CPMD

The CPMD code is a parallelized plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.

Prerequisites to use CPMD on the cluster system

In order to use CPMD on the cluster system, you need a valid license, which is usually granted free of charge to members of academic institutions for non-profit, non-transferable personal usage after an application on their web site.

After you receive your license, please let us know (`cluster-help@luis.uni-hannover.de`, please also include your user account name). We will then ask the CPMD consortium to validate your license and thereafter add you to the unix group `cpmd` that has access to the software.

Using CPMD on the cluster

To list all installed CPMD versions, run `module spider cpmd`.

If you want to access CPMD version 4.3, you have to load all modules recommended by the command `module spider CPMD/4.3`:

```
module load GCC/8.3.0 OpenMPI/3.1.4 CPMD/4.3
```

In a sample job-script below you will need to set an input file and provide the location to pseudo-potential that are available for download from CPMD website after authentication.

SLURM script

cpmd-job.sh

```
#!/bin/bash -l
#SBATCH --job-name=cpmd_job
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=20
#SBATCH --mem=120G
#SBATCH --time=1:00:00
#SBATCH --mail-user=user@uni-hannover.de
#SBATCH --mail-type=END

# Compute node the job ran on
echo "Job ran on:" $HOSTNAME

# Load modules
```

```
module load GCC/8.3.0 OpenMPI/3.1.4 CPMD/4.3

# Change to work dir
cd $SLURM_SUBMIT_DIR

CPMD_INPUT=<your input file>
CPMD_OUTPUT=cpmd-job-${SLURM_JOB_ID}.log
PP_PATH=<path to the location of pseudo-potentials>

srun cpmd.x ${CPMD_INPUT} ${PP_PATH} > ${CPMD_OUTPUT}
```

Further Reading

- CPMD home page
- CPMD manual
- CPMD pseudo-potentials