

Quantum Espresso tutorial

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Workshop schedule

Second floor rooms H284 Tokyo Institute of Technology Ookayama Campus Main Building Location:

Tokyo, Meguro-ku, Ookayama 2-12-1 (Tokyu Meguro Line-Oimachi Ookayama station)

<http://www.titech.ac.jp/maps/ookayama/index.html>

<http://www.titech.ac.jp/maps/ookayama/campus/index.html>

Schedule

February 27, 2014 (Thursday)

10:00-12:00	Advance preparation (only applicant)*
13:00-13:20	Introduction of quantum ESPRESSO and first-principles calculation
13:20-14:40	Calculation example of the band structure of graphene
14:40-15:00	Break
15:00-16:30	Training
16:30-17:30	For density functional theory
18:00-	(2000 yen entrance fee) Banquet

February 28, 2014 (Friday)

9:00-12:00 Practice questions and answers

- In preparation, we will respond individually Compiling the quantum ESPRESSO and how to log in to the remote machine, for and how to use the Unix command. If it is possible to come to the 10:00 to 12:00, staff will support the preparation of the seminar you are concerned about the contents of these.

quantum ESPRESSO tutorial (preliminary version: 2014.1.31)

It is the material of workshops to enable you to experience the first-principles calculations in quantum ESPRESSO.

First of all, please fix the execution environment of the quantum ESPRESSO in reference to Chapter 2 Chapter 1. In Section 3, for example the calculation of the density of states and band structure of graphene, however, the value in appearance for the first-principles calculation method using ESPRESSO, then you read this chapter first If you are not having used the ESPRESSO still, Try to flow calculations. When calculating for some substance in fact, we have introduced for check of convergence that are always required in Chapter 4. 5 chapters, so we introduce the various calculations such as the calculation of the phonon structure and optimization, please see from where you are interested.

Note:

In quantum ESPRESSO, the results will come out in its own way even with the input a little wrong. It now also be described and that the user should be careful as much as possible, experience some degree of validation and from various angles is required to determine the results came out in the end is correct. Please note that not bear any responsibility for any problems related to the calculation results obtained with reference to the contents of this site.

Workshop schedule

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Reference

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- [Tetrahedron for law](#)

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1. Advance preparation

In this workshop , it is intended that we will try to move the actual quantum-ESPRESSO, and ask them to calculate the band structure of such graphene . Because sure you have the linux server where you installed the quantum-ESPRESSO the venue , you will be asked to use it to log in to there . Please come fix only environment where you can log in to the server to reference the 1.1 anyone who wants to try only the duration of the training sessions simply . Provide here some people (Chapter 2 and 1.2 . Is fine and I have you ignored) is fine and I am back to have to copy the file that you use in meeting training , being able to install it yourself in linux machine later I think you'll be using the server you have .

On the other hand , it is possible to install a quantum-ESPRESSO and Mac Windows. For someone who is looking to try to move with their laptops , please refer to it because I introduced some way . I think that in any case , and want to start on the assumption that it is in the situation that has access to the machine on which the quantum ESPRESSO is contained in the training session from 13:00 . The one with the uneasiness with advance preparation , because it will help with preparation from 10:00 on the day , please come a little early .

1.1 Environment to log in to the server

- For Windows

it is necessary to introduce the environment of X and ssh. Recommendation is to install a 1) cygwin / X, but requires a capacity of 100MB number in HDD. If there is a limit to the file size, try the person of 2) putty + xming.

1. Install the cygwin / X

from the site of cygwin, you can download and run the setup-x86_64.exe or setup-x86.exe.

Please refer to the <http://x.cygwin.com/docs/ug/setup.html#setup-cygwin-x-installing>.

In particular, the package selection screen,

- x11/xorg-server
- x11/xinit
- Net/openssh

Minimal environment is ready if you choose the three

After, X-Window will start Start cygwin from the icon created on the desktop, by typing the command and startx.

the contents of the above because it is described in the image with the <http://tsubame.gsic.titech.ac.jp/node/360>, please refer to that place.

2. Install the putty + xming

Page, so you come out a number if search putty xming in google, please look there for the details.

For Mac

If ssh for Mac contains the standard. For X, Applications - it is OK if there is Xquartz.app or X11.app in the > Utilities. If not, please download and install from the <http://xquartz.macosforge.org/> Xquartz.

1.2. Preparing to install the quantum ESPRESSO to PC

Compiling with cygwin is supported once. Start the setup-x86.exe of cygwin, the Devel following screen package selection

gcc-core, gcc-fortran, patch, libtool, autoconf, automake

Make sure you've installed the per.

