Introduction to VASP (1)

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

What is VASP?

The Vienna Ab initio Simulation Package (VASP) is a **computer program for atomic scale materials modelling**, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

VASP computes an approximate solution to the **many-body Schrödinger equation**, either within density functional theory (DFT), solving the Kohn-Sham equations, or within the Hartree-Fock (HF) approximation, solving the Roothaan equations. Hybrid functionals that mix the Hartree-Fock approach with density functional theory are implemented as well. Furthermore, Green's functions methods (GW quasiparticles, and ACFDT-RPA) and many-body perturbation theory (2nd-order Møller-Plesset) are available in VASP.

In VASP, central quantities, like the one-electron orbitals, the electronic charge density, and the local potential are expressed in **plane wave basis sets**. The interactions between the electrons and ions (+ core electrons) are described using norm-conserving or ultrasoft pseudopotentials, or the projector-augmented-wave method.

To determine the electronic ground state, VASP makes use of efficient iterative matrix diagonalisation techniques, like the residual minimisation method with direct inversion of the iterative subspace (RMM-DIIS) or blocked Davidson algorithms. These are coupled to highly efficient Broyden and Pulay density mixing schemes to speed up the self-consistency cycle.

https://www.vasp.at/

Log in C238

Use MobaXterm or ssh Secure Shell to login because they have interface to do download

```
ssh username@workstation
```

Username:
Workstation:
Password:

IAMS_peap

pleiosaur@gmail.com -> kt01

snajman@gmail.com -> kt02

amor_2100@yahoo.com -> kt03

yafen.hsiao@gmail.com -> kt04

longnguyenqtr@gmail.com -> kt05

ilikejenny920729@gmail.com -> kt06

neige7675@gmail.com -> kt07

VASP Input Files

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

POSCAR	This file contains the lattice geometry and the ionic positions, optionally also starting velocities and predictor-corrector coordinates for a MD-run.
INCAR	It determines 'what to do and how to do it', and can contain a relatively large number of parameters. Most of these parameters have convenient defaults, and a user unaware of their meaning should not change any of the default values. Be very careful in dealing with the INCAR file, it is the main source of errors and false results
POTCAR	This file contains the pseudopotential for each atomic species used in the calculation. If the number of species is larger than one simply concats the POTCAR files of the species.
KPOINTS	The file KPOINTS must contain the k-point coordinates and weights or the mesh size for creating the k-point grid.

POSCAR (1)

```
Graphene
   1.000
    1.2300000000    -2.1304224933     0.0000000000
    1.2300000000     2.1304224933     0.0000000000
    0.0000000000     0.0000000000    20.0000000000
  C
  2
Selective dynamics
Cartesian
 0.0000000000  0.0000000000  0.0000000000   F  F  F
 1.2300000000  0.7101408311  0.0000000000   F  F  F
```

Ratio parameter, usually I use 1.0 only; it is powerful when you try to manually find out the best lattice constants

Unit vectors of your PBC simulation model

1st type atom's name, optional for VASP 5; but this line should not be there in VASP 4

