First-principles calculation code

based on real-space finite-difference method

(for electronic structure calculation)

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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" developed in the Hirose Laboratory, Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, is summarized. All examples in this manual are premised on the execution using the Pentium 4 cluster in our laboratory. When these example calculations are to be performed using other computers described in Section 1.1, or computers other than those listed in Section 1.2.

1.1 Operation confirmed machine models

Operation of this program has been confirmed on the following machine models.
• Pentium 4 cluster
• NEC SX7 (Information Synergy Center, Tohoku University)
• Hitachi SR11000 (Institute for Solid State Physics, the University of Tokyo)

1.2 Contact information

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

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2 Outline of the code

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 molecular-dynamics simulations are not explained in this manual, refer to other references for explanations of unfamiliar terms and other details.

2.1 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)

2.2 Boundary conditions

The current program is divided into four types depending on the setting of boundary conditions.
- version40$\cdots x$, y and z all belong to the isolated system
- version41$\cdots x$ belongs to the periodic system; y and z belong to the isolated system
- version42$\cdots x$ and y belong to the periodic system; z belongs to the isolated system
- version43$\cdots x$, y and z all belong to the periodic system

Select an appropriate program in accordance with the model to be calculated. Ascii input/output data are compatible with all four versions. Binary input/output data for version 40 are incompatible with other versions because of the lack of an imaginary part in wave functions.

2.3 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.

2.4 Pseudopotentials

This code uses the pseudopotential databease NCPS97, whose format is also modified for this code. The NCPS97 database is developed by Dr. Kazuaki Kobayashi of National Institute for Materials Science, Japan. For NCPS databases, see http://www.geocities.co.jp/Technopolis/4765/INFO/

2.5 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.

1.Shared-memory parallel computer

A single computer is equipped with a large-capacity memory and plural processors, wherein each of the processors shares the memory in the computer. Accordingly, while this computer has the merit that a processor can instantaneously refer to another processor 's calculation results in the computer, it also has the demerit of a limitation in the scale of calculation due to the limitation in the memory capacity and the number of processors that can be mounted in a single computer. A unit that shares the memory with other units is called a *node*. By utilizing plural nodes, the parallelization described below is also possible.

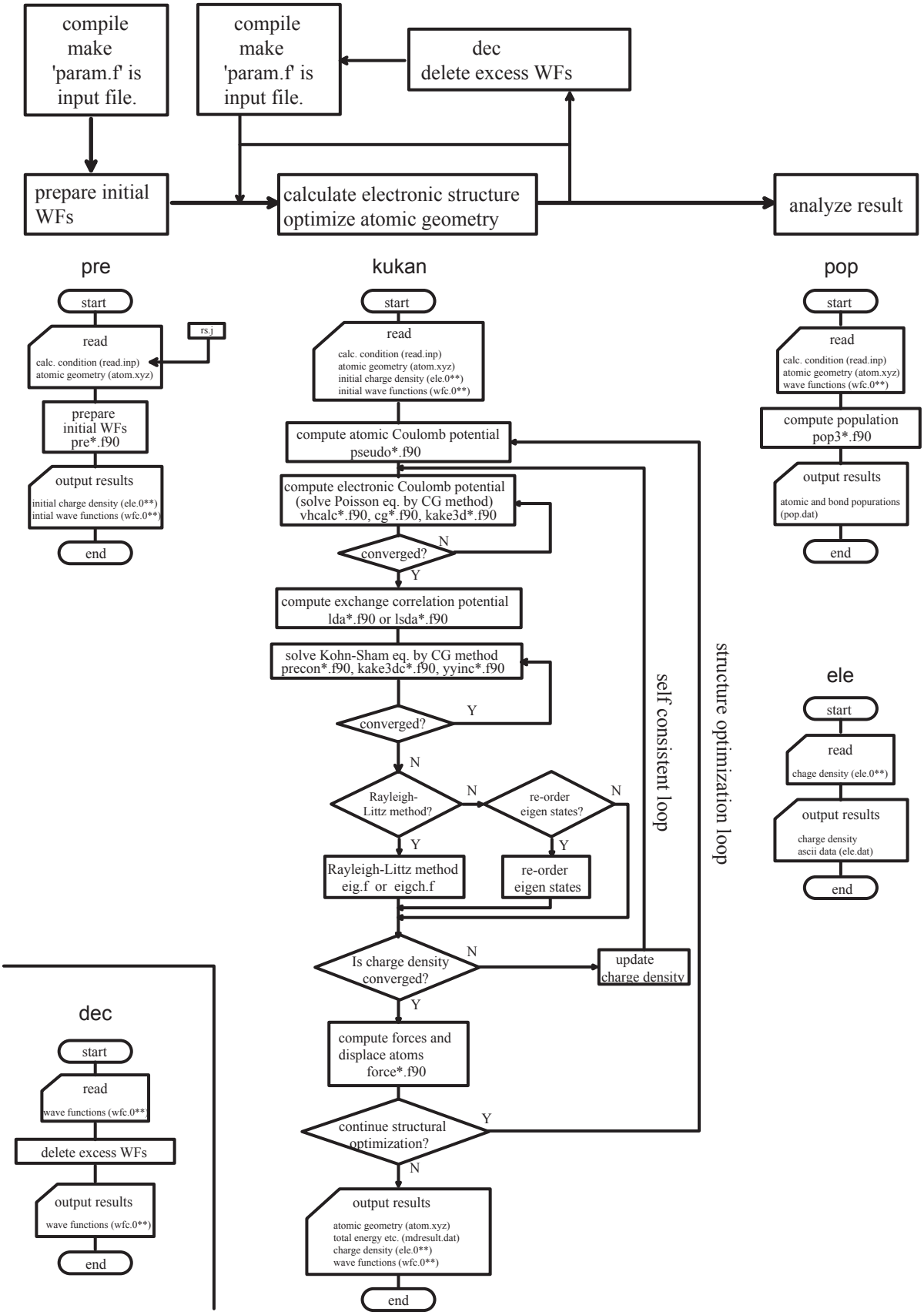

Figure 1: flowchart

2.Massively parallel computer

In this type of computer, plural computers (nodes) are connected via network cables to form a cluster. Calculations are shared and performed by plural nodes, and calculation results are transferred to other nodes via the network cables. Most examples of the early parallelization were of this type. When a program requires a large amount of data transfer relative to the amount of calculation, its performance does not improve due to the bottleneck of data communication; however, when a program requires a small amount of data transfer, the performance improves in proportion to the number of nodes in the cluster.

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.
Parallelization using *plural processors*: use method 1.
Parallelization using *plural nodes*: use method 2.[1]
Parallelization: use both methods 1 and 2.
Parallelization using *m processors*: use method 1 with m processors.
Parallelization using *n nodes*: use method 2 with n nodes.
Parallelization by $m \times n$: use n nodes with m processors per one node. Perform parallelization using a total of m×n processors.
In this manual, the above examples are applied unless otherwise stated.

