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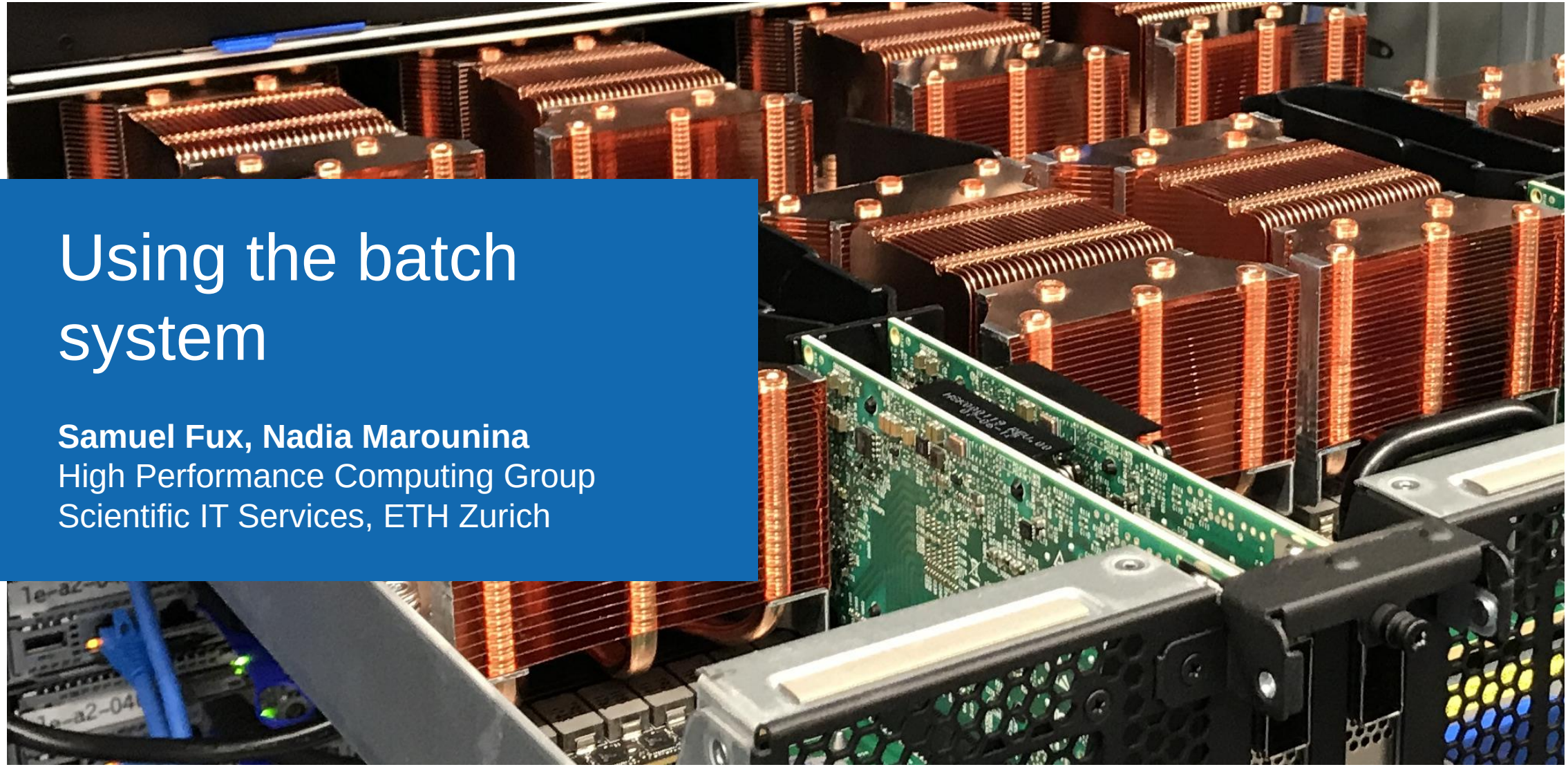
Scientific IT Services
High Performance Computing



