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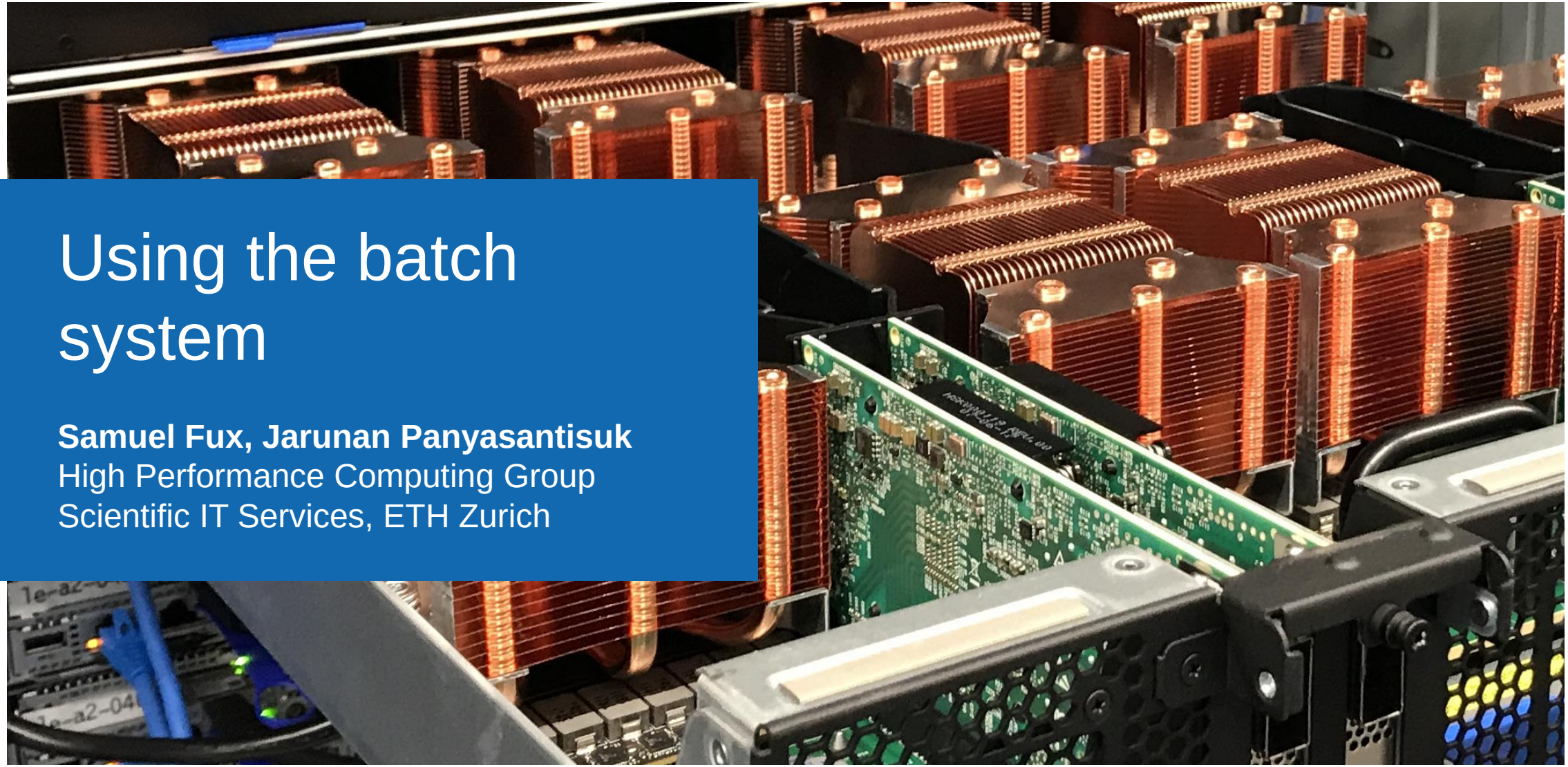
Scientific IT Services
High Performance Computing



