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Tutorial:
Advanced (Batch) Job Scripting

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How to read the following slides

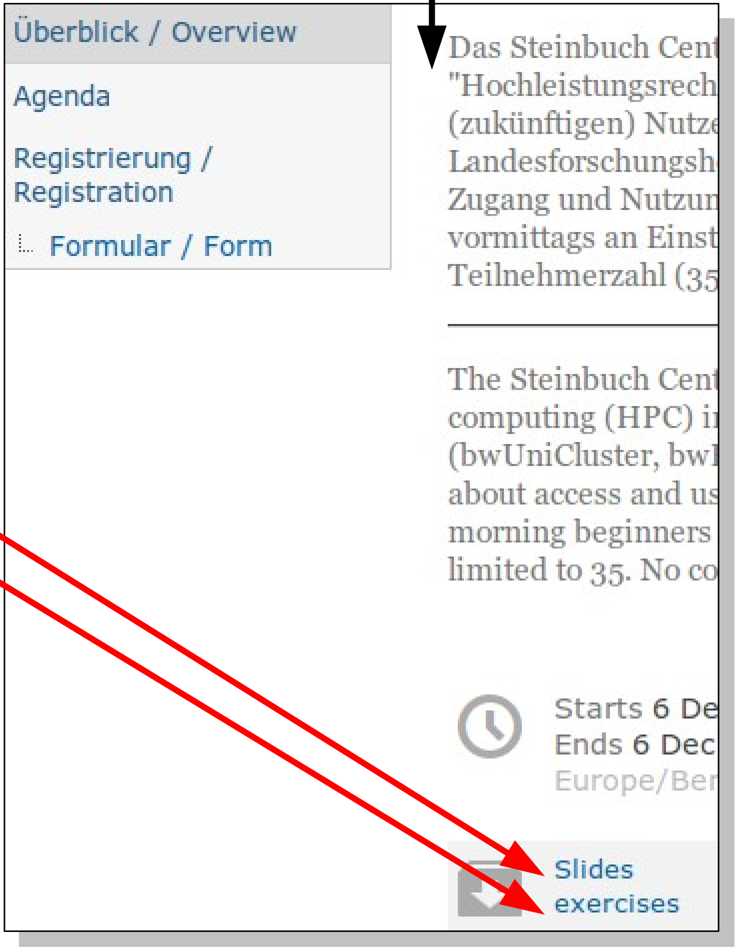
Abbreviation/Colour code	Full meaning
`$ command -opt value`	`$` = prompt of the interactive shell The full prompt may look like: `user@machine:path $` The command has been entered in the interactive shell session

`<integer>`
`<string>`
	`<>` = Placeholder for integer, string etc

`foo, bar`	Metasyntactic variables
`${WORKSHOP}`	`/pfs/data1/software_uc1/bwhpc/kit/workshop/2018-10-10`

Where to get the slides and exercises?

- https://indico.scc.kit.edu/e/bwhpc_course_2018-10-10 or
  uc1:/pfs/data1/software_uc1/bwhpc/kit/workshop/2018-10-10
  - Slides
  - Exercises



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Goal

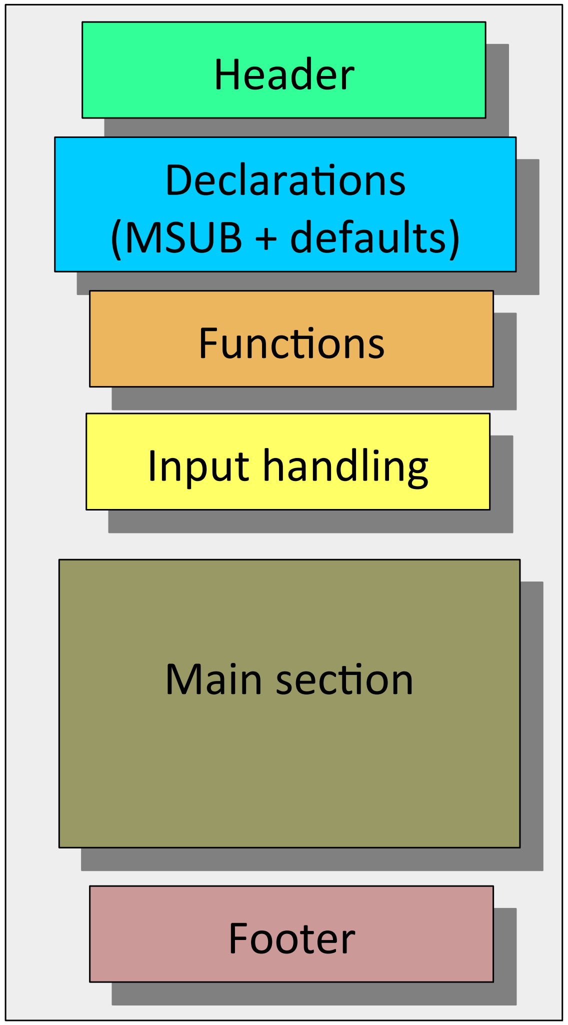
- Be descriptive!
  - Comment your code
    - e.g. via headers sections of script and functions.
  - Decipherable names for variables and functions