Number of 1st type atom

You can omit this line, but all atoms are free to move

Atom coordinates are presented in cartesian x, y, z

Atoms' coordinates

F means fixed, T means free to move

POSCAR (2)

```
 Graphene
   1.00000000000000
     1.2300000000000000   -2.1304224933000002    0.0000000000000000
     1.2300000000000000    2.1304224933000002    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
   C
     2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000   F   F   F
  0.3333333333333357  0.6666666666666643  0.0000000000000000   F   F   F

  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

Atom coordinates are presented in direct coordinates

velocities

POSCAR (3) - the relation between cartesian and direct representation

Unit vectors: (a1, a2, a3)
(b1, b2, b3)
(c1, c2, c3)

Coordinates in Cartesian: (x, y, z) $\xleftrightarrow{?}$ Coordinates in Direct: (i, j, k)

$$x = i *a1 + j*b1 + k*c1$$
$$y = i*a2 + j*b2 + b*c2$$
$$z = i*a3 + j*b3+ k*c3$$

Homework1: What is the reverse translation?

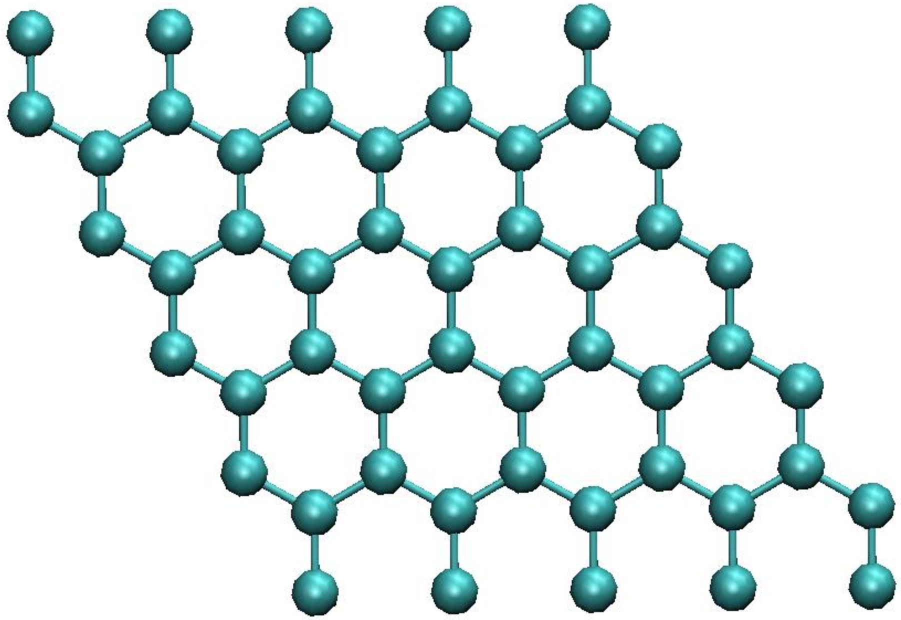
