bw|HPC

Batch System – Best Practices

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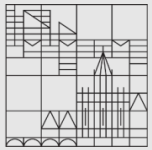

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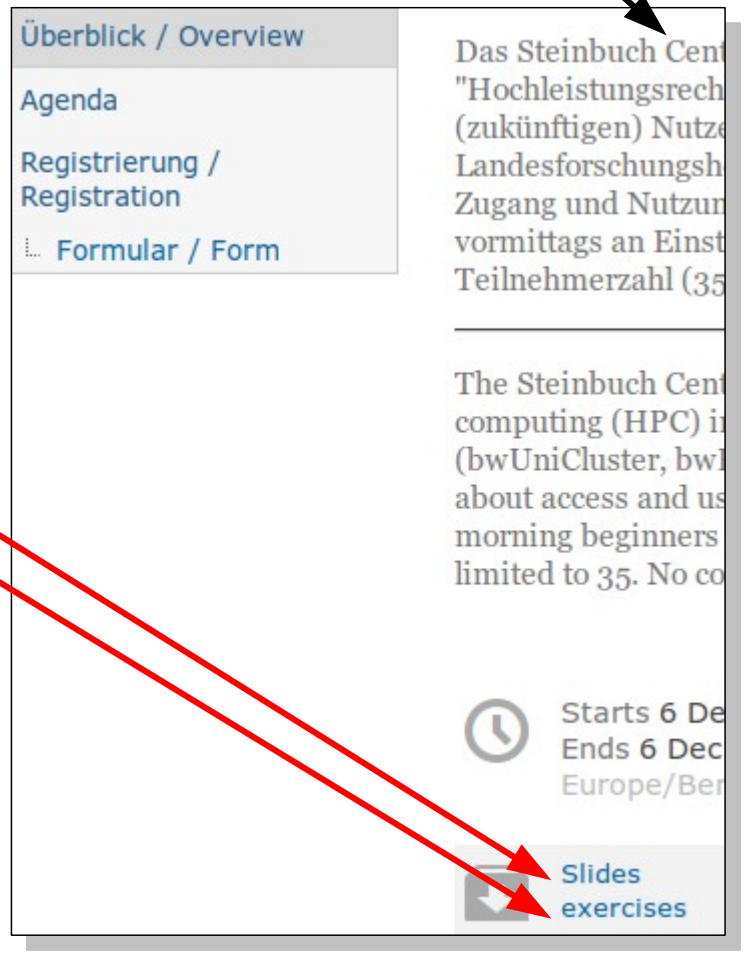
How to read the following slides

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/2019-04-10`

- MOAB: more info can be found at http://bwhpc.de/wiki in article:
  - Batch_Jobs
- SLURM: more info can be found at http://wiki.scc.kit.edu/hpc in article:
  - Batch_Jobs

Where to get the slides/exercises/reservation?

- https://indico.scc.kit.edu/e/bwhpc_course_2019-04-10 or
  bwUniCluster: /pfs/data1/software_uc1/bwhpc/kit/workshop/2019-04-10
  - Slides
  - Exercises



- Workshop reservation:
  single node:

```
msub -A workshop
-l advres=bwhpc-workshop_single.97
```

- multi node:

```
msub -A workshop
-l advres=bwhpc-workshop_multi.98
```

How to do excerices?

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

```
$ ws_allocate bwhpc-course 30
Workspace created. Duration is 720 hours.
Further extensions available: 3
/pfs/work2/workspace/scratch/xy1234-bwhpc-course-0
```

- Copy examples to your workspace

```
$ WORKSHOP=/pfs/data1/software_uc1/bwhpc/kit/workshop/2019-04-10
$ cd $(ws_find bwhpc-course)
$ mkdir -v 2019-04-10; cd 2019-04-10
$ cp -pr ${WORKSHOP}/exercises/04 ./
```

- Submit jobs from your workspace

```
$ cd $(ws_find bwhpc-course)/2019-04-10/04
$ msub <jobscript>
```

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_single.89

## 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=...

Sbatch Directives

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

```
#!/bin/bash

#SBATCH -N 1
#SBATCH -t 00:01:00
#SBATCH --mem=50mb
#SBATCH -p singlenode
#SBATCH -J serial-test
#SBATCH --mail-type=BEGIN,FAIL,END
#SBATCH --mail-user=<my_email_address>

## to access today's standing reservation
#SBATCH -A workshop
#SBATCH --reservation=<name>

printenv
```

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

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
```

- @ 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

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)*

Ressource specifications (3)

- @ SLURM (ForHLR I/II)
  - `node` = computer server
  - `task` = number of „instances“ of your command to be executed, default: max tasks per node is equal max cores (exception: overcommit)
  - `cpu` = *CPU Cores*Threads* (e.g. hyperthreading)
  - `thread` = number of processing units on each core (not number of application tasks launched per core; default: on per *CPU core*

Examples:

1) Addressing 2 CPU cores (@1 task) on 1 node:

