bw|HPC

Batch System Introduction

Thorsten Zirwes, SCC, KIT

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386

UNI FREIBURG

UNIVERSITÄT HOHENHEIM 1818

Hochschule Esslingen
University of Applied Sciences

Universität Konstanz

UNIVERSITÄT MANNHEIM

Universität Stuttgart

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

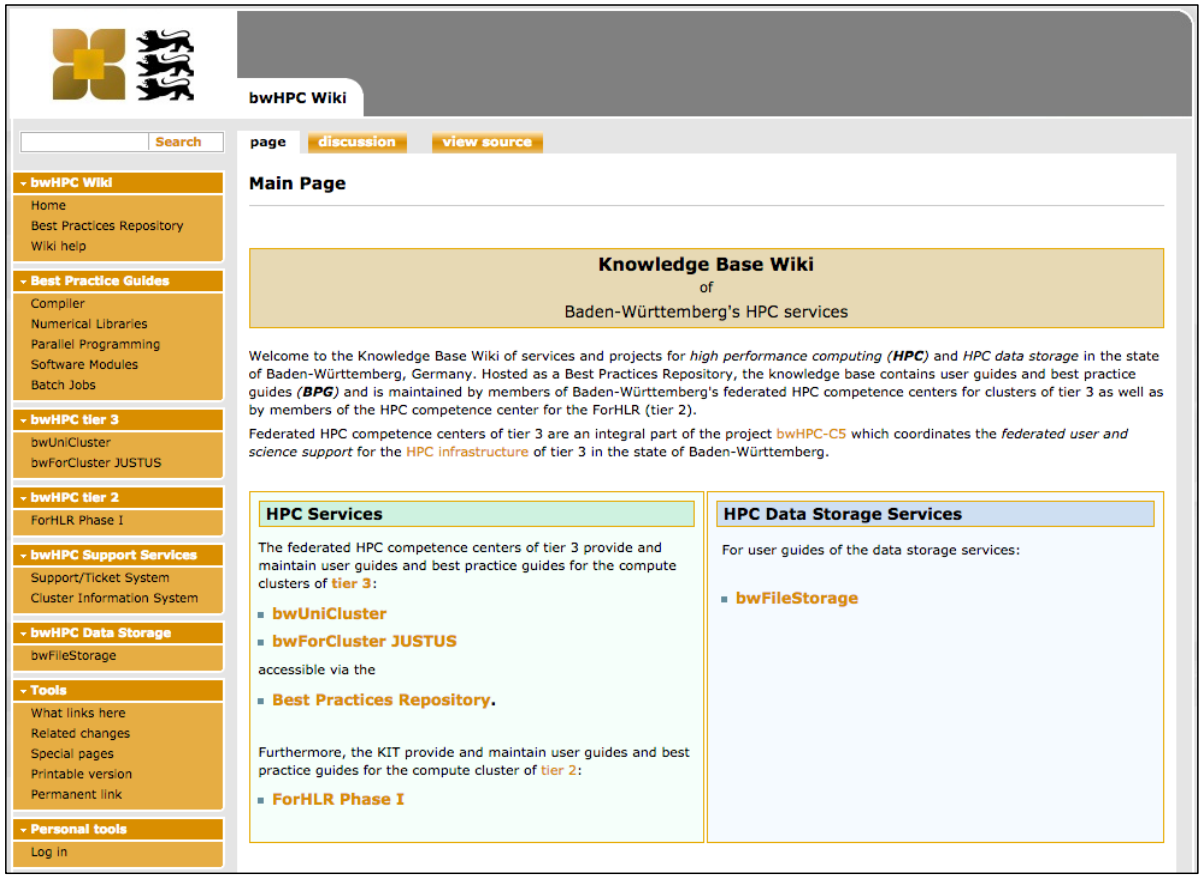
KIT Karlsruher Institut für Technologie

ulm university universität ulm

Funding: Baden-Württemberg MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

Reference: bwHPC-C5 Best Practices Repository

- All information given in this talk can be found at http://bwhpc.de/wiki:
  - Batch_Jobs



Material: Slides & Scripts

- https://indico.scc.kit.edu/e/bwhpc_course_2019-04-09
- @bwUniCluster:

