CP2K

Purpose: Ab initio
Latest version: 9.1.0
License: Free of use
GNU GPL _ext-link
Website: *https://www.cp2k.org/_ext-link*

CP2K is a program for ab initio electronic structure calculations and molecular dynamics.

CP2K is geared towards, but not restricted to, massive parallel computations using mixed plane-wave/Gaussian bases and pseudopotentials. It can implement a variety of methods, including semiempirical, HF, DFT (LDA, GGA, meta-GGA, hybrid), MP2 and TD-DFT, for molecular and periodic systems.

It can also perform both classical and ab initio molecular dynamics, Monte Carlo, and minimum energy path calculations.

SLURM Submit script example

For more information use the ***Job Script Generator***.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the sterr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submited.
- **-n**: Number of tasks.

cp2k_example.slm

```
#!/bin/bash
#SBATCH -J cp2k_example
#SBATCH -e cp2k_example.err
#SBATCH -o cp2k_example.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 0-02:00

module load apps/cp2k/6.1

##
#  Modify the input and output files
INPUT_FILE=cp2k_example.inp
OUTPUT_FILE=cp2k_example.out

cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

##
#  cp2k.version where version is usually one of:
#  sopt – Serial
#  popt – Parallel (MPI)
#
srun cp2k.version -i ${INPUT_FILE} -o
${OUTPUT_FILE}

cp ./${OUTPUT_FILE} ${SLURM_SUBMIT_DIR}
```

- **-c**: Number of cores per task.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

Software execution information:

There are different CP2K binaries deppending on the calculation type. The binary is called ***cp2k.version*** where version is usually one of: :

- **sopt** – Serial, optimised.
- **popt** – Parallel (MPI), optimised.