# MANUAL OVERVIEW

This document describes the function and use of the ‘hpcq’ script at AAM. This script is used as a backup for job submission of Abaqus, Nastran, StartCCM+, Optistruct and Magma jobs to the CAE compute clusters at WHQ, PBO, and EHQ.

In addition , this version supports ADAMS and OPTISTRUCT on the CAE WHQ cluster.

The batch manager is IBM LSF for most jobs (Abaqus and Nastran). Optistruct and StarCCM+ jobs can also be submitted to the Altair cluster at WHQ (AltairApp/hwul2).

## MANUAL

The HPCQ CAE batch job submission script **hpcq** is located in ***/usr/local/bin/*** on each of the following servers:-

whqlx40, punlx07,fralx07 – **Production** whqlx20 - **Development**

The script has a help option (-h) that lists out all the command line options:

**Example:** mckenns@whqlx20:~> hpcq.v17 -h

cmd -v -a -i -q -m -n –p -j -s –c –b -h --

-v verbose displays some additional messages, mostly used for debugging.

-a Application to run, Abaqus Check, Abaqus Solve

Nastran, Optistruct, StarCCM+ etc...

-i Input file name (current directory, or FQ directory/filename)

-q LSF batch queue name. e.g. q16

-m host ( generally a ‘lsfchoice’ or an LSF host group for the type of job

e.g. twin\_oct for 16 core servers)

-n Number of CPUs . e.g. 16

-h help

-b ask for a date and time to run your job, or enter a date immediately after ‘-b’

e.g. ‘-b “tomorrow 8am”

-b date=(pretty free format, but with rules of ‘date’ command)

-c HPCQ configuration file to use, it not the default one.

-f FORTRAN subroutine file name (obsoleted)

(More options for ABAQUS and OPTISTRUCT jobs on the following pages

These are invoked with ‘-j {some option} and a value or sometimes ‘=value’)

If none of the above are entered , the script will prompt via a series of menus determined by a configuration file for the information needed to submit a job. A minimum of an Application, input file and number of CPUs are required for all jobs. In some cases, the options are mandatory, in other cases optional, depending on how the option is save in the configuration file.

The LSF queue may be calculated by the script, or left up to LSF to choose.

The other options, may, or may not be requested, depending on the Application and type of job.

The script reads in a configuration file (from /usr/local/SAetc named hpcq.conf), which

Controls which applications and options a user can pick. The same script can use different configuration files for different purposes.

*As of 7.6, config file is /usr/local/SAetc/hpcq.conf.menu2 and /usr/local/SAetc/magma.env for Magma environment variables.*

ABAQUS JOB OPTIONS

-j Job options

* Submodels multiple submodel input files are embedded in the input file.

These are copied to the compute host as part of the job.

* Fortran files ‘-j user=xxx.f’ file ‘xxx.f’ being a FORTRAN source file which is

copied to the compute node and compiled as part of the job.

* Old Job ‘oldjob=yyy.odb’. The current directory is searched for the ‘yyy.odb’ file

And all files named ‘yyy.\*’ are copied to the compute node as part of the job. Multiple ‘oldjob’ options are allowed.

* Precision ‘-j double=zzz’ where ‘zzz’ is one of {explicit|both|off|Constraint}.
* GPU ‘-j gpu=1’ a compute node with a GPU is required for this job.
* Global Model ‘-j globalmodel=aaa.inp’ (not sure about this. S.M.)

-p ‘parallel’ job. Default is ‘domain’

-s Model (q2mx) or small job (q2)

OPTISTRUCT JOB OPTIONS

-j Job options

* GPU ‘-j gpu=Y’ a compute node with a GPU is required for this job.
* MMO ‘-j mmo’ The user will be prompted for THREADS (-nt x) and PROCS (-np y) options

**Using the HPCQ script**

*The following are the steps that are executed to use the tool:*

*The below if for the ‘prompting’ usage.*

1. **/usr/local/bin** should part of every user’s **PATH** environment. if not, type

**export PATH=$PATH:/usr/local/bin**

1. Execute **hpcq** command

**Example:**

HPC queuing submit command.