For Mac

Quantum ESPRESSO also can be compiled if I put gfortran by using fink or Macports on Mac. However, XCrysdn also below can be installed with fink, it is recommended to use the fink.

I will describe the installation of fink below. If you want to install the fink, it takes time considerably to compile the source, please be careful. (Depending on the performance of the PC, but you must wait at least a few hours)

First, in accordance with <http://www.finkproject.org/download/srcdist.php>, please install the fink. I think the questions asked during the installation there is no problem using the default value of all.

It is may use it if you are already put the fink but, <http://www.finkproject.org/download/10.9-upgrade.php?phpLang> with reference to the following page of any problems you encounter if = keep in creating a list of packages that are en installed, please try removing and then reloading the fink.

it is in the pages of the installation of fink

```
% ./bootstrap
```

When you are finished is

```
./sw/bin/init.sh
```

You configure the fink as. (Preferences. Are performed automatically each time you log in. If you leave and write to. Profile This command) then

```
% fink selfupdate
```

I want to state up-to-date as fink. Then I install the fortran.

```
%fink install gcc48
```

Now, to prepare for ESPRESSO compilation is complete from the installation of fink. In addition, please keep in installed here also XCrysden needed later.

```
% fink install xcrysden
```

2. Installation

Here, I will explain how to install the quantum ESPRESSO. Because there is also information on the following pages regarding the installation method, please refer to that place.

2.1 Download the latest version

I download the latest version from the page of the quantum ESPRESSO. 5.0.3 because it is currently the latest, I will download the patch from 5.0.3 to 5.0.2 and 5.0.2. On account of the patch, download the following three files.

- Espresso-502.tar.gz
- Phonon-5.02.tare.gz
- Espresso-5.0.2-diff

2.2. And patch deployment of files

On placing the three files above to the directory where you want to deploy, you can apply the patch by expanding the file as follows:

```
tar zxvf espresso-5.0.2.tar.gz
cd espresso-5.0.2
tar zxvf ../PHonon-5.0.2.tar.gz
patch -p1 < ../espresso-5.0.2-5.0.3.diff
```

2.3. configure

I make make.sys by examining the environment, such as a compiler. In a situation by the gcc compiler or the intel, gfortran is on,

```
./configure
```

In the case to go well there are many. If you are using the fink

```
CC=/sw/bin/gcc-4 ./configure
```

You must provide hinting in an explicit gcc of fink as.

You will be looking at automatic library as well such as LAPACK and FFT, but if you want to set for yourself, you must edit the appropriate make.sys that was created with. / Configure. In addition, please note that this make.sys so will be overwritten each time you want to configure.

2.4 make

The output appears as follows: Now, typing just make.

to install, type at the shell prompt:

to install, type at the shell prompt:

```
./configure
make target
where target is one of the following:
pw          basic code for scf, structure optimization, MD
ph          phonon code, Gamma-only version and third-order
derivatives
pwcond     ballistic conductance
neb        code for Nudged Elastic Band method
pp         postprocessing programs
cp         CP code: CP MD with ultrasoft pseudopotentials
ld1        utilities for pseudopotential generation
upf        utilities for pseudopotential conversion
tddfpt     time dependent dft code
gui        Graphical User Interface
pwall      same as "make pw ph pp pwcond neb"
all        same as "make pwall cp ld1 upf tddfpt"
xspectra   X-ray core-hole spectroscopy calculations
gipaw      NMR and EPR spectra
w90        Maximally localised Wannier Functions
want       Quantum Transport with Wannier functions
yambo      electronic excitations with plane waves
plumed     Metadynamics plugin for pw or cp
clean      remove executables and objects
veryclean  revert distribution to the original status
tar        create a tarball of the source tree
doc        build documentation
links     create links to all executables in bin/
```


3. Density of states and band structure of graphene

First, as a simple calculation example, let's ask for the density of states and band structure of graphene. Both scf calculation - will be the trend of > post-processing -> non-scf calculation.

