First-principles calculation code based on real-space finite-difference method RSPACE

(for electronic structure calculation)

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Graduate School of Engineering, Kobe University

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1 Introduction

In this manual, the basic usage of the "first-principles molecular-dynamics simulation program based on the real-space finite difference method (RSPACE)" developed in the Ono Laboratory, Graduate School of Engineering, Kobe University, is summarized. The examples in this document are explained under the assumption that computers in which Intel Fortran Compiler and Sun Grid Engine are installed are used. When these example calculations are to be performed using other computers described in Section 1.1, or computers other than those listed in Section 1.1, contact the address indicated in Section 1.2.

1.1 Operation confirmed machine models

Operation of this program has been confirmed on the following machine models.
• Fugaku computer
• Ohtaka, ISSP, Univ. Tokyo

1.2 Contact information

When bugs of this program or misprints in this manual are found, contact:

Tomoya Ono
Department of Electrical and Electronic Engineering, Kobe University
1-1, Rokkodai-cho, Nada, Kobe, 657-0851, Japan
e-mail:t.ono@eedept.kobe-u.ac.jp

1.3 License

1.4 Reference

Please use the following references for the electronic-structure calculation method of RSPACE code when results are published.
• K. Hirose, T. Ono, Y. Fujimoto, and S. Tsukamoto, *First-Principles Calculations in Real-Space Formalism, Electronic Configurations and Transport Properties of Nanostructures* (Imperial College, London, 2005).
• T. Ono, M. Heide, N. Atodiresei, P. Baumeister, S. Tsukamoto, and S. Blügel, Phys. Rev. B **82**, 205115 (2010).
In addition, norm-conserving pseudopotentials are used, please cite
• K. Kobayashi, Comput. Mater. Sci. **14**, 72 (1999).

2 Compile of source code

This section introduces the procedure to obtain the code and compile the code. In addition, the pseudopotentials used in RSPACE are explained.

2.1 Copy of source code

Directory RSPACEes taken from https://github.com/onotmy/RSPACEdist or unzipped RSPACEes.zip distributed in workshops is copied on the any directory of the computer. In the directory where the code is expanded, the directories kukan, PAW and NCPS are generated. kukan is the directory storing the source code and PAW and NCPS are those containing pseudopotentials for excise.

2.2 Setup of makefile

For compile of the source code, makefile has to be modified. In the directory kukan, makefile is stored. Initial values are set for computer where Intel Fortran Compiler is installed and the forth line of makefile is as follows.

```
system = xeon
```

When the computer with Intel Fortran Compiler is used, it is not necessary to modify the makefile. The other computers, which are introduced in Chap. 1.1, makefile is modified following Table 1.

Table 1: Setup of makefile. Since ohtaka uses Intel compiler, the same option with PC cluster is available.

Computer	Option
Fugaku	`kei`
PC cluster using Intel compiler	`xeon`
Ohtaka, issp, Univ. Tokyo	`xeon`

2.3 Compile

Input
`make`
in the directory kukan. After the compile is completed, check whether "kukan8", "ele", "dos", "ldos", and "orbcharge" are generated.

2.4 Pseudopotentials

This code uses projector augmented-wave method to describe the interaction between atomic nucleus and electron. For some elements, this code uses the norm-conserving pseudopotential, in which the first line of `paw.***` is "`# ncpp pseudopotential ...`" Note that even if the norm-conserving pseudopotentials are stored, the file names are `paw.***`. In addition, the norm-conserving pseudopotentials which are commented "`# ncpp pseudopotential converted by ncps_convert`" are taken from the norm-conserving pseudopotential database (NCPS97) developed by Dr. Kazuaki Kobayashi of National Institute for Materials Science, Japan. For NCPS97 databases, see
https://www.nims.go.jp/cmsc/staff/kobayak/NCPS/ncps2kplusE.html. The norm-conserving pseudopotentials taken from NCPS97 are not included in the distributed version at the moment. If you need pseudopotentials modified from NCPS97, please e-mail to the contact address.

3 Outline of the electronic structure calculation

In this chapter, the flowchart necessary for the determination of parameters upon the execution of simulations using the "first-principles molecular-dynamics simulation program based on the real-space finite difference method" and the description format unique to this program are summarized. Since the terms and description formats generally used in First-principles calculation are not explained in this manual, refer to other references for explanations of unfamiliar terms and other details.

3.1 Unit

The atomic unit (a.u. or Hartree) system is used in this program. In the atomic unit system, the following definitions are applied.

Electron mass	m	$\rightarrow$	1
Electron charge	e^2	$\rightarrow$	1
Planck's constant	$\hbar$	$\rightarrow$	1
Dielectric constant in vacuum	ε_0	$\rightarrow$	$\frac{1}{4\pi}$

Therefore, the following physical quantities are expressed as follows in the atomic unit system.

Length	1 (a.u.)	$\rightarrow$	5.2918×10^{-11}(m)
Mass	1 (a.u.)	$\rightarrow$	9.1094×10^{-31}(kg)
Time	1 (a.u.)	$\rightarrow$	2.4189×10^{-17} (sec)
Energy	1 (a.u.)	$\rightarrow$	27.212(eV)

3.2 Boundary conditions

In this code, four types of boundary conditions, (i) x, y and z all belong to the periodic system, (ii) x and y belong to the periodic system; z belongs to the isolated system, (iii) x belongs to the periodic system; y and z belong to the isolated system, and (iv) x, y and z all belong to the isolated system, are available. Select an appropriate boundary condition in accordance with the model to be calculated. Ascii input/output data are compatible with all four boundary conditions. Binary input/output data for type (iv) are incompatible with other types because of the lack of an imaginary part in wave functions.

3.3 Flowchart

Figure 1 shows a flowchart of this program. Terms appearing in the figure will be used in the parameter setting; refer to this figure when necessary.

3.4 Expression of parallel processing

This program has been developed with the aim of performing a large-scale calculation at high speed. Accordingly, parallel processing is conducted using plural processors. In this section, the parallelization technique is explained and terms related to the parallelization in this manual are defined.

The current parallel computers can be roughly divided into the following two types.

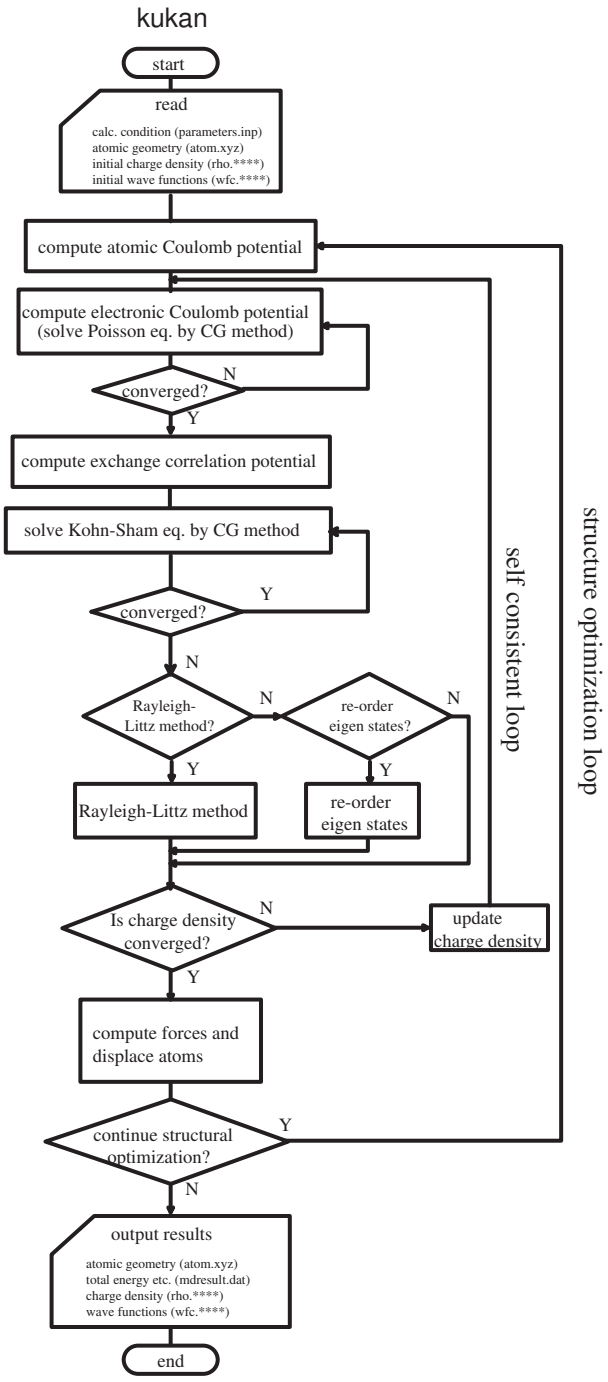

Figure 1: flowchart

1. Process parallelization Computations are divided into plural number of processes. The processes do not share the memory space and execute computation independently. When the process needs to referrer the results in other processes, calculation results are transferred to other processes via the network cables.

2. Thread parallelization One process uses the plural number of cores (threads). The memory space is occupied by each process and shared by threads. When the communications between threads are required, calculation results are transferred in the hardware memory, which is not time consuming. Since the maximum size of the hardware memory and the number of cores belong to the same hardware memory are limited, the computational scale is limited by the hardware memory size and the number of cores.

The current program has been coded so that both types of parallel processing are possible. However, there is a difference in the methods of compilation and execution between the two types of parallel processing. Examples describing execution conditions are shown below.
Process parallelization. $\cdots$ use method **1**.
Thread parallelization. $\cdots$ use method **2.**
Parallelization: use both methods **1** and **2**.
Parallelized by m processes. $\cdots$ use method 1 with m processes.
Parallelized by n threads. $\cdots$ use method **2** with n threads.
Parallelized by n$\times$m $\cdots$ use n threads for 1 process and the number of processes is m. Totally n$\times$m cores are involved for calculation. This type of parallelization is hybrid parallelization.

In this manual, the above examples are applied unless otherwise stated.

4 Simple molecule calculation

First of all, as a simple example, the electronic structure of a CO molecule under the isolated boundary condition using 1$\times$1parallelization.

4.1 Preparation of the directory

First, create an execution directory "$\sim$/CO" under your home directory (which here is indicated by "$\sim$/"), then create "pspaw($\sim$/CO/pspaw)" ' under "$\sim$/CO". Then, copy "kukan8", "parameters.inp", "atom.xyz", and "job.sh" to $\sim$/CO from the directory, where the source codes are compiled. Next, copy the pseudopotential files "paw.006" and "paw.008" for carbon and oxygen, respectively, to $\sim$/CO/pspaw from the PAW directory.