Please choose one of the following applications:

1. Abaqus syntax check

2. Abaqus

3. Nastran

4. Optistruct

5. Magma

6. StarCCM+

7. ADAMS

q. Quit

**( Optistruct, Magma, and StarCCM+ options will not show up unless the user is part of the corresponding ‘optistruct’, ‘magma’, or ‘starccm’ Unix groups)**

1. Abaqus syntax check (calls /usr/local/bin/abaquscheck2017\_v2.1.sh -i $INPUT -v ${ABAQUS\_VER}

**Example:**

Please enter your choice [2]:1

Select one of the following files or key in a complete file specification...

teptu-op1-rev.inp

A list on files with a ‘inp’ extension in the current directory is provided.

Double click on to select it and paste it after cursor.

Please enter Input file:teptu-op1-rev.inp

creating job submission script for input file teptu-op1-rev.inp...

/tmp/hks.mckenns.3110

copying script to server...

hks.mckenns.3110 100% 2659 2.6KB/s 00:00

submitting script to LFS on server...

Job <146452> is submitted to queue <q1>.

An Abaqus syntax check job is submitted via IBM LSF to the current CAE cluster

The job terminates and sends and email to the requestor, if the ‘.forward’ is setup for their Unix account, otherwise it is left on the execution host.

**Example(c’t’d):**

mckenns@whqlx02:~> bjobs -l 146452

Job <146452>, User <mckenns>, Project <default>, Job Group </teptu-op1-rev.inp.

3110>, Status <DONE>, Queue <q1>, Command </tmp/hks.mckenn

s.3110>

Wed Aug 15 10:21:35: Submitted from host <whqlx02.aam.net>, CWD <$HOME>, Copy F

iles "/tmp/hks.mckenns.3110 > /tmp/hks.mckenns.3110", Spec

ified Hosts <abaqchk>;

Wed Aug 15 10:21:38: Started on <whqlx04.aam.net>, Execution Home </home/mckenn

s>, Execution CWD </home/mckenns>;

Wed Aug 15 10:21:42: Done successfully. The CPU time used is 0.9 seconds.

SCHEDULING PARAMETERS:

r15s r1m r15m ut pg io ls it tmp swp mem

loadSched - - - - - - - - - - -

loadStop - - - - - - - - - - -

RESOURCE REQUIREMENT DETAILS:

Combined: select[type == any] order[r15s:pg]

Effective: select[ type == any] order[r15s:pg]

1. Abaqus solve options (calls /usr/local/bin/qabaq2.2017\_v3.5.sh -i ${INPUT} -q $QUEUE -n $CPUS ${JOB\_OPTIONS} ${PARALLEL} -v ${ABAQUS\_VER} -m ${HOST}

**Example:**

Please enter your choice [2]:2

Enter the number of processors to use:

1. Four

2. Four with FORTRAN subroutine

3. Twelve

4. Twelve with Model Validation (run time <= 60 minutes

5. Sixteen

6. Sixteen with Explicit run queue

7. Sixteen with FORTRAN subroutines

8. Sixteen with submodels

q. Quit

Please enter your choice :

* The above options, and others are customized to sites by reading in a configuration file

(/usr/local/SAetc/hpcq.conf.menu2) . (see Appendix 1)

* Options with FORTRAN will prompt for an additional FORTRAN subroutine file (extension ‘.f’) and this will be copied to the execution host and the Abaqus options added to the script that is submitted.
* Options with ‘Explicit’ can now run on any 16/24 core HPE or Dell compue node, using the ‘mp\_mode=threads’ option on the ABAQUS command line.
* Options with ‘submodels’ will prompt the user for any files with extension (\*.odb) that they wish to attach to the job. (\*.odb files are created as output from Abaqus solve jobs, so these files were created previously and are now being used as part of this job)
* Options with ‘Oldjob’ will prompt for a file name with extension (.odb), however all of the files of the same name will be copied and included in this job.
* User can enter an input file name from the current working directory, or a fully qualified file name, =including directory path to file name.
* All scratch output, excepting the log file is copied back to the input location on termination.
* If the input location, (e.g. /caehome/user/..) is mounted on the compute node where the job is running, the output is copied to the input location directly over NFS, rather than ‘scp’ .

