bw|HPC

KIT | NHR
National High-Performance Computing Center

Advanced (Batch) Job Scripting

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How to read the following slides

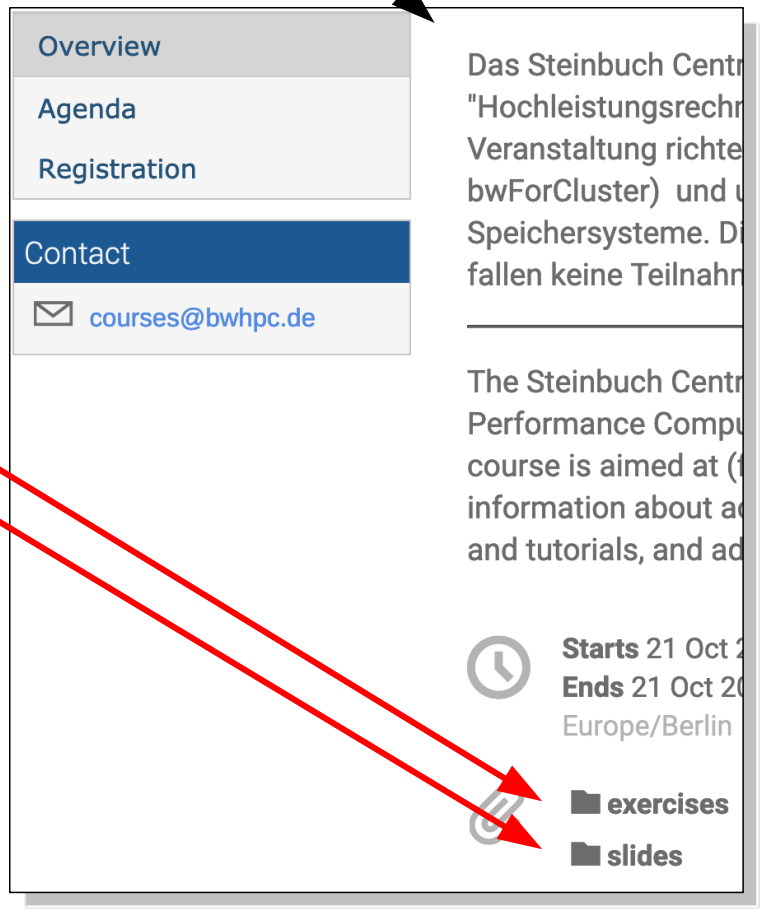
Abbreviation/Colour code	Full meaning
`$ command -opt value`	`$` = prompt of the interactive shell The full prompt may look like: `user@machine:path $` The command has been entered in the interactive shell session
`<integer>` `<string>`	<> = Placeholder for integer, string etc
`foo, bar`	Metasyntactic variables
`${WORKSHOP}`	`@uc2:/opt/bwhpc/common/workshops/2024-10-17` `@hk:/software/all/workshops/2024-10-17`

Where to get the slides/exercises/reservation?

- https://indico.scc.kit.edu/e/hpc_course_2024-10-17 or

  bwUniCluster: /opt/bwhpc/common/workshops/2024-10-17

  horeka:/software/all/workshops/2024-10-17
  - exercises
  - slides



- Workshop reservation:
  single node:

```
sbatch -p single --res=ws
```

- multi node:

```
sbatch -p multiple --res=ws
```

How to do excerices?

- Login to cluster & Generate workspace „bwhpc-course“

```
$ ws_allocate bwhpc-course 30
Info: creating workspace
/pfs/work7/workspace/scratch/ab1234-bwhpc-course
remaining extensions  : 3
remaining time in days: 30
```

- Copy examples to your workspace

```
$ WORKSHOP=/opt/bwhpc/common/workshops/2024-10-17
$ cd $(ws_find bwhpc-course)
$ mkdir -v 2024-10-17; cd 2024-10-17
$ cp -vpr ${WORKSHOP}/exercises/02  ./
```

