

HPCC - Hrothgar

Getting Started User Guide – Abaqus



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User Guide

1. Introduction

Abaqus software suite delivers accurate, robust, high-performance solutions for challenging nonlinear problems, large-scale linear dynamics applications, and routine design simulations. Its unmatched integration of implicit and explicit FEA capabilities enables you to use the results of one simulation directly in a subsequent analysis to capture the effects of prior history, such as manufacturing processes on product performance. Abaqus software suite's official website is http://www.simulia.com/products/abaqus_fea.html. Currently the Abaqus 6.9-2 is installed on Hrothgar. This is a licensed application. Users should obtain authorization to use it from Mechanical Engineering department.

2. Setting the environment

Hrothgar is equipped with SoftEnv to set up the environment with minimum work by users. The use of SoftEnv is not required but highly recommended by HPCC staff. For more information about Softenv, please refer to the user guide "User's Environment" at HPCC user guides page <http://www.hpcc.ttu.edu/php/NewUser.php>.

First, users can check whether the environment variables for Abaqus are set by command *which abaqus*. If it returns `/lustre/work/apps/abaqus/Commands/abaqus` like the screen shot below, the environment variables are set correctly, skip this section and go to Section 3 Job Submission.



```
1:hrothgar.hpcc.ttu.edu - default - SSH Secure S...
File Edit View Window Help
[Icons]
Quick Connect Profiles
hrothgar:~$ which abaqus
/lustre/work/apps/abaqus/Commands/abaqus
hrothgar:~$
Connected to hrothgar.hpcc.ttu.edu  SSH2 - aes128-cbc - hmac-md5
```

If it returns message like "no abaqus found", then follow the below steps to set up the environment variables.

To set up abaqus environment variables in current session:

\$ soft add +abaqus

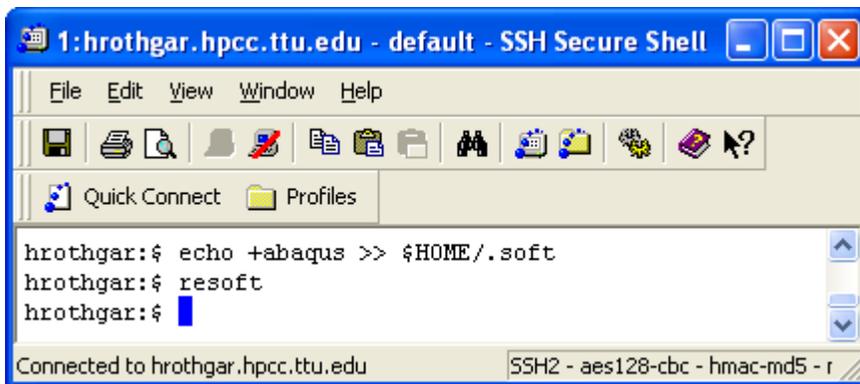
Type “which abaqus” to verify that abaqus command can be found as in the screen shot. In this way the environment variables is valid only in the current session. It expires when the user logs out.

To set up abaqus environment variables permanently:

To make path changes permanent and consisted across all nodes, execute the following commands:

```
$ echo +abaqus >> $HOME/.soft
```

```
$ resoft
```



The screenshot shows a terminal window titled "1:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell". The terminal displays the following commands and their outputs:

```
hrothgar:$ echo +abaqus >> $HOME/.soft
hrothgar:$ resoft
hrothgar:$
```

The status bar at the bottom of the window indicates "Connected to hrothgar.hpcc.ttu.edu" and "SSH2 - aes128-cbc - hmac-md5 - r".

3. Job Submission

3.1. Non-interactive (batch) jobs

An example of job submission script and input file is available at `/lustre/work/apps/examples/abaqus`.