4.2 Preparation of input parameter file "parameters.inp"

Modify parameters.inp in $\sim$/CO as follows. The lines written by red color are those which are often revised. The meanings of the parameters will be explained later.

Example of parameters.inp

```
 1:  &nml_inp_prm_kukan
 2:  nprocx = 1
 3:  nprocy = 1
 4:  nprocz = 1
 5:  xmax = 10.0d0
 6:  ymax = 10.0d0
 7:  zmax = 10.0d0
 8:  nxmax = 30
 9:  nymax = 30
10:  nzmax = 30
11:  neigmx = 8
12:  natom = 2
13:  nperi = 0
14:  eta = 0.2d0
15:  npre = 1
```

```
16:  nspv = 1
17:  /
```

Since there is the possibility that the sample file has been changed depending on the program version, check all the parameters. The meaning of each parameter is listed below.

nproc{x,y,z,k}	For the control of parallel calculations. Refer to Chap. 5. In the calculation described in the present chapter, set all the values to 1.
{x,y,z}max	The range from -(x,y,z)max to +(x,y,z)max is the calculation range. When setting isolated boundary conditions, this calculation range should be set such that all the atomic coordinates determined by "atom.xyz" (refer to Sec. 4.3) maintain a distance of 9-15 (a.u.) from the boundary surface.
n{x,y,z}max	The number of grid points; must be an integer. 2×nxmax is the number of grid points in the x direction, and xmax/nxmax is the grid width "dx". For the grid width setting, refer to Appendix.
neigmx	The number of wave functions to be calculated. Set this parameter to the number of atoms ×4 when transition metals are not included, and to the number of atoms ×9 when transition metals are included.
natom	The number of atoms.
nperi	Setting for boundary conditions. x, y and z all belong to the isolated system: nperi = 0. x belongs to the periodic system; y and z belong to the isolated system:1, x and y belong to the periodic system; z belongs to the isolated system:2, x, y and z all belong to the periodic system:3.
numk {x,y,z}	Th enumber of k point for each direction. Set this parameter to 1 when isolated boundary conditions are applied in all of the x, y and z directions. When the plural number of k points are sampled, list the information of k points after line 33. In addition, numkx is numkx × numky × numkz and the others are 1, in the excise of this text.
nspv	When the effect of spin on the exchange-correlation potential is neglected, nspv=1, and when it is to be considered, nspv=2.
eta	mixing ratio of charge density for the self-consistent field calculation.
looplimit	The maximum number of iterations for the self-consistent field calculation.
tmstep	Time step for structural optimization of atomic geometry.
nmd_end	The number of iterations for structural optimization.
ngdiis	The number of previous structural optimization steps for Pulay method. When this parameters is set at 1, the atomic coordinates are simply updated following force acting on atoms.
npre	Control parameters for initial charge density and wave functions. Read:0, generate:1.

4.3 Preparation of the atomic-coordinates file

Next, create the file "atom.xyz" in which information such as atomic coordinates is described. In the current calculation, the file should be set as follows. The numbers below indicate, from the left, atom's x coordinate, y coordinate, z coordinate, atomic number, x-direction switch of structure optimization, y-direction switch of structure optimization[1], z-direction switch of structure optimization, and mass of the atom [atomic weight × proton mass (1838 a.u.)]. When the structure optimization switch is 0, the atom is not moved in that direction. Initially, set all the switches to 0, because electronic structures alone will be calculated first. When plural atoms are present, add a data line for each atom at the bottom. Accordingly, for N atoms, this file requires N lines.

```
Example of atom.xyz(only the first 3 lines)
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2:   0.5500000000000000D+00  0.5500000000000000D+00  0.5500000000000000D+00 6 0 0 0 22056.00 00 1 1a
3:  -0.5500000000000000D+00 -0.5500000000000000D+00 -0.5500000000000000D+00 8 0 0 0 29408.00 00 1 2a
```

Although the equilibrium interatomic distance of the CO molecule is 2.13∼2.14 (a.u.), this value should be set smaller than the experimental value, because the current calculation aims at obtaining electronic structures and equilibrium interatomic distances using an optimization calculation of atomic structures.

4.4 Visualization of atomic structure

The visualization tools for atomic structures are provided in https://uemoto1.github.io/rsview/. You can check the atomic geometry by pasting "parameters.inp" and "atom.xyz" to the boxes in the page.

4.5 Preparation of job script file

The job script file is prepared to execute the kukan program. Here, we assume that the computer in which the Sun Grid Engine is installed is used. When one uses the other computers, the script file which is suitable for the computer should be prepared.

In this job script, one needs to input the number of cores, which corresponds to $n \times m$ in Sec. 3.4, at the 2nd line and the number of threads per process, which is n in Sec. 3.4, at the 6th line. The number of processes, which is m in Sec. 3.4, is automatically calculated in this script file.

```
Example of job.sh
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 1
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=1
 7:  i=0
 8:  for bbbb in $(cat $USER.$PE.$JOB_ID.2)
 9:  do
10:  i=$(( i+1 ))
11:  done
12:  export I_MPI_PERHOST=$(( NSLOTS/OMP_NUM_THREADS/i ))
13:  export I_MPI_HYDRA_HOST_FILE=hostfile
14:  cut $PE_HOSTFILE -d " " -f 1 > hostfile
15:  mpiexec.hydra ./kukan8
```

4.6 Execute electronic-structure calculation program

To submit s job, one needs to use qsub command.

```
qsub job.sh
```

[1] At the moment, only simple structural optimization is available.

If there are no jobs in queue, “kukan8” is immediately executed. When this program is completed, the files rho.00000, vht.00000, wfc.00000.000, and mdresult.dat are generated.
`cat mdresult.dat`
The contents of “mdresult.dat” are listed below.

```
computed by kukan8f 10/07/2021-01
==========  data from nml_inp_prm_kukan  ==========
ndisp       :          66
catmfn      :atom.xyz
nprocx      :           1
nprocy      :           1
nprocz      :           1
nprock      :           1
xmax        :   10.0000000000000
ymax        :   10.0000000000000
zmax        :   10.0000000000000
nxmax       :          30
nymax       :          30
nzmax       :          30
npxmax      :          -1
npymax      :          -1
npzmax      :          -1
nso         :           0
socang      :    0.000E+00  0.000E+00  0.000E+00
nsym        :           0
neigmx      :           8
natom       :           2
num_atcell  :           2
num_ppcell  :           2
num_ppcell_d:           2
gmaxps      :   20.0000000000000
nperi       :           0
npopshow    :           0
numkx       :           1
numky       :           1
numkz       :           1
ksym        :           0
kband       :           0
cexco       :    vwn
nspv        :           1
epsvh       :  1.000000000000000E-012
epssd       :  1.000000000000000E-006
ratio_diis  :  0.300000000000000
eps_scf     :  1.000000000000000E-006
ncgmin      :           1
ncgmax      :         800
ncgres      :         801
nprecon_cg  :           1
nprecon_diis:           1
nsdmax      :           4
nkscg       :           1
ndiismax    :           4
ncgscf      :         200
nretcg      :        2000
nrrz        :           1
nchange     :           1
eta         :  0.200000000000000
etamag      :  0.2000E-01  0.2000E+01
looplimit   :        1000
nbrydn      :          20
tmstep      :  0.000000000000000E+000
nmd_start   :           0
nmd_end     :           1
ngdiis      :           1
sconst      :  0.000000000000000E+000
biasx       :  0.000000000000000E+000
biasy       :  0.000000000000000E+000
biasz       :  0.000000000000000E+000
tf          :  3.000000000000000E-003
tfmin       :  -300.000000000000
```

```
tfmax       :   300.000000000000
chrgd       :  0.000000000000000E+000
npolcon     :           0
polconocc   :   2.70000000000000
endjel      :  0.000000000000000E+000
chrjel      :  0.000000000000000E+000
fcut        :  1.000000000000000E-005
npre        :           1
nevhist     :           3
northo      :           1
lveffout    : F
eps         :  1.000000000000000E-016
eps_eig_diis:  1.000000000000000E-014
alambda_diis:  0.500000000000000
alambda_min :  0.100000000000000
alambda_max :   1.00000000000000
nradmx      :        1502
nrprjmx     :           6
nprjmx      :          18
lsphel      :           8
nlmax       :           4
lrhomx      :          25
nfiltyp     :           1
psctoff     :   1.05000000000000
nqmx        :         400
psftrad     :   10.0000000000000
psctrat     :   1.00000000000000
psext       :   2.00000000000000
filpp       :  2.000000000000000E-002
rctpcc      :   2.00000000000000
nmesh       :           2
npmesh      :           2
veta        :  0.200000000000000
new_pwx     :           0
new_pwy     :           0
new_pwz     :           0
new_rsx     :           0
new_rsy     :           0
new_rsz     :           0
nint1dmax   :        1000
nf          :           4
nfdg        :           4
nfh         :           4
zs_pre      :  0.500000000000000
pol_pre     :   1.50000000000000
=====================================================
Filtering of pseudopotentials is implemented by Fermi distribution.
Filtering of pseudopotentials is implemented by Fermi distribution.
npxmax, npymax, and npzmax are updated below.
==========  data computed by listvecdim  ==========
npxmax      :           8
npymax      :           8
npzmax      :           8
=====================================================
cell size [lx,ly,lz (a.u.)]
  0.200000000D+02   0.200000000D+02   0.200000000D+02
coarse grid spacing [hx,hy,hz (a.u.)]
  0.333333333D+00   0.333333333D+00   0.333333333D+00
dense grid spacing [hx,hy,hz (a.u.)]
  0.166666667D+00   0.166666667D+00   0.166666667D+00
cutoff energy of wave functions [gmax_coarse,gmax_dense (Ry)]
  0.888264396D+02   0.355305758D+03
number of electron       charge         spin
  0.100000000D+02   0.000000000D+00   0.100000000D+01
electric field [ex,ey,ez (a.u./a.u.)]
  0.000000000D+00   0.000000000D+00   0.000000000D+00
time step (a.u.)  (fs)
  0.000000000D+00   0.000000000D+00
thermo (k)    kt (a.u.)
  0.947268709D+03   0.300000000D-02
cufoff of force acting on atoms (a.u.)
  0.100000000D-04
```

```
 charge mixing ratio of scf
   0.200000000D+00
 Wavefunctions & electron density are generated automatically.
 total charge   10.0000000000000      (electrons)
 fermi level -0.146484375000000      (hartree)
 atomic charge(electrons)
           1   3.96705399526238
           2   6.03294602603470

   k,spin,  band ,     eigen value    ,    residual norm  ,    occupation
   1    1      1    -0.1146279824E+01    0.1681287489E-03    0.1000000000E+01
   1    1      2    -0.5206011957E+00    0.9081387779E-04    0.1000000000E+01
   1    1      3    -0.4881479723E+00    0.7834659643E-05    0.1000000000E+01
   1    1      4    -0.4881479722E+00    0.7834809456E-05    0.1000000000E+01
   1    1      5    -0.3228845234E+00    0.9546005133E-04    0.1000000000E+01
   1    1      6    -0.3492088515E-01    0.3120994796E-02    0.7071811229E-16
   1    1      7    -0.3492088510E-01    0.3120994834E-02    0.7071811099E-16
   1    1      8     0.2411643271E-01    0.4101883778E-01    0.2009109160E-24
Scf=  19   dp=    0.7195235888D-06
    one electron energy       -5.93212297431056      (hartree)
 exchange correlation energy  -5.93119093855571      (hartree)
    hartree       energy      -29.8581863228309      (hartree)
    ewald         energy       12.5967331459555      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -29.1247670897417      (hartree)
    Total         energy      -29.1247670897417      (hartree)
 atomic force
    1   0.2582586348585816D+00   0.2582586348586007D+00   0.2582586348207829D+00
    2  -0.2582586348585816D+00  -0.2582586348586007D+00  -0.2582586348207829D+00
 mdstep=           1
 atom coordinate (input)
   0.5500000000000000D+00   0.5500000000000000D+00   0.5500000000000000D+00   6   0   0   0  22056.00   11  1    1a
  -0.5500000000000000D+00  -0.5500000000000000D+00  -0.5500000000000000D+00   8   0   0   0  29408.00   11  1    2a
 atom coordinate (output)
   0.5500000000000000D+00   0.5500000000000000D+00   0.5500000000000000D+00   6   0   0   0  22056.00   11  1    1a
  -0.5500000000000000D+00  -0.5500000000000000D+00  -0.5500000000000000D+00   8   0   0   0  29408.00   11  1    2a
 real time   511.450775861740      (sec)
 com. time  8.787584304809570E-002 (sec)
 com. vol.  0.000000000000000E+000 (byte)
```

