

# Introduction to Electronic Structure Calculations using VASP

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Present document is an introduction manual of how to use VASP on HPC systems for material science or physics related problems. VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) based on density functional theory (DFT) using pseudopotentials and a plane wave basis set. The approach implemented in VASP is based on a local-density approximation and an exact evaluation of the instantaneous electronic ground state that use efficient matrix diagonalization schemes and an efficient Pulay mixing. These techniques avoid all previous problems occurring in the original Car-Parrinello method which is based on the simultaneous integration of electronic and ionic equations of motion. The interaction between ions and electrons is described using ultrasoft Vanderbilt pseudopotentials (US-PP) or the projector augmented wave method (PAW) or the generalised gradient approximation (GGA). All techniques allow a considerable reduction of the necessary number of plane-waves per atom for transition metals and first row elements. Forces and stress can be calculated with VASP and used to relax atoms into their instantaneous groundstate.

This particular document includes:

- a) An introduction
- b) Setup
- c) Input files
- d) Running VASP
- e) References
- f) Appendix (Related scripts)

## **Introduction**

**VASP** is a complex package for performing ab-initio quantum-mechanical simulations based on density functional theory (DFT) using pseudopotentials or the projector-augmented wave method and a plane wave basis set. The approach implemented in VASP is based on the local-density approximation with the free energy as a variational quantity and instantaneous electronic ground state is evaluated. Beginners are advised to read slides prepared for the [hand-on sections](#). The [User guide](#) provides more details for experienced users.

## **Setup**

To use **VASP** you need to have a license, currently only Prof. Seong-Gon Kim has his license and the license is not for the HPC group users.

Current installations includes **VASP** version 4.6.

## Input Files

There are four essential input files, and must exist in the present working directory before VASP can be executed. The following is a sample input for MnBi magnetic system.

- INCAR file

The INCAR file is the central input file of VASP. It determines what to do and how to do it. It is a tagged format free-ASCII file: Each line consists of a tag (i.e. a string) the equation sign '=' and one or several values. Defaults are supplied for most parameters.

```
IBRION = 2  
ISIF = 3  
LWAVE = .FALSE.  
LCHARG = .FALSE.
```

- POSCAR

The POSCAR file contains the positions of the ions. For the Ni example, the POSCAR file contains the following lines:

```
Ni_FCC                                comment line  
1                                       universal scaling factor  
4.00 0.00 0.00                          first Bravais lattice vector  
0.00 4.00 0.00                          second Bravais lattice vector  
0.00 0.00 4.00                          third Bravais lattice vector  
4                                       number of atoms per species, be consistent  
Direct                                direct or cartesian, only first letter is significant  
0.00000000 0.00000000 0.00000000      positions  
0.50000000 0.00000000 0.50000000  
0.50000000 0.50000000 0.00000000  
0.00000000 0.50000000 0.50000000
```

The positions can be given in direct (fractional) or Cartesian coordinates. In the second case, positions will be scaled by the universal scaling factor supplied in the second line.

The lattice vectors are always scaled by the universal scaling factor. File is free formatted.

- KPOINTS

The KPOINTS file determines the k-points setting

```
K-Points      Comment
  0           0 = automatic generation of k-points
Monkhorst     M use Monkhorst Pack
  11 11 11    grid 11x11x11
  0  0  0     shift (usually 0 0 0)
```

The first line is a comment. If the second line equals zero, k-points are generated automatically using the Monkhorst-Pack's technique (first character in third line equals M). With Supplied KPOINTS file a 11X11X11 Monkhorst-Pack grid is used for the calculations.

