bw|HPC

KIT | NHR
National High-Performance Computing Center

Batch system – introduction

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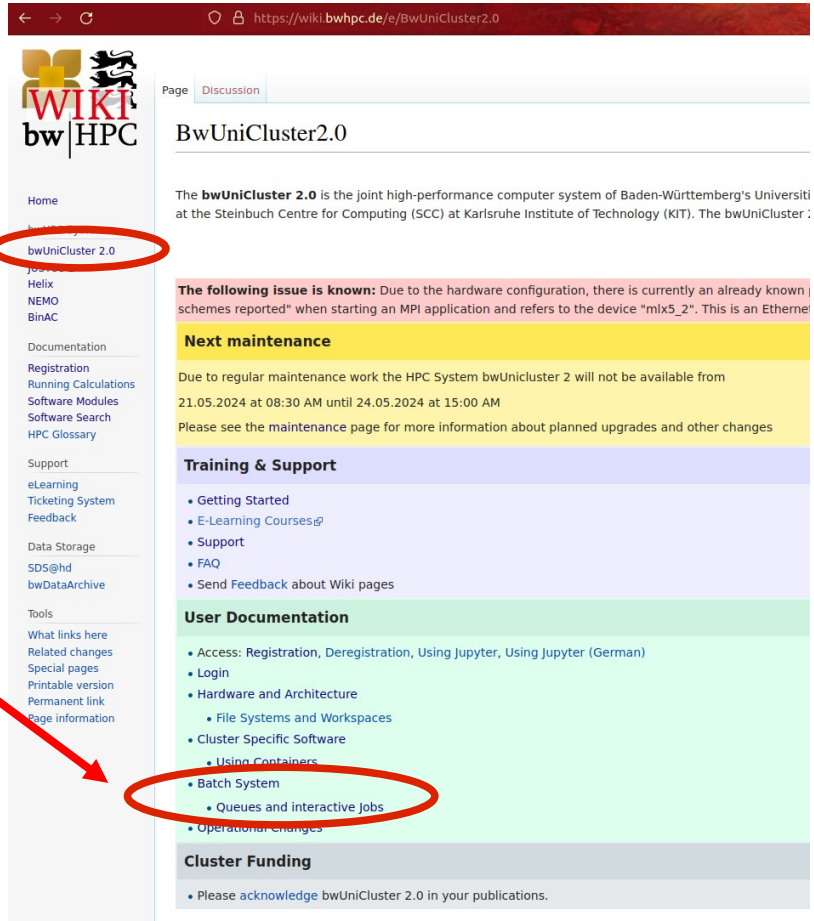
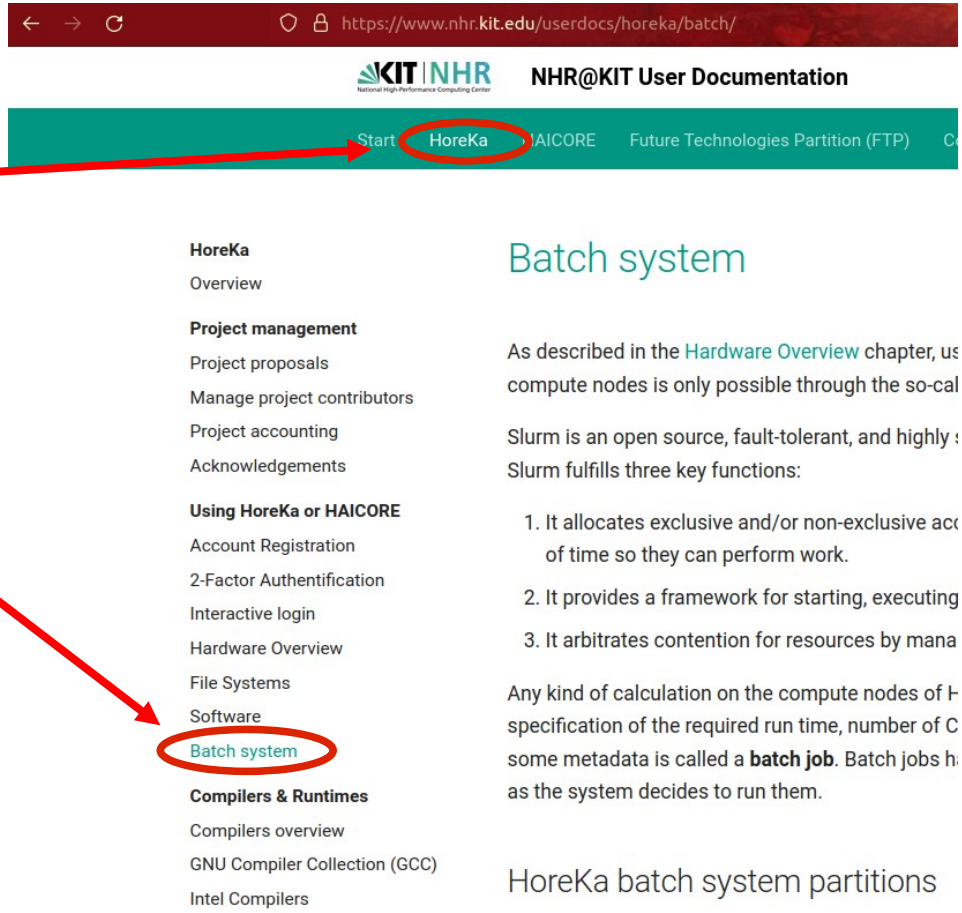
Reference: bwHPC Wiki

