

Using Job Arrays on Hydra (slides, long version)

In the intro portion of the workshop you will learn:

- What are job arrays, when and why use them?
- How to write job arrays scripts.
- How to submit job arrays:
 - task range, increment and limit concurrent tasks.
- Job arrays tips and tricks.
- Parallel job arrays.
- How to consolidate small tasks in job arrays.
- How to manage job arrays:
 - `qstat(+)`, `qdel`, `qalter`, `qacct(+)`.
- HPC wiki on job arrays:
 - <https://confluence.si.edu/display/HPC/Job+Arrays>

Introduction

What are job arrays, when and why use them?

- Job arrays allow you to run the same job file multiple times in a single job submission.
- They are typically used for running a given analysis on different input files or parameters.
- They allow you to use the same job file and a single qsub to run a type of analysis instead of writing a myriad of very similar job files.
- Job arrays have each a unique job id with multiple task ids

How to write job arrays scripts

A trivial example

- Job array scripts, or job files, are like any other job file, except that they have a task identifier stored in the variable `SGE_TASK_ID`
- Example:

```
echo + `date` $JOB_NAME started on $HOSTNAME in $QUEUE \  
  with jobID=$JOB_ID and taskID=$SGE_TASK_ID  
model < model.$SGE_TASK_ID.inp  
echo = `date` $JOB_NAME for taskID=$SGE_TASK_ID done.
```

this example runs `model` using the input file `model.N.inp`

How to submit job arrays

That trivial example can be queued on 100 tasks with

```
qsub -t 1-100 trivial_example.job
```

Your job-array NNNNNN.1-100:1 ("trivial_example.job") has 1

this queues one job with 100 tasks, or the equivalent of 100 job files with

```
model < model.1.inp
```

in test1.job

```
model < model.2.inp
```

in test2.job, etc..., up to

```
model < model.100.inp
```

in test100.job - hence one job file instead of 100.

this assumes that you have 100 input files called model.1.inp, model.2.inp, ... , model.100.inp

A more complete job array file

task range and limit concurrent tasks: csh syntax

```
# /bin/csh
#
## -N model-100 -cwd -j y -o model.$TASK_ID.log
## -t 1-1000 -tc 100
#
echo + `date` $JOB_NAME started on $HOSTNAME in $QUEUE \
  with jobID=$JOB_ID and taskID=$SGE_TASK_ID
#
set INPUT  = model.$SGE_TASK_ID.inp
set OUTPUT = model.$SGE_TASK_ID.out
./model < $INPUT > $OUTPUT
#
echo = `date` $JOB_NAME for taskID=$SGE_TASK_ID done.
```

task range and limit concurrent tasks: sh syntax

```
# /bin/sh
#
## -N model-100 -cwd -j y -o model.$TASK_ID.log
## -t 1-1000 -tc 100
#
echo + `date` $JOB_NAME started on $HOSTNAME in $QUEUE \
  with jobID=$JOB_ID and taskID=$SGE_TASK_ID
#
INPUT=model.$SGE_TASK_ID.inp
OUTPUT=model.$SGE_TASK_ID.out
./model < $INPUT > $OUTPUT
#
echo = `date` $JOB_NAME for taskID=$SGE_TASK_ID done.
```

Note

- Task range and max concurrent task embedded in the script
`-t 1-1000 -tc 100`
- Different log file and output file for each task
`-o model.$TASK_ID.log`

```
INPUT=model.$SGE_TASK_ID.inp  
OUTPUT=model.$SGE_TASK_ID.out  
./model < $INPUT > $OUTPUT
```

- Also:
 - use `$TASK_ID` in embedded `-o` directive
 - use `$SGE_TASK_ID` in the script

Job arrays tips and tricks

Various ways of using the task id `$SGE_TASK_ID`

- 1 formatting trick
- 2 using `awk`
- 3 using `sed`
- 4 using `bc`
- 5 using `cd`
- 6 using `<<EOF`
- 7 using your own tool (`sh`, `csch`, `awk`, `perl`, `python`, `C`, `Fortran`, ...)

Formatting: replacing 1,2,...,100 by 001,002,...,100

- csh syntax

```
@ i = $SGE_TASK_ID  
set I = `echo $i | awk '{printf "%3.3d", $1}'`
```

- sh syntax

```
let i=$SGE_TASK_ID  
I=$(echo $i | awk '{printf "%3.3d", $1}')
```

Using awk to extract parameters from a single file

- csh syntax

```
@ i = $SGE_TASK_ID  
set P = (`awk "NR==$i" parameters-list.txt`)
```

- sh syntax

```
let i=$SGE_TASK_ID  
P=$(awk "NR==$i" parameters-list.txt)
```

- the variable P will hold the content of the i-th line of parameters-list.txt, and can be used as:

```
./compute $P  
assuming compute takes parameters.
```

Using sed and a template

- to replace NNN in the template by the task id

- csh syntax

```
@ i = $SGE_TASK_ID
sed "s/NNN/$i/" input-template.inp > model.$i.inp
model < model.$i.inp > model.$i.out
```