- POTCAR

The POTCAR file contains the pseudopotentials (for more than one species simply concatenate POTCAR files using the UNIX command cat, if compressed, use zcat). The POTCAR file also contains information about the atoms (i.e. their mass, their valence, the energy of the atomic reference configuration for which the pseudopotential was created etc.).

```
> gunzip /usr/local/vasp/potpaw_GGA/Ni/POTCAR.Z > POTCAR_Ni
> gunzip /usr/local/vasp/potpaw_GGA/Mn/POTCAR.Z > POTCAR_Mn
> cat POTCAR_Mn POTCAR_Ni > POTCAR
```

For a case where you want to generate a system of MnNi, remember since your POTCAR file contains Mn first and then Ni, you should be consistent while putting the positions in POSCAR file, ie, write the positions for Mn first and then Ni.

Potentials are available in the following directory:

**/usr/local/vasp**

Depending on what kind of potential you are looking for, you have to go further to choose your directory, such as if you want to use GGA potential you should grab /usr/local/vasp/potpaw\_GGA/Ni/POTCAR.Z Also, there are typically soft and hard potential for each element. Depending on your application you should choose them.

## Running VASP

### Interactively

1) To run VASP **interactively**, make sure the corresponding modules has been loaded, the change to the working directory containing all the input files and execute the command, i.e. vasp\_raptor

After starting VASP, you will get a output similar to

```
running on 1 nodes
distr: one band on 1 nodes, 1 groups
vasp.4.6.36 17Feb09 complex
POSCAR found : 1 types and 4 ions
LDA part: xc-table for Ceperly-Alder, standard interpolation
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: wrap around errors must be expected
FFT: planning ... 1
reading WAVECAR
entering main loop
```

	N	E	dE	d eps	ncg	rms
rms(c)						
DAV:	1	0.171904832619E+03	0.17190E+03	-0.12785E+04	2688	
		0.132E+03				
DAV:	2	-0.139486735106E+02	-0.18585E+03	-0.18195E+03	2816	
		0.297E+02				
DAV:	3	-0.219597939772E+02	-0.80111E+01	-0.77212E+01	3120	
		0.754E+01				
DAV:	4	-0.221560634061E+02	-0.19627E+00	-0.19475E+00	2816	
		0.106E+01				
DAV:	5	-0.221585319930E+02	-0.24686E-02	-0.24677E-02	2888	0.931E-
		0.148E+01				
DAV:	6	-0.220787802645E+02	0.79752E-01	-0.60216E+01	2792	
		0.935E+01	0.138E+01			
DAV:	7	-0.188888548414E+02	0.31899E+01	-0.16576E+01	2800	
		0.455E+01	0.929E-01			
DAV:	8	-0.188797520710E+02	0.91028E-02	-0.11630E-01	2720	
		0.260E+00	0.476E-01			
DAV:	9	-0.188758089926E+02	0.39431E-02	-0.86160E-03	3208	0.981E-
		0.651E-02				
DAV:	10	-0.188757571416E+02	0.51851E-04	-0.38206E-04	2496	0.180E-

1 F= -.18875757E+02 E0= -.18853669E+02 d E =-.662648E-01

VASP uses a self-consistency cycle with a Pulay mixer and an iterative matrix diagonalisation scheme to calculate the Kohn Sham (KS) ground-state. Each line corresponds to one electronic step, and in each step the wavefunctions are iteratively improved a little bit, and the charge density is refined once. A copy of stdout (that's what you see on the screen) is also written to the file OSZICAR.

The columns have the following meaning: Column N is counter for the electronic iteration step, E is the current free energy, dE the change of the free energy between two steps, and d eps the

change of the band-structure energy. The column `ncg` indicates how often the Hamilton operator is applied to the wavefunctions. The column `rms` gives the initial norm of the residual vector that is summed over all occupied bands, and is an indication how well the wave-functions are converged. Finally the column `rms(c)` indicates the difference between the input and output charge density. During the first four steps, the density and the potentials are not updated to pre-converge the wavefunctions (therefore `rms(c)` is not shown). After the first four iterations, the update of the charge density starts. The final line shows the free electronic energy `F` after convergence has been reached.

More information (for instance the forces and the stress tensor) can be found in the `OUTCAR` file. Please check this file in order to get an impression which information can be found on the `OUTCAR` file.