3 Simple molecular calculation

In this chapter, as a simple example, a 1×1 atomic structure optimization calculation of CO molecule is performed using a program in which isolated boundary conditions are applied in all directions.

3.1 Create the directory

First, create an execution directory "∼/CO" under your home directory (which here is indicated by "∼/"), then create "source(∼/CO/source)" and "exe(∼/CO/exe)" under "∼/CO". Next, send a source file to "∼/CO/source" by FTP or by copying the file. When this operation cannot be executed properly, ask the advice of someone familiar with Linux.

3.2 Create the parameter file and compilation

Before compilation, create the parameter file "param.f." A sample file "param.f" has already been created under "∼/CO/source"; therefore, change lines 1 to 24 of this sample file in accordance with the following examples. 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.

[1]Most shared-memory computers can perform parallel processing by generating plural processes within one node. In this case, even when only one node is used, this type of parallelization is applied.

NPROC(X,Y,Z)	$\cdots$	For the control of parallel calculations. Refer to Chapter 4. In the calculation described in the present chapter, set all the values to 1.
(X,Y,Z)MAX	$\cdots$	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 Section 3.3) maintain a distance of 9-15 (a.u.) from the boundary surface.
N(X,Y,Z)MAX	$\cdots$	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.
NP(X,Y,Z)MAX	$\cdots$	The number of grid points included in a pseudopotential nonlocal region; must be an integer. It should be selected such that the (NPXMAX-4)×DX approximately equals the cut-off radius of the pseudopotential. For the setting of the cut-off radius of the pseudopotential, refer to Appendix.
NEIGMX	$\cdots$	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	$\cdots$	The number of atoms.
NUMK	$\cdots$	The number of sampling k-points. Set this parameter to 1 when isolated boundary conditions are applied in all of the x, y and z directions.
NUMS	$\cdots$	When the effect of spin on the exchange-correlation potential is neglected, NUMS=1, and when it is to be considered, NUMS=2.
NMESH	$\cdots$	The width of the dense grid (DX/NMESH) in a double-grid technique. NMESH=3 is preferable.
NPERI	$\cdots$	Setting for boundary conditions. Isolated boundary conditions: NPERI = 0. Periodic boundary conditions in 1 direction: NPERI=1. Periodic boundary conditions in 2 directions: NPERI=2. Periodic boundary conditions in 3 directions: NPERI=3.
NRAS(X,Y,Z)	$\cdots$	Setting for spiral boundary conditions. Set this parameter to 0; no explanation is given here.
NUMK(X,Y,Z)	$\cdots$	The numbers of sampling k-points in x, y and z directions. Since these are used only in the calculation under the application of electric field, always set these parameters to 1 in the current calculation.
ENDJEL	$\cdots$	Setting for "jellium". Set this value to 0.0D0; no explanation is given here.
CHRJEL	$\cdots$	Setting for "jellium". Set this value to 0.0D0; no explanation is given here.
MACHINE	$\cdots$	Setting for type of computer. Scalar: 0, vector: 1.

`example of param.f (only the first 24 lines)`

```
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=1,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=10.0D0,YMAX=10.0D0,ZMAX=10.0D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=30,NYMAX=30,NZMAX=30)
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=9,NPYMAX=9,NPZMAX=9)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=8,NATOM=2,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=1,NUMS=1)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=0)
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)
```

Compilation is performed by "makefile". Type as follows under "∼/CO/source":
>`make -f make.dragons lda0`[2][3]
When the compilation is completed, check and confirm that files "kukan40", "pre", "ele" and "pop" have been created in "∼/CO/source".
Next, create the execution-condition input file "read.inp". Download the "read.inp" file by FTP, etc. into the client computer, edit it using a text editor, and send it again to "∼/CO/source". In the current calculation, this file should be set as follows.[4]

```
example of read.inp
#    convergency for CG (P. eq.)   convergency for CG (KS eq.)   convergency of SCF
     1.0D-12                       1.0D-12                       1.0D-8
#    min. it. for CG (P. eq.)      max. it. for CG (P. eq.)      restart for CG (P. eq.):N (1/N its.)
     1                             400                           500
#    max. it. for CG (KS eq.)      switch for CG (KS eq.)(0;no 1;yes)
     2                             1
#    mixing ratio of SCF           max. it. of SCF
     0.10D0                        200
#    time step of MD (a.u.)        Num. it. of MD:Ns(start)      Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     0.0D0                         0                             1
#    Elec. Field in X (a.u.)       Elec. Field in Y (a.u.)       Elec. Field in Z (a.u.)
     0.0D0                         0.0D0                         0.0D0
#    k point (write all k points)
#    X                             Y                             Z                             weight
     0.00D0                        0.00D0                        0.00D0                        1
#    Fermi temperature(KT) (a.u.)  min. of eigenvalues (a.u.)    max. of eigenvalues (a.u.)
     0.0001D0                      -1000.0D0                     1000.0D0
#    Rayleigh-Ritz:N (1/N scf)     re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                             1                                 0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2
```

[2] ">" indicates a prompt; do not input ">".

[3] The number after "lda" indicates the version number; input 0 for version 40, 1 for version 41, 2 for version 42, and 3 for version 43.

[4] Text written in Japanese characters may cause error depending on the type of computer. In such cases, delete the entire comment text.

3.3 Create 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 MD, y-direction switch of molecular dynamic (MD)[5], z-direction switch of MD, and mass of the atom [atomic weight × proton mass (1838 a.u.)]. When the MD 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
  0.5500000E+00  0.5500000E+00  0.5500000E+00   6   0   0   0   22056.00
 -0.5500000E+00 -0.5500000E+00 -0.5500000E+00   8   0   0   0   29408.00
```

Although the equilibrium interatomic distance of the CO molecule is 2.1 (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.

3.4 Copy files necessary for execution

Finally, copy the files necessary for the execution directory "∼/CO/exe". Here, assuming that the current directory is "∼/CO/source", type the following.

```
>cd ..
>cp source/pre exe
>cp source/kukan40 exe
>cp source/read.inp exe
>cp source/atom.xyz exe
```

The execution environment is now ready.

3.5 Execute electronic-structure calculation program

Before performing an electronic-structure calculation for the first time, input wave functions must be assumed by hand.[6]Here, assuming that the current directory is "∼/CO", type the following.

```
>cd exe
>bsub -n 1 -q S -e errfile -o outfile "mpijob mpirun pre"
```

When the program is executed, initial wave function files "ele.000" and "wfc.000" are created in "∼/CO/exe" by "pre".[7][8]Next, type the following to execute the electronic-structure calculation program.