- Submit jobs from your workspace

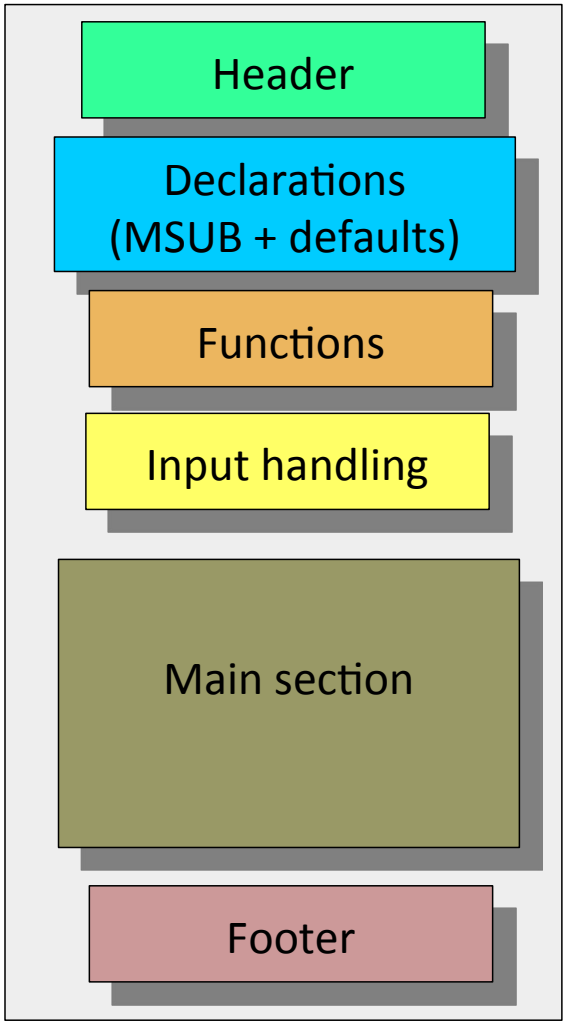
```
$ cd $(ws_find bwhpc-course)/2024-10-17/02
$ sbatch -p {single|cpuonly} --res=ws <jobscript>
```

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 Slurm



Typical Issues & Cases (1)

- Singlenode Issues
  - (Parallel) File System Issues
    - Workflow for job on a different Filesystem (on $TMPDIR/BEEOND, Case 1)
  - *OpenMP Jobs (cf. Afternoon – talk no. 4)*
- Multinode Issues
  - Parallel File System Issues
  - *MPI Jobs (cf. Afternoon – talk no. 4)*
- Walltime Issues
  - Job abortion (Case 2)
- Task Issues
  - Bulk Jobs (Case 3)
  - Array Jobs (Case 4)
  - Chain Jobs (Case 5)

Typical Issues & Cases (2)

- Login Node Issues
  - @bwUniCluster, we have 4 Login nodes but over 2000! users
  - „only want to test fast/interactively“ slows the login nodes

  → Do not Run your code, application, job on login nodes / in `${HOME}`:
    - for interactive jobs use sacct
    - For development use develop queue

SLURM variables (bwUniCluster 2.0, HoreKa)

- bwHPC Wiki , excerpt:

Environment	Brief explanation
SLURM_JOB_CPUS_PER_NODE	Number of processes per node dedicated to the job
SLURM_JOB_NODELIST	List of nodes dedicated to the job
SLURM_JOB_NUM_NODES	Number of nodes dedicated to the job
SLURM_MEM_PER_NODE	Memory per node dedicated to the job
SLURM_NPROCS	Total number of processes dedicated to the job
SLURM_CLUSTER_NAME	Name of the cluster executing the job
SLURM_CPUS_PER_TASK	Number of CPUs requested per task
SLURM_JOB_ACCOUNT	Account name
SLURM_JOB_ID	Job ID

- SLURM Submit options (excerpt):

`${WORKSHOP}/exercises/02/00_switch.sh`

```
#!/bin/bash
#SBATCH -J test
#SBATCH -N1 -n1 --mem=50
#SBATCH -t 00:05:00
#SBATCH --mail-type=all
#SBATCH --export="my_own_variable=arguments"

if [ ! -z ${SLURM_JOB_NAME} ] ; then
   printenv 2>&1 | grep -e "(SLURM|my_own_variable)"
else
   printenv 2>&1 | grep 'TMPDIR'
fi
```

File system issues (1)

- Multinode Job:
  - For most cases

    → use *workspaces*

    But: Producing Tbyte of scratch files & >10000 File?
    Change your application code

    Need help for that? Apply for Tiger Team Support.

  - A lot of I/O over all nodes

    → opt out to local parallel file system (FS) instead of global one

    use `BeeOND`: but requires a „workflow“
- Singlenode Job:
  - A lot of I/O?

