OpenMX Calculations: A Case Study of Hydrogen Molecule

Truong Vinh Truong Duy

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Abstract

In this document we introduce the behaviour of OpenMX calculations. Hydrogen molecule is chosen as the sample input for the calculations as it is among the simplest and most popular elements. We will use this case study as an opportunity to derive the OpenMX calltree and present a number of important subroutines involving the calculations. In reality, even with this simplest element, the calculations turn out to be remarkably complicated and the details described here is inadequate. This document is still evolving, however, it is expected to serve as an introduction to beginner developers about how calculations are performed in OpenMX.

Contents

Listings

Chapter 1

Getting Started: Running OpenMX

1.1 Execution Parameters

- Version of OpenMX: the latest version of 3.6.
- Input file: openmx3.6/work/force_example/H2_LDA.dat.
- level.of.stdout 2
- level.of.fileout 2
- Definition.of.Atomic.Species
  H H5.0-s1 H_CA11
- scf.XcType LDA
- scf.energycutoff 100.0
- scf.EigenvalueSolver cluster
- Execution hosts: Cray XT5 of JAIST.
- The number of MPI processes: 1 and 2. Results are presented for the first case only.
- Program profiler: Craypat and HPCToolkit.

1.2 Running OpenMX

Listing 1.1: The number of threads

```
1 The number of threads in each node for OpenMP
    parallelization is 1.
```

Listing 1.2: Welcome to OpenMX

```
*******************************************************
*******************************************************
 Welcome to OpenMX   Ver. 3.6
 Copyright (C), 2002-2011, T. Ozaki
 OpenMX comes with ABSOLUTELY NO WARRANTY.
 This is free software, and you are welcome to
 redistribute it under the constitution of the GNU-GPL.
*******************************************************
*******************************************************
```

Listing 1.3: SpeBasisName

```
<Input_std>  SpeBasisName=H5.0
<Input_std>  p= 0 l= 0 Primitive=  1
<Input_std>  p= 0 l= 1 Primitive=  0
<Input_std>  p= 0 l= 2 Primitive=  0
<Input_std>  p= 0 l= 3 Primitive=  0
<Input_std>  p= 0 l= 4 Primitive=  0

<Input_std>  0 Name  H
<Input_std>  0 Basis H5.0-s1
<Input_std>  0 VPS   H_CA11
<Input_std>  ct_AN= 1 WhatSpecies= 0 USpin= 0.5000 DSpin=
    0.5000
<Input_std>  ct_AN= 2 WhatSpecies= 0 USpin= 0.5000 DSpin=
    0.5000
Band.Nkpath=0


<Input_std>  Your input file was normally read.
<Input_std>  The system includes 1 species and 2 atoms.
proc=   0  Species_Top=   0  Species_End=   0
myid=0  MSpeciesNum=1
```

Listing 1.4: PAO and VPS

```
*******************************************************
                      PAO and VPS
*******************************************************

<Read_PAO>  spe= 0  AtomNum= 1
<Read_PAO>  spe= 0  Spe_Num_Mesh_PAO=500
<Read_PAO>  spe= 0  AtomNum= 1
<Read_PAO>  spe= 0  Spe_Num_Mesh_PAO=500
<SetPara_DFT>  PAOs of species H were normally found.
<Read_VPS>  VPS of H_CA11 was a format of ADPACK1.7
<Read_VPS>  spe= 0  Spe_Total_VPS_Pro=12
<Read_VPS>  spe= 0  Spe_Num_RVPS= 6
```

```
<Read_VPS>  VPS of H_CA11 was a format of ADPACK1.7
<Read_VPS>   i= 0   Spe_VPS_List= 0
<Read_VPS>   i= 1   Spe_VPS_List= 0
<Read_VPS>   i= 2   Spe_VPS_List= 0
<Read_VPS>   i= 3   Spe_VPS_List= 1
<Read_VPS>   i= 4   Spe_VPS_List= 1
<Read_VPS>   i= 5   Spe_VPS_List= 1
<Read_VPS>  spe= 0   Spe_Total_VPS_Pro=12
<Read_VPS>  spe= 0   Spe_Num_RVPS= 6
<SetPara_DFT>  VPSs of species H were normally found.
               H_CA11.vps is j-dependent.
               In case of scf.SpinOrbit.Coupling=off,
               j-dependent pseudo potentials are averaged
                  by j-degeneracy,
               which corresponds to a scalar relativistic
                  treatment.
<ReadPara_DFT>  YOUSO19= 8 YOUSO20=14
```

Listing 1.5: Fourier transform of PAO and projectors of VNL

```
*******************************************************
     Fourier transform of PAO and projectors of VNL
*******************************************************

<FT_PAO>           Fourier transform of pseudo atomic
   orbitals
<FT_NLP>           Fourier transform of non-local projectors
<FT_ProExpn_VNA>   Fourier transform of VNA separable
   projectors
<FT_VNA>           Fourier transform of VNA potentials
<FT_ProductPAO>    Fourier transform of product of PAOs
 Gc_AN=1 G2ID=0
 Gc_AN=2 G2ID=0
 proc =   0 elapsed time =          0.00000
<Estimate_NL>  ct_AN= 1 FNAN SNAN  2  2
<Estimate_NL>  ct_AN= 2 FNAN SNAN  2  2
 Gc_AN=1 G2ID=0
 Gc_AN=2 G2ID=0
```

Listing 1.6: Allocation of atoms to proccesors at MD_iter

```
*******************************************************
  Allocation of atoms to proccesors at MD_iter=    1
*******************************************************

 proc =   0  # of atoms=   2  estimated weight=
    0.00400
```

Listing 1.7: Truncation and setting of grids

```
1  ****************************************************
2              Truncation and setting of grids
3  ****************************************************
4
5  <truncation>  Logically truncation of the whole system
6  <physical truncation> CpyCell= 1 ct_AN= 1 FNAN SNAN  1  0
7  <physical truncation> CpyCell= 1 ct_AN= 2 FNAN SNAN  1  0
8  <physical truncation> myid=   0 CpyCell= 1 ct_AN=   1 FNAN
       SNAN   1   0
9  <physical truncation> myid=   0 CpyCell= 1 ct_AN=   2 FNAN
       SNAN   1   0
10    myid=0 ct_AN=1  FNAN= 1  SNAN= 0
11    myid=0 ct_AN=2  FNAN= 1  SNAN= 0
12 TFNAN=       2   Average FNAN=   1.00000
13 TSNAN=       0   Average SNAN=   0.00000
14 <logical truncation> myid=   0 CpyCell= 1 ct_AN=   1 FNAN
       SNAN   1   0
15 <logical truncation> myid=   0 CpyCell= 1 ct_AN=   2 FNAN
       SNAN   1   0
16 <physical truncation> CpyCell= 2 ct_AN= 1 FNAN SNAN  1  0
17 <physical truncation> CpyCell= 2 ct_AN= 2 FNAN SNAN  1  0
18 <physical truncation> myid=   0 CpyCell= 2 ct_AN=   1 FNAN
       SNAN   1   0
19 <physical truncation> myid=   0 CpyCell= 2 ct_AN=   2 FNAN
       SNAN   1   0
20    myid=0 ct_AN=1  FNAN= 1  SNAN= 0
21    myid=0 ct_AN=2  FNAN= 1  SNAN= 0
22 TFNAN=       2   Average FNAN=   1.00000
23 TSNAN=       0   Average SNAN=   0.00000
24 <logical truncation> myid=   0 CpyCell= 2 ct_AN=   1 FNAN
       SNAN   1   0
25 <logical truncation> myid=   0 CpyCell= 2 ct_AN=   2 FNAN
       SNAN   1   0
26 <physical truncation> CpyCell= 2 ct_AN= 1 FNAN SNAN  1  0
27 <physical truncation> CpyCell= 2 ct_AN= 2 FNAN SNAN  1  0
28 <physical truncation> myid=   0 CpyCell= 2 ct_AN=   1 FNAN
       SNAN   1   0
29 <physical truncation> myid=   0 CpyCell= 2 ct_AN=   2 FNAN
       SNAN   1   0
30    myid=0 ct_AN=1  FNAN= 1  SNAN= 0
31    myid=0 ct_AN=2  FNAN= 1  SNAN= 0
32 TFNAN=       2   Average FNAN=   1.00000
33 TSNAN=       0   Average SNAN=   0.00000
34 <logical truncation> myid=   0 CpyCell= 2 ct_AN=   1 FNAN
       SNAN   1   0
35 <logical truncation> myid=   0 CpyCell= 2 ct_AN=   2 FNAN
       SNAN   1   0
36 List_YOUSO[4]= 2
37 <Check_System> The system is molecule.
```

Listing 1.8: UCell_Box(MD_iter,1,CpyCell)

```
***** UCell_Box(MD_iter,1,CpyCell) *****
lattice vectors (bohr)
A = 18.897259885789,  0.000000000000,  0.000000000000
B =  0.000000000000, 18.897259885789,  0.000000000000
C =  0.000000000000,  0.000000000000, 18.897259885789
reciprocal lattice vectors (bohr^-1)
RA =  0.332491871581,  0.000000000000,  0.000000000000
RB =  0.000000000000,  0.332491871581,  0.000000000000
RB =  0.000000000000,  0.000000000000,  0.332491871581
Trial cutoff energies (a,b,c) =   7.075 (16),   7.075 (16),
      7.075 (16)
Trial cutoff energies (a,b,c) =  28.301 (32),  28.301 (32),
     28.301 (32)
Trial cutoff energies (a,b,c) =  63.677 (48),  63.677 (48),
     63.677 (48)
Trial cutoff energies (a,b,c) = 113.204 (64), 113.204 (64),
    113.204 (64)
UCell_Box: Cutoff=113.204065(64) 113.204065(64)
   113.204065(64)
UCell_Box: (tuned) Cutoff=109.694076(63) 109.694076(63)
   109.694076(63)
Required cutoff energy (Ryd) for 3D-grids = 100.0000
    Used cutoff energy (Ryd) for 3D-grids = 109.6941,
        109.6941, 109.6941
Num. of grids of a-, b-, and c-axes = 63, 63, 63
Grid_Origin -8.920706492117 -9.015192791546 -9.771083186978
Cell_Gxyz   1   0.472063492063  0.477063492063
   0.517063492063
Cell_Gxyz   2   0.512063492063  0.507063492063
   0.467063492063
Cell_Volume =   6748.333037104149 (Bohr^3)
GridVol     =      0.026988258356 (Bohr^3)
Cell vectors (bohr) of the grid cell (gtv)
  gtv_a =  0.299956506124,  0.000000000000,  0.000000000000
  gtv_b =  0.000000000000,  0.299956506124,  0.000000000000
  gtv_c =  0.000000000000,  0.000000000000,  0.299956506124
  |gtv_a| =  0.299956506124
  |gtv_b| =  0.299956506124
  |gtv_c| =  0.299956506124
Max_OneD_Grids=63
```

Listing 1.9: UCell_Box(MD_iter,2,CpyCell)

```
***** UCell_Box(MD_iter,2,CpyCell) *****
Grid_Origin -8.920706492117 -9.015192791546 -9.771083186978
Cell_Volume =   6748.333037104149 (Bohr^3)
GridVol     =      0.026988258356 (Bohr^3)
Cell vectors (bohr) of the grid cell (gtv)
```

```
  gtv_a =  0.299956506124,  0.000000000000,  0.000000000000
  gtv_b =  0.000000000000,  0.299956506124,  0.000000000000
  gtv_c =  0.000000000000,  0.000000000000,  0.299956506124
  |gtv_a| =  0.299956506124
  |gtv_b| =  0.299956506124
  |gtv_c| =  0.299956506124
Num. of grids overlapping between atoms  1 (G) and  0 (L) =
    19386
Num. of grids overlapping between atoms  1 (G) and  1 (L) =
    15529
Num. of grids overlapping between atoms  2 (G) and  0 (L) =
    19386
Num. of grids overlapping between atoms  2 (G) and  1 (L) =
    15529
YOUSO11=23264 YOUSO12=23264 YOUSO17=75
<UCell_Box> Info. of cutoff energy and num. of grids
lattice vectors (bohr)
A  = 18.897259885789,  0.000000000000,  0.000000000000
B  =  0.000000000000, 18.897259885789,  0.000000000000
C  =  0.000000000000,  0.000000000000, 18.897259885789
reciprocal lattice vectors (bohr^-1)
RA =  0.332491871581,  0.000000000000,  0.000000000000
RB =  0.000000000000,  0.332491871581,  0.000000000000
RB =  0.000000000000,  0.000000000000,  0.332491871581
Trial cutoff energies (a,b,c) =   7.075 (16),   7.075 (16),
     7.075 (16)
Trial cutoff energies (a,b,c) =  28.301 (32),  28.301 (32),
    28.301 (32)
Trial cutoff energies (a,b,c) =  63.677 (48),  63.677 (48),
    63.677 (48)
Trial cutoff energies (a,b,c) = 113.204 (64), 113.204 (64),
    113.204 (64)
UCell_Box: Cutoff=113.204065(64) 113.204065(64)
   113.204065(64)
UCell_Box: (tuned) Cutoff=109.694076(63) 109.694076(63)
   109.694076(63)
Required cutoff energy (Ryd) for 3D-grids = 100.0000
    Used cutoff energy (Ryd) for 3D-grids = 109.6941,
       109.6941, 109.6941
Num. of grids of a-, b-, and c-axes = 63, 63, 63
Grid_Origin -8.920706492117 -9.015192791546 -9.771083186978
Cell_Gxyz   1   0.472063492063  0.477063492063
   0.517063492063
Cell_Gxyz   2   0.512063492063  0.507063492063
   0.467063492063
Cell_Volume =   6748.333037104149 (Bohr^3)
GridVol     =      0.026988258356 (Bohr^3)
Cell vectors (bohr) of the grid cell (gtv)
  gtv_a =  0.299956506124,  0.000000000000,  0.000000000000
```

```
  gtv_b =  0.000000000000,  0.299956506124,  0.000000000000
  gtv_c =  0.000000000000,  0.000000000000,  0.299956506124
  |gtv_a| =  0.299956506124
  |gtv_b| =  0.299956506124
  |gtv_c| =  0.299956506124
Num. of grids overlapping with atom    1 = 19386
Num. of grids overlapping with atom    2 = 19386
Num. of grids overlapping between atoms  1 (G) and  0 (L) =
    19386
Num. of grids overlapping between atoms  1 (G) and  1 (L) =
    15529
Num. of grids overlapping between atoms  2 (G) and  0 (L) =
    19386
Num. of grids overlapping between atoms  2 (G) and  1 (L) =
    15529
```

Listing 1.10: SCF calculation 1 at MD = 1

```
*******************************************************
            SCF calculation at MD = 1
*******************************************************

<MD= 1>  Calculation of the overlap matrix
<MD= 1>  Calculation of the nonlocal matrix
<MD= 1>  Calculation of the VNA projector matrix

****************** MD= 1  SCF= 1 ******************
  Mc_AN=  1 Gc_AN=  1 ocupcy_u= 0.500000000000 ocupcy_d=
      0.500000000000
  Mc_AN=  2 Gc_AN=  2 ocupcy_u= 0.500000000000 ocupcy_d=
      0.500000000000
<Cluster>  Solving the eigenvalue problem...
  Eigenvalues of OLP   1   0.240978994092259
  Eigenvalues of OLP   2   1.759020904003656
  Eigenvalues of Kohn-Sham  1 -0.445643207069
      -0.445643207069
  Eigenvalues of Kohn-Sham  2  0.187811903205
      0.187811903205
ChemP= 0.000000000000 TZ= 2.000000000000 Num_state=
    2.000000000000
  ChemP= 0.000000000000
  HOMO =  1
     1    H  MulP   0.5000  0.5000 sum   1.0000
     2    H  MulP   0.5000  0.5000 sum   1.0000
 Sum of MulP: up   =     1.00000 down          =
     1.00000
                total=     2.00000 ideal(neutral)=
                    2.00000
<DFT>  Total Spin Moment (muB) =  0.000000000000
<DFT>  Mixing_weight= 0.000100000000
```

```
26 <DFT> Uele = -0.891286414137 dUele =
       1.000000000000
27 <DFT> NormRD = 1.000000000000 Criterion =
       0.000000000100
```

Listing 1.11: SCF calculation 2 at MD = 1

```
1  ****************** MD= 1  SCF= 2 ******************
2  <Poisson> Poisson's equation using FFT...
3  <Set_Hamiltonian>  Hamiltonian matrix for VNA+dVH+Vxc...
4  <Cluster>  Solving the eigenvalue problem...
5    Eigenvalues of Kohn-Sham  1 -0.424793245755
       -0.424793245755
6    Eigenvalues of Kohn-Sham  2  0.206931358315
       0.206931358315
7  ChemP= 0.000000000000 TZ= 2.000000000000 Num_state=
       2.000000000000
8    ChemP= 0.000000000000
9    HOMO=  1
10   1    H  MulP   0.5000   0.5000 sum   1.0000
11   2    H  MulP   0.5000   0.5000 sum   1.0000
12 Sum of MulP: up   =     1.00000 down          =
       1.00000
13             total=     2.00000 ideal(neutral)=
       2.00000
14 <DFT>  Total Spin Moment (muB) =  0.000000000000
15 <DFT>  Mixing_weight= 0.000100000000
16 <DFT>  Uele   =   -0.849586491510  dUele    =
       0.041699922627
17 <DFT>  NormRD =    0.000000000000  Criterion =
       0.000000000100
```

