

# Slurm Submit Script Examples for Slurm

In this page, there is a list of examples of slurm scripts for launching different software in Altamira.

## VASP

### VASP Example for INTEL OneApi 2021

```
#!/bin/bash -l

#SBATCH --job-name=vasp_test
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --ntasks=64
#SBATCH --cpus-per-task=1
#SBATCH --nodes=4 # > 1, If you put 1, VASP ends with a segmentation fault
#SBATCH --time=72:00:00
#SBATCH --partition=res # Put res if you comes from RES, omit it for general projects

module load VASP/5.4.4_INTEL
source /gpfs/res_apps/INTEL/oneapi/2021.3/setvars.sh

ulimit -s unlimited

myJobName=$SLURM_JOB_NAME.$SLURM_JOBID
mkdir $myJobName && cd $myJobName

myBinFile=vasp_std
myWrkLoad=/home/uc00/uc00108/test/VASP_test/Pd04
cp $myWrkLoad/INCAR .; cp $myWrkLoad/KPOINTS .; cp $myWrkLoad/POSCAR .; cp $myWrkLoad/POTCAR .

echo "-- Running $myBinFile --"
mpirun $myBinFile
```