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

(for transport-property 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 (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:

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1.3 License

1.4 Reference

Please use the following references for the transport-property 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, Y. Egami, K. Hirose, Phys. Rev. B **86**, 195406 (2012).
For the database of norm-conserving pseudopotentials NCPS97, 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 RSPACEtr taken from https://github.com/onotmy/RSPACEdist or unzipped RSPACEtr.zip distributed in workshops is copied on the any directory of the computer. In the directory where the code is expanded, the directories kukan, inverse, genbloch, negf_sclapck, and NCPS are generated. The directories kukan, inverse, genbloch, negf_sclapck are the directory storing the source code and the latter is that containing pseudopotentials for excise.

2.2 Setup of makefile

For compile of the source code, makefiles in directories kukan, inverse, genbloch, and negf_sclapck have to be modified. In the expanded directory, 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 each directory. After the compile is completed, check whether "kukan8", "inverse", "genbloch", and "negf" are generated.

2.4 Pseudopotentials

Transport-property calculations require the use of norm-conserving pseudopotentials. The pseudopotentials for transport-property calculations are stored in the NCPS directry, which is generated by unzip source code. Make sure that 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 for transport-property calculations

The model for the transport-property calculation consists of three parts: the left and right electrode regions and the scattering region, as shown in Fig. 1. The coordinate axes shown in black in Fig. 1 are those of the entire system. The potential of the left electrode region is calculated using the blue coordinate axes, and the potential of the right electrode region is calculated using the coordinate axes and supercells shown by green lines. To calculate the potential of the scattering region, the coordinate axes and supercells with red lines are used. The model should also be created so that the junction surface of the electrode and scattering regions is not crossed by a nonlocal region of pseudopotential. Figure 2 shows the junction of

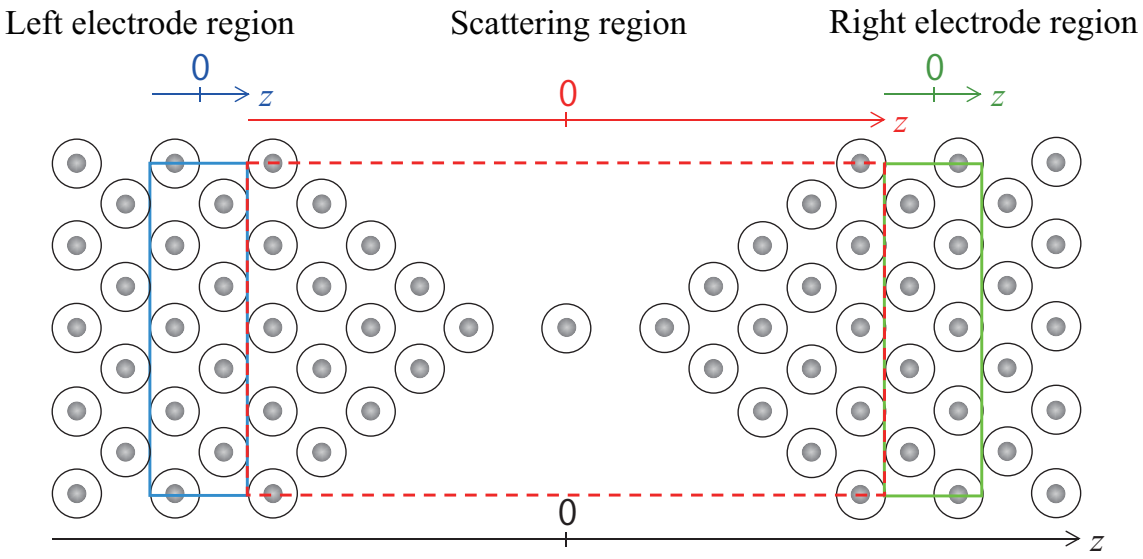

Figure 1: Model for transport-property calculations. The blue lines show the coordinate axes and supercells for the left electrode region calculation. The green lines show the coordinate axes and supercells for the right electrode region calculation. Red lines are coordinate axes and supercells for scattering region calculation. Gray spheres represent atoms. The black circles surrounding the gray sphere are the nonlocal regions of the pseudopotential of the atom.

the left electrode region and the scattering region. A magnified view of the interface is shown, where `npzmax` is the number of grids corresponding to the radius of the nonlocal region of the pseudopotential. Therefore, the junction interface is set at a distance of `npzmax` from the atoms.