  /pfs/data1/software_uc1/bwhpc/kit/workshop/2019-04-09

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

Batch System

Resource management

- Jobs are **not** executed by the user

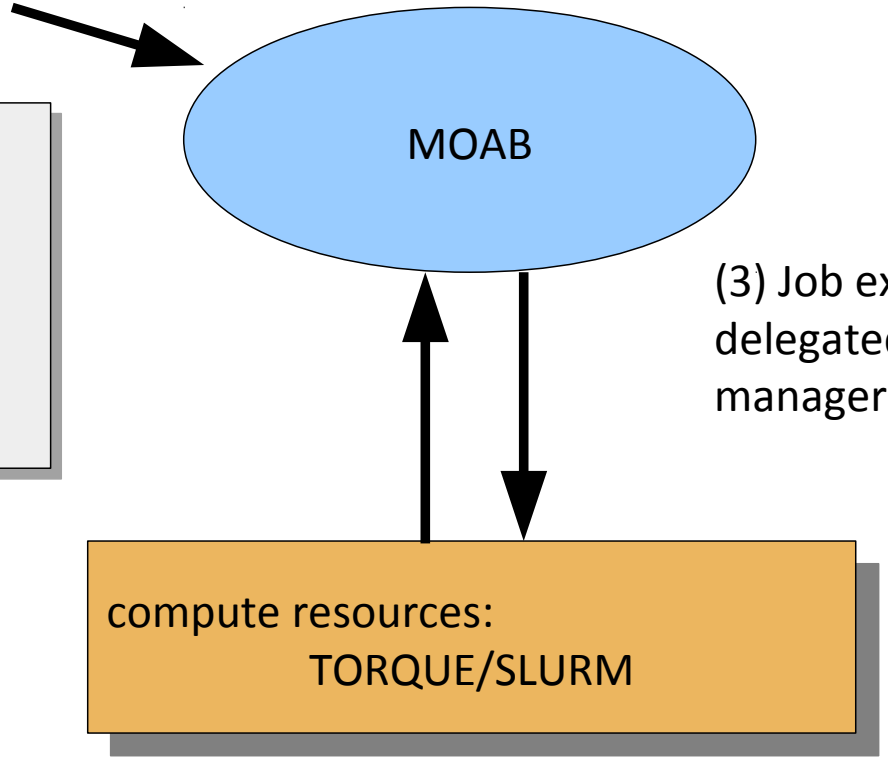
- Instead, there is a management system (Batch System)
  - **workload manager (scheduler)**
    - scheduling, managing, monitoring, reporting
    - MOAB
  - **resource manager**
    - control over jobs and distributed compute nodes
    - SLURM (bwUniCluster, ForHLR I)
    - TORQUE (ForHLR II, all bwForClusters)

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
```



(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_script.sh**:

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

./your_simulation
```

1) Options for the job

2) Actual work to be exectuted on the cluster

2. Submit job **ONLY with "msub"**

```
$ msub job_script.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  : <jobscriptname>.o<job_ID>
bwForCl. BinAC        : <jobscriptname>.o<job_ID>
```

1. Job Submit: msub options

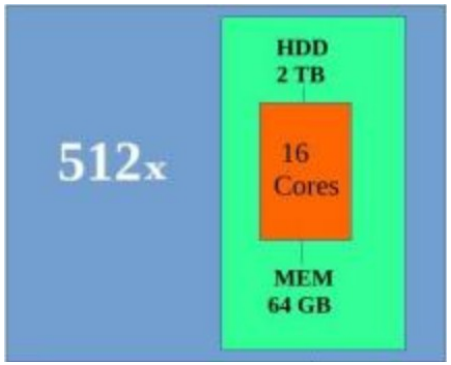
- http://www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#msub_Command
- msub options: command line or in your job script