- Most information given by this talk can be found at https://wiki.bwhpc.de
  - select cluster
  - then select Batch System



Reference: NHR@KIT User Documentation

- Most information given by this talk can be found at https://www.nhr.kit.edu/userdocs
  - select cluster
  - then select Batch System



Material: Slides & Scripts

- https://indico.scc.kit.edu/e/hpc_course_2024-04-09
- BwUniCluster 2.0: /opt/bwhpc/common/workshops/2024-04-09/
- HoreKa: /software/all/workshop/2024-04-09/

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
`foo, bar`	Metasyntactic variables

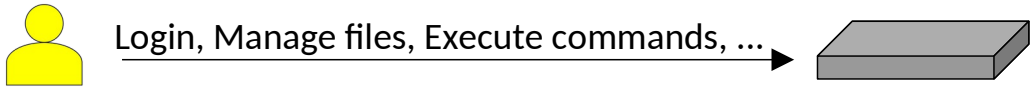
Outline

- Batch system – Why we need it and what it does.
- Job’s life cycle
- 1./2. Preparation and Submission
- 3. Processing
- 4. Post processing
- Interactive jobs

Batch System

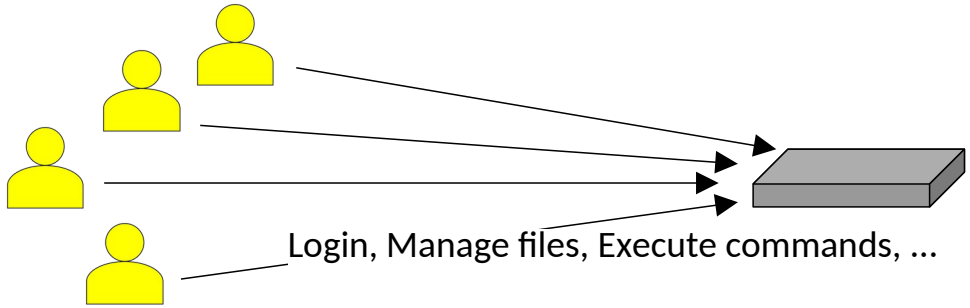
Resource management (1)

- Individual computer: single user, single node



- Shared workstation: multiple users, single node
  - All users can execute commands
  - Concurrent tasks can cause slowdown of system

