bw|HPC

Batch System – Best Practices

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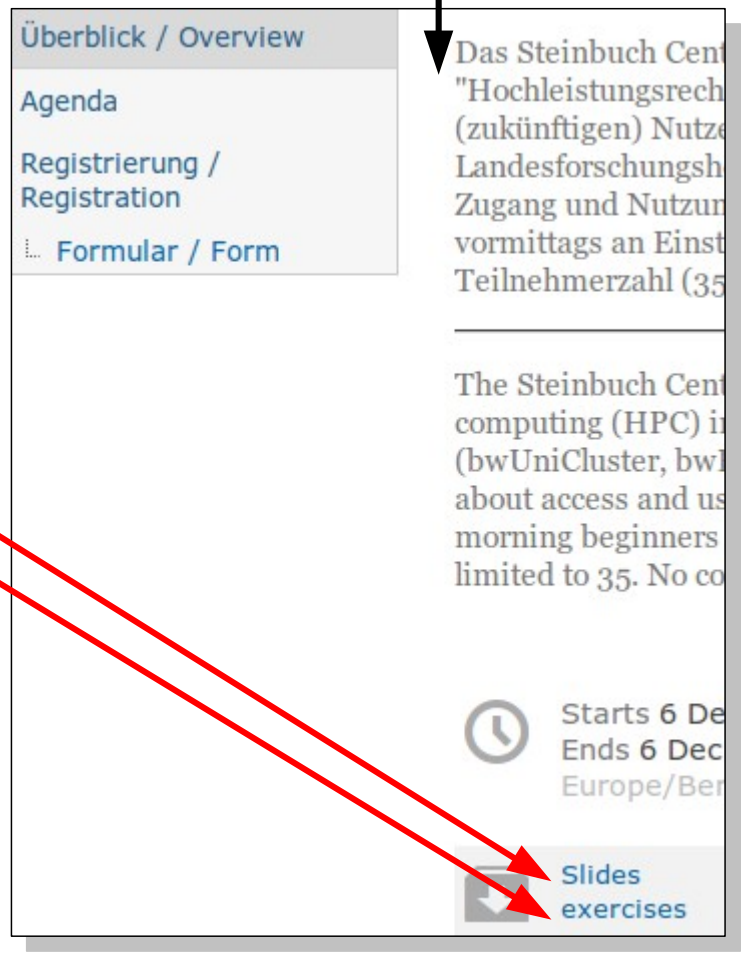
How to read the following slides

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`

- Most information given by this talk can be found at http://bwhpc.de/wiki under the article:
  - Batch_Jobs

Where to get the slides and exercises?

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



- How to do exercises?
  1. Generate workspace
  2. Copy examples to workspace
  3. Submit from workspace

Job Preparation

Msub Directives (1)

- Write msub defaults in your script, overwrite time interactively via CLI, e.g.: **msub -N newname <script>**

```
#!/bin/bash

#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb
#MSUB -q develop
#MSUB -N serial-test
#MSUB -m bea
#MSUB -M my_email_address

## to access today's standing reservation
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

printenv
```

Msub Directives (2)

- Use alternative directive prefixes to store multiple „defaults“ in your run script and use them via: **msub -C '#Prefix'**
  - Pitfall 1: undefined msub options in #Prefix will be filled with defined #MSUB options

```
...
## Default
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb
#MSUB -N default
#MSUB -v runtype=1
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

## Alternative msub directives, to use via: msub -C '#MALT'
#MALT -l nodes=1:ppn=1
#MALT -l walltime=00:02:00
#MALT -l mem=200mb
#MALT -N alternative
#MALT -v runtype=2

if [[ ${runtype:-0} -eq 1 ]] ; then
   echo "Run default"; printenv
else
   echo "Run alternative"; printenv
fi
```

${WORKSHOP}/exercises/04/01_msubdirectives.sh

Attention!!!
#MALT uses from #MSUB:
-A workshop & -l advres=...

Job Script: Structuring (1)

- Howto?

