Parts of a VASP code

INPUTS

      INCAR: Sets the parameters of the simulation. This is where you will set the temperature. TEBEG and TEEND, for most simulations, set them both to your desired temperature. NSW: number of steps.

      POSCAR: Think of this as the "position" of the atoms in your simulation cell. You can open this in vesta and ovito to move atoms around, look at them from different angles, ect. If you are making your own simulation cell, this is likely the input that you will need to start from scratch.

      POTCAR: gives the pseudopotentials for each atom. You should NOT need to modify this.

      KPOINTS: This gives the simulation the spacing of each atom, typically, you will not need to modify this. You will likely use regular mesh, though there are other modes that may be needed.

      Jobfile.job: Here you can name your simulations, tell it how long to run, how many nodes and how many cores per node. To change the name, you can change everything that comes after "j o e" to the name you desire. This helps you keep track of what is currently running.

```
#!/bin/bash
#SBATCH -J Fe
#SBATCH -o Fe.o%j
#SBATCH -e Fe.e%j
#SBATCH --ntasks-per-node=40
#SBATCH -N 3
#SBATCH --partition=cmpg
time mpirun $VASP_INTEL_EXE > logError
```

OUTPUTS

      XDATCAR: This is the "movie" of your simulations. To watch your simulation you can dump this in ovito. Often, if you want to run something for example 50 pico seconds, you will need only the last snap shot. In this case, go to the end of the "movie" and export the file. Name it POSCAR and ensure that it is saved as a poscar file. This will be your new starting position for your next simulation. All the other files can be the same.

      OSZICAR: gives you the temperature and energy output of each timestep. If you are analyzing this as the simulation progresses, grep the desired result.

OUTCAR: gives the pressure and volume outputs. Treat the same as OSZICAR

CONTCAR: This file is written after each step and is a way for the simulation to know how fast and where to different atoms are moving. Copy this over for the new run so it can "start where it left off"

Things to be copied over for each "run" in Al-Sc-x
The new poscar from xdatcar, jobfile, kpoints, potcar, contcar, incar.