    => users have to manage resources on their own



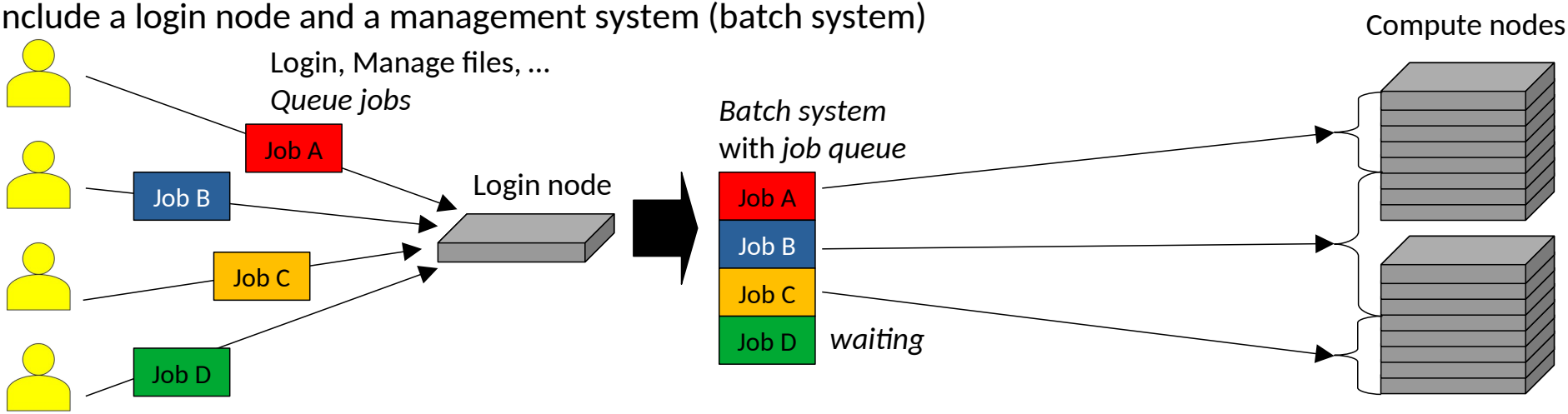
- HPC cluster: lots of users, lots of nodes
  - Users (as a group) cannot manage resources by hand: too many users and resources

    => Resource management required

Resource management (2)

- HPC cluster: lots of users, lots of nodes

- Include a login node and a management system (batch system)



Resource management (3)

- User logs on to a designated **login node**, not a **compute node**
- Jobs are **not** executed by the user directly, but put into a **queue**

- **Batch system** manages distribution of jobs to resources
- Batch system consists of two parts
  - Workload manager (scheduler)
    - Scheduling, managing, monitoring, reporting
    - SLURM (HoreKa, bwUniCluster 2.0, JUSTUS 2, Helix)
    - MOAB (NEMO, BinAC)
  - Resource manager
    - Control over jobs and distributed compute nodes
    - SLURM
    - TORQUE (for systems with MOAB)

Waiting time for jobs depends on:

- Job resource demands
- Demand history
- ONLY bwUniCluster 2.0: share of university

All examples here are for SLURM, MOAB works similarly but with different commands.

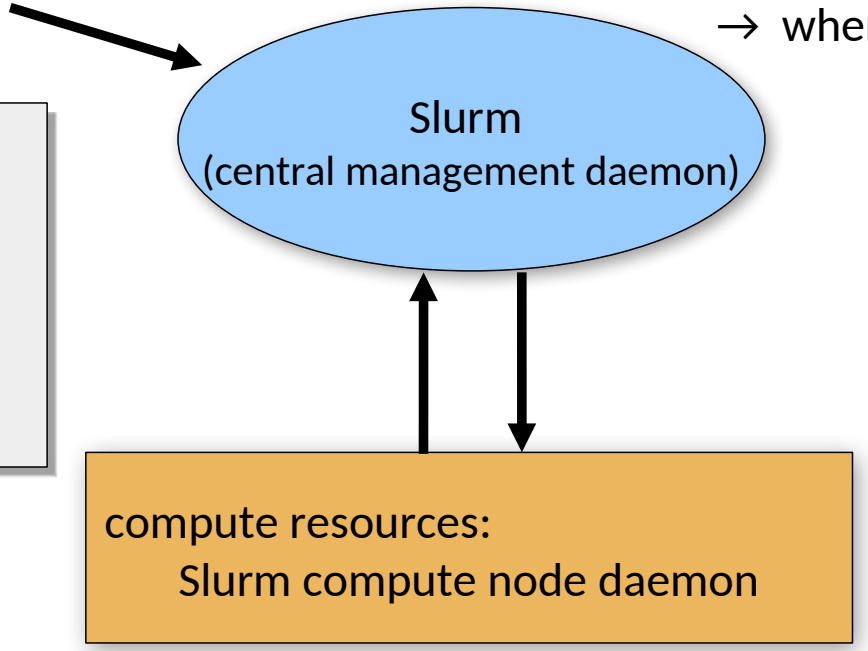
Job’s life cycle

Job's life cycle (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=500

./your_simulation
```



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

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

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

Job's life cycle (2)

1. Preprocessing: setup **job_script.sh**:

