Workshop Agenda – Feb 25th 2015

Time	Presenter	Title
09:30	T. König	Talk – bwHPC Concept & bwHPC-C5 - Federated User Support Activities
09:45	R. Walter	Talk – bwHPC architecture (bwUniCluster, bwForCluster JUSTUS, ForHLR Phase I)
10:00	A. Fuchs	Talk – Cluster: Access, Data Transfer and Storage, GUI
10:30		*Break*
10:45	R. Barthel	Talk – File System, Software System (modulefiles), Batch System
11:10	A. Fuchs	Tutorial – bwUniCluster: Access, Data Transfer, Compiling, Modulefiles, Batch Job Scripting
11:50		*Lunch Break*
13:00	R. Barthel	Talk – Advanced Bash Scripting
13:30	R. Barthel	Tutorial – Advanced (Batch) Job Scripting
14:15		*Break*
14:30	A. Fuchs	Tutorial – Compiling, Makefile, Parallelising
15:15		User Forum – Solving User Cases
16:00		*End*

bw|HPC – C5

Tutorial:
Advanced (Batch) Job Scripting

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How to read the following slides

Abbreviation/Colour code	Full meaning
`$ command -option 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

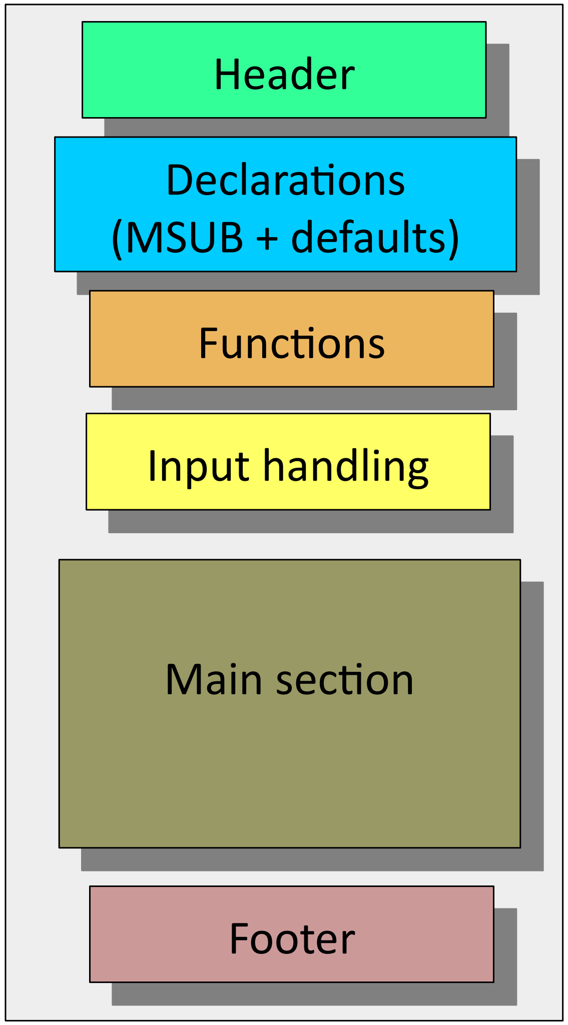
`foo, bar`	Metasyntactic variables
`${WORKSHOP}`	`/pfs/data1/software_uc1/bwhpc/kit/workshop/2015-02-25`

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 modules
    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
- Singlenode Job:
  - use `${TMPDIR}`: HowTo → Case 1
- Chain jobs
  - HowTo → Case 2
- Many sequential tiny jobs:
  - Bundle to one big job: HowTo → Case 3

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?
  - Compare: Examples

```
${WORKSHOP}/exercises/bash/job_run_under_local_tmpdir.sh
+
${WORKSHOP}/exercises/bash/{gen_files,gen_files.inp}
```

Case 1: Jobs @ $TMPDIR (2)

- Code snip: `${WORKSHOP}/exercises/bash/job_run_under_local_tmpdir.sh`

```
#!/bin/bash

#MSUB -N test
#MSUB -l advres=workshop.54,nodes=1:ppn=1,mem=50mb
#MSUB -l walltime=00:05:00
#MSUB -m n

## a) Tutorial ToDo: load modules if necessary

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

## c) Tutorial ToDo: Check existance of run_DIR

## d) copy files from submit_DIR to run_DIR
cd $MOAB_SUBMITDIR
cp -pv gen_files gen_files.inp "${TMP}/${USER}.${MOAB_JOBID:-$$}"

## e) cd to run_DIR and start "binary" together with input file
cd "${TMP}/${USER}.${MOAB_JOBID:-$$}"
./gen_files 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
* Write code for a,c,f,h
* Generalise blue code
  avoiding repetition
* Redirect output of binary
```

Case 1: Jobs @ $TMP (3)

- Header: `${WORKSHOP}/exercises/bash/solutions/generalised_job_run_under_local_tmpdir.sh`