```
#SBATCH --nodes=1 --ntasks=1 --cpus-per-task=2
```

2) 40 Tasks on 1 node:

```
#SBATCH -N1 --ntasks=40 --overcommit
```

Ressource specifications (2)

- @ SLURM (ForHLR I/II)
  - `--mem` = Memory per node (Check defaults: „scontrol show config“)
  - `--mem-per-cpu` = Minimum memory per allocated cpu,
    if exceeding MaxMemPerCPU, do workaround with mem,
    ntasks and cpus-per-task
  - Node access policies

    ForHLR I/II: **singlejob** *(=exclusively for your job)*

Job Script: Templates

- 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

```
#!/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

- MOAB: Not allowed:

```
$ msub job.sh -x argument
```

→ msub will interprete -x as an own option

- SLURM: allowed:

```
$ sbatch job.sh -x argument
```

→ sbatch assumes that everything after stating the script name are user's arguments

- 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

MOAB: 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** working 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

- Coures:
  - @KIT: OpenMP (10.07.19) as part of lecture „Parallelrechner & Parallelprogrammierung“
  - @Uni Stuttgart: Oct 14-18 2019, https://www.hlrs.de/training/2019/PAR

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

    → Normally 1 thread is to be pinned to 1 core
  - Process binding

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_single.97

# 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 is restricted to 1 node.
- Do not define number of threads explicitely. Use environment variables.

OpenMP parallel jobs: Pinning

- Using Intel OpenMP Thread Affinity for Pinning Threads differently

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

```
#!/bin/bash
#MSUB -l nodes=1:ppn=4
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop_single.97

# 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!**
- Coures:
  - @KIT: OpenMP (10.07.19) as part of lecture „Parallelrechner & Parallelprogrammierung“
  - @Uni Stuttgart: Oct 14-18 2019, https://www.hlrs.de/training/2019/PAR

MPI process binding

- Compute-bound MPI
  - As many MPI tasks per node as cores available
- Memory-bound MPI
  - One MPI task per socket/node
- Hybrid MPI + OpenMP
  - One MPI task per „domain“, multithreaded process over the whole domain

Compute-bound: Intel-MPI parallel jobs

- 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_single.97

# Set executable name to variable
exe=./hello_impi
# Load modules
module load mpi/impi/2017-intel-17.0

# 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_multi.94**
- For testing example, copy the executable to submit directory
- Adds automatically the corresponding Intel compiler module
- Use mpirun to execute the binary, print details of task pinning.

Compute-bound: OpenMPI parallel jobs

- 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_single.97

# Set executable name to variable
exe=./hello_openmpi
# Load modules
module load 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 -display-map ${exe}
```

Memory-bound: Intel-MPI parallel jobs

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

```
#!/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_multi.98
# Set executable name to variable
exe=./hello_impi
# Load modules
module load compiler/intel mpi/impi


# Printout number of nodes = MPI tasks
echo "No.MPI tasks = ${MOAB_NODECOUNT}"
# Spawn only one MPI task per node
export I_MPI_JOB_RESPECT_PROCESS_PLACEMENT=0
mpirun -perhost 1 -binding domain=node -print-rank-map ${exe}
```

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

- Preset of MOAB must be overwriten by: `I_MPI_JOB….=0`
- Assign to each MPI task the full node as its domain

Memory-bound: OpenMPI parallel jobs

- 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_multi.98

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

# Define domain size of each MPI task
domain_size=$((${MOAB_PROCCOUNT}/${MOAB_NODECOUNT}))
# Printout number of MPI tasks and domain size
echo "No.MPI tasks = ${MOAB_NODECOUNT}"
echo "Domain size  = ${domain_size}"

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

- Autoloads corresponding Intel compiler
- Assign to each MPI task the full node as its domain

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
#MSUB -l walltime=00:01:00
#MSUM -l pmem=200mb
#MSUB -A workshop
#MSUB -l advres=bwhpc-workshop_multi.98

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

# Define domain size of each MPI task
domain_size=$((${MOAB_PROCCOUNT}/${MOAB_NODECOUNT}))
# Printout number of MPI tasks and domain size
echo "No.MPI tasks = ${MOAB_NODECOUNT}"
echo "Domain size  = ${domain_size}"

# Spawn only one MPI task per node; set variables
export OMP_NUM_THREADS=${domain_size}
export I_MPI_JOB_RESPECT_PROCESS_PLACEMENT=0
mpirun -genvall -perhost 1 -binding domain=node -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_multi.98

# 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!

Questions?