- sh syntax

```
let i=$SGE_TASK_ID
sed "s/NNN/$i/" input-template.inp > model.$i.inp
model < model.$i.inp > model.$i.out
```

Using bc to run models on temperatures grid

- start at 23.72 and increase by 2.43 increments,
- replace TP by the temperature and NNN by the task id

csH syntax

```
@ i = $SGE_TASK_ID
set tp = `echo "23.72 + $i*2.43" | bc`
sed -e "s/NNN/$i/" -e "s/TP/$tp/" input-template.inp \
    > model.$i.inp
```

sh syntax

```
let i=$SGE_TASK_ID
tp=$(echo "23.72 + $i*2.43" | bc)
sed -e "s/NNN/$i/" -e "s/TP/$tp/" input-template.inp \
    > model.$i.inp
```

Using cd and different directories for each task

■ csh syntax

```
@ i = $SGE_TASK_ID  
cd task.$i  
model < model.inp > model.out
```

■ sh syntax

```
let i=$SGE_TASK_ID  
cd task.$i  
model < model.inp > model.out
```

assumes there is a model.inp file in each task.N directory

Using the <<EOF construct

■ csh syntax

```
@ i = $SGE_TASK_ID
set tp = `echo "23.72 + $i*2.43" | bc`
model <<EOF > model.$out
temp=$tp
EOF
```

■ sh syntax

```
let i=$SGE_TASK_ID
tp=$(echo "23.72 + $i*2.43" | bc)
model <<EOF > model.$out
temp=$tp
EOF
```

Using your own tool, `mytool`, to convert a task id to parameters

- csh syntax

```
@ i = $SGE_TASK_ID
set P = (`./mytool $i`)
./compute $P
```

- sh syntax

```
i=$SGE_TASK_ID
P=$(./mytool $i)
./compute $P
```

- `mytool` can be anything you want:

- any shell script, awk, perl, python, C, fortran, ...

How to consolidate small tasks in job arrays.

Why?

- Each task is started like a job, hence has the same overhead as starting one job
- Users should avoid running lots of very short tasks ($< 10\text{-}30\text{m}$)
- It is relatively easy to consolidate short tasks into longer ones, using the task increment:
 - `qsub -t 200-500:20` will run tasks with `id=200,220,240,...,500`

How?

- use the variables:

`$SGE_TASK_FIRST`

`$SGE_TASK_LAST`

`$SGE_TASK_STEPSIZE`

`$SGE_TASK_ID`

Example to consolidate short tasks

■ csh syntax

```
@ iFr = $SGE_TASK_ID
@ iTo = $iFr + $SGE_TASK_STEPSIZE - 1
if ($iTo > $SGE_TASK_LAST) @ iTo = $SGE_TASK_LAST
#
echo running model.csh for taskIDs $iFr to $iTo
@ i = $iFr
while ($i <= $iTo)
    ./model.csh $i >& model-$i.log
    @ i++
end
```

Example to consolidate short tasks

■ sh syntax

```
let iFr=$SGE_TASK_ID
let iTo=$iFr+$SGE_TASK_STEPSIZE-1
if [ $iTo -gt $SGE_TASK_LAST ]; then
    let iTo=$SGE_TASK_LAST
fi
#
echo running model.sh for taskIDs $iFr to $iTo
let i=$iFr
for ((i=$iFr; i<=iTo; i++)); do
    ./model.sh $i >& model.$i.log
done
```

assuming that

- the script `model.csh` or `model.sh` do the work and takes one argument: the id.

Parallel job arrays

Job arrays can run parallel tasks

- Each task request a parallel environment, as per the `-pe` specification:
 - `-pe mthread N` for multi-threaded
 - `-pe mpich N` or `-pe orte N` for MPI
- Check the HPC wiki for more info at <https://confluence.si.edu/display/HPC/Job+Arrays>

How to manage job arrays

job status with `qstat` or `qstat+`

- list task id(s) for running jobs - single job id
- remaining task range for queued jobs

job deletion with `qdel`

- can delete specific tasks w/ `-t` flags
- otherwise delete all the tasks: running and queued!

job modification with qalter

- supports -t and -tc flags
- use -tc if and when needed, can be used to increase its value progressively

job accounting with qacct or qacct+

- use -t flag to get info on specific task(s)
- otherwise return info on all the tasks (can be (very) long)

Also remember

Can run a lot of concurrent tasks

- separate name spaces
 - some of the tasks will run at the same time
 - should not write in the same file
- I/O contention:
 - concurrent tasks read the same file(s)?
- manage the results files
 - esp. if a lot are created in the same directory
- test on a small set of tasks first
- avoid sending emails with `-m` `abe`
 - it applies to each task (lots of emails).

Resource limits:

- * Limit of 10,000 tasks per job array,
- * Limit of 2,500 jobs per user in the queue, and
- * Limit of 25,000 jobs in the queue (for all users).

HPC wiki on job arrays

- goto <https://confluence.si.edu/display/HPC/Job+Arrays>

Hands on portion