Homework2: Edit a unit cell of (bcc, fcc, hcp, diamond) by your self. Use Direct or Cartesian coordinates to edit is easier?

POSCAR (4) – How to visualize the simulation structure

1. By hand drawing
2. By imagination

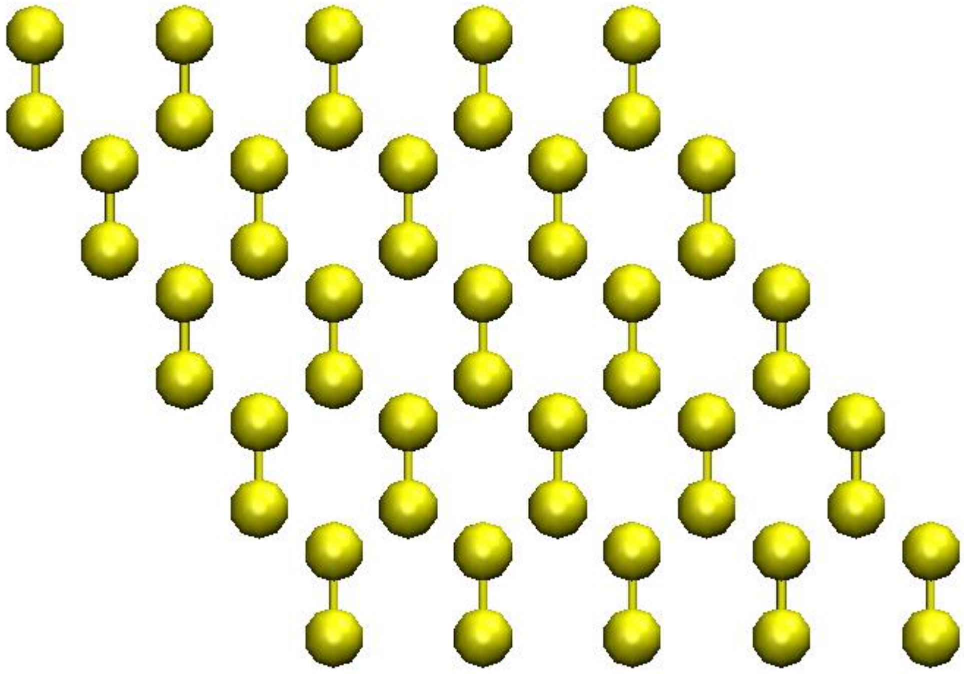
3. With the aid of some software

- VMD (Visual Molecular Dynamics) http://www.ks.uiuc.edu/Research/vmd/
- VESTA (Visualization for Electronic and Structural Analyisis http://jp-minerals.org/vesta/en/



POSCAR (4) – VMD

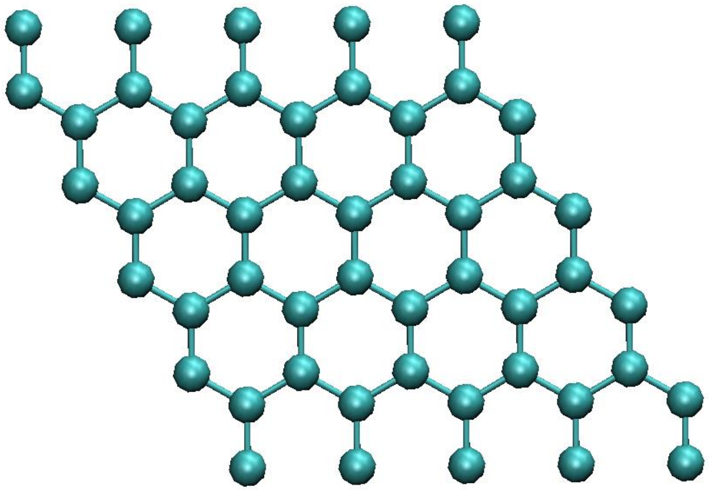
1. Download VMD and install it.
2. Download POSCAR or CONTCAR via Secure Shell or MobaXterm to some temp directory on your computer.
3. Open VMD and “file” -> “New Molecule” -> choose correct file and select “file type” as VASP_POSCAR -> load
4. Click “Graphic” -> “Representation” -> choose CPK for “Drawing method” and click periodic in +x, -x, +y, -y



POSCAR (4) – VMD

5. You also can use my small program “DOUB” to convert POSCAR into *.xyz (follow the text on right hand side)

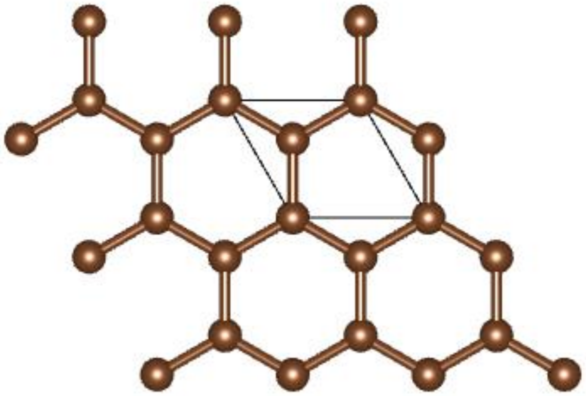
*.xyz is a general file type for displaying configurations.

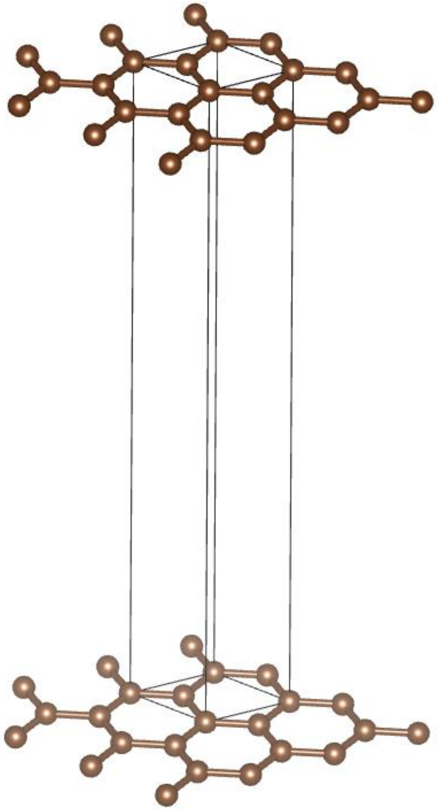


