Karlsruhe Institute of Technology

Batch System Introduction

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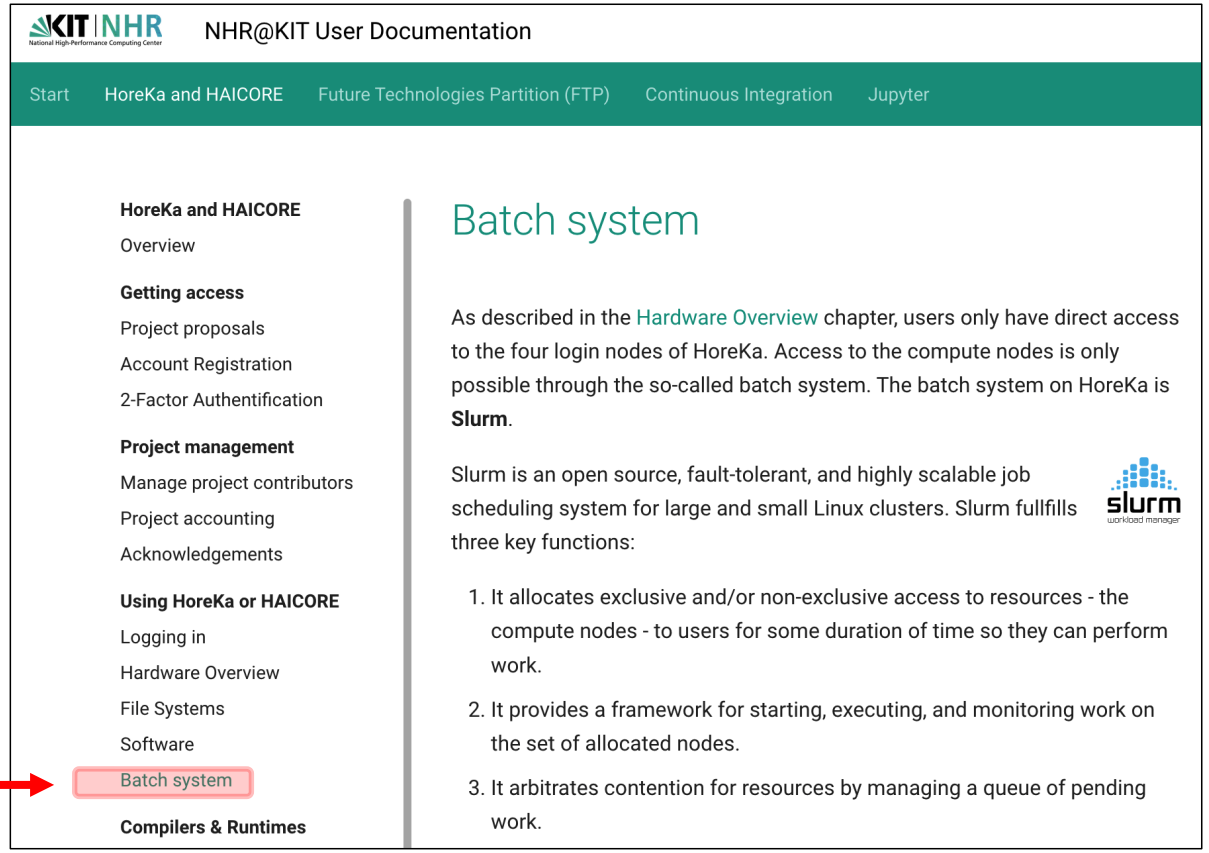
Reference: NHR@KIT User Documentation

- All information given in this talk can be found at: https://www.nhr.kit.edu/userdocs/horeka/batch/



Material: Slides & Scripts

- https://indico.scc.kit.edu/e/nhr-kit_course_2022-10-12
- @horeka:
  - /software/all/workshop/2022-10-12

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
    - SLURM (HoreKa, bwUniCluster 2.0, 2x bwForCluster)
    - MOAB (2x bwForCluster)
  - **resource manager**
    - control over jobs and distributed compute nodes
    - SLURM (HoreKa, bwUniCluster 2.0, 2x bwForCluster)
    - TORQUE (2x bwForCluster)

