



bw | HPC – C5

Batch System Introduction

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Reference: bwHPC-C5 Best Practices Repository

- Most information given by this talk can be found at <http://bwhpc-c5.de/wiki>:

- Batch_Jobs



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Knowledge Base Wiki
of
Baden-Württemberg's HPC services

Welcome to the Knowledge Base Wiki of services and projects for *high performance computing (HPC)* and *HPC data storage* in the state of Baden-Württemberg, Germany. Hosted as a Best Practices Repository, the knowledge base contains user guides and best practice guides (**BPG**) and is maintained by members of Baden-Württemberg's federated HPC competence centers for clusters of tier 3 as well as by members of the HPC competence center for the ForHLR (tier 2).

Federated HPC competence centers of tier 3 are an integral part of the project **bwHPC-C5** which coordinates the *federated user and science support* for the **HPC infrastructure** of tier 3 in the state of Baden-Württemberg.

HPC Services

The federated HPC competence centers of tier 3 provide and maintain user guides and best practice guides for the compute clusters of **tier 3**:

- **bwUniCluster**
- **bwForCluster JUSTUS**

accessible via the

- **Best Practices Repository.**

Furthermore, the KIT provide and maintain user guides and best practice guides for the compute cluster of **tier 2**:

- **ForHLR Phase I**

HPC Data Storage Services

For user guides of the data storage services:

- **bwFileStorage**

Material: Slides & Scripts

- <https://indico.scc.kit.edu/indico/event/310/>
- @bwUniCluster/ForHLR I/ForHLR II:
/pfs/data1/software_uc1/bwhpc/kit/workshop/2017-10-10

How to read the following slides

Abbreviation/Colour code	Full meaning
<code>\$ command -option value</code>	<code>\$</code> = prompt of the interactive shell The full prompt may look like: user@machine:path\$ The command has been entered in the interactive shell session
<code><integer></code> <code><string></code>	<code><></code> = Placeholder for integer, string etc

Batch System

Resource management

- Jobs are **not** executed by the user
- Instead, there is a management system (Batch System)
 - **workload manager (scheduler)**
 - scheduling, managing, monitoring, reporting
 - MOAB
 - **resource manager**
 - control over jobs and distributed compute nodes
 - SLURM (bwUniCluster, ForHLR I)
 - TORQUE (ForHLR II, all bwForClusters)

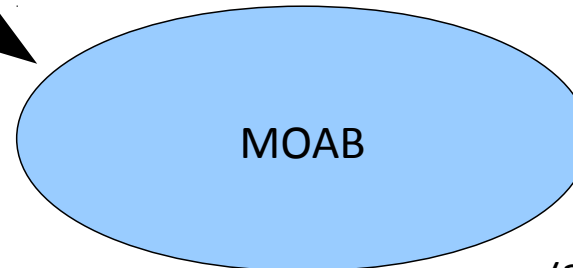
Resource and workload manager (1)

(1) User creates a **job script** and submits it to MOAB via the “**msub**” command

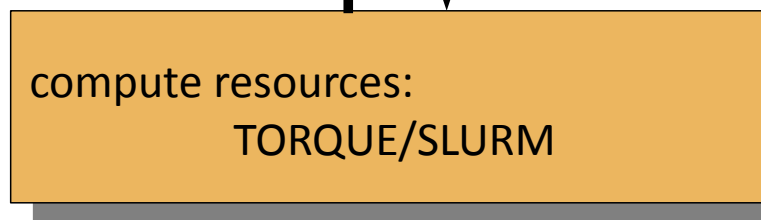
```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb

./your_simulation
```

(2) MOAB parses the job script:
→ where & when to run job



(3) Job execution:
delegated to resource
manager on the node



(4) The resource manager (TORQUE/SLURM) executes the job and communicates status information to MOAB

Resource and workload manager (2)

- All clusters:
 - compute job will **only** be processed by the batch system
 - Running jobs on login nodes not allowed