3.1. scf calculation

Before you go any further calculation, it is necessary to obtain the (charge density) charge density by scf calculation first. graphene.scf.in input file is the following files needed for scf calculation. Download this file for the time being, put into an appropriate directory.

```
&control
  calculation = 'scf'
  prefix='graphene',
  tstress = .true.
  tprnfor = .true.
  pseudo_dir = './',
  outdir='./work/'
/
&system
 ibrav = 4,
  celldm(1) = 4.602,
  celldm(3) = 4,
  nat = 2,
  ntyp = 1,
  ecutwfc = 30.0,
  ecutrho = 150.0,
  occupations = 'smearing'
  smearing = 'm-p'
  degauss = 0.01
/
&electrons
  mixing_beta = 0.7
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C 12.0107 C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {automatic}
12 12 1 0 0 0
```

Particularly important parameters are as follows.

- Structure of the unit cell

```
ibrav = 4,
cell dm(1) = 4.602,
cell dm(3) = 4,
```

It has a (ibrav = 4) hexagonal structure, $a_1 = a(1,0,0)$, $a_2 = a(-1/2, \sqrt{3}/2, 0)$, $a_3 = a(0,0, c/a)$. It has: (a_B , $1A \sim 0.529177a_B$ Bohr radius units), and $c/a = 4a = 4.602$ when it was.

- Atom type and number of elements

```
nat = 2,
ntyp = 1,
```

One carbon (ntyp = 1), the number of atoms of the unit cell 2 (nat = 2)

- Atom position

```
• ATOMIC_POSITIONS {alat}
• C 0.00 0.00 0.00
• C 0.00 0.57735026918962576451 0.00
```

Specifies the (alat) atomic positions in units of ($= 4.602$) a in the xyz coordinate

(0,0,0), (0, $1/\sqrt{3}$), 0)

When you put the two points, graphene is completed.

- Cutoff energy

```
ecutwfc = 30.0,
ecutrho = 150.0,
```

ecutwfc The cut-off energy when it is deployed in the plane wave wave function. Units Ry. ecutrho cut off when you expand the charge density. It is not necessary to set for ecutrho is $ecutrho = 4 * ecutwfc$ automatically if you are using a pseudo-potential of norm-conserving, but better taken in larger than $4 * ecutwfc$ good in the case of ultra soft.

- K How to get a point

```
K_POINTS {automatic}
```

```
12 12 1 0 0 0
```

And this represents a taking the k point 12x12x1. 0 0 0 on whether to shift the overall mesh, and it is a mesh that contains the Γ point in this case. If it is 12 12 1 1 1 0, Γ point comes at the center of the mesh

- Pseudopotential

```
C 12.0107 C.pz-van_ak.UPF
```

It means that you use the file C.pz-van_ak.UPF of pseudopotential for carbon. This is one of the files that can be downloaded from the website of the quantum ESPRESSO. The contents of pseudopotential, there is a simple description at the beginning of this file, but, C.pz-van_ak.UPF has become the ultrasoft pseudopotential of type using the LDA using the parameters of the Perdew-Zunger. 12.0107 is the mass of carbon, but will not be used for this calculation.

Note:

Here, You can use this file as a pseudopotential of carbon, but please keep in mind that it does not have recommended the use of this pseudopotential for carbon. In order to come also related to the calculation and the amount of physical quantity selection of pseudopotential (created) are trying to compute, must be examined in each case.

The above contents are described often if paper is doing a first-principles calculation, the contents of the calculation almost determined by this.

Refer to INPUT_PW.html For more information about the meaning of each parameter.

Note:

A number of parameters can be set also very parameters other than the set here. It is omitted because it is not a problem in the value of the default in this calculation, it is recommended that it should be read the INPUT_PW.html If you want to calculate in earnest.

You must be located in the directory you have set in the file pseudo_dir C.pz-van_ak.upf of pseudopotential further in order to flow the calculation. In this case, place the C.pz-van_ak.upf in current directory pseudo_dir = Because it is './'. Scf calculation is done by executing the following command in this state.

```
% ~/espresso-5.0.2/bin/pw.x < graphene.scf.in > graphene.scf.out
```

The results are output to graphene.scf.out. Near the end to look at this file

```
the Fermi energy is -0.4661 ev
```

```
! total energy = -22.84944326 Ry
  Harris-Foulkes estimate = -22.84944326 Ry
  estimated scf accuracy < 7.1E-10 Ry
```

```
The total energy is the sum of the following terms:
```

```
one-electron contribution = -89.64903894 Ry
hartree contribution = 46.53466683 Ry
xc contribution = -6.97848167 Ry
ewald contribution = 27.24348888 Ry
smearing contrib. (-TS) = -0.00007836 Ry
```

```
convergence has been achieved in 6 iterations
```

We can compute well as long as. It should be noted that the energy of graphene obtained by this calculation

```
% grep -a "^\\!" graphene.scf.out
```

If it is valid, I can also be seen from the command line.