If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful. The order of the calculation is affected by the compiler, the quantities more than 10 digits might not correspond to the above contents.

5 Parallalization of calculation

As described in Sec. 3.4, there are two types of parallelization: parallelization only within one node, and parallelization using plural nodes. In this chapter, both types of parallelization are introduced. The solution to the example problem in this chapter is identical to that in Chap. 4. However, due to an alteration of the computation sequence due to parallelization, some of the computation results in this chapter may be slightly different from those in Chap. 4.

5.1 Thread parallelization by 4×1

First, parallelization processing is performed within a single node. "parameters.inp", "atom.xyz" files are the same as those in Chap. 4. The job script file "job.sh" is different. The following is the example of the creation of "job.sh". Revisions from Chap. 4 are shown by red characters.

Example of job.sh

```
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 4
 4:  #$ -cwd
```

```
 5:  #$ -V
 6:  export OMP_NUM_THREADS=4
 7:  i=0
 8:  for bbbb in $(cat $USER.$PE.$JOB_ID.2)
 9:  do
10:  i=$(( i+1 ))
11:  done
12:  export I_MPI_PERHOST=$(( NSLOTS/OMP_NUM_THREADS/i ))
13:  export I_MPI_HYDRA_HOST_FILE=hostfile
14:  cut $PE_HOSTFILE -d " " -f 1 > hostfile
15:  mpiexec.hydra ./kukan8
```

In the computer we assume to use here, the submission command of the job is identical to that in Chap. 4. However, since the parallelization requires much computer resources, the submission command is not identical to the job using single core. For the detail, refer the instruction of the computer which one uses. The calculation result can be found in mdresult.dat. If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful. In addition, confirm that "real time '' , which is 3rd line from the bottom, in mdresult.dat decreases from that in Chap. 4 due to the parallelization.

5.2 Process parallelization by 1×8

Parallelization processing by generating 8 processes within one node is explained. "atom.xyz" is identical to that in Chap. 4. Now, the parameters for the parallelization in "parameters.inp" are revised as follows:

```
Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  xmax = 10.0d0
 6:  ymax = 10.0d0
 7:  zmax = 10.0d0
 8:  nxmax = 30
 9:  nymax = 30
10:  nzmax = 30
11:  neigmx = 8
12:  natom = 2
13:  nperi = 0
14:  eta = 0.2d0
15:  npre = 1
16:  nspv = 1
17:  /
```

Here, we assume that the computational region is divided into 2 parts in x, y, and z direction, yielding 8 sub regions, and 1 process is assigned for each sub region. Be careful that the number of grids in one direction should be divided by the number of processes in the direction ($2\times$`nxmax`/`nprocx` must be integer.). The revision from that in Chap. 4 is expressed by red characters.

The sample of the job script "job.sh" is also provided. The revision from Chap. 4 is represented by red characters.

```
Example of job.sh
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 8
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=1
 7:  i=0
 8:  for bbbb in $(cat $USER.$PE.$JOB_ID.2)
 9:  do
10:  i=$(( i+1 ))
11:  done
12:  export I_MPI_PERHOST=$(( NSLOTS/OMP_NUM_THREADS/i ))
13:  export I_MPI_HYDRA_HOST_FILE=hostfile
14:  cut $PE_HOSTFILE -d " " -f 1 > hostfile
15:  mpiexec.hydra ./kukan8
```

The submission procedure of jobs and the confirmation method of the calculation result are the same with those in Sec. 5.1.

5.3 Hybrid parallelization by 4×8

The parallelization method by 4×8 is introduced. "parameters.inp" and "atom.xyz" are the same with those in Sec. 5.1, whereas "job.sh" is not the same. The following is an example of the creation of "job.sh", in which the revisions from Sec. 4 are expressed by red characters.

```
Example of job.sh
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 32
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=4
 7:  i=0
 8:  for bbbb in $(cat $USER.$PE.$JOB_ID.2)
 9:  do
10:  i=$(( i+1 ))
11:  done
12:  export I_MPI_PERHOST=$(( NSLOTS/OMP_NUM_THREADS/i ))
13:  export I_MPI_HYDRA_HOST_FILE=hostfile
14:  cut $PE_HOSTFILE -d " " -f 1 > hostfile
15:  mpiexec.hydra ./kukan8
```

The submission procedure of jobs and the confirmation method of the calculation result are the same with those in Sec. 5.1.

6 Atomic structure optimization

6.1 preparation of parameters files

"parameters.inp" and "atom.xyz" have to be revised for the atomic structure optimization. Following is an example of the creation of "parameters.inp". Revisions from Sec. 5.3 are shown by red characters.

```
Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  xmax = 10.0d0
 6:  ymax = 10.0d0
 7:  zmax = 10.0d0
 8:  nxmax = 30
 9:  nymax = 30
10:  nzmax = 30
11:  neigmx = 8
12:  natom = 2
13:  nperi = 0
14:  eta = 0.2d0
15:  npre = 1
16:  nspv = 1
17:  tmstep = 80.0d0
18:  nmd_end = 20
19:  /
```

Next, an example of the creation of "atom.xyz" is shown. Here, since the position of atoms are optimized for all the direction, the flags for all the directions are set to be 1.

```
Example of atom.xyz(only the first 3 lines)
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2: 0.55000000000000000D+00  0.55000000000000000D+00  0.55000000000000000D+00 6 1 1 1 22056.00 00 1 1a
3:-0.55000000000000000D+00 -0.55000000000000000D+00 -0.55000000000000000D+00 8 1 1 1 29408.00 00 1 2a
```

6.2 Execution of kukan8

After the revision of the parameter files, the electronic structure calculation can be executed. The execution of "kukan8" can be achieved by submitting "job.sh", which is used in Sec. 5.3.

After "kukan8" is executed, the total energy and atomic structure for each structural optimization step are output in mdresult.dat. If the total energy is *ca* -29.1705565(a.u.) and the inter atomic distance calculated from atomic coordinate (output) is *ca* 2.14(a.u.) at the last step of the structural optimization, mdstep=20, then the calculation is successful.

7 Electronic structure calculation for spin-polarized system

Most atoms, ions, O_2 molecules and S_2 molecules show spin polarization, therefore, they should be handled with a calculation that takes the spin into consideration. Here, a method is explained, using an electronic structure calculation of O_2 molecules as an example.

7.1 Preparation of directory

In the similar manner for Chap. 4, the preparation of the directory and copy of the execution files are carried out. In the pspaw directory, "paw.008", which is for oxygen atom, is copied.

7.2 Preparation of parameter files

"parameters.inp" and "atom.xyz" have to be revised to calculate an O_2 molecule. The following is an example of the creation of "parameters.inp". Revisions from Sec. 5.3 are shown by red characters.

```
Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  xmax = 10.0d0
 6:  ymax = 10.0d0
 7:  zmax = 10.0d0
 8:  nxmax = 30
 9:  nymax = 30
10:  nzmax = 30
11:  neigmx = 8
12:  natom = 2
13:  nperi = 0
14:  eta = 0.2d0
15:  npre = 1
16:  nspv = 2
17:  pol_pre = 2.5d0
18:  /
```

Then, an example of the creation of "atom.xyz" is described.

```
Example of atom.xyz(only the first 3 lines)
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2: 0.11000000000000000D+01 0.00000000000000000D+00 0.00000000000000000D+00 8 1 1 1 29408.00 00 1 1a
3:-0.11000000000000000D+01 0.00000000000000000D+00 0.00000000000000000D+00 8 1 1 1 29408.00 00 1 2a
```

7.3 Execution of kukan8

After the revision of the parameter files, the electronic structure calculation can be executed. The execution of "kukan8" can be achieved by submitting "job.sh", which is used in Sec. 5.3.