Using the batch system

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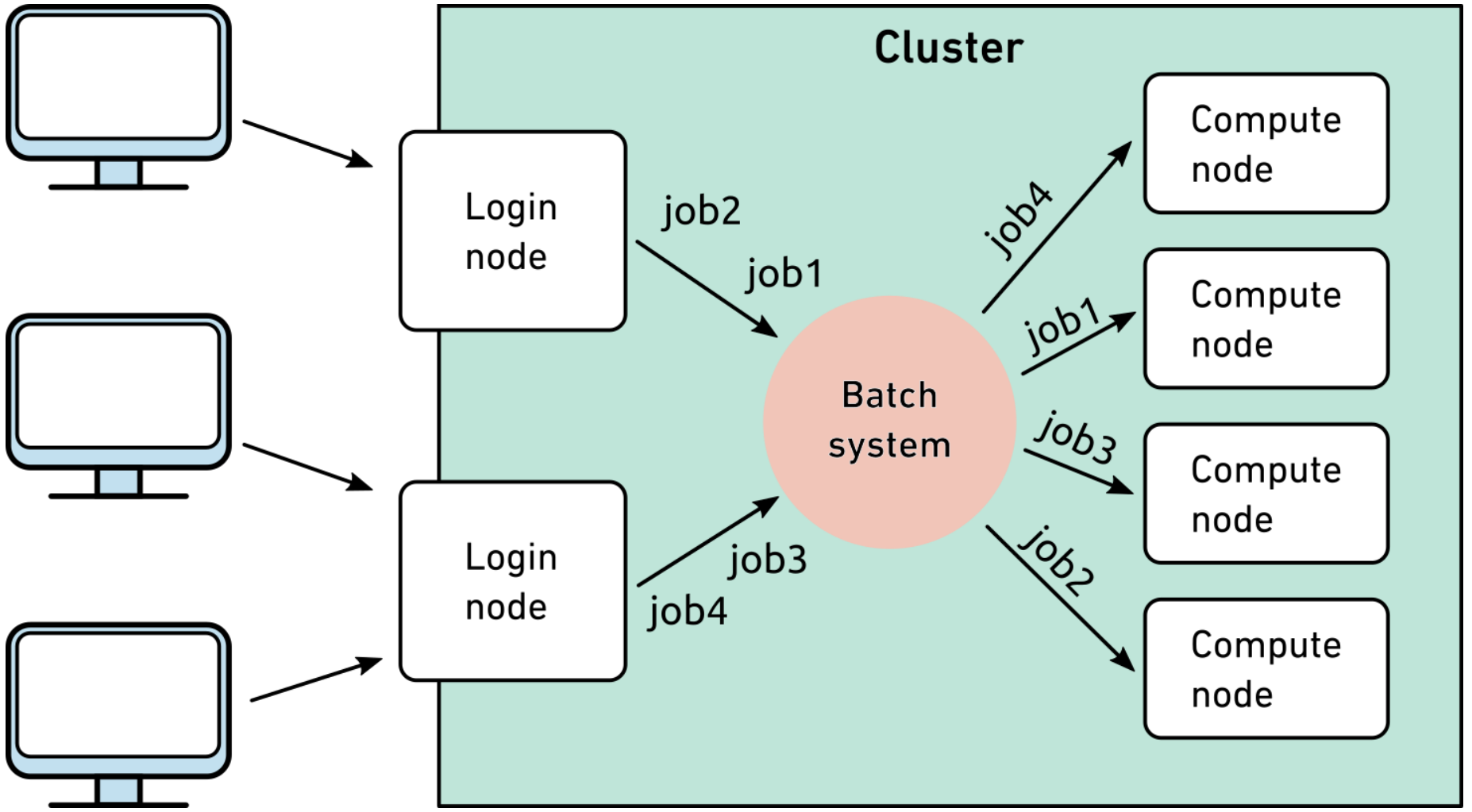
Batch > Overview



Batch > Overview

- The batch system of Euler is called **Slurm** (Simple Linux Utility for Resource Management)
- Slurm manages all resources available on the cluster and allocates them to user jobs
  - Ensures that resources are used as efficiently as possible
  - Calculates user/job priorities based on a fair share principle
- All computations must be submitted to the batch system
  - There is no other way to access the cluster's compute nodes
- Please do not run computations on the login nodes
  - Login nodes may only be used for file transfer, compilation, code testing and debugging, and quick pre- and post-processing