Using the batch system

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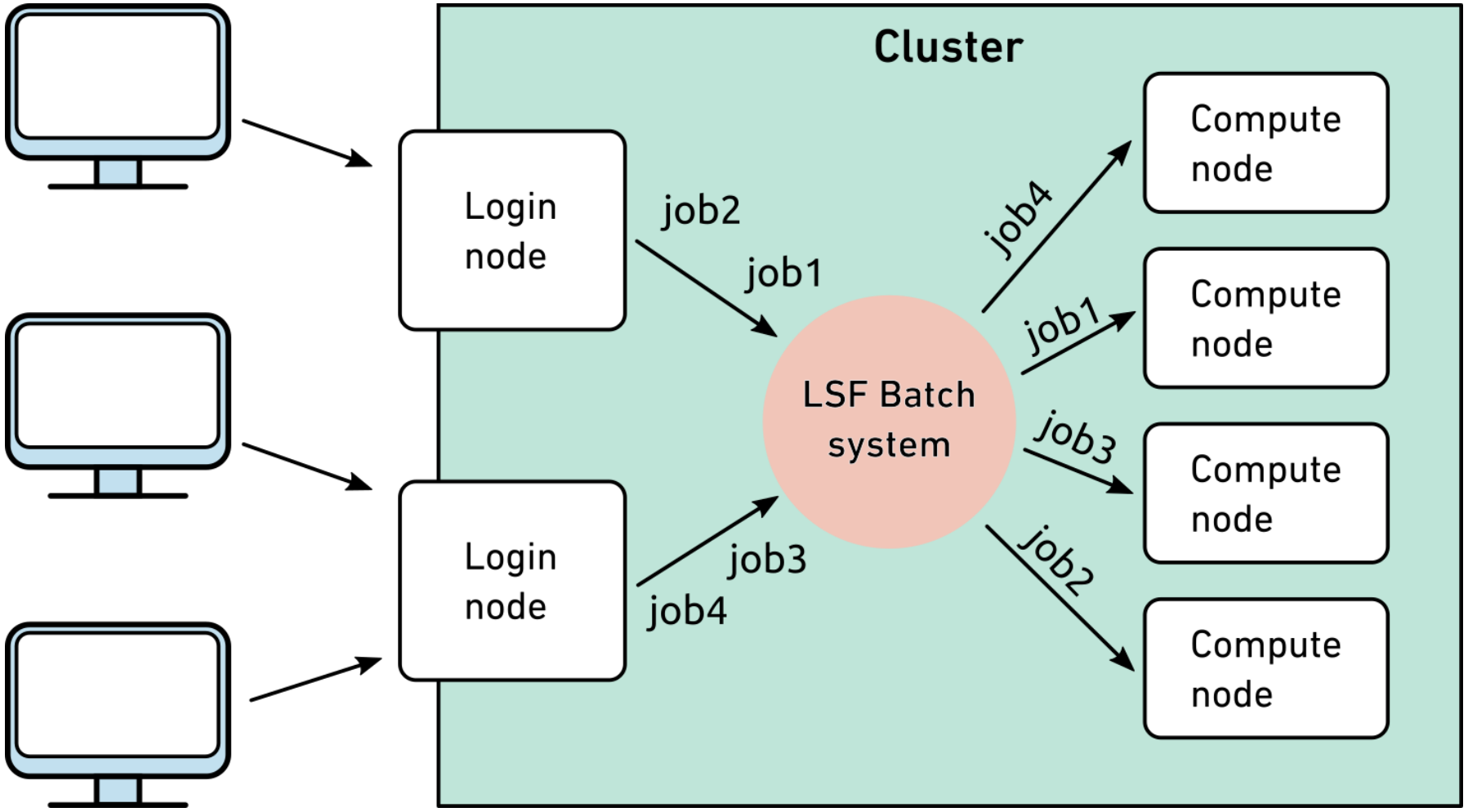
Batch > Overview



Batch > Overview

- The batch system of Euler is called *LSF* (Load Sharing Facility)
- LSF manages all resources available on the cluster and allocates them to users' 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 `bsub` to submit a job to the batch system

  ```
  bsub [LSF options] job
  ```

- A *job* can be either …
  - a single Linux command
  - a shell script, passed via “<”
  - a here document, passed via “<<”
  - a program, with its path
  - a command or program, with its arguments
  - multiple commands, enclosed in quotes
  - piped commands, enclosed in quotes
  - a command with I/O redirection, quoted

```
cmd
< script
<< EOF ... EOF
/path/to/program
cmd arg1 arg2
"cmd1 ; cmd2"
"cmd1 | cmd2"
"cmd <in >out"
```

