

PBS Pro and Ansys

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Introduction

ANSYS Mechanical software is a comprehensive finite element analysis (FEA) tool for structural analysis, including linear, nonlinear, dynamic, hydrodynamic and explicit studies. If provides a complete set of elements behaviour, material models and equation solvers for a wide range of mechanical design problems.

Submitting an Ansys job via PBS

By default, Ansys is run interactively via Ansys Workbench. This should be kept to a minimum when developing programs, as it affects other users of the login node. When you wish to execute jobs, especially jobs that run for a reasonable amount of time, the job should be submitted to execute on a queue of the "Cluster" in batch mode or run non-interactively.

If you execute large jobs on the "Head or Login" node, this will slow down its usability and will impact other users. The following guide provides details on how to submit an Ansys job to the HPC cluster. In order to submit an Ansys job to the cluster, you need to write a script file similar to the one below. Lines beginning with "##" represents comments. Replace the username in the directory structure with your username (eg, userr) and the email address to your email address. Change the Ansys Script File Name to the name of the Ansys file that you want to be executed on the cluster.

Please Note: For CFX and Fluent, the basic license will allow CFX or Fluent to use up to 4 cpus (or cores) without additional licenses.

Fluent Example

```
#!/bin/bash -1
#
#### set shell
#PBS -S [Name of shell including full path]
#
#### job name & output files
#PBS -N [Name of Job]
#
#### select resources
#PBS -1 select=[number of nodes or chunks required];ncpus=[number of cpus required]
#PBS -1 mem=[amount of memory required]
#PBS -1 walltime=[how long the job should run for, hh:mm:ss]
#
#### redirect error & output files
#PBS -e /home/[username]/[location]/[input (standard out) file name]
```

```
#PBS -o /home/[username]/[location]/[output (standard out) file name]
#### mail options
#PBS -m ae
#PBS -M [your email address]
#### select queue
#PBS -q default
#### load ansys module (setup environment)
module load ansys
#### specifies number of CPUs for parallel computing (must match nodes X ppn total)
nCPU=[nodes X ppn]
#### specifies the version of ANSYS FLUENT (2d: 2-Dimension; 3d: 3-Dimension)
version=[2d or 3d]
#### specifies journal file (simulation input)
journal=[journal name]
#### change to current working directory
cd $PBS O WORKDIR
#### execute program
fluent $version -t${NPROCS} -cnf=$PBS NODEFILE -g -i $journal
```

Executing script on the cluster

The USQ HPC Cluster uses a job scheduler that allows you to schedule and run jobs on the various compute nodes. To submit a job, simply execute the command: *qsub* [*pbs_script_file*]. A handy command, to check if your job is running, queued or completed is by using the command qstat.

Setting Up Ansys for the first time

Before being able to use any of the software above for the first time, each user needs to set his/her own license to "academic license". This is only need to be done once.

Here is how, open up the license manager by running this executable:

/usr/local/ansys_inc/shared_files/licensing/lic_admin/anslic_admin It will open ANSLIC_ADMIN Utility (GUI interface), then:

- select "Set License Preferences for User XXXXX" button
- select "12.1"
- Under Global settings, select "Use Academic Licenses"
- Click "Ok"
- Close the ANSLIC_ADMIN Utility by clicking on the top right "X"

References:

- 1. Ansys Fluent Website
- 2. <u>CFD Lab BluWiki</u>
- 3. CFX Tutorials
- 4. Ansys CFX v13 Tutorial