7.4 Confirmation of calculated result

After "kukan8" is executed, the total energy and atomic structure for each structural optimization step are output in mdresult.dat. The following is the contents of mdresult.dat.

```
 computed by kukan8f 10/07/2021-01
 ==========  data from nml_inp_prm_kukan  ==========
 ndisp       :          66
 catmfn      :atom.xyz
 nprocx      :           2
 nprocy      :           2
 nprocz      :           2
 nprock      :           1
 xmax        :   10.0000000000000
```

```
ymax         :   10.0000000000000
zmax         :   10.0000000000000
nxmax        :           30
nymax        :           30
nzmax        :           30
npxmax       :           -1
npymax       :           -1
npzmax       :           -1
nso          :            0
socang       :    0.000E+00  0.000E+00  0.000E+00
nsym         :            0
neigmx       :            8
natom        :            2
num_atcell   :            2
num_ppcell   :            2
num_ppcell_d:            2
gmaxps       :   20.0000000000000
nperi        :            0
npopshow     :            0
numkx        :            1
numky        :            1
numkz        :            1
ksym         :            0
kband        :            0
cexco        :    vwn
nspv         :            2
epsvh        :  1.000000000000000E-012
epssd        :  1.000000000000000E-006
ratio_diis   :  0.300000000000000
eps_scf      :  1.000000000000000E-006
ncgmin       :            1
ncgmax       :          800
ncgres       :          801
nprecon_cg   :            1
nprecon_diis:            1
nsdmax       :            4
nkscg        :            1
ndiismax     :            4
ncgscf       :          200
nretcg       :         2000
nrrz         :            1
nchange      :            1
eta          :  0.200000000000000
etamag       :  0.2000E-01  0.2000E+01
looplimit    :         1000
nbrydn       :           20
tmstep       :  0.000000000000000E+000
nmd_start    :            0
nmd_end      :            1
ngdiis       :            1
sconst       :  0.000000000000000E+000
biasx        :  0.000000000000000E+000
biasy        :  0.000000000000000E+000
biasz        :  0.000000000000000E+000
tf           :  3.000000000000000E-003
tfmin        :  -300.000000000000
tfmax        :   300.000000000000
chrgd        :  0.000000000000000E+000
npolcon      :            0
polconocc    :   2.70000000000000
endjel       :  0.000000000000000E+000
chrjel       :  0.000000000000000E+000
fcut         :  1.000000000000000E-005
npre         :            1
nevhist      :            3
northo       :            1
lveffout     : F
eps          :  1.000000000000000E-016
eps_eig_diis:  1.000000000000000E-014
alambda_diis:  0.500000000000000
alambda_min :  0.100000000000000
alambda_max :   1.00000000000000
```

```
nradmx      :        1502
nrprjmx     :           6
nprjmx      :          18
lsphel      :           8
nlmax       :           4
lrhomx      :          25
nfiltyp     :           1
psctoff     :   1.05000000000000
nqmx        :         400
psftrad     :   10.0000000000000
psctrat     :   1.00000000000000
psext       :   2.00000000000000
filpp       :  2.000000000000000E-002
rctpcc      :   2.00000000000000
nmesh       :           2
npmesh      :           2
veta        :  0.200000000000000
new_pwx     :           0
new_pwy     :           0
new_pwz     :           0
new_rsx     :           0
new_rsy     :           0
new_rsz     :           0
nint1dmax   :        1000
nf          :           4
nfdg        :           4
nfh         :           4
zs_pre      :  0.500000000000000
pol_pre     :   2.50000000000000
================================================
Filtering of pseudopotentials is implemented by Fermi distribution.
npxmax, npymax, and npzmax are updated below.
==========  data computed by listvecdim  ==========
npxmax      :           8
npymax      :           8
npzmax      :           8
================================================
cell size [lx,ly,lz (a.u.)]
  0.200000000D+02   0.200000000D+02   0.200000000D+02
coarse grid spacing [hx,hy,hz (a.u.)]
  0.333333333D+00   0.333333333D+00   0.333333333D+00
dense grid spacing [hx,hy,hz (a.u.)]
  0.166666667D+00   0.166666667D+00   0.166666667D+00
cutoff energy of wave functions [gmax_coarse,gmax_dense (Ry)]
  0.888264396D+02   0.355305758D+03
number of electron       charge         spin
  0.120000000D+02   0.000000000D+00   0.200000000D+01
electric field [ex,ey,ez (a.u./a.u.)]
  0.000000000D+00   0.000000000D+00   0.000000000D+00
time step (a.u.)  (fs)
  0.000000000D+00   0.000000000D+00
thermo (k)    kt (a.u.)
  0.947268709D+03   0.300000000D-02
cufoff of force acting on atoms (a.u.)
  0.100000000D-04
charge mixing ratio of scf
  0.200000000D+00
mag. mix. rat., weight of mag. in F_broyd
  0.200000000D-01   0.200000000D+01
Wavefunctions & electron density are generated automatically.
total charge   12.0000000000000      (electrons)
fermi level -0.200965734984493      (hartree)
spin polarization   1.99998396976344      (\mu_B)
atomic charge(electrons)
          1   6.00004021338838
          2   5.99995931855053

  k,spin,  band ,     eigen value    ,    residual norm  ,    occupation
  1    1      1    -0.1254558746E+01    0.5590606172E-05    0.1000000000E+01
  1    1      2    -0.7390836051E+00    0.1294065611E-04    0.1000000000E+01
  1    1      3    -0.5193703883E+00    0.7873743224E-05    0.1000000000E+01
  1    1      4    -0.5193703484E+00    0.7874100050E-05    0.1000000000E+01
```

```
   1    1      5    -0.5132127947E+00    0.1428824583E-04    0.1000000000E+01
   1    1      6    -0.2382477208E+00    0.1192830194E-04    0.9999959925E+00
   1    1      7    -0.2382476806E+00    0.1191613510E-04    0.9999959924E+00
   1    1      8     0.3152630366E-01    0.3053279321E-01    0.2204601893E-33
   1    2      1    -0.1208810858E+01    0.5126299216E-05    0.1000000000E+01
   1    2      2    -0.6768262849E+00    0.7934150386E-05    0.1000000000E+01
   1    2      3    -0.4707029973E+00    0.1238054324E-04    0.1000000000E+01
   1    2      4    -0.4570515823E+00    0.6177505055E-05    0.1000000000E+01
   1    2      5    -0.4570515778E+00    0.6175992292E-05    0.1000000000E+01
   1    2      6    -0.1636837748E+00    0.1597780821E-04    0.4007575659E-05
   1    2      7    -0.1636837634E+00    0.1603078993E-04    0.4007560499E-05
   1    2      8     0.2068322922E-01    0.3022580374E-01    0.8185137418E-32
Scf=  56   dp=    0.7707854778D-06
    one electron energy       -7.29253398590822      (hartree)
 exchange correlation energy  -6.53042635624750      (hartree)
    hartree       energy      -43.0469428896086      (hartree)
    ewald         energy       16.3636363636364      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -40.5062675138589      (hartree)
    Total         energy      -40.5062668681279      (hartree)
 atomic force
    1   0.7857619123930881D-01   0.2595831478657828D-06   0.6006352215592869D-07
    2  -0.7857619123930881D-01  -0.2595831478657828D-06  -0.6006352215592869D-07
 mdstep=           1
 atom coordinate (input)
   0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00   11  1    1a
  -0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00   11  1    2a
 atom coordinate (output)
   0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00   11  1    1a
  -0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00   11  1    2a
 real time   92.2596390247345      (sec)
 com. time   29.5566251277924      (sec)
 com. vol.   44391988224.0000      (byte)
```

If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful.

For the atomic structure optimization, the procedure is the same with that in Chap. 6.

8 Calculate electronic structure of crystal or surface

Calculations performed up to Chap. 5 are the calculations to obtain electronic structures of isolated clusters. In Chap. 8, a calculation method for crystals and surfaces having a periodic structure is explained.

8.1 Supercell

For the calculation of crystals and surfaces having a periodic structure, a supercell, in which one period of the crystal or surface is equivalent to one unit, is used. As an example, a single layer of a thin film in which atoms are aligned regularly, as shown in Fig. 2, is considered. In this figure, a white circle indicates an atom. The thin film has a periodic structure with a minimum unit of the square shown at the center in Fig. 2. In this case, results can be obtained by calculations within only this square, without the need to perform calculations for all atoms. Here, note that the number of atoms involved in the calculation is 2, not 5, because atoms B, C and D are copies of atom A when atom A is taken to be at the center. This is easily understood when we see that atom A is superimposed with atoms B, C and D upon parallel shifting of the supercell in the up, down, left or right direction by one period. Thus, there are many cases in which the number of atoms to be calculated is smaller than it seems when using a supercell.

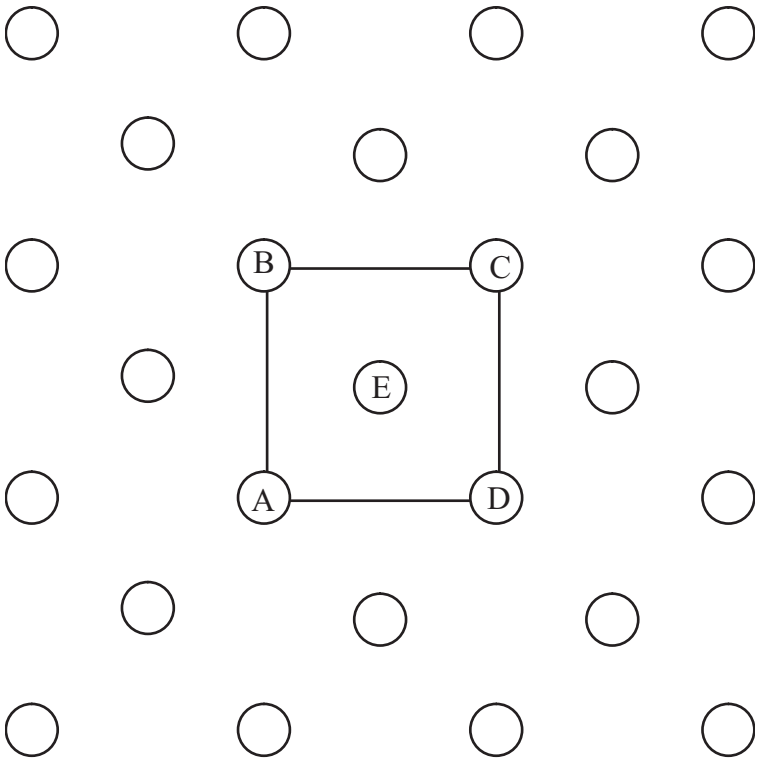

Figure 2: Supercell

When making a model, take care to avoid superimposition of atoms by parallel shifting of a supercell by one period.

8.2 Electronic structure calculation of Li bulk

The atomic structure of crystals are periodic in x, y, and z directions. Therefore, `nperi` in "parameters.inp", which determines the boundary condition, should be `3`. Similar to Chap. 4, the preparation of the directory and copy of the execution files are carried out. In the pspaw directory, "paw.003", which is for lithium atom, is copied.