Batch > Basic job submission

- Use `sbatch` to submit a job to the batch system
- `sbatch [Slurm options] --wrap="job"`
- A *job* can be either …
  - a single Linux command — `cmd`
  - a shell script, passed via “<” — `< script`
  - a here document, passed via “<<” — `<< EOF ... EOF`
  - a program, with its path — `/path/to/program`
  - a command or program, with its arguments — `cmd arg1 arg2`
  - multiple commands, enclosed in quotes — `"cmd1 ; cmd2"`
  - piped commands, enclosed in quotes — `"cmd1 | cmd2"`
  - a command with I/O redirection, quoted — `"cmd <in >out"`
- We’ll talk about `sbatch`’s options later

Batch > Basic job submission

- When you submit a job via `sbatch`, the batch system analyzes it and dispatches it to a batch queue
  - Slurm always selects the best queue for your job
  - You can not select a queue yourself
- If all goes well, `sbatch` tells you
  - The job's unique identifier ("job ID") – e.g. "1010171"
- The jobid is important to check, monitor or terminate a job
- If you report a problem with a job (pending, running or done) to cluster support, then **always** provide the corresponding jobid

Batch > Basic job submission > Examples

```
[sfux@eu-login-03 ~]$ sbatch --wrap="echo hello"
Submitted batch job 1010112

[sfux@eu-login-03 ~]$ sbatch < hello.sh
Submitted batch job 1010113

[sfux@eu-login-03 ~]$ sbatch --wrap="./bin/hello"
Submitted batch job 1010114

[sfux@eu-login-03 ~]$ sbatch --wrap="date; pwd; ls -l"
Submitted batch job 1010115

[sfux@eu-login-03 ~]$ sbatch --wrap="du -sk /scratch > du.out"
Submitted batch job 1010116
```

Batch > Resource requirements

- The batch system of Euler works like a black box
  - You do not need to know anything about queues, hosts, user groups, priorities, etc. to use it
  - You only need to specify the resources needed by your job
- The two most important resources are
  - Maximal run-time and the number of processors for parallel jobs
- These resources are passed to `bsub` using options

```
sbatch --time=HH:MM:SS --ntasks=number_of_processors --warp="command"
```

- By default, a job will get 1 processor for 4 hour
  - If you need more time and/or processors, you must request them
  - Standard run-time limits are 4h, 24h, 120h

Batch > Advanced resource requirements

- Memory
  - By default Slurm gives you 1000 MB of memory per processor (core)
  - If you need more, you must request it
  - For example, to request 2000 MB per processor (core):

```
sbatch --mem-per-cpu=2000 --wrap="command"
```

- Scratch space
  - LSF does not allocate any local scratch space to batch jobs
  - If your job writes temporary files into the local `/scratch` file system, you **must** request it
  - For example, to request 10,000 MB of scratch space:

```
sbatch --tmp=10000 --wrap="command"
```

- If you don't specify any unit, then the integer value will be interpreted as MB. If you specify values in GB, then you need to add the suffix "g" (in the example above, you would write 2g instead of 2000)

Batch > `sbatch` options

`--ntasks=N`	request *N* cores (*`--nodes=1`* allocates all cores on a single node)
`--time=HH:MM:SS`	request *a runtime of* *`HH:MM:SS`*
`--output="filename"`	redirect job's standard output to *`filename`*
`--error="filename"`	redirect job's error messages to *`filename`*
`--mem-per-cpu=YYY`	request *`YYY`* MB memory per core (or add suffix "g" to specify GBs)
`--tmp=YYY`	request *`YYY`* MB of local scratch space (or add suffix "g" to specify GBs)
`--job-name="jobname"`	assign a *`jobname`* to the job
`--account="share"`	run job under a particular Euler share *`"share"`*
`--mail-type=BEGIN`	send an email when the job begins
`--mail-type=END,FAIL`	send an email when the job ends (finishes successfully or fails)

Batch > `sbatch` GPU options

`--gpus=N`	request *N* gpus
`--gpus=MODEL:N`	request *N* gpus of model *MODEL* (for instance `--gpus=rxt_3090:1`)
`--gres=gpumem:XXg`	request a GPU with at least *XX* GB GPU memory

- Currently we only have the following GPU models available in Slurm:
  - Nvidia GTX 1080 (*gtx_1080*)
  - Nvidia RTX 3090 (*rtx_3090*)
- More models will be added soon

Batch > Parallel job submission

Shared memory job (OpenMP)

- Runs on a single compute node
- Can use up to 24 processors
- To compile an openMP code

```
$ module load gcc/6.3.0
$ gcc –o hello_omp hello_omp.c
```