1. Nastran options

calls /usr/local/bin/qnxnastran1102.3.sh -i $INPUT -node ${HOST} -v ${NXNAST\_VER} ${JOB\_OPTIONS}

Prompts for a file with either (.dat) or (.pdf) extension.

* It may prompt for a Nastran Version if there are multiple versions listed in the configuration file

/usr/local/SAetc/hpcq.conf.

…

3. Nastran

…

Please enter your choice [2]:3

Select one of the following files or key in a complete file specification...

Cant.dat

teptu-op2-rev.dat

Please enter Input file:Cant.dat

copying script to server...

mckenns.14484 100% 1821 1.8KB/s 00:00

submitting script to LFS on server...

Job <150817> is submitted to queue <q3>.

1. Optistruct options

For the Altair cluster (hwul2 head node)

calls /usr/local/bin/qoptistruct\_v5.sh with options -i $INPUT -v ${OS\_VER}

For the CAE WHQ cluster (whqlsf head node)

/usr/local/bin/qoptistruct\_v1.sh -i $INPUT -v ${OS\_VER} ${JOB\_OPTIONS}

…

4. Optistruct

Please chose Optistruct version :

1. Optistruct 2019.1

2. Optistruct 2019.2

q. Quit

Please enter your choice [1]:

Please enter your choice [1]:

1

Please chose Cluster :

1. 2019.1 on WHQ

2. 2019.1 on hwul2

q. Quit

Please enter your choice [1]:

**(1)For the CAE WHQ cluster (whqlsf head node)**

Please chose if you want to submit an OPTISTRUCT MMO job:

1. Yes

2. No

q. Quit

Please enter your choice [1]:

Enter the number of OPTISTRUCT THREADS (default 4) :

1. Four

2. Eight

q. Quit

Please enter your choice [1]:

Enter the number of OPTISTRUCT MMO PROCS (default 4) :

1. Four

2. Eight

q. Quit

Please enter your choice [1]:

Select one of the following files or key in a complete file specification...

beam\_test\_file\_copy.fem

Please enter Input file:

**Continues to submit an Optistruct MMO job to CAE WHQ cluster)**

**If the user enters 2/N/n for the ‘Optistruct MMO’ option**

Please chose if you want to submit an OPTISTRUCT MMO job:

1. Yes

2. No

q. Quit

Please enter your choice [1]:

2

Enter the number of processors to use:

1. 10 cores

2. 16 cores

q. Quit

Please enter your choice :

**(continue to prompt for an input file and submit an LSF job to CAE WHQ cluster)**

**(2)For the Altair cluster (hwul2 head node)**

Select one of the following files or key in a complete file specification...

beam\_test\_file\_copy.fem

Please enter Input file:beam\_test\_file\_copy.fem

copying script to server...

mckenns.14369 100% 1099 1.1KB/s 00:00

submitting script to PBS on server...

Response from PAS server

878.admin

1. Magma options

Calls /usr/local/bin/magma5\_v5.4.1.sh -i ${INPUT} -q $QUEUE -n $CPUS -v ${MAGMA5\_VER} -m ${HOST} -r ${CAE\_MAGMA\_OPT}

* In addition, there is a new, 72 core (64 cores licensed for MAGMA), whqlx49.
* All MAGMA jobs will be dispatched to this server from now on.
* The MAGMA license manager still runs on whqlx777 for now.
* MAGMA DOE is enabled now with the Start/Restart menu below.
* The MAGMA user selected the number of cores via their client when they create either the

MAGMA 5.3.1 (magma5.log) file or the MAGMA 5.4.0 (magmasoft.log) file.