    → opt out to local file system instead of global one

    use `${TMPDIR}/BeeOND`: but requires a „workflow“

Jobs @ local/private FS (1)

- If temporary files of job > Gbyte
  → Run your job at `local/private Filesystem`

- Basic script recipe:
  1. Set “declarations“/defaults
  2. Use “private“ subdirectory, assign to `${run_DIR}`
  3. Prepare `${run_DIR}` or Copy “things“ to `${run_DIR}`
  4. Change to `${run_DIR}` & start your application
  5. Copy results back to `DIR` where job was submitted

- How?
  - Start with templates:

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

Jobs @ local/private FS (2)

- Code snip: `${WORKSHOP}/exercises/02/01_job_run_under_local_fs.sh`

```
#!/bin/bash
...
## 1.a-f) Declaration: defaults + load modules

## 2) Define your run private local filesystem
##    Interactive / NODES=1 / NODES>1:
mkdir -pv "${TMPDIR}/${USER}.${SLURM_JOB_ID:-$$}"
run_DIR=???

## 3.a) Check existence of run directory

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

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

## 5.a) Check run status

## 5.b) Transfer files to submit directory
cp -pv files_*.out "${SLURM_SUBMIT_DIR}"

## 5.c) Cleanup run_DIR
```

TASK/ToDo:
* Generalise blue code avoiding repetition
* Write code for 1-5
* Redirect output of binary

Jobs @ local/private FS (3)

- Part 1/3:

${WORKSHOP}/solutions/02/01_job_run_under_local_fs_solv.sh

```
## 1.a) Define your binary
submitdir=${SLURM_SUBMIT_DIR:-${PWD}}
EXE="01_gen_files.x"

## 1.b) Define output file
##    = Name of executable wo extension + JOBID or PID
output="$(basename ${EXE/.*})_${SLURM_JOB_ID:-$$}.log"

## 1.c) Define full path input files
Input="01_gen_files.inp"

## 1.d) Define input files to be copied
copy_list="${EXE} ${input}"

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

## 1.f) Load modules INTEL+MKL
for mod in compiler/intel numlib/mkl ; do
   module load "${mod}"
done
```

Solution!

Jobs @ local/private FS (4)

- Part 2/3: `${WORKSHOP}/solutions/02/01_job_run_under_local_fs_solv.sh`

Solution!

```
## 2) Define your run directory and and generate via mkdir
##    Nodes=1 -> TMPDIR option: run_DIR <=> tmpdir + username + JobID or PID
##    Nodes>1 -> BEEOND option: run_DIR <=> path to BEEOND directories
if [ ! -z ${SLURM_JOB_NAME} ] ; then
   if [ ${SLURM_NNODES:-1} -gt 1 ] ; then
      run_DIR=/mnt/odfs/${SLURM_JOB_ID}/stripe_16/
   else
      run_DIR=${TMPDIR}
   fi
else
   run_DIR="${TMPDIR}/${USER}.${SLURM_JOB_ID:-$$}"
   mkdir -pv "${run_DIR}"
fi

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

## 3.b) Change to Submit Dir or PWD / Copy files from submit_DIR to run_DIR
cd "${submitdir}"
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
```

Jobs @ local/private FS (5)

- Part 3/3:

${WORKSHOP}/solutions/02/01_job_run_under_local_fs_solv.sh

```
## 4) 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

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

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

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

Solution!

Walltime Issues (1)

- Revision:
  - Jobs have limited runtime (=walltime)
  - Define walltime by your own, cf. sbatch `-t D-HH:MM:SS`

- Issue:
  - Executable needs more time than given walltime

    → queueing system is terminating your jobscript and its child processes

- Solution:
  - `sbatch --signal=B:<sigint>@<seconds>` , e.g. 120 before walltime send sigterm (15)

```
TASK/ToDo:
* combine "sbatch --signal" & "trap" to trigger message and "exit 1"
```

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

Walltime Issues (2)

- Use: „`sbatch --signal`“ and „trap“ to abort job on own terms

Solution!

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

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

#SBATCH -n 1 -t 00:01:00
#SBATCH --mem=100
#SBATCH --signal=B:15@10
#SBATCH -p ws

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

trap cleanup 15

echo "Repeating \"sleep 1\" loop until SIGTERM"
i=1
while true ; do
  sleep 1; echo $i; let i+=1
done
```

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

Bulk Jobs (1)

- Many (>100) „independent“ jobs with very short runtime
  - Solution:

    → Pack in one multinode/multitask job with long runtime

    HowTo?
    - Assign resources for „parallel“ task processing, aka „workers“
    - Load balance „workers“, i.e., and assign step by step free „workers“ with jobs