```
>bsub -n 1 -q S -e errfile -o outfile "mpijob mpirun kukan40"
```

When this program is completed, the files "ele.000" and "wfc.000" in "∼/CO/exe" are updated

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

[6]Calculation results do not depend on the wave functions assumed. However, since the current calculation is convergent, the computation time may be extremely long depending on the way in which wave functions are assumed. Here, wave functions close to the solution should be assumed.

[7]The number and characters after -n, -q, -e and -o indicate the number of processes, the execution QUEUE name, the error file name, and the standard-output file name, respectively.

[8]Job execution is confirmed by "bjobs".

and “mdresult.dat” is created. The calculation result can be confirmed by inputting the following.

>`cat mdresult.dat`

The contents of “mdresult.dat” are listed below.

```
example of mdresult.dat
 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.)]
   0.111111111D+00   0.111111111D+00   0.111111111D+00
 nonlocal region [vnlx,vnly,vnlz (a.u.)]
   0.600000000D+01   0.600000000D+01   0.600000000D+01
 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.)
   0.315756236D+02   0.100000000D-03
 cufoff of the force (a.u.)
   0.500000000D-02
 mixing ratio of scf
   0.100000000D+00
 nrasy,nrasz
           0           0
 total charge   10.0000000000000
 fermi level -0.244140625000000      (hartree)
 atomic charge
           1   3.97034710203453
           2   6.02965289796599
  1   1   1 eigen value =   -0.1138159053D+01    0.1210809104D-09    0.2000000000D+01
  1   1   2 eigen value =   -0.5232890463D+00    0.9447984641D-11    0.2000000000D+01
  1   1   3 eigen value =   -0.4875246388D+00    0.7255293815D-11    0.2000000000D+01
  1   1   4 eigen value =   -0.4875246123D+00    0.2651612204D-10    0.2000000000D+01
  1   1   5 eigen value =   -0.3252261010D+00    0.1516331236D-09    0.2000000000D+01
  1   1   6 eigen value =   -0.3528477697D-01    0.1775874064D-09    0.0000000000D+00
  1   1   7 eigen value =   -0.3528471655D-01    0.8456857513D-08    0.0000000000D+00
  1   1   8 eigen value =    0.1491283425D-01    0.1573650079D-06    0.0000000000D+00
scf= 107   dp=    0.8672886747D-08
    one electoron energy      -5.92344690344374      (hartree)
 exchange correlation energy   1.57745576380013      (hartree)
    hartree       energy      -29.8137255676793      (hartree)
    ewald         energy       12.5967331459555      (hartree)
    field correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -21.5629835613674      (hartree)
    total         energy      -21.5629835613674      (hartree)
 mdstep=           1
 atom coordinate (input)
  1   0.5500000000000000D+00   0.5500000000000000D+00   0.5500000000000000D+00   6   0   0   0  22056.00
  2  -0.5500000000000000D+00  -0.5500000000000000D+00  -0.5500000000000000D+00   8   0   0   0  29408.00
 atom coordinate (output)
  1   0.5500000000000000D+00   0.5500000000000000D+00   0.5500000000000000D+00   6   0   0   0  22056.00
  2  -0.5500000000000000D+00  -0.5500000000000000D+00  -0.5500000000000000D+00   8   0   0   0  29408.00
 atomic force
  1   0.1995570983038144D+00   0.1995570995934819D+00   0.1995571384730521D+00
  2  -0.1995570983038144D+00  -0.1995570995934819D+00  -0.1995571384730521D+00
 real time   483.160570859909      (sec)
 com. time  3.999900817871094E-002 (sec)
 com. vol.  0.000000000000000E+000 (byte)
 ======================================================================
 This calculation was executed using pseudopotential database NCPS97.
 For NCPS database, see K.Kobayashi, Comput. Mater. Sci. 14, 72 (1999).
```

If the “total energy” part and “atom force” part of “mdresult.dat” are identical to the above contents, then the calculation is successful.

3.6 Execute atomic-structure optimization program

Following the electronic-structure calculation, the optimization of atomic structures is performed. For the execution of atomic-structure optimization, change the contents of "atom.xyz" and "read.inp" as follows.

```
example of read.inp
#    convergency for CG (P. eq.)   convergency for CG (KS eq.)   convergency of SCF
     1.0D-12                       1.0D-12                       1.0D-8
#    min. it. for CG (P. eq.)      max. it. for CG (P. eq.)      restart for CG (P. eq.):N (1/N its.)
     1                             400                           500
#    max. it. for CG (KS eq.)      switch for CG (KS eq.)(0;no 1;yes)
     2                             1
#    mixing ratio of SCF           max. it. of SCF
     0.10D0                        200
#    time step of MD (a.u.)        Num. it. of MD:Ns(start)      Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     80.0D0                        0                             40
#    Elec. Field in X (a.u.)       Elec. Field in Y (a.u.)       Elec. Field in Z (a.u.)
     0.0D0                         0.0D0                         0.0D0
#    k point (write all k points)
#    X                             Y                             Z                             weight
     0.00D0                        0.00D0                        0.00D0                        1
#    Fermi temperature(KT) (a.u.)  min. of eigenvalues (a.u.)    max. of eigenvalues (a.u.)
     0.0001D0                      -1000.0D0                     1000.0D0
#    Rayleigh-Ritz:N (1/N scf)     re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                             1                                 0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2

example of atom.xyz
  0.6000000E+00  0.6000000E+00  0.6000000E+00   6   1   1   1   22056.00
 -0.6000000E+00 -0.6000000E+00 -0.6000000E+00   8   1   1   1   29408.00
```

After the completion of copying, initial wave functions should be created; however, since the results obtained in Section 3.5 are close to the solution, these results are used without assuming new wave functions this time. Now type

`>bsub -n 1 -q S -e errfile -o outfile "mpijob mpirun kukan40"`

to execute the atomic-structure optimization calculation program.

When the program is completed, information on electronic structures at each MD (structural optimization) step is output to "mdresult.dat". When the "total energy" is approximately -21.6000 (a.u.) at mdstep=40, the last part of "mdresult.dat", and the distance between two atoms is approximately 2.1 (a.u.) in the column of "atom coordinate (output)", the calculation is successful.

4 Parallelization using plural processors

As described in Section 2.5, 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 Chapter 3. However, due to an alteration of the computation sequence by parallelization, some of the computation results in this chapter may be slightly different from those in Chapter 3.

4.1 2×1 parallelization processing

First, parallelization processing is performed within a single node. This operation is basically the same as that in Chapter 3. Instead of

>`make -f make.dragons lda0`
input in Section 3.2, type the following.
>`make -f make.dragonp lda0`
Other operations are identical to those in Chapter 3.

4.2 1×2 parallelization processing within one node

Parallelization processing by generating 2 processes within one node is explained. When actually executing parallelization using 2 nodes or more, refer to Section 4.3.

First, after the completion of the operation up to Section 3.1 in Chapter 3, change the current directory to "∼/CO/source". Open "param.f" with the editor and change the parameter to NPROCX=2. With this, the region of -XMAX<0 is operated by the process 0, and the region of 0<-XMAX is operated by the process 1. Although it is not performed here, a similar division is performed when NPROC(Y,Z) is altered. The total number of nodes is NPROCX × NPROCY × NPROCZ. For parallelization, the restrictions that 2×N(X,Y,Z)MAX are divisible by the respective NPROC(X,Y,Z), and that NPROC(X,Y,Z) are either 1 or even numbers apply.