**Example**

mckenns@whqlx40:~> hpcq

Please choose one of the following applications [2]::

…

5. Magma

…

Please enter your choice [1]:

5

Please enter your choice:

1. Start a normal Magma job

2. Restart a previous Magma job that was dumped/stopped

q. Quit

Please enter your choice [1]:

1. StarCCM+(CMF) options

* If requesting a job on the Altair cluster

calls /usr/local/bin/qstarccmplust\_v5.sh -i $INPUT -m ${HOST} -n $CPUS -v ${STARCCM\_VER}

If requesting a job on the 64 core DL980s whqlx34/whqlx35 at WHQ

calls /usr/local/bin/qstarccmplust\_v4.2.6.sh -i $INPUT -m ${HOST} -n $CPUS -v ${STARCCM\_VER} ${JOB\_OPTIONS}

HPC queuing submit command.

Please choose one of the following applications:

…

6. StarCCM+

…

Please enter your choice [2]:6

Please choose STARCCM+ version:

1. STARCCM+12.04.010

2. STARCCM+12.04.010 on hwul2

q. Quit

Please enter your choice [1]:

Enter the number of processors to use:

1. Four

2. Eight

3. Sixteen

4. Thirty two

5. Forty eight

6. Sixty four

q. Quit

Please enter your choice :

or [2]

Please enter your choice [1]:2

Enter the number of processors to use:

1. Twenty eight

2. Fifty six

3. Eighty four

4. One Hundred and twelve

q. Quit

Please enter your choice :

1. ADAMS 2019.2

Calls /usr/local/bin/qadams\_v1.sh -i $INPUT -v ${ADAMS\_VER}

ADAMS uses 8 tokens/cores, so 3 ADAMS jobs can run on a 24 core server, 2 on a 16 core server

7. ADAMS 2019.2

q. Quit

Please enter your choice [1]:

7

Select one of the following files or key in a complete file specification...

bar10.acf

…

Host name: whqlx20

SERVER: whqlsf

creating job submission script for input file bar10.acf...

Input : bar10.acf

Input File: bar10.acf

Job Group:bar10.acf.23561

Current Directory:/caehome/mckenns/CAE\_Folder/adams

INCNAME: whqlx20://caehome/mckenns/CAE\_Folder/adams/bar10

copying script to server...

adams.mckenns.23561 100% 4131 4.0KB/s 00:00

submitting script to LSF on server...

Job <202702> is submitted to queue <q8adams>.

1. Glossary:
   1. HPC – High Performance Cluster. Generally refers to either or both WHQ and PUNE HPC servers list earlier.
   2. LSF – Platform LSF is an IBM product to manage batch job submission for

e.g. Abaqus, Nastran, StartCCM, etc Engineering jobs.

* 1. SIO – Southfield Michigan IT office

# CHANGE LOG

Add change log information whenever approved procedure is changed.

|  |  |  |  |
| --- | --- | --- | --- |
| DATE | CHANGED BY | CHANGE DESCRIPTION | VERSION |
| 02/08/2019 | S. McKenna | Created Man page | 7.6 |
| 02/08/2019 | S. McKenna | Updated for Explicit and MAGMA DOE | 7.6.1 |
| 04/30/2020 | S.McKenna | Updated to v17 with ADAMS and OPTISTRUCT at WHQ | 17 |

**Appendix 1. (hpcq.conf or similar configuration file)**

BOL="-n"

# ------------------------------------------------------------------------- #

# CAE\_APPS="abaqchk,abaq,nxnastran,optistruct" #

# This variable controls which applications the user can select from the #

# menu. The valid options are listed above, so 'xoptistruct' will not match #

# and will not show up as a valid selection. #

# If the user forces the option (enters 4), the script will exit with #

# an error message. S. McKenna. #

# ------------------------------------------------------------------------- #

# LSF head node and cluster name. Possible values below #

# export CLUSTER="AAM\_WHQ\_cluster1 AAM\_PBO\_cluster1 AAM\_EHQ\_cluster1" #

# export HEAD\_NODE="whqlx02 punlx01 fralx03" #

# ------------------------------------------------------------------------- #

export CLUSTER="AAM\_WHQ\_cluster1"

export HEAD\_NODE="whqlx02"

# ------------------------------------------------------------------------- #

# Main menu of applications: This is an array of values of applications and #

# their descriptions that will show on the corresponding menus below. #

# The array below will control how the applications are displayed to the #

# user for the new hpcq.v7 version #

# ------------------------------------------------------------------------- #

CAE\_APPS\_OK=( Y Y Y Y Y Y N N N)

