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Large-Scale Parallel Computing

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EXERCISE 1

Lichtenberg-cluster - basics

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- How to use the HPC system?
  - An HPC system consists of different types of nodes
    - Login nodes, compute nodes, I/O nodes
  - A user remotely logs into the system via ssh
    - User gets access to a login node
    - Login node used for code compilation and job submission
  - Executing a program
    - After a program is compiled on the login node
    - The program is submitted for execution on compute nodes via a batch system
    - A batch job specifies: num nodes to use, expected execution time

Lichtenberg-cluster - access

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- Everyone should have access to the system by now
  - Please hand in the signed forms if you haven't by now
- Login
  - `ssh <TU_id>@lclusterN.hrz.tu-darmstadt.de`
  - N can be from 1 to 8
  - Example:
    - `ssh ab12cdef@lcluster5.hrz.tu-darmstadt.de`
  - Will give access to a login node

Lichtenberg-cluster – compiling code

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- Many different types of build systems/runtime environments available on the system
  - Compilers: gcc, intel, etc
  - MPI: OpenMPI, compiled with intel, gcc compilers, etc
  - OpenMP flavors
  - All have different versions installed on the system
  - Many utilities also available for usage
    - Debuggers, profilers, utility libraries, etc.
- Is there any easy way to switch between different programming environments?

Lichtenberg-cluster – module system

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- The module command allows to easily load/unload different software
- Usage
  - Load a module: `module load <utility name>`
  - Unload a module: `module unload <utility name>`
  - How to know if a module is present on the system
    - `module avail`
  - List of modules already loaded
    - `module list`

Lichtenberg-cluster – job submission

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- Parallel jobs have to be submitted through a batch system for execution on compute nodes
- Job submission:
  - `bsub < job_script`
- See the status of the job
  - `bjobs -l job_id`
- Cancel a job
  - `bkill job_id`

Lichtenberg-cluster – example script

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```
#BSUB -J test_job
#BSUB -o test_job.out
#BSUB -e test_job.err
#BSUB -W 00:05
#BSUB -n 4
#BSUB -a openmpi
#BSUB -u shah@cs.tu-darmstadt.de
#BSUB -N

module load openmpi
mpirun ./test_app
```