- 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 on login nodes / in `${HOME}` :

- for interactive jobs use msub -I -V

Multinode Job:

- use *workspaces*
- Producing Tbyte of scratch files & >10000 File: Change your application code

  Need help? Apply for Tiger Team Support.

Singlenode Job:

- use `${TMPDIR}`: HowTo → Case 1

Chain jobs: HowTo → Case 2

Many sequential tiny jobs:

- Bundle to one big job: HowTo → Case 3

Handling walltime based job aborts: HowTo → Case 4

Use of MPI/OpenMP Parallelisation in jobs: *see slides of next talk*

Job Arrays: Howto → Case 5

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 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/02/01_job_run_under_local_tmpdir.sh
+
${WORKSHOP}/exercises/02/{01_gen_files,01_gen_files.inp}
```

Case 1: Jobs @ $TMPDIR (2)

- Code snip: `${WORKSHOP}/exercises/02/01_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 "${TMPDIR}/${USER}.${MOAB_JOBID:-$$}"

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

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

## 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/02/01_generalised_job_run_under_local_tmpdir.sh`

Solution!

```
## 1) Define full path of your binary
EXE="${MOAB_SUBMITDIR:-${PWD}}/01_gen_files.x"

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

## 3) Define full path input files
Input="${MOAB_SUBMITDIR:-${PWD}}/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 and generate via mkdir
run_DIR="${TMPDIR}/${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/02/01_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/02/02_chain_job.sh
```

Case 2: Chain Jobs (2)

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

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

```bash
#!/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
```

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

```
TASK/ToDo:5 min
* add the parts 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
```

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
```

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

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

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Case 2: Chain Jobs (4)

- moab_chain_job.sh + interactive_chain_job.sh =

```
${WORKSHOP}/solutions/02/02_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/02/02_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/02/02_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 occured
   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 + joblist.txt

`${WORKSHOP}/exercises/02/03_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
```

`${WORKSHOP}/exercises/02/03_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"
```

Case 4: Handling walltime based job aborts

- Revision:
  - Jobs have limited runtime (=walltime)
  - Define walltime by your own, cf. `msub -l walltime=D:HH:MM:SS`
- Issue:
  - Executable needs more time than given walltime
    → queueing system is terminating your jobscript and its child processes
- Solution:
  - `msub -l signal=<sigint>@<seconds>` , e.g. 120 before walltime send sigterm (15)

```
TASK/ToDo:10 min
* combine "msub -l signal" & "trap" to trigger message and "exit 1"
```

- template: `${WORKSHOP}/exercises/02/04_handle_aborts.sh`

Case 4: Handling walltime based job aborts

Solution!

- Use: „msub -l signal“ and „trap“ to abort job on own terms

${WORKSHOP}/solutions/02/04_handle_aborts.sh

```
#!/bin/bash
## Pre-termination via MOAB
## sending signal with defined offset

#MSUB -l nodes=1:ppn=1,walltime=00:01:00,mem=100mb
#MSUB -l signal=15@10
#MSUB -l advres=bwhpc-workshop.64
#MSUB -A workshop

cleanup(){
  echo "Cleanup before walltime reached"
  exit 0
}

trap cleanup 15

echo "Repeating \"sleep 10\" loop until SIGTERM"
while true ; do
  sleep 10
done
```

MOAB sends SIGTERM (kill -15) 10 seconds before walltime is reached

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!