CAE\_APPS=( "abaqck" "abaq" "nxnastran" "optistruct" "magma" "starccm" \

"seven" "Eight" "Nine" )

# ------------------------------------------------------------------------- #

# Descriptions that will show on the menu that correspond to the above #

# ------------------------------------------------------------------------- #

# Note: we can have up to 9 applications, hence the last three names #

# "Seven", "Eight", and "Nine" are just placeholders. #

# ------------------------------------------------------------------------- #

#

#CAE\_APPSA=( "Abaqus syntax check" "Abaqus Solve" "Nastran" "Optistruct" "Magma" "StarCCM+" "Seven" "Eight" "Nine" )

CAE\_APPSA=( "Abaqus syntax check" "Abaqus Solve" "Nastran" "Optistruct" \

"Magma" "StarCCM+" "Seven" "Eight" "Nine" )

# ------------------------------------------------------------------------- #

# These variables determine the various ABAQUS jobs/CPU combinations that #

# can be submitted by the user. An entry of "N" means it will not show up #

# and is not selectable by the user. #

# ------------------------------------------------------------------------- #

ABAQ\_CPUS=( Y Y N N Y Y Y Y N )

ABAQ\_CPUS=( Y Y N N Y Y Y Y Y N )

ABAQ\_CPUSnum=( 4 4 12 12 16 16 16 16 16 16)

ABAQ\_FORTRAN=( N Y N N N N Y N N Y )

ABAQ\_SUBMODEL=( N N N N N N N Y N N )

ABAQ\_OLDJOB=( N Y N N N N Y N Y Y )

#ABAQ\_CPUSA=( "Four" "Four with FORTRAN subroutine" "Twelve " "Twelve with Model Validation (run time <= 60 minutes" "Sixteen" "Sixteen with Explicit run queue" "Sixteen with FORTRAN subroutines" "Sixteen with subroutines" "job")

ABAQ\_CPUSA=( "Four" "Four with FORTRAN subroutine and OLDJOB" "Twelve " \

"Twelve with Model Validation (run time <= 60 minutes" "Sixteen" \

"Sixteen with Explicit on any 16 core node" "Sixteen with FORTRAN subroutines and OLDJOB" \

"Sixteen with submodel (odb)" "Sixteen with Explicit on any node with restart (oldjob)" "16 core with FORTRAN and oldjob" )

#ABAQ\_CPUSque=( q2 q2 q5 q5mx q16 q16explicit q16 q16 q16test )

ABAQ\_CPUSque=( q2 q2 q5 q5mx q16 q16 q16 q16 q16 q16 )

# ------------------------------------------------------------------------- #

# The only reason for the below array is to align with the menu options for #

# 'Explicit' ABAQUS solves and change the mp\_mode to 'threads' so that the #

# jobs don't loop on IB connected compute nodes and run forever. #

# q16explicit above is changed to q16 so we can run 'explicit' jobs on any #

# of the ABAQUS compute nodes, not just the HPE ones. #

# ------------------------------------------------------------------------- #

ABAQ\_CPUSexpl=( N N N N N Y N N Y N )

ABAQ\_CPUShost=( twin\_dual twin\_dual lsfchoice )

# ------------------------------------------------------------------------- #

# It's possible to have multiple application versions show up in a menu #

# if the xxx\_VERS array is only one entry, the user will not be prompted #

# to select a version #

# ------------------------------------------------------------------------- #

ABAQUS\_VERSA=( "ABAQUS 6.14.2" "ABAQUS 2017" )

ABAQUS\_VERS=(abq6142 abq2017 )

# ------------------------------------------------------------------------- #

# overwrite with a single version. see above

# ------------------------------------------------------------------------- #

ABAQUS\_VERS=(abq2017 )

ABAQUS\_VER="abq6142"

NXNAST\_VER="nxnastran91"