- Waiting time:
 - fairshare based queue
 - depends on:
 - your job demands
 - your demand history
 - your university's share (bwUniCluster only)

Job's life circle

1. Setup `job.sh`:

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb

./your_simulation
```

Options for the job

Actual work to be executed on the cluster

2. Submit job **ONLY** with “msub”

```
$ msub job.sh
<job_ID>
```

3. Job pending/running

```
$ showq
<job_ID> state "Idle" → "Running"
```

4. Job is finished → check output (default job name)

```
bwUniCluster/ForHLR1/2: job_{uc1,fh1,fh2}<job_ID>.out
bwForCl. JUSTUS/NEMO   : <jobscripname>.o<job_ID>
bwForCl. BinAC         : <jobscripname>.o<job_ID>
```


1. Job Submit: msub options

- http://www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#msub_Command
- msub options: command line or in your job script

Command line	Script	Purpose
<code>-l resources</code>	<code>#MSUB -l resources</code>	Defines the resources that are required by the job. See the description below for this important flag.
<code>-N name</code>	<code>#MSUB -N name</code>	Gives a user specified name to the job.
<code>-q queue</code>	<code>#MSUB -q queue</code>	Defines the queue class
<code>-m bea</code>	<code>#MSUB -m bea</code>	Send email when job begins (b), ends (e) or aborts (a).

1. Job Submit: *resource_list*

■ http://www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#msub_-l_resource_list

Resource	Purpose
-l nodes=2:ppn=16	Number of nodes and number of processes per node
-l walltime=600	Wall-clock time (seconds)
-l walltime=00:01:30:00	DD:HH:MM:SS format
-l pmem=1000mb	Max. amount of physical memory used by one process of the job (kb,mb,gb)
-l mem=1000mb	Max. total physical memory used by the job

Use these options in the job script:

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb
...
```

Or use them with msub:

```
$ msub -l nodes=1:ppn=1,walltime=00:01:00,pmem=1gb <job_script>
```

`msub -q queues (bwUniCluster)`

■ www.bwhpc-c5.de/wiki/index.php/Batch_Jobs_-_bwUniCluster_Features#msub_-q_queues

<i>queue</i>	<i>default resources</i>	<i>MIN resources</i>	<i>MAX resources</i>
automatic queue routing			
develop	<i>procs=1, pmem=4000mb</i>	<i>nodes=1</i>	<i>walltime=00:30:00, nodes=1:ppn=16</i>
singlenode	<i>procs=1, pmem=4000mb</i>	<i>walltime=00:30:01, nodes=1</i>	<i>walltime=3:00:00:00, nodes=1:ppn=16</i>
multinode	<i>procs=1, pmem=4000mb</i>	<i>nodes=2</i>	<i>walltime=2:00:00:00, nodes=128:ppn=28</i>
Manual queue selection			
verylong	<i>procs=1, pmem=4000mb</i>	<i>walltime=3:00:00:01, nodes=1</i>	<i>walltime=6:00:00:00, nodes=1:ppn=16</i>
fat	<i>procs=1, pmem=32000mb</i>	<i>nodes=1</i>	<i>walltime=3:00:00:00, nodes=1:ppn=32</i>

■ **Automatic queue choosing** - walltime, nodes, processes

Tutorial 1a

- **Goal:** Use the Batch System to execute “`printenv`” on the cluster
- **1)** Create a file „`submit_script.sh`“ and set the following options in the submit script:
 - `nodes=1:ppn=1`
 - `pmem=50mb`
 - `walltime=00:01:00`
- **2)** After defining these options, write the command to be executed in the jobscript (“`printenv`”)
- **3)** Save the jobscript and submit it to the Batch System with

```
$ msub -l advres=workshop_single.50 submit_script.sh
```
- You can use “`showq`” to see the status of your job
- **4)** Look in the output file of your job (`job_uc1_<jobID>.out`) for variables starting with „**MOAB_**“. These can be used to get information on how the job was started

