



bw|HPC – C5

Tutorial: Advanced (Batch) Job Scripting

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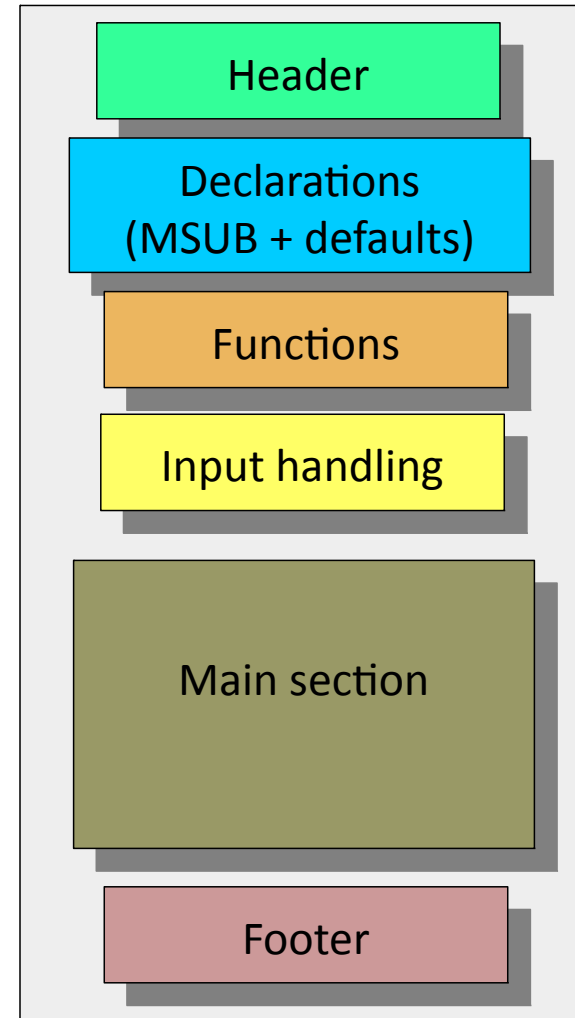
How to read the following slides

Abbreviation/Colour code	Full meaning
<code>\$ command -option value</code>	<code>\$</code> = prompt of the interactive shell The full prompt may look like: <code>user@machine:path\$</code> The <code>command</code> has been entered in the interactive shell session
<code><integer> <string></code>	<code><></code> = Placeholder for integer, string etc
<code>foo, bar</code>	Metasyntactic variables
<code>\${WORKSHOP}</code>	<code>/opt/bwhpc/kit/workshop/2016-12-06</code>



Goal

- Be descriptive!
 - Comment your code
 - e.g. via headers sections of script and functions.
 - Decipherable names for variables and functions
- Organise and structure!
 - Break complex scripts into simpler blocks e.g. use functions
 - Use exit codes
 - Use standardized parameter flags for script invocation.
- Write job script that runs **interactively**
 - Then add part for MOAB



Best Practises – Common Problems (1)

- Do not Run your code/application/job in `${HOME}`
- Multinode Job:
 - use `${WORK}`
 - Producing Tbyte of scratch files + <10000 File: [Change your application code](#)
if you do not know how:
Apply for Tiger Team Support (https://www.bwhpc-c5.de/en/zas_info_tigerteamsupport.php)
- Singlenode Job:
 - use `${TMPDIR}`: [HowTo](#) → [Case 1](#)
- Chain jobs
 - [HowTo](#) → [Case 2](#)
- Many sequential tiny jobs:
 - [Bundle to one big job: HowTo](#) → [Case 3](#)
- *Use of MPI/OpenMP Parallelisation in jobs:*
 - *[Tutorial „best practice - parallelization and compiling“](#)*

Rev: MOAB variables

■ http://www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#Moab_Environment_Variables

MOAB variables	
Environment variables	Description
MOAB_CLASS	Class name
MOAB_GROUP	Group name
MOAB_JOBID	Job ID
MOAB_JOBNAME	Job name
MOAB_NODECOUNT	Number of nodes allocated to job
MOAB_PARTITION	Partition name the job is running in
MOAB_PROCCOUNT	Number of processors allocated to job
MOAB_SUBMITDIR	Directory of job submission
MOAB_USER	User name

■ MSUB variables:

```
#!/bin/bash

#MSUB -N test
#MSUB -l advres=workshop.8,nodes=1:ppn=1,mem=50mb
#MSUB -l walltime=00:05:00
#MSUB -m n
#MSUB -v my_own_variables="arguments"
```