4 Transport-Property Calculation Flow

Transport calculations are performed in the following steps: 1) electronic state calculations for the electrode and scattering region, 2) Green's function calculations for the electrode and scattering region, 3) generalized Bloch wave calculations for the electrode region, and 4) scattering wave function calculations (transmission property calculations). In this section, we investigate the transport properties of a monoatomic chain of C atoms. First, in Chap. 5, we calculate the transport properties for a model in which the electrode and scattering region are exactly the same, as shown in Fig. 3. Next, in Chap. 6, we calculate the transport properties of a model

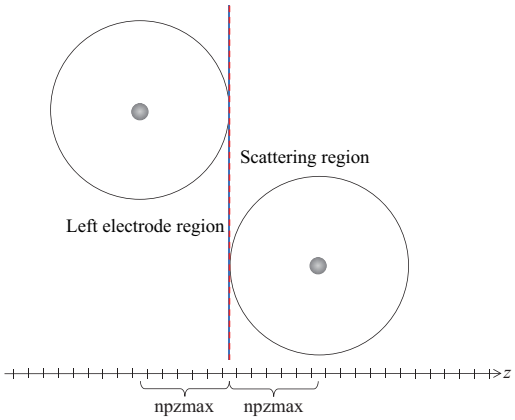

Figure 2: Junction interface between the left electrode region and the scattering region.

in which the structure used in Chap. 5 is used as the electrode, and the position of the C atom in the scattering region is slightly changed as shown in Fig. 4, so that the electrode region and the scattering region are different.

5 Calculation of transport properties when the electrode region and scattering region are the same

5.1 Calculation of electronic structure in the electrode (scattering) region

Create a calculation directory electrode for the electrode region and copy `kukan8` from `~/RSPACE/kukan` to the execution directory in it, referring to the electronic structure calculation section. Create a calculation condition setting file `parameters.inp` and an atom coordinate file `atom.xyz` as shown below. Note that each of the scattering region and electrode region has its own coordinate origin, as shown in Fig. 3.

```
    Example of a parameters.inp file.
 1:  &nml_inp_prm_kukan
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  xmax = 5.2d0
 6:  ymax = 5.2d0
 7:  zmax = 1.4d0
 8:  nxmax = 8
 9:  nymax = 8
10:  nzmax = 4
11:  npxmax = 4
12:  npymax = 4
13:  npzmax = 4
14:  neigmx = 4
15:  natom = 1
16:  lveffout = .true.
17:  /

Example of atom.xyz file (first 2 lines only).
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2:   0.00000000000000000D+00  0.00000000000000000D+00  0.00000000000000000D+00 6 0 0 0 22056.00 00 1 1a
```

Create a directory `pspaw` under the directory electrode and copy the normconserving pseudopotentials for C atoms into it.

Then, create the execution script `job.sh` as follows.

Example of job.sh file

```
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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
```

After that, submit the script `job.sh` by

`qsub -q mm job.sh`

The `-q` option specifies the execution queue. Specify a queue appropriate for the job to be submitted.

When the electronic structure calculation is completed, `rho.0000*`, `vht.0000*`, `wfc.00000.00*`, `mdresult.dat`, `Potential.txt` are created. * is a number from 0 to 7. The calculation results can be checked by entering