```
example of param.f (only the first 24 lines)
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=2,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=10.0D0,YMAX=10.0D0,ZMAX=10.0D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=30,NYMAX=30,NZMAX=30)
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=9,NPYMAX=9,NPZMAX=9)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=8,NATOM=2,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=1,NUMS=1)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=0)
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)
```

The contents of other files are identical to those in Chapter 3. The same operations as in Chapter 3 are performed for compilation and file copying. Type
>`bsub -n 2 -R "span[ptile=2]" -q S -e errfile -o outfile "mpijob mpirun pre"`
at "∼/CO/exe" to create the initial wave functions. Here, the numbers after "-n" and "ptile=" are the number of nodes and the number of processors per node, respectively. Accordingly, in the $m \times n$ parallelization, "n" corresponds to the number of nodes, and "m" corresponds to the number of processors.[9] After the completion of the above operations, "ele.000", "ele.001", "wfc.000" and "wfc.001" should be created in "∼/CO/exe", where the numbers expressed by * in "ele.00*" and "wfc.00*" are the numbers allocated to each process. "ele.000" and "wfc.000" are input/output by process 0, and "ele.001" and "wfc.001" are input/output by process 1.

Next, type
>`bsub -n 2 -R "span[ptile=2]" -q S -e errfile -o outfile "mpijob mpirun kukan40"`

[9]When no designation is made, "span[ptile=2]" is assumed.

to execute the electronic-structure calculation program. Output results are identical to those in Chapter 3.

4.3 1×2 parallelization processing with two nodes

Here, parallelization using two or more nodes is explained. Type

```
>bsub -n 2 -R "span[ptile=1]" -q P4 -e errfile -o outfile "mpijob mpirun pre"
>bsub -n 2 -R "span[ptile=1]" -q P4 -e errfile -o outfile "mpijob mpirun kukan40"
```

to execute the programs for the generation of initial wave functions and the calculation of electronic structures.[10]

5 Calculate electronic structure of crystal or surface

Calculations performed up to Chapter 4 are the calculations to obtain electronic structures of isolated clusters. In Chapter 5, a calculation method for crystals and surfaces having a periodic structure is explained. All the calculations in this chapter are performed with one processor because of the small model size.

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

5.2 Calculate electronic structure of lithium crystal

A crystal has periodicity in all the x, y and z directions. Accordingly, the program used in the calculation of electronic structures of crystals is version 43. The directories are created as in Chapter 3; first, create "param.f" as follows.

```
example of param.f (only the first 24 lines)
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=1,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=3.32D0,YMAX=3.32D0,ZMAX=3.32D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=10,NYMAX=10,NZMAX=10)
```

[10] When 2 or more nodes are used, parallel calculation is performed with que P4 or P8.

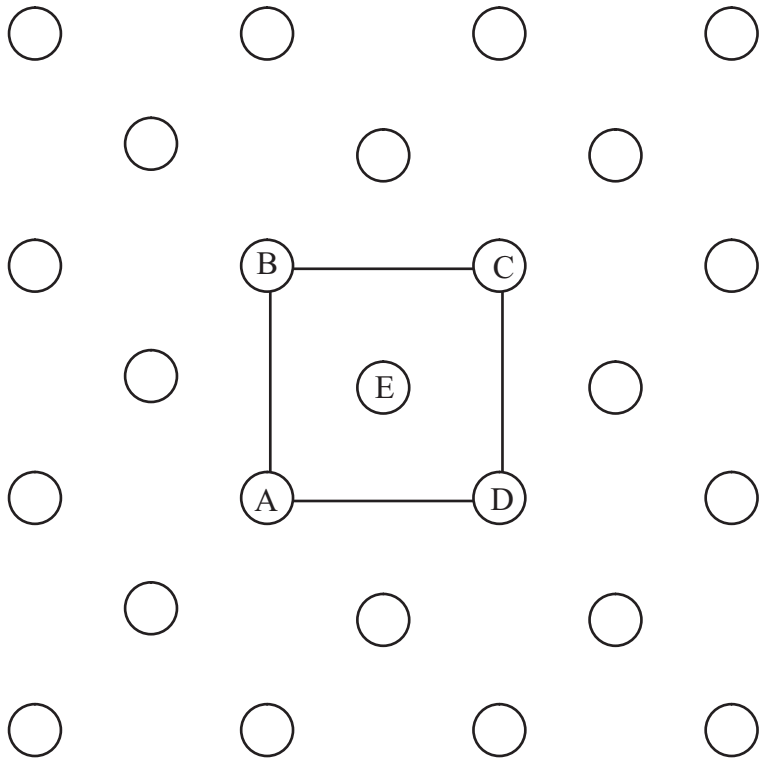

Figure 2: Supercell

```
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=10,NPYMAX=10,NPZMAX=10)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=8,NATOM=2,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=1,NUMS=1)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=3)
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)
```

Since the lattice constant of lithium is 6.64 (a.u.), designate (X,Y,Z)MAX=3.32 so that the calculation region 2×(X,Y,Z)MAX becomes 6.64 (a.u.). For compilation, type the following.
`>make -f make.dragons lda3`
Then, copy the necessary files "pre" and "kukan43" into the execution directory.

```
example of read.inp
#    convergency for CG (P. eq.)   convergency for CG (KS eq.)   convergency of SCF
     1.0D-12                       1.0D-12                       1.0D-8
#    min. it. for CG (P. eq.)      max. it. for CG (P. eq.)      restart for CG (P. eq.):N (1/N its.)
     1                             400                           500
#    max. it. for CG (KS eq.)      switch for CG (KS eq.)(0;no 1;yes)
     2                             1
#    mixing ratio of SCF           max. it. of SCF
     0.10D0                        200
#    time step of MD (a.u.)        Num. it. of MD:Ns(start)      Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     0.0D0                         0                             1
#    Elec. Field in X (a.u.)       Elec. Field in Y (a.u.)       Elec. Field in Z (a.u.)
     0.0D0                         0.0D0                         0.0D0
```

```
#    k point (write all k points)
#    X                          Y                          Z                          ウエイト
     0.0D0                      0.0D0                      0.0D0                      1
#    Fermi temperature(KT) (a.u.)  min. of eigenvalues (a.u.)    max. of eigenvalues (a.u.)
     0.0001D0                   -1000.0D0                  1000.0D0
#    Rayleigh-Ritz:N (1/N scf)     re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                          1                              0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2
```

After creating "read.inp", create the atomic-coordinate file "atom.xyz". As described in Section 5.1, because lithium is a body-centered-cubic crystal, the number of atoms required for the minimum unit cell is 2; therefore, the coordinate file is defined as follows.