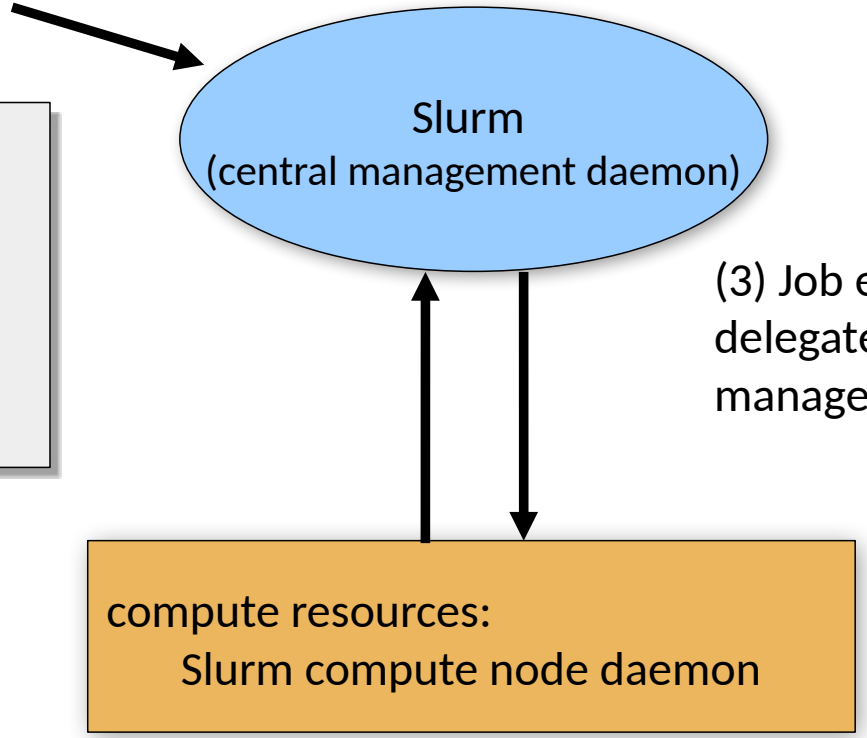
Resource and workload manager (1)

(1) User creates a **job script** and submits it to Slurm via the "**sbatch**" command

```
#!/bin/bash
#SBATCH -p dev_cpuonly
#SBATCH -N 1 -n 1
#SBATCH -t 00:01:00
#SBATCH -mem-per-cpu=50

./your_simulation
```

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



(4) The resource manager executes the job and communicates status information to nodes

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:
  - depends on:
    - your job demands
    - your demand history
    - ONLY bwUniCluster 2.0: your university's share

Job's life cycle

- 1. Preprocessing: Setup **job_script.sh**:

```
#!/bin/bash
#SBATCH -p dev_cpuonly
#SBATCH -N 1 -n 1
#SBATCH -t 00:01:00
#SBATCH -mem-per-cpu=50

./your_simulation
```

1) Options for the job

2) Actual work to be exectuted on the cluster

- 2. Submit: ONLY with "**sbatch**" (for interactive jobs: "**salloc**")

```
$ sbatch job_script.sh
<job_ID>
```

- 3. Processing:

```
$ squeue
<job_ID> STATE: "PENDING" → "RUNNING" → "COMPLETED"
```

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

```
bwUniCluster: slurm-<job_ID>.out
HoreKa      : slurm-<job_ID>.out
```

1./2. Job Submit: Sbatch options

- https://wiki.bwhpc.de/e/BwUniCluster_2.0_Slurm_common_Features#sbatch_Command_Parameters
  on bwUniCluster 2.0 and
- https://www.nhr.kit.edu/userdocs/horeka/batch/
  on HoreKa respectively.
- sbatch options: command line or in your job script

Command line	Script	Purpose
`-N` *nodes*	`#SBATCH --nodes=`*nodes*	**Number of nodes to be used.**
`-n` *tasks*	`#SBATCH --ntasks=`*tasks*	**Number of tasks to be launched.**
`-J` *name*	`#SBATCH --job-name=`*name*	**Gives a user specified name to the job.**
`-p` *queue*	`#SBATCH --partition=`*queue*	**Defines the queue class**
`--mail-type=`*type*	`#SBATCH --mail-type=`*type*	**Send email when job begins (BEGIN), ends (END), aborts (FAIL), at each event (ALL) ...**