`cat mdresult.dat .`

The contents of `mdresult.dat` are shown below.

```
Example output from mdresult.dat (last 26 lines only)
    one electron energy       -1.98428247580907      (hartree)
 exchange correlation energy  0.503128486008291      (hartree)
    hartree       energy      -3.87149552432593      (hartree)
    ewald         energy     -0.653017442586121      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
  energy offset of ps. pot.   0.000000000000000E+000 (hartree)
  energy jellium/ions         0.000000000000000E+000 (hartree)
   helmholtz free energy      -6.00566695673548      (hartree)
    Total         energy      -6.00566695671283      (hartree)
 atomic force
    1   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00
 mdstep=           1
 atom coordinate (input)
   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   6   0   0   0  22056.00   11  0    1a
 atom coordinate (output)
   0.0000000000000000D+00   0.0000000000000000D+00   0.0000000000000000D+00   6   0   0   0  22056.00   11  0    1a
 real time   1.50830888748169      (sec)
 com. time  0.363945007324219      (sec)
 com. vol.   610557952.000000      (byte)
```

The calculation is successful if the total energy and atom force in `mdresult.dat` agree with the above results by about 10 digits. Since the computation order differs depending on the compiler, the results may differ from the above results for the part after 10 digits.

5.2 Green's function calculation for electrode (scattering) region

Copy `inverse` and `gfcdir.sh` from `~/RSPACE/inverse` under the directory for the electrode region. Add the execution characteristics with `gfcdir.sh`.

`chmod +x gfcdir.sh`

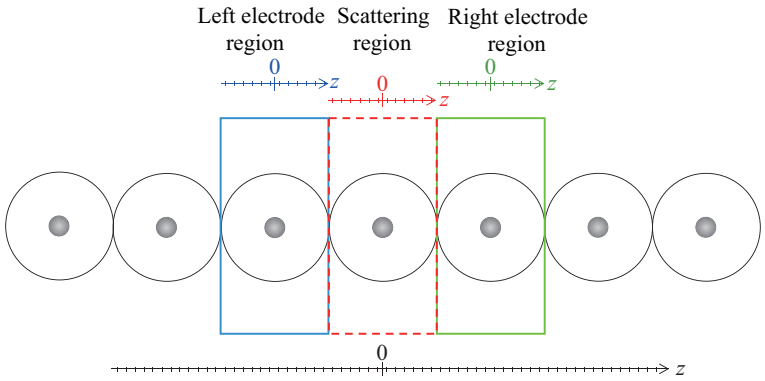

Figure 3: Model with the same structure of electrode and scattering region. The gray sphere is the C atom, and the short line on the z-axis represents the grid point. Other symbols are the same as in Fig. 1.

Then, add the following to `parameters.inp` file created in Sec. 5.1.

```
   Example of a parameters.inp file (only added lines).
 1:  &nml_inp_prm_inv
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  nprocg = 1
 6:  nshift = 5
 7:  deshift = 0.00367485d0
 8:  /
```

where `nprocg` is the number of parallel processes in the column direction of the Green's function, and `nprocx` × `nprocy` × `nprocz` × `nprocg` corresponds to the number of all MPI processes. `nshift` is the number of energy sampling points, from index 0 to `nshift` − 1 is the number of energy samples, where `nshift`/2 (rounded up to the nearest whole number) corresponds to the Fermi level. `deshift` is the interval between energy meshes. The execution script `job.sh` is created as follows.

```
   Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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 ./inverse > output_inverse.txt
```

The red text above shows the changes from Sec. 5.1. Finally, the execution script `job.sh` has been submitted by

```
qsub -q mm job.sh
```

When the calculation of the Green's function is completed, the directories `gfcll`, `gfclr`, `gfcrl`, `gfcrr`, and `gfc` are created and the Green's function information is stored in them. By typing

`tail output_inverse.txt`
the following information will be displayed.

```
Example output from output_inverse.txt (last 10 lines only).
 2045th Green function is converged. # of its     140  elapsed time    0.15705E-01(sec.) 2045/ 2048
 2046th Green function is converged. # of its     140  elapsed time    0.15720E-01(sec.) 2046/ 2048
 2047th Green function is converged. # of its     140  elapsed time    0.15687E-01(sec.) 2047/ 2048
 2048th Green function is converged. # of its     134  elapsed time    0.14973E-01(sec.) 2048/ 2048
 computation of Green function has been completed before the elapsed time limit.
 Green functions have been calculated.
  Elapsed time=  0.3294042E+02   (sec)
 program ended.
 carried out by the version of 12/24/2021-01
  Total elapsed time=  0.3362157E+02  (sec.)
```

