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 -I nodes=1:ppn=16:cluster,walltime=02:30:00

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

 \rightarrow qsub -I -X -I nodes=1:ppn=16:cluster+1:ppn=244:booster,walltime=02:30:00

• Leave the interactive session:

 \rightarrow exit

• Submit a batch job:

 \rightarrow qsub job_script.sh

- Specify the nodes you want to use:
 - → -I nodes=x:ppn=y:cluster will allocate DEEP Cluster Nodes
 - → -I nodes=x:ppn=y:booster will allocate DEEP Booster Nodes
 - → -I nodes=x:ppn=y:sdv will allocate SDV Cluster Nodes
 - \rightarrow -/ nodes=x:ppn=y:knl will allocate (randomly) SDV KNL Nodes
 - \rightarrow -I nodes=x:ppn=y:knl:extoll will allocate SDV KNL Nodes with EXTOLL
 - \rightarrow -*l* nodes=x:ppn=y:knl: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 -1 nodes=[number of nodes]:ppn=[number of processes per node]:[nodetype] #PBS -1 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

- $pbstop \rightarrow$ Shows system load and job overview.
- pbsnodes -nl \rightarrow Shows information on nodes, that are currently not available.
- showres \rightarrow Shows reservations. (Only on deepm)
- $showq \rightarrow Lists$ active, idle and blocked jobs. (Only on deepm)
- qstat -u USER \rightarrow 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 \rightarrow Provides an estimated start time for a certain job. (Only on deepm)