Case 1: Jobs @ \$TMPDIR (1)

- If temporary files of job > Gbyte → Run your job at `${TMPDIR}`
 - but ONLY if single node jobs
- What to do:
 - Generate subdirectory under `${TMPDIR}` => `${run_DIR}`
 - Copy to `${run_DIR}`
 - Change to `${run_DIR}` & program execution
 - Copy results to start DIR
- How?
 - Start with templates:

```
${WORKSHOP}/exercises/07/01_job_run_under_local_tmpdir.sh  
+  
${WORKSHOP}/exercises/07/{01_gen_files,01_gen_files.inp}
```

Case 1: Jobs @ \$TMPDIR (2)

Code snip: `${WORKSHOP}/exercises/07/01_job_run_under_local_tmpdir.sh`

```
#!/bin/bash
...
## a) Tutorial ToDo: load modules INTEL+MKL
    if not loaded

## b) Define your run directory under tmpdir
##     incorporating username and JobID/PID
mkdir -pv "${TMP}/${USER}.${MOAB_JOBID:-$$}"

## c) Tutorial ToDo: Check existence of run directory

## d) Copy files from submit directory
##     to run directory
cd $MOAB_SUBMITDIR
cp -pv gen_files.x "${TMP}/${USER}.${MOAB_JOBID:-$$}"
##     Check if copy succeeded
cp -pv gen_files.inp "${TMP}/${USER}.${MOAB_JOBID:-$$}"

## e) Change to run directory (check if succeeded) and start binary + input file
cd "${TMP}/${USER}.${MOAB_JOBID}"
./01_gen_files.x 01_gen_files.inp

## f) Tutorial ToDo: check run status

## g) transfer files to submit directory
cp -pv files_*.out "${MOAB_SUBMITDIR}"

## h) Tutorial ToDo: cleanup run_DIR
```

TASK/ToDo: 10min
* Generalise blue code
 avoiding repetition
* Write code for a-h
* Redirect output of binary



Case 1: Jobs @ \$TMP (3)

Decl. + a-c:

```
${WORKSHOP}/solutions/07/01_generalised_job_run_under_local_tmpdir.sh
```

Solution!

```
## 1) Define full path of your binary
EXE="01_gen_files.x"

## 2) Define output file
##     = Name of executable + JOBID or PID
output="$(basename ${EXE})_${MOAB_JOBID:-$$.log"

## 3) Define input files
input="01_gen_files.inp"

## 4) Define input files to be copied
copy_list="${EXE} ${input}"

## 5) Define files to be copied back after run, i.e. output file
save_list="${output} files_*.out"

## a) Load modules INTEL+MKL if not loaded
for mod in compiler/intel numlib/mkl ; do
    module list 2>&1 | grep "${mod}" >/dev/null || module load "${mod}"
done

## b) Define your run directory and generate via mkdir
run_DIR="$TMP/${USER}.${MOAB_JOBID:-$}"
mkdir -pv "${run_DIR}"

## c) Check existence of run directory
if [ ! -d "${run_DIR}" ] ; then
    echo "ERROR: Run DIR = ${run_DIR} does not exist"; exit 1
fi
```



Case 1: Jobs @ \$TMP (4)

Part d-h:

```
${WORKSHOP}/solutions/07/01_generalised_job_run_under_local_tmpdir.sh
```

Solution!

```
## d) Change to Submit Dir or PWD / Copy files from submit_DIR to run_DIR
cd "${MOAB_SUBMITDIR:-${PWD}}"
for X in ${copy_list} ; do
    cp -pv "${X}" "${run_DIR}"
    if [ $? -ne 0 ] ; then echo "ERROR: Copy of ${X} failed"; exit 1; fi
done

## e) Change to runDIR and start binary
cd "${run_DIR}"
if [ $? -ne 0 ] ; then echo "ERROR: Entering ${run_DIR} failed"; exit 1; fi
./$EXE ${input} > $output 2>&1

## f) Check run status
if [ $? -ne 0 ] ; then
    echo "WARNING: ${EXE} did not run properly!"
fi

## g) Transfer output files to submit directory
cd "${run_DIR}"
for X in ${save_list} ; do
    cp -pv "${X}" "${MOAB_SUBMITDIR}"
    if [ $? -ne 0 ] ; then echo "WARNING: Copy of ${X} failed"; fi
done

## h) Cleanup run directory
rm -f ${run_DIR}/*; rmdir ${run_DIR}; exit 0
```



