Introduction to VASP

Vienna Ab initio **S**imulation **P**ackage

Univ. Wien: Kresse, Marsman, Furthmüller …

http://www.vasp.at

The most used software package for computational materials modelling solid/liquid materials from first principles.

My description of VASP in one sentence

Geometry optimization and molecular dynamics using density functional theory (LDA/GGA/Hybrid-GGA) with periodic boundary conditions and a projector-augmented wave basis set (“PAW” method).

VASP features

- **Functionals**
  - LDA, GGAs, metaGGAs
  - Hartree-Fock, Hartree-Fock/DFT hybrids
- **First derivatives**
  - Forces and stress tensor for DFT, Hartree-Fock, and hybrid functionals
- **Dynamics and relaxation**
  - Born-Oppenheimer molecular dynamics
  - Relaxation using conjugate gradient, Quasi-Newton or damped molecular dynamics
  - Nudged elastic band methods (transition states search)
- **Magnetism**
  - Collinear and non-collinear
  - Spin-orbit coupling
  - Constrained magnetic moments approach.
- **Linear response to electric fields** (Dielectric properties)
- **Linear response to ionic displacements** (Phonons)
- **Optical properties**
  - Frequency dependent dielectric tensors in the independent particle approximation
  - Frequency dependent tensors in the RPA and TD-DFT
  - Cassida's equation for TD-DFT and TD-Hartree-Fock
- **Berry phases**
  - Macroscopic polarization
  - Finite electric fields
- **Green's function methods**
  - GW quasiparticles
  - ACFDT total energies in the RPA
- **Many-body perturbation theory (MP2)**
- **...**

How expensive are VASP calculations?

Fe(bcc) - *1 atom*
100 k-points: 10 seconds on 16 cores

Li_2FeSiO_4 - *64 atom supercell*
*G*amma point: 30 seconds on 64 cores

MgO supercell - *63 atoms*
HSE06 - 4 kpts: 1600 seconds on 128 cores

Carbon nanotube fragment - *512 atoms*
Gamma point: 500 seconds on 256 cores

VASP workflow

Input files:

INCAR

POSCAR

POTCAR

KPOINTS

```
$ mpirun -np 64 vasp
```

Output files:

OUTCAR

OSZICAR

DOSCAR

...

POSCAR: geometry

Arbitrary description

"Lattice constant"

x-vector

y-vector

z-vector

Number of atoms for each species

"Direct" or "Cartesian" coordinates

Position 1 (x,y,z)

Position 2 (x,y,z)

...

```
diamond
1.00
5.428835   0.000000 0.000000
0.000000   5.428835 0.000000
0.000000   0.000000 5.428835
8
Direct
0.000000   0.000000 0.000000
0.000000   0.500000 0.500000
0.500000   0.500000 0.000000
0.500000   0.000000 0.500000
0.750000   0.250000 0.250000
0.750000   0.750000 0.750000
0.250000   0.750000 0.250000
0.250000   0.250000 0.750000
```

POTCAR: “potentials” (basis)

```
[pla@triolith1 Li2FeSiO4]$ grep TITEL POTCAR
   TITEL  = PAW_PBE Li_sv 10Sep2004
   TITEL  = PAW_PBE Mn_sv 23Jul2007
   TITEL  = PAW_PBE Fe_sv 23Jul2007
   TITEL  = PAW_PBE Si 05Jan2001
   TITEL  = PAW_PBE O 08Apr2002
```

POTCAR files contain a list of "atomic" POTCAR files, one for each species.

```
$ cat /potpaw_PBE/Li_sv/POTCAR
    /potpaw_PBE/Mn_sv/POTCAR
    /potpaw_PBE/Fe_sv/POTCAR
    /potpaw_PBE/Si/POTCAR
    /potpaw_PBE/O/POTCAR
    >> POTCAR
```

INCAR: simulation parameters

```
[pla@triolith1 Si-cd]$ cat INCAR
ISTART = 0
ICHARG = 2

PREC = Accurate
ENCUT = 350

ALGO = fast
EDIFF = 1.0E-5
ISMEAR = -5

LCHARG = .FALSE.
LWAVE = .FALSE.

ISPIN = 1
NCORE = 16
```

Start calc. from scratch

First charge density from atom superpositions

Size of main FFT grids for charge density

Size of basis set (cut-off in eV)

Don't forget ENCUT!