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

1. Job Submit: *resource_list*

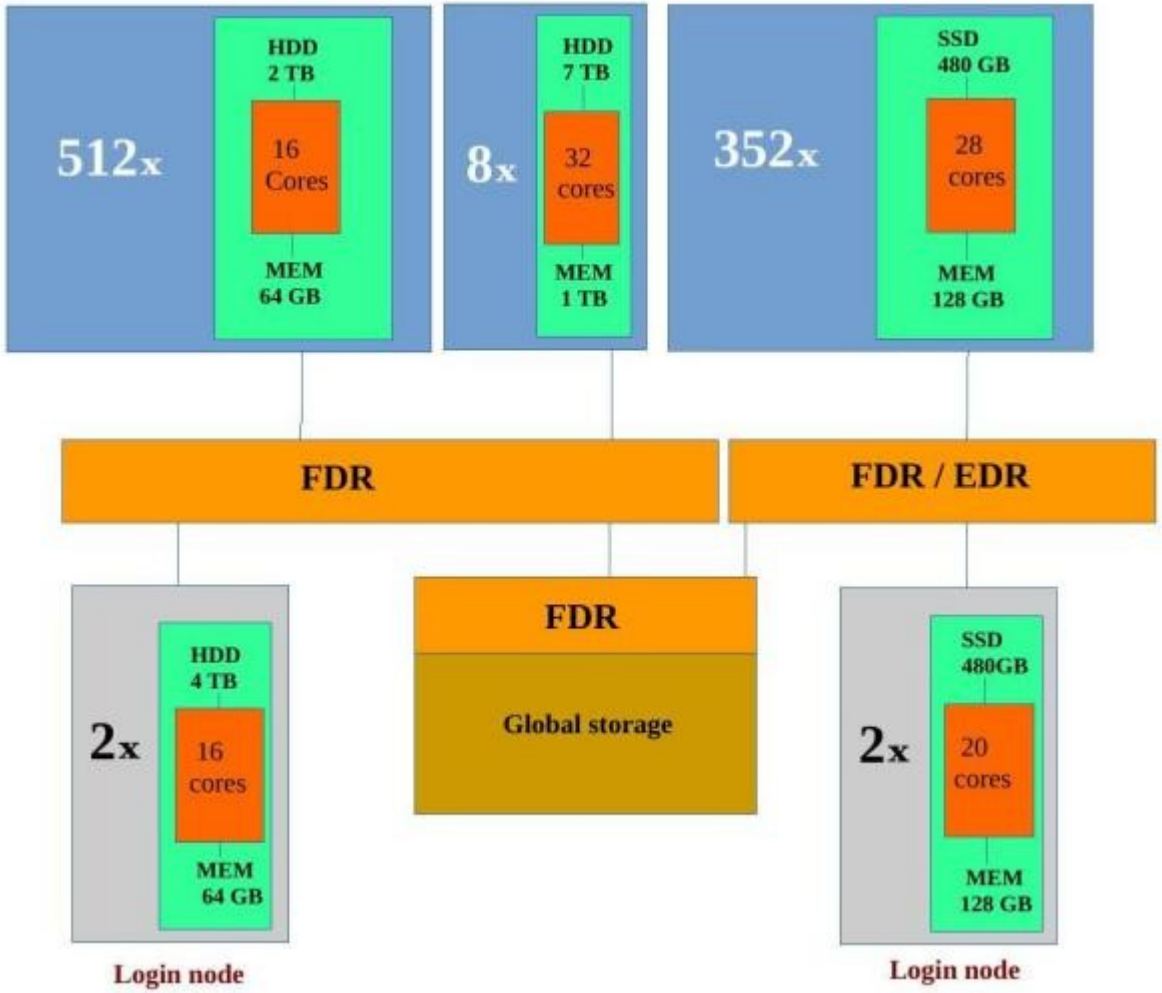
- http://www.bwhpc-c5.de/wiki/index.php/Batch_Jobs#msub_-l_resource_list

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



Example for bwUni cluster:
The cluster consists of 512 compute nodes
Each compute node has two CPUs with 8 cores each

bwUniCluster



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

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

- **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

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

[?????]
```

2) After defining these options, insert the command to be exectuted at the end of the jobscript ("`printenv`")

3) Save the jobscript and submit it to the Batch System with

```
$ msub -A workshop -l advres=workshop_single.97 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 -A workshop -l advres=workshop_single.97 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 -A workshop -l advres=workshop_single.89 -l nodes=1:ppn=2 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 directly 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 -A workshop -l advres=workshop_single.89 -l nodes=1:ppn=2 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-exectuion 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 <jobscript>
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:

limits for **university_X**!

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

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>	cancel the job (new command)
mjobctl -c -w state=**Idle**	cancel ALL idle jobs
mjobctl -c -w state=**Running**	cancel ALL running jobs
mjobctl -c -w state=**BatchHold**	cancel ALL hold jobs
mjobctl -c -w user=$USER	**cancel ALL your jobs!**

Tutorial 2

- 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 with **msub**
- Use **showq** to check the status of your job
- 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 -A workshop -l advres=workshop_single.97 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

- **Jobs on login nodes are not permitted**
- **Solution: interactive moab jobs**
  - Access 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

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:
```

Job running. You are now on a compute node

Requested time for the interactive job ran out

Back on the login node

MOAB vs. SLURM

- On ForHLR I and II, „**SLURM**“ instead of MOAB is used as batch system
  - Jobscripts need to be modified!
  - All details can be found on the ForHLR wiki

MOAB

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


./program
```

SLURM

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --cpus-per-task=1
#SBATCH --time=0:10:00
#SBATCH --mem=500m

./program
```

- Submit the job with:

```
$ msub submit_script.sh
```

```
$ sbatch submit_script.sh
```