Solution!

```
. . .
## a) Load modules if necessary
module load compiler/intel
module load numlib/mkl

## b) Define full path of your binary
EXE="gen_files"

## c) Define output file
output="$(basename ${EXE})_${MOAB_JOBID:-$$}.log"

## d) Define input files
input="gen_files.inp"

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

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

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

Case 1: Jobs @ $TMP (4)

- Body + Footer: `${WORKSHOP}/exercises/bash/solutions/generalised_job_run_under_local_tmpdir.sh`

Solution!

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

## i) Copy files from submit_DIR to run_DIR
cd "${MOAB_SUBMITDIR}"
for X in ${copy_list} ; do
   cp -pv "${X}" "${run_DIR}"
done

## j) cd to runDIR and start binary
cd "${run_DIR}"
./$EXE ${input} > $output 2>&1

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

## l) Transfer files to submit directory
cd "${run_DIR}"
for X in ${save_list} ; do
   cp -pv "${X}" "${MOAB_SUBMITDIR}"
done

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

Case 2: Chain Jobs (1)

- Idea:
  - Split ***N*** consecutive Jobs into ***N*** MOAB Batch Jobs
- Goal:
  - Do everything in one script
  - Submit only once to MOAB

- „Pre-step“: generate script that runs interactively
  - Result:

```
${WORKSHOP}/exercises/bash/interactive_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
```

```
$ export myloop_counter=0
$ ./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} ./moab_chain_job.sh
   else
      ## Terminate chain
      echo "  ERROR: ${cmd} of chain job no. ${myloop_counter} terminated unexpectedly"
      exit 1
   fi
fi
```

```
$ msub -v myloop_counter=0 ./moab_chain_job.sh
```

Case 2: Chain Jobs (4)

- moab_chain_job.sh + interactive_chain_job.sh =

```
${WORKSHOP}/exercises/bash/solutions/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

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

- Prestep: Schedule N jobs to one slot:

```
TASK: 10min
* Write Loop that executes 10 times para_slave.sh but:

  a) the execution waits until file lock does NOT exist

  b) the execution generates the file lock

  c) the successful termination of para_slave.sh removes
     the lock file
```

```
USE the templates:
${WORKSHOP}/exercises/bash/para_master.sh
${WORKSHOP}/exercises/bash/para_slave.sh
```

Case 3: Pseudo Parallelisation (2)

Solution!

${WORKSHOP}/exercises/bash/solutions/para_master.sh

```
no_loop=10
slave_sh=para_slave.sh
lock_file=lock

## LOOP ##
i=1
while (( $i <= ${no_loop} ))  ; do
   ## If lock does not exists -> execute slave job
   if [ ! -e "${lock_file}" ] ; then
      ## generate lock
      touch "${lock_file}"
      ## generate logfile name
      log_file=${slave_sh%.sh}_${i}.log

      ## execute job + options
      echo "Starting Job $i of ${slave_sh}"
      ./${slave_sh} "${lock_file}" "${log_file}"
      ##
      ## increase counter
      let i+=1
   fi

   ## Do not finish current iteration until lock disappears
   while [ $(ls ${lock_file} 2>/dev/null | wc -l) -ge 1 ] ; do
      sleep 2
   done

done
```

Case 3: Pseudo Parallelisation (3)

Solution!

${WORKSHOP}/exercises/bash/solutions/para_master.sh

```
lock_file=${1}
log_file=${2}
cmd="sleep 2"          ## user command for this tutorial

## Execute command (cmd) and protocol execution time and finishing time to log file
echo "Starting  time: $(date)" > ${log_file}
${cmd} >> ${log_file} 2>&1

## Determine exit status of command
stat_cmd=$?

## Remove lock file
if [ "${stat_cmd}" -eq 0 ] ; then
   echo "Job successfully finished" >> ${log_file}
   rm -f "${lock_file}"
else
   echo "Job finished with error" >> ${log_file}
fi
echo "Finishing time: $(date)" >> ${log_file}
```

Case 3: Pseudo Parallelisation (4)

- Further generalisation of para_master.sh & para_slave.sh
  - inner loop over number of slots = number of core of MOAB job
  - Generate para_slave.sh automatically
  - Allow input your subjobs

  - Example: bwUniCluster_pseudo-parallel.sh
    - run with 2 cores per 2 nodes:

```
$ cp ${WORKSHOP}/exercises/bash/solutions/{bwUniCluster_pseudo-parallel.sh,jobfile.txt} .

$ ./bwUniCluster_pseudo-parallel.sh -h  # read help
$ nano jobfile.txt                      # edit jobs

$ msub bwUniCluster_pseudo-parallel.sh jobfile.txt
```

Batch jobs with input parsing

- Not working:
  - msub [options] *your_script* -x *argument*

    → msub will interprete -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
  - Do not use if your job solely does MPI:

    mpirun –machinefile=file binary

    mpirun -n <int> binary
  - Correct, (because the resource manager tells mpirun what to do):
    - mpirun binary

- 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!