Scheme used to diagonalize Hamiltonian

SCF convergence criteria (eV)

Smearing/partial occupancies

Save charge density to disk

(the "CHGCAR" file)

Save Kohn-Sham orbitals to disk

(the "WAVECAR" file)

Spin polarized? (1=no, 2=yes)

For Band parallelization

KPOINTS: Brillouin-zone sampling

Number of k-points
K-point generation scheme
Grid size (x y z)
Mesh shift

```
Comment line
 0
Monkhorst Pack
 4  4  4
 0  0  0
```

"0" has no meaning here due to automatic generation

4x4x4 Monkhorst Pack grid

- You can also specify each k-point manually.
- There is a special "line mode" for generating k-points for e.g. band plots. Described in the manual.

Demo: Si (cubic diamond)

OUTCAR: main output

```
---------------------------------------- Iteration    1(  11)  ---------------
[...]
Free energy of the ion-electron system (eV)
  ---------------------------------------------------
  alpha Z        PSCENC =        13.46525406
  Ewald energy   TEWEN  =      -914.45032677
  -1/2 Hartree   DENC   =       -59.70036230
  -exchange  EXHF       =         0.00000000
  -V(xc)+E(xc)   XCENC  =       -71.82231490
  PAW double counting   =      3536.86238241    -3397.02569318
  entropy T*S    EENTRO =         0.00000000
  eigenvalues    EBANDS =        24.78760960
  atomic energy  EATOM  =       824.52501657
  ---------------------------------------------------
  free energy    TOTEN  =       -43.35843450 eV
[...]
```

- The output file is designed to be used with the Unix "grep" utility.

OUTCAR: main output

```
[pla@triolith1 Si-cd]$ grep "free energy" OUTCAR
  free energy    TOTEN  =        55.91217646 eV
  free energy    TOTEN  =       -39.11715826 eV
  free energy    TOTEN  =       -43.97635596 eV
  free energy    TOTEN  =       -44.07892152 eV
  free energy    TOTEN  =       -44.08260409 eV
  free energy    TOTEN  =       -43.58101946 eV
  free energy    TOTEN  =       -43.35400878 eV
  free energy    TOTEN  =       -43.35749971 eV
  free energy    TOTEN  =       -43.35831228 eV
  free energy    TOTEN  =       -43.35843450 eV
  free energy    TOTEN  =       -43.35842932 eV
  free energy    TOTEN  =       -43.35842796 eV
  free energy    TOTEN  =       -43.35842838 eV
```

Two blank spaces. Clever!

```
[pla@triolith1 Si-cd]$ grep "free  energy" OUTCAR
  free  energy   TOTEN  =       -43.35842838 eV
```

OUTCAR: main output

```
$ tail OUTCAR
                                  User time (sec):      9714.723
                                System time (sec):       164.176
                               Elapsed time (sec):      9924.793

                         Maximum memory used (kb):       414440.
                         Average memory used (kb):            0.

                              Minor page faults:        8697122
                              Major page faults:              0
                            Voluntary context switches:       51906
```

- Useful for estimating what time to request in the job script.
- Don’t trust the memory estimates!