```
#!/bin/bash
#SBATCH -p dev_single
#SBATCH -N 1 -n 1
#SBATCH -t 00:01:00
#SBATCH -mem-per-cpu=500

./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. Post processing: job is finished → check output
   Default: **slurm-<job_ID>.out**

1./2. Job submission

1./2. Job submission: important resource parameters

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 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 MB) per node
`--mem-per-cpu=`*MB_value*	`#SBATCH --mem-per-cpu=`*MB_value*	Memory per allocated core
`-p` *queue*	`#SBATCH --partition=`*queue*	Queue class to be used

- List of most used parameters can be found in the documentation
- Long and short options can be mixed arbitrarily but recommended as above

1./2. Job submission: partitions / queues

- A partition defines a specific **queue**
  => submitted jobs will only wait for jobs in the same queue

- Partitions are used for different
  - Types of hardware (e.g. nodes with/without GPUs)
  - Purposes (e.g. development, production)

- Let’s take a look at the hardware!

1./2. Job submission: hardware of bwUniCluster 2.0

	HPC nodes (Thin / HPC / IceLake)	Fat nodes	GPU nodes	IceLake + GPUx4
Number of nodes	200+60 / 360 / 272	6	14 (4 GPUs each) 10 (8 GPUs each)	15 (4 GPUs each)
Sockets per node	2 / 2 / 2	4	2	2
Cores per node	40 / 40 / 64	80	40	64
Main memory per node	96 GB, 192 GB / 96 GB / 256 GB	3 TB	384 GB 768 GB	512 GB
Local SSD	960 GB SATA / 1.8 TB NVMe	4.8 TB NVMe	3.2 TB NVMe 6.4 TB NVMe	6.4 TB NVMe
Interconnect (InfiniBand)	HDR 100 (blocking) / HDR 100 / HDR 200	HDR	HDR	HDR
GPUs	-	-	NVIDIA Tesla V100	NVIDIA A100 NVIDIA H100

1./2. Job submission: partitions of bwUniCluster 2.0 (selection)

Partition	Default resources	Min. resources	Max. resources
dev_single	time=10, mem-per-cpu=1125MB		time=00:30:00, nodes=1, mem=180000MB, ntasks-per-node=40
single	time=30, mem-per-cpu=1125MB		time=72:00:00, nodes=1, mem=180000MB, ntasks-per-node=40
multiple	time=30, mem-per-cpu=1125MB	nodes=2	time=72:00:00, nodes=128, mem=180000MB, ntasks-per-node=40
gpu_4	time=10, mem-per-cpu=2178MB, cpu-per-gpu=20		time=48:00:00, nodes=14, mem=376000MB, ntasks-per-node=40
fat	time=10, mem-per-cpu=18750MB		time=72:00:00, nodes=1, ntasks-per-node=80

- Full list availbale at https://wiki.bwhpc.de/e/BwUniCluster2.0/Batch_Queues

1./2. Job submission: hardware of Horeka

	CPU only nodes	Extra-large nodes	GPU nodes
Number of nodes	570 + 32	8	167
Sockets per node	2	2	2
Cores per node	76	76	76
Main memory per node	256/512 GB	4096 GB	512 GB
Local SSD	960 GB NVMe	7x3.84 TB NVMe	960 GB NVMe
Interconnect (InfiniBand)	HDR	HDR	HDR
GPUs	-	-	NVIDIA A40 / A100