Tutorial 1a - Solution

- Create a file named „**submit_script.sh**“ with the following content:

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb

printenv
```

- Save the file and submit it with

```
$ msub -l advres=workshop_single.50 submit_script.sh
```

- In the output file, you can find the MOAB variables:

- For example: „**MOAB_CLASS=develop**“ means:

In the job script, we have not defined a queue class but the job was automatically submitted to the „develop“ queue

Tutorial 1b

- **1)** Modify your submit script so that instead of “`printenv`” the value of „**MOAB_PROCCOUNT**“ is printed (Hint: Use **echo**)
- Submit your job again, but this time use `msub` to specify the number of processes:

```
$ msub -1 nodes=1:ppn=2 -l advres=workshop_single.50 submit_script.sh
```

- **2)** Check in your output file if the number of processes is 1 as specified in the submit script or 2 as specified with **msub**

Tutorial 1b - Solution

- Modify your submit script to print the variable **MOAB_PROCCOUNT**

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:01:00
#MSUB -l pmem=50mb

echo $MOAB_PROCCOUNT
```

- Save the file and submit it with

```
$ msub -l nodes=1:ppn=2 -l advres=workshop_single.50 submit_script.sh
```

- In the output file the number of processes is printed:

```
job_uc1_<job-ID>.out
```

```
2
```

The options given directly to msub take precedence over the options in the submit script

Read also: www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#Environment_Variables_for_Batch_Jobs

Check status of your jobs (1)

- after submission → msub returns <job-ID>

```
$ msub job.sh
```

```
659562
```

- **commands:**

\$ showq	Show status of all your jobs
\$ showq -n	Show status of all your jobs, showing job names
\$ showq -r \$ showq -i \$ showq -b \$ showq -c	All your active (running) jobs eligible(idle) jobs blocked jobs completed jobs
\$ checkjob <job-ID>	Get detailed information of your job → explains why your job is pending
\$ canceljob <job-ID>	Cancel the job with <job-ID>

Check status of your jobs (2)

■ Command “showq”:

```
$ showq
```

active jobs-----

JOBID	USERNAME	STATE	PROCS	REMAINING	STARTTIME
12345	xy_ab1234	Running	1	00:04:58	Thu Jan 22 19:21:56

1 active job

eligible jobs-----

JOBID	USERNAME	STATE	PROCS	WCLIMIT	QUEUETIME
12346	xy_ab1234	Idle	1	00:05:00	Thu Jan 22 19:21:47

1 eligible job

blocked jobs-----

JOBID	USERNAME	STATE	PROCS	WCLIMIT	QUEUETIME
12347	xy_ab1234	Idle	1	00:05:00	Thu Jan 22 19:21:47

1 blocked job

■ Check why job can not start:

```
checkjob <job_ID>
```

get information of your job

```
checkjob -v -v -v <job_ID>
```

All detailed information

Check status of your jobs (3)

■ STATES:

■ Pre-execution states:

- Idle Job is waiting for free resources
- Deferred Job cannot be scheduled right now
- BatchHold Job is blocked by scheduler.
Reasons: no resources,limits,failure

```
Idle → Running → Canceling == OK
```

```
Idle → Deferred → Idle → Deferred → ... → BatchHold → Canceling
```

■ Execution states

- Starting Job is starting
- Running Job is running
- Suspended Job has exceeded specified walltime

Check status of your jobs (4)

example: MAXPROC limit

■ Submitted job (bwUniCluster)

```
$ msub -l nodes=1:ppn=32 -q fat <jobscript>
12345
```

showq:

```
blocked jobs-----
JOBID          USERNAME          STATE PROCS      WCLIMIT          QUEUETIME
12345          xy_ab1234         Idle   32             00:05:00  Fri Jan 23 15:31:05
```

checkjob -v -v -v 12345:

```
State: Idle
Creds:  user:xy_ab1234  group:xyz  account:kit  class:fat
...
NOTE:  job violates constraints for partition uc1 (job 12345 violates active
HARD MAXPROC limit of 64 for class fat user partition ALL (Req: 32  InUse: 64))

BLOCK MSG:  job 12345 violates active HARD MAXPROC limit of 64 for class fat
user partition ALL (Req: 32  InUse: 64) (recorded at last scheduling iteration)
```