- We’ll talk about `bsub`’s options later

Batch > Basic job submission

- When you submit a job via `bsub`, the batch system analyzes it and dispatches it to a batch queue
  - LSF always selects the best queue for your job
  - You can not select a queue yourself
- If all goes well, `bsub` tells you
  - The kind of job you have submitted – e.g. “Generic job”
  - The job’s unique identifier (“job ID”) – e.g. “8146539”
  - The queue were the job was dispatched – e.g. “normal.4h”

Batch > Basic job submission > Examples

```
[sfux@eu-login-03 ~]$ bsub echo hello
Generic job.
Job <8146539> is submitted to queue <normal.4h>.

[sfux@eu-login-03 ~]$ bsub < hello.sh
Generic job.
Job <8146540> is submitted to queue <normal.4h>.

[sfux@eu-login-03 ~]$ bsub ./bin/hello
Generic job.
Job <8146541> is submitted to queue <normal.4h>.

[sfux@eu-login-03 ~]$ bsub "date; pwd; ls -l"
Generic job.
Job <8146542> is submitted to queue <normal.4h>.

[sfux@eu-login-03 ~]$ bsub "du -sk /scratch > du.out"
Generic job.
Job <8146543> is submitted to queue <normal.4h>.
```

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

  `bsub -W` *`HH:MM`* `-n` *`number_of_processors`* …
- 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 and 30 days

Batch > Advanced resource requirements

- Memory
  - By default LSF gives you 1024 MB of memory per processor (core)
  - If you need more, you must request it
  - For example, to request 2048 MB per processor (core):

    ```
    bsub -R "rusage[mem=2048]" …
    ```
- 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:

    ```
    bsub -R "rusage[scratch=10000]" …
    ```
- Both requirements can be combined

  ```
  bsub -R "rusage[mem=2048,scratch=10000]" …
  ```

Batch > Requesting GPUs in Euler

- Selecting by GPU model

```
bsub -n 1 -R "rusage[ngpus_excl_p=1]" -R "select[gpu_model0==TITANRTX]" ./my_cuda_program
```

- Selecting by GPU memory

```
bsub -n 1 -R "rusage[ngpus_excl_p=1]" -R "select[gpu_mtotal0>=10240]" ./my_cuda_program
```

GPU Model	Specifier	GPU memory	CPU cores	CPU memory
NVIDIA GeForce RTX 2080 Ti	GeForceRTX2080Ti	11 GiB	36	384 GiB
NVIDIA GeForce RTX 2080 Ti	GeForceRTX2080Ti	11 GiB	128	512 GiB
NVIDIA TITAN RTX	TITANRTX	24 GiB	128	512 GiB
NVIDIA Tesla V100-SXM2 32 GB	TeslaV100_SXM2_32GB	32 GiB	48	768 GiB

Batch > Other bsub options

`-o` *`outfile`*	append job's standard output to *outfile*
`-e` *`errfile`*	append job's error messages to *errfile*
`-R "rusage[…]"`	advanced resource requirement (memory,…)
`-J` *`jobname`*	assign a *jobname* to the job
`-w "`*`depcond`*`"`	*wait* until dependency condition is satisfied
`-Is`	submit an *interactive* job with pseudo-terminal
`-B / -N`	send an email when the job begins/ends
`-u` *`user@domain`*	use this address instead of *username*@ethz.ch

Batch > Parallel job submission

- Shared memory job (OpenMP)
  - Runs on a single compute node
  - Can use up to 24 processors
  - Number of processors must be defined in `$OMP_NUM_THREADS`

```
export OMP_NUM_THREADS=8
bsub -n 8 ./program
```

- Distributed memory job (MPI)
  - Runs on multiple compute nodes
  - Can use tens or even hundreds of processors
  - Program must be launched using `mpirun`

```
module load compiler
module load mpi_library
bsub -n 240 mpirun ./program
```

Batch > Parallel job submission > Examples

```
[sfux@eu-login-03 ~]$ export OMP_NUM_THREADS=8
[sfux@eu-login-03 ~]$ bsub -n 8 ./hello_omp
Generic job.
Job <8147290> is submitted to queue <normal.4h>.

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

[sfux@eu-login-03 ~]$ bsub -n 240 mpirun ./hello_mpi
MPI job.
Your environment is not configured for MPI.
Please load the module(s) needed by your job before executing 'bsub'.
Request aborted by esub. Job not submitted.

[sfux@eu-login-03 ~]$ module load intel open_mpi
[sfux@eu-login-03 ~]$ bsub -n 240 mpirun ./hello_mpi
MPI job.
Job <8147303> is submitted to queue <normal.4h>.
```