Listing 1.12: SCF calculation 3 at MD = 1

```
1  ****************** MD= 1  SCF= 3 ******************
2  <Poisson> Poisson's equation using FFT...
3  <Set_Hamiltonian>  Hamiltonian matrix for VNA+dVH+Vxc...
4  <Cluster>  Solving the eigenvalue problem...
5    Eigenvalues of Kohn-Sham  1 -0.424793245755
       -0.424793245755
6    Eigenvalues of Kohn-Sham  2  0.206931358315
       0.206931358315
7  ChemP= 0.000000000000 TZ= 2.000000000000 Num_state=
       2.000000000000
8    ChemP= 0.000000000000
9    HOMO=  1
10   1    H  MulP   0.5000   0.5000 sum   1.0000
11   2    H  MulP   0.5000   0.5000 sum   1.0000
12 Sum of MulP: up   =     1.00000 down          =
       1.00000
```

```
13 ␣␣␣␣␣␣␣␣␣␣␣␣␣␣total=␣␣␣␣␣2.00000␣ideal(neutral)=␣␣␣␣␣
       2.00000
14 <DFT>␣␣Total␣Spin␣Moment␣(muB)␣=␣␣0.000000000000
15 <DFT>␣␣Mixing_weight=␣0.000100000000
16 <DFT>␣␣Uele␣␣␣=␣␣␣−0.849586491510␣␣dUele␣␣␣␣=␣␣␣
       0.000000000000
17 <DFT>␣␣NormRD␣=␣␣␣␣0.000000000000␣␣Criterion␣=␣␣␣
       0.000000000100
18 write␣eigenvalues
19 write␣eigenvectors
20 <MD=␣1>␣␣Force␣calculation
21 ␣␣Force␣calculation␣#1
22 <Force>␣␣force(1)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣␣
       0.016934198825␣␣0.012697431438␣−0.021158048413
23 <Force>␣␣force(1)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣
       −0.016934198825␣−0.012697431438␣␣0.021158048413
24 ␣␣Force␣calculation␣#2
25 <Force>␣␣force(2)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣␣
       0.192004840585␣␣0.144003630439␣−0.240006050731
26 <Force>␣␣force(2)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣
       −0.192004840585␣−0.144003630439␣␣0.240006050731
27 ␣␣Force␣calculation␣#3
28 <Force>␣␣force(3)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣
       −0.088256376434␣−0.066180645714␣␣0.110312051520
29 <Force>␣␣force(3)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣␣
       0.088256376434␣␣0.066180645714␣−0.110312051520
30 ␣␣Force␣calculation␣#4
31 <Force>␣␣force(4B)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣
       −0.345886901541␣−0.259415167684␣␣0.432358618455
32 <Force>␣␣force(4B)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣␣
       0.345886901541␣␣0.259415167684␣−0.432358618455
33 ␣␣Force␣calculation␣#5
34 <Force>␣␣force(5)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣␣
       0.078269566025␣␣0.058702174519␣−0.097836957531
35 <Force>␣␣force(5)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣
       −0.078269566025␣−0.058702174519␣␣0.097836957531
36 <MD=␣1>␣␣Total␣Energy
37 ␣␣Force␣calculation␣#6
38 <Total_Ene>␣␣force(6)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣␣
       0.316816150895␣␣0.237612113171␣−0.396020188619
39 <Total_Ene>␣␣force(6)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣
       −0.316816150895␣−0.237612113171␣␣0.396020188619
40 <Calc_EH0>␣A␣spe=␣0␣1D−grids=127␣3D−grids=19050
41 <Calc_EH0>␣B␣spe=␣0␣1D−grids=127␣3D−grids=19050
42 ␣␣Force␣calculation␣#7
43 <Total_Ene>␣␣force(7)␣myid=␣0␣␣Mc_AN=␣1␣Gc_AN=␣1␣␣
       −0.071184495454␣−0.053388371590␣␣0.088980619317
44 <Total_Ene>␣␣force(7)␣myid=␣0␣␣Mc_AN=␣2␣Gc_AN=␣2␣␣␣
       0.071184495454␣␣0.053388371590␣−0.088980619317
```

```
45 <Total_Ene>  force(8) myid= 0  Mc_AN= 1 Gc_AN= 1
       -0.026297677244 -0.019723255253  0.032872093133
46 <Total_Ene>  force(8) myid= 0  Mc_AN= 2 Gc_AN= 2
       0.026297676122  0.019723259771 -0.032872093024
47 <Total_Ene>  force(t) myid= 0 Gc_AN= 1    0.072399305658
       0.054307909326 -0.090497862870
48 <Total_Ene>  force(t) myid= 0 Gc_AN= 2  -0.072399306780
       -0.054307904808  0.090497862979
```

Listing 1.13: Dipole moment (Debye)

```
1  ****************************************************
2                    Dipole moment (Debye)
3  ****************************************************
4
5   Absolute D          0.00000039
6
7                             Dx                Dy
                                 Dz
8   Total                 0.00000022        0.00000016
        -0.00000027
9   Core                  1.92128272        1.44096204
        -2.40160340
10  Electron             -1.92128250       -1.44096188
        2.40160313
11  Back ground           0.00000000        0.00000000
        0.00000000
```

Listing 1.14: Total Energy (Hartree) at MD = 1

```
1  ****************************************************
2                  Total Energy (Hartree) at MD = 1
3  ****************************************************
4
5    Uele   =        -0.849586491510
6
7    Ukin   =         0.867294836322
8    UH0    =        -1.126624865574
9    UH1    =         0.002131136124
10   Una    =        -1.143875598977
11   Unl    =         0.153152502541
12   Uxc0   =        -0.297105686293
13   Uxc1   =        -0.297105686293
14   Ucore  =         0.748369642435
15   Uhub   =         0.000000000000
16   Ucs    =         0.000000000000
17   Uzs    =         0.000000000000
18   Uzo    =         0.000000000000
19   Uef    =         0.000000000000
20   UvdW   =         0.000000000000
```

```
21  Utot  =     -1.09376371971380
22
23  Note:
24
25  Utot = Ukin+UH0+UH1+Una+Unl+Uxc0+Uxc1+Ucore+Uhub+Ucs+Uzs+
        Uzo+Uef+UvdW
26
27  Uele:   band energy
28  Ukin:   kinetic energy
29  UH0:    electric part of screened Coulomb energy
30  UH1:    difference electron-electron Coulomb energy
31  Una:    neutral atom potential energy
32  Unl:    non-local potential energy
33  Uxc0:   exchange-correlation energy for alpha spin
34  Uxc1:   exchange-correlation energy for beta spin
35  Ucore:  core-core Coulomb energy
36  Uhub:   LDA+U energy
37  Ucs:    constraint energy for spin orientation
38  Uzs:    Zeeman term for spin magnetic moment
39  Uzo:    Zeeman term for orbital magnetic moment
40  Uef:    electric energy by electric field
41  UvdW:   semi-empirical vdW energy
42
43  (see also PRB 72, 045121(2005) for the energy
        contributions)
```

Listing 1.15: Computational times (s) at MD = 1

```
1  ****************************************************
2            Computational times (s) at MD = 1
3  ****************************************************
4
5   DFT in total       =    1.19688
6
7   Set_OLP_Kin        =    0.17402
8   Set_Nonlocal       =    0.12352
9   Set_Hamiltonian    =    0.02677
10  Poisson            =    0.09745
11  diagonalization    =    0.00447
12  Mixing_DM          =    0.00026
13  Force              =    0.11963
14  Total_Energy       =    0.49827
15  Set_Aden_Grid      =    0.02145
16  Set_Orbitals_Grid  =    0.05433
17  Set_Density_Grid   =    0.00917
```

Listing 1.16: MD or geometry opt. at MD = 1

```
1  ****************************************************
2              MD or geometry opt. at MD = 1
```

```
3  ***************************************************
4
5  <Steepest_Descent>  SD_scaling= 0.944862993551
6  <Steepest_Descent>  |Maximum force| (Hartree/Bohr) =
       0.127987779335
7  <Steepest_Descent>  Criterion       (Hartree/Bohr) =
       0.000100000000
8
9    atom=  1, XYZ(ang) Fxyz(a.u.)=   0.0000    0.0000
         0.0000     0.0724    0.0543   -0.0905
10   atom=  2, XYZ(ang) Fxyz(a.u.)=   0.4000    0.3000
        -0.5000    -0.0724   -0.0543    0.0905
11
12 outputting data on grids to files...
13
14 Save the scfout file (H2_LDA/1MPI/pure/H2_LDA.scfout)
```

Listing 1.17: Computational Time (second)

```
1  ***********************************************************
2  ***********************************************************
3                  Computational Time (second)
4  ***********************************************************
5  ***********************************************************
6
7                                  Min_ID     Min_Time     Max_ID
                                                  Max_Time
8     Total Computational Time =  0          10.360       0
              10.360
9     readfile                 =  0           6.652       0
               6.652
10    truncation               =  0           0.766       0
               0.766
11    MD_pac                   =  0           0.003       0
               0.003
12    DFT                      =  0           1.197       0
               1.197
13
14 *** In DFT ***
15
16    Set_OLP_Kin              =  0           0.174       0
               0.174
17    Set_Nonlocal             =  0           0.124       0
               0.124
18    Set_Hamiltonian          =  0           0.027       0
               0.027
19    Poisson                  =  0           0.097       0
               0.097
20    Diagonalization          =  0           0.004       0
               0.004
```

```
21    Mixing_DM                =  0          0.000          0
                0.000
22    Force                    =  0          0.120          0
                0.120
23    Total_Energy             =  0          0.498          0
                0.498
24    Set_Aden_Grid            =  0          0.021          0
                0.021
25    Set_Orbitals_Grid        =  0          0.054          0
                0.054
26    Set_Density_Grid         =  0          0.009          0
                0.009
27    Others                   =  0          0.068          0
                0.068
```

Listing 1.18: Program execution result

```
1 The calculation was normally finished. (proc=   0)
2 Application 175934 resources: utime 0, stime 0
```

Chapter 2

OpenMX Calltree

2.1 Input

2.1.1 Initial checks

Upon execution, OpenMX checks some initial configurations, such as the number of OpenMP threads, runtest, maketest, force test, memory leak, etc. It then initializes the List_YOUSO and alloc_first by calling Init_List_YOUSO() and init_alloc_first(). Between them, setup_CPU_group() is called to input the eigenvalue solver, the number of atoms, energy cutoff, and sets up a new MPI process group in case there are fewer atoms than MPI processes.

Listing 2.1: Initial checks.

```
Time % |        Time |Calltree
       |             | PE=0='HIDE'

 100.0% | 92.797543 |Total
|-------------------------------
|   0.0% |  0.000189 |main:openmx.c:line.89
|   0.0% |  0.000008 |main:openmx.c:line.99
||------------------------------
||  0.0% |  0.000002 |MPI_Init:...:line.0
||  0.0% |  0.000001 |MPI_Comm_rank:...:line.0
||  0.0% |  0.000002 |MPI_Comm_size:...:line.0
||  0.0% |  0.000004 |dtime:dtime.c:line.15
||==============================
|   0.0% |  0.000010 |main:openmx.c:line.144
||------------------------------
||  0.0% |  0.000006 |MPI_Bcast:...:line.0
||  0.0% |  0.000004 |MPI_Bcast(sync):...:line.0
||==============================
|   0.0% |  0.044252 |main:openmx.c:line.348
||------------------------------
||  0.0% |  0.000012 |neb_check:neb_check.c:line.36
||  0.0% |  0.000536 |neb_check:neb_check.c:line.41
```

```
23 | 3|          |              | input_open:Inputtools.c:line.24
24 | ||    0.0% |   0.043613 |neb_check:neb_check.c:line.46
25 | 3|          |              | input_string2int:Inputtools.c:line
   |     .316
26 | ||    0.0% |   0.000090 |neb_check:neb_check.c:line.68
27 | 3|          |              | input_close:Inputtools.c:line.49
28 | ╠═══════════════════════════════════
29 | |   33.2% | 30.792857 |main:openmx.c:line.372
30 | ╠-----------------------------------
31 | ||    0.0% |   0.000008 |Init_List_YOUSO:Init_List_YOUSO.c:
   |     line.6
32 | ||    0.0% |   0.000014 |setup_CPU_group:setup_CPU_group.c:
   |     line.15
33 | ||    0.0% |   0.000157 |setup_CPU_group:setup_CPU_group.c:
   |     line.18
34 | |||--------------------------------
35 | 3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
36 | 3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
37 | 3||    0.0% |   0.000154 |input_open:Inputtools.c:line.24
38 | |||================================
39 | ||    0.0% |   0.000070 |setup_CPU_group:setup_CPU_group.c:
   |     line.29
40 | 3|          |              | input_close:Inputtools.c:line.49
41 | ||    0.0% |   0.000278 |setup_CPU_group:setup_CPU_group.c:
   |     line.34
42 | |||--------------------------------
43 | 3||    0.0% |   0.000025 |input_double:Inputtools.c:line.241
44 | 3||    0.0% |   0.000012 |input_int:Inputtools.c:line.203
45 | 3||    0.0% |   0.000060 |input_logical:Inputtools.c:line.160
46 | 3||    0.0% |   0.000127 |input_open:Inputtools.c:line.24
47 | 3||    0.0% |   0.000054 |input_string2int:Inputtools.c:line
   |     .316
48 | |||================================
49 | ||    0.0% |   0.000075 |setup_CPU_group:setup_CPU_group.c:
   |     line.83
50 | 3|          |              | input_close:Inputtools.c:line.49
51 | ||    0.0% |   0.000008 |setup_CPU_group:setup_CPU_group.c:
   |     line.87
52 | |||--------------------------------
53 | 3||    0.0% |   0.000004 |MPI_Bcast:...:line.0
54 | 3||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
55 | |||================================
56 | ||    0.0% |   0.000005 |init_alloc_first:init_alloc_first.c:
   |     line.18
57 | ||    0.0% |   0.000237 |readfile:readfile.c:line.29
58 | ||    0.0% |   0.000005 |readfile:readfile.c:line.37
59 | |||--------------------------------
60 | 3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
61 | 3||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
```

```
3||    0.0%  |   0.000003  |dtime:dtime.c:line.15
|||=================================
```

2.1.2 Main input subroutine: readfile()

readfile() is the main subroutine for reading the input file or restart file. It actually calls several subroutines for inputting data, including Input_std(), Allocate_Arrays(), Set_Allocate_Atom2CPU(), SetPara_DFT(), TRAN_Check_Input().

2.1.3 Called by readfile(): Input_std()

Input_std() reads the input file and initializes the corresponding parameters accordingly. It makes use of input_int(), input_string(), input_double(), input_logical(), etc. defined in Inputtools.c. Some parameters require invoking Allocate_Arrays().