Case 2: Chain Jobs (1)

- Idea:
 - Do **N** consecutive Jobs via **N** MOAB Batch Jobs
- Goal:
 - Do everything in one script
 - Submit only at the beginning
- „Pre-step“: generate script that runs interactively
 - Result: `${WORKSHOP}/exercises/07/02_chain_job.sh`

Case 2: Chain Jobs (2)

```
#!/bin/bash
## Defaults
loop_max=10
cmd='sleep 2'

## Check if counter environment variable is set
if [ -z "${myloop_counter}" ] ; then
    echo " ERROR: myloop_counter is undefined, stop chain job"; exit 1
fi
## Only continue if below loop_max
if [ ${myloop_counter} -lt ${loop_max} ] ; then
    ## Increase counter
    let myloop_counter+=1
    ## Print current Job number
    echo " Chain job iteration = ${myloop_counter}"
    ## Execute your command
    echo " -> executing ${cmd}"
    ${cmd}

    if [ $? -eq 0 ] ; then
        ## Continue only if last command was successful
        export myloop_counter=${myloop_counter}
        ./${0}
    else
        ## Terminate chain
        echo " ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
        exit 1
    fi
fi
fi
```

```
${WORKSHOP}/exercises/07/02_chain_job.sh
```

```
$ export myloop_counter=0
$ ./02_interactive_chain_job
```

Case 2: Chain Jobs (2) → How for MOAB?

```
#!/bin/bash
#MSUB ...
## Defaults
loop_max=10
cmd='sleep 2'

## Check if counter environment variable is set
if [ -z "${myloop_counter}" ] ; then
    echo " ERROR: myloop_counter is undefined, stop chain job"; exit 1
fi
## only continue if below loop_max
if [ ${myloop_counter} -lt ${loop_max} ] ; then
    ## increase counter
    let myloop_counter+=1
    ## print current Job number
    echo " Chain job iteration = ${myloop_counter}"
    ## Execute your command
    echo " -> executing ${cmd}"
    ${cmd}

    if [ $? -eq 0 ] ; then
        ## continue only if last command was successful
        export myloop_counter=${myloop_counter}
        ./${0}
    else
        ## Terminate chain
        echo " ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
        exit 1
    fi
fi
```

TASK/ToDo:5 min
* add the parts for MOAB



Case 2: Chain Jobs (3) → Solution! for Moab

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1,walltime=00:00:05,pmem=50mb
## Defaults
loop_max=10
cmd='sleep 2'

## Check if counter environment variable is set
if [ -z "${myloop_counter}" ] ; then
    echo " ERROR: myloop_counter is undefined, stop chain job"; exit 1
fi
## only continue if below loop_max
if [ ${myloop_counter} -lt ${loop_max} ] ; then
    ## increase counter
    let myloop_counter+=1
    ## print current Job number
    echo " Chain job iteration = ${myloop_counter}"
    ## Execute your command
    echo " -> executing ${cmd}"
    ${cmd}

    if [ $? -eq 0 ] ; then
        ## continue only if last command was successful
        msub -v myloop_counter=${myloop_counter} ./02_chain_job.sh
    else
        ## Terminate chain
        echo " ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
        exit 1
    fi
fi
```

Solution!

`${WORKSHOP}/solutions/07/02_chain_job.sh`

`$ msub -v myloop_counter=0 ./02_chain_job.sh`

Case 2: Chain Jobs (4)

■ moab_chain_job.sh + interactive_chain_job.sh =

```
${WORKSHOP}/solutions/07/02_generalised_chain_job.sh
```

```
. . .
. . .
if [ $? -eq 0 ] ; then
  ## continue only if last command was successful
  if [ ! -z ${MOAB_JOBNAME} ] ; then
    ## If MOAB_JOBNAME environment variable is defined
    ## -> this script is under MOAB "control"
    msub -v myloop_counter=${myloop_counter} ./generalised_chain_job.sh
  else
    export myloop_counter=${myloop_counter}
    ./${0}
  fi
else
  ## Terminate chain
  echo "  ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
  exit 1
fi
. . .
. . .
```

→ USE bash programming to **generalise** and **unify** your batch job scripts

Chain Jobs – Alternative (1)

- Problem of `moab_chain_job.sh`: **Waiting time!**

- Solution: two scripts + `msub -l depend=afterok:<jobID>`

- 1. script: `${WORKSHOP}/solutions/07/02_chain_link_job.sh`

```
#!/bin/bash
#MSUB ...