The computation is successful if the 6th line from the bottom displays "`computation of Green function has been completed before the elapsed time limit.`"

5.3 Generalized Bloch wave calculation for electrode region

Copy `genbloch` and `gbwdir.sh` from `~/RSPACE/genbloch` under the directory for the electrode region. Add the execution characteristics with `gbwdir.sh`.
`chmod +x gbwdir.sh`
Then, add the following to the `parameters.inp` file created in Sec. 5.2.

```
    Example of a parameters.inp file (only added lines).
 1:  &nml_inp_prm_genbl
 2:  nprocx = 1
 3:  nprocy = 1
 4:  nprocz = 1
 5:  nprocrhpt = 8
 6:  /
```

where `nprocrhpt` is the number of parallel processes for the integration points in the Sakurai-Sugiura method of integration around a circle. `nprocx`×`nprocy`×`nprocz`×`nprocrhpt` corresponds to the number of all MPI processes. The execution script `job.sh` is created as follows.

```
    Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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 ./genbloch > output_genbloch.txt
```

The red text above shows the changes from Sec. 5.2. Finally, the execution script `job.sh` has been submitted by
`qsub -q mm job.sh`

When the calculation of the generalized Bloch wave is completed, the directory `gbwdir` is created and the electrode information is stored in it. By typing
`tail output_genbloch.txt`
the following information will be displayed

```
Example output from output_genbloch.txt (last 10 lines only).
```

```
 Now simultaneous equations are being solved.
 BiCG ended.
 Simultaneous equations have been solved.
  BiCG  0.1112206E+01  (sec.)
BL and BR are being calculated.
BL and BR have been calculated.  0.4599609E+00  (sec.)
  SS method (incl. check)  0.2045255E+02  (sec.)
 all ratio matrices are converged.
 carried out by the version of 12/24/2021-01
  total elapsed time  0.2205640E+02  (sec.)
```

The calculation is successful if "`all ratio matrices are converged.`" is displayed on the third line from the bottom.

5.4 Scattering wave function calculation (transmission property calculation)

After executing `genbloch`, the directory `gbwdir` containing the generalized Bloch waves of the electrodes is created, so link `gbwdir` to `gbwl` for the left electrode and to `gbwr` for the right electrode.

```
ln -s gbwdir gbwl; ln -s gbwdir gbwr
```

Copy `negf` from `~/RSPACE/negf_sclpck` under the directory for the electrode region. Then, add the following to the calculation condition setting file `parameters.inp` created in Sec. 5.3.

```
    Example of a parameters.inp file (only added lines).
 1:  &nml_inp_prm_negf
 2:  /
```

Also, create the execution script `job.sh` as follows.

```
    Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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 ./negf > output_negf.txt
```

The red text above shows the changes from Sec. 5.3. Finally, the execution script `job.sh` has been submitted by

```
qsub -q mm job.sh
```

When the calculation of scattering wavefunctions is completed, the `output_negf.txt.000*` is created and the conductance information is stored in it. The ** is a number from 0 to 4, corresponding to the index of the energy point. By typing

```
tail output_negf.txt
```

the following information will be displayed.

```
Example output from output_negf.txt (last 10 lines only).
 lcalch : T
 *****************************************
Computed by negf.f90 03/26/2021-01.  0.8265972E-02(sec.)
Computed by negf.f90 03/26/2021-01.  0.8724928E-02(sec.)
Computed by negf.f90 03/26/2021-01.  0.8724928E-02(sec.)
```

```
Computed by negf.f90 03/26/2021-01.  0.4714772E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.4787703E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.5115573E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.5655939E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.5758747E+01(sec.)
```

If the display shows "`Computed by negf.f90`" for the number of processes, the computation was successful.