```
example of atom.xyz
 -0.3320000E+01 -0.3320000E+01 -0.3320000E+01   3   0   0   0    12866.00
  0.0000000E+00  0.0000000E+00  0.0000000E+00   3   0   0   0    12866.00
```

Here, the positive/negative sign of the coordinate of the atom in line 1 is arbitrary; however, since it is automatically altered by the program to the values such as those shown above, the altered data[11] are output to the output files such as "mdresult.dat". Copying of the files and execution are performed as in Chapter 3; note that "kukan40" is altered to "kukan43." Finally, execution result of the electronic structure calculation "mdresult.dat" is displayed. If the "total energy" part is identical to the contents shown below, then the calculation is successful.

```
 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.)]
   0.110666667D+00   0.110666667D+00   0.110666667D+00
 nonlocal region [vnlx,vnly,vnlz (a.u.)]
   0.664000000D+01   0.664000000D+01   0.664000000D+01
 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.)
   0.315756236D+02   0.100000000D-03
 cufoff of the force (a.u.)
   0.500000000D-02
 mixing ratio of scf
   0.100000000D+00
 nrasy,nrasz
           0           0
 total charge   2.00000000000000
 fermi level  0.000000000000000E+000 (hartree)
 atomic charge
           1   1.00000803902034
           2  0.999991960979647
  1   1   1 eigen value =   -0.1178122856D+00    0.2073869768D-11    0.2000000000D+01
  1   1   2 eigen value =    0.1995609987D+00    0.5303687887D-11    0.0000000000D+00
  1   1   3 eigen value =    0.1995609987D+00    0.9593338376D-11    0.0000000000D+00
  1   1   4 eigen value =    0.1995609987D+00    0.9980901767D-11    0.0000000000D+00
  1   1   5 eigen value =    0.4638158146D+00    0.2989061296D-10    0.0000000000D+00
  1   1   6 eigen value =    0.5167489683D+00    0.2050917370D-10    0.0000000000D+00
  1   1   7 eigen value =    0.5167489683D+00    0.2063266407D-10    0.0000000000D+00
  1   1   8 eigen value =    0.5167489683D+00    0.4127189397D-10    0.0000000000D+00
scf=  68   dp=    0.9340968942D-08
    one electoron energy     -0.235624571166907      (hartree)
```

[11] When periodic boundary conditions are applied, data are altered so that atoms are within $-\mathrm{XMAX}-\mathrm{DX}/2 \leq x \leq +\mathrm{XMAX}-\mathrm{DX}/2$ in the program.

```
 exchange correlation energy -5.386069972278303E-003 (hartree)
    hartree       energy     -1.621170951704844E-003 (hartree)
    ewald         energy     -0.548077326733235      (hartree)
    field correction          0.000000000000000E+000 (hartree)
   helmholtz free energy     -0.790709138824125      (hartree)
    total         energy     -0.790709138824125      (hartree)
 mdstep=           1
 atom coordinate (input)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.3320000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  12866.00
 atom coordinate (output)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.3320000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  12866.00
 atomic force
  1   0.8770383276775760D-17  -0.1502306554972619D-16  -0.4150725315750125D-16
  2  -0.8770383276775760D-17   0.1502306554972619D-16   0.4150725315750125D-16
 real time   28.4494550228119      (sec)
 com. time  9.999990463256836E-003 (sec)
 com. vol.  0.000000000000000E+000 (byte)
 ======================================================================
 This calculation was executed using pseudopotential database NCPS97.
 For NCPS database, see K.Kobayashi, Comput. Mater. Sci. 14, 72 (1999).
```

5.3 Calculate electronic structure of lithium surface

Next, the electronic structure of the lithium surface is calculated. No first-principles electronic structure calculation method 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, has 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. Accordingly, the program used for the electronic structure calculation of thin films is version 42. Directories are created in a manner identical to that in Chapter 3. Then, first create "param.f", as described in Chapter 3, as follows.

```
example of param.f (only the first 24 lines)
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=1,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=3.32D0,YMAX=3.32D0,ZMAX=13.28D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=10,NYMAX=10,NZMAX=40)
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=10,NPYMAX=10,NPZMAX=10)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=16,NATOM=4,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=1,NUMS=1)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=2)
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)
```

Since the lattice constant of lithium is 6.64 (a.u.), designate (X,Y,Z)MAX=3.32 so that the calculation region 2×(X,Y,Z)MAX becomes 6.64 (a.u.). The calculation region in the z direction with no periodicity should be set slightly longer than this value, because the boundary surface must be detached from atoms. Create "read.inp" as follows.

```
example of read.inp
```

```
#    convergency for CG inerration (P. eq.)       convergency for CG inerration (KS eq.)     SCF の収束判定
     1.0D-12                       1.0D-12                       1.0D-8
#    min. it. for CG (P. eq.)      max. it. for CG (P. eq.)      restart for CG (P. eq.):N (1/N its.)
     1                             400                           500
#    max. it. for CG (KS eq.)      switch for CG (KS eq.)(0;no 1;yes)
     2                             1
#    mixing ratio of SCF           max. it. of SCF
     0.05D0                        200
#    time step of MD (a.u.)        Num. it. of MD:Ns(start)      Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     0.0D0                         0                             1
#    Elec. Field in X (a.u.)       Elec. Field in Y (a.u.)       Elec. Field in Z (a.u.)
     0.0D0                         0.0D0                         0.0D0
#    k point (write all k points)
#    X                             Y                             Z                             weight
     0.0D0                         0.0D0                         0.0D0                         1
#    Fermi temperature(KT) (a.u.)  min. of eigenvalues (a.u.)    max. of eigenvalues (a.u.)
     0.0001D0                      -1000.0D0                     1000.0D0
#    Rayleigh-Ritz:N (1/N scf)     re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                             1                                 0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2
```

After creating “read.inp” and compilation, create the atomic coordinate file “atom.xyz.” The number of atoms necessary for the minimum unit cell is 4, and the coordinate file is made as follows.

```
example of atom.xyz
 -0.3320000E+01 -0.3320000E+01 -0.4980000E+01   3   0   0   0    12866.00
  0.0000000E+00  0.0000000E+00 -0.1660000E+01   3   0   0   0    12866.00
 -0.3320000E+01 -0.3320000E+01  0.1660000E+01   3   0   0   0    12866.00
  0.0000000E+00  0.0000000E+00  0.4980000E+01   3   0   0   0    12866.00
```

Copying of the file and execution are performed as in Chapter 3, but be sure to the alteration from “kukan40” to “kukan42”. Finally, execution result “mdresult.dat” of the electronic structure calculation is displayed. If the “total energy” part and “atom force” part are identical to the contents shown below, then the calculation is successful.