OSZICAR: condensed output

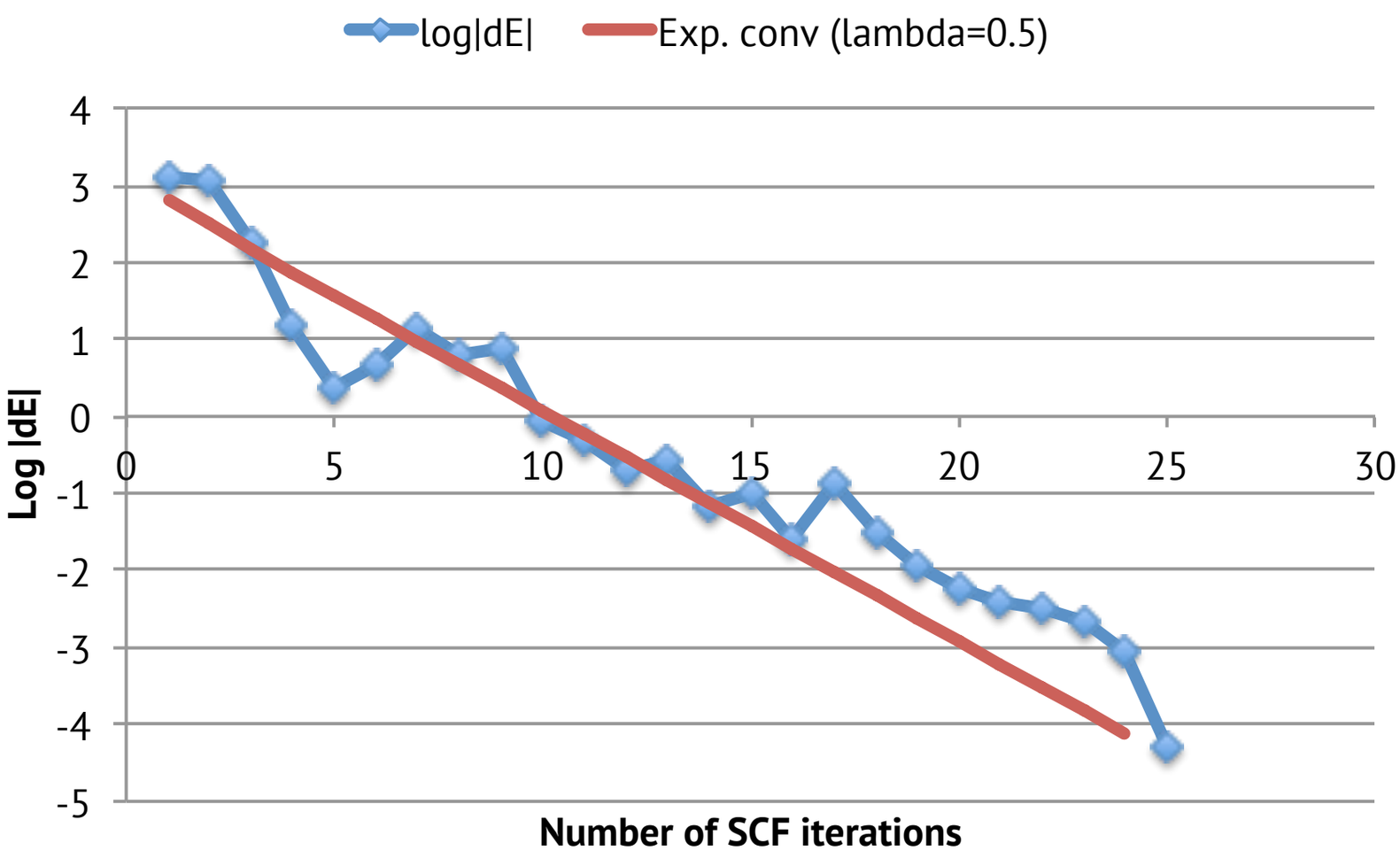
```
[pla@triolith1 Si-cd]$ cat OSZICAR
```

SCF iteration | Energy (eV) | delta E | Residual vector | Residual v. charge density

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	0.559121764629E+02	0.55912E+02	-0.96389E+03	168	0.900E+02	
DAV:	2	-0.391171582601E+02	-0.95029E+02	-0.87841E+02	217	0.142E+02	
DAV:	3	-0.439763559607E+02	-0.48592E+01	-0.47727E+01	216	0.317E+01	
DAV:	4	-0.440789215218E+02	-0.10257E+00	-0.10230E+00	198	0.571E+00	
DAV:	5	-0.440826040933E+02	-0.36826E-02	-0.36817E-02	219	0.862E-01	0.983E+00
RMM:	6	-0.435810194607E+02	0.50158E+00	-0.28100E-01	168	0.223E+00	0.604E+00
RMM:	7	-0.433540087813E+02	0.22701E+00	-0.64361E-01	170	0.346E+00	0.338E-01
RMM:	8	-0.433574997067E+02	-0.34909E-02	-0.18428E-02	188	0.609E-01	0.147E-01
RMM:	9	-0.433583122811E+02	-0.81257E-03	-0.16625E-03	192	0.217E-01	0.984E-02
RMM:	10	-0.433584345042E+02	-0.12222E-03	-0.30341E-04	192	0.919E-02	0.236E-02
RMM:	11	-0.433584293241E+02	0.51801E-05	-0.45215E-05	191	0.330E-02	0.346E-03
RMM:	12	-0.433584279602E+02	0.13640E-05	-0.30600E-06	151	0.906E-03	0.523E-03
RMM:	13	-0.433584283769E+02	-0.41674E-06	-0.44608E-07	118	0.410E-03	

```
   1 F= -.43358428E+02 E0= -.43358428E+02  d E =0.000000E+00 mag=    -0.0001
```

Magnetic moment of the cell appears here.



Neat trick: plot log|dE| vs SCF

$$|e_{n+1}| \approx \lambda |e_n|^{\alpha}$$

Final remark

Read every page in the manual.

Really!

http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html