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 between brackets to distinguish between individual jobs in an array
  - LSF stores job index and array size in environment variables
  - Each job can have its own standard output
- Examples:

```
bsub -J "array_name[1-N]" ./program  # submit N jobs at once
bjobs -J array_name                  # all jobs in an array
bjobs -J jobID                       # all jobs in an array
bjobs -J array_name[index]           # specific job in an array
bjobs -J jobID[index]                # specific job in an array
```

Batch > Job array > Example

```
[sfux@eu-login-03 ~] bsub -J "hello[1-8]"
bsub> echo "Hello, I am job $LSB_JOBINDEX of $LSB_JOBINDEX_END"
bsub> ctrl-D
Job array.
Job <29976045> is submitted to queue <normal.4h>.
[sfux@eu-login-03 ~]$ bjobs
JOBID      USER  STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
29976045   sfux  PEND  normal.4h  euler03                 hello[1]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[2]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[3]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[4]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[5]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[6]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[7]   Oct 10 11:03
29976045   sfux  PEND  normal.4h  euler03                 hello[8]   Oct 10 11:03
[leonhard@euler03 ~]$ bjobs -J hello[6]
JOBID      USER  STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
29976045   sfux  PEND  normal.4h  euler03                 hello[6]   Oct 10 11:03
```

Batch > #BSUB pragmas

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

```
#!/bin/bash
#BSUB -n 24                          # 24 cores
#BSUB -W 8:00                        # 8-hour run-time
#BSUB -R "rusage[mem=4000]"          # 4000 MB per core
cd /path/to/execution/folder
command arg1 arg2
```

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

```
bsub < script
```

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

```
bsub -n 48 < script
```

Batch > Light-weight job

- Light-weight jobs are jobs that do not consume a lot of CPU time, for example
  - Master process in some type of parallel jobs
  - File transfer program
  - Interactive shell
- Some compute nodes are specially configured for light-weight jobs
  - They allow multiple light-weight jobs to run on the same core at the same time
  - This is more efficient than allocating 100% of a core to a job that would use only 10%
- Use the option “-R light” to submit a light-weight job
  - Example: submit a 15-minute interactive bash shell

    ```
    bsub -W 15 -Is -R light /bin/bash
    ```
  - Do not forget to logout (type “logout” or “exit”) when you’re done

Batch > Light-weight job > Example

```
[sfux@eu-login-03 ~]$ bsub -W 15 -Is -R light /bin/bash
Generic job.
Job <27877012> is submitted to queue <light.5d>.
<<Waiting for dispatch ...>>
<<Starting on eu-c7-133-05>>
[sfux@eu-c7-133-05 ~]$ pwd
/cluster/home/sfux
[sfux@eu-c7-133-05 ~]$ hostname
eu-c7-133-05
[sfux@eu-c7-133-05 ~]$ exit
exit
[sfux@eu-login-03 ~]$
```

Batch > Job control commands

`busers`	user limits, number of pending and running jobs
`bqueues`	queues status (open/closed; active/inactive)
`bjobs`	more or less detailed information about pending and running jobs, and recently finished jobs
`bbjobs`	better bjobs ☺
`bhist`	info about jobs finished in the last hours/days
`bpeek`	display the standard output of a given job
`lsf_load`	show the CPU load of all nodes used by a job
`bjob_connect`	login to a node where your job is running
`bkill`	kill a job

Commands shown in red are not standard LSF command but specific to the HPC clusters at ETH

Batch > Job control > Main bjobs options

(no option)	list all your jobs in all queues
`-p`	list only *pending* (waiting) jobs and indicate why they are pending
`-r`	list only *running* jobs
`-d`	list only *done* job (finished within the last hour)
`-l`	display status in *long* format
`-w`	display status in *wide* format
`-o "`*`format`*`"`	use custom *output* format (see LSF documentation for details)
`-J` *`jobname`*	show only job(s) called *jobname*
`-q` *`queue`*	show only jobs in a specific *queue*
`job-ID(s)`	list of job-IDs (this **must** be the last option)