```
example of mdresult.dat
 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.)]
   0.110666667D+00   0.110666667D+00   0.110666667D+00
 nonlocal region [vnlx,vnly,vnlz (a.u.)]
   0.664000000D+01   0.664000000D+01   0.664000000D+01
 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.)
   0.315756236D+02   0.100000000D-03
 cufoff of the force (a.u.)
   0.500000000D-02
 mixing ratio of scf
   0.500000000D-01
 nrasy,nrasz
           0           0
 total charge   4.00000000000000
 fermi level -0.152587890625000      (hartree)
 atomic charge
```

```
          1  0.967249575076897
          2   1.03275143049763
          3   1.03275062842039
          4  0.967248366005066
  1   1   1 eigen value =   -0.2196704018D+00    0.6853601472D-12    0.2000000000D+01
  1   1   2 eigen value =   -0.1768975089D+00    0.6728713433D-11    0.2000000000D+01
  1   1   3 eigen value =   -0.1266419235D+00    0.1790864275D-11    0.0000000000D+00
  1   1   4 eigen value =   -0.7439854043D-01    0.3724121012D-11    0.0000000000D+00
  1   1   5 eigen value =   -0.1110562288D-01    0.3347725756D-11    0.0000000000D+00
  1   1   6 eigen value =    0.8068451685D-01    0.1832362815D-09    0.0000000000D+00
  1   1   7 eigen value =    0.1004363050D+00    0.7532717841D-12    0.0000000000D+00
  1   1   8 eigen value =    0.1004363050D+00    0.9460792198D-12    0.0000000000D+00
  1   1   9 eigen value =    0.1219676673D+00    0.2811960464D-10    0.0000000000D+00
  1   1  10 eigen value =    0.1519722048D+00    0.7256278434D-12    0.0000000000D+00
  1   1  11 eigen value =    0.1519722048D+00    0.4901169071D-11    0.0000000000D+00
  1   1  12 eigen value =    0.2269131077D+00    0.5608559071D-12    0.0000000000D+00
  1   1  13 eigen value =    0.2269131078D+00    0.2327435943D-10    0.0000000000D+00
  1   1  14 eigen value =    0.2383325693D+00    0.1261513382D-08    0.0000000000D+00
  1   1  15 eigen value =    0.3192690808D+00    0.1792683991D-10    0.0000000000D+00
  1   1  16 eigen value =    0.3192690809D+00    0.6374910847D-09    0.0000000000D+00
scf= 142   dp=    0.9268376643D-08
    one electoron energy     -0.793135821317456      (hartree)
 exchange correlation energy -2.020703521583506E-002 (hartree)
    hartree       energy       5.33767415324447      (hartree)
    ewald         energy      -5.96650333694423      (hartree)
    field correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -1.44217204023306      (hartree)
    total         energy      -1.44217204023306      (hartree)
 mdstep=           1
 atom coordinate (input)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.4980000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00  -0.1660000000000000D+01   3   0   0   0  12866.00
  3  -0.3320000000000000D+01  -0.3320000000000000D+01   0.1660000000000000D+01   3   0   0   0  12866.00
  4   0.0000000000000000D+00   0.0000000000000000D+00   0.4980000000000000D+01   3   0   0   0  12866.00
 atom coordinate (output)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.4980000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00  -0.1660000000000000D+01   3   0   0   0  12866.00
  3  -0.3320000000000000D+01  -0.3320000000000000D+01   0.1660000000000000D+01   3   0   0   0  12866.00
  4   0.0000000000000000D+00   0.0000000000000000D+00   0.4980000000000000D+01   3   0   0   0  12866.00
 atomic force
  1  -0.8407493306262627D-16   0.2804451702379245D-16  -0.2554335266887098D-02
  2  -0.5458557017826061D-16   0.2985089337772781D-18   0.1253766698119486D-02
  3   0.4371815274932037D-17   0.4886340272487307D-16  -0.1253688155347638D-02
  4   0.1342886879659548D-15  -0.7720642868244279D-16   0.2554256724115250D-02
 real time   277.704668998718      (sec)
 com. time  3.999137878417969E-002 (sec)
 com. vol.  0.000000000000000E+000 (byte)
 ======================================================================
 This calculation was executed using pseudopotential database NCPS97.
 For NCPS database, see K.Kobayashi, Comput. Mater. Sci. 14, 72 (1999).
```

6 More accurate first-principles calculation

The calculations described up to the previous section are the simplest, in other words, the rough approximate first-principles electronic structure calculations. To improve the accuracy of calculation, there are methods of considering spins and of increasing the number of sampling k-points in a periodic model. In this chapter, such methods are explained.

6.1 Electronic structure calculation with consideration of spin

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. Create "param.f", "read.inp" and "atom.xyz" as follows.

```
example of param.f (only the first 24 lines)
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=1,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=8.0D0,YMAX=8.0D0,ZMAX=8.0D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=24,NYMAX=24,NZMAX=24)
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=9,NPYMAX=9,NPZMAX=9)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=8,NATOM=2,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=1,NUMS=2)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=0)
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)

example of read.inp
#    convergency for CG inerration (P. eq.)       convergency for CG inerration (KS eq.)     SCF の収束判定
     1.0D-12                      1.0D-12                      1.0D-8
#    min. it. for CG (P. eq.)     max. it. for CG (P. eq.)     restart for CG (P. eq.):N (1/N its.)
     1                            400                          500
#    max. it. for CG (KS eq.)     switch for CG (KS eq.)(0;no 1;yes)
     2                            1
#    mixing ratio of SCF          max. it. of SCF
     0.10D0                       200
#    time step of MD (a.u.)       Num. it. of MD:Ns(start)     Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     0.0D0                        0                            1
#    Elec. Field in X (a.u.)      Elec. Field in Y (a.u.)      Elec. Field in Z (a.u.)
     0.0D0                        0.0D0                        0.0D0
#    k point (write all k points)
#    X                            Y                            Z                            weight
     0.00D0                       0.00D0                       0.00D0                       1
#    Fermi temperature(KT) (a.u.) min. of eigenvalues (a.u.)   max. of eigenvalues (a.u.)
     0.0001D0                     -1000.0D0                    1000.0D0
#    Rayleigh-Ritz:N (1/N scf)    re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                            1                                 0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2

example of atom.xyz
  0.1100000E+01  0.0000000E+00  0.0000000E+00   8   0   0   0   29408.00
 -0.1100000E+01  0.0000000E+00  0.0000000E+00   8   0   0   0   29408.00
```

The operations are basically similar to those in Chapter 3, but it should be noted that NUMS in "param.f" has been set to 2. Input the following for compilation.

`>make -f make.dragons lsda0`

Make sure to type "lsda" instead of "lda". Other than this, the operations are identical to those in Chapter 3. The output result "mdresult.dat" is shown below:

```
example of mdresult.dat
 cell size [lx,ly,lz (a.u.)]
   0.160000000D+02   0.160000000D+02   0.160000000D+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.)]
   0.111111111D+00   0.111111111D+00   0.111111111D+00
 nonlocal region [vnlx,vnly,vnlz (a.u.)]
```

