we use `qstat`

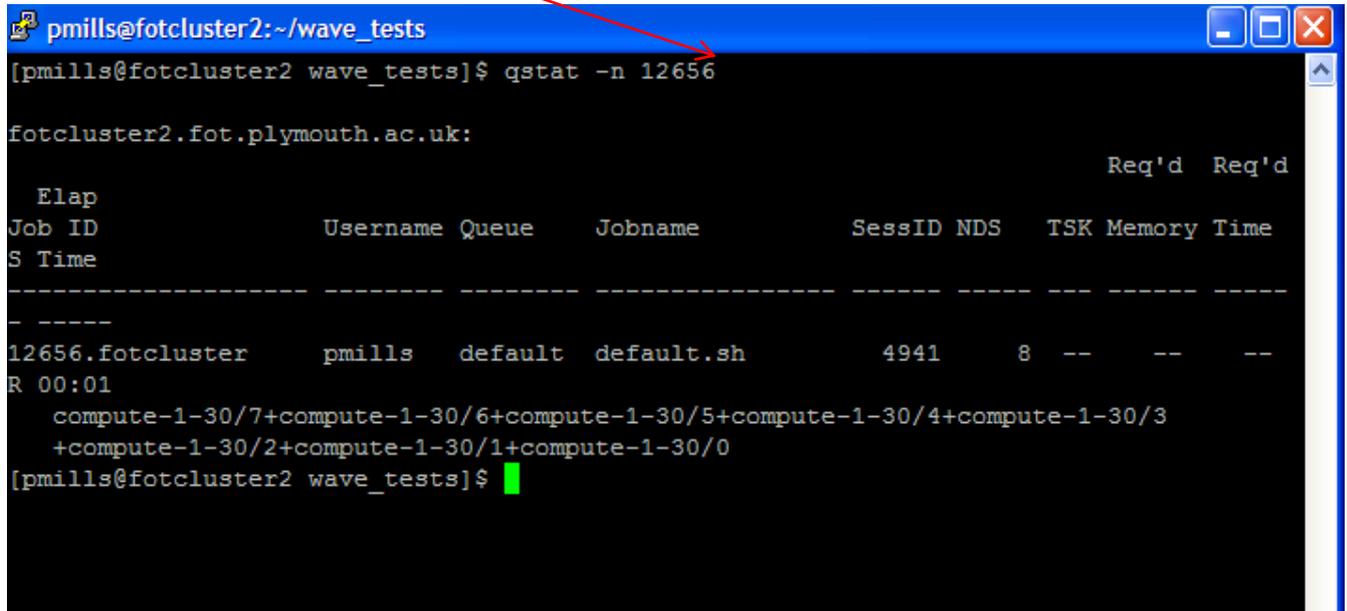


A terminal window titled 'pmills@fotcluster2:~/wave_tests'. The prompt is '[pmills@fotcluster2 wave_tests]\$'. The user enters 'qsub default.sh'. The output is '12656.fotcluster2.fot.plymouth.ac.uk'. The user then enters 'qstat'. The output is a table of job information.

```
pmills@fotcluster2:~/wave_tests
[pmills@fotcluster2 wave_tests]$ qsub default.sh
12656.fotcluster2.fot.plymouth.ac.uk
[pmills@fotcluster2 wave_tests]$ qstat
Job id          Name                User              Time Use S Queue
-----
12553.fotcluster2  waveBreakOnshore  tsomerville      2100:04: R default
12574.fotcluster2  oceanM             troc              39330:02 R default
12630.fotcluster2  w1_heat7_u1_10    klangfeld        938:39:5  R infiniband
12631.fotcluster2  w1_heat7_u1_12    klangfeld        1945:38:  R infiniband
12652.fotcluster2  Celtic            vvlasenko        315:06:5  R default
12655.fotcluster2  default.sh        pmills           00:31:25  R default
12656.fotcluster2  default.sh        pmills           00:01:42  R default
[pmills@fotcluster2 wave_tests]$
```