Listing 2.2: Input_std() called by readfile() (Note that this is not an exhausted listing and the execution order is incorrect).

```
||    0.0%  |   0.007424  |readfile:readfile.c:line.49
|||---------------------------------
3||    0.0%  |   0.000003  |Input_std:Input_std.c:line.60
||||-------------------------------
4|||    0.0%  |   0.000001  |MPI_Comm_rank:...:line.0
4|||    0.0%  |   0.000002  |MPI_Comm_size:...:line.0
||||===============================
3||    0.0%  |   0.000009  |Input_std:Input_std.c:line.94
4||          |             | input_open:Inputtools.c:line.24
3||    0.0%  |   0.000115  |Input_std:Input_std.c:line.99
||||-------------------------------
4|||    0.0%  |   0.000022  |input_int:Inputtools.c:line.203
4|||    0.0%  |   0.000094  |input_string:Inputtools.c:line.279
|||=================================
3||    0.0%  |   0.000005  |Input_std:Input_std.c:line.1023
4||          |             | Species2int:Input_std.c:line.3392
5||          |             |  SEQ:openmx_common.c:line.435
3||    0.0%  |   0.000002  |Input_std:Input_std.c:line.1036
4||          |             | input_last:Inputtools.c:line.514
3||    0.0%  |   0.000024  |Input_std:Input_std.c:line.1064
||||-------------------------------
4|||    0.0%  |   0.000010  |input_find:Inputtools.c:line.493
4|||    0.0%  |   0.000013  |input_string2int:Inputtools.c:line
    .316
||||===============================
3||    0.0%  |   0.000002  |Input_std:Input_std.c:line.1072
4||          |             | input_last:Inputtools.c:line.514
3||    0.0%  |   0.000361  |Input_std:Input_std.c:line.119
||||-------------------------------
```

```
4|||    0.0% |   0.000031 |input_double:Inputtools.c:line.241
4|||    0.0% |   0.000124 |input_int:Inputtools.c:line.203
4|||    0.0% |   0.000058 |input_intv:Inputtools.c:line.446
4|||    0.0% |   0.000147 |input_logical:Inputtools.c:line
    .160
|||=================================
3||    0.0% |   0.000061 |Input_std:Input_std.c:line.1377
4||         |            | input_logical:Inputtools.c:line
    .160
3||    0.0% |   0.000057 |Input_std:Input_std.c:line.1434
4||         |            | input_find:Inputtools.c:line.493
3||    0.0% |   0.000056 |Input_std:Input_std.c:line.1452
4||         |            | input_find:Inputtools.c:line.493
3||    0.0% |   0.000029 |Input_std:Input_std.c:line.1547
4||         |            | input_int:Inputtools.c:line.203
3||    0.0% |   0.000058 |Input_std:Input_std.c:line.1557
4||         |            | input_int:Inputtools.c:line.203
3||    0.0% |   0.000249 |Input_std:Input_std.c:line.1567
|||---------------------------------
4|||    0.0% |   0.000066 |input_double:Inputtools.c:line.241
4|||    0.0% |   0.000077 |input_int:Inputtools.c:line.203
4|||    0.0% |   0.000105 |input_logical:Inputtools.c:line
    .160
|||=================================
3||    0.0% |   0.000094 |Input_std:Input_std.c:line.1685
|||---------------------------------
4|||    0.0% |   0.000031 |input_double:Inputtools.c:line.241
4|||    0.0% |   0.000063 |input_int:Inputtools.c:line.203
|||=================================
3||    0.0% |   0.000589 |Input_std:Input_std.c:line.1728
|||---------------------------------
4|||    0.0% |   0.000135 |input_double:Inputtools.c:line.241
4|||    0.0% |   0.000293 |input_int:Inputtools.c:line.203
4|||    0.0% |   0.000067 |input_logical:Inputtools.c:line
    .160
4|||    0.0% |   0.000094 |input_string2int:Inputtools.c:line
    .316
|||=================================
3||    0.0% |   0.000441 |Input_std:Input_std.c:line.1757
|||---------------------------------
4|||    0.0% |   0.000055 |input_find:Inputtools.c:line.493
4|||    0.0% |   0.000123 |input_int:Inputtools.c:line.203
4|||    0.0% |   0.000263 |input_logical:Inputtools.c:line
    .160
|||=================================
3||    0.0% |   0.000633 |Input_std:Input_std.c:line.1811
|||---------------------------------
4|||    0.0% |   0.000130 |input_double:Inputtools.c:line.241
4|||    0.0% |   0.000329 |input_int:Inputtools.c:line.203
```

```
72 | 4|||    0.0% |   0.000052 |input_logical:Inputtools.c:line
       .160
73 | 4|||    0.0% |   0.000123 |input_string2int:Inputtools.c:line
       .316
74 | ||||==========================================
75 | 3||    0.0% |   0.000057 |Input_std:Input_std.c:line.1868
76 | 4||         |            | input_int:Inputtools.c:line.203
77 | 3||    0.0% |   0.000058 |Input_std:Input_std.c:line.1890
78 | ||||------------------------------
79 | 4|||    0.0% |   0.000002 |Allocate_Arrays:Allocate_Arrays.c:
       line.7
80 | 4|||    0.0% |   0.000056 |input_find:Inputtools.c:line.493
81 | ||||==========================================
82 | 3||    0.0% |   0.000042 |Input_std:Input_std.c:line.1916
83 | 4||         |            | input_logical:Inputtools.c:line
       .160
84 | 3||    0.0% |   0.000048 |Input_std:Input_std.c:line.1947
85 | 4||         |            | input_doublev:Inputtools.c:line
       .399
86 | 3||    0.0% |   0.000016 |Input_std:Input_std.c:line.200
87 | 4||         |            | input_int:Inputtools.c:line.203
88 | 3||    0.0% |   0.000307 |Input_std:Input_std.c:line.2008
89 | ||||------------------------------
90 | 4|||    0.0% |   0.000065 |input_double:Inputtools.c:line.241
91 | 4|||    0.0% |   0.000065 |input_int:Inputtools.c:line.203
92 | 4|||    0.0% |   0.000176 |input_logical:Inputtools.c:line
       .160
93 | ||||==========================================
94 | 3||    0.0% |   0.000145 |Input_std:Input_std.c:line.2036
95 | ||||------------------------------
96 | 4|||    0.0% |   0.000048 |input_doublev:Inputtools.c:line
       .399
97 | 4|||    0.0% |   0.000039 |input_intv:Inputtools.c:line.446
98 | 4|||    0.0% |   0.000057 |input_logical:Inputtools.c:line
       .160
99 | ||||==========================================
100| 3||    0.0% |   0.000310 |Input_std:Input_std.c:line.2071
101| ||||------------------------------
102| 4|||    0.0% |   0.000066 |input_double:Inputtools.c:line.241
103| 4|||    0.0% |   0.000244 |input_logical:Inputtools.c:line
       .160
104| ||||==========================================
105| 3||    0.0% |   0.000172 |Input_std:Input_std.c:line.209
106| ||||------------------------------
107| 4|||    0.0% |   0.000007 |Allocate_Arrays:Allocate_Arrays.c:
       line.7
108| 4|||    0.0% |   0.000058 |input_logical:Inputtools.c:line
       .160
109| 4|||    0.0% |   0.000106 |input_string2int:Inputtools.c:line
```

```
    |     .316
110 ||||==========================================
111 | 3||    0.0% |   0.000676 |Input_std:Input_std.c:line.2482
112 ||||------------------------------
113 | 4|||    0.0% |   0.000012 |input_close:Inputtools.c:line.49
114 | 4|||    0.0% |   0.000137 |input_double:Inputtools.c:line.241
115 | 4|||    0.0% |   0.000196 |input_int:Inputtools.c:line.203
116 | 4|||    0.0% |   0.000261 |input_logical:Inputtools.c:line
    |     .160
117 | 4|||    0.0% |   0.000070 |input_string:Inputtools.c:line.279
118 ||||==========================================
119 | 3||    0.0% |   0.000007 |Input_std:Input_std.c:line.249
120 | 4||         |            | input_find:Inputtools.c:line.493
121 | 3||    0.0% |   0.000002 |Input_std:Input_std.c:line.2500
122 | 4||         |            | input_errorCount:Inputtools.c:line
    |     .152
123 | 3||    0.0% |   0.000003 |Input_std:Input_std.c:line.261
124 | 4||         |            | SpeciesString2int:Input_std.c:line
    |     .3215
125 |||||------------------------------
126 | 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
127 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
128 ||||==========================================
129 | 3||    0.0% |   0.000003 |Input_std:Input_std.c:line.265
130 | 4||         |            | input_last:Inputtools.c:line.514
131 | 3||    0.0% |   0.000041 |Input_std:Input_std.c:line.290
132 | 4||         |            | input_string2int:Inputtools.c:line
    |     .316
133 | 3||    0.0% |   0.000040 |Input_std:Input_std.c:line.345
134 | 4||         |            | input_int:Inputtools.c:line.203
135 | 3||    0.0% |   0.000041 |Input_std:Input_std.c:line.351
136 | 4||         |            | input_double:Inputtools.c:line.241
137 | 3||    0.0% |   0.000296 |Input_std:Input_std.c:line.357
138 ||||------------------------------
139 | 4|||    0.0% |   0.000108 |input_double:Inputtools.c:line.241
140 | 4|||    0.0% |   0.000188 |input_int:Inputtools.c:line.203
141 ||||==========================================
142 | 3||    0.0% |   0.000055 |Input_std:Input_std.c:line.421
143 | 4||         |            | input_find:Inputtools.c:line.493
144 | 3||    0.0% |   0.000094 |Input_std:Input_std.c:line.433
145 ||||------------------------------
146 | 4|||    0.0% |   0.000066 |input_double:Inputtools.c:line.241
147 | 4|||    0.0% |   0.000029 |input_string2int:Inputtools.c:line
    |     .316
148 ||||==========================================
149 | 3||    0.0% |   0.000057 |Input_std:Input_std.c:line.467
150 | 4||         |            | input_string2int:Inputtools.c:line
    |     .316
151 | 3||    0.0% |   0.000131 |Input_std:Input_std.c:line.484
```

```
152 ||||------------------------------
153  4|||    0.0% |   0.000065 |input_double:Inputtools.c:line.241
154  4|||    0.0% |   0.000066 |input_string2int:Inputtools.c:line
        .316
155 ||||==============================
156  3||    0.0% |   0.000172 |Input_std:Input_std.c:line.504
157 ||||------------------------------
158  4|||    0.0% |   0.000130 |input_logical:Inputtools.c:line
        .160
159  4|||    0.0% |   0.000043 |input_string2int:Inputtools.c:line
        .316
160 ||||==============================
161  3||    0.0% |   0.000056 |Input_std:Input_std.c:line.540
162  4||         |            | input_logical:Inputtools.c:line
        .160
163  3||    0.0% |   0.000128 |Input_std:Input_std.c:line.55
164  3||    0.0% |   0.000130 |Input_std:Input_std.c:line.560
165 ||||------------------------------
166  4|||    0.0% |   0.000065 |input_double:Inputtools.c:line.241
167  4|||    0.0% |   0.000065 |input_logical:Inputtools.c:line
        .160
168 ||||==============================
169  3||    0.0% |   0.000065 |Input_std:Input_std.c:line.577
170  4||         |            | input_logical:Inputtools.c:line
        .160
171  3||    0.0% |   0.000066 |Input_std:Input_std.c:line.589
172  4||         |            | input_logical:Inputtools.c:line
        .160
173  3||    0.0% |   0.000130 |Input_std:Input_std.c:line.618
174 ||||------------------------------
175  4|||    0.0% |   0.000065 |input_double:Inputtools.c:line.241
176  4|||    0.0% |   0.000065 |input_logical:Inputtools.c:line
        .160
177 ||||==============================
178  3||    0.0% |   0.000065 |Input_std:Input_std.c:line.658
179  4||         |            | input_double:Inputtools.c:line.241
180  3||    0.0% |   0.000028 |Input_std:Input_std.c:line.672
181  4||         |            | input_intv:Inputtools.c:line.446
182  3||    0.0% |   0.000038 |Input_std:Input_std.c:line.715
183 ||||------------------------------
184  4|||    0.0% |   0.000018 |input_double:Inputtools.c:line.241
185  4|||    0.0% |   0.000020 |input_string2int:Inputtools.c:line
        .316
186 ||||==============================
187  3||    0.0% |   0.000358 |Input_std:Input_std.c:line.727
188 ||||------------------------------
189  4|||    0.0% |   0.000119 |input_double:Inputtools.c:line.241
190  4|||    0.0% |   0.000174 |input_int:Inputtools.c:line.203
191  4|||    0.0% |   0.000064 |input_logical:Inputtools.c:line
```

```
    .160
192 ||||==========================================
193 3||    0.0% |   0.000033 |Input_std:Input_std.c:line.757
194 4||         |            | input_double:Inputtools.c:line.241
195 3||    0.0% |   0.000454 |Input_std:Input_std.c:line.763
196 ||||------------------------------
197 4|||    0.0% |   0.000007 |__ipaps_TRAN_Input_std:
    TRAN_Input_std.c:line.44
198 4|||    0.0% |   0.000202 |__ipaps_TRAN_Input_std:
    TRAN_Input_std.c:line.53
199 |||||----------------------------
200 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
201 5||||    0.0% |   0.000133 |input_logical:Inputtools.c:line
    .160
202 5||||    0.0% |   0.000067 |input_string:Inputtools.c:line
    .279
203 |||||==============================
204 4|||    0.0% |   0.000056 |input_double:Inputtools.c:line.241
205 4|||    0.0% |   0.000057 |input_doublev:Inputtools.c:line
    .399
206 4|||    0.0% |   0.000132 |input_string2int:Inputtools.c:line
    .316
207 ||||==========================================
208 3||    0.0% |   0.000067 |Input_std:Input_std.c:line.843
209 4||         |            | input_double:Inputtools.c:line.241
210 3||    0.0% |   0.000069 |Input_std:Input_std.c:line.857
211 4||         |            | input_double:Inputtools.c:line.241
212 3||    0.0% |   0.000131 |Input_std:Input_std.c:line.885
213 ||||------------------------------
214 4|||    0.0% |   0.000065 |input_double:Inputtools.c:line.241
215 4|||    0.0% |   0.000066 |input_string2int:Inputtools.c:line
    .316
216 ||||==========================================
217 3||    0.0% |   0.000019 |Input_std:Input_std.c:line.912
218 4||         |            | input_int:Inputtools.c:line.203
219 3||    0.0% |   0.000031 |Input_std:Input_std.c:line.922
220 ||||------------------------------
221 4|||    0.0% |   0.000011 |Allocate_Arrays:Allocate_Arrays.c:
    line.7
222 4|||    0.0% |   0.000009 |input_find:Inputtools.c:line.493
223 4|||    0.0% |   0.000011 |input_string2int:Inputtools.c:line
    .316
224 ||||==========================================
```

2.1.4 Called by readfile(): SetPara_DFT()

SetPara_DFT() itself includes several subroutines:

- ReadPara_DFT(): to read the data of pseudo atomic orbitals and

density and output information to standard output.

- Read_PAO(): to read the data of pseudo atomic orbitals and density. In particular, data are stored in
  - double **Spe_PAO_XV (radial mesh (x=log(r)) for PAO, size: Spe_PAO_XV[List_YOUSO[18]][List_YOUSO[21]])
  - double **Spe_PAO_RV (logarithmic radial mesh (r=exp(r)) for PAO, size: Spe_PAO_XV[List_YOUSO[18]][List_YOUSO[21]])
  - double ****Spe_PAO_RWF (radial parts of basis orbitals on radial mesh of PAO, size: Spe_PAO_RWF[List_YOUSO[18]][List_YOUSO[25]+1] [List_YOUSO[24]][List_YOUSO[21]])
  - double **Spe_Atomic_Den (atomic charge densities on radial mesh of PAO, size: Spe_Atomic_Den[List_YOUSO[18]][List_YOUSO[21]])
- Read_VPS(): to read the data of pseudopotentials and partial correction core pcc. In particular:
  - Re-normalization of atomic charge density double **Spe_Atomic_Den (atomic charge densities on radial mesh of PAO, size: Spe_Atomic_Den [List_YOUSO[18]][List_YOUSO[21]]
  - double ***Spe_VNLE (projection energies of projectors of non-local potentials on radial mesh of VPS, size: Spe_VNLE[SO_switch+1] [List_YOUSO[18]][List_YOUSO[19]]
  - int **Spe_VPS_List (angular momentum numbers of projectors of non-local potentials, size: Spe_VPS_List[List_YOUSO[18]][List_YOUSO[19]])
  - double **Spe_VPS_XV (radial mesh (x=log(r)) for VPS, size: Spe_VPS_XV[List_YOUSO[18]][List_YOUSO[22]])
  - double **Spe_VPS_RV (logarithmic radial mesh (r=exp(x)) for VPS, size: Spe_VPS_RV[List_YOUSO[18]][List_YOUSO[22]])
  - double ****Spe_VNL (radial parts of projectors of non-local potentials on radial mesh of VPS, size: Spe_VNL[SO_switch+1][List_YOUSO[18]] [List_YOUSO[19]][List_YOUSO[22]])
  - double **Spe_Atomic_PCC (partial core correction charge densities on radial mesh of VPS, size: Spe_Atomic_PCC[List_YOUSO[18]][List_YOUSO[22]])
  - double **Spe_VH_Atom (Hartree potentials of atomic charge densities on radial mesh of VPS, size: Spe_VH_Atom[List_YOUSO[18]][List_YOUSO[22]])
  - double **Spe_Vna (neutral atom potentials on radial mesh of VPS, size: Spe_Vna[List_YOUSO[18]][List_YOUSO[22]])
  - double ***Projector_VNA (Projectors for a projector expansion of VNA, size: Projector_VNA[List_YOUSO[18]][YOUSO35+1][YOUSO34] [List_YOUSO[22]])

  - double **VNA_proj_ene (Projector energy for a projector expansion of VNA, size: VNA_proj_ene[List_YOUSO[18]][YOUSO35+1][YOUSO34])
  - V_Hart_atom(): called by Read_VPS() for calculating inside and outside contributions to an atom by Gauss-Legendre. It in turn invokes AtomicDenF() in AtomicDenF.c for the calculation of the atomic charge density of one atom specified "Gensi" at R.
  - RadialF() (in RadialF.c): called by Read_VPS() for calculating the radial function of pseudo atomic orbital specified by "l" for atomic species "Gensi" at R.
  - Int_phi0_phi1(): called by Read_VPS() the calculation of projector expansion of VNA.

- Set_Comp2Real(): to initialize dcomplex Comp2Real[YOUSO36+1][2*(YOUSO36+1)+1][2*(YOUSO36+1)+1] for describing s, p, d, f, etc. This subroutine calls Complex() in openmx_common.c.

- output_structures(): to output data to the .cif and .xyz files. Performed by only the host/master process.

- FT_PAO() (in FT_PAO.c): is a subroutine to Fourier transform pseudo atomic orbitals.

  - Spherical_Bessel() (in Spherical_Bessel.c): called to calculate the spherical Bessel functions and its derivative from 0 to lmax.
  - double ****Spe_RF_Bessel (radial parts of basis orbitals on radial mesh in the momentum space, size: Spe_RF_Bessel[List_YOUSO[18]][List_YOUSO[25]+1][List_YOUSO[24]][List_YOUSO[15]])
  - RadialF() in RadialF.c.

- FT_NLP() (in FT_NLP.c): is a subroutine to Fourier transform projectors of nonlocal potentials.

  - Spherical_Bessel() (in Spherical_Bessel.c).
  - double ****Spe_NLRF_Bessel (radial parts of projectors of nonlocal potentials on radial mesh in the momentum space, size: Spe_RF_Bessel[SO_switch+1][List_YOUSO[18]][List_YOUSO[19]+2][List_YOUSO[15]])
  - Nonlocal_RadialF() (in Nonlocal_RadialF.c): for calculating the radial function of onlocal potentials.

- FT_ProExpn_VNA(): is a subroutine to Fourier transform VNA separable projectors.

  - Spherical_Bessel() (in Spherical_Bessel.c).

  - double ***Spe_VNA_Bessel (radial parts of projectors of VNA on radial mesh in the momentum space, size: Spe_VNA_Bessel[List_YOUSO[18]] [YOUSO35+1][YOUSO34][List_YOUSO[15]])
  - PhiF() (in PhiF.c): is a subroutine to calculate the value of a radial function at R.

- FT_VNA() (in FT_VNA.c): is a subroutine to Fourier transform VNA potentials.
  - Spherical_Bessel() (in Spherical_Bessel.c).
  - double **Spe_CrudeVNA_Bessel (radial parts of crude VNA potentials on Gauss-Legendre radial mesh in the momentum space, size: Spe_CrudeVNA_Bessel[List_YOUSO[18]][GL_Mesh+2])
  - VNAF() (in VNAF.c): is a subroutine to calculate the neutral atom potential of one atom specified by "Gensi".

- FT_ProductPAO() (in FT_ProductPAO.c): is a subroutine to Fourier transform the product of two pseudo atomic orbitals.
  - RadialF() in RadialF.c.
  - Spherical_Bessel() (in Spherical_Bessel.c).
  - double *******Spe_ProductRF_Bessel (radial parts of product of two PAOs on Gauss-Legendre radial mesh in the momentum space, size: Spe_ProductRF_Bessel[List_YOUSO[18]][Spe_MaxL_Basis[i]+1] [Spe_Num_Basis[i][j]][Spe_MaxL_Basis[i]+1][Spe_Num_Basis[i][l]][Lmax+1][GL_Mesh+2])

2.1.5 Called by readfile(): Set_Allocate_Atom2CPU()

Set_Allocate_Atom2CPU.c is a subroutine to allocate atoms to processors for the MPI parallel computation. It includes several subroutines.

- Conventional_Allocation(): to partition the system by the one-dimensional domain decomposition. It counts the number of atoms with a weight factor, which can be the number of orbitals powered to 1, 2, or 3, or the elapsed times at the previous MD step.

- Estimate_NL(): to estimate the nearest neighbour list.

- double **Cell_Gxyz (atomic global coordinates spanned by the unit cell vectors, size: Cell_Gxyz[atomnum+1][4]).

- int *Species_Top, *Species_End (give global indices of the first and last species in species allocated to each processor, size: Species_Top[numprocs], Species_End[numprocs]).

- int *G2ID (gives a proccesor ID allocated to each atom with a global atom index, size: G2ID[atomnum+1]).
- int *M2G (gives a conversion from the medium index to the global indices of atoms, size: M2G[Matomnum+1]).