1./2. Job Submit: Important Resource Parameters

Sbatch Resource Options		
Command line	Script	Purpose
`-t` *time*	`#SBATCH --time=`*time*	Wallclock time limit
`-N` *nodes*	`#SBATCH --node=`*nodes*	Number of nodes to be used
`-n` *tasks*	`#SBATCH --ntasks=`*tasks*	Number of tasks to be launched
`-c` *count*	`#SBATCH --cpus-per-task=`*count*	Number of CPUs required per (MPI-)task
`--ntasks-per-node=`*count*	`#SBATCH --ntasks-per-node=`*count*	Number of (MPI-)tasks per node
`--mem=`*MB_value*	`#SBATCH --mem=`*MB_value*	Memory in MegaByte per node
`--mem-per-cpu=`*MB_value*	`#SBATCH --mem-per-cpu=`*MB_value*	Memory required per allocated core

- https://wiki.bwhpc.de/e/BwUniCluster_2.0_Slurm_common_Features#sbatch_Command_Parameters
  on bwUniCluster 2.0 and
- https://www.nhr.kit.edu/userdocs/horeka/batch/
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1./2. Job Submit: Important Resource Parameters

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`-n` *tasks*	`#SBATCH --ntasks=`*tasks*	Number of tasks to be launched
`-c` *count*	`#SBATCH --cpus-per-task=`*count*	Number of CPUs required per (MPI-)task
`--ntasks-per-node=`*count*	`#SBATCH --ntasks-per-node=`*count*	Number of (MPI-)tasks per node
`--mem=`*MB_value*	`#SBATCH --mem=`*MB_value*	Memory in MegaByte per node
`--mem-per-cpu=`*MB_value*	`#SBATCH --mem-per-cpu=`*MB_value*	Memory required per allocated core

Use these options in the job script:

```
#!/bin/bash
#SBATCH --N 1
#SBATCH --n 20
#SBATCH --time=00:02:00
#SBATCH --mem=500mb
...
```

Or use them with sbatch:

```
$ sbatch -N 1 -n 20 -t 2 --mem=500  <job_script>
```

HoreKa

	Thin nodes	Fat nodes	Accelerator nodes
Number of nodes	570	32	167
Sockets per node	2	2	2
Number of cores per node	76	76	76
Main memory per node	256 GB	512 GB	512 GB
Interconnect (InfiniBand)	HDR	HDR	HDR

- 4 login nodes
- Accelerator nodes incorporate 4 NVIDIA A100-40 GPUs

sbatch -p *queues* (All queues of HoreKa)

queue	*default resources*	*MIN resources*	*MAX resources*
dev_cpuonly	time=10, ntasks=1, mem-per-cpu=1600mb	nodes=1, ntasks=1	time=60, nodes=2, mem=243200mb, ntasks=152
cpuonly	time=10, ntasks=152, mem-per-cpu=1600mb, mem=243200mb	nodes=1, ntasks=152	time=72:00:00, nodes=192, mem=501600mb, ntasks=152
dev_accelerated	time=10, ntasks=1, grep=gpu:1, mem-per-cpu=3300mb, def-mem-per-gpu=125400mb, def-cpu-per-gpu=38	nodes=1, ntasks=1, gres=gpu:1	time=1:00:00, nodes=1, mem=501600mb, ntasks=152, gres=gpu:4
accelerated	time=10, ntasks=152, grep=gpu:4, mem=501600mb, mem-per-cpu=3300mb, def-mem-per-gpu=125400mb, def-cpu-per-gpu=38	nodes=1, ntasks=152, gres=gpu:4	time=48:00:00, nodes=56, ntasks=152, gres=gpu:4, mem=501600mb

- https://www.nhr.kit.edu/userdocs/horeka/batch/
- Time and memory will be automatically chosen if not set

Available Resources

- **Check available resources via**

```
$ sinfo_t_idle
```

```
[ab1234@hkn1993 bwKURS-intro]$ sinfo_t_idle
Partition dev_cpuonly   :       1 nodes idle
Partition cpuonly       :     101 nodes idle
Partition dev_accelerate:       1 nodes idle
Partition accelerated   :      83 nodes idle
Partition haicore-gpu4  :       3 nodes idle
Partition haicore-gpu8  :       0 nodes idle
```

Tutorial 1a – HoreKa

- **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:
  - 1 task
  - 500 MB memory
  - Time: 5 minutes

```
#!/bin/bash
#SBATCH  [???]
#SBATCH --time=00:05:00
#SBATCH --mem=500

[?????]
```

- **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

```
$ sbatch  -p cpuonly --reservation=ws submit_script.sh
```