First, "parameters.inp" is revised as follows:

```
Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  xmax = 3.32d0
 3:  ymax = 3.32d0
 4:  zmax = 3.32d0
 5:  nxmax = 10
 6:  nymax = 10
 7:  nzmax = 10
 8:  neigmx = 8
 9:  natom = 2
10:  nperi = 3
11:  eta = 0.2d0
12:  npre = 1
13:  nspv = 1
14:  /
```

Since a lattice constant of lithium bulk is 6.64 (a.u.), `{x,y,z}max` are set to be `3.32`,so that 2×`{x,y,z}max` is 6.64 (a.u.). Next, "atom.xyz" is revised as follows:

```
Example of atom.xyz(only the first 3 lines)
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2:0.33200000000000000D+01 0.33200000000000000D+01 0.33200000000000000D+01 3 0 0 0 12866.00 00 1 1a
3:0.00000000000000000D+00 0.00000000000000000D+00 0.00000000000000000D+00 3 0 0 0 12866.00 00 1 2a
```

As introduced in Sec. 8.1, lithium forms body centered cubic, the number of atoms in the smallest cubic cell is 2. Thus, "atom.xyz" is expressed as shown above. Here, although the plus or minus sign of the atomic coordinate of the 1st atom does not matter, the electronic structure

calculation code automatically changes to plus and output the changed one to mdresult.dat. Note that in the case of periodic boundary condition, the electronic structure calculation code shift the atomic geometry so that the atoms exist at `-xmax+dx/2` $\leq$ `x` $\leq$ `+xmax+dx/2`. The execution of "kukan8" can be achieved by submitting "job.sh", which is used in Sec. 5.1. The contents of mdresult.dat are shown below. If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful.

```
computed by kukan8f 10/07/2021-01
==========  data from nml_inp_prm_kukan  ==========
ndisp       :          66
catmfn      :atom.xyz
nprocx      :           2
nprocy      :           2
nprocz      :           2
nprock      :           1
xmax        :   3.32000000000000
ymax        :   3.32000000000000
zmax        :   3.32000000000000
nxmax       :          10
nymax       :          10
nzmax       :          10
npxmax      :          -1
npymax      :          -1
npzmax      :          -1
nso         :           0
socang      :    0.000E+00  0.000E+00  0.000E+00
nsym        :           0
neigmx      :           8
natom       :           2
num_atcell  :           2
num_ppcell  :           2
num_ppcell_d:           2
gmaxps      :   20.0000000000000
nperi       :           3
npopshow    :           0
numkx       :           1
numky       :           1
numkz       :           1
ksym        :           0
kband       :           0
cexco       :    vwn
nspv        :           1
epsvh       :  1.000000000000000E-012
epssd       :  1.000000000000000E-006
ratio_diis  :  0.300000000000000
eps_scf     :  1.000000000000000E-006
ncgmin      :           1
ncgmax      :         800
ncgres      :         801
nprecon_cg  :           1
nprecon_diis:           1
nsdmax      :           4
nkscg       :           1
ndiismax    :           4
ncgscf      :         200
nretcg      :        2000
nrrz        :           1
nchange     :           1
eta         :  0.200000000000000
etamag      :  0.2000E-01  0.2000E+01
looplimit   :        1000
nbrydn      :          20
tmstep      :  0.000000000000000E+000
nmd_start   :           0
nmd_end     :           1
ngdiis      :           1
sconst      :  0.000000000000000E+000
biasx       :  0.000000000000000E+000
biasy       :  0.000000000000000E+000
biasz       :  0.000000000000000E+000
tf          :  3.000000000000000E-003
```

```
tfmin       :  -300.000000000000
tfmax       :   300.000000000000
chrgd       :  0.000000000000000E+000
npolcon     :           0
polconocc   :   2.70000000000000
endjel      :  0.000000000000000E+000
chrjel      :  0.000000000000000E+000
fcut        :  1.000000000000000E-005
npre        :           1
nevhist     :           3
northo      :           1
lveffout    : F
eps         :  1.000000000000000E-016
eps_eig_diis:  1.000000000000000E-014
alambda_diis:  0.500000000000000
alambda_min :  0.100000000000000
alambda_max :   1.00000000000000
nradmx      :        1502
nrprjmx     :           6
nprjmx      :          18
lsphel      :           8
nlmax       :           4
lrhomx      :          25
nfiltyp     :           1
psctoff     :   1.05000000000000
nqmx        :         400
psftrad     :   10.0000000000000
psctrat     :   1.00000000000000
psext       :   2.00000000000000
filpp       :  2.000000000000000E-002
rctpcc      :   2.00000000000000
nmesh       :           2
npmesh      :           2
veta        :  0.200000000000000
new_pwx     :          11
new_pwy     :          11
new_pwz     :          11
new_rsx     :          11
new_rsy     :          11
new_rsz     :          11
nint1dmax   :        1000
nf          :           4
nfdg        :           4
nfh         :           4
zs_pre      :  0.500000000000000
pol_pre     :   1.50000000000000
==================================================
Filtering of pseudopotentials is implemented by Fermi distribution.
npxmax, npymax, and npzmax are updated below.
==========  data computed by listvecdim  ==========
npxmax      :          13
npymax      :          13
npzmax      :          13
==================================================
cell size [lx,ly,lz (a.u.)]
  0.664000000D+01   0.664000000D+01   0.664000000D+01
coarse grid spacing [hx,hy,hz (a.u.)]
  0.332000000D+00   0.332000000D+00   0.332000000D+00
dense grid spacing [hx,hy,hz (a.u.)]
  0.166000000D+00   0.166000000D+00   0.166000000D+00
cutoff energy of wave functions [gmax_coarse,gmax_dense (Ry)]
  0.895413376D+02   0.358165351D+03
sample k point [skx,sky,skz (2pi/l)]  weight
  0.000000000D+00   0.000000000D+00   0.000000000D+00     1
number of electron       charge         spin
  0.200000000D+01   0.000000000D+00   0.100000000D+01
electric field [ex,ey,ez (a.u./a.u.)]
  0.000000000D+00   0.000000000D+00   0.000000000D+00
time step (a.u.)  (fs)
  0.000000000D+00   0.000000000D+00
thermo (k)    kt (a.u.)
  0.947268709D+03   0.300000000D-02
```

```
 cufoff of force acting on atoms (a.u.)
   0.100000000D-04
 charge mixing ratio of scf
   0.200000000D+00
 Wavefunctions & electron density are generated automatically.
 total charge   2.00000000000000      (electrons)
 fermi level  0.000000000000000E+000 (hartree)

   k,spin,  band ,     eigen value    ,    residual norm  ,    occupation
   1    1      1    -0.1167088071E+00    0.2221946831E-04    0.1000000000E+01
   1    1      2     0.2003278374E+00    0.1977575511E-05    0.9990223598E-29
   1    1      3     0.2003278374E+00    0.1977592983E-05    0.9990223584E-29
   1    1      4     0.2003278374E+00    0.1977562067E-05    0.9990223584E-29
   1    1      5     0.4749742779E+00    0.2674800751E-03    0.0000000000E+00
   1    1      6     0.5117627206E+00    0.7047456468E-05    0.0000000000E+00
   1    1      7     0.5117627206E+00    0.7047539705E-05    0.0000000000E+00
   1    1      8     0.5117627206E+00    0.7047510236E-05    0.0000000000E+00
Scf=  14   dp=    0.5914206410D-06
    one electron energy      -0.233417614152484      (hartree)
 exchange correlation energy  -2.94987040832271      (hartree)
    hartree       energy     -2.729458074090454E-003 (hartree)
    ewald         energy     -0.548077326733232      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
  energy offset of ps. pot.  -8.985135182183986E-004 (hartree)
  energy jellium/ions         0.000000000000000E+000 (hartree)
   helmholtz free energy      -3.73499332080073      (hartree)
    Total         energy      -3.73499332080073      (hartree)
 atomic force
    1  -0.1647987302177967D-16  -0.4857225732735060D-16  -0.3469446951953614D-17
    2   0.1647987302177967D-16   0.4857225732735060D-16   0.3469446951953614D-17
 mdstep=           1
 atom coordinate (input)
   0.3320000000000000D+01   0.3320000000000000D+01   0.3320000000000000D+01   3   0   0   0  22056.00   00  1    1a
   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  29408.00   00  1    2a
 atom coordinate (output)
   0.3320000000000000D+01   0.3320000000000000D+01   0.3320000000000000D+01   3   0   0   0  22056.00   00  1    1a
   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  29408.00   00  1    2a
 real time   2.73188090324402      (sec)
 com. time  0.337303638458252      (sec)
 com. vol.   734042112.000000      (byte)
```

8.3 Electronic structure calculation of Li surface

Next, the electronic structure of the lithium surface is calculated. No first-principles electronic structure calculation methods for an object such as a surface, in which one side of the plane-vertical direction is a vacuum and the other side is an infinite continuation of crystal, have yet been practically established. Therefore, in the calculation of surfaces, a thin film in which multiple atomic layers are accumulated is considered to be a surface. Here, the electronic structure calculation of a 4-atomic-layer thin film of lithium (001) is performed. A thin film has periodicity in x and y directions. This, the parameter for the boundary condition `nperi` in "parameters.inp" is 2. Similar to Sec. 8.2, the preparation of the directory and copy of the execution files are carried out. Then, in the similar manner with that in Sec. 8.2, revise "parameters.inp" and "atom.xyz" as follows:

```
    Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  xmax = 3.32d0
 3:  ymax = 3.32d0
 4:  zmax =13.28d0
 5:  nxmax = 10
 6:  nymax = 10
 7:  nzmax = 40
 8:  neigmx = 16
 9:  natom = 4
10:  nperi = 2
11:  eta = 0.2d0
12:  npre = 1
13:  nspv = 1
14:  /
```

Revisions from Sec. 8.2 are shown by red characters. Since lattice constant of lithium bulk is 6.64 (a.u.), {x,y,z }max are set to be 3.32 so that 2×{x,y,z }max is 6.64 (a.u.). In addition, zmax, which is the direction without periodicity, is taken to be enough large so as to keep the distance between atoms and boundary planes. Moreover, the number of atoms in the supercell is 4 because the number of atomic layers is 4.

```
    Example of atom.xyz (only first 5 lines)
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2:  0.33200000000000000D+01 0.33200000000000000D+01 -0.49800000000000000D+01 3 0 0 0 12866.00 00 1 1a
3:  0.00000000000000000D+00 0.00000000000000000D+00 -0.16600000000000000D+01 3 0 0 0 12866.00 00 1 2a
4:  0.33200000000000000D+01 0.33200000000000000D+01  0.16600000000000000D+01 3 0 0 0 12866.00 00 1 3a
5:  0.00000000000000000D+00 0.00000000000000000D+00  0.49800000000000000D+01 3 0 0 0 12866.00 00 1 4a
```

