SIESTA

Purpose: Ab initio electronic structure, Molecular Dynamics
Latest version: 4.1
License: Free of use for academics users
Mixed
Website: *https://departments.icmab.es/_ext-link*

SIESTA is a program for ab initio electronic structure and molecular dynamics of solids and molecules.

SIESTA applies DFT hamiltonians (LDA, GGA) to strictly localized numerical basis sets and non-local pseudopotentials to obtain electronic structures. From these it can compute solid properties (band structure, DOS, k-space sampling, dielectric polarisation, phonons), perform Born-Oppenheimer molecular dynamics (NVT and NPT), and, in recent versions, Van der Waals potentials and ballistic electron transport properties (TranSIESTA).

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 stderr redirection filename.
- **-o**: Name of the stdout redirection filename.

siesta_example.slm

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

module load apps/siesta/4.1

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

##
#  You don't need to modify nothing more
cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

srun siesta < ${INPUT_FILE} > ${OUTPUT_FILE}

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

- **-p**: Name of the partition (queue) where the job will be submitted.
- **-n**: Number of tasks.
- **-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.