  - You can use "`squeue`" to see the status of your job
- **4)** Look in the output file of your job (**slurm-<jobID>.out**) for variables starting with „**SLURM_**". 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
#SBATCH -n 1
#SBATCH --time=00:05:00
#SBATCH --mem=500

printenv
```

- Save the file and submit it with („**--reservation=ws**” only for this workshop)

```
$ sbatch -p cpuonly --reservation=ws submit_script.sh
```

- In the output file, you can find the SLURM variables:
  - For example: „**SLURM_JOB_PARTITION=cpuonly**“ means:
    - In the job script, we have not defined a partition but the job was submitted to the „cpuonly“ partition with sbatch command

Tutorial 1b

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

```
$ sbatch -p cpuonly --reservation=ws -n 4 submit_script.sh
```

- **2)** Check in your output file if the number of processes is „1“ as specified in the submit script or „4“ as specified directly with **sbatch**

Tutorial 1b - Solution

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

```
#!/bin/bash
#SBATCH -n 1
#SBATCH --time=00:01:00
#SBATCH --mem=500

echo $SLURM_NPROCS
```

- Save the file and submit it with

```
$ sbatch -p cpuonly --reservation=ws -n 4 submit_script.sh
```

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

  slurm-<job-ID>.out

```
4
```

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

Job life cycle: 3. Processing (1)

- After submit command: if successful it returns <job-ID>

```
$ sbatch submit_script.sh

Submitted batch job 1487560
```

- „Monitoring“ via:
  - 3.a.

    ```
    scontrol show job <job-ID>
    ```

  - 3.b.

    ```
    squeue
    ```

  - 3.c. Login to compute node:

    ```
    srun --jobid=<id> --pty [--overlap] /usr/bin/bash
    ```

- „Modifying“ via:
  - 4. Cancel your job

    ```
    scancel <job-ID>
    ```

3.a. Processing – scontrol show job (1)

- After submission of your script **submit_script.sh**

```
$ scontrol show job <job-ID>

JobId=1487569 JobName=submit_script.sh
   UserId=ab1234(27049) GroupId=hk-project-scs(501119) .
   Priority=1 Nice=0 Account=hk-project-scs QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:00:19 TimeLimit=00:10:00 TimeMin=N/A
   SubmitTime=2021-10-13T00:06:58 EligibleTime=2021-10-13...
   AccrueTime=2021-10-13T00:06:59
   StartTime=2021-10-13T00:06:59 EndTime=2021-10-13T00:16:59 ...
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=...
   Partition=dev_cpuonly AllocNode:Sid=hkn1999:2170796
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=hkn0301
   BatchHost=hkn0301
   ...
```

1) Your project acronym

2) Your job state

3) Your time logging

4) Your selected partition

5) Your node list and Node on which job started

3.a. Processing – scontrol show job (2)

- After submission of your script **submit_script.sh**

```
$ scontrol show job <job-ID>

JobId=1487569 JobName=submit_script.sh
   ...
   NumNodes=1 NumCPUs=2 NumTasks=1 CPUs/Task=1 ...
   TRES=cpu=2,mem=3200M,node=1,billing=2
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:1 CoreSpec=*
   MinCPUsNode=1 MinMemoryCPU=1600M MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) ...
   Command=/hkfs/home/hk-project-scs/ab1234/submit-script.sh
   WorkDir=/hkfs/home/project/hk-project-scs/ab1234
   StdErr=/hkfs/home/hk-project-scs/ab1234/slurm-1487569.out
   StdIn=/dev/null
   StdOut=/hkfs/home/hk-project-scs/ab1234/slurm-1487569.out
   Power=
   NtasksPerTRES:0
```

1) Your requested nodes & CPU cores

2) Your job memory

3) Actual node policy

4) Your submit directory & submit script

5) Your job standard output and error log file

3.b. Processing – squeue

- After submission of your script **submit_script.sh**

```
$ squeue

   JOBID   PARTITION     NAME     USER    ST     TIME  NODES NODELIST(REASON)
 1487570   dev_cpuon   submit_s   ab1234  R         0:05      1            hkn0301
```

```
$ squeue --long

  JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
1487570 dev_cpuon submit_s   ab1234  RUNNING       2:49      10:00      1 hkn0301
```

- Job states:
  - PD = PENDING
  - R = RUNNING
  - CD = COMPLETED

  ...
  - F = FAILED
  - CA = CANCELLED

- When job is pending: **expected start time?**

```
$ squeue --start

   JOBID ...           START_TIME   SCHEDNODES
 1487570 ... 2021-10-14T10:10:10      hkn0301
```

3.b. Processing – sacct

- After submission of your script **submit_script.sh**
  - Display accounting data of your job and job steps?