```
  0.600000000D+01   0.600000000D+01   0.600000000D+01
 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.)
  0.315756236D+02   0.100000000D-03
 cufoff of the force (a.u.)
  0.500000000D-02
 mixing ratio of scf
  0.100000000D+00
 nrasy,nrasz
          0           0
 total charge   12.0000000000000
 fermi level -0.183105468750000      (hartree)
 atomic charge
          1   6.00000124907822
          2   5.99999875092187
  1   1   1 eigen value =   -0.1250449843D+01    0.9853324659D-12    0.1000000000D+01
  1   1   2 eigen value =   -0.7358900948D+00    0.7557513382D-12    0.1000000000D+01
  1   1   3 eigen value =   -0.5204972613D+00    0.8099017100D-11    0.1000000000D+01
  1   1   4 eigen value =   -0.5204972358D+00    0.7842062476D-11    0.1000000000D+01
  1   1   5 eigen value =   -0.5145541678D+00    0.7139757295D-12    0.1000000000D+01
  1   1   6 eigen value =   -0.2402934242D+00    0.6102861955D-11    0.1000000000D+01
  1   1   7 eigen value =   -0.2402933938D+00    0.5418164983D-11    0.1000000000D+01
  1   1   8 eigen value =    0.6012055962D-01    0.3413178094D-04    0.0000000000D+00
  1   2   1 eigen value =   -0.1201854523D+01    0.9270068382D-12    0.1000000000D+01
  1   2   2 eigen value =   -0.6707397602D+00    0.4974411436D-11    0.1000000000D+01
  1   2   3 eigen value =   -0.4708171441D+00    0.7836487258D-12    0.1000000000D+01
  1   2   4 eigen value =   -0.4561860939D+00    0.1666281538D-10    0.1000000000D+01
  1   2   5 eigen value =   -0.4561860124D+00    0.1540088571D-10    0.1000000000D+01
  1   2   6 eigen value =   -0.1632235824D+00    0.6376329410D-11    0.0000000000D+00
  1   2   7 eigen value =   -0.1632234930D+00    0.1620357289D-10    0.0000000000D+00
  1   2   8 eigen value =    0.2828060391D-01    0.1443861832D-03    0.0000000000D+00
scf= 106   dp=    0.8882018574D-08
    one electoron energy      -7.27825895479820      (hartree)
 exchange correlation energy   2.08449247570767      (hartree)
    hartree       energy      -42.8905266088814      (hartree)
    ewald         energy       16.3636363636364      (hartree)
    field correction          0.000000000000000E+000 (hartree)
   helmholtz free energy      -31.7206567243356      (hartree)
    total         energy      -31.7206567243356      (hartree)
 mdstep=           1
 atom coordinate (input)
  1   0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00
  2  -0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00
 atom coordinate (output)
  1   0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00
  2  -0.1100000000000000D+01   0.0000000000000000D+00   0.0000000000000000D+00   8   0   0   0  29408.00
 atomic force
  1   0.7898879336295694D-01   0.2620224698811231D-14   0.1005343984723030D-13
  2  -0.7898879336295694D-01  -0.2620224698811232D-14  -0.1005343984723030D-13
 real time   249.685297966003      (sec)
 com. time  2.999567985534668E-002 (sec)
 com. vol.  0.000000000000000E+000 (byte)
 ======================================================================
 This calculation was executed using pseudopotential database NCPS97.
 For NCPS database, see K.Kobayashi, Comput. Mater. Sci. 14, 72 (1999).
```

Next, for atomic-structure optimization, change the contents of “read.inp” and “atom.xyz” as in Chapter 3, then execute “kukan40”.

6.2 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 Sections 5.2 and 5.3 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. Here, the electronic structure of a lithium crystal is calculated with 64 k-points.

Creation of "read.inp" In order to increase the number of sampling k-points, manually input the value of k-points to be calculated into the calculation-condition setting file "read.inp". 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}{llll}
\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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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}{2}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 "read.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.

```
#    convergency for CG (P. eq.)   convergency for CG (KS eq.)   convergency of SCF
     1.0D-12                       1.0D-12                       1.0D-8
#    min. it. for CG (P. eq.)      max. it. for CG (P. eq.)      restart for CG (P. eq.):N (1/N its.)
     1                             400                           500
#    max. it. for CG (KS eq.)      switch for CG (KS eq.)(0;no 1;yes)
     2                             1
#    mixing ratio of SCF           max. it. of SCF
     0.10D0                        200
#    time step of MD (a.u.)        Num. it. of MD:Ns(start)      Num. it. of MD:Ne(end) (Ne-Nsis the total number of it. of MD
     0.0D0                         0                             1
#    Elec. Field in X (a.u.)       Elec. Field in Y (a.u.)       Elec. Field in Z (a.u.)
     0.0D0                         0.0D0                         0.0D0
#    k point (write all k points)
```

```
#    X                            Y                            Z                            weight
     -0.50D0                      -0.50D0                      -0.50D0                      1
     -0.25D0                      -0.50D0                      -0.50D0                      2
      0.00D0                      -0.50D0                      -0.50D0                      1
     -0.50D0                      -0.25D0                      -0.50D0                      2
     -0.25D0                      -0.25D0                      -0.50D0                      2
      0.00D0                      -0.25D0                      -0.50D0                      2
      0.25D0                      -0.25D0                      -0.50D0                      2
     -0.50D0                       0.00D0                      -0.50D0                      1
     -0.25D0                       0.00D0                      -0.50D0                      2
      0.00D0                       0.00D0                      -0.50D0                      1
     -0.50D0                      -0.50D0                      -0.25D0                      2
     -0.25D0                      -0.50D0                      -0.25D0                      2
      0.00D0                      -0.50D0                      -0.25D0                      2
      0.25D0                      -0.50D0                      -0.25D0                      2
     -0.50D0                      -0.25D0                      -0.25D0                      2
     -0.25D0                      -0.25D0                      -0.25D0                      2
      0.00D0                      -0.25D0                      -0.25D0                      2
      0.25D0                      -0.25D0                      -0.25D0                      2
     -0.50D0                       0.00D0                      -0.25D0                      2
     -0.25D0                       0.00D0                      -0.25D0                      2
      0.00D0                       0.00D0                      -0.25D0                      2
      0.25D0                       0.00D0                      -0.25D0                      2
     -0.50D0                       0.25D0                      -0.25D0                      2
     -0.25D0                       0.25D0                      -0.25D0                      2
      0.00D0                       0.25D0                      -0.25D0                      2
      0.25D0                       0.25D0                      -0.25D0                      2
     -0.50D0                      -0.50D0                       0.00D0                      1
     -0.25D0                      -0.50D0                       0.00D0                      2
      0.00D0                      -0.50D0                       0.00D0                      1
     -0.50D0                      -0.25D0                       0.00D0                      2
     -0.25D0                      -0.25D0                       0.00D0                      2
      0.00D0                      -0.25D0                       0.00D0                      2
      0.25D0                      -0.25D0                       0.00D0                      2
     -0.50D0                       0.00D0                       0.00D0                      1
     -0.25D0                       0.00D0                       0.00D0                      2
      0.00D0                       0.00D0                       0.00D0                      1
#    Fermi temperature(KT) (a.u.) min. of eigenvalues (a.u.)   max. of eigenvalues (a.u.)
     0.0001D0                     -1000.0D0                    1000.0D0
#    Rayleigh-Ritz:N (1/N scf)    re-order eigenstates:N (1/N scf)  omit the comp. of Coulomb pot. of fixed atoms (0;no 2;yes
     1                            1                                 0
#    total negative charge - total positive charge
     0.0D0
#    cutoff of force
     0.5D-2
```

Creation of other files Next, create the parameter file. The point of difference compared with Section 5.2 is the "NUMK" value of 36 on line 9. An example of the creation of the parameter file is shown below.