3.2. bands calculation

Next, calculate the energy of the Kohn-Sham orbitals for k any point by using the charge density as calculated in scf. Please create a file called graphene.nscf.in you have changed only line you highlight the following from graphene.scf.in of using the scf calculation.

```
&control
  calculation = 'bands'
  prefix='graphene',
  tstress = .true.
  tprnfor = .true.
  pseudo_dir = './',
  outdir='./work/'
/
&system
```

```
ibrav = 4,
```

```
celldm(1) = 4.602,
celldm(3) = 4,
nat = 2,
```

```

ntyp = 1,
ecutwfc = 30.0,
ecutrho = 150.0,
occupations = 'smearing'
smearing = 'm-p'
degauss = 0.01
/
&electrons
  mixing_beta = 0.7
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C 12.0107 C.pz-van_ak.upf
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {tpiba_b}
4
0.00000000 0.00000000 0.00000000 20
0.66666667 0.00000000 0.00000000 20
0.50000000 0.28867500 0.00000000 20
0.00000000 0.00000000 0.00000000 20

```

Line 5 of the last, each 20 points on the line $((3, 0, 1/2, 1/2\sqrt{3}))$ of Γ Γ (0,0,0)-K (2/3, 0,0)-M it specifies to compute each. `tpiba_b` represents the use in units of $2\pi/a$ to the coordinates given. In the same place and directory you scf calculating this file

```
% ~/espresso-5.0.2/bin/pw.x < graphene.nscf.in > graphene.nscf.out
```

It is a band calculation end do it with. After, are summarized in the file Kohn-Sham energy of the calculation. Because there is a program `bands.x` its own, I will prepare the input file `graphene.band.in` as follows.

```

&bands
  outdir = './work/',
  prefix='graphene',
  filband='graphene.band',
  lsym=.true.
/

```

In previous ver.4 of espresso, the first line will be `&inputpp` instead of `&bands`.

`bands.x` does not work well with 5.0.2 ver. Please apply the patch to 5.0.3 without fail.

Run the following command using this file.

```
% ~/espresso-5.0.2/bin/bands.x < graphene.band.in > graphene.band.out
```

This file called graphene.band should be able to. This file contains a list of the Kohn-Sham energy is being output for each k for each point as follows.

```
&plot nbnd= 8, nks= 61 /
  0.000000 0.000000 0.000000
-20.113 -8.374 -3.513 -3.513 2.628 4.431 5.452 8.033
  0.033333 0.000000 0.000000
-20.093 -8.349 -3.594 -3.558 2.656 4.458 5.479 8.047
  0.066667 0.000000 0.000000
-20.033 -8.276 -3.827 -3.692 2.738 4.540 5.560 8.088
  0.100000 0.000000 0.000000
-19.933 -8.155 -4.190 -3.911 2.874 4.675 5.695 8.159
  0.133333 0.000000 0.000000
-19.794 -7.986 -4.652 -4.206 3.066 4.864 5.884 8.266
  0.166667 0.000000 0.000000
-19.615 -7.769 -5.186 -4.568 3.312 5.107 6.128 8.410
  0.200000 0.000000 0.000000
-19.396 -7.505 -5.765 -4.988 3.613 5.403 6.426 8.597
  0.233333 0.000000 0.000000
-19.139 -7.195 -6.370 -5.452 3.969 5.751 6.779 8.373
  0.266667 0.000000 0.000000
-18.842 -6.987 -6.841 -5.951 4.379 6.151 7.186 7.640
  0.300000 0.000000 0.000000
-18.508 -7.603 -6.474 -6.443 4.844 6.600 6.882 7.647
...
```

I can make a band diagram to do it by processing it as their favorite this file, but as a program of its own, two programs that plotband.x and band_plot.x are also available. Both the work of similar, I'll try using a band_plot.x here.

```
% ~/espresso-5.0.2/bin/band_plot.x  
  
Number of bands to be plotted:  
  
8  
  
Fermi level (eV):  
  
-0.4661  
  
Name of the bands file (produced by band.x):  
  
graphene.band  
  
Name of the output file:  
  
band.dat
```

And if I answer the questions as described above, the file that is easy to plot (band.dat) is created.