  → Cf. today's talk no. 1 (adv. bash scripting) and 2 (adv. job scripting)

- Print out what your script is doing
- Do Bash Scripting (assign variables, use conditionals, functions)
- Use modulefile statements
- Use Global Environment Variables
  - Understand them!

```
cleanup(){
  <do_stuff_here> ; exit 0
}
# Check existance of input
my_input=${HOME}/input
if [ ! -e ${my_input} ] ; then
   echo "ERROR: ${my_input} does not
exist"
   exit 1
fi

# Printing all environment variable
echo "Current available env. vars"
printenv
# Printing job resources
echo "Number nodes = ${MOAB_NODECOUNT}"
echo "Number cores = ${MOAB_PROCCOUNT}"
```

What is PROC?

Ressource specifications (1)

- @ MOAB
  - Node

    = computer server
  - Proc

    = „processors“ → Cores
  - *Task*

    = atomic collection of resources, such as processors, memory, or local disk, which must be found on the same node
- @ OpenMP
  - Thread

    = smallest sequence of instructions managed independently by a OS scheduler

    → Normally 1 thread is pinned to 1 core
- @ MPI
  - Task

    = is 1 process excuted by the OS

    → smallest useful unit: 1 MPI task per node

Examples:

1) Addressing 2 cores on 1 node:

```
msub -l nodes=1:ppn=2
```

2) two cores on nodes 1,2 + four cores on node 3:

```
msub -l nodes=2:ppn=2+1:ppn=4
```

Ressource specifications (2)

- @ MOAB
  - **mem**
    = Working memory for total job
  - **pmem**
    = Working memory per cores

Example:

Addressing 4GB for 2cores on 1 node:

```
msub -l nodes=1:ppn=2,pmem=2gb
or
msub -l nodes=1:ppn=2,mem=4gb
```

- Node access policies

bwUniCluster: **shared** *(with other users' jobs)*
how to get whole node? → e.g.:

```
msub -l nodes=1:ppn=16   or
msub -l naccesspolicy=singlejob
```

bwForClusters: shared, **singleuser** *(=shared with other own jobs),*
singlejob *(=exclusively for your job)*

ForHLR: singlejob
→ Addressing not max cores/mem per node is wasting resources!

Job Script: Structuring (2)

- Use templates for job scripts
  - Provided by many installed software packages
    - cf. help description of SW

Example:

- How to get? Search in description for example directory, or e.g. Turbomole

```
$ module show chem/turbomole 2>&1 | grep "EXA_DIR"
→ shows path:
/opt/bwhpc/common/chem/turbomole/7.2.1_tmolex432/bwhpc-examples
```

bwHPC_turbomole_single-node_tmpdir_example.sh

```
#!/bin/bash

## Purpose: Turbomole JOB example script for bwHPC, such as bw{For,Uni}Cluster
##          for   S I N G L E   N O D E   runs   O N L Y
...
...
```

Best Practises – Job setup (1)

- Directory:
  - Running your code/application/job in ${HOME} is not permitted

    Valid destinations are:

    1. Workspaces (`ws_allocate`)
    2. $TMPDIR (not suitable for multinode jobs)

  - Issues:
    - Workspaces:
      - Does not handle well codes producing Tbyte of scratch files and more then 10000 files. Solution: Change your application code, Apply for Tiger Team Support.
    - $TMPDIR:
      - Requires job script setup to handle data transfer (cf. case 1 of previous talk)

```
#!/bin/bash
#MSUB ...
cp -pr ${MOAB_SUBMITDIR}/<file> ${TMPDIR}
...
cp -pr ${TMPDIR}/<results>* ${MOAB_SUBMITDIR}
```

Best Practises – Job setup (2)

- Directory: (cont.)
  - Potential problems:
    - During job run, binaries/inputfiles etc not found

      → give full path to binaries/inputfiles

      → change DIR in jobscript

```
#!/bin/bash
#MSUB ...
# Change to job submission directory
cd ${MOAB_SUBMITDIR}
```

- Record resource usage to optimise resource requests
  - Walltime:

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

# Record runtime of executed program
SECONDS=0
time ./program
...
echo $SECONDS
```

Job submission

Job Submit

- Not working:
  - msub ***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
```

Job execution

Best Practices – Job „Observation“

- Do NOT run script that submits every second commands like:
  - **`checkjob`**
  - **`showq -n`**
  - **`tail -f  <Global_file_system>/<file>`**
    - Change to „**`tail -f -s 10"`** etc.