Bulk Jobs: MPI based solution (1)

- Parbatch → MPI task based

Example: job script

`${WORKSHOP}/exercises/02/03_parbatch.sh`

```
#!/bin/bash

#SBATCH -n 4 -N 1
#SBATCH --mem=150
#SBATCH -t 00:03:00

module load system/parbatch

parbatch joblist.txt
```

+ joblist.txt

`${WORKSHOP}/exercises/02/03_joblist.txt`

```
echo "Subjob 01"; hostname
echo "Subjob 02"; hostname
echo "Subjob 03"; hostname
echo "Subjob 04"; hostname
echo "Subjob 05"; hostname
echo "Subjob 06"; hostname
echo "Subjob 07"; hostname
echo "Subjob 08"; hostname
```

TASK/ToDo:

- Prepare joblist with 10 jobs each running max. 15 seconds and submit it with *„workers“*

Bulk Jobs: MPI based solution (2)

Solution!

- Parbatch → MPI task based

  Example: job script

```
#!/bin/bash

#SBATCH -n 2 -N 1
#SBATCH --mem=150
#SBATCH -t 00:03:00

module load system/parbatch

parbatch joblist.txt
```

\+ joblist.txt

${WORKSHOP}/exercises/02/03_joblist.txt

```
sleep 10; echo 'Hello'; sleep 5
sleep 10; echo 'World'; sleep 5
sleep 10; echo 'today'; sleep 5
sleep 10; echo 'it is'; sleep 5
sleep 10; echo 'time'; sleep 5
sleep 10; echo 'for'; sleep 5
sleep 10; echo 'something'; sleep 5
sleep 10; echo 'new'; sleep 5
```

Job Arrays (1)

- Jobs with a „task range“
  - with the same executable and ressource requirements
    → but different input (files)
  - Interactive setup (aka „pure“ bash script setup):
    - Master script:
      - Translating index setup into list, excuting each index value as a job
  - Slurm:
    - Available as submit feature:

```
sbatch --array [<indexlist>]:<delim> job.sh
```

    → makes master script obsolete & groups Job IDs (= easier to handle)
    → **`job.sh`** gets index value via **`$SLURM_ARRAY_TASK_ID`**

Job Arrays (2)

- Simple slurm array example: `${WORKSHOP}/exercises/02/05_slurm_array.sh`

```
#!/bin/bash

#SBATCH -J ws_array
#SBATCH -N1 -n2
#SBATCH -t 00:01:00
#SBATCH --array=0-10:2
#SBATCH --output=array_%A-%2a.out

printenv | grep "SLURM_ARRAY"

## Generate real number, e.g. via exp fct.
echo ${SLURM_ARRAY_TASK_ID} | awk '{printf "%.4f\n",exp($X)}'
sleep 2
```

List from 0 to 10 with increment of 2

Default is: `slurm-%A_%a.out`, but generates here:
`slurm-12346_0.out`
`...`
`slurm-123456_10.out`

%2a = pads one-digit numbers with zeros

current array task ID

Bash based Job Array (3)

- Without array submit features → approach:
  - a.) handle each index value as one job/task
  - b.) handle as one (=master) sbatch job

```
export IARR="0-10:2"
${WORKSHOP}/exercises/02/05_master_job_array.sh
```

```
#!/bin/bash

#SBATCH --export="All,IARR=2-10:2"   # index setup: min-max:inc

# Define subjob script
subjob="./05_array_task.sh"
# Decipher index setup:
IARR=${IARR:-1-5:1}
if [[ ${IARR/://} = ${IARR} ]] ; then inc=1 ; else inc=${IARR/*:} ; fi
IARR=${IARR/:*}
if [[ ${IARR/-//} = ${IARR} ]] ; then max=1 ; else max=${IARR/*-} ; fi
min=${IARR/-*}
ndm="${#max}" ## Number of digits of max

echo "Generate index list from ${min} to ${max} with increment ${inc}"
while [[ $min -le $max ]] ; do
   printf "  Execute ${subjob} %0${ndm}d\n" "${min}"
   #${subjob} $(printf "%0${ndm}d" "${min}")
   let min+=${inc}
done
```

Automatic padding digits with zeros

Bash based Job Array (4)

TASK/ToDo:

- Modify `05_master_job_array.sh`
  - To do parallel (use parbatch):
- `05_array_task.sh` writes index value to indexed output

`${WORKSHOP}/exercises/02/05_array_task.sh`

```
#!/bin/bash

## Get index value via positional parameter
value="??"

## Define name of output file, array_<jobid>-<task-id>.out
outputfile="??"

## Write value to file
??
```

Bash based Job Array (4)

Solution!