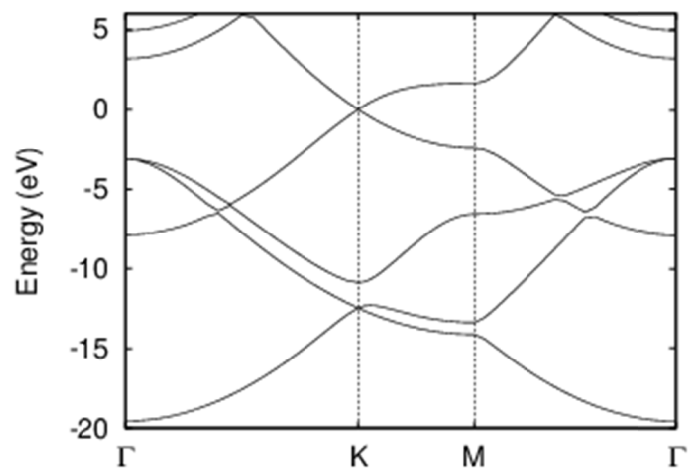
Note:

The Fermi energy has been brought out in graphene.scf.out. However, but because it was speculated that using the k-point discrete only, priority should be given to there if you know and let them use of the energy of the K-point exactly as graphene.

And plot it using a file called band.plt in gnuplot this. I think this (the side that he where there is a style by each person. The reference level to the end.

```
% gnuplot band.plt
```

Now, the following files are generated



3.3 DOS calculation

Now let's ask for the density of states. In a separate directory from the directory that you band calculation, please scf calculation

```
% ~/espresso-5.0.2/bin/pw.x < graphene.scf.in > graphene.scf.out
```

Please create a file called graphene.nscf.in you have changed only line you highlight the following from graphene.scf.in which was then used in the scf calculation.

```
&control
  calculation = 'nscf'
  prefix='graphene',
  tstress = .true.
  tprnfor = .true.
  pseudo_dir = './',
  outdir='./work/'
/
&system
 ibrav = 4,
  celldm(1) = 4.602,
  celldm(3) = 4,
  nat = 2,
  ntyp = 1,
  ecutwfc = 30.0,
  ecutrho = 150.0,
  occupations = 'tetrahedra'
/
&electrons
  mixing_beta = 0.7
  conv_thr = 1.0d-8
/
ATOMIC_SPECIES
C 12.0107 C.pz-van_ak.UPF
ATOMIC_POSITIONS {alat}
C 0.00 0.00 0.00
C 0.00 0.57735026918962576451 0.00
K_POINTS {automatic}
36 36 1 0 0 0
```

The final two lines, it specifies to calculate the k-point mesh of 36x36x1. It reduces the number of k points is calculated using the symmetry in practice. In addition, you specify that you want to use the tetrahedron method as occupations. For more information about the tetrahedron method, please see the About tetrahedron method. It is a technique very useful in carrying out the approximate calculation of the integral in k-space information from the k-point mesh is not limited to first-principles calculations, limited.

Make nscf calculated using this file.

```
% ~/espresso-5.0.2/bin/pw.x < graphene.nscf.in > graphene.nscf.out
```

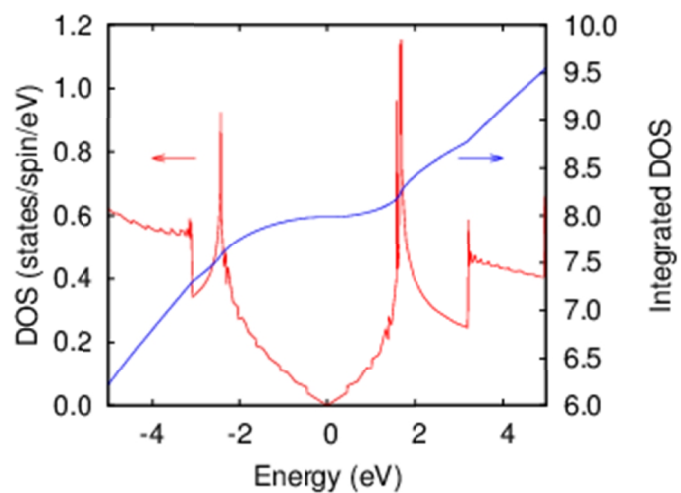
After that, perform the calculation of the DOS together the energy was calculated. As input program dos.x dedicated, I will provide a file graphene.dos.in as follows.

```
&dos
  outdir = './work/',
  prefix='graphene',
  fildos='graphene.dos',
/
```

If you run the dos.x using this file,

```
% ~/espresso-5.0.2/bin/dos.x < graphene.dos.in > graphene.dos.out
```

file called graphene.dos should be able to. This figure is obtained as follows: if the plot as it is.