Listing 2.3: SetPara_DFT() and Set_Allocate_Atom2CPU() called by readfile().

```
1  ||   33.2% | 30.777885 |readfile:readfile.c:line.61
2  |||--------------------------------
3  3||    0.0% |  0.000006 |Allocate_Arrays:Allocate_Arrays.c:
       line.7
4  3||    0.0% |  0.000016 |Set_Allocate_Atom2CPU:
       Set_Allocate_Atom2CPU.c:line.39
5  3||    0.0% |  0.000003 |Set_Allocate_Atom2CPU:
       Set_Allocate_Atom2CPU.c:line.52
6  4||         |           | Conventional_Allocation:
       Set_Allocate_Atom2CPU.c:line.1198
7  |||||------------------------------
8  5||||    0.0% |  0.000001 |MPI_Comm_rank:...:line.0
9  5||||    0.0% |  0.000002 |MPI_Comm_size:...:line.0
10 |||||==============================
11 3||    0.4% |  0.367262 |SetPara_DFT:SetPara_DFT.c:line.44
12 3||    0.0% |  0.000003 |SetPara_DFT:SetPara_DFT.c:line.50
13 ||||-------------------------------
14 4|||    0.0% |  0.000001 |MPI_Comm_rank:...:line.0
15 4|||    0.0% |  0.000001 |MPI_Comm_size:...:line.0
16 ||||===============================
17 3||    3.2% |  2.980455 |SetPara_DFT:SetPara_DFT.c:line.66
18 ||||-------------------------------
19 4|||    0.0% |  0.000003 |ReadPara_DFT:SetPara_DFT.c:line
       .248
20 |||||------------------------------
21 5||||    0.0% |  0.000001 |MPI_Comm_rank:...:line.0
22 5||||    0.0% |  0.000002 |MPI_Comm_size:...:line.0
23 |||||==============================
24 4|||    0.0% |  0.000002 |ReadPara_DFT:SetPara_DFT.c:line
       .281
25 5|||         |           | fnjoint2:openmx_common.c:line.389
26 4|||    0.1% |  0.048502 |ReadPara_DFT:SetPara_DFT.c:line
       .288
27 |||||------------------------------
28 5||||    0.1% |  0.047632 |__ipas_Read_PAO:SetPara_DFT.c:
       line.469
29 ||||||-----------------------------
30 6|||||    0.1% |  0.047364 |input_double:Inputtools.c:line
       .241
31 6|||||    0.0% |  0.000066 |input_int:Inputtools.c:line.203
```

```
32 | 6|||||    0.0% |   0.000202 |input_open:Inputtools.c:line.24
33 | ||||||================================
34 | 5||||    0.0% |   0.000837 |__ipas_Read_PAO:SetPara_DFT.c:
       line.517
35 | ||||||----------------------------
36 | 6|||||    0.0% |   0.000093 |input_double:Inputtools.c:line
       .241
37 | 6|||||    0.0% |   0.000745 |input_int:Inputtools.c:line.203
38 | ||||||================================
39 | 5||||    0.0% |   0.000033 |__ipas_Read_PAO:SetPara_DFT.c:
       line.569
40 | 6||||          |            | input_close:Inputtools.c:line.49
41 | ||||================================
42 | 4|||    0.0% |   0.000189 |ReadPara_DFT:SetPara_DFT.c:line
       .299
43 | 5|||          |            | Allocate_Arrays:Allocate_Arrays.c
       :line.7
44 | 4|||    0.0% |   0.000002 |ReadPara_DFT:SetPara_DFT.c:line
       .309
45 | 5|||          |            | fnjoint2:openmx_common.c:line.389
46 | 4|||    0.0% |   0.005185 |ReadPara_DFT:SetPara_DFT.c:line
       .316
47 | |||||----------------------------
48 | 5||||    0.0% |   0.000676 |__ipas_Read_PAO:SetPara_DFT.c:
       line.469
49 | ||||||----------------------------
50 | 6|||||    0.0% |   0.000604 |input_double:Inputtools.c:line
       .241
51 | 6|||||    0.0% |   0.000064 |input_int:Inputtools.c:line.203
52 | 6|||||    0.0% |   0.000009 |input_open:Inputtools.c:line.24
53 | ||||||================================
54 | 5||||    0.0% |   0.000121 |__ipas_Read_PAO:SetPara_DFT.c:
       line.493
55 | 6||||          |            | input_find:Inputtools.c:line.493
56 | 5||||    0.0% |   0.000002 |__ipas_Read_PAO:SetPara_DFT.c:
       line.506
57 | 6||||          |            | input_last:Inputtools.c:line.514
58 | 5||||    0.0% |   0.000822 |__ipas_Read_PAO:SetPara_DFT.c:
       line.517
59 | ||||||----------------------------
60 | 6|||||    0.0% |   0.000084 |input_double:Inputtools.c:line
       .241
61 | 6|||||    0.0% |   0.000738 |input_int:Inputtools.c:line.203
62 | ||||||================================
63 | 5||||    0.0% |   0.003518 |__ipas_Read_PAO:SetPara_DFT.c:
       line.536
64 | 6||||          |            | input_find:Inputtools.c:line.493
65 | 5||||    0.0% |   0.000012 |__ipas_Read_PAO:SetPara_DFT.c:
       line.557
```

```
66  6|||| |  | input_last:Inputtools.c:line.514
67  5||||  0.0% |  0.000033 |__ipas_Read_PAO:SetPara_DFT.c:
        line.569
68  6|||| |  | input_close:Inputtools.c:line.49
69  |||||==========================
70  4|||  0.0% |  0.000002 |ReadPara_DFT:SetPara_DFT.c:line
        .358
71  5|||  |  | fnjoint2:openmx_common.c:line.389
72  4|||  0.0% |  0.028508 |ReadPara_DFT:SetPara_DFT.c:line
        .364
73  |||||--------------------------
74  5||||  0.0% |  0.000020 |__ipas_Read_VPS:SetPara_DFT.c:
        line.1007
75  6|||| |  | input_close:Inputtools.c:line.49
76  5||||  0.0% |  0.000004 |__ipas_Read_VPS:SetPara_DFT.c:
        line.589
77  ||||||------------------------
78  6|||||  0.0% |  0.000002 |MPI_Comm_rank:...:line.0
79  6|||||  0.0% |  0.000003 |MPI_Comm_size:...:line.0
80  ||||||========================
81  5||||  0.0% |  0.028299 |__ipas_Read_VPS:SetPara_DFT.c:
        line.618
82  ||||||------------------------
83  6|||||  0.0% |  0.028103 |input_double:Inputtools.c:line
        .241
84  6|||||  0.0% |  0.000195 |input_open:Inputtools.c:line.24
85  ||||||========================
86  5||||  0.0% |  0.000047 |__ipas_Read_VPS:SetPara_DFT.c:
        line.643
87  ||||||------------------------
88  6|||||  0.0% |  0.000028 |input_double:Inputtools.c:line
        .241
89  6|||||  0.0% |  0.000018 |input_int:Inputtools.c:line.203
90  ||||||========================
91  5||||  0.0% |  0.000136 |__ipas_Read_VPS:SetPara_DFT.c:
        line.674
92  ||||||------------------------
93  6|||||  0.0% |  0.000062 |input_find:Inputtools.c:line.493
94  6|||||  0.0% |  0.000074 |input_logical:Inputtools.c:line
        .160
95  ||||||========================
96  5||||  0.0% |  0.000002 |__ipas_Read_VPS:SetPara_DFT.c:
        line.757
97  6|||| |  | input_last:Inputtools.c:line.514
98  |||||==========================
99  4|||  0.0% |  0.000206 |ReadPara_DFT:SetPara_DFT.c:line
        .375
100 5|||  |  | Allocate_Arrays:Allocate_Arrays.c
        :line.7
```

```
101 | 4|||    0.0% |   0.000002 |ReadPara_DFT:SetPara_DFT.c:line
    |    .384
102 | 5|||         |            | fnjoint2:openmx_common.c:line.389
103 | 4|||    3.1% |   2.859272 |ReadPara_DFT:SetPara_DFT.c:line
    |    .391
104 | |||||-------------------------
105 | 5||||    0.0% |   0.000017 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1007
106 | 6||||         |            | input_close:Inputtools.c:line.49
107 | 5||||    2.7% |   2.483385 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1024
108 | ||||||-----------------------
109 | 6|||||    1.3% |   1.222610 |V_Hart_atom:SetPara_DFT.c:line
    |    .1368
110 | 7|||||         |            | AtomicDenF:AtomicDenF.c:line.18
111 | 6|||||    1.4% |   1.260775 |V_Hart_atom:SetPara_DFT.c:line
    |    .1411
112 | 7|||||         |            | AtomicDenF:AtomicDenF.c:line.18
113 | ||||||=========================
114 | 5||||    0.0% |   0.021921 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1102
115 | 6||||         |            | RadialF:RadialF.c:line.19
116 | 5||||    0.0% |   0.016477 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1116
117 | 6||||         |            | RadialF:RadialF.c:line.19
118 | 5||||    0.0% |   0.045710 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1134
119 | 6||||         |            | Int_phi0_phi1:SetPara_DFT.c:line
    |    .1313
120 | 7||||         |            |  PhiF:PhiF.c:line.14
121 | 5||||    0.0% |   0.005719 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1147
122 | 6||||         |            | Int_phi0_phi1:SetPara_DFT.c:line
    |    .1313
123 | 7||||         |            |  PhiF:PhiF.c:line.14
124 | 5||||    0.2% |   0.173282 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1176
125 | 6||||         |            | Int_phi0_phi1:SetPara_DFT.c:line
    |    .1313
126 | 7||||         |            |  PhiF:PhiF.c:line.14
127 | 5||||    0.1% |   0.053218 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1190
128 | 6||||         |            | Int_phi0_phi1:SetPara_DFT.c:line
    |    .1313
129 | 7||||         |            |  PhiF:PhiF.c:line.14
130 | 5||||    0.1% |   0.059061 |__ipas_Read_VPS:SetPara_DFT.c:
    |    line.1212
131 | 6||||         |            | Int_phi0_phi1:SetPara_DFT.c:line
    |    .1313
```

```
132 | 7|||| |  | PhiF:PhiF.c:line.14
133 | 5|||| 0.0% | 0.000004 |__ipas_Read_VPS:SetPara_DFT.c:
    line.589
134 | ||||||----------
135 | 6||||| 0.0% | 0.000001 |MPI_Comm_rank:...:line.0
136 | 6||||| 0.0% | 0.000003 |MPI_Comm_size:...:line.0
137 | ||||||==========
138 | 5|||| 0.0% | 0.000184 |__ipas_Read_VPS:SetPara_DFT.c:
    line.618
139 | ||||||----------
140 | 6||||| 0.0% | 0.000176 |input_double:Inputtools.c:line
    .241
141 | 6||||| 0.0% | 0.000008 |input_open:Inputtools.c:line.24
142 | ||||||==========
143 | 5|||| 0.0% | 0.000044 |__ipas_Read_VPS:SetPara_DFT.c:
    line.643
144 | ||||||----------
145 | 6||||| 0.0% | 0.000027 |input_double:Inputtools.c:line
    .241
146 | 6||||| 0.0% | 0.000018 |input_int:Inputtools.c:line.203
147 | ||||||==========
148 | 5|||| 0.0% | 0.000135 |__ipas_Read_VPS:SetPara_DFT.c:
    line.674
149 | ||||||----------
150 | 6||||| 0.0% | 0.000061 |input_find:Inputtools.c:line.493
151 | 6||||| 0.0% | 0.000074 |input_logical:Inputtools.c:line
    .160
152 | ||||||==========
153 | 5|||| 0.0% | 0.000002 |__ipas_Read_VPS:SetPara_DFT.c:
    line.757
154 | 6|||| |  | input_last:Inputtools.c:line.514
155 | 5|||| 0.0% | 0.000074 |__ipas_Read_VPS:SetPara_DFT.c:
    line.767
156 | 6|||| |  | input_find:Inputtools.c:line.493
157 | 5|||| 0.0% | 0.000003 |__ipas_Read_VPS:SetPara_DFT.c:
    line.819
158 | 6|||| |  | input_last:Inputtools.c:line.514
159 | 5|||| 0.0% | 0.000036 |__ipas_Read_VPS:SetPara_DFT.c:
    line.968
160 | 6|||| |  | input_logical:Inputtools.c:line
    .160
161 | ||||==========
162 | 4||| 0.0% | 0.000133 |Set_Comp2Real:SetPara_DFT.c:line
    .1601
163 | 5||| |  | Complex:openmx_common.c:line.91
164 | 4||| 0.0% | 0.005513 |Set_Comp2Real:SetPara_DFT.c:line
    .1712
165 | 5||| |  | Complex:openmx_common.c:line.91
```

```
166 | 4|||    0.0% |   0.000014 |Set_Comp2Real:SetPara_DFT.c:line
    .1715
167 | 5|||         |            | Complex:openmx_common.c:line.91
168 | 4|||    0.0% |   0.000133 |Set_Comp2Real:SetPara_DFT.c:line
    .1720
169 | 5|||         |            | Complex:openmx_common.c:line.91
170 | 4|||    0.0% |   0.000119 |Set_Comp2Real:SetPara_DFT.c:line
    .1727
171 | 5|||         |            | Complex:openmx_common.c:line.91
172 | 4|||    0.0% |   0.000132 |Set_Comp2Real:SetPara_DFT.c:line
    .1734
173 | 5|||         |            | Complex:openmx_common.c:line.91
174 | 4|||    0.0% |   0.000119 |Set_Comp2Real:SetPara_DFT.c:line
    .1741
175 | 5|||         |            | Complex:openmx_common.c:line.91
176 | 4|||    0.0% |   0.032418 |__ipas_Gauss_Legendre:
    Gauss_Legendre.c:line.25
177 |||=================================
178 | 3||    0.0% |   0.000006 |SetPara_DFT:SetPara_DFT.c:line.109
179 | 4||        |            | output_structures:SetPara_DFT.c:
    line.2224
180 | 5||        |            |   Cross_Product:openmx_common.c:
    line.68
181 | 3||   17.8% |  16.493565 |SetPara_DFT:SetPara_DFT.c:line.118
182 ||||-----------------------------
183 | 4|||    0.0% |   0.001632 |FT_PAO:FT_PAO.c:line.40
184 | 4|||    0.0% |   0.000003 |FT_PAO:FT_PAO.c:line.41
185 | 5|||         |            | dtime:dtime.c:line.15
186 | 4|||    0.0% |   0.000004 |FT_PAO:FT_PAO.c:line.68
187 |||||---------------------------
188 | 5||||   0.0% |   0.000002 |MPI_Comm_rank:...:line.0
189 | 5||||   0.0% |   0.000002 |MPI_Comm_size:...:line.0
190 | 4|||    0.3% |   0.268966 |FT_PAO:FT_PAO.c:line.136
191 | 4|||    3.4% |   3.157631 |FT_PAO:FT_PAO.c:line.160
192 | 5|||         |            | Spherical_Bessel:Spherical_Bessel
    .c:line.21
193 | 4|||    1.4% |   1.290456 |FT_PAO:FT_PAO.c:line.190
194 | 5|||         |            | RadialF:RadialF.c:line.19
195 | 4|||    0.0% |   0.000012 |FT_PAO:FT_PAO.c:line.234
196 |||||---------------------------
197 | 5||||   0.0% |   0.000005 |MPI_Bcast:...:line.0
198 | 5||||   0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
199 | 5||||   0.0% |   0.000001 |MPI_Barrier:...:line.0
200 | 5||||   0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
201 ||||=================================
202 | 4|||    0.0% |   0.000007 |FT_PAO:FT_PAO.c:line.278
203 | 5|||         |            | dtime:dtime.c:line.15
204 ||||=================================
205 | 4|||    0.0% |   0.001673 |FT_NLP:FT_NLP.c:line.40
```

```
206 | 4|||    0.0% |   0.000002 |FT_NLP:FT_NLP.c:line.41
207 | 5|||         |            |  dtime:dtime.c:line.15
208 | 4|||    0.0% |   0.000003 |FT_NLP:FT_NLP.c:line.66
209 | |||||----------------------------
210 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
211 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
212 | 4|||    1.0% |   0.942579 |FT_NLP:FT_NLP.c:line.134
213 | 4|||    3.6% |   3.304627 |FT_NLP:FT_NLP.c:line.164
214 | 5|||         |            |  Spherical_Bessel:Spherical_Bessel
    |     .c:line.21
215 | 4|||    8.1% |   7.525941 |FT_NLP:FT_NLP.c:line.196
216 | 5|||         |            |  Nonlocal_RadialF:Nonlocal_RadialF
    |     .c:line.6
217 | 4|||    0.0% |   0.000023 |FT_NLP:FT_NLP.c:line.243
218 | |||||----------------------------
219 | 5||||    0.0% |   0.000012 |MPI_Bcast:...:line.0
220 | 5||||    0.0% |   0.000011 |MPI_Bcast(sync):...:line.0
221 | |||||============================
222 | 4|||    0.0% |   0.000007 |FT_NLP:FT_NLP.c:line.282
223 | 5|||         |            |  dtime:dtime.c:line.15
224 | |||||============================
225 | 3||   11.8% |  10.936564 |SetPara_DFT:SetPara_DFT.c:line.122
226 | ||||----------------------------
227 | 4|||    0.0% |   0.001885 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.40
228 | 4|||    0.0% |   0.000002 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.41
229 | 5|||         |            |  dtime:dtime.c:line.15
230 | 4|||    0.0% |   0.000004 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.71
231 | |||||----------------------------
232 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
233 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
234 | 4|||    0.9% |   0.876138 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.155
235 | 4|||    0.4% |   0.401717 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.181
236 | 5|||         |            |  Spherical_Bessel:Spherical_Bessel
    |     .c:line.21
237 | 4|||    8.4% |   7.811978 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.208
238 | 5|||         |            |  PhiF:PhiF.c:line.14
239 | 4|||    0.0% |   0.000150 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    |     line.262
240 | |||||----------------------------
241 | 5||||    0.0% |   0.000078 |MPI_Bcast:...:line.0
242 | 5||||    0.0% |   0.000072 |MPI_Bcast(sync):...:line.0
243 | |||||============================
```

```
244 | 4|||    0.0% |   0.000007 |FT_ProExpn_VNA:FT_ProExpn_VNA.c:
    line.301
245 | 5|||         |            | dtime:dtime.c:line.15
246 | |||||=============================
247 | 4|||    0.0% |   0.001350 |FT_VNA:FT_VNA.c:line.39
248 | 4|||    0.0% |   0.000002 |FT_VNA:FT_VNA.c:line.40
249 | 5|||         |            | dtime:dtime.c:line.15
250 | 4|||    0.0% |   0.000004 |FT_VNA:FT_VNA.c:line.67
251 | |||||-----------------------------
252 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
253 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
254 | 4|||    0.1% |   0.097845 |FT_VNA:FT_VNA.c:line.150
255 | 4|||    0.9% |   0.861045 |FT_VNA:FT_VNA.c:line.176
256 | 5|||         |            | Spherical_Bessel:Spherical_Bessel
    .c:line.21
257 | 4|||    0.0% |   0.000816 |FT_VNA:FT_VNA.c:line.183
258 | 5|||         |            | VNAF:VNAF.c:line.18
259 | 4|||    0.5% |   0.498871 |FT_VNA:FT_VNA.c:line.186
260 | 5|||         |            | VNAF:VNAF.c:line.18
261 | 4|||    0.0% |   0.000010 |FT_VNA:FT_VNA.c:line.224
262 | |||||-----------------------------
263 | 5||||    0.0% |   0.000005 |MPI_Bcast:...:line.0
264 | 5||||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
265 | |||||=============================
266 | 4|||    0.0% |   0.000006 |FT_VNA:FT_VNA.c:line.258
267 | 5|||         |            | dtime:dtime.c:line.15
268 | ||||==============================
269 | 4|||    0.0% |   0.001319 |FT_ProductPAO:FT_ProductPAO.c:line
    .39
270 | 4|||    0.0% |   0.000002 |FT_ProductPAO:FT_ProductPAO.c:line
    .40
271 | 5|||         |            | dtime:dtime.c:line.15
272 | 4|||    0.0% |   0.000003 |FT_ProductPAO:FT_ProductPAO.c:line
    .72
273 | |||||-----------------------------
274 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
275 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
276 | 4|||    0.0% |   0.015467 |FT_ProductPAO:FT_ProductPAO.c:line
    .168
277 | 4|||    0.0% |   0.000417 |FT_ProductPAO:FT_ProductPAO.c:line
    .188
278 | 5|||         |            | RadialF:RadialF.c:line.19
279 | 4|||    0.4% |   0.367510 |FT_ProductPAO:FT_ProductPAO.c:line
    .219
280 | 5|||         |            | Spherical_Bessel:Spherical_Bessel
    .c:line.21
281 | 4|||    0.0% |   0.000012 |FT_ProductPAO:FT_ProductPAO.c:line
    .318
282 | |||||-----------------------------
```

```
283 | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
284 | 5||||    0.0% |   0.000005 |MPI_Barrier(sync):...:line.0
285 | 5||||    0.0% |   0.000005 |MPI_Bcast:...:line.0
286 | 5||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
287 | ||||================================
288 | 4|||    0.0% |   0.000006 |FT_ProductPAO:FT_ProductPAO.c:line
    |     .375
289 | 5|||         |            | dtime:dtime.c:line.15
290 | ||||================================
291 | 3||    0.0% |   0.000004 |__ipap_TRAN_Check_Region_Lead:
    |     TRAN_Check_Region_Lead.c:line.32
292 | |||===============================
293 | ||    0.0% |   0.000080 |readfile:readfile.c:line.80
294 | |||-------------------------------
295 | 3||    0.0% |   0.000034 |Set_Allocate_Atom2CPU:
    |     Set_Allocate_Atom2CPU.c:line.39
296 | 3||    0.0% |   0.000045 |Set_Allocate_Atom2CPU:
    |     Set_Allocate_Atom2CPU.c:line.61
297 | ||||-----------------------------
298 | 4|||    0.0% |   0.000004 |Conventional_Allocation:
    |     Set_Allocate_Atom2CPU.c:line.1198
299 | |||||---------------------------
300 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
301 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
302 | ||||================================
303 | 4|||    0.0% |   0.000006 |Conventional_Allocation:
    |     Set_Allocate_Atom2CPU.c:line.1229
304 | 5|||         |            | Cross_Product:openmx_common.c:
    |     line.68
305 | 4|||    0.0% |   0.000027 |Conventional_Allocation:
    |     Set_Allocate_Atom2CPU.c:line.1248
306 | |||||---------------------------
307 | 5||||    0.0% |   0.000009 |MPI_Bcast:...:line.0
308 | 5||||    0.0% |   0.000008 |MPI_Bcast(sync):...:line.0
309 | 5||||    0.0% |   0.000010 |rnd:openmx_common.c:line.303
310 | ||||================================
311 | 4|||    0.0% |   0.000006 |Conventional_Allocation:
    |     Set_Allocate_Atom2CPU.c:line.1520
312 | |||||---------------------------
313 | 5||||    0.0% |   0.000003 |MPI_Bcast:...:line.0
314 | 5||||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
315 | ||||================================
316 | 4|||    0.0% |   0.000003 |Conventional_Allocation:
    |     Set_Allocate_Atom2CPU.c:line.1566
317 | |||||---------------------------
318 | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
319 | 5||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
320 | |||===============================
321 | ||    0.0% |   0.000145 |readfile:readfile.c:line.91
```

```
322 |||-------------------------------
323 | 3||    0.0% |   0.000049 |Set_Allocate_Atom2CPU:
    |    Set_Allocate_Atom2CPU.c:line.39
324 | 3||    0.0% |   0.000096 |Set_Allocate_Atom2CPU:
    |    Set_Allocate_Atom2CPU.c:line.61
325 ||||-------------------------------
326 | 4|||    0.0% |   0.000003 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1198
327 |||||-------------------------------
328 | 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
329 | 5||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
330 ||||===============================
331 | 4|||    0.0% |   0.000003 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1216
332 |||||-------------------------------
333 | 5||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
334 | 5||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
335 ||||===============================
336 | 4|||    0.0% |   0.000010 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1229
337 | 5|||         |            | Cross_Product:openmx_common.c:
    |    line.68
338 | 4|||    0.0% |   0.000038 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1248
339 |||||-------------------------------
340 | 5||||    0.0% |   0.000008 |MPI_Bcast:...:line.0
341 | 5||||    0.0% |   0.000008 |MPI_Bcast(sync):...:line.0
342 | 5||||    0.0% |   0.000022 |rnd:openmx_common.c:line.303
343 ||||===============================
344 | 4|||    0.0% |   0.000035 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1281
345 |||||-------------------------------
346 | 5||||    0.0% |   0.000003 |Estimate_NL:Set_Allocate_Atom2CPU
    |    .c:line.1650
347 ||||||-------------------------------
348 | 6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
349 | 6|||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
350 ||||||===============================
351 | 5||||    0.0% |   0.000021 |Estimate_NL:Set_Allocate_Atom2CPU
    |    .c:line.1701
352 | 5||||    0.0% |   0.000011 |Estimate_NL:Set_Allocate_Atom2CPU
    |    .c:line.1766
353 ||||||-------------------------------
354 | 6|||||    0.0% |   0.000006 |MPI_Bcast:...:line.0
355 | 6|||||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
356 ||||===============================
357 | 4|||    0.0% |   0.000006 |Conventional_Allocation:
    |    Set_Allocate_Atom2CPU.c:line.1520
358 |||||-------------------------------
```

```
359 | 5|||| 0.0% | 0.000003 |MPI_Bcast:...:line.0
360 | 5|||| 0.0% | 0.000003 |MPI_Bcast(sync):...:line.0
361 |||||=============================
362 | 4||| 0.0% | 0.000003 |Conventional_Allocation:
        Set_Allocate_Atom2CPU.c:line.1566
363 |||||-----------------------------
364 | 5|||| 0.0% | 0.000001 |MPI_Barrier:...:line.0
365 | 5|||| 0.0% | 0.000001 |MPI_Barrier(sync):...:line.0
366 |||============================================
367 | || 0.0% | 0.000004 |readfile:readfile.c:line.99
368 |||-----------------------------------------
369 | 3|| 0.0% | 0.000002 |TRAN_Check_Input:TRAN_Check_Input.c
        :line.30
370 | 3|| 0.0% | 0.000002 |dtime:dtime.c:line.15
371 |||============================================
```