```
[tigp@c238-1 codes]$ ./DOUB
 Enter the file name to read
POSCAR
 Enter the file name to write
tt1.xyz
 How many atoms?
2
 What is the input file type?(DLPOLY/Siesta/s-
input/VASP/PWSCF/xyz/GULP = 1/2/3/4/5/6/7)
4
 You want double or triple the size?(2/3)
5
 In x-direction?(y/n = 1/2)
1
 In y-direction?(y/n = 1/2)
1
 In z-direction?(y/n = 1/2)
2
 How many kinds of atom species?
1
 What is the name of           1 atom species?
C
 The number of C  atom is?
2
```

POSCAR (4) – VESTA

1. Download VESTA and install it.
2. Download POSCAR or CONTCAR via Secure Shell or MobaXterm to some temp directory on your computer.
3. Open VMESTA and “file” -> “open” -> load CONTCAR
4. Click “Edit” -> “Bond…” - > “New”; Click “Object” -> “Boundary…” -> xmin = -1, ymin = -1





INCAR

All list at http://cms.mpi.univie.ac.at/vasp/vasp/All_parameters_or_at_least_most.html

Important parameters

- ISTART = 0, 1, 2, or 3
- ICHARG = 0, 1, 2, 11, or 12
- ISYM = 0, 1, 2, or 3
- NELM = 60 or larger integer number
- EDIFF = 10^{-4} or some smaller number
- ENCUT = largest ENMAX or larger number
- ISPIN = 1, 2
- MAGMOM = specify the magnetization of each atom
- PREC = low, medium, high, nornal, accurate
- ISMEAR = -5, -4, -3, -2, 0, 1, 2 ..., 5
- SIGMA = 0.2 or smaller number
- NSW = some integer, the total ionic steps for configuration change
- EDIFFG = some small number (like 10^{-4} or -0.01)
- IBRION = -1, 0, 1, 2, 3, 5, 6, 7, 8
- POTIM = 0.5 or some number, size for atoms' moving
- ISIF = 0, 1, 2, 3, 4, 5, 6

- LWAVE = .F. or .T.
- LCHARG = .F. or .T.
- NPAR = some integer

INCAR (1)

- ISTART = 0, 1, 2, or 3

  0: Start job: begin 'from scratch'. Initialize the orbitals according to the flag INIWAV

  (usually choose this one)

  1: restart with constant energy cut-off''. Continuation job -- read orbitals from file WAVECAR

  2: 'restart with constant basis set': Continuation job -- read orbitals from the file WAVECAR

  3: 'full restart including orbitals and charge prediction' ; Same as ISTART=2 but in addition a valid file TMPCAR must exist

- ICHARG = 0, 1, 2, 11, or 12

  0: Calculate charge density from initial orbitals. (WAVCAR)

  1: Read the charge density from file CHGCAR

  2: Take superposition of atomic charge densities (usually choose this one)

  11: To obtain the eigenvalues (for band structure plots) or the DOS for a given charge density read from CHGCAR.

  12: Non-selfconsistent calculations for a superposition of atomic charge densities.

INCAR (2)

- ISYM = 0, 1, 2, or 3

  Switch symmetry on (ISYM=1, 2 or 3) or off (ISYM=0). For ISYM=2 a more efficient, memory conserving symmetrisation of the charge density is used. For ISYM=3, the forces and the stress tensor only are symmetrized, whereas the charge density is left unsymmetrized (VASP.5.1 only).

- NELM = 60 or larger integer number; too big (like 200) is already not OK for SC steps

  NELM gives the maximum number of electronic SC (self consistency) steps which may be performed.

