VASP

Purpose: ab initio Molecular Dynamics
Latest version: 6.1.2
License: ⚠ Must be provided by the user
Proprietary
Website: *https://www.vasp.at/_ext-link*

Vienna Ab-Initio Simulation Package (VASP) is a program for plane-wave ab initio molecular dynamics.

VASP is a package to perform Born-Oppenheimer ab initio molecular dynamics (MD) simulations, employing a plane-wave DFT approach (LDA, GGA, meta-GGA, hybrids) to electronic structure. It implements either Vanderbilt pseudopotentials or the projector-augmented wave (PAW) method and Pulay-Broyden convergence to compute the ground electronic state at each step, as opposed to Car-Parrinello molecular dynamics.

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.

vasp_example.slm

```
#!/bin/bash
#SBATCH -J vasp_example
#SBATCH -e vasp_example.err
#SBATCH -o vasp_example.out
#SBATCH -p std
#SBATCH -n 8
#SBATCH -t 0-01:00

module load apps/vasp/5.4.4
ulimit -s unlimited

##
#  Modify the input and output files!
INPUT_FILE={INCAR,KPOINTS,POTCAR,POSCAR}
OUTPUT_FILE=OUTCAR

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

srun $(which vasp_std)

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.