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#!/bin/bash
### This is a SBATCH submission file.
### VASP job will run on 20 processors for a maximun of 72 hours on the
defq queue.
### The job use home directory.
#SBATCH -J CR2_2_equilibre
#SBATCH -n 20
#SBATCH -t 72:00:00
#SBATCH -p defq
#SBATCH --output slurm-%j.txt
#SBATCH --error slurm-error%j.txt
module purge
module load shared
module load slurm intel/openmpi-for-intel/1.8
intel/compiler/64/15.0/2015.0.090
module load vasp/5-3-5
echo Running on $(hostname)
echo Available nodes: $SLURM_NODELIST
echo Slurm_submit_dir: $SLURM_SUBMIT_DIR
echo Start time: $(date)
mpirun vasp
```