

Information about the batch system

Ressource allocation

- Start an interactive session for example on one DEEP Cluster Node for 2.5 hours:

→ `qsub -I -X -l nodes=1:ppn=16:cluster,walltime=02:30:00`

- Leave the interactive session:

→ `exit`

- Submit a batch job:

→ `qsub job_script.sh`

- Specify the nodes you want to use:

→ `-l nodes=x:ppn=y:cluster` will allocate DEEP Cluster Nodes

→ `-l nodes=x:ppn=y:booster` will allocate DEEP Booster Nodes

→ `-l nodes=x:ppn=y:sdv` will allocate SDV Cluster Nodes

→ `-l nodes=x:ppn=y:kn1` will allocate (randomly) SDV KNL Nodes

→ `-l nodes=x:ppn=y:kn1:extoll` will allocate SDV KNL Nodes with EXTOLL

→ `-l nodes=x:ppn=y:kn1:nvme` will allocate SDV KNL Nodes with NVMe

- The following job script can be used as a template for your own jobs:

```
#!/bin/bash
#PBS -S /bin/bash
#PBS -l nodes=[number of nodes]:ppn=[number of processes per node]:[nodetype]
#PBS -l walltime=[hours]:[minutes]:[seconds]
#PBS -e [path to your errorfiles]
#PBS -o [path to your outputfiles]
#PBS -m e
#PBS -M [your mail address]
#PBS -N [name of your program]
#PBS -d [path to your working directory]
#PBS -v LD_LIBRARY_PATH
module load parastation
[load all the modules you need]
mpiexec -np [number of processes] [executable]
```

Some useful commands

- `pbstop` → Shows system load and job overview.
- `pbsnodes -nl` → Shows information on nodes, that are currently not available.
- `showres` → Shows reservations. (Only on deepm)
- `showq` → Lists active, idle and blocked jobs. (Only on deepm)
- `qstat -u USER` → Shows jobs of a certain user.
- `qstat -f JOBID` → Shows detailed information about a certain job (job id can be obtained by `qstat -u`).
- `showstart JOBID` → Provides an estimated start time for a certain job. (Only on deepm)