```
$ sbatch submit_script.sh
Submitted batch job 1487652

$ sacct -j 1487652
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
1487652      submit_sc+ dev_cpuon+ hk-projec+          2    RUNNING      0:0
1487652.bat+      batch            hk-projec+          2    RUNNING      0:0
1487652.ext+     extern            hk-projec+          2    RUNNING      0:0
1487652.0      hostname            hk-projec+          2  COMPLETED      0:0
1487652.1          bash            hk-projec+          2    RUNNING      0:0
```

3.c. Processing – Compute node login

- Once your job is running (state=R),
  - login to dededicated nodes is possible:

```
ab1234@hkn1990:~$ sbatch submit_script.sh
Submitted batch job 1487652

ab1234@hkn1990:~$ squeue
  JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
1487652 dev_cpuon submit_s   ab1234  R       2:42      1 hkn0301

ab1234@hkn1990:~$ srun --jobid=1487652 --pty [--overlap] /usr/bin/bash
ab1234@hkn0301:~$
```

- The command srun adds another step to your job,
  - Once main jobs finishs, this job step is cancelled automatically:

```
ab1234@hkn0301:~$
slurmstepd: error: *** STEP 1487652.2 ON hkn0301 CANCELLED AT 2021-10-13T10:35:52 ***
exit
srun: Job step aborted: Waiting up to 32 seconds for job step to finish.

ab1234@hkn1990:~$
```

3.d. Processing – Change status of your job

- Once your job is submitted (state=**PD or R**),
  - You can cancel your job

```
$ sbatch submit_script.sh
Submitted batch job 1487683

$ scancel 1487683
  JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
1487683 dev_cpuon submit_s   ab1234  R       2:42      1 hkn0301
```

  - Check with `sacct` :

```
$ sacct -j 1487683
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
1487683      submit_sc+ dev_cpuon+ hk-projec+          2 CANCELLED+      0:0
1487683.bat+      batch            hk-projec+          2  CANCELLED
1487683.ext+     extern            hk-projec+          2  CANCELLED
```

Tutorial 2

- Modify your submit script so that it executes a command to wait for 600 seconds (**sleep 600**)
- Set **walltime** to **10 minutes** and give your job a name
- Submit your job script with **sbatch**
- Use **squeue** to check the status of your job
- Use **scontrol show job** to see from which directory you started your job
- Use **scancel <job-ID>** to cancel your job

Tutorial 2 - Solution

- Modify your submit script

```
#!/bin/bash
#SBATCH -N 1 -n 1
#SBATCH -t 00:10:00
#SBATCH --mem-per-cpu=50
#SBATCH -J myJobName

sleep 600
```

- Save the file and submit it with

```
$ sbatch -p cpuonly --reservation=ws submit_script.sh
```

- Get your start directory of your jobs

```
$ scontrol show job 1487685 | grep WorkDir
   WorkDir=/hkfs/home/project/hk-project-scs/ab1234/workshop
```

- Use **`scancel <job-ID>`** to cancel your job

Interactive jobs

- Jobs on login nodes are not permitted
- **Solution: interactive slurm jobs**
  - Access compute nodes and work on them interactively

```
ab1234@hkn1990$ salloc -p cpuonly -n 1 -t 10 --mem=2000

salloc: Granted job allocation 1487738
salloc: Waiting for resource configuration
salloc: Nodes hkn0301 are ready for job

ab1234@hkn0301:~$ {Now you can work on the compute node}

salloc: Job 1487738 has exceeded its time limit and its allocation has been revoked.
srun: Job step aborted: Waiting up to 32 seconds for job step to finish.
slurmstepd: error: *** STEP 1487738.interactive ON hkn0301 CANCELLED AT 2021-10-
13T13:02:41 DUE TO TIME LIMIT ***
exit
srun: error: hkn0301: task 0: Exited with exit code 127

ab1234@hkn1990:~$
```

Job is waiting to start, Do Not interupt the command

Job running. You are now on a compute node

Requested time for the interactive job ran out

Back on the login node