3.1.1. Step 1 – copy examples as test programs

To test this example, first copy the directory to the user’s work space by the following command:

```
$cp -r /lustre/work/apps/examples/abaqus abaqus
```

There are two files in this directory, `abaqus.sh` and `tutorial.inp`. `tutorial.inp` is the input file, and it is obtained from an Abaqus tutorial web page <http://www.engin.brown.edu/courses/en175/abagustut/abagustut.htm>. `abaqus.sh` is used for submitting an Abaqus job with input file `tutorial.inp`.

```

hrothgar:/examples$ cp -r /lustre/work/apps/examples/abaqus abaqus
hrothgar:/examples$ cd abaqus
hrothgar:/examples/abaqus$ ls
abaqus.sh  tutorial.inp

```

The file `abaqus.sh` looks like the below. The lines starting with “#” are Sun Grid Engine settings. In this case, the job’s name is `abaqus` (`# -N abaqus`), the job is submitted to “normal” queue (`# -q normal`), and it requested for 12 cores (`# -pe fill 12`). The command line is “`abaqus job=tutorial input=tutorial.inp scratch=$SCRATCH cpus=$NSLOTS interactive`”. Users may modify the command line for their own input files.

```

#!/bin/sh
#$ -V
#$ -cwd
#$ -S /bin/bash
#$ -N abaqus
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q normal
#$ -pe fill 12
#$ -P hrothgar
abaqus job=tutorial input=tutorial.inp scratch=$SCRATCH
cpus=$NSLOTS interactive

```

3.1.2. Step 2 – `qsub` to submit jobs

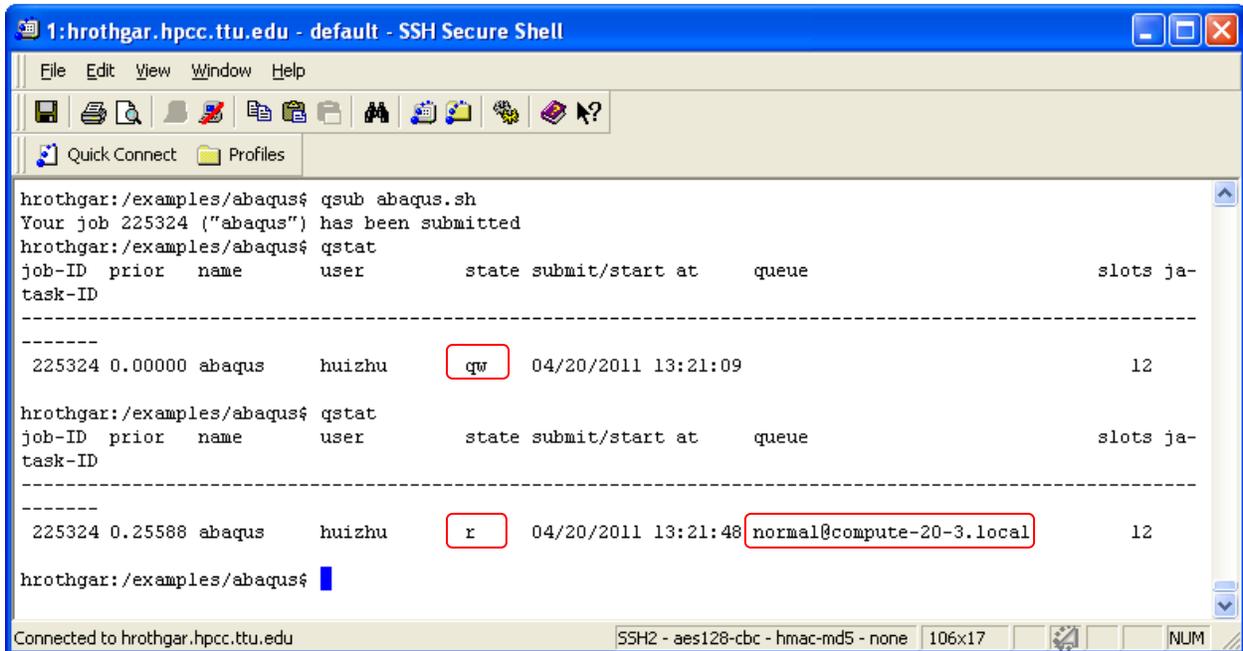
To submit the job, run command:

```
$ qsub abaqus.sh
```