## Define your command
cmd='sleep 30'

## Execute your command
echo "  -> executing ${cmd}"
${cmd}

## Do you check if correctly terminated
if [ $? -ne 0 ] ; then
  ## Terminate chain
  echo "  ERROR: ${cmd} of chain job no. ${myloop_counter:-1} terminated unexpectedly"
  exit 1
fi
```

Chain Jobs – Alternative (2)

- 2. script: `${WORKSHOP}/solutions/07/02_moab_submitter_f_chain_job.sh`

```
#!/bin/bash
max_nojob=${1:-5}
chain_link_job=${PWD}/02_chain_link_job.sh
dep_type="${2:-afterok}"

counter=1
while [ ${counter} -le ${max_nojob} ] ; do
    ## Differ msub_opt depending on chain link number
    if [ ${counter} -eq 1 ] ; then
        msub_opt=""
    else
        msub_opt="-l depend=${dep_type}:${jobID}"
    fi

    echo "Chain job iteration = ${counter}"
    echo "    msub -v myloop_counter=${counter} ${msub_opt} ${chain_link_job}"
    ## Store job ID for next iteration by storing output of msub command with empty lines
    jobID=$(msub -v myloop_counter=${counter} ${msub_opt} ${chain_link_job} 2>&1 | sed '/^$/d')

    ## Check if ERROR occurred
    if [[ "${jobID}" =~ "ERROR" ]] ; then
        echo "    -> submission failed!" ; exit 1
    else
        echo "    -> job number = ${jobID}"
    fi

    ## Increase counter
    let counter+=1
done
```


Case 3: Pseudo Parallelisation (1)

- If you have many (>100) tiny jobs (subjobs)
 - Pack in one job (masterjob) doing:
 - Define number of Cores got by queueing system
 - Queue subjobs and assign step by step to free Cores of masterjob

Case 3: Pseudo Parallelisation - Alternative

- Parbatch → MPI task based

Example: job script

```
`${WORKSHOP}/exercises/07/03_msub_parbatch.sh
```

```
#!/bin/bash

#MSUB -l nodes=1:ppn=4
#MSUB -l mem=150mb
#MSUB -l walltime=00:03:00

module load system/parbatch

parbatch joblist.txt
```

+ joblist.txt

```
`${WORKSHOP}/exercises/07/03_joblist.txt
```

```
hostname ; sleep 2; echo "Hello 1-a"
hostname ; sleep 2; echo "Hello 2-b"
hostname ; sleep 2; echo "Hello 3-c"
hostname ; sleep 2; echo "Hello 4-d"
hostname ; sleep 2; echo "Hello 5-e"
hostname ; sleep 2; echo "Hello 6-f"
hostname ; sleep 2; echo "Hello 7-g"
hostname ; sleep 2; echo "Hello 8-h"
```

Best Practises – Batch jobs with input parsing

■ Not working:

- msub ***your_script -x argument***
→ msub will interpret -x as an own option

■ Solution:

(A) Submit wrapper script:

```
#!/bin/bash
your_script -x argument
```

(B) Export your script options and arguments to environment variable; read in that variable during runtime of script, cf. [wiki](#)

```
if [ -n "${SCRIPT_FLAGS}" ] ; then
  if [ -z "${*}" ] ; then
    set -- ${SCRIPT_FLAGS}
  fi
fi
```

(C) Use msub wrapper via:

```
$ module load system/msub_addon/1.0
$ msub <options> job.sh
```

Best Practises – Common problems (2)

- Manual defining of MPI tasks for mpirun?

- **False: Do not use if your job solely does MPI:**

- `mpirun –machinefile=file binary`

- `mpirun -n <int> binary`

- **Correct way:**

- `mpirun binary` (*because the resource manager tells mpirun what to do*)

- If you want to know about job allocated hosts in your script to:

- (A) Use msub wrapper via:

```
$ module load system/msub_addon/1.0  
$ msub <options> job.sh
```

- (B) Write loop into your batch job script → returns hostname of each task:

```
for tasks in $(srun hostname) ; do  
    echo $tasks  
done
```

Thank you for your attention!