2.1.6 Completion of readfile() and final preparations for entering the main computation loop

At this point, readfile() has completed, and some final preparations for entering the main computation loop are performed.

- PrintMemory() (in PrintMemory.c): is a subroutine to save memory size of each array.
- PrintMemory_Fix() (in PrintMemory_Fix.c): is a subroutine to print the size of arrays with fixed sizes.
- init() (in init.c): is a subroutine to initialize several parameters at the starting point of calculations, such as correction position and force flags, atomic weight settings and transformation, and initial Ukc calculation.
- double **Gxyz (atomic global coordinates, velocities, and gradients of the total energy with respect to the atomic coordinates, size: Gxyz[atomnum+1][YOUSO26]).

Listing 2.4: Final preparations for entering the main computation loop

```
1 | || 0.0% | 0.000001 |MPI_Barrier:...:line.0
2 | || 0.0% | 0.000001 |MPI_Barrier(sync):...:line.0
3 | || 0.0% | 0.000848 |PrintMemory:PrintMemory.c:line.19
4 | || 0.0% | 0.000009 |PrintMemory_Fix:PrintMemory_Fix.c:
      line.19
5 | || 0.0% | 0.005601 |PrintMemory_Fix:PrintMemory_Fix.c:
      line.28
6 | 3| | | PrintMemory:PrintMemory.c:line.19
```

```
 7 ||    0.0% |   0.000004 |init:init.c:line.64
 8 3|         |            | InitV:init.c:line.525
 9 ||||------------------------------
10 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
11 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
12 ||||==================================
13 |    0.0% |   0.000004 |main:openmx.c:line.401
14 |         |            | __ipap_fnjoint:openmx_common.c:line
       .358
15 |    0.0% |   0.000007 |main:openmx.c:line.416
16 ||---------------------------------
17 ||    0.0% |   0.000004 |MPI_Bcast:...:line.0
18 ||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
19 ||================================
20 |    0.0% |   0.000005 |main:openmx.c:line.434
21 ||---------------------------------
22 ||    0.0% |   0.000003 |MPI_Bcast:...:line.0
23 ||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
24 ||================================
```

2.2 Main Computation Loop

2.2.1 truncation

truncation() (in truncation.c): is a subroutine to divide a large system into smaller systems and set grid data.

- free_arrays_truncation0(): to free and prepare the arrays for this round of calculations, including H0, CntH0, HNL, iCntHNL, OLP, CntOLP, H, CntH, DS_NL, CntDS_NL, DM, ResidualDM, EDM, PDM, IOLP, CntCoes, HVNA, DS_VNA, HVNA2, CntHVNA2, DM_onsite, v_eff, NC_OcpN, NC_v_eff, GListTAtoms0, GListTCells0, GListTAtoms1, GListTAtoms2, GListTAtoms3, Density_Grid, ADensity_Grid, PCC-Density_Grid, Vxc_Grid, RefVxc_Grid, VNA_Grid, dVHart_Grid, Vpot_Grid, Orbs_Grid, COrbs_Grid, VEF_Grid, NumOLG, RMI1, RMI2, ratv, atv, atv_ijk, GridListAtom, CellListAtom, MGridListAtom, F_M2G, S_M2G, etc.

- Set_Periodic(): to allocates atv, ratv, atv_ijk, R_index1, R_index2, CellDis and calls Generation_ATV() in openmx_common.c to generate atv, ratv, atv_ijk.

- Estimate_Trn_System(): to find Max_FSNAN by the physical truncation for allocation of natn, ncn, and Dis. FNAN, SNAN, Max_FNAN, Max_FSNAN are determined by the physical truncation.

- Allocate_Arrays() (in Allocate_Arrays.c): to allocate natn, ncn, and Dis.
- Trn_System(): to find TFNAN and TSNAN.
- Set_Inf_SndRcv(): to find the following information for send and receive.
  - int *F_Rcv_Num (gives the number of atoms of which informations, related by FNAN, are received at myid from ID. size: F_Rcv_Num[numprocs])
  - int *S_Rcv_Num (gives the number of atoms of which informations, related by SNAN, are recieved at myid from ID. size: S_Rcv_Num[numprocs])
  - int *F_Snd_Num (gives the number of atoms of which informations, related by FNAN, are transfered from myid to ID. size: F_Snd_Num[numprocs])
  - int *S_Snd_Num (gives the number of atoms of which informations, related by SNAN, are transfered from myid to ID. size: S_Snd_Num[numprocs])
  - int **Rcv_GAN (a global atom index cell index of which information is received at myid from a processor ID. size: Rcv_GAN[numprocs] [F_Rcv_Num[ID]+S_Rcv_Num[ID]])
  - int **Snd_MAN (an intermediate atom index of which information is sent to a processor ID. size: Snd_MAN[numprocs][FS_Snd_Num[ID]])
  - int **Snd_GAN (a global atom index of which information is sent to a processor ID. size: Snd_GAN[numprocs][FS_Snd_Num[ID]])
  - int *F_TopMAN,*S_TopMAN (give the first intermediate atom number in atoms sent from ID in the size of F_Rcv_Num[ID] and F_Rcv_Num[ID] + S_Rcv_Num[ID], respectively. size: F_TopMAN[numprocs], S_TopMAN[numprocs])
  - int *F_G2M,*S_G2M (give a conversion from the global atom number to the medium atom number for atoms sent from ID in the size of F_Rcv_Num[ID] and F_Rcv_Num[ID] + S_Rcv_Num[ID], respectively. size: F_G2M[atomnum+1],S_G2M[atomnum+1])
  - int **Pro_Snd_GAtom (gives the global atomic number used for MPI communication of DS_VNA and DS_NL size: Pro_Snd_GAtom [numprocs][Num_Pro_Snd[ID]])
  - int **Pro_Snd_MAtom (gives the intermedium atomic number used for MPI communication of DS_VNA and DS_NL size: Pro_Snd_MAtom [numprocs][Num_Pro_Snd[ID]])

  - int **Pro_Snd_LAtom (gives the local atomic number used for MPI communication of DS_VNA and DS_NL size: Pro_Snd_LAtom [numprocs][Num_Pro_Snd[ID]])
  - int **Pro_Snd_LAtom2 (gives the local atomic number used for MPI communication of DS_VNA and DS_NL, and tells us the position of array which should be stored. size: Pro_Snd_LAtom2[numprocs] [Num_Pro_Snd[ID]])
  - qsort_int3() (in QuickSort.c): quick sorting of the array Pro_Snd_GAtom.

- Set_RMI(): RMI[Mc_AN][i][j] is a array which specifies the position of arrays storing hopping and overlap integrals between atoms i and j.
  - int ***RMI1 (a table which converts local atomic index to global atomic index. size: RMI1[Matomnum+1] [FNAN[Gc_AN]+SNAN[Gc_AN]+1] [FNAN[Gc_AN]+SNAN[Gc_AN]+1])
  - int ***RMI2 (a table which converts local atomic index to global atomic index. size: RMI2[Matomnum+1] [FNAN[Gc_AN]+SNAN[Gc_AN]+1] [FNAN[Gc_AN]+SNAN[Gc_AN]+1])

- UCell_Box(): xyz-coordinate to cell-coordinate, finds grids overlapping to each atom, outputs informations on grids to the .UCell file, finds overlap grids between two orbitals, finds grids that each processor has to know and setting of grids (intermediate).
  - Reciprocal lattice vectors rtv
  - set real space grids with gtv, rgtv
  - Find_ApproxFactN() (in Find_ApproxFactN.c): is a subroutine to find the number of grids along the a-, b-, and c-axes which satisfies the required cutoff energy approximately.
  - double **Cell_Gxyz; atomic global coordinates spanned by the unit cell vectors size: Cell_Gxyz[atomnum+1][4]
  - int **MGridListAtom; neighboring grid points (medium variable) of an atom Mc_AN size: MGridListAtom[Matomnum+MatomnumF+1] [Max_GridN_Atom*ScaleSize+1]
  - Get_Grid_XYZ() (in openmx_common.c):
  - GN2N() (in openmx_common.c):
  - R_atv() (in openmx_common.c):
  - Find_CGrids() (in Find_CGrids.c): gives the coordinates in the translated cell or in the original cell.
  - int *GridN_Atom; the number of grids overlaping to each atom size: GridN_Atom[atomnum+1]

- int **GridListAtom; neighboring grid points of an atom Mc_AN size: GridListAtom[Matomnum+1][Max_GridN_Atom*ScaleSize+1]
- int **CellListAtom; cell number of neighboring grid points of an atom Mc_AN size: CellListAtom[Matomnum+MatomnumF+1] [Max_GridN_Atom*ScaleSize+1]
- int ***GListTAtoms0; grid index (grobal) overlaping between two orbitals size: GListTAtoms0[Matomnum+1] [FNAN[Gc_AN]+1] [NumOLG[Gc_AN][h_AN]]
- int ***GListTCells0; cell index (grobal) overlaping between two orbitals size: GListTCells0[Matomnum+1] [FNAN[Gc_AN]+1] [NumOLG[Gc_AN][h_AN]]
- int ***GListTAtoms1; grid index (local for ct_AN) overlaping between two orbitals size: GListTAtoms1[Matomnum+1] [FNAN[Gc_AN]+1] [NumOLG[Gc_AN][h_AN]]
- int ***GListTAtoms2; grid index (local for h_AN) overlaping between two orbitals size: GListTAtoms2[Matomnum+1] [FNAN[Gc_AN]+1] [NumOLG[Gc_AN][h_AN]]
- int ***GListTAtoms3; grid index (medium1) overlaping between two orbitals size: GListTAtoms3[Matomnum+1] [FNAN[Gc_AN]+1] [NumOLG[Gc_AN][h_AN]]
- int **NumOLG; the number of overlapping grids between atom Mc_AN and atom Lh_AN size: NumOLG[Matomnum+1] [FNAN[Gc_AN]+1]
- allocate_grids2atoms(): find the unit vector perpendicular to the bc-plane, find the minimum and maximum grid numbers of a-axis,
- int *My_Cell0 My_Cell0 gives a flag for the grids of a-axis that a processor ID has to know. size: My_Cell0[Ngrid1];
- int *My_Cell1 My_Cell1 gives the global grids of a-axis that a processor ID has to know. size: My_Cell1[Num_Cells0];
- int *Cell_ID0 Cell_ID0 gives a processor ID which computes electron densities on the grids of a-axis. size: Cell_ID0[Ngrids1];
- int *edge_block edge_block specifies the boundary cell of My_Cell0 size: edge_block[Ngrids1];
- int *Start_Grid1,*End_Grid1; Start_Grid1 and End_Grid1 give the first and final grid numbers of the a-axis allocated to a processor ID. size: Start_Grid1[numprocs],End_Grid1[numprocs]
- int *Start_Grid2,*End_Grid2; Start_Grid1 and End_Grid1 give the first and final grid numbers of the b-axis allocated to a processor ID. size: Start_Grid1[numprocs],End_Grid1[numprocs]