The execution of "kukan8" can be achieved by submitting "job.sh", which is used in Sec. 5.1. The contents of mdresult.dat are shown below. If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful.

```
computed by kukan8f 10/07/2021-01
==========  data from nml_inp_prm_kukan  ==========
ndisp       :          66
catmfn      :atom.xyz
nprocx      :           1
nprocy      :           1
nprocz      :           1
nprock      :           1
xmax        :   3.32000000000000
ymax        :   3.32000000000000
zmax        :   13.2800000000000
nxmax       :          10
nymax       :          10
nzmax       :          40
npxmax      :          -1
npymax      :          -1
npzmax      :          -1
nso         :           0
socang      :    0.000E+00  0.000E+00  0.000E+00
nsym        :           0
neigmx      :          16
natom       :           4
num_atcell  :           4
num_ppcell  :           4
num_ppcell_d:           4
gmaxps      :   20.0000000000000
nperi       :           2
npopshow    :           0
numkx       :           1
numky       :           1
numkz       :           1
ksym        :           0
kband       :           0
cexco       :    vwn
nspv        :           1
epsvh       :  1.000000000000000E-012
epssd       :  1.000000000000000E-006
ratio_diis  :  0.300000000000000
eps_scf     :  1.000000000000000E-006
ncgmin      :           1
ncgmax      :         800
ncgres      :         801
nprecon_cg  :           1
nprecon_diis:           1
nsdmax      :           4
nkscg       :           1
ndiismax    :           4
ncgscf      :         200
nretcg      :        2000
nrrz        :           1
nchange     :           1
eta         :  0.200000000000000
etamag      :  0.2000E-01  0.2000E+01
looplimit   :        1000
```

```
nbrydn      :          20
tmstep      :  0.000000000000000E+000
nmd_start   :           0
nmd_end     :           1
ngdiis      :           1
sconst      :  0.000000000000000E+000
biasx       :  0.000000000000000E+000
biasy       :  0.000000000000000E+000
biasz       :  0.000000000000000E+000
tf          :  3.000000000000000E-003
tfmin       :  -300.000000000000
tfmax       :   300.000000000000
chrgd       :  0.000000000000000E+000
npolcon     :           0
polconocc   :   2.70000000000000
endjel      :  0.000000000000000E+000
chrjel      :  0.000000000000000E+000
fcut        :  1.000000000000000E-005
npre        :           1
nevhist     :           3
northo      :           1
lveffout    : F
eps         :  1.000000000000000E-016
eps_eig_diis:  1.000000000000000E-014
alambda_diis:  0.500000000000000
alambda_min :  0.100000000000000
alambda_max :   1.00000000000000
nradmx      :        1502
nrprjmx     :           6
nprjmx      :          18
lsphel      :           8
nlmax       :           4
lrhomx      :          25
nfiltyp     :           1
psctoff     :   1.05000000000000
nqmx        :         400
psftrad     :   10.0000000000000
psctrat     :   1.00000000000000
psext       :   2.00000000000000
filpp       :  2.000000000000000E-002
rctpcc      :   2.00000000000000
nmesh       :           2
npmesh      :           2
veta        :  0.200000000000000
new_pwx     :          11
new_pwy     :          11
new_pwz     :           0
new_rsx     :          11
new_rsy     :          11
new_rsz     :           0
nint1dmax   :        1000
nf          :           4
nfdg        :           4
nfh         :           4
zs_pre      :  0.500000000000000
pol_pre     :   1.50000000000000
=================================================
Filtering of pseudopotentials is implemented by Fermi distribution.
npxmax, npymax, and npzmax are updated below.
==========  data computed by listvecdim  ==========
npxmax      :          13
npymax      :          13
npzmax      :          13
=================================================
cell size [lx,ly,lz (a.u.)]
  0.664000000D+01   0.664000000D+01   0.265600000D+02
coarse grid spacing [hx,hy,hz (a.u.)]
  0.332000000D+00   0.332000000D+00   0.332000000D+00
dense grid spacing [hx,hy,hz (a.u.)]
  0.166000000D+00   0.166000000D+00   0.166000000D+00
cutoff energy of wave functions [gmax_coarse,gmax_dense (Ry)]
  0.895413376D+02   0.358165351D+03
```

```
 sample k point [skx,sky,skz (2pi/l)]  weight
   0.000000000D+00   0.000000000D+00   0.000000000D+00     1
 number of electron       charge         spin
   0.400000000D+01   0.000000000D+00   0.100000000D+01
 electric field [ex,ey,ez (a.u./a.u.)]
   0.000000000D+00   0.000000000D+00   0.000000000D+00
 time step (a.u.)  (fs)
   0.000000000D+00   0.000000000D+00
 thermo (k)    kt (a.u.)
   0.947268709D+03   0.300000000D-02
 cufoff of force acting on atoms (a.u.)
   0.100000000D-04
 charge mixing ratio of scf
   0.200000000D+00
 Wavefunctions & electron density are generated automatically.
 total charge   4.00000000000000      (electrons)
 fermi level -0.150663681074548      (hartree)
 atomic charge(electrons)
           1  0.966898864781597
           2   1.03309398965166
           3   1.03305383620344
           4  0.966953309316269

   k,spin,  band ,     eigen value    ,    residual norm  ,    occupation
   1    1      1    -0.2175963215E+00    0.9255817490E-05    0.9999999998E+00
   1    1      2    -0.1755385413E+00    0.2024381528E-04    0.9997494547E+00
   1    1      3    -0.1257888232E+00    0.3148168486E-04    0.2505455374E-03
   1    1      4    -0.7435455586E-01    0.4629599606E-04    0.8976823099E-11
   1    1      5    -0.1128622627E-01    0.7191272051E-04    0.6653448908E-20
   1    1      6     0.8106096692E-01    0.4539199539E-03    0.2847222140E-33
   1    1      7     0.9699623738E-01    0.2043024361E-04    0.1404606508E-35
   1    1      8     0.9699623738E-01    0.2050212873E-04    0.1404606506E-35
   1    1      9     0.1215723704E+00    0.4009765298E-03    0.3888615650E-39
   1    1     10     0.1475499445E+00    0.1702896075E-04    0.6747703575E-43
   1    1     11     0.1475499445E+00    0.1703836743E-04    0.6747703542E-43
   1    1     12     0.2221841004E+00    0.3874937010E-04    0.0000000000E+00
   1    1     13     0.2221841008E+00    0.4047717571E-04    0.0000000000E+00
   1    1     14     0.2411123012E+00    0.2117652680E-01    0.0000000000E+00
   1    1     15     0.3131105300E+00    0.2871026352E-02    0.0000000000E+00
   1    1     16     0.3131106430E+00    0.2904394717E-02    0.0000000000E+00
Scf=  33   dp=    0.9108212353D-06
    one electron energy      -0.786244796380038      (hartree)
 exchange correlation energy  -5.90841119173525      (hartree)
    hartree       energy       5.33747058567152      (hartree)
    ewald         energy      -5.96650333694422      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -7.32371667544123      (hartree)
    Total         energy      -7.32368873938799      (hartree)
 atomic force
    1  -0.1349743305877592D-09  -0.1349936736619608D-09  -0.3026876386059786D-02
    2  -0.9367655185173021D-09  -0.9367523694166422D-09   0.1474398973778331D-02
    3   0.2790416561554850D-09   0.2790489703501150D-09  -0.1470765827326505D-02
    4   0.7926981929495763D-09   0.7926970727284881D-09   0.3023243239607960D-02
 mdstep=           1
 atom coordinate (input)
   0.3320000000000000D+01   0.3320000000000000D+01  -0.4980000000000000D+01   3   0   0   0  12866.00   00  1    1a
   0.0000000000000000D+00   0.0000000000000000D+00  -0.1660000000000000D+01   3   0   0   0  12866.00   00  1    2a
   0.3320000000000000D+01   0.3320000000000000D+01   0.1660000000000000D+01   3   0   0   0  12866.00   00  1    3a
   0.0000000000000000D+00   0.0000000000000000D+00   0.4980000000000000D+01   3   0   0   0  12866.00   00  1    4a
 atom coordinate (output)
   0.3320000000000000D+01   0.3320000000000000D+01  -0.4980000000000000D+01   3   0   0   0  12866.00   00  1    1a
   0.0000000000000000D+00   0.0000000000000000D+00  -0.1660000000000000D+01   3   0   0   0  12866.00   00  1    2a
   0.3320000000000000D+01   0.3320000000000000D+01   0.1660000000000000D+01   3   0   0   0  12866.00   00  1    3a
   0.0000000000000000D+00   0.0000000000000000D+00   0.4980000000000000D+01   3   0   0   0  12866.00   00  1    4a
 real time   64.8970191478729      (sec)
 com. time   22.5335934162140      (sec)
 com. vol.  0.000000000000000E+000 (byte)
```

8.4 Increase the number of sampling k points

In a crystal, we have to consider that electrons having all kinds of wave-number vectors (periodicities) are present. Namely, the wave function whose periodicity is identical to that of the lattice (components of the wave-number vector are integers) is only one of the wave functions in the Brillouin region. The calculations performed in Secs. 8.2 and 8.3 are only for those having integer components of wave-number vectors among multiple wave functions. However, strictly speaking, all the wave functions within the Brillouin region must be handled. To increase the number of sampling k-points, divide the Brillouin region with meshes in order to consider all the wave functions; the finer the meshes, the more accurate the calculation becomes. However, since the calculation time increases as the number of divisions increases, the number of sampling k-points should be determined with consideration given to the size of the model to be calculated.