- How to follow **live** the job progress on compute node?
  - **`ssh`** on given compute node does
    - **NOT** work on bwUniCluster
    - Work on bwForCluster JUSTUS
    - ...

  → cf. bwHPC Wiki

Parallel Jobs

OpenMP parallel jobs (1)

- OpenMP = Open Multi-Processing)

  → compiler directives, lib routines, environment variables to enable multithreading on shared-memory multiprocessor platforms

  - https://www.openmp.org

- Training info:
  - @Uni Stuttgart: Oct 15-19 2018, https://www.hlrs.de/training/2018-10-15-par/
  - @KIT: June/July 2019 as part of lecture „Parallelrechner & Parallelprogrammierung“

- Typical issues:
  - Number of threads not matching given ressources

    → Normally 1 thread is to be pinned to 1 core

OpenMP parallel jobs (2)

- Example: `${WORKSHOP}/exercises/04/parallel/omp.sh`

```
#!/bin/bash
#MSUB -l nodes=1:ppn=2
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

# Set executable name to variable
exe=./hello_omp
# Load modules
module load compiler/intel
# Setup OpenMP environment variable
export OMP_NUM_THREADS=${MOAB_PROCCOUNT}
# Printout number of threads
echo "No.threads = ${OMP_NUM_THREADS}"
# Execute program
${exe}
```

- Shared memory restricts to 1 node.
- Do not define number of threads explicitely. Use MOAB variables.

OpenMP parallel jobs (3)

- Using Intel OpenMP Thread Affinity for Pinning Threads differently

${WORKSHOP}/exercises/04/parallel/omp_v2.sh

```
#!/bin/bash

#MSUB -l nodes=1:ppn=2
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

# Set executable name to variable
exe=./hello_omp
# Load modules
module load compiler/intel

# Setup OpenMP environment variable
export OMP_NUM_THREADS=${MOAB_PROCCOUNT}
# Use different pinning: none, scatter, compact
export KMP_AFFINITY=verbose,scatter

# Printout number of threads
echo "No.threads = ${OMP_NUM_THREADS}"

# Execute program
${exe}
```

TASK/ToDo: 5 min

- Submit script with different pinnings
- Compare results

MPI parallel jobs (1)

- MPI = Message Passing Interface
  - → To enable programs parallelly running on a distributed memory system
  - MPI tutorial from Livermore Computing Center (https://computing.llnl.gov/tutorials/mpi/)
  - MPI Standards on http://www.mpi-forum.org
- Variants @ Clusters
  - Intel-MPI (impi → modules: mpi/impi/<version>)
  - OpenMPI (openmpi → modules: mpi/openmpi/<version>)
  - Dependencies?
    - **Versions depend on compilers!**
- Training info:
  - @Uni Stuttgart: Oct 15-19 2018, https://www.hlrs.de/training/2018-10-15-par/
  - @KIT: June/July 2019 as part of lecture „Parallelrechner & Parallelprogrammierung“

Intel-MPI parallel jobs (1)

- Example: `${WORKSHOP}/exercises/04/parallel/impi.sh`

```
#!/bin/bash
#MSUB -l nodes=1:ppn=2
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

# Set executable name to variable
exe=./hello_impi
# Load modules
module load compiler/intel mpi/impi

# Printout number of tasks
echo "No.MPI tasks = ${MOAB_PROCCOUNT}"
# Spawn for each core 1 MPI task
mpirun -print-rank-map ${exe}
```

- For computations on more than 1 node use **`bwhpc-workshop.77`**
- For testing example, copy the executable to submit directory
- The corresponding MPI module has to be loaded on the compute nodes.
- Use mpirun to execute the binary.

OpenMPI parallel jobs (1)

- Difference to OpenMPI?