- int *Num_Rcv_Grid1; Num_Rcv_Grid1 gives the number of grids on the a-axis for myid to recieve from ID. size: Num_Rcv_Grid1[numprocs];
- int *Num_Snd_Grid1; Num_Snd_Grid1 gives the number of grids on the a-axis for myid to send to ID. size: Num_Snd_Grid1[numprocs];
- int **Rcv_Grid1; Rcv_Grid1 gives the grids on the a-axis for myid to recieve from ID. size: Rcv_Grid1[numprocs][Num_Rcv_Grid1[ID]];
- int **Snd_Grid1; Snd_Grid1 gives the grids on the a-axis for myid to send to ID. size: Snd_Grid1[numprocs][Num_Snd_Grid1[ID]];
- int *Num_IRcv_Grid1; Num_IRcv_Grid1 gives the number of grids on the a-axis for myid to recieve from ID for converting Poisson's grid to atom's grid. size: Num_IRcv_Grid1[numprocs];
- int *Num_ISnd_Grid1; Num_ISnd_Grid1 gives the number of grids on the a-axis for myid to send to ID for converting Poisson's grid to atom's grid. size: Num_ISnd_Grid1[numprocs];
- int **IRcv_Grid1; IRcv_Grid1 gives the grids on the a-axis for myid to recieve from ID for converting Poisson's grid to atom's grid. size: IRcv_Grid1[numprocs][Num_IRcv_Grid1[ID]];
- int **ISnd_Grid1; ISnd_Grid1 gives the grids on the a-axis for myid to send to ID for converting Poisson's grid to atom's grid. size: ISnd_Grid1[numprocs][Num_ISnd_Grid1[ID]];
- int *TopMAN2_Grid; TopMAN2_Grid gives the first medium grid number in grids sent from ID in the size of Num_Rcv_FNAN2_Grid[ID]. size: TopMAN2_Grid[numprocs]
- int *Num_Rcv_FNAN2_Grid Num_Rcv_FNAN2_Grid gives the number of grids for myid to recieve from ID in terms of FNAN2. size: Num_Rcv_FNAN2_Grid[numprocs]
- int *Num_Snd_FNAN2_Grid Num_Snd_FNAN2_Grid gives the number of grids for myid to send to ID in terms of FNAN2. size: Num_Snd_FNAN2_Grid[numprocs]
- int **Snd_FNAN2_At Snd_FNAN2_At gives the global atom number which are sent from myid to ID in terms of FNAN2. size: Snd_FNAN2_At[numprocs][Num_Snd_FNAN2_Grid[ID]]
- int **Snd_FNAN2_Nc Snd_FNAN2_Nc gives the medium grid number which are sent from myid to ID in terms of FNAN2. size: Snd_FNAN2_Nc[numprocs][Num_Snd_FNAN2_Grid[ID]]
- int *Rcv_FNAN2_GA Rcv_FNAN2_GA gives the global atom number which are sent from the other IDs in terms of FNAN2. size: Rcv_FNAN2_GA[FNAN2_Grid]
- int *Rcv_FNAN2_MN Rcv_FNAN2_MN gives a medium grid number sent in terms of FNAN2 size: Rcv_FNAN2_MN[numprocs]

– int *Rcv_FNAN2_GRc Rcv_FNAN2_GRc gives a global grid number sent in terms of FNAN2 size: Rcv_FNAN2_GRc[numprocs]

Listing 2.5: truncation.c

```
1  |   45.4% |  42.087852 |main:openmx.c:line.460
2  ||---------------------------------
3  ||    0.0% |   0.020698 |__ipai_truncation:truncation.c:line
       .63
4  ||=================================
5  ||    0.0% |   0.000003 |__ipai_truncation:truncation.c:line
       .102
6  |||-------------------------------
7  3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
8  3||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
9  |||===============================
10 ||    0.0% |   0.000002 |__ipai_truncation:truncation.c:line
       .112
11 3|         |            | dtime:dtime.c:line.15
12 ||    0.0% |   0.000005 |__ipai_truncation:truncation.c:line
       .119
13 |||-------------------------------
14 3||    0.0% |   0.000003 |MPI_Bcast:...:line.0
15 3||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
16 |||===============================
17 ||    0.0% |   0.000003 |__ipai_truncation:truncation.c:line
       .122
18 3|         |            | free_arrays_truncation0:truncation.
       c:line.5035
19 ||||-----------------------------
20 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
21 4|||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
22 ||||===========================
23 ||    0.0% |   0.001324 |__ipai_truncation:truncation.c:line
       .221
24 |||-------------------------------
25 3||    0.0% |   0.000350 |__ipai_Set_Periodic:truncation.c:
       line.4901
26 4||         |            | PrintMemory:PrintMemory.c:line.19
27 3||    0.0% |   0.000007 |__ipai_Set_Periodic:truncation.c:
       line.4923
28 4||         |            | Generation_ATV:openmx_common.c:
       line.27
29 3||    0.0% |   0.000006 |Estimate_Trn_System:truncation.c:
       line.2852
30 ||||-----------------------------
31 4|||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
32 4|||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
33 ||||===========================
```

```
34 | 3||    0.0% |   0.000147 |Estimate_Trn_System:truncation.c:
       line.2872
35 | 3||    0.0% |   0.000018 |Estimate_Trn_System:truncation.c:
       line.2955
36 | ||||------------------------------
37 | 4|||    0.0% |   0.000015 |MPI_Allreduce:...:line.0
38 | 4|||    0.0% |   0.000004 |MPI_Allreduce(sync):...:line.0
39 | ||||==============================
40 | 3||    0.0% |   0.000039 |Estimate_Trn_System:truncation.c:
       line.2987
41 | ||||------------------------------
42 | 4|||    0.0% |   0.000018 |MPI_Reduce:...:line.0
43 | 4|||    0.0% |   0.000005 |MPI_Reduce(sync):...:line.0
44 | 4|||    0.0% |   0.000006 |MPI_Bcast:...:line.0
45 | 4|||    0.0% |   0.000010 |MPI_Bcast(sync):...:line.0
46 | ||||==============================
47 | 3||    0.0% |   0.000005 |Allocate_Arrays:Allocate_Arrays.c:
       line.7
48 | 3||    0.0% |   0.000006 |__ipai_Trn_System:truncation.c:line
       .2483
49 | ||||------------------------------
50 | 4|||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
51 | 4|||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
52 | ||||==============================
53 | 3||    0.0% |   0.000142 |__ipai_Trn_System:truncation.c:line
       .2497
54 | 3||    0.0% |   0.000055 |__ipai_Trn_System:truncation.c:line
       .2614
55 | ||||------------------------------
56 | 4|||    0.0% |   0.000027 |MPI_Bcast:...:line.0
57 | 4|||    0.0% |   0.000028 |MPI_Bcast(sync):...:line.0
58 | ||||==============================
59 | 3||    0.0% |   0.000247 |__ipai_Trn_System:truncation.c:line
       .2641
60 | ||||------------------------------
61 | 4|||    0.0% |   0.000010 |__ipai_LT:truncation.c:line.3273
62 | |||||----------------------------
63 | 5||||    0.0% |   0.000007 |MPI_Comm_rank:...:line.0
64 | 5||||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
65 | |||||============================
66 | 4|||    0.0% |   0.000111 |__ipai_LT:truncation.c:line.3281
67 | 4|||    0.0% |   0.000112 |__ipai_LT:truncation.c:line.3293
68 | 4|||    0.0% |   0.000014 |__ipai_LT:truncation.c:line.3300
69 | 5|||         |            | dtime:dtime.c:line.15
70 | ||||==============================
71 | 3||    0.0% |   0.000097 |__ipai_Trn_System:truncation.c:line
       .2645
72 | 3||    0.0% |   0.000025 |__ipai_Trn_System:truncation.c:line
       .2760
```

```
|||+-------------------------------
4|||    0.0% |   0.000006 |MPI_Bcast:...:line.0
4|||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
4|||    0.0% |   0.000008 |MPI_Reduce:...:line.0
4|||    0.0% |   0.000006 |MPI_Reduce(sync):...:line.0
|||=================================
3||    0.0% |   0.000064 |__ipai_Trn_System:truncation.c:line
    .2788
|||+-------------------------------
4|||    0.0% |   0.000032 |MPI_Bcast:...:line.0
4|||    0.0% |   0.000032 |MPI_Bcast(sync):...:line.0
|||=================================
3||    0.0% |   0.000116 |__ipai_Trn_System:truncation.c:line
    .2819
||=================================
||    0.0% |   0.000470 |__ipai_truncation:truncation.c:line
    .273
||+-------------------------------
3||    0.0% |   0.000007 |__ipai_Set_Periodic:truncation.c:
    line.4923
4||         |            | Generation_ATV:openmx_common.c:
    line.27
3||    0.0% |   0.000003 |__ipai_Trn_System:truncation.c:line
    .2483
|||+-------------------------------
4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
4|||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
|||=================================
3||    0.0% |   0.000003 |Estimate_Trn_System:truncation.c:
    line.2852
|||+-------------------------------
4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
|||=================================
3||    0.0% |   0.000064 |Estimate_Trn_System:truncation.c:
    line.2872
3||    0.0% |   0.000004 |Estimate_Trn_System:truncation.c:
    line.2955
|||+-------------------------------
4|||    0.0% |   0.000002 |MPI_Allreduce:...:line.0
4|||    0.0% |   0.000002 |MPI_Allreduce(sync):...:line.0
|||=================================
3||    0.0% |   0.000012 |Estimate_Trn_System:truncation.c:
    line.2987
|||+-------------------------------
4|||    0.0% |   0.000003 |MPI_Bcast:...:line.0
4|||    0.0% |   0.000002 |MPI_Bcast(sync):...:line.0
4|||    0.0% |   0.000004 |MPI_Reduce:...:line.0
4|||    0.0% |   0.000002 |MPI_Reduce(sync):...:line.0
```

```
112 ||||==========================================
113 3||    0.0% |   0.000002 |Allocate_Arrays:Allocate_Arrays.c:
        line.7
114 3||    0.0% |   0.000072 |__ipai_Trn_System:truncation.c:line
        .2497
115 3||    0.0% |   0.000030 |__ipai_Trn_System:truncation.c:line
        .2614
116 ||||------------------------------
117 4|||    0.0% |   0.000018 |MPI_Bcast:...:line.0
118 4|||    0.0% |   0.000013 |MPI_Bcast(sync):...:line.0
119 ||||==========================================
120 3||    0.0% |   0.000119 |__ipai_Trn_System:truncation.c:line
        .2641
121 ||||------------------------------
122 4|||    0.0% |   0.000003 |__ipai_LT:truncation.c:line.3273
123 |||||----------------------------
124 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
125 5||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
126 ||||==================================
127 4|||    0.0% |   0.000053 |__ipai_LT:truncation.c:line.3281
128 4|||    0.0% |   0.000056 |__ipai_LT:truncation.c:line.3293
129 4|||    0.0% |   0.000007 |__ipai_LT:truncation.c:line.3300
130 5|||         |            | dtime:dtime.c:line.15
131 ||||==========================================
132 3||    0.0% |   0.000053 |__ipai_Trn_System:truncation.c:line
        .2645
133 3||    0.0% |   0.000013 |__ipai_Trn_System:truncation.c:line
        .2760
134 ||||------------------------------
135 4|||    0.0% |   0.000003 |MPI_Bcast:...:line.0
136 4|||    0.0% |   0.000002 |MPI_Bcast(sync):...:line.0
137 4|||    0.0% |   0.000004 |MPI_Reduce:...:line.0
138 4|||    0.0% |   0.000003 |MPI_Reduce(sync):...:line.0
139 ||||==========================================
140 3||    0.0% |   0.000033 |__ipai_Trn_System:truncation.c:line
        .2788
141 ||||------------------------------
142 4|||    0.0% |   0.000016 |MPI_Bcast:...:line.0
143 4|||    0.0% |   0.000017 |MPI_Bcast(sync):...:line.0
144 ||||==========================================
145 3||    0.0% |   0.000057 |__ipai_Trn_System:truncation.c:line
        .2819
146 |||=======================================
147 ||    0.0% |   0.000808 |__ipai_truncation:truncation.c:line
        .282
148 |||---------------------------------
149 3||    0.0% |   0.000003 |Set_Inf_SndRcv:truncation.c:line
        .6753
150 ||||------------------------------
```

```
151 | 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
152 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
153 ||||==========================================
154 | 3||    0.0% |   0.000003 |Set_Inf_SndRcv:truncation.c:line
    |     .6912
155 ||||------------------------------
156 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
157 | 4|||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
158 ||||==========================================
159 | 3||    0.0% |   0.000003 |Set_Inf_SndRcv:truncation.c:line
    |     .6946
160 ||||------------------------------
161 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
162 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
163 ||||==========================================
164 | 3||    0.0% |   0.000003 |Set_Inf_SndRcv:truncation.c:line
    |     .7275
165 | 4||         |            | qsort_int3:QuickSort.c:line.66
166 | 3||    0.0% |   0.000003 |Set_RMI:truncation.c:line.3073
167 ||||------------------------------
168 | 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
169 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
170 ||||==========================================
171 | 3||    0.0% |   0.000728 |Set_RMI:truncation.c:line.3122
172 | 4||         |            | PrintMemory:PrintMemory.c:line.19
173 | 3||    0.0% |   0.000057 |Set_RMI:truncation.c:line.3132
174 | 3||    0.0% |   0.000004 |Set_RMI:truncation.c:line.3140
175 | 4||         |            | dtime:dtime.c:line.15
176 | 3||    0.0% |   0.000003 |Set_RMI:truncation.c:line.3214
177 | 4||         |            | dtime:dtime.c:line.15
178 |||==========================================
179 | ||    0.0% |   0.000351 |__ipai_truncation:truncation.c:line
    |     .326
180 | 3|         |            | PrintMemory:PrintMemory.c:line.19
181 | ||    0.0% |   0.000358 |__ipai_truncation:truncation.c:line
    |     .330
182 | 3|         |            | PrintMemory:PrintMemory.c:line.19
183 | ||    0.0% |   0.000002 |__ipai_truncation:truncation.c:line
    |     .336
184 | 3|         |            | Check_System:truncation.c:line.3011
185 | 4|         |            |  MPI_Comm_rank:...:line.0
186 | ||   12.9% |  11.936993 |__ipai_truncation:truncation.c:line
    |     .354
187 |||------------------------------
188 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.3527
189 ||||------------------------------
190 | 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
191 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
192 ||||==========================================
```

```
193 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.3547
194 | 4||         |            | Cross_Product:openmx_common.c:line
    |     .68
195 | 3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.3586
196 | ||||-------------------------------
197 | 4|||    0.0% |   0.000003 |largest:openmx_common.c:line.487
198 | 4|||    0.0% |   0.000003 |smallest:openmx_common.c:line.496
199 | ||||===============================
200 | 3||    0.0% |   0.000025 |UCell_Box:truncation.c:line.3608
201 | 4||         |            | Cross_Product:openmx_common.c:line
    |     .68
202 | 3||    0.0% |   0.000025 |UCell_Box:truncation.c:line.3677
203 | ||||-------------------------------
204 | 4|||    0.0% |   0.000020 |__ipap_Find_ApproxFactN:
    |     Find_ApproxFactN.c:line.35
205 | 4|||    0.0% |   0.000005 |__ipap_Find_ApproxFactN:
    |     Find_ApproxFactN.c:line.39
206 | |||||-----------------------------
207 | 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
208 | 5||||    0.0% |   0.000004 |MPI_Comm_size:...:line.0
209 | ||||===============================
210 | 3||    0.0% |   0.000009 |UCell_Box:truncation.c:line.3685
211 | 4||         |            | Cross_Product:openmx_common.c:line
    |     .68
212 | 3||    0.0% |   0.000076 |UCell_Box:truncation.c:line.3957
213 | 3||    0.0% |   0.000008 |UCell_Box:truncation.c:line.3991
214 | ||||-------------------------------
215 | 4|||    0.0% |   0.000004 |MPI_Bcast:...:line.0
216 | 4|||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
217 | ||||===============================
218 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.4003
219 | 4||         |            | Cross_Product:openmx_common.c:line
    |     .68
220 | 3||    0.6% |   0.596576 |UCell_Box:truncation.c:line.4114
221 | 3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4135
222 | 4||         |            | dtime:dtime.c:line.15
223 | 3||    0.4% |   0.339875 |UCell_Box:truncation.c:line.4149
224 | 4||         |            | Get_Grid_XYZ:openmx_common.c:line
    |     .866
225 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4172
226 | 4||         |            | Get_Grid_XYZ:openmx_common.c:line
    |     .866
227 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4199
228 | 4||         |            | GN2N:openmx_common.c:line.808
229 | 3||   11.9% |  10.999415 |UCell_Box:truncation.c:line.4211
230 | ||||-------------------------------
231 | 4|||    5.5% |   5.090195 |__ipai_Find_CGrids:Find_CGrids.c:
    |     line.11
```

```
4|||    6.4% |   5.909219 |__ipai_Find_CGrids:Find_CGrids.c:
    line.52
5|||         |            | R_atv:openmx_common.c:line.83
||||==========================================
3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.4275
4||         |            | dtime:dtime.c:line.15
3||    0.0% |   0.000012 |UCell_Box:truncation.c:line.4309
||||------------------------------
4|||    0.0% |   0.000007 |MPI_Bcast:...:line.0
4|||    0.0% |   0.000006 |MPI_Bcast(sync):...:line.0
||||==========================================
3||    0.0% |   0.000904 |UCell_Box:truncation.c:line.4337
4||         |            | PrintMemory:PrintMemory.c:line.19
3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4350
||||------------------------------
4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
4|||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
||||==========================================
3||    0.0% |   0.000002 |UCell_Box:truncation.c:line.4418
||||------------------------------
4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
||||==========================================
3||    0.0% |   0.000002 |UCell_Box:truncation.c:line.4721
||||------------------------------
4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
||||==========================================
3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4830
||||------------------------------
4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
4|||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
|||==========================================
3||    0.0% |   0.000011 |MPI_Reduce:...:line.0
3||    0.0% |   0.000004 |MPI_Reduce(sync):...:line.0
3||    0.0% |   0.000003 |MPI_Bcast:...:line.0
3||    0.0% |   0.000002 |MPI_Bcast(sync):...:line.0
3||    0.0% |   0.000007 |MPI_Reduce:...:line.0
3||    0.0% |   0.000003 |MPI_Reduce(sync):...:line.0
3||    0.0% |   0.000004 |MPI_Bcast:...:line.0
3||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
||   19.4% | 17.985050 |__ipai_truncation:truncation.c:line
    .381
|||------------------------------
3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.3527
||||------------------------------
4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
||||==========================================
```

```
279 | 3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.4003
280 | 4||         |            | Cross_Product:openmx_common.c:line
    |     .68
281 | 3||    1.0% |   0.884904 |UCell_Box:truncation.c:line.4114
282 | 3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4135
283 | 4||         |            | dtime:dtime.c:line.15
284 | 3||    0.4% |   0.339045 |UCell_Box:truncation.c:line.4149
285 | 4||         |            | Get_Grid_XYZ:openmx_common.c:line
    |     .866
286 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4172
287 | 4||         |            | Get_Grid_XYZ:openmx_common.c:line
    |     .866
288 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4199
289 | 4||         |            | GN2N:openmx_common.c:line.808
290 | 3||   17.9% |  16.638245 |UCell_Box:truncation.c:line.4211
291 ||||-----------------------------
292 | 4|||   11.0% |  10.162730 |__ipai_Find_CGrids:Find_CGrids.c:
    |     line.11
293 | 4|||    7.0% |   6.475515 |__ipai_Find_CGrids:Find_CGrids.c:
    |     line.52
294 | 5|||         |            | R_atv:openmx_common.c:line.83
295 ||||=============================
296 | 3||    0.0% |   0.003162 |UCell_Box:truncation.c:line.4266
297 | 4||         |            | qsort_int:QuickSort.c:line.42
298 | 3||    0.0% |   0.000007 |UCell_Box:truncation.c:line.4275
299 | 4||         |            | dtime:dtime.c:line.15
300 | 3||    0.0% |   0.000012 |UCell_Box:truncation.c:line.4309
301 ||||-----------------------------
302 | 4|||    0.0% |   0.000006 |MPI_Bcast:...:line.0
303 | 4|||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
304 ||||=============================
305 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4350
306 ||||-----------------------------
307 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
308 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
309 ||||=============================
310 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4418
311 ||||-----------------------------
312 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
313 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
314 ||||=============================
315 | 3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4443
316 | 4||         |            | dtime:dtime.c:line.15
317 | 3||    0.0% |   0.014309 |UCell_Box:truncation.c:line.4493
318 | 3||    0.1% |   0.105298 |UCell_Box:truncation.c:line.4560
319 | 4||         |            | R_atv:openmx_common.c:line.83
320 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.4683
321 | 4||         |            | dtime:dtime.c:line.15
322 | 3||    0.0% |   0.000014 |UCell_Box:truncation.c:line.4711
```

```
323 ||||------------------------------
324  4|||    0.0% |   0.000009 |MPI_Allreduce:...:line.0
325  4|||    0.0% |   0.000004 |MPI_Allreduce(sync):...:line.0
326 ||||==============================
327  3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4721
328 ||||------------------------------
329  4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
330  4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
331 ||||==============================
332  3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4830
333 ||||------------------------------
334  4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
335  4|||    0.0% |   0.000003 |MPI_Barrier(sync):...:line.0
336  3||    0.0% |   0.000009 |MPI_Reduce:...:line.0
337  3||    0.0% |   0.000003 |MPI_Reduce(sync):...:line.0
338  3||    0.0% |   0.000004 |MPI_Bcast:...:line.0
339  3||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
340 |||============================
341  ||   13.1% | 12.134898 |__ipai_truncation:truncation.c:line
        .405
342 |||------------------------------
343  3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.3527
344 ||||------------------------------
345  4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
346  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
347 ||||==============================
348  3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.3547
349  4||         |            | Cross_Product:openmx_common.c:line
        .68
350  3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.3586
351 ||||------------------------------
352  4|||    0.0% |   0.000003 |largest:openmx_common.c:line.487
353  4|||    0.0% |   0.000003 |smallest:openmx_common.c:line.496
354 ||||==============================
355  3||    0.0% |   0.000020 |UCell_Box:truncation.c:line.3608
356  4||         |            | Cross_Product:openmx_common.c:line
        .68
357  3||    0.0% |   0.000023 |UCell_Box:truncation.c:line.3677
358 ||||------------------------------
359  4|||    0.0% |   0.000019 |__ipap_Find_ApproxFactN:
        Find_ApproxFactN.c:line.35
360  4|||    0.0% |   0.000003 |__ipap_Find_ApproxFactN:
        Find_ApproxFactN.c:line.39
361 |||||----------------------------
362  5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
363  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
364 ||||==============================
365  3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.3685
```

```
366 | 4||          |              | Cross_Product:openmx_common.c:line
    .68
367 | 3||    0.0% |   0.000106 |UCell_Box:truncation.c:line.3957
368 | 3||    0.0% |   0.000008 |UCell_Box:truncation.c:line.3991
369 | ||||------------------------------
370 | 4|||    0.0% |   0.000004 |MPI_Bcast:...:line.0
371 | 4|||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
372 | ||||==============================
373 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.4003
374 | 4||          |              | Cross_Product:openmx_common.c:line
    .68
375 | 3||    0.6% |   0.598306 |UCell_Box:truncation.c:line.4114
376 | 3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4135
377 | 4||          |              | dtime:dtime.c:line.15
378 | 3||    0.4% |   0.340119 |UCell_Box:truncation.c:line.4149
379 | 4||          |              | Get_Grid_XYZ:openmx_common.c:line
    .866
380 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4172
381 | 4||          |              | Get_Grid_XYZ:openmx_common.c:line
    .866
382 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4199
383 | 4||          |              | GN2N:openmx_common.c:line.808
384 | 3||   11.9% |  11.002538 |UCell_Box:truncation.c:line.4211
385 | ||||------------------------------
386 | 4|||    6.3% |   5.878089 |__ipai_Find_CGrids:Find_CGrids.c:
    line.11
387 | 4|||    5.5% |   5.124449 |__ipai_Find_CGrids:Find_CGrids.c:
    line.52
388 | 5|||         |              | R_atv:openmx_common.c:line.83
389 | ||||==============================
390 | 3||    0.0% |   0.003108 |UCell_Box:truncation.c:line.4266
391 | 4||          |              | qsort_int:QuickSort.c:line.42
392 | 3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.4275
393 | 4||          |              | dtime:dtime.c:line.15
394 | 3||    0.0% |   0.000012 |UCell_Box:truncation.c:line.4309
395 | ||||------------------------------
396 | 4|||    0.0% |   0.000007 |MPI_Bcast:...:line.0
397 | 4|||    0.0% |   0.000006 |MPI_Bcast(sync):...:line.0
398 | ||||==============================
399 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4350
400 | ||||------------------------------
401 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
402 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
403 | ||||==============================
404 | 3||    0.0% |   0.000002 |UCell_Box:truncation.c:line.4418
405 | ||||------------------------------
406 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
407 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
408 | ||||==============================
```

```
409 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.4443
410 | 4||         |            | dtime:dtime.c:line.15
411 | 3||    0.0% |   0.016346 |UCell_Box:truncation.c:line.4493
412 | 3||    0.1% |   0.119907 |UCell_Box:truncation.c:line.4560
413 | 4||         |            | R_atv:openmx_common.c:line.83
414 | 3||    0.0% |   0.000006 |UCell_Box:truncation.c:line.4683
415 | 4||         |            | dtime:dtime.c:line.15
416 | 3||    0.0% |   0.000013 |UCell_Box:truncation.c:line.4711
417 ||||-------------------------------
418 | 4|||    0.0% |   0.000009 |MPI_Allreduce:...:line.0
419 | 4|||    0.0% |   0.000004 |MPI_Allreduce(sync):...:line.0
420 ||||===============================
421 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4721
422 ||||-------------------------------
423 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
424 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
425 ||||===============================
426 | 3||    0.0% |   0.000192 |UCell_Box:truncation.c:line.4754
427 ||||-------------------------------
428 | 4|||    0.0% |   0.000006 |allocate_grids2atoms:truncation.c:
        line.7386
429 |||||-----------------------------
430 | 5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
431 | 5||||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
432 | 5||||    0.0% |   0.000002 |Cross_Product:openmx_common.c:
        line.68
433 ||||===============================
434 | 4|||    0.0% |   0.000181 |allocate_grids2atoms:truncation.c:
        line.7576
435 |||||-----------------------------
436 | 5||||    0.0% |   0.000103 |MPI_Reduce:...:line.0
437 | 5||||    0.0% |   0.000078 |MPI_Reduce(sync):...:line.0
438 |||||============================
439 | 4|||    0.0% |   0.000005 |allocate_grids2atoms:truncation.c:
        line.7585
440 |||||-----------------------------
441 | 5||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
442 | 5||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
443 ||||===============================
444 | 3||    0.0% |   0.000003 |UCell_Box:truncation.c:line.4790
445 | 4||         |            | dtime:dtime.c:line.15
446 | 3||    0.0% |   0.006475 |UCell_Box:truncation.c:line.4797
447 | 3||    0.1% |   0.047635 |UCell_Box:truncation.c:line.4805
448 | 4||         |            | GN2N:openmx_common.c:line.808
449 | 3||    0.0% |   0.000004 |UCell_Box:truncation.c:line.4824
450 | 4||         |            | dtime:dtime.c:line.15
451 | 3||    0.0% |   0.000005 |UCell_Box:truncation.c:line.4830
452 ||||-------------------------------
453 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
```

```
454 | 4|||    0.0% |   0.000003 |MPI_Barrier(sync):...:line.0
455 |||=================================
456 ||   0.0% |   0.003774 |__ipai_truncation:truncation.c:line
    .2200
457 | 3|         |            | PrintMemory:PrintMemory.c:line.19
458 ||   0.0% |   0.000666 |__ipai_truncation:truncation.c:line
    .2226
459 | 3|         |            | PrintMemory:PrintMemory.c:line.19
460 ||   0.0% |   0.000010 |__ipai_truncation:truncation.c:line
    .2278
461 |||---------------------------------
462 | 3||   0.0% |   0.000005 |MPI_Reduce:...:line.0
463 | 3||   0.0% |   0.000002 |MPI_Reduce(sync):...:line.0
464 | 3||   0.0% |   0.000002 |MPI_Bcast:...:line.0
465 | 3||   0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
466 |||=================================
467 ||   0.0% |   0.002215 |__ipai_truncation:truncation.c:line
    .2411
468 | 3|         |            | PrintMemory:PrintMemory.c:line.19
469 ||   0.0% |   0.000215 |__ipai_truncation:truncation.c:line
    .2424
470 | 3|         |            | PrintMemory:PrintMemory.c:line.19
471 ||   0.0% |   0.000003 |__ipai_truncation:truncation.c:line
    .2434
472 | 3|         |            | __ipap_fnjoint:openmx_common.c:line
    .358
473 ||   0.0% |   0.000003 |__ipai_truncation:truncation.c:line
    .2457
474 | 3|         |            | dtime:dtime.c:line.15
```