In the current calculation, the first Brillouin region is divided by $4 \times 4 \times 4$ meshes. The coordinates of each mesh point in the Brillouin region become as follows, assuming that $c_x = \frac{2\pi}{L_x}$, $c_y = \frac{2\pi}{L_y}$, $c_z = \frac{2\pi}{L_z}$.

$$
\begin{array}{cccc}
\left(-\frac{1}{2}c_x, -\frac{1}{2}c_y, -\frac{1}{2}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{2}c_y, -\frac{1}{2}c_z\right), & \left(0, -\frac{1}{2}c_y, -\frac{1}{2}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{2}c_y, -\frac{1}{2}c_z\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(0, -\frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{4}c_y, -\frac{1}{2}c_z\right) \\
\left(-\frac{1}{2}c_x, 0, -\frac{1}{2}c_z\right), & \left(-\frac{1}{4}c_x, 0, -\frac{1}{2}c_z\right), & \left(0, 0, -\frac{1}{2}c_z\right), & \left(\frac{1}{4}c_x, 0, -\frac{1}{2}c_z\right) \\
\left(-\frac{1}{2}c_x, \frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(-\frac{1}{4}c_x, \frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(0, \frac{1}{4}c_y, -\frac{1}{2}c_z\right), & \left(\frac{1}{4}c_x, \frac{1}{4}c_y, -\frac{1}{2}c_z\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{2}c_y, -\frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{2}c_y, -\frac{1}{4}c_z\right), & \left(0, -\frac{1}{2}c_y, -\frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{2}c_y, -\frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(0, -\frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{4}c_y, -\frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, 0, -\frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, 0, -\frac{1}{4}c_z\right), & \left(0, 0, -\frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, 0, -\frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, \frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, \frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(0, \frac{1}{4}c_y, -\frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, \frac{1}{4}c_y, -\frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{2}c_y, 0\right), & \left(-\frac{1}{4}c_x, -\frac{1}{2}c_y, 0\right), & \left(0, -\frac{1}{2}c_y, 0\right), & \left(\frac{1}{4}c_x, -\frac{1}{2}c_y, 0\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{4}c_y, 0\right), & \left(-\frac{1}{4}c_x, -\frac{1}{4}c_y, 0\right), & \left(0, -\frac{1}{4}c_y, 0\right), & \left(\frac{1}{4}c_x, -\frac{1}{4}c_y, 0\right) \\
\left(-\frac{1}{2}c_x, 0, 0\right), & \left(-\frac{1}{4}c_x, 0, 0\right), & (0, 0, 0), & \left(\frac{1}{4}c_x, 0, 0\right) \\
\left(-\frac{1}{2}c_x, \frac{1}{4}c_y, 0\right), & \left(-\frac{1}{4}c_x, \frac{1}{4}c_y, 0\right), & \left(0, \frac{1}{4}c_y, 0\right), & \left(\frac{1}{4}c_x, \frac{1}{4}c_y, 0\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{2}c_y, \frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{2}c_y, \frac{1}{4}c_z\right), & \left(0, -\frac{1}{2}c_y, \frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{2}c_y, \frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, -\frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, -\frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(0, -\frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, -\frac{1}{4}c_y, \frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, 0, \frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, 0, \frac{1}{4}c_z\right), & \left(0, 0, \frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, 0, \frac{1}{4}c_z\right) \\
\left(-\frac{1}{2}c_x, \frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(-\frac{1}{4}c_x, \frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(0, \frac{1}{4}c_y, \frac{1}{4}c_z\right), & \left(\frac{1}{4}c_x, \frac{1}{4}c_y, \frac{1}{4}c_z\right)
\end{array}
$$

Calculations should be performed for all these points, but when using the complex conjugate relationship between the wave functions of (k_x, k_y, k_z) and $(-k_x, -k_y, -k_z)$, calculations for only (k_x, k_y, k_z) are sufficient. Therefore, the number of points actually required in the calculation can be reduced from 64 points to 36 points in the above example.

Input the coordinates within the Brillouin region, into "parameters.inp", excluding coefficients c_x, c_y, and c_z. With respect to the points that are skipped in the calculation using the complex conjugate relationship, input 2 in their weight column. An example of the creation of "parameters.inp" is shown below. Revisions from Sec. 8.2 are shown by red characters.

```
   Example of parameters.inp
 1:  &nml_inp_prm_kukan
 2:  xmax = 3.32d0
 3:  ymax = 3.32d0
 4:  zmax = 3.32d0
 5:  nxmax = 10
 6:  nymax = 10
 7:  nzmax = 10
 8:  neigmx = 8
 9:  natom = 2
10:  nperi = 3
11:  eta = 0.2d0
12:  npre = 1
13:  nspv = 1
14:  numkx = 36
15:  skpx( 1)=-0.50D0
16:  skpy( 1)=-0.50D0
17:  skpz( 1)=-0.50D0
18:  nwkp( 1)=1
19:  skpx( 2)=-0.25D0
20:  skpy( 2)=-0.50D0
21:  skpz( 2)=-0.50D0
```

```
 22:  nwkp( 2)= 2
 23:  skpx( 3)= 0.00D0
 24:  skpy( 3)=-0.50D0
 25:  skpz( 3)=-0.50D0
 26:  nwkp( 3)= 1
 27:  skpx( 4)=-0.50D0
 28:  skpy( 4)=-0.25D0
 29:  skpz( 4)=-0.50D0
 30:  nwkp( 4)= 2
 31:  skpx( 5)=-0.25D0
 32:  skpy( 5)=-0.25D0
 33:  skpz( 5)=-0.50D0
 34:  nwkp( 5)= 2
 35:  skpx( 6)= 0.00D0
 36:  skpy( 6)=-0.25D0
 37:  skpz( 6)=-0.50D0
 38:  nwkp( 6)= 2
 39:  skpx( 7)= 0.25D0
 40:  skpy( 7)=-0.25D0
 41:  skpz( 7)=-0.50D0
 42:  nwkp( 7)= 2
 43:  skpx( 8)=-0.50D0
 44:  skpy( 8)= 0.00D0
 45:  skpz( 8)=-0.50D0
 46:  nwkp( 8)= 1
 47:  skpx( 9)=-0.25D0
 48:  skpy( 9)= 0.00D0
 49:  skpz( 9)=-0.50D0
 50:  nwkp( 9)= 2
 51:  skpx(10)= 0.00D0
 52:  skpy(10)= 0.00D0
 53:  skpz(10)=-0.50D0
 54:  nwkp(10)= 1
 55:  skpx(11)=-0.50D0
 56:  skpy(11)=-0.50D0
 57:  skpz(11)=-0.25D0
 58:  nwkp(11)= 2
 59:  skpx(12)=-0.25D0
 60:  skpy(12)=-0.50D0
 61:  skpz(12)=-0.25D0
 62:  nwkp(12)= 2
 63:  skpx(13)= 0.00D0
 64:  skpy(13)=-0.50D0
 65:  skpz(13)=-0.25D0
 66:  nwkp(13)= 2
 67:  skpx(14)= 0.25D0
 68:  skpy(14)=-0.50D0
 69:  skpz(14)=-0.25D0
 70:  nwkp(14)= 2
 71:  skpx(15)=-0.50D0
 72:  skpy(15)=-0.25D0
 73:  skpz(15)=-0.25D0
 74:  nwkp(15)= 2
 75:  skpx(16)=-0.25D0
 76:  skpy(16)=-0.25D0
 77:  skpz(16)=-0.25D0
 78:  nwkp(16)= 2
 79:  skpx(17)= 0.00D0
 80:  skpy(17)=-0.25D0
 81:  skpz(17)=-0.25D0
 82:  nwkp(17)= 2
 83:  skpx(18)= 0.25D0
 84:  skpy(18)=-0.25D0
 85:  skpz(18)=-0.25D0
 86:  nwkp(18)= 2
 87:  skpx(19)=-0.50D0
 88:  skpy(19)= 0.00D0
 89:  skpz(19)=-0.25D0
 90:  nwkp(19)= 2
 91:  skpx(20)=-0.25D0
 92:  skpy(20)= 0.00D0
 93:  skpz(20)=-0.25D0
 94:  nwkp(20)= 2
 95:  skpx(21)= 0.00D0
 96:  skpy(21)= 0.00D0
 97:  skpz(21)=-0.25D0
 98:  nwkp(21)= 2
 99:  skpx(22)= 0.25D0
100:  skpy(22)= 0.00D0
101:  skpz(22)=-0.25D0
102:  nwkp(22)= 2
103:  skpx(23)=-0.50D0
104:  skpy(23)= 0.25D0
105:  skpz(23)=-0.25D0
106:  nwkp(23)= 2
107:  skpx(24)=-0.25D0
108:  skpy(24)= 0.25D0
109:  skpz(24)=-0.25D0
110:  nwkp(24)= 2
111:  skpx(25)= 0.00D0
112:  skpy(25)= 0.25D0
113:  skpz(25)=-0.25D0
114:  nwkp(25)= 2
115:  skpx(26)= 0.25D0
116:  skpy(26)= 0.25D0
117:  skpz(26)=-0.25D0
118:  nwkp(26)= 2
119:  skpx(27)=-0.50D0
120:  skpy(27)=-0.50D0
121:  skpz(27)= 0.00D0
122:  nwkp(27)= 1
123:  skpx(28)=-0.25D0
124:  skpy(28)=-0.50D0
125:  skpz(28)= 0.00D0
126:  nwkp(28)= 2
127:  skpx(29)= 0.00D0
128:  skpy(29)=-0.50D0
129:  skpz(29)= 0.00D0
130:  nwkp(29)= 1
131:  skpx(30)=-0.50D0
132:  skpy(30)=-0.25D0
133:  skpz(30)= 0.00D0
134:  nwkp(30)= 2
135:  skpx(31)=-0.25D0
```

```
136:  skpy(31)=-0.25D0
137:  skpz(31)= 0.00D0
138:  nwkp(31)= 2
139:  skpx(32)= 0.00D0
140:  skpy(32)=-0.25D0
141:  skpz(32)= 0.00D0
142:  nwkp(32)= 2
143:  skpx(33)= 0.25D0
144:  skpy(33)=-0.25D0
145:  skpz(33)= 0.00D0
146:  nwkp(33)= 2
147:  skpx(34)=-0.50D0
148:  skpy(34)= 0.00D0
149:  skpz(34)= 0.00D0
150:  nwkp(34)= 1
151:  skpx(35)=-0.25D0
152:  skpy(35)= 0.00D0
153:  skpz(35)= 0.00D0
154:  nwkp(35)= 2
155:  skpx(36)= 0.00D0
156:  skpy(36)= 0.00D0
157:  skpz(36)= 0.00D0
158:  nwkp(36)= 1
159:  /
```

