Vienna Ab-initio Software Package (VASP)

- *The input files:*

INCAR
POTCAR
KPOINTS
POSCAR

Note: Please make sure that all these four files are in the directory where you run VASP.

- *The output files:*

OUTCAR **A detail information about your simulation**

OSZICAR **A brief information about the total energy calculation**

CONTCAR **the final (optimized) position of atoms**

CHG
CHGCAR
DOSCAR
PCDAT
XDATCAR
WAVECAR
EIGENVAL

file: POSCAR

It contains:

- Lattice constant
- Lattice vectors
- Atom positions
- Number of species
- Number of atoms
- Dynamics atoms

Example: Pd, surface (100), 1x1 unit cell and 5 layers.

```
Ag: atom
3.96000
  0.5000000   0.5000000   0.0000000
 -0.5000000   0.5000000   0.0000000
  0.0000000   0.0000000   5.5000000
  5
Selective dynamics
Cartesian
  0.0000000   0.0000000   0.0000000   F  F  F
  0.0000000   0.5000000   0.5000000   F  F  F
  0.0000000   0.0000000   1.0000000   F  F  F
  0.0000000   0.5000000   1.5000000   T  T  T
  0.0000000   0.0000000   2.0000000   T  T  T
```

First line is just an explanation about the simulation you are doing

Lattice constant in Angstrom

Bravais lattice vectors

Total number of atoms species

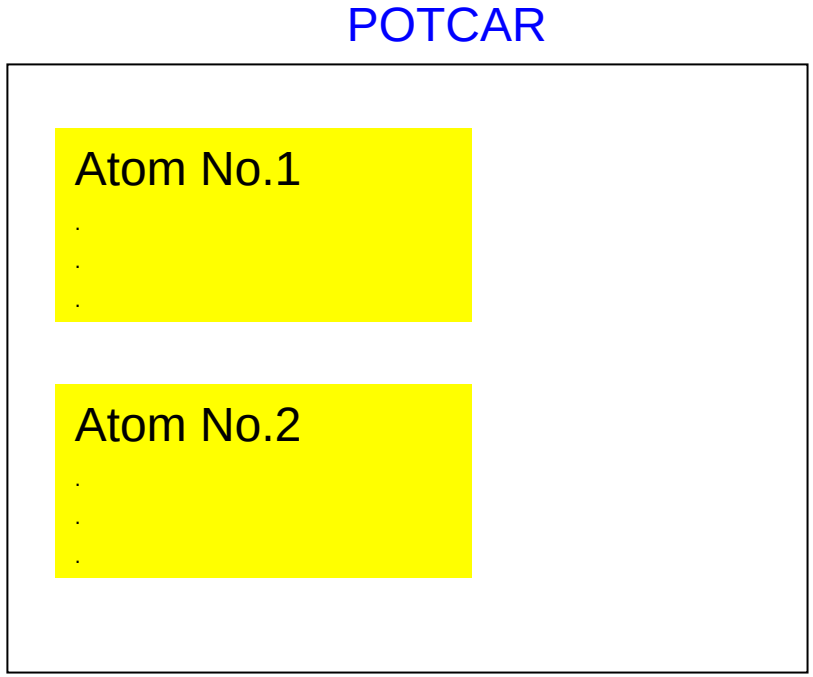
It can be Cartesian or Direct. Cartesian indicates that atoms positions are in Cartesian coordinates leave it as it is.

Atoms positions. F F F means that the atom can not move in any direction x, y and z during the simulation and T T T means that the atom moves in all three directions x, y and z. **Note: The atom positions in Cartesian is given by these numbers time the lattice constant.**

Question: In this example how much is the vacuum thickness?

file: POTCAR

It contains information about electron-ion interactions for each ion



Note: Please make sure that you have chosen the proper POTCAR.

The output files:

An example of the file OSZICAR

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	-0.230935226871E+02	-0.23094E+02	-0.37664E+00	240	0.918E+00	0.550E-01
DAV:	2	-0.238342830187E+02	-0.74076E+00	-0.21118E+00	360	0.163E+01	0.710E+00
DAV:	3	-0.230635031639E+02	0.77078E+00	-0.91365E-01	298	0.137E+01	0.266E+00
DAV:	4	-0.230838138798E+02	-0.20311E-01	-0.96000E-02	310	0.542E+00	0.669E-01
DAV:	5	-0.230923806448E+02	-0.85668E-02	-0.25679E-02	264	0.195E+00	0.276E-01
DAV:	6	-0.230929268276E+02	-0.54618E-03	-0.74028E-03	266	0.124E+00	0.233E-01
DAV:	7	-0.230928147303E+02	0.11210E-03	-0.22522E-03	280	0.725E-01	0.136E-01
DAV:	8	-0.230925894262E+02	0.22530E-03	-0.59306E-04	232	0.460E-01	0.278E-02
DAV:	9	-0.230926065494E+02	-0.17123E-04	-0.73637E-05	144	0.898E-02	

Electronic optimization loop

1 F= -.23092607E+02 E0= -.23091337E+02 d E =-.163432E-01

Ionic iterations

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	-0.231229799239E+02	-0.23123E+02	-0.34604E+01	240	0.281E+01	0.177E+00
DAV:	2	-0.231104231630E+02	-0.47056E-02	-0.87377E-02	258	0.341E+00	0.420E-01
DAV:	3	-0.231145483907E+02	-0.41252E-02	-0.10203E-02	246	0.118E+00	0.284E-01
DAV:	4	-0.231149788729E+02	-0.43048E-03	-0.70637E-03	264	0.731E-01	0.364E-01
DAV:	5	-0.231141994908E+02	0.77938E-03	-0.27052E-03	240	0.590E-01	0.702E-02
DAV:	6	-0.231142681055E+02	-0.68615E-04	-0.18824E-04	172	0.200E-01	