  → compare: `${WORKSHOP}/exercises/04/parallel/openmpi.sh`

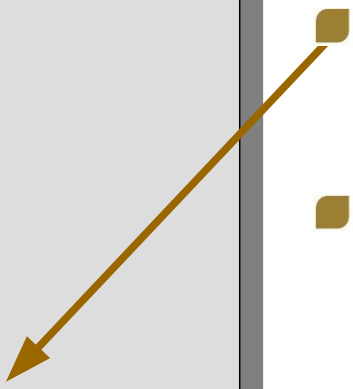
```
#!/bin/bash

#MSUB -l nodes=1:ppn=2
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.75

# Set executable name to variable
exe=./hello_openmpi
# Load modules
module load compiler/intel mpi/openmpi/3.1-intel-17.0

# Printout number of tasks
echo "No.MPI tasks = ${MOAB_PROCCOUNT}"

# Spawn for each core 1 MPI task
mpirun -report-bindings ${exe}
```

Intel-MPI parallel jobs (2)

- Spawning **only 1 MPI task per node**
  - Pitfalls: a) `mpirun -n ${MOAB_NODECOUNT}` b) `mpirun -perhost 1` c) ...

`${WORKSHOP}/exercises/04/parallel/impi_v2.sh`

```
#!/bin/bash
#MSUB -l nodes=2:ppn=28
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.77
# Set executable name to variable
exe=./hello_impi
# Load modules
module load compiler/intel mpi/impi
# Set up list for tasks to be spawned
mylist=./hostlist_${MOAB_JOBID:-$$}.txt
srun hostname -s | sort | uniq > $mylist
# Printout number of nodes = MPI tasks
echo "No.MPI tasks = ${MOAB_NODECOUNT}"
# Spawn only one MPI task per node
mpirun -machinefile ${mylist} -print-rank-map ${exe}
```



- This only works on bwUniCluster and ForHLR 1
- On Torque based systems use **`cat $PBS_NODEFILE`**

OpenMPI parallel jobs (2)

- Spawning only 1 MPI task per node
  - Difference to Intel-MPI?

`${WORKSHOP}/exercises/04/parallel/openmpi_v2.sh`

```
#!/bin/bash

#MSUB -l nodes=2:ppn=28
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.77

# Set executable name to variable
exe=./hello_openmpi
# Load modules
module load compiler/intel mpi/openmpi/3.1-intel-17.0



# Printout number of nodes = MPI tasks
echo "No.MPI tasks = ${MOAB_NODECOUNT}"


# Spawn only one MPI task per node
mpirun --map-by ppr:1:node:pe=28 -report-bindings ${exe}
```

Hybrid parallel jobs: Intel-MPI + OpenMP

- Spawning only 1 MPI task per node, and n OpenMP thread per MPI task

${WORKSHOP}/exercises/04/parallel/hybrid_impi_omp.sh

```
#!/bin/bash

#MSUB -l nodes=2:ppn=28,walltime=00:01:00,pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.77

# Set executable name to variable
exe=./hello_impi_omp
# Load modules
module load compiler/intel mpi/impi

# Set up list for tasks to be spawned
mylist=./hostlist_${MOAB_JOBID:-$$}.txt
srun hostname -s | sort | uniq > $mylist
# Setup OpenMP env variable
export OMP_NUM_THREADS=$((${MOAB_PROCCOUNT}/${MOAB_NODECOUNT}))

# Printout number of nodes = MPI tasks
echo "No. MPI tasks (nodes) = ${MOAB_NODECOUNT}"
echo "No. threads per node  = ${OMP_NUM_THREADS}"
# Spawn only one MPI task per node
mpirun -machinefile ${mylist} -print-rank-map ${exe}
```

Hybrid parallel jobs: OpenMPI + OpenMP

- Spawning only 1 MPI task per node, and n OpenMP thread per MPI task
  - Difference to Intel-MPI?

${WORKSHOP}/exercises/04/parallel/hybrid_openmpi_omp.sh

```
#!/bin/bash
#MSUB -l nodes=2:ppn=28,walltime=00:01:00,pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop.77

# Set executable name to variable
exe=./hello_openmpi_omp
# Load modules
module load compiler/intel mpi/openmpi/3.1-intel-17.0



# Setup OpenMP env variable
export OMP_NUM_THREADS=$((${MOAB_PROCCOUNT}/${MOAB_NODECOUNT}))
# Printout number of nodes = MPI tasks
echo "No. MPI tasks (nodes) = ${MOAB_NODECOUNT}"
echo "No. threads per node  = ${OMP_NUM_THREADS}"
# Spawn only one MPI task per node
mpirun --map-by ppr:1:node:pe=${OMP_NUM_THREADS} -report-bindings ${exe}
```

Thank you for your attention!