Another important file is the `WAVECAR` file which stores the final wave functions. To speed up calculations, VASP usually tries to read this file upon startup. At the end of calculations, the file is written (or if it exists, overwritten).

## **PBS job**

2) To run VASP in parallel mode, it is better to use PBS script to submit job.

First, add the corresponding modules load to your `.bashrc` file, i.e. add line

```
"swsetup openmpi-intel-64".
```

The PBS script would look like the following.

```
#!/bin/bash
#PBS -N NiSystem
#PBS -l nodes=4:ppn=4
#PBS -l walltime=45:00:00
# PBS -q q64p48h@raptor
#PBS -mea
#PBS -r n
#PBS -V
cd $PBS_O_WORKDIR
mpirun -np 16 vasp_raptor
```

## References

Please remember to cite the following references when publishing results obtained with VASP:

- G. Kresse and J. Hafner. Ab initio molecular dynamics for liquid metals. *Phys. Rev. B*, 47:558, 1993.
- G. Kresse and J. Hafner. Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium. *Phys. Rev. B*, 49:14251, 1994.
- G. Kresse and J. Furthmüller. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mat. Sci.*, 6:15, 1996.
- G. Kresse and J. Furthmüller. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *Phys. Rev. B*, 54:11169, 1996.

Depending on the potentials used you should also include the following citations:

### *Ultra-soft pseudopotentials*

- D. Vanderbilt. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Phys. Rev. B*, 41:7892, 1990.
- G. Kresse and J. Hafner. Norm-conserving and ultrasoft pseudopotentials for first-row and transition-elements. *J. Phys.: Condens. Matter*, 6:8245, 1994.

### *PAW potentials*

- P. E. Blochl. Projector augmented-wave method. *Phys. Rev. B*, 50:17953, 1994.
- G. Kresse and D. Joubert. From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B*, 59:1758, 1999.

The references to the exchange and correlation approximations implemented in VASP are:

### *Local Density Approximation (LDA)*

- J. P. Perdew and A. Zunger. Self-interaction correction to density-functional approximations for many-electron systems. *Phys. Rev. B*, 23:5048, 1981.

### *Generalized Gradient Approximation PW91 (GGA-PW91)*

- J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, and C. Fiolhais. Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. *Phys. Rev. B*, 46:6671, 1992.
- J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, and C. Fiolhais. Erratum: Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. *Phys. Rev. B*, 48:4978, 1993.

### *Generalized Gradient Approximation PBE (GGA-PBE)*

- J. P. Perdew, K. Burke, and M. Ernzerhof. Generalized gradient approximation made simple. *Phys. Rev. Lett.*, 77:3865, 1996.
- J. P. Perdew, K. Burke, and M. Ernzerhof. Erratum: Generalized gradient approximation made simple. *Phys. Rev. Lett.*, 78:1396, 1997.

## Further Information

- <http://cms.mpi.univie.ac.at/vasp/>  
The official VASP web page have further news and information.

## Appendix

To generate a simple Volume~Energy curve, you may use the following script iteratively, below is shown for a Nickel (fcc) system:

```
rm Summary latconst energies evfit.*
```

```
for a in `seq -w 3.0 0.02 4.0`
do
echo "a= $a"
```

```
cat >POSCAR <<!
```

```
Ni_FCC
```

```
1
```

```
$a 0.00 0.00
```

```
0.00 $a 0.00
```

```
0.00 0.00 $a
```

```
4
```

```
Direct
```

```
0.00000000 0.00000000 0.00000000
```

```
0.50000000 0.00000000 0.50000000
```

```
0.50000000 0.50000000 0.00000000
```

```
0.00000000 0.50000000 0.50000000
```

```
!
```

```
mpirun -np 4 vasp-64-mpi
```

```
E=`tail -n 2 OSZICAR | awk '{ print $3}'`
```

```
echo $a $E >> Summary
```

```
cleanvaspfiles
```

```
done
```