4. Check of convergence

In this section, we will introduce how to check the calculation whether converge properly

4.1. scf Convergence condition of the loop

First, I'll take a look at the conditions for the convergence of loop scf. Please take a look at the graphene.scf.out.

```
iteration # 1      ecut=    65.00 Ry      beta=0.70
Davidson diagonalization with overlap
ethr = 1.00E-02,  avg # of iterations = 5.3

total cpu time spent up to now is      2.1 secs

total energy          =    -22.83943110 Ry
Harris-Foulkes estimate =    -22.99140928 Ry
estimated scf accuracy <      0.23683536 Ry
```

I can see that the total energy and is calculated once per loop feel like. Scf loop ends when the total energy is obtained with higher accuracy than conv_thr. Once, it would be good to try when loop or end up play around the conv_thr. conv_thr is the balance between computation time and accuracy of what you want to find, but I think conv_thr = 1.d-6 of default as weak as some convergence condition. Because not converge when you tight convergence condition much to the contrary, It is important to note. (There are only about 16 digits of accuracy in the first place is a double-precision real number that is commonly used.)

4.2. The convergence to the cutoff energy

4.3. The convergence for k-point mesh

4.4. Convergence for (degauss) width of Smearing

FAQ

Please refer to the head family also `FAQ <<http://www.quantum-espresso.org/faq/>>` . Below is a based on my personal experience .scf calculation does not convergel considered several causes .

The first is when the structure of the input is wrong is there often . May not converge if there atoms and are isolated interatomic distance , or close abnormally . Please check the structure XCrysdn.

If you do not want to converge repeatedly or smaller estimated scf accuracy may be increased even after repeated loop of scf, try to reduce the mixing_beta. When creating a new charge density in the loop of scf, this value represents the level to maintain the percentage of how much the old charge density . It means that smaller , we will be converged slowly If it is less , but the vibration is less likely to occur .

You may also vibration is likely to occur even if you have set the degauss too small in spite of metal , or alternatively , not specified occupations. on the setting , set the appropriate degauss the occupations = "smearing".

If you do not converge well anyway , as a way to convergence of scf, try the CG method rather than the method of daivdson default. (diagonalization = "cg") calculation is quite slow , but it is to converge in a stable manner .

In any case , I think if the structure itself is not very stable so often when the experience , it is difficult to converge . Computation or a meaningful calculation itself , please try to check carefully

About tetrahedron method

The tetrahedron method is a technique used when determining the integral value of k-space from the physical quantity obtained in the k point on discrete. Specifically, let's look at an example calculation of density of states. Definition of the density of states $D(E)$ is

$$D(E) = \sum_k d(E - e_k)$$

It is given by. However, it becomes a state density unrealistic with only a finite number delta function. You can use this simple formula when on the k-point discrete, ϵ_k is known. To avoid this problem most easily,

$$d : \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(E - e_k)^2}{2\sigma^2}\right)$$

I think that it would be approximated by a Gaussian delta function as. Take fine mesh spacing of k points, it will be a reasonably decent approximation if it does by selecting the appropriate σ to match it fact. (By calculating in accordance with the remains of occupations = 'smearing', the density of states in this way can be obtained. value of degauss is. corresponds to σ), however, such as the van Hove singularity will get dull pretty, band it would be hard to say the value of the gap as well as would look small amount of σ , very clean state density can be obtained. It is a tetrahedron method to avoid this problem.

I consider the one-dimensional system for simplicity first. When ϵ_k is given for k discrete points, the simplest is to interpolate a straight line between the point k as a discrete approximation of ϵ_k for k continuous. Approximate this: math: If you do it by running the integration of $D(E)$ analytically using the ϵ_k , you can obtain D step function as $D(E)$. Using this method, if we finer mesh, and will approach the $D(E)$ ensures faster than when using the Gaussian, and the gap values on a mesh with discrete is reflected as the gap. This is the one-dimensional version of the tetrahedron method.

To extend this method to three-dimensional, it means that you may be a similar linear interpolation in three dimensions on. However, it is not possible to interpolate linear as it is in the cube. So, I'll do I split six tetrahedrons in (tetrahedron) further cube. (This is. Is the origin of the name of the tetrahedron method) Then, within each tetrahedron, linear interpolation is possible. Thus, the interpolated in each tetrahedron the body: you may have to do it by integrating the $D(E)$ analytically using the ϵ_k , density of states by the tetrahedron method is obtained: math.

For more information, please visit and Bloch et al..