- EDIFF = 10^{-4} or some smaller number

  Specifies the global break condition for the electronic SC-loop.

- ENCUT = largest ENMAX or larger number

  Cut-off energy for plane wave basis set in eV. All plane-waves with a kinetic energy smaller than ENCUT are included in the basis set: i.e.

$$\psi_{j,\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{j,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}. \qquad |\mathbf{G}+\mathbf{k}| < G_{\mathrm{cut}} \quad \text{with} \qquad E_{\mathrm{cut}} = \frac{\hbar^2}{2m} G_{\mathrm{cut}}^2$$

INCAR (3)

- ISPIN = 1, 2

  ISPIN=1 non spin polarized calculations are performed; ISPIN=2 spin polarized calculations are performed.

- MAGMOM = specify the magnetization of each atom

  Default: all atoms are assigned with magnetization 1.0 for ISPIN = 2

- PREC = low, medium, high, nornal, accurate

  Setting the detail number of plane waves expansion according to ENCUT and this tag.

- ISMEAR = -5, -4, -3, -2, 0, 1, 2 ..., 5

  Determines how the partial occupancies are set for each orbital; each number indicates one method.

- SIGMA = 0.2 or smaller number

  The smearing width parameter.

INCAR (4)

- NSW = some integer, the total ionic steps for configuration change

  NSW sets the maximum number of ionic steps.

- EDIFFG = some small number (like 10^{-4} or -0.01)

  Optimization break criteria; positive: total energy difference, negative: force on each atom.

- IBRION = -1, 0, 1, 2, 3, 5, 6, 7, 8

  -1: fix all atoms; 0: molecular dynamics; 1: quasi-Newton (variable metric) algorithm optimization, 2: conjugate-gradient algorithm, 5~8: determine the Hessian matrix

- POTIM = 0.5 or some number, size for atoms' moving

- LWAVE = .F. or .T. (print out the WAVECAR (wave functions) or not)

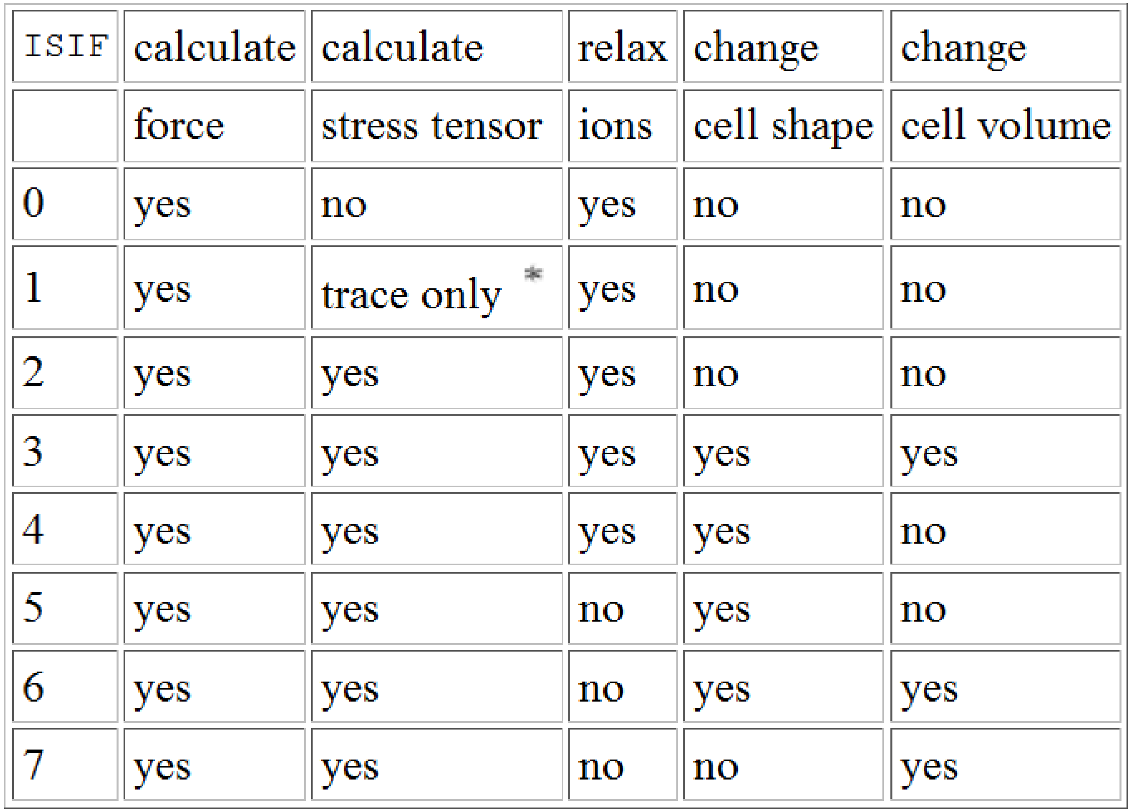
- LCHARG = .F. or .T. (print out the CHGCAR (charge density) or not)

INCAR (5)

- NPAR = some integer

  NPAR is set to 1. This implies distribution over plane wave coefficients only: all cores will work on every individual band, by distributing the plane wave coefficients over all cores. NPAR usually is set to be about the square root of the total cpu number. Then NPAR bands will run in MPI with NCORE/NPAR on one band.

- ISIF = 0, 1, 2, 3, 4, 5, 6



ISIF	calculate	calculate	relax	change	change
	force	stress tensor	ions	cell shape	cell volume
0	yes	no	yes	no	no
1	yes	trace only *	yes	no	no
2	yes	yes	yes	no	no
3	yes	yes	yes	yes	yes
4	yes	yes	yes	yes	no
5	yes	yes	no	yes	no
6	yes	yes	no	yes	yes
7	yes	yes	no	no	yes

POTCAR (1)

The pseudopotential for each atomic species are in data base at some where in c238. Basically, If your system has many type of atom species, you need to concat them in one file with name of POTCAR. The sequence is important and needs to be the same as in POSCAR.

There are two type of POTCAR flavors: (i) Ultra-soft (ii) PAW (projected augmented wave). The 2nd one is more popular now.

In POTCAR, the information of ENMAX is written in, which can be used for ENCUT.

POTCAR (2)