1./2. Job submission: partitions of HoreKa

Partition	Default resources	Min. resources	Max. resources
dev_cpuonly	time=10, ntasks=1, mem-per-cpu=1600MB	nodes=1, ntasks=152	time=04:00:00, nodes=12, mem=243200MB, ntasks-per-node=152
cpuonly	time=10, ntasks=152, mem-per-cpu=1600MB, mem=243200MB	nodes=1, ntasks=152	time=3-00:00:00, nodes=192, mem=501600MB, ntasks-per-node=152
dev_accelerated	time=30, ntasks=1 cpu-per-gpu=38, gres=gpu:1	nodes=1, ntasks=152, gres=gpu:1	time=01:00:00, nodes=1, mem=501600MB, ntasks-per-node=152, gres=gpu:4
accelerated	time=30, ntasks=152, mem=501600MB, cpu-per-gpu=38, gres=gpu:4	nodes=1, ntasks=152, gres=gpu:4	time=2-00:00:00, nodes=128, mem=501600MB, ntasks-per-node=152, gres=gpu:4
large	time=10, ntasks=1, mem-per-cpu=27130MB	nodes=1, ntasks=1	time=2-00:00:00, nodes=8, mem=4123930MB, ntasks-per-node=152

1./2. Job submission: available resources

- Check available resources via `$ sinfo_t_idle`
- Be careful: a node planned for another job is counted “idle” but will not start a job

```
xy_ab1234@bwunicluster:~$ sinfo_t_idle

Partition dev_single    :      6 nodes idle
Partition single        :      0 nodes idle
Partition dev_multiple  :      8 nodes idle
Partition multiple      :      3 nodes idle
Partition fat           :      0 nodes idle
Partition dev_multiple_e:      8 nodes idle
Partition multiple_e    :      3 nodes idle
Partition dev_special   :      2 nodes idle
Partition special       :      0 nodes idle
Partition gpu_4         :      0 nodes idle
Partition dev_gpu_4     :      1 nodes idle
Partition gpu_8         :      0 nodes idle
```

```
xy_ab1234@horeka:~$ sinfo_t_idle

Partition dev_cpuonly    :    1 nodes idle
Partition cpuonly        :  101 nodes idle
Partition dev_accelerate :    1 nodes idle
Partition accelerate     :   83 nodes idle
```

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 for the batch system
  - 1 task
  - 500 MB memory
  - Wall time: 5 minutes

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

[?????]
```

- 2. Insert the command to be executed at the end of the jobscript
- 3. Save the jobscript and submit it to the batch system with

```
$ sbatch  -p single --reservation=ws submit_script.sh                # bwunicluster
```

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

  - You can use **`squeue`** to see the status of the 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.

(Errors can occur when copying commands from the pdf, as not all dashes "-" are dashes in the pdf.)

Tutorial 1a - Solution

- **Goal:** use the batch system to execute **printenv** on the cluster
- 1. Create a file "**submit_script.sh**" and set the following options for the batch system
  - 1 task
  - 500 MB memory
  - Wall time: 5 minutes

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --time=00:05:00
#SBATCH --mem=500

printenv
```

- 2. Insert the command to be executed at the end of the jobscript
- 3. Save the jobscript and submit it to the batch system with

```
$ sbatch  -p single --reservation=ws submit_script.sh                # bwunicluster
```

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

  - You can use **squeue** to see the status of the 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.
  - Example: "**SLURM_JOB_PARTITION=cpuonly**" means: the job was submitted to the partition "**cpuonly**". We specified this on the command line but not on the script.

Tutorial 1b

- **Goal**: learn about option precedence.
- 1. Modify your script so that instead of executing **`printenv`**, the value of "**`SLURM_NPROCS`**" is printed (Hint: use **`echo`**)
- 2. Submit your job again, but this time use **`sbatch`** to specify the number of processes:

```
$ sbatch  -p single --reservation=ws -n 4 submit_script.sh          # bwunicluster
```

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

- 3. Check in your output file what the number of processes used is:
  - "1" as specified in the script
  - "4" as specified on the command line

Tutorial 1b - Solution

- **Goal**: learn about option precedence.
- 1. Modify your script so that instead of executing **`printenv`**, the value of "**`SLURM_NPROCS`**" is printed (Hint: use **`echo`**)
- 2. Submit your job again, but this time use **`sbatch`** to specify the number of processes:

```
$ sbatch  -p single --reservation=ws -n 4 submit_script.sh          # bwunicluster
```