```
example of param.f (only the first 24 lines)
 1:!     **********  param.f 05/02/2011-01  **********
 2:      IMPLICIT REAL*8 (A-H,O-Z)
 3:      INCLUDE 'mpif.h'
 4:! number of processors (nodes)
 5:      PARAMETER (NPROCX=1,NPROCY=1,NPROCZ=1)
 6:! size of supercell
 7:      PARAMETER (XMAX=3.32D0,YMAX=3.32D0,ZMAX=3.32D0)
 8:! number of grid points
 9:      PARAMETER (NXMAX=10,NYMAX=10,NZMAX=10)
10:! number of grid points in core region
11:      PARAMETER (NPXMAX=10,NPYMAX=10,NPZMAX=10)
12:! number of wave functions, number of wave atoms, number grid points for spiral boundary conditions
13:      PARAMETER (NEIGMX=8,NATOM=2,NRASXY=0,NRASXZ=0,NRASYZ=0)
14:! number of sampling k-pints, electron spin
15:      PARAMETER (NUMKX=1,NUMKY=1,NUMKZ=1,NUMK=36,NUMS=1)
16:! number of grid points for double grid technique
17:      PARAMETER (NMESH=3)
18:! switch for periodic boundary conditions
19:      PARAMETER (NPERI=3)
```

```
20:! charge of jellium (if you do not use jellium, set CHRJEL to be zero.)
21:      PARAMETER (ENDJEL=0.0D0,CHRJEL=0.0D0)
22:
23:! switch for the type of computer (scalar;0, vector;1)
24:      PARAMETER (MACHINE=0)
```

The atomic coordinates file “atom.xyz” is identical to that in Section 5.2. Compilation and execution are also performed identically to those in Section 5.2. Below is an example of the output of the electronic-structure calculation result “mdresult.dat”.

```
example of mdresult.dat
 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.)]
   0.110666667D+00   0.110666667D+00   0.110666667D+00
 nonlocal region [vnlx,vnly,vnlz (a.u.)]
   0.664000000D+01   0.664000000D+01   0.664000000D+01
 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.)
   0.315756236D+02   0.100000000D-03
 cufoff of the force (a.u.)
   0.500000000D-02
 mixing ratio of scf
   0.100000000D+00
 nrasy,nrasz
           0           0
```

```
 total charge   1.99999999999993
 fermi level  7.14978657779170E-003 (hartree)
 atomic charge
           1  0.999997434689555
           2   1.00000256531064
  1   1   1 eigen value =    0.1271181160D+00    0.1083547447D-10    0.0000000000D+00
  1   1   2 eigen value =    0.1271183920D+00    0.1713894363D-10    0.0000000000D+00
  1   1   3 eigen value =    0.1271198154D+00    0.4268511246D-11    0.0000000000D+00
  1   1   4 eigen value =    0.1271200480D+00    0.3571187958D-11    0.0000000000D+00
  1   1   5 eigen value =    0.1271217278D+00    0.1533725279D-10    0.0000000000D+00
  1   1   6 eigen value =    0.1271219741D+00    0.5014411299D-11    0.0000000000D+00
  1   1   7 eigen value =    0.2946099298D+00    0.1855425777D-10    0.0000000000D+00
  1   1   8 eigen value =    0.2946100753D+00    0.6763772503D-10    0.0000000000D+00

                                                 ............
                                                 ............
                                                 ............

 36   1   1 eigen value =   -0.1175039808D+00    0.1286537827D-10    0.3125000000D-01
 36   1   2 eigen value =    0.1996909149D+00    0.1417640513D-10    0.0000000000D+00
 36   1   3 eigen value =    0.1996938022D+00    0.8841951083D-11    0.0000000000D+00
 36   1   4 eigen value =    0.1996971599D+00    0.7549029704D-11    0.0000000000D+00
 36   1   5 eigen value =    0.2923582235D+00    0.6749380587D-02    0.0000000000D+00
 36   1   6 eigen value =    0.5164111164D+00    0.9270942044D-10    0.0000000000D+00
 36   1   7 eigen value =    0.5164138899D+00    0.4742088553D-10    0.0000000000D+00
 36   1   8 eigen value =    0.5164167871D+00    0.6850669262D-11    0.0000000000D+00
scf=  68   dp=    0.9186551643D-08
    one electoron energy     -7.842581501942483E-002 (hartree)
 exchange correlation energy -6.650449821272245E-003 (hartree)
    hartree       energy     -9.416134072745397E-004 (hartree)
    ewald         energy     -0.548077326733235      (hartree)
    field correction          0.000000000000000E+000 (hartree)
   helmholtz free energy     -0.634140477571235      (hartree)
    total         energy     -0.634095204981207      (hartree)
 mdstep=           1
 atom coordinate (input)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.3320000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  12866.00
 atom coordinate (output)
  1  -0.3320000000000000D+01  -0.3320000000000000D+01  -0.3320000000000000D+01   3   0   0   0  12866.00
  2   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   3   0   0   0  12866.00
 atomic force
  1   0.2852771071137328D-12  -0.1347960982550435D-12   0.1335356698440086D-12
  2  -0.2852771071137320D-12   0.1347960982550435D-12  -0.1335356698440086D-12
 real time   470.199990034103      (sec)
 com. time  0.109968900680542      (sec)
 com. vol.  0.000000000000000E+000 (byte)
 ======================================================================
 This calculation was executed using pseudopotential database NCPS97.
 For NCPS database, see K.Kobayashi, Comput. Mater. Sci. 14, 72 (1999).
```

A Determination of grid width

Regarding the grid width DX, DY, and DZ, 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.[12]

[12]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.

DX, DY, and DZ (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.

B Determination of cut-off radius of pseudopotential

For the cut-off radius of pseudopotential, a value larger than the maximum cut-off radius required for atoms contained in a cell should be used. The cut-off radius required for each atom is listed below.

Atom	Cut-off radius(a.u.)	Atom	Cut-off radius(a.u.)
H	0.951	Al	2.500
Li	2.800	Si	2.300
C	1.450	S	1.750
N	1.240	Cl	1.950
O	1.519	Fe	2.550
F	1.256	Cu	2.600
Na	4.200	W	2.800

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