- Modify `05_master_job_array.sh`
  - To do parallel (use parbatch):
- `05_array_task.sh` writes index value to indexed output

`${WORKSHOP}/solutions/02/05_array_task_solv.sh`

```
#!/bin/bash

## Get index value via positional parameter
value="${1:?missing_value}
## Define name of output file
outputfile="array_${SLURM_JOB_ID:-$$}-${value}.out"
## Write value to file
echo ${value} > ${outputfile}
```

`${WORKSHOP}/solutions/02/05_master_job_array_solv.sh`

```
module load system/parbatch
...
joblist=joblist_${SLURM_JOB_ID:-$$}.txt
while [[ $min -le $max ]] ; do
   printf "  Execute ${subjob} %0${ndm}d\n" "${min}"
   echo "${subjob}" $(printf "%0${ndm}d" "${min}") >> ${joblist}
   let min+=${inc}
done
# Execute parbatch
parbatch ${joblist}
```

Bonus: Chain Jobs (1)

- Idea:
  - Do ***N*** consecutive Jobs via ***N*** 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
```

Bonus: Bash script based Chain Jobs (2)

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

```
$ export myloop_counter=0
$ ./02_chain_job.sh
```

loop

```
#!/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
```

Bonus: Chain Jobs (3) → How for Slurm?

```
#!/bin/bash
#SBATCH ...
## 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
```

loop

TASK/ToDo:
* add the parts for Slurm

Bonus: Chain Jobs (4) → Solution! for Slurm

```
#!/bin/bash
#SBATCH -N1 -n1 -t 00:00:05 -mem=250 -p ws
## 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 [ $? -eq 0 ] ; then
      ## continue only if last command was successful
       sbatch --export=myloop_counter=${myloop_counter} ./02_chain_job_solv.sh
   else
      ## Terminate chain
      echo "  ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
      exit 1
   fi
fi
```

loop

${WORKSHOP}/solutions/02/02_chain_job_solv.sh

```
$ sbatch --export=myloop_counter=0 ./02_chain_job_solv.sh
```

Bonus: Chain Jobs (5)

- Slurm + interactive script =

  `${WORKSHOP}/solutions/02/02_gen_chain_job_solv.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} ./02_gen_chain_job_solv.sh
     elif [ ! -z ${SLURM_JOB_NAME} ] ; then
        sbatch --export="myloop_counter=${myloop_counter}" ./02_gen_chain_job_solv.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

Bonus: Chain Jobs: Optimization (1)

- Problem of 02_generalised_chain_job.sh: **Waiting time**!
  - Solution: two scripts (master + links) + `sbatch -d afterok:<jobID>`
  - 1. script - links: `${WORKSHOP}/solutions/02/02_chain_link_job_solv.sh`

```
#!/bin/bash
#SBATCH ...

## 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
```

Bonus: Chain Jobs: Optimization (2)

- 2. script - master: `${WORKSHOP}/solutions/02/02_submitter_f_chain_job_solv.sh`

loop

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

myloop_counter=1
while [ ${myloop_counter} -le ${max_nojob} ] ; do
   if [ ${myloop_counter} -eq 1 ] ; then
      slurm_opt=""
   else
      slurm_opt="-d ${dep_type}:${jobID}"
   fi

   echo "Chain job iteration = ${myloop_counter}"
   echo "   sbatch --export=myloop_counter=${myloop_counter} ${slurm_opt} ${chain_link_job}"
   ## Store job ID for next iteration by storing output of msub command with empty lines
   jobID=$(sbatch --export=myloop_counter=${myloop_counter} ${slurm_opt} ${chain_link_job}
           2>&1 | sed 's/[S,a-z]* //g')

   ## Check if ERROR occured
   if [[ "${jobID}" =~ "ERROR" ]] ; then
      echo "   -> submission failed!" ; exit 1
   else
      echo "   -> job number = ${jobID}"
   fi
   ## Increase counter
   let myloop_counter+=1
done
```

Your Workflows?

- Tell us about your typical workflow
  - Preprocessing methods
  - Input methods
  - Data staging methods
  - I/O management
  - Postprocessing methods
  -
  - If you have issue, please contact us via:

    https://www.bwhpc.de/supportportal.php

Thank you for your attention!

Questions?