To check the status of the job:

```
$qstat
```

The following snapshot shows the procedure of submitting a job and checking its status. The first `qstat` command shows that the job is in state “`qw`”, which means the job is waiting in the queue. The second `qstat` command shows that the job is in state “`r`”, which means it is running in normal queue, on the node `compute-20-3.local`.



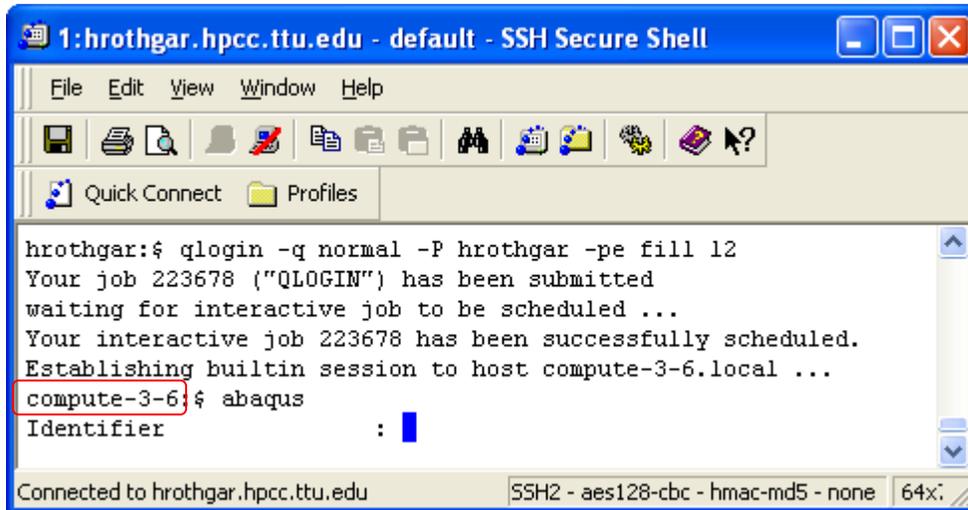
```
1:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
hrothgar:/examples/abaqus$ qsub abaqus.sh
Your job 225324 ("abaqus") has been submitted
hrothgar:/examples/abaqus$ qstat
job-ID prior name user state submit/start at queue slots ja-
task-ID
-----
225324 0.00000 abaqus huizhu qw 04/20/2011 13:21:09 12
hrothgar:/examples/abaqus$ qstat
job-ID prior name user state submit/start at queue slots ja-
task-ID
-----
225324 0.25588 abaqus huizhu r 04/20/2011 13:21:48 normal@compute-20-3.local 12
hrothgar:/examples/abaqus$
Connected to hrothgar.hpcc.ttu.edu SSH2 - aes128-cbc - hmac-md5 - none 106x17 NUM
```

3.2. Interactive jobs

3.2.1. Non-GUI jobs

A user can start using Abaqus without the graphical user interface (GUI) by submitting an interactive job. Run the following command `qlogin -q normal -P hrothgar -pe fill 12` to start an interactive job, if there are available nodes, the system will schedule the job to a compute node shortly. Otherwise the user has to wait and check back where there are available nodes.

The screen shot below illustrated the procedure. In this particular case, the job is scheduled to node compute-3-6. The user may type “abaqus” or other commands to start an Abqus job. When the job finishes, the user can start another abaqus job, or end the interactive job by command “*exit*”.



```
1:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
hrothgar:~$ qlogin -q normal -P hrothgar -pe fill 12
Your job 223678 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 223678 has been successfully scheduled.
Establishing builtin session to host compute-3-6.local ...
compute-3-6:~$ abaqus
Identifier          :
```

3.2.2. GUI jobs

To take advantage of Abaqus's graphical user interface, one can submit interactive jobs with X window. The following steps submit an interactive job to a node, and the user can invoke Abaqus's graphical interface on that node.