Electronic optimization loop

2 F= -.23114268E+02 E0= -.23111404E+02 d E =-.380048E-01

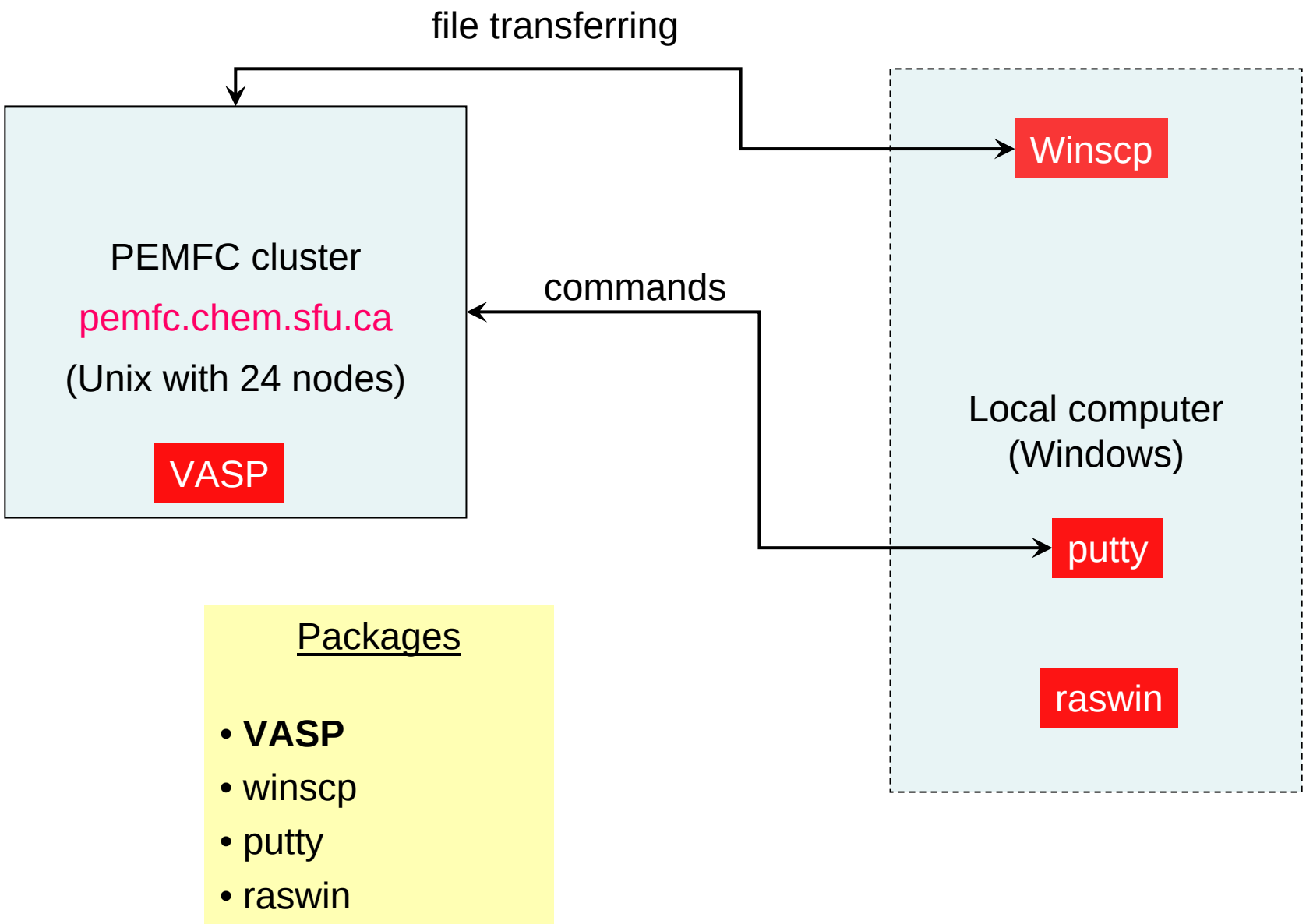
The final total energy

An example of the file CONTCAR

Pd, surface (100), 1x1 unit cell and 5 layers.

```
Ag: atom
   3.960000000000000
    0.5000000000000000    0.5000000000000000    0.0000000000000000
   -0.5000000000000000    0.5000000000000000    0.0000000000000000
    0.0000000000000000    0.0000000000000000    5.5000000000000000
  5
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
 0.5000000000000000  0.5000000000000000  0.0909090909090935   F   F   F
 0.0000000000000000  0.0000000000000000  0.1818181818181799   F   F   F
 0.5000000000000000  0.5000000000000000  0.2724375420314517   T   T   T
 0.0000000000000000  0.0000000000000000  0.3622611262789428   T   T   T
```

Connection to PEMFC cluster



Packages

- **VASP**
- winscp
- putty
- raswin

Some practice with winscp and putty

The aim is to visualize your POSCAR

- ✓ The raswin package is used.
- ✓ In raswin the input file has to be in a special format (pdb format).
- ✓ To convert our POSCAR to pdb format we have to use a program called “pdb” in PEMFC cluster.

> The file PSCAR has to be transferred to pemfc (winscp)
> run “pdb” (putty)
> move back the file PSCAR to local computer (winscp)
> run raswin

Practice with raswin

To get more information about rasmol please visit the website:

http://www.bernstein-plus-sons.com/software/rasmol/doc/rasmol.html

Raswin has two shells:

command shell
graphic shell

For those who are interested to know about command shell here is the most important commands in rasmol are:

1. select [atom name]
2. spacefill [radius]
3. write vectps [output file].ps
4. color [color]