By typing

`cat output_negf.txt.0000`

the transmission information for the 0th energy point is displayed. The number behind "transmission" at the 15th line is the conductance.

```
Generalized Bloch waves of electrodes are being read.
Generalized Bloch waves have been read.  0.1027203E-01(sec.)
Ratio matrices are being read.
Ratio matrices have been read.  0.3162122E-01(sec.)
offdiagonal elements are being read.
offdiagonal elements have been read.  0.1991701E-01(sec.)
Green functions are being read.
Green functions have been read.  0.6935692E-01 (sec)
Self energies are being computed.
Self energies have been computed.  0.3151560E+00(sec.)
Green functions are being computed.
Green functions have been computed.  0.1639958E+01(sec.)
Conductance is being computed by Fisher Lee formula.
 ****************************************
 transmission=   2.00000000000000      (by Fisher Lee)
 ****************************************
```

In `output_negf.txt.0000`, transmission appears three times. In the exercises in this section, no scattering occurs in the scattering region because the electrode region and the scattering region have the same atomic structure. Therefore, it is obvious that the conductance will be an integer.

6 Calculation of transport properties when the electrode region and scattering region are different

6.1 Electronic structure calculations in the scattering region

Here, one atom of the C atom chain, which is neatly lined up with C atoms, is slightly moved to form the scattering region. In order to make the connection between the electrode region and the potential as smooth as possible, a buffer atom is placed on each side of the moved atom, making a cell containing three atoms in the scattering region. Create a directory `scat` for the calculation of scattering region at the same level as electrode. Copy `kukan8` from `~/RSPACE/kukan` to the execution directory. Create a file for setting the calculation conditions, `parameters.inp`, and an atomic coordinates file, `atom.xyz`, as shown below. Note that each of the scattering region and electrode region has its own coordinate origin, as shown in Fig. 4.

```
    Example of a parameters.inp file.
 1:  &nml_inp_prm_kukan
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  xmax = 5.2d0
 6:  ymax = 5.2d0
 7:  zmax = 4.2d0
 8:  nxmax = 8
```

```
 9:  nymax = 8
10:  nzmax = 12
11:  npxmax = 4
12:  npymax = 4
13:  npzmax = 4
14:  neigmx = 12
15:  natom = 3
16:  lveffout = .true.
17:  /

Example of atom.xyz file (first 4 lines only).
1:!  [x], [y], [z], [atom number], switch [x], [y], [z], [weight], switches [soc], [pp], [na]
2:   0.0000000000000000D+00  0.0000000000000000D+00 -2.8000000000000000D+00 6 0 0 0 22056.00 00 1 1a
3:   0.5000000000000000D+00  0.5000000000000000D+00  0.0000000000000000D+00 6 0 0 0 22056.00 00 1 2a
4:   0.0000000000000000D+00  0.0000000000000000D+00  2.8000000000000000D+00 6 0 0 0 22056.00 00 1 3a
```

Create a directory `pspaw` under the directory scat and copy the normconserving pseudopotentials for the C atom into it.

Create the execution script `job.sh` as follows.

```
    Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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
```

After that, the execution script `job.sh` has been submitted by

```
qsub -q mm job.sh
```

When the calculation of electronic structure is completed, `rho.0000*`, `vht.0000*`, `wfc.00000.00*`, `mdresult.dat`, `Potential.txt` are created. * is a number from 0 to 7. By typing

```
cat mdresult.dat
```