The atomic coordinates "atom.xyz" is identical to that in Sec. 8.2. Execution is also performed identically to those in Sec, 8.2. Below is an example of the output of the electronic-structure calculation result mdresult.dat. If the "free energy" part and "FORCE" part of "mdresult.dat" are identical to the above contents by 10 digits, then the calculation is successful.

```
computed by kukan8f 10/07/2021-01
==========  data from nml_inp_prm_kukan  ==========
ndisp       :          66
catmfn      :atom.xyz
nprocx      :           1
nprocy      :           1
nprocz      :           1
nprock      :           1
xmax        :   3.32000000000000
ymax        :   3.32000000000000
zmax        :   3.32000000000000
nxmax       :          10
nymax       :          10
nzmax       :          10
npxmax      :          -1
npymax      :          -1
npzmax      :          -1
nso         :           0
socang      :    0.000E+00  0.000E+00  0.000E+00
nsym        :           0
neigmx      :           8
natom       :           2
num_atcell  :           2
num_ppcell  :           2
num_ppcell_d:           2
gmaxps      :   20.0000000000000
nperi       :           3
npopshow    :           0
numkx       :          36
numky       :           1
numkz       :           1
ksym        :           0
kband       :           0
cexco       :    vwn
nspv        :           1
epsvh       :  1.000000000000000E-012
epssd       :  1.000000000000000E-006
ratio_diis  :  0.300000000000000
eps_scf     :  1.000000000000000E-006
ncgmin      :           1
ncgmax      :         800
ncgres      :         801
nprecon_cg  :           1
nprecon_diis:           1
nsdmax      :           4
nkscg       :           1
ndiismax    :           4
```

```
ncgscf      :         200
nretcg      :        2000
nrrz        :           1
nchange     :           1
eta         :  0.200000000000000
etamag      :  0.2000E-01  0.2000E+01
looplimit   :        1000
nbrydn      :          20
tmstep      :  0.000000000000000E+000
nmd_start   :           0
nmd_end     :           1
ngdiis      :           1
sconst      :  0.000000000000000E+000
biasx       :  0.000000000000000E+000
biasy       :  0.000000000000000E+000
biasz       :  0.000000000000000E+000
tf          :  3.000000000000000E-003
tfmin       :  -300.000000000000
tfmax       :   300.000000000000
chrgd       :  0.000000000000000E+000
npolcon     :           0
polconocc   :   2.70000000000000
endjel      :  0.000000000000000E+000
chrjel      :  0.000000000000000E+000
fcut        :  1.000000000000000E-005
npre        :           1
nevhist     :           3
northo      :           1
lveffout    : F
eps         :  1.000000000000000E-016
eps_eig_diis:  1.000000000000000E-014
alambda_diis:  0.500000000000000
alambda_min :  0.100000000000000
alambda_max :   1.00000000000000
nradmx      :        1502
nrprjmx     :           6
nprjmx      :          18
lsphel      :           8
nlmax       :           4
lrhomx      :          25
nfiltyp     :           1
psctoff     :   1.05000000000000
nqmx        :         400
psftrad     :   10.0000000000000
psctrat     :   1.00000000000000
psext       :   2.00000000000000
filpp       :  2.000000000000000E-002
rctpcc      :   2.00000000000000
nmesh       :           2
npmesh      :           2
veta        :  0.200000000000000
new_pwx     :          11
new_pwy     :          11
new_pwz     :          11
new_rsx     :          11
new_rsy     :          11
new_rsz     :          11
nint1dmax   :        1000
nf          :           4
nfdg        :           4
nfh         :           4
zs_pre      :  0.500000000000000
pol_pre     :   1.50000000000000
=====================================================
Filtering of pseudopotentials is implemented by Fermi distribution.
npxmax, npymax, and npzmax are updated below.
==========  data computed by listvecdim  ==========
npxmax      :          13
npymax      :          13
npzmax      :          13
=====================================================
cell size [lx,ly,lz (a.u.)]
```

```
  0.664000000D+01   0.664000000D+01   0.664000000D+01
coarse grid spacing [hx,hy,hz (a.u.)]
  0.332000000D+00   0.332000000D+00   0.332000000D+00
dense grid spacing [hx,hy,hz (a.u.)]
  0.166000000D+00   0.166000000D+00   0.166000000D+00
cutoff energy of wave functions [gmax_coarse,gmax_dense (Ry)]
  0.895413376D+02   0.358165351D+03
sample k point [skx,sky,skz (2pi/l)]  weight
 -0.500000000D+00  -0.500000000D+00  -0.500000000D+00     1
 -0.250000000D+00  -0.500000000D+00  -0.500000000D+00     2
  0.000000000D+00  -0.500000000D+00  -0.500000000D+00     1
 -0.500000000D+00  -0.250000000D+00  -0.500000000D+00     2
 -0.250000000D+00  -0.250000000D+00  -0.500000000D+00     2
  0.000000000D+00  -0.250000000D+00  -0.500000000D+00     2
  0.250000000D+00  -0.250000000D+00  -0.500000000D+00     2
 -0.500000000D+00   0.000000000D+00  -0.500000000D+00     1
 -0.250000000D+00   0.000000000D+00  -0.500000000D+00     2
  0.000000000D+00   0.000000000D+00  -0.500000000D+00     1
 -0.500000000D+00  -0.500000000D+00  -0.250000000D+00     2
 -0.250000000D+00  -0.500000000D+00  -0.250000000D+00     2
  0.000000000D+00  -0.500000000D+00  -0.250000000D+00     2
  0.250000000D+00  -0.500000000D+00  -0.250000000D+00     2
 -0.500000000D+00  -0.250000000D+00  -0.250000000D+00     2
 -0.250000000D+00  -0.250000000D+00  -0.250000000D+00     2
  0.000000000D+00  -0.250000000D+00  -0.250000000D+00     2
  0.250000000D+00  -0.250000000D+00  -0.250000000D+00     2
 -0.500000000D+00   0.000000000D+00  -0.250000000D+00     2
 -0.250000000D+00   0.000000000D+00  -0.250000000D+00     2
  0.000000000D+00   0.000000000D+00  -0.250000000D+00     2
  0.250000000D+00   0.000000000D+00  -0.250000000D+00     2
 -0.500000000D+00   0.250000000D+00  -0.250000000D+00     2
 -0.250000000D+00   0.250000000D+00  -0.250000000D+00     2
  0.000000000D+00   0.250000000D+00  -0.250000000D+00     2
  0.250000000D+00   0.250000000D+00  -0.250000000D+00     2
 -0.500000000D+00  -0.500000000D+00   0.000000000D+00     1
 -0.250000000D+00  -0.500000000D+00   0.000000000D+00     2
  0.000000000D+00  -0.500000000D+00   0.000000000D+00     1
 -0.500000000D+00  -0.250000000D+00   0.000000000D+00     2
 -0.250000000D+00  -0.250000000D+00   0.000000000D+00     2
  0.000000000D+00  -0.250000000D+00   0.000000000D+00     2
  0.250000000D+00  -0.250000000D+00   0.000000000D+00     2
 -0.500000000D+00   0.000000000D+00   0.000000000D+00     1
 -0.250000000D+00   0.000000000D+00   0.000000000D+00     2
  0.000000000D+00   0.000000000D+00   0.000000000D+00     1
number of electron       charge         spin
  0.200000000D+01   0.000000000D+00   0.100000000D+01
electric field [ex,ey,ez (a.u./a.u.)]
  0.000000000D+00   0.000000000D+00   0.000000000D+00
time step (a.u.)  (fs)
  0.000000000D+00   0.000000000D+00
thermo (k)    kt (a.u.)
  0.947268709D+03   0.300000000D-02
cufoff of force acting on atoms (a.u.)
  0.100000000D-04
charge mixing ratio of scf
  0.200000000D+00
Wavefunctions & electron density are generated automatically.
total charge   2.00000000000000      (electrons)
fermi level  4.990245136382576E-003 (hartree)

  k,spin,  band ,     eigen value    ,    residual norm  ,    occupation
  1    1      1     0.1276911619E+00    0.1795303845E-04    0.1726724182E-17
  1    1      2     0.1276912156E+00    0.2885103797E-05    0.1726693314E-17
  1    1      3     0.1276912204E+00    0.3603082316E-05    0.1726690530E-17
  1    1      4     0.1276914590E+00    0.1206592195E-04    0.1726553231E-17
  1    1      5     0.1276914869E+00    0.2236848053E-05    0.1726537142E-17
  1    1      6     0.1276914951E+00    0.2104691340E-05    0.1726532419E-17
  1    1      7     0.2960137168E+00    0.3023006586E-04    0.7413740556E-42
  1    1      8     0.2960142583E+00    0.3675556895E-04    0.7412402605E-42

                                        ............
```

```
. . . . . .
. . . . . .

  36    1      1    -0.1171184730E+00    0.2232957757E-05    0.1000000000E+01
  36    1      2     0.1998659527E+00    0.1486899586E-05    0.6149670471E-28
  36    1      3     0.1998660252E+00    0.1489569316E-05    0.6149521950E-28
  36    1      4     0.1998660361E+00    0.1461062073E-05    0.6149499586E-28
  36    1      5     0.4733944586E+00    0.3582212652E-04    0.0000000000E+00
  36    1      6     0.5106320514E+00    0.1338804452E-05    0.0000000000E+00
  36    1      7     0.5106320707E+00    0.1740284669E-05    0.0000000000E+00
  36    1      8     0.5106320856E+00    0.1652332926E-05    0.0000000000E+00
Scf=  18   dp=    0.2711104473D-06
    one electron energy      -7.767047846717511E-002 (hartree)
 exchange correlation energy  -2.95120062202080      (hartree)
    hartree       energy     -1.176430860117228E-003 (hartree)
    ewald         energy     -0.548077326733234      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
  energy offset of ps. pot.  -3.459068569757674E-004 (hartree)
  energy jellium/ions         0.000000000000000E+000 (hartree)
   helmholtz free energy      -3.57990357875921       (hartree)
    Total         energy      -3.57847076493830       (hartree)
 atomic force
    1  -0.5041052564346475D-17  -0.7344548290402406D-17  -0.1386461481169671D-15
    2   0.5041052564346475D-17   0.7344548290402408D-17   0.1386461481169670D-15
 mdstep=           1
 atom coordinate (input)
   0.33200000000000000D+01   0.33200000000000000D+01   0.33200000000000000D+01   3   0   0   0  22056.00   00  1    1a
   0.00000000000000000D+00   0.00000000000000000D+00   0.00000000000000000D+00   3   0   0   0  29408.00   00  1    2a
 atom coordinate (output)
   0.33200000000000000D+01   0.33200000000000000D+01   0.33200000000000000D+01   3   0   0   0  22056.00   00  1    1a
   0.00000000000000000D+00   0.00000000000000000D+00   0.00000000000000000D+00   3   0   0   0  29408.00   00  1    2a
 real time   36.2784969806671      (sec)
 com. time   9.13151669502258      (sec)
 com. vol.  0.000000000000000E+000 (byte)
```

A Determination of grid width

Regarding the grid width `dx`, a value smaller than the minimum grid width required for atoms contained in a cell should be used. The grid width required for each atom is listed below.[2]

dx (a.u.)	Atom
0.27	Cu
0.30	Fe,W
0.33	C,N,F,Cl
0.35	O,S,(C)
0.50	Li,Na
0.60	H,Al,Si

Here, for elements not listed in the above table, confirm the values at the contact address.

[2]When a soft-type potential is used, the value within parentheses can be used for the C atom; this value was used in the example in this manual.