# ------------------------------------------------------------------------- #

# It's possible to have multiple application versions show up in a menu #

# if the xxx\_VERS array is only one entry, the user will not be prompted #

# to select a version #

# ------------------------------------------------------------------------- #

NXNAST\_VERSA=( "NASTRAN 9.1" "NASTRAN 11.0.2" )

NXNAST\_VERS=( nxnastran91 nxnastran11.0.2 )

#NXNAST\_VERS=( nxnastran91 )

NXNAST\_VERS=( nxnastran91 )

# ------------------------------------------------------------------------- #

# #

# ------------------------------------------------------------------------- #

MAGMA\_VER="v5.3.1"

# ------------------------------------------------------------------------- #

# Optistruct application on the Altair appliance (head node hwul2) #

# ------------------------------------------------------------------------- #

#OS\_VER="12.0.212" # Legacy Optistruct HM version

OS\_VER="13.0"

OS\_VERS=( 12.0.212 13.0 )

OS\_VERS=( 13.0 )

OS\_VERSA=( "Optistruct 12.0.212" "Optistruct 13.0" )

# ------------------------------------------------------------------------- #

# It's possible to have multiple application versions show up in a menu #

# ------------------------------------------------------------------------- #

STARCCM\_VER="12.04.010-R8"

STARCCM\_VERS=( 12.04.010-R8 12.04.010-R8 )

STARCCM\_VERS=( 12.04.010-R8 )

STARCCM\_VERSA=( "STARCCM+12.04.010-Rx" "STARCCM+12.04.010-R8" )

STARCCM\_Cluster=( "on WHQ 64 core systems" "on Altair Appliance(hwul2)" )

STARCCM\_Cluster=( "" "on hwul2" )

# ------------------------------------------------------------------------- #

# The following variables are used to manage the STARCCM+ menus

# ------------------------------------------------------------------------- #

STARCCM\_CPUS=( N N Y Y Y Y )

STARCCM\_CPUS=( Y Y Y Y Y Y )

STARCCM\_CPUSnum=( 4 8 16 32 48 64 )

#STARCCM\_CPUSmenu=( 1 2 3 4 5 6 )

STARCCM\_CPUSA=( 'Four' 'Eight' 'Sixteen' 'Thirty two' 'Forty eight' 'Sixty four' )

# ------------------------------------------------------------------------- #

# The following variables are used to manage the ALTAIR STARCCM+ menus

# ------------------------------------------------------------------------- #

STARCCM\_CPUS\_Altair=( Y Y Y Y )

STARCCM\_CPUSnum\_Altair=( 28 56 84 112 )

#STARCCM\_CPUSmenu\_Altair=( 1 2 3 4 )

STARCCM\_CPUSA\_Altair=( 'Twenty eight' 'Fifty six' 'Eighty four' 'One Hundred and twelve' )

#CAE\_APP="abaqchk"

# ------------------------------------------------------------------------- #

# Some default environment variables for the HPCQ script #

# ------------------------------------------------------------------------- #

CAE\_APP=""

QUEUE="q2"

CPUS=""

EOL="\c"

FESAFE\_EXE="N"

FILE\_SEARCH="\*.inp"

HOST="lsfchoice"

INPUT=""

JOB\_OPTIONS=""

SUB\_HOST=$(uname -n)

USER=$(whoami)

**Appendix 2. (magma.env or similar file)**

MAGMA\_VER="v5.3.1"

MAGMA\_VER="v5.4.0"

MAGMA\_VERS=( "v5.3.1" )

MAGMA\_VERS=( "v5.3.1" "v5.4.0" )

MAGMA\_VERSA=( "MAGMA 5.3.1" "MAGMA 5.4" )

MAGMA\_Cluster=( "on WHQ 16 core queue " "on WHQ 64 core server (whqlx49)" )

#MAGMA\_Cluster=( "" "on hwul2" )

# The following variables are used to manage the MAGMA+ menus

MAGMA\_CPUS=( N Y )

MAGMA\_CPUSnum=( 16 64 )

MAGMA\_CPUSA=( 'Sixteen on any MAGMA compute node' 'Sixty four on whqlx49' )

MAGMA\_CPUSque=( q16m q64m )