the calculation results can be checked. The contents of `mdresult.dat` are shown below.

```
Example output from mdresult.dat (last 30 lines only)
    one electron energy       -4.42126517940423      (hartree)
 exchange correlation energy   1.43546009002026      (hartree)
    hartree       energy      -11.4133984518028      (hartree)
    ewald         energy      -2.30899188167952      (hartree)
    field correction          0.000000000000000E+000 (hartree)
    B_con correction          0.000000000000000E+000 (hartree)
  energy offset of ps. pot.   0.000000000000000E+000 (hartree)
  energy jellium/ions         0.000000000000000E+000 (hartree)
   helmholtz free energy      -16.7174051015430      (hartree)
    Total         energy      -16.7081954228663      (hartree)
 atomic force
    1  -0.5004831433636606D-01  -0.5004831424587112D-01  -0.3428957091978465D-01
    2   0.1001011372392719D+00   0.1001011370422020D+00   0.1928804633492357D-04
    3  -0.5005282290290586D-01  -0.5005282279633087D-01   0.3427028287344972D-01
 mdstep=           1
 atom coordinate (input)
   0.0000000000000000D+00   0.0000000000000000D+00  -0.2800000000000000D+01   6   0   0   0  22056.00   11  0    1a
   0.5000000000000000D+00   0.5000000000000000D+00   0.0000000000000000D+00   6   0   0   0  22056.00   11  0    2a
   0.0000000000000000D+00   0.0000000000000000D+00   0.2800000000000000D+01   6   0   0   0  22056.00   11  0    3a
 atom coordinate (output)
   0.0000000000000000D+00   0.0000000000000000D+00  -0.2800000000000000D+01   6   0   0   0  22056.00   11  0    1a
   0.5000000000000000D+00   0.5000000000000000D+00   0.0000000000000000D+00   6   0   0   0  22056.00   11  0    2a
   0.0000000000000000D+00   0.0000000000000000D+00   0.2800000000000000D+01   6   0   0   0  22056.00   11  0    3a
 real time   17.5159118175507      (sec)
```

```
com. time    5.65586304664612      (sec)
com. vol.    10140364800.0000      (byte)
```

The calculation is successful if the total energy and atom force in `mdresult.dat` agree with the above results by about 10 digits. Since the computation order differs depending on the compiler, the results may differ from the above results for the part after 10 digits.

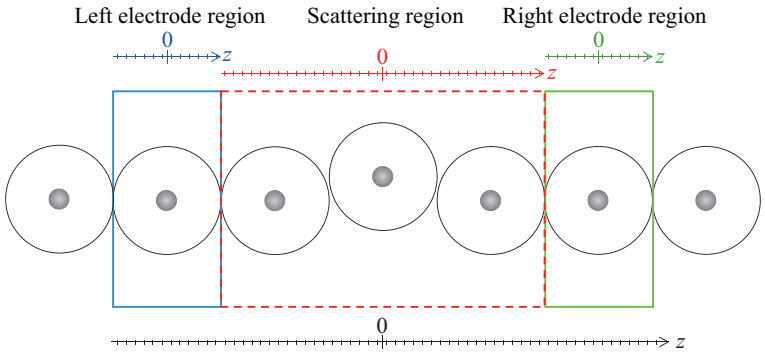

Figure 4: Model with different electrode and scattering region structures. Symbols in the figure are the same as in Fig. 3.

6.2 Green's function calculation in the scattering region

Copy `inverse` and `gfcdir.sh` from `~/RSPACE/inverse` under the directory `scat` for the scattering region. Add the execution characteristics with `gfcdir.sh` by

`chmod +x gfcdir.sh`

Then, add the following to the `parameters.inp` file created in Sec. 6.1.

```
   Example of a parameters.inp file (only added lines).
 1:  &nml_inp_prm_inv
 2:  nprocx = 2
 3:  nprocy = 2
 4:  nprocz = 2
 5:  nprocg = 1
 6:  nshift = 5
 7:  deshift = 0.00367485d0
 8:  /
```

The number of energy sample points `nshift` and the energy mesh spacing `deshift` should match those for which the electrodes were calculated. The execution script `job.sh` is created as follows.

```
   Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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 ./inverse > output_inverse.txt
```

The red text above shows the changes from Sec. 6.1. Finally, the execution script `job.sh` has been submitted by
`qsub -q mm job.sh`

When the calculation of the Green's function calculation is completed, the directories `gfcll`, `gfclr`, `gfcrl`, `gfcrr`, and `gfc` are created and the information of Green's function information is stored in them. By typing
`tail output_inverse.txt`
the following information will be displayed.

```
Example output from output_inverse.txt (last 10 lines only)
2047th Green function. Seed is switched to 3 at itr 38
 2047th Green function. Seed is switched to   3 at itr     384
 2047th Green function is converged. # of its     435  elapsed time    0.62642E-01(sec.) 2047/ 2048
 2048th Green function. Seed is switched to   3 at itr     358
 2048th Green function is converged. # of its     375  elapsed time    0.55043E-01(sec.) 2048/ 2048
 computation of Green function has been completed before the elapsed time limit.
 Green functions have been calculated.
  Elapsed time=  0.1555100E+03   (sec)
 program ended.
 carried out by the version of 12/24/2021-01
  Total elapsed time=  0.1562588E+03  (sec.)
```

The computation is successful if the 6th line from the bottom displays "`computation of Green function has been completed before the elapsed time limit.`".