- To run an openMP code, define number of processors in `$OMP_NUM_THREADS`

```
$ module load gcc/6.3.0
$ export OMP_NUM_THREADS=8
$ sbatch --ntasks=8 ./hello_omp
```

Distributed memory job (MPI)

- Runs on multiple compute nodes
- Can use tens or even hundreds of processors
- To compile an MPI code

```
$ module load gcc/6.3.0
$ module load openmpi/4.0.2
$ mpicc –o hello_mpi hello_mpi.c
```

- Program must be launched using `mpirun`

```
$ module load gcc/6.3.0
$ module load openmpi/4.0.2
$ sbatch --ntasks=240
--wrap="mpirun hello_mpi"
```

Batch > Parallel job submission > Examples

```
[sfux@eu-login-03 ~]$ export OMP_NUM_THREADS=8

[sfux@eu-login-03 ~]$ sbatch --ntasks=8 --wrap="./hello_omp"

Submitted batch job 1010900

[sfux@eu-login-03 ~]$ unset OMP_NUM_THREADS

[sfux@eu-login-03 ~]$ module load gcc/8.2.0 openmpi/4.1.4

[sfux@eu-login-03 ~]$ sbatch -n 240 --wrap="mpirun ./hello_mpi"

Submitted batch job 1010901
```

Batch > Job array

- Multiple similar jobs can be submitted at once using a so-called “job array”
  - All jobs in an array share the same jobid
  - Use job index to distinguish between individual jobs in an array
  - Slurm stores array parameters in environment variables that can be used inside the jobs:

$SLURM_ARRAY_TASK_COUNT	Number of Slurm jobs in the array
$SLURM_ARRAY_TASK_ID	Array index of the elements in the array
$SLURM_ARRAY_TASK_MIN	Minimum index in the job array
$SLURM_ARRAY_TASK_MAX	Maximum index in the job array

- Examples:

```
sbatch --array=1-8 --wrap="echo Hello I am job \$SLURM_ARRAY_TASK_ID out
of \$SLURM_ARRAY_TASK_COUNT"
```

Batch > Job array

- You can specify the range by using the format *start-end:step*
- This way you can map parameters (in a parameter study) in your job to the job array index
- It is also possible to use the jobid (%A) and the element number (%a) as part of the output or error files for the individual jobs in a job array:

```
sbatch --array=1-4 --output="out.%A.%a" --error "err.%A.%a" --wrap="…"
```

- For monitoring job arrays you can use the jobid and the element number
  - Using just the jobid will refer to all jobs in the array
  - Using jobid_element will refer to the single job in the array

Batch > Job array > Example

```
[sfux@eu-login-41 ~]$ sbatch --wrap="echo \"Hello, I am job \$SLURM_ARRAY_TASK_ID of
\$SLURM_ARRAY_TASK_COUNT"
Submitted batch job 1424960
[sfux@eu-login-41 ~]$ squeue -j 1424960
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         1424960_4 normal.4h     wrap     sfux  R       0:45      1 eu-a2p-517
         1424960_3 normal.4h     wrap     sfux  R       0:45      1 eu-a2p-517
         1424960_2 normal.4h     wrap     sfux  R       0:45      1 eu-a2p-517
         1424960_1 normal.4h     wrap     sfux  R       0:45      1 eu-a2p-517
[sfux@eu-login-41 ~]$ squeue -j 1424960_4
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         1424960_4 normal.4h     wrap     sfux  R       0:48      1 eu-a2p-517
```

Batch > Exercise 3: Job array

Tasks	Commands
Go to the `hpc-examples` folder	`cd hpc-examples/job_arrays/ex1`
Submit a job array	`sbatch --array=1-4 --wrap="echo \$SLURM_ARRAY_TASK_ID"`
	`sbatch --array=1-4 --wrap="echo \$((SLURM_ARRAY_TASK_ID*2))`
Load module	`module load gcc/6.3.0 python/3.8.5`
Submit a job	`sbatch --array=1-4 --wrap="python read_input.py"`