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

- 3. Check in your output file what the number of processes used is:
  - "1" as specified in the script
  - "4" as specified on the command line

  => The output file contains:

```
4
```

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --time=00:05:00
#SBATCH --mem=500

echo "$SLURM_NPROCS"
```

=> The options given on the command line take precedence over the options provided in the script.

3. Processing

3. Processing

- After job submission: job-ID is printed if successful

```
$ sbatch submit_script.sh
Submitted batch job 1487560
```

- “Monitoring” via:
  - 3.a Simple information on job status

```
squeue
```

```
sacct
```

  - 3.b Extensive details on the job

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

  - 3.c Login onto the compute node

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

- “Modifying” via:
  - 3.d Cancel the job

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

3.a Processing - squeue

- Check status of a job after submission

```
$ 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
  - ...

- While job is pending: what is the **expected start time?**

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

3.a Processing - sacct

- Obtain accounting information of a job

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

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

3.b Processing – scontrol show job (1)

- Obtain detailed information on the job

```
$ scontrol show job <job-ID>
JobId=1487569 JobName=submit_script.sh
   UserId=ab1234(27049) GroupId=scc(12345) ...
   Priority=4298 Nice=0 Account=kit QOS=normal
   JobState=RUNNING Reason=Prolong 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_single AllocNode:Sid=uc2n997:2170796
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=uc2n362
   BatchHost=uc2n362
   ...
```

1) Consumed resources will be booked on your university / project

2) Your job state

3) Your time logging

4) Your selected partition

5) Your node list and Node on which job started

3.b Processing – scontrol show job (2)

- Obtain detailed information on the job

```
$ scontrol show job <job-ID>
JobId=1487569 JobName=submit_script.sh
   ...
   NumNodes=1 NumCPUs=2 NumTasks=1 CPUs/Task=1 ...
   TRES=cpu=2,mem=2250M,node=1,billing=2
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:1 CoreSpec=*
   MinCPUsNode=1 MinMemoryCPU=1125M MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) ...
   Command=/pfs/data5/home/kit/scc/ab1234/submit_script.sh
   WorkDir=/pfs/data5/home/kit/scc/ab1234
   StdErr=/pfs/data5/home/kit/scc/ab1234/slurm-1487569.out
   StdIn=/dev/null
   StdOut=/pfs/data5/home/kit/scc/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.c Processing – Login onto compute node

- While the job is running (state = **R**): login to dedicated compute 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:~$
```

- **srun** adds another step to your job. Once **main job finishs**, 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 – Cancel the job

- You can cancel your job, e.g. if
  - Submitted wrongly
  - Job does not behave as expected

```
$ 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

- **Goal:** practice monitoring and cancelling of jobs.
- 1. Modify your script such that it executes a command to wait for 600 seconds (**`sleep 600`**)
- 2. Set a walltime of 10 minutes and give a name to your job.
- 3. Submit your job script with **`sbatch`**.
- 4. Use **`squeue`** to check the status.
- 5. Use **`scontrol show job`** to see from which directory you started the job.
- 6. Use **`scancel <job-ID>`** to cancel your job.

Tutorial 2 - Solution

- **Goal:** practice monitoring and cancelling of jobs.
- 1. Modify your script such that it executes a command to wait for 600 seconds (**`sleep 600`**)
- 2. Set a walltime of 10 minutes and give a name to your job.
- 3. Submit your job script with **`sbatch`**.

```
#!/bin/bash
#SBATCH -N 1 -n 1
#SBATCH -t 00:10:00
#SBATCH --mem-per-cpu=500
#SBATCH -J myJobName

sleep 600
```

```
$ sbatch  -p single --reservation=ws submit_script.sh                # bwunicluster
```

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

- 4. Use **`squeue`** to check the status.
- 5. Use **`scontrol show job`** to see from which directory you started the job.

```
$ scontrol show job 1487685 | grep WorkDir
   WorkDir=/pfs/data5/home/kit/scc/ab1234/workshop
```

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

Interactive jobs

Interactive jobs

- Jobs on login nodes are not permitted
- Sometimes interactive access is required (e.g. for debugging, heavy compilation jobs, etc.)
  => **interactive slurm jobs**

```
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

Thank you for your attention.

Questions?