To check to see which nodes the job is running on we use the command

- `qstat -n <job number>`



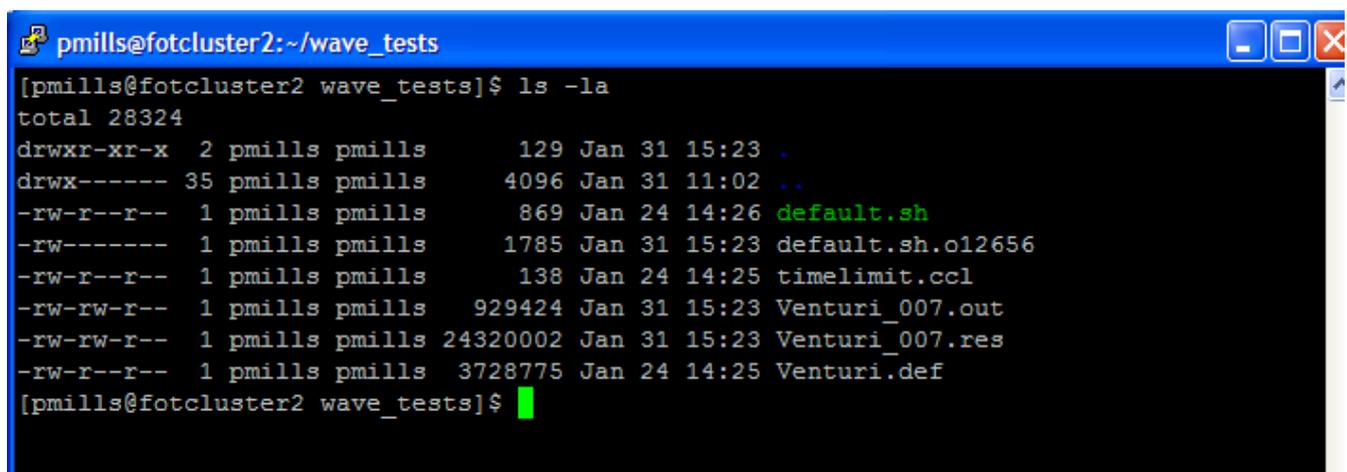
```
pmills@fotcluster2:~/wave_tests
[pmills@fotcluster2 wave_tests]$ qstat -n 12656

fotcluster2.fot.plymouth.ac.uk:

      Elap                               Req'd  Req'd
Job ID                               SessID NDS   TSK Memory Time
S Time
-----
12656.fotcluster      pmills  default  default.sh      4941    8  --   --   --
R 00:01
  compute-1-30/7+compute-1-30/6+compute-1-30/5+compute-1-30/4+compute-1-30/3
  +compute-1-30/2+compute-1-30/1+compute-1-30/0
[pmills@fotcluster2 wave_tests]$
```

Once the job has finished, we can go back to our home folder and we should now have the additional files

- 1) `.res` (results) file. This is the file that you would download to your local machine.
- 2) `.out` (output)file. Output summary of the job submission.
- 3) `.sh.o12656` file. Copy of script file, with job number appended to the name.



```
pmills@fotcluster2:~/wave_tests
[pmills@fotcluster2 wave_tests]$ ls -la
total 28324
drwxr-xr-x  2 pmills pmills    129 Jan 31 15:23 .
drwx----- 35 pmills pmills   4096 Jan 31 11:02 ..
-rw-r--r--  1 pmills pmills    869 Jan 24 14:26 default.sh
-rw-----  1 pmills pmills   1785 Jan 31 15:23 default.sh.o12656
-rw-r--r--  1 pmills pmills    138 Jan 24 14:25 timelimit.ccl
-rw-rw-r--  1 pmills pmills  929424 Jan 31 15:23 Venturi_007.out
-rw-rw-r--  1 pmills pmills 24320002 Jan 31 15:23 Venturi_007.res
-rw-r--r--  1 pmills pmills 3728775 Jan 24 14:25 Venturi.def
[pmills@fotcluster2 wave_tests]$
```

The output and results file can now be copied back to your local machine so that you are able to see the output details.