Batch > Job dependencies

- If you have a workflow or a pipeline, then sometimes tasks depend on each other
- A simple way to chain two jobs is to add the command to submit job 2 at the end of job 1
  - Not recommended because it is error-prone and may lead to infinite loops.
- A more robust solution is to use **job dependencies**
  - Store the jobid of the first job in a variable and specify the job dependency condition for the second
  - Possible dependency conditions: after, afterany, afterok, afternotok

```
[sfux@eu-login-15 ~]$ myjobid=$(sbatch --parsable --job-name="job1" --wrap="sleep 360")
[sfux@eu-login-15 ~]$ sbatch --job-name="job2" -d afterany:$myjobid --wrap="sleep 120"
Submitted batch job 1525788
[sfux@eu-login-15 ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1525788 normal.4h     job2     sfux PD       0:00      1 (Dependency)
           1525785 normal.4h     job1     sfux  R       0:43      1 eu-a2p-530
[sfux@eu-login-15 ~]$
```

Batch > #SBATCH pragmas

- `sbatch` options can be specified either on the command line or inside a job script using the #SBATCH pragma, for example

```
#!/bin/bash
#SBATCH --ntasks=24                    # 24 cores
#SBATCH --time=8:00:00                 # 8-hour run-time
#SBATCH --mem-per-cpu=4000             # 4000 MB per core
cd /path/to/execution/folder
module load gcc/6.3.0 openmpi/4.0.2
mpirun myprogram arg1
```

- In this case, the script can be submitted using the “<” operator

```
$ sbatch < script
```

- `bsub` options specified on the command line override those inside the script

```
$ sbatch --ntasks=48 < script
```

Batch > Job monitoring > commands

`squeue`	check the state of a job in the queue
`scontrol`	check resource usage of a job
`sstat`	check information about a running job
`sacct`	detailed information about pending, running and finished jobs
`scancel`	kill a job

Batch > Job monitoring > `squeue`

- After submitting a job, the job will wait in a queue to be run on a compute node and has the pending status (PD). You can check the job status with the `squeue` command

```
[sfux@eu-login-41 ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1433323 normal.4h     wrap     sfux  PD       0:04      1 eu-g1-026-2
           1433322 normal.4h     wrap     sfux  R        0:11      1 eu-a2p-483
```

- You can also check only for running jobs (R) or for pending jobs (PD):

```
[sfux@eu-login-41 ~]$ squeue -t RUNNING
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1433322 normal.4h     wrap     sfux  R        0:28      1 eu-a2p-483
[sfux@eu-login-41 ~]$ squeue -t PENDING
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1433323 normal.4h     wrap     sfux  PD       0:21      1 eu-g1-026-2
[sfux@eu-login-41 ~]$
```

Batch > Job monitoring > `scontrol`

```
[sfux@eu-login-15 ~]$ squeue -u sfux
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1498523 normal.4h     wrap     sfux  R       0:28      1 eu-a2p-528
[sfux@eu-login-15 ~]$ scontrol show jobid -dd 1498523
JobId=1498523 JobName=wrap
   UserId=sfux(40093) GroupId=sfux-group(104222) MCS_label=N/A
   Priority=1769 Nice=0 Account=normal/es_hpc QOS=es_hpc/normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=0 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   DerivedExitCode=0:0
   RunTime=00:00:38 TimeLimit=01:00:00 TimeMin=N/A
   SubmitTime=2022-10-27T11:44:30 EligibleTime=2022-10-27T11:44:30
   AccrueTime=2022-10-27T11:44:30
   StartTime=2022-10-27T11:44:31 EndTime=2022-10-27T12:44:31 Deadline=N/A
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2022-10-27T11:44:31 Scheduler=Main
   Partition=normal.4h AllocNode:Sid=eu-login-15:26645
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=eu-a2p-528
   BatchHost=eu-a2p-528
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   TRES=cpu=1,mem=1G,node=1,billing=1
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:1 CoreSpec=*
   JOB_GRES=(null)
     Nodes=eu-a2p-528 CPU_IDs=127 Mem=1024 GRES=
   MinCPUsNode=1 MinMemoryCPU=1G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=(null)
   WorkDir=/cluster/home/sfux
   StdErr=/cluster/home/sfux/slurm-1498523.out
   StdIn=/dev/null
   StdOut=/cluster/home/sfux/slurm-1498523.out
   Power=
```