6.3 Scattering wave function calculation (transmission property calculation)

It is not necessary to calculate the generalized Bloch waves for the scattering region. The generalized Bloch waves for the electrodes have already been calculated in Sec. 5.3, so the `gbwdir` under electrode is changed to the link `gbwl` for the left electrode, `gbwr` for the right electrode.
`ln -s ../electrode/gbwdir gbwl; ln -s ../electrode/gbwdir gbwr`
Copy `negf` from `~/RSPACE/negf_sclpck` under the directory `scat` for scattering region. Then, add the following to the file `parameters.inp` created in Sec. 6.2.

```
   Example of a parameters.inp file (only added lines).
 1:  &nml_inp_prm_negf
 2:  /
```

Also, create the execution script `job.sh` as follows.

```
   Example of job.sh file.
 1:  #!/bin/bash
 2:  #$ -S /bin/bash
 3:  #$ -pe mpi 64
 4:  #$ -cwd
 5:  #$ -V
 6:  export OMP_NUM_THREADS=8
 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 ./negf > output_negf.txt
```

The red text above shows the changes from Sec. 6.2. Finally, the execution script `job.sh` has been submitted by

```
qsub -q mm job.sh
```

When the calculation for scattering wavefunction is completed, the `output_negf.txt.000*` is created and the conductance information is stored in it. The ** is a number from 0 to 4, corresponding to the index of the energy point. By typing

```
tail output_negf.txt
```

the following information will be displayed.

```
Example output from output_negf.txt (last 10 lines only).
 lcalch : T
 ****************************************
Computed by negf.f90 03/26/2021-01.  0.6978035E-02(sec.)
Computed by negf.f90 03/26/2021-01.  0.7871866E-02(sec.)
Computed by negf.f90 03/26/2021-01.  0.8123875E-02(sec.)
Computed by negf.f90 03/26/2021-01.  0.8749112E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.9594602E+01(sec.)
Computed by negf.f90 03/26/2021-01.  0.1020803E+02(sec.)
Computed by negf.f90 03/26/2021-01.  0.1038002E+02(sec.)
Computed by negf.f90 03/26/2021-01.  0.1057339E+02(sec.)
```

If the display shows "`Computed by negf.f90`" for the number of processes, the computation was successful. By typing

```
cat output_negf.txt.0000
```

the transmission information for the 0th energy point is displayed. The number behind "transmission" at the 15th line is the conductance.

```
Example output from output_negf.txt.0000 (first 16 lines only)
Generalized Bloch waves of electrodes are being read.
Generalized Bloch waves have been read.  0.2075791E-01(sec.)
Ratio matrices are being read.
Ratio matrices have been read.  0.2291341E+01(sec.)
offdiagonal elements are being read.
offdiagonal elements have been read.  0.1054244E+01(sec.)
Green functions are being read.
Green functions have been read.  0.1806390E+01 (sec)
Self energies are being computed.
Self energies have been computed.  0.3305230E+00(sec.)
Green functions are being computed.
Green functions have been computed.  0.1577935E+01(sec.)
Conductance is being computed by Fisher Lee formula.
 ****************************************
 transmission=   1.88977404371895      (by Fisher Lee)
 ****************************************
```

In `output_negf.txt.0000`, transmission appears three times, but for elementary exercises, only the number on line 15 needs to be referenced. In the exercises in this section, scattering occurs in the scattering region because the atomic structures of the electrode region and the scattering region are different. Therefore, the conductance is smaller than the result in Sec. 5.4.