First, set up X-win32 for X window forwarding. Refer to the user guide Installing X-Windows server on the user guides page <http://www.hpcc.ttu.edu/php/NewUser.php>.

Second, figure out the IP address of the local computer.

```
env | grep SSH_CLIENT
```

This command returns the IP address of the local computer like:

```
SSH_CLIENT=129.118.104.202 2735 22, where 129.118.104.202 is the required IP address.
```

Third, run command qlogin to start an interactive job.

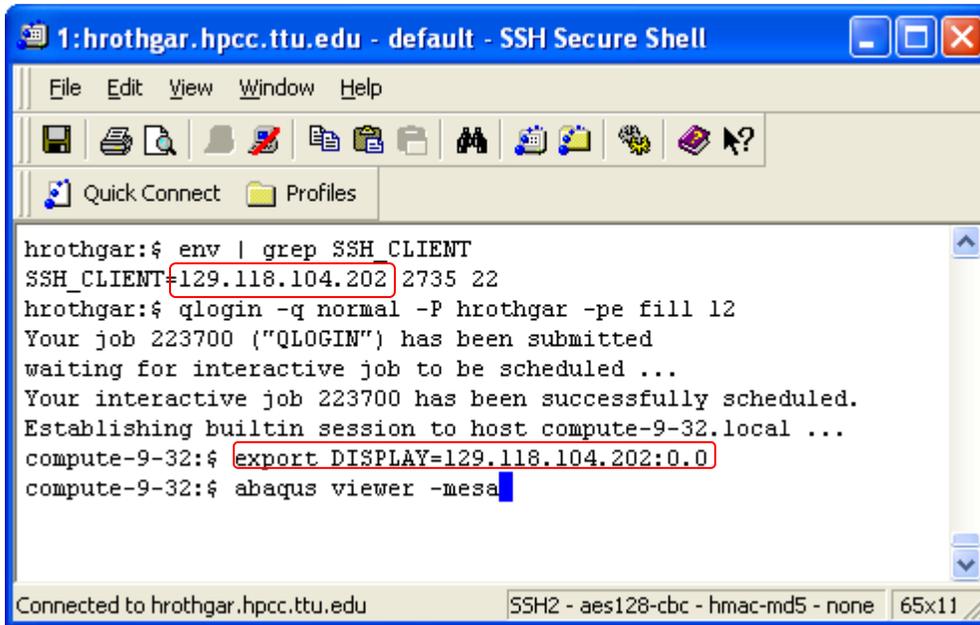
```
qlogin -q normal -P hrothgar -pe fill 12
```

Sun Grid Engine will schedule a free node for his job. When the terminal is brought to a specific node, the user needs to export the DISPLAY environment variable by the command:

```
export DISPLAY=<IP>:0.0
```

The <IP> field in the command is the IP address figured out by the above step.

Now the user can invoke Abaqus/Viewer by typing the command **abaqus viewer -mesa**, or invoke Abaqus/CAE by command **abaqus cae -mesa**.



```
1:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
hrothgar:~$ env | grep SSH_CLIENT
SSH_CLIENT=129.118.104.202 2735 22
hrothgar:~$ qlogin -q normal -P hrothgar -pe fill 12
Your job 223700 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 223700 has been successfully scheduled.
Establishing builtin session to host compute-9-32.local ...
compute-9-32:~$ export DISPLAY=129.118.104.202:0.0
compute-9-32:~$ abaqus viewer -mesa
```

Connected to hrothgar.hpcc.ttu.edu SSH2 - aes128-cbc - hmac-md5 - none 65x11

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For Additional Assistance Contact: hpccsupport@ttu.edu

For Comments/Suggestions on user guide hpcc@ttu.edu