2.2.2 DFT

DFT.c is a subroutine to perform self-consistent calculations within LDA or GGA. It first allocates arrays for data on grid and orbital optimization, and prints out the their memory usage. It then invokes the following subroutines.

- Set_OLP_Kin() (in Set_OLP_Kin.c) is a subroutine to calculate the overlap matrix and the matrix for the kinetic operator in momentum space.
  - double *****OLP; overlap matrix elements of basis orbitals size: OLP[4] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]]
  - double *****H0; matrix elements of basis orbitals for T+VNL size: H0[4] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]]

- double *****OLP_L; $< i|lx, ly, lz|j >$ overlap matrix elements with lx,y,z operator of basis orbitals which are used to calculate orbital moment. size: OLP_L[3] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]]
- xyz2spherical() (in xyz2spherical.c): a subroutine to transform xyz coordinates to spherical coordinates.
- Spherical_Bessel() (in Spherical_Bessel.c): a subroutine to calculate the spherical Bessel functions and its derivative from 0 to lmax.
- RF_BesselF() (in RF_BesselF.c): a subroutine to calculate radial part of PAO of atom specified by "Gensi" in k-space.

Listing 2.6: DFT: Set_OLP_Kin()

```
1  |   18.9% |  17.581981 |main:openmx.c:line.473
2  ||---------------------------------
3  ||    0.0% |   0.000002 |DFT:DFT.c:line.136
4  3|         |            | dtime:dtime.c:line.15
5  ||    0.0% |   0.000003 |DFT:DFT.c:line.141
6  |||--------------------------------
7  3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
8  3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
9  |||================================
10 ||    0.0% |   0.008685 |DFT:DFT.c:line.40
11 ||    0.0% |   0.001065 |DFT:DFT.c:line.603
12 3|         |            | PrintMemory:PrintMemory.c:line
       .19
13 ||    0.0% |   0.000004 |DFT:DFT.c:line.654
14 3|         |            | __ipap_fnjoint:openmx_common.c:
       line.358
15 ||    9.4% |   8.761327 |DFT:DFT.c:line.683
16 |||--------------------------------
17 3||    0.0% |   0.000024 |Set_OLP_Kin:Set_OLP_Kin.c:line
       .35
18 3||    0.0% |   0.000024 |Set_OLP_Kin:Set_OLP_Kin.c:line
       .51
19 ||||-------------------------------
20 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
21 4|||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
22 4|||    0.0% |   0.000014 |MPI_Barrier:...:line.0
23 4|||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
24 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
25 ||||===============================
26 3||    1.2% |   1.073071 |Set_OLP_Kin:Set_OLP_Kin.c:line
       .111
27 3||    1.1% |   0.978257 |Set_OLP_Kin:Set_OLP_Kin.c:line
       .178
```

```
28 | 4||          |             | Complex:openmx_common.c:line
   .91
29 | 3||    1.0% |   0.951827  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .196
30 | 4||          |             | Complex:openmx_common.c:line
   .91
31 | 3||    1.0% |   0.952894  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .214
32 | 4||          |             | Complex:openmx_common.c:line
   .91
33 | 3||    1.0% |   0.964796  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .232
34 | 4||          |             | Complex:openmx_common.c:line
   .91
35 | 3||    1.0% |   0.950800  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .250
36 | 4||          |             | Complex:openmx_common.c:line
   .91
37 | 3||    1.0% |   0.949774  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .268
38 | 4||          |             | Complex:openmx_common.c:line
   .91
39 | 3||    1.0% |   0.965853  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .286
40 | 4||          |             | Complex:openmx_common.c:line
   .91
41 | 3||    1.0% |   0.951407  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .304
42 | 4||          |             | Complex:openmx_common.c:line
   .91
43 | 3||    0.0% |   0.000144  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .363
44 | 4||          |             | Complex:openmx_common.c:line
   .91
45 | 3||    0.0% |   0.000142  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .369
46 | 4||          |             | Complex:openmx_common.c:line
   .91
47 | 3||    0.0% |   0.000143  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .375
48 | 4||          |             | Complex:openmx_common.c:line
   .91
49 | 3||    0.0% |   0.000143  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .381
50 | 4||          |             | Complex:openmx_common.c:line
   .91
51 | 3||    0.0% |   0.000142  |Set_OLP_Kin:Set_OLP_Kin.c:line
   .387
52 | 4||          |             | Complex:openmx_common.c:line
```

```
    .91
53  3||    0.0%  |   0.000143  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .393
54  4||          |             | Complex:openmx_common.c:line
    .91
55  3||    0.0%  |   0.000142  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .399
56  4||          |             | Complex:openmx_common.c:line
    .91
57  3||    0.0%  |   0.000142  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .405
58  4||          |             | Complex:openmx_common.c:line
    .91
59  3||    0.0%  |   0.000026  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .416
60  ||||------------------------------
61  4|||    0.0%  |   0.000009  |dtime:dtime.c:line.15
62  4|||    0.0%  |   0.000016  |xyz2spherical:xyz2spherical.c:
    line.20
63  ||||==============================
64  3||    0.0%  |   0.000040  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .475
65  4||          |             | Complex:openmx_common.c:line
    .91
66  3||    0.0%  |   0.008578  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .518
67  4||          |             | Spherical_Bessel:
    Spherical_Bessel.c:line.21
68  3||    0.0%  |   0.004920  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .560
69  4||          |             | RF_BesselF:RF_BesselF.c:line
    .18
70  3||    0.0%  |   0.004804  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .569
71  4||          |             | RF_BesselF:RF_BesselF.c:line
    .18
72  3||    0.0%  |   0.000022  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .613
73  ||||------------------------------
74  4|||    0.0%  |   0.000015  |Complex:openmx_common.c:line
    .91
75  4|||    0.0%  |   0.000007  |ComplexSH:openmx_common.c:line
    .615
76  ||||==============================
77  3||    0.0%  |   0.000020  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .633
78  ||||------------------------------
79  4|||    0.0%  |   0.000015  |Cmul:openmx_common.c:line.115
80  4|||    0.0%  |   0.000005  |Im_pow:openmx_common.c:line
```

```
    .770
81  ||||==========================================
82  3||    0.0%  |   0.000089  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .644
83  ||||------------------------------
84  4|||    0.0%  |   0.000040  |CRmul:openmx_common.c:line.261
85  4|||    0.0%  |   0.000039  |Cadd:openmx_common.c:line.99
86  4|||    0.0%  |   0.000011  |Gaunt:Gaunt.c:line.22
87  ||||==========================================
88  3||    0.0%  |   0.002686  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .66
89  4||          |             | PrintMemory:PrintMemory.c:line
    .19
90  3||    0.0%  |   0.000039  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .738
91  4||          |             | Complex:openmx_common.c:line
    .91
92  3||    0.0%  |   0.000083  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .750
93  ||||------------------------------
94  4|||    0.0%  |   0.000039  |Cadd:openmx_common.c:line.99
95  4|||    0.0%  |   0.000039  |Cmul:openmx_common.c:line.115
96  4|||    0.0%  |   0.000005  |Conjg:openmx_common.c:line.123
97  ||||==========================================
98  3||    0.0%  |   0.000054  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .817
99  4||          |             | Complex:openmx_common.c:line
    .91
100 3||    0.0%  |   0.000087  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .876
101 ||||------------------------------
102 4|||    0.0%  |   0.000044  |Cadd:openmx_common.c:line.99
103 4|||    0.0%  |   0.000044  |Cmul:openmx_common.c:line.115
104 ||||==========================================
105 3||    0.0%  |   0.000006  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .999
106 4||          |             | dtime:dtime.c:line.15
107 3||    0.0%  |   0.000003  |Set_OLP_Kin:Set_OLP_Kin.c:line
    .1274
108 4||          |             | dtime:dtime.c:line.15
109 ||==========================================
```