Batch > Job monitoring > `sacct`

- The command `sacct` provides you information about running or finished jobs:

```
[sfux@eu-login-15 ~]$ sacct --format JobID,State,AllocCPUS,Elapsed,NNodes,NTasks,TotalCPU,REQMEM,MaxRSS,NodeList -j
1525037
JobID             State  AllocCPUS    Elapsed   NNodes   NTasks   TotalCPU     ReqMem     MaxRSS        NodeList
------------ ---------- ---------- ---------- -------- -------- ---------- ---------- ---------- ---------------
1525037         RUNNING          4   00:01:27        1            00:00:00     16000M                eu-a2p-373
1525037.bat+    RUNNING          4   00:01:27        1        1   00:00:00                           eu-a2p-373
1525037.ext+    RUNNING          4   00:01:27        1        1   00:00:00                           eu-a2p-373
```

- Possible format options for `sacct`:

Account,AdminComment,AllocCPUS,AllocNodes,AllocTRES,AssocID,AveCPU,AveCPUFreq,AveDiskRead,AveDiskWrite,AvePages,AveRSS,AveVMSize,BlockID,Cluster,Comment,Constraints,ConsumedEnergy,ConsumedEnergyRaw,Container,CPUTime,CPUTimeRAW,DBIndex,DerivedExitCode,Elapsed,ElapsedRaw,Eligible,End,ExitCode,Flags,GID,Group,JobID,JobIDRaw,JobName,Layout,MaxDiskRead,MaxDiskReadNode,MaxDiskReadTask,MaxDiskWrite,MaxDiskWriteNode,MaxDiskWriteTask,MaxPages,MaxPagesNode,MaxPagesTask,MaxRSS,MaxRSSNode,MaxRSSTask,MaxVMSize,MaxVMSizeNode,MaxVMSizeTask,McsLabel,MinCPU,MinCPUNode,MinCPUTask,NCPUS,NNodes,NodeList,NTasks,Partition,Priority,QOS,QOSRAW,Reason,ReqCPUFreq,ReqCPUFreqGov,ReqCPUFreqMax,ReqCPUFreqMin,ReqCPUS,ReqMem,ReqNodes,ReqTRES,Reservation,ReservationId,Reserved,ResvCPU,ResvCPURAW,Start,State,Submit,SubmitLine,Suspended,SystemComment,SystemCPU,Timelimit,TimelimitRaw,TotalCPU,TRESUsageInAve,TRESUsageInMax,TRESUsageInMaxNode,TRESUsageInMaxTask,TRESUsageInMin,TRESUsageInMinNode,TRESUsageInMinTask,TRESUsageInTot,TRESUsageOutAve,TRESUsageOutMax,TRESUsageOutMaxNode,TRESUsageOutMaxTask,TRESUsageOutMin,TRESUsageOutMinNode,TRESUsageOutMinTask,TRESUsageOutTot,UID,User,UserCPU,WCKey,WCKeyID,WorkDir

Batch > Job monitoring > `scancel`

```
[sfux@eu-login-15 ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           1525589 normal.24   sbatch     sfux  R       0:11      1 eu-a2p-373
[sfux@eu-login-15 ~]$ scancel 1525589
[sfux@eu-login-15 ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
[sfux@eu-login-15 ~]$
```

Options:

job-ID	kill *job-ID*
--name=*jobname*	kill <u>all</u> jobs with name *jobname*
--user=*username*	kill all jobs from user *username*
--state=state	kill all jobs in state *state* (states: PENDING, RUNNING or SUSPENDED)

Batch > Job output

- Each Slurm job creates a file Slurm-*JOBID*.out in the directory where you submitted the job from
- The Slurm log file contains the stdout and stderr of your job if you did not redirect it
- If a job fails, then you can find the error message in the Slurm-*JOBID*.out file
- If you report a problem about a job to cluster support, then always provide the corresponding Slurm file with the job output

Dos and don’ts

Dos

- Understand what you are doing
- Ask for help if you don’t understand what you are doing
- Optimize your workflow to make it as efficient as possible
- Keep in mind that our clusters are shared by many users
- Choose the file system you want to use carefully

Don’ts

- Don’t waste CPU time or disk space
- Don’t run applications on the login nodes
- Don’t write large amounts of data to standard output
- Don’t create millions of small files
- Don’t run hundreds of small jobs if the same work can be done in a single job

Getting help

- Wiki: https://scicomp.ethz.ch

- Ticket system
  - https://smartdesk.ethz.ch (ETH account authentication)
  - Please describe your problem as accurately as possible

- E-mail
  - cluster-support@id.ethz.ch
  - Please do not send questions to individual members of the team

- Person-to-person (not during COVID 19)
  - Contact us to set up an appointment at your place
  - Visit us at Binzmühlestrasse 130

Questions?