Batch > Job control > bbjobs

- Displays more human-friendly information than `bjobs`
  - Requested number of cores, memory and scratch
  - Queue wait time
  - Wall-clock time
  - Number of tasks
- Shows the efficiency of a job
  - CPU utilization
  - Memory utilization

```
[sfux@eu-login-05 ~]$ bbjobs 146773638
 Job ID                                : 146773638
  Status                               : RUNNING
  Running on node                      : 24*eu-c7-113-09
  User                                 : sfux
  Queue                                : normal.120h
  Command                              : python
launch_solver.py -p /cluster/home/sfux[...]
  Working directory                    :
$HOME/python/solver/test1
Requested resources
  Requested cores                      : 24
  Requested runtime                    : 120 h 0 min
  Requested memory                     : 2500 MB per core,
60000 MB total
  Requested scratch                    : not specified
  Dependency                           : -
Job history
  Submitted at                         : 10:03 2020-10-13
  Started at                           : 10:03 2020-10-13
  Queue wait time                      : 18 sec
Resource usage
  Updated at                           : 11:44 2020-10-13
  Wall-clock                           : 1 h 41 min
  Tasks                                : 52
  Total CPU time                       : 39 h 47 min
  CPU utilization                      : 98.4 %
  Sys/Kernel time                      : 0.0 %
  Total resident Memory                : 40788 MB
  Resident memory utilization          : 68.0 %
```

Batch > Job control > Main bkill options

`job-ID`	kill *job-ID*
`0`	kill all jobs (yours only)
`-J jobname`	kill most recent job called *jobname*
`-J jobname 0`	kill all jobs called *jobname*
`-q queue`	kill most recent job in *queue*
`-q queue 0`	kill all jobs in *queue*

Batch > Job output

- By default a job's output is stored in a file named "lsf.o*job-ID*" located in the submission directory
- In addition to your program’s standard output, this file shows
  - The command that you submitted to the batch system
  - The queue where the job was dispatched
  - The date and time when the job started/ended
  - The name(s) of the compute node(s) that executed the job
  - The directory where your program ran
  - The CPU time and memory used by the job
  - The number of processes and threads executed by the job
- This can be used to fine-tune the resources requirements of your next jobs

```
Sender: LSF System <lsfadmin@eu-ms-024-36>
Subject: Job 146799736: <./test.py> in cluster <euler> Done

Job <./test.py> was submitted from host <eu-login-30> by user <sfux> in cluster <euler> at Tue Oct 13 11:28:50 2020
Job was executed on host(s) <eu-ms-024-36>, in queue <normal.4h>, as user <sfux> in cluster <euler> at Tue Oct 13 11:29:00
2020
</cluster/home/sfux> was used as the home directory.
</cluster/home/sfux/test/python/matplotlib> was used as the working directory.
Started at Tue Oct 13 11:29:00 2020
Terminated at Tue Oct 13 11:29:02 2020
Results reported at Tue Oct 13 11:29:02 2020

Your job looked like:

------------------------------------------------------------
# LSBATCH: User input
./test.py
------------------------------------------------------------

Successfully completed.

Resource usage summary:

    CPU time :                                   16182 sec.
    Max Memory :                                 879.00 MB
    Average Memory :                             602.00 MB
    Total Requested Memory :                     1000.00 MB
    Delta Memory :                               121.00 MB
    Max Swap :                                     -
    Max Processes :                              4
    Max Threads :                                5
    Run time :                                   18423 sec.
    Turnaround time :                            19004 sec.

The output (if any) follows:
```

Batch > Troubleshooting

- `bsub` rejects my job
  - If the error message is not self-explanatory, please report it to cluster-support@id.ethz.ch
- My job is stuck in the queue since XXX hours/days
  - Use `bjobs -p` to find out why your job is pending
  - “Individual host-based reasons” means that the resources requested by your jobs are not available at this time
  - Some resources may *never* become available (e.g. mem=10000000)
  - Some resource requirements may be *mutually exclusive*
- My job was sent to the “purgatory” queue
  - This queue is designed to catch jobs that were not submitted properly, either due to a user error or a bug in the batch system
  - **Always** report this type of problem to cluster-support@id.ethz.ch

Questions?