```
PAW C 31May2000
4.00000000000000000
parameters from PSCTR are:
  VRHFIN =C: s2p2
  LEXCH  = CA
  EATOM  =   146.6877 eV,   10.7812 Ry

  TITEL  = PAW C 31May2000
  LULTRA =        F    use ultrasoft PP ?
  IUNSCR =        0    unscreen: 0-lin 1-nonlin 2-no
  RPACOR =     .000    partial core radius
  POMASS =   12.011; ZVAL   =    4.000    mass and valenz
  RCORE  =    1.500    outmost cutoff radius
  RWIGS  =    1.630; RWIGS  =     .863    wigner-seitz radius (au A)
  ENMAX  =  400.000; ENMIN  =  300.000 eV
  ICORE  =        2    local potential
  LCOR   =        T    correct aug charges
  LPAW   =        T    paw PP
  EAUG   =  644.873
  DEXC   =     .000
  RMAX   =    2.266    core radius for proj-oper
  RAUG   =    1.300    factor for augmentation sphere
  RDEP   =    1.501    radius for radial grids
  RDEPT  =    1.300    core radius for aug-charge
  QCUT   =   -5.516; QGAM   =   11.032    optimization parameters
```

POTCAR (3)

```
 Description
   l     E      TYP  RCUT    TYP  RCUT
   0   .000     23  1.200
   0   .000     23  1.200
   1   .000     23  1.500
   1  2.500     23  1.500
   2   .000      7  1.500
  Error from kinetic energy argument (eV)
  NDATA  =      100
  STEP   =   20.000   1.050
 50.8      49.0      48.1      46.3      45.4      43.7      42.0      41.1
 39.5      37.8      37.0      35.5      34.0      32.5      31.1      29.8
 28.5      27.2      26.0      24.2      23.1      22.0      20.5      19.6
 18.6      17.3      16.1      15.3      14.2      13.1      12.2      11.2
 10.4      9.57      8.82      8.11      7.24      6.64      5.90      5.39
 4.77      4.20      3.69      3.23      2.81      2.44      2.11      1.75
 1.49      1.22      .988      .830      .661      .521      .386      .297
 .226      .160      .111      .756E-01  .508E-01  .339E-01  .227E-01  .148E-01
 .109E-01  .856E-02  .744E-02  .691E-02  .649E-02  .608E-02  .546E-02  .470E-02
 .388E-02  .310E-02  .233E-02  .181E-02  .139E-02  .115E-02  .102E-02  .967E-03
 .935E-03  .888E-03  .809E-03  .689E-03  .554E-03  .429E-03  .332E-03  .266E-03
 .238E-03  .231E-03  .229E-03  .221E-03  .196E-03  .163E-03  .127E-03  .987E-04
 .822E-04  .771E-04  .761E-04  .735E-04
END of PSCTR-controll parameters
 local part
 124.721915246208937
  .18943348E+02   .18940802E+02   .18938005E+02   .18933335E+02   .18926784E+02
```

KPOINTS (1)

There are 3 ways to prepare a KPOINTS file:

- Entering all k-points explicitly
- Strings of k-points for band structure calculations
- Automatic k-mesh generation

For band structure calculation.

In most cases, doing optimization, prepare a CHGCAR …

- Automatic k-mesh generation

```
Automatic Generation
 0                     number of k-points = 0 ->automatic generation scheme
Gamma                  Gamma ! generate a Gamma centered grid
  9   9   1            subdivisions N_1, N_2 and N_3 along reciprocal vectors
 0.0  0.0  0.0         optional shift of the mesh (s_1, s_2, s_3)
```

KPOINTS (2)

- Automatic k-mesh generation

  The Gamma can be replaced by Monkhorst. The difference is

In Gamma case,

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1}{N_1} + \vec{b}_2 \frac{n_2 + s_2}{N_2} + \vec{b}_3 \frac{n_3 + s_3}{N_3}.$$

In Monkhorst case,

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1 + 1/2}{N_1} + \vec{b}_2 \frac{n_2 + s_2 + 1/2}{N_2} + \vec{b}_3 \frac{n_3 + s_3 + 1/2}{N_3}.$$

KPOINTS (3)

- Strings of k-points for band structure calculations

k-points along high symmetry lines

61

! 61 intersections

Line-mode

rec

! reciprocal space; you can use “car”, cartesian space (not usually used)

0 0 0

0.5 0.0 0

Who can draw these vectors with respect to the unit cell vectors?

0.5 0.0 0

0.33333333333333333333 0.33333333333333333333 0

0.33333333333333333333 0.33333333333333333333 0

0 0 0