Check status of your jobs (6)

example: organisation limits

Submitted job (bwUniCluster)

```
$ msub -l nodes=1:ppn=1 <jobscrip>  
55555
```

showq:

```
blocked jobs-----  
JOBID          USERNAME      STATE  PROCS   WCLIMIT      QUEUETIME  
55555          xy_ab1234     Idle   1       00:10:00    Fri Jan 21 15:31:05
```

checkjob -v -v -v 55555:

```
State: Idle  
class:develop  
...
```

limits for university_X!

```
BLOCK MSG: job 55555 violates active SOFT MAXPROC limit of 1000  
for acct university_X partition ALL (Req: 1 InUse: 1010) ...
```

Change status of your jobs

■ Change command: **mjobctl**

`mjobctl -c <job_ID>`

`mjobctl -c -w state=Idle`

`mjobctl -c -w state=Running`

`mjobctl -c -w state=BatchHold`

`mjobctl -c -w user=$USER`

cancel the job (new command)

cancel ALL idle jobs

cancel ALL running jobs

cancel ALL hold jobs

cancel ALL your jobs!

Tutorial 2

- **1)** Modify your submit script so that it executes a command to wait for 600 seconds (**sleep 600**)
- Increase the **walltime** to 10 minutes and give your job a name
- Submit your job script
- Use **showq** to check where your job is
- Use **showq -n** to see the name of your job
- Use **canceljob <job-ID>** or **mjobctl -c <job-ID>** to cancel your job

Tutorial 2 - Solution

■ Modify your submit script

```
#!/bin/bash
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:10:00
#MSUB -l pmem=50mb
#MSUB -N myJobName

sleep 600
```

■ Save the file and submit it with

```
$ msub -l advres=workshop_single.50 submit_script.sh
```

■ Show the status of your jobs with **showq**

```
active jobs-----
JOBID          USERNAME      STATE  PROCS  REMAINING      STARTTIME
11705861      mb1337      Running    1    00:08:12  Tue Apr  5 14:30:01
```

- Use **checkjob -v -v -v <job-ID>** to see further information
- Use **canceljob <job-ID>** or **mjobctl -c <job-ID>** to cancel your job

Moab: Interactive jobs

- **Interactive jobs on login nodes are not permitted**

- **Solution: interactive moab jobs**

- Access to compute nodes and work on them interactively

- HowTo:

```
$ msub -I -V -l nodes=1:ppn=1,walltime=02:00:00
```

Attention: Restrictions may apply (shared nodes, single node etc.)

-I = interactive

-V = all environment variables are exported to the compute node

- **Details @ bwUniCluster**

- www.bwhpc-c5.de/wiki/index.php/Batch_Jobs_-_bwUniCluster_Features#Interactive_Jobs

- **Details @ bwForClusters**

- see bwHPC Wiki for bwForCluster of interest

Moab: Interactive jobs (Example)

```
mb1337@uc1n996: msub -I -V -l nodes=1:ppn=1,walltime=00:02:00
```

Job is waiting to start

```
salloc: Job is in held state, pending scheduler release  
salloc: Pending job allocation 11631324  
salloc: job 11631324 queued and waiting for resources
```

```
salloc: job 11631324 has been allocated resources  
salloc: Granted job allocation 11631324
```

Job running. You are now on a compute node

```
mb1337@uc1n257$ {Now you can work on the compute node}
```

```
allocation has been revoked.  
srun: Job step aborted: Waiting up to 32 seconds  
for job step to finish.  
srun: error: uc1n257: task 0: Killed  
mb1337@uc1n996:
```

Requested time for the interactive job ran out

Back on the login node