- Set_Nonlocal() (in Set_Nonlocal.c) is a subroutine to calculate matrix elements and the derivatives of nonlocal potentials in the momentum space.
  - double *****HNL; real matrix elements of basis orbitals for nonlocal VPS. size: HNL[List_YOUSO[5]] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]]

– double ******DS_NL; overlap matrix elements between projectors, of non-local potentials, and basis orbitals. size: DS_NL[SO_switch+1] [4] [Matomnum+MatomnumF+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_VPS_Pro[Hwan]+2]

Listing 2.7: DFT: Set_Nonlocal()

```
1  ||    0.1% |   0.058919 |DFT:DFT.c:line.689
2  |||-------------------------------
3  3||    0.0% |   0.000020 |Set_Nonlocal:Set_Nonlocal.c:
       line.36
4  3||    0.1% |   0.058899 |Set_Nonlocal:Set_Nonlocal.c:
       line.39
5  ||||------------------------------
6  4|||    0.0% |   0.000004 |Nonlocal0:Set_Nonlocal.c:line
       .78
7  |||||-----------------------------
8  5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
9  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
10 |||||==============================
11 4|||    0.0% |   0.002296 |Nonlocal0:Set_Nonlocal.c:line
       .98
12 4|||    0.0% |   0.015321 |Nonlocal0:Set_Nonlocal.c:line
       .135
13 4|||    0.0% |   0.000018 |Nonlocal0:Set_Nonlocal.c:line
       .272
14 |||||-----------------------------
15 5||||    0.0% |   0.000009 |dtime:dtime.c:line.15
16 5||||    0.0% |   0.000009 |xyz2spherical:xyz2spherical.c
       :line.20
17 |||||==============================
18 4|||    0.0% |   0.000238 |Nonlocal0:Set_Nonlocal.c:line
       .330
19 5|||         |            | Complex:openmx_common.c:line
       .91
20 4|||    0.0% |   0.009043 |Nonlocal0:Set_Nonlocal.c:line
       .369
21 5|||         |            | Spherical_Bessel:
       Spherical_Bessel.c:line.21
22 4|||    0.0% |   0.028424 |Nonlocal0:Set_Nonlocal.c:line
       .406
23 5|||         |            | RF_BesselF:RF_BesselF.c:line
       .18
24 4|||    0.0% |   0.000191 |Nonlocal0:Set_Nonlocal.c:line
       .444
25 |||||-----------------------------
26 5||||    0.0% |   0.000133 |Complex:openmx_common.c:line
       .91
27 5||||    0.0% |   0.000057 |ComplexSH:openmx_common.c:
       line.615
```

```
28 |||||=================================
29  4|||    0.0%  |   0.000240  |Nonlocal0:Set_Nonlocal.c:line
       .464
30 |||||---------------------------
31  5||||    0.0%  |   0.000178  |Cmul:openmx_common.c:line.115
32  5||||    0.0%  |   0.000062  |Im_pow:openmx_common.c:line
       .770
33 |||||=================================
34  4|||    0.0%  |   0.000572  |Nonlocal0:Set_Nonlocal.c:line
       .475
35 |||||---------------------------
36  5||||    0.0%  |   0.000235  |CRmul:openmx_common.c:line
       .261
37  5||||    0.0%  |   0.000235  |Cadd:openmx_common.c:line.99
38  5||||    0.0%  |   0.000102  |Gaunt:Gaunt.c:line.22
39 |||||=================================
40  4|||    0.0%  |   0.000243  |Nonlocal0:Set_Nonlocal.c:line
       .540
41  5|||          |             | Complex:openmx_common.c:line
       .91
42  4|||    0.0%  |   0.000527  |Nonlocal0:Set_Nonlocal.c:line
       .547
43 |||||---------------------------
44  5||||    0.0%  |   0.000234  |Cadd:openmx_common.c:line.99
45  5||||    0.0%  |   0.000234  |Cmul:openmx_common.c:line.115
46  5||||    0.0%  |   0.000059  |Conjg:openmx_common.c:line
       .123
47 |||||=================================
48  4|||    0.0%  |   0.000238  |Nonlocal0:Set_Nonlocal.c:line
       .585
49  5|||          |             | Complex:openmx_common.c:line
       .91
50  4|||    0.0%  |   0.001173  |Nonlocal0:Set_Nonlocal.c:line
       .592
51 |||||---------------------------
52  5||||    0.0%  |   0.000586  |Cadd:openmx_common.c:line.99
53  5||||    0.0%  |   0.000587  |Cmul:openmx_common.c:line.115
54 |||||=================================
55  4|||    0.0%  |   0.000007  |Nonlocal0:Set_Nonlocal.c:line
       .664
56  5|||          |             | dtime:dtime.c:line.15
57  5|||          |             | PrintMemory:PrintMemory.c:
       line.19
58  4|||    0.0%  |   0.000331  |Nonlocal0:Set_Nonlocal.c:line
       .955
59  4|||    0.0%  |   0.000008  |Nonlocal0:Set_Nonlocal.c:line
       .987
60  5|||          |             | dtime:dtime.c:line.15
61  4|||    0.0%  |   0.000010  |Nonlocal0:Set_Nonlocal.c:line
```

```
    .1359
62  5|||          |              | dampingF:dampingF.c:line.21
63  4|||    0.0%  |   0.000006   |Nonlocal0:Set_Nonlocal.c:line
    .1383
64  5|||          |              | dtime:dtime.c:line.15
65  4|||    0.0%  |   0.000005   |Nonlocal0:Set_Nonlocal.c:line
    .1409
66  |||||---------------------------
67  5||||    0.0%  |   0.000001   |MPI_Barrier:...:line.0
68  5||||    0.0%  |   0.000004   |MPI_Barrier(sync):...:line.0
69  |||||===========================
70  4|||    0.0%  |   0.000003   |dtime:dtime.c:line.15
71  |||=================================
```

- Set_ProExpn_VNA() (in Set_ProExpn_VNA.c) is a subroutine to calculate matrix elements and the derivatives of VNA projector expansion in the momentum space.
  - double ****HVNA; real matrix elements of basis orbitals for VNA projectors. size: HVNA[Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]]
  - double ****HVNA2; real matrix elements of basis orbitals for VNA projectors. size: HVNA2[4] [Matomnum+MatomnumF+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Cwan]]
  - Type_DS_VNA *****DS_VNA; overlap matrix elements between projectors of VNA potentials, and basis orbitals. size: DS_VNA[4] [Matomnum+4] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [(YOUSO35+1)*(YOUSO35+1
    Type_DS_VNA is defined as float.
  - Set_ProExpn() (in Set_ProExpn_VNA.c): to evaluate matrix elements of neutral atom potential in the KB or Blochl separable form in momentum space.
  - Set_VNA12() (in Set_ProExpn_VNA.c): to evaluate matrix elements of one-center (orbitals) but two-center integrals for neutral atom potentials in the momentum space.

Listing 2.8: DFT: Set_ProExpn_VNA()

```
1  ||     0.1%  |   0.137008   |DFT:DFT.c:line.695
2  |||-------------------------------
3  3||    0.0%  |   0.000044   |Set_ProExpn_VNA:Set_ProExpn_VNA
   .c:line.45
4  3||    0.1%  |   0.136965   |Set_ProExpn_VNA:Set_ProExpn_VNA
   .c:line.50
5  ||||-----------------------------
6  4|||    0.0%  |   0.000005   |Set_ProExpn:Set_ProExpn_VNA.c:
   line.105
```

```
7  |||||----------------------------
8  5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
9  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
10 5||||    0.0% |   0.000002 |dtime:dtime.c:line.15
11 |||||============================
12 4|||    0.0% |   0.001459 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.150
13 5|||          |            | PrintMemory:PrintMemory.c:
       line.19
14 4|||    0.0% |   0.000109 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.198
15 4|||    0.0% |   0.000408 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.208
16 5|||          |            | RF_BesselF:RF_BesselF.c:line
       .18
17 4|||    0.0% |   0.038642 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.254
18 4|||    0.0% |   0.000023 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.396
19 |||||----------------------------
20 5||||    0.0% |   0.000014 |dtime:dtime.c:line.15
21 5||||    0.0% |   0.000009 |xyz2spherical:xyz2spherical.c
       :line.20
22 |||||============================
23 4|||    0.0% |   0.007660 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.457
24 5|||          |            | Complex:openmx_common.c:line
       .91
25 4|||    0.0% |   0.003315 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.479
26 5|||          |            | Spherical_Bessel:
       Spherical_Bessel.c:line.21
27 4|||    0.0% |   0.003571 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.560
28 |||||----------------------------
29 5||||    0.0% |   0.002475 |Complex:openmx_common.c:line
       .91
30 5||||    0.0% |   0.001096 |ComplexSH:openmx_common.c:
       line.615
31 |||||============================
32 4|||    0.0% |   0.007711 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.581
33 |||||----------------------------
34 5||||    0.0% |   0.005754 |Cmul:openmx_common.c:line.115
35 5||||    0.0% |   0.001957 |Im_pow:openmx_common.c:line
       .770
36 |||||============================
37 4|||    0.0% |   0.002993 |Set_ProExpn:Set_ProExpn_VNA.c:
       line.592
```

```
38 | 5|||          |             | Gaunt:Gaunt.c:line.22
39 | 4|||    0.0% |   0.007857  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.648
40 | 5|||          |             | Complex:openmx_common.c:line
       .91
41 | 4|||    0.0% |   0.017275  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.655
42 |||||----------------------------
43 | 5||||    0.0% |   0.007683  |Cadd:openmx_common.c:line.99
44 | 5||||    0.0% |   0.007670  |Cmul:openmx_common.c:line.115
45 | 5||||    0.0% |   0.001922  |Conjg:openmx_common.c:line
       .123
46 |||||============================
47 | 4|||    0.0% |   0.007673  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.694
48 | 5|||          |             | Complex:openmx_common.c:line
       .91
49 | 4|||    0.0% |   0.000007  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.783
50 | 5|||          |             | dtime:dtime.c:line.15
51 | 4|||    0.0% |   0.000007  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.905
52 |||||----------------------------
53 | 5||||    0.0% |   0.000002  |MPI_Barrier:...:line.0
54 | 5||||    0.0% |   0.000006  |MPI_Barrier(sync):...:line.0
55 | 4|||    0.0% |   0.000154  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.1215
56 | 4|||    0.0% |   0.000004  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.1238
57 | 5|||          |             | dtime:dtime.c:line.15
58 | 4|||    0.0% |   0.000008  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.1297
59 | 5|||          |             | dampingF:dampingF.c:line.21
60 | 4|||    0.0% |   0.000003  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.1312
61 | 5|||          |             | dtime:dtime.c:line.15
62 | 4|||    0.0% |   0.000002  |Set_ProExpn:Set_ProExpn_VNA.c:
       line.1369
63 | 5|||          |             | dtime:dtime.c:line.15
64 |||||============================
65 | 4|||    0.0% |   0.000005  |Set_VNA12:Set_ProExpn_VNA.c:
       line.1418
66 |||||----------------------------
67 | 5||||    0.0% |   0.000002  |MPI_Comm_rank:...:line.0
68 | 5||||    0.0% |   0.000002  |MPI_Comm_size:...:line.0
69 | 5||||    0.0% |   0.000001  |dtime:dtime.c:line.15
70 |||||============================
71 | 4|||    0.0% |   0.001055  |Set_VNA12:Set_ProExpn_VNA.c:
       line.1438
```

```
72 | 5|||          |              | PrintMemory:PrintMemory.c:
       line.19
73 | 4|||    0.0% |   0.033677 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1470
74 | 4|||    0.0% |   0.000024 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1597
75 |||||-------------------------
76 | 5||||    0.0% |   0.000015 |dtime:dtime.c:line.15
77 | 5||||    0.0% |   0.000009 |xyz2spherical:xyz2spherical.c
       :line.20
78 |||||=============================
79 | 4|||    0.0% |   0.000020 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1655
80 | 5|||          |              | Complex:openmx_common.c:line
       .91
81 | 4|||    0.0% |   0.003014 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1686
82 | 5|||          |              | Spherical_Bessel:
       Spherical_Bessel.c:line.21
83 | 4|||    0.0% |   0.000020 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1737
84 | 5|||          |              | Complex:openmx_common.c:line
       .91
85 | 4|||    0.0% |   0.000063 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1748
86 |||||-------------------------
87 | 5||||    0.0% |   0.000015 |CRmul:openmx_common.c:line
       .261
88 | 5||||    0.0% |   0.000015 |Cadd:openmx_common.c:line.99
89 | 5||||    0.0% |   0.000015 |Complex:openmx_common.c:line
       .91
90 | 5||||    0.0% |   0.000007 |ComplexSH:openmx_common.c:
       line.615
91 | 5||||    0.0% |   0.000011 |Gaunt:Gaunt.c:line.22
92 |||||=============================
93 | 4|||    0.0% |   0.000039 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1771
94 |||||-------------------------
95 | 5||||    0.0% |   0.000020 |CRmul:openmx_common.c:line
       .261
96 | 5||||    0.0% |   0.000020 |Cadd:openmx_common.c:line.99
97 |||||=============================
98 | 4|||    0.0% |   0.000020 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1822
99 | 5|||          |              | Conjg:openmx_common.c:line
       .123
100| 4|||    0.0% |   0.000020 |Set_VNA12:Set_ProExpn_VNA.c:
       line.1857
101| 5|||          |              | Complex:openmx_common.c:line
```

```
    .91
102 4|||    0.0%  |   0.000044  |Set_VNA12:Set_ProExpn_VNA.c:
    line.1864
103 |||||----------------------------
104 5||||    0.0%  |   0.000020  |Cadd:openmx_common.c:line.99
105 5||||    0.0%  |   0.000020  |Cmul:openmx_common.c:line.115
106 5||||    0.0%  |   0.000005  |Conjg:openmx_common.c:line
    .123
107 |||||============================
108 4|||    0.0%  |   0.000020  |Set_VNA12:Set_ProExpn_VNA.c:
    line.1903
109 5|||          |             | Complex:openmx_common.c:line
    .91
110 4|||    0.0%  |   0.000039  |Set_VNA12:Set_ProExpn_VNA.c:
    line.1910
111 |||||----------------------------
112 5||||    0.0%  |   0.000020  |Cadd:openmx_common.c:line.99
113 5||||    0.0%  |   0.000020  |Cmul:openmx_common.c:line.115
114 |||||============================
115 4|||    0.0%  |   0.000006  |Set_VNA12:Set_ProExpn_VNA.c:
    line.1979
116 5|||          |             | dtime:dtime.c:line.15
117 4|||    0.0%  |   0.000009  |Set_VNA12:Set_ProExpn_VNA.c:
    line.2244
118 |||||----------------------------
119 5||||    0.0%  |   0.000002  |MPI_Barrier:...:line.0
120 5||||    0.0%  |   0.000006  |MPI_Barrier(sync):...:line.0
121 5||||    0.0%  |   0.000002  |dtime:dtime.c:line.15
122 |||=================================
```

- Set_Aden_Grid() (in Set_Aden_Grid.c): a subroutine to calculate a charge density superposed atomic densities on grid.
  - double **Density_Grid; electron densities on grids. size: Density_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
  - double *ADensity_Grid; electron densities by the superposition of atomic densities on grids. size: ADensity_Grid[Num_Cells0*Ngrid2*Ngrid3].
  - double *PCCDensity_Grid; electron densities by the superposition of partial core correction densities on grids. size: PCCDensity_Grid[Num_Cells0*Ngrid2*Ngrid3].

Listing 2.9: DFT: Set_Aden_Grid()

```
1 ||    0.2%  |   0.229197  |DFT:DFT.c:line.780
2 |||----------------------------
3 3||    0.0%  |   0.004159  |__ipai_Set_Aden_Grid:
    Set_Aden_Grid.c:line.33
```

```
 4 | 3||    0.0% |   0.000005 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.72
 5 |||||-------------------------------
 6 | 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
 7 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
 8 | 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
 9 | |||=================================
10 | 3||    0.0% |   0.000640 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.112
11 | 4||         |            | PrintMemory:PrintMemory.c:line
       .19
12 | 3||    0.0% |   0.000006 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.155
13 | 4||         |            | dtime:dtime.c:line.15
14 | 3||    0.0% |   0.022140 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.163
15 | 3||    0.1% |   0.120957 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.171
16 | |||||-------------------------------
17 | 4|||    0.1% |   0.056830 |AtomicDenF:AtomicDenF.c:line
       .18
18 | 4|||    0.1% |   0.064128 |Get_Grid_XYZ:openmx_common.c:
       line.866
19 | |||||=================================
20 | 3||    0.1% |   0.081256 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.190
21 | 4||         |            | AtomicPCCF:AtomicPCCF.c:line
       .18
22 | 3||    0.0% |   0.000005 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.196
23 | 4||         |            | dtime:dtime.c:line.15
24 | 3||    0.0% |   0.000015 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.250
25 | |||||-------------------------------
26 | 4|||    0.0% |   0.000011 |MPI_Allreduce:...:line.0
27 | 4|||    0.0% |   0.000004 |MPI_Allreduce(sync):...:line.0
28 | |||||=================================
29 | 3||    0.0% |   0.000003 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.401
30 | 4||         |            | dtime:dtime.c:line.15
31 | 3||    0.0% |   0.000008 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.474
32 | 4||         |            | dtime:dtime.c:line.15
33 | 3||    0.0% |   0.000002 |__ipai_Set_Aden_Grid:
       Set_Aden_Grid.c:line.719
34 | 4||         |            | dtime:dtime.c:line.15
```

- Set_Orbitals_Grid() (in Set_Orbitals_Grid.c): a subroutine to calculate the value of basis functions on each grid point.

– Get_Orbitals() (in Get_Orbitals.c): a subroutine to calculate basis orbitals.

– Type_Orbs_Grid ***Orbs_Grid; values of basis orbitals on grids. size: Orbs_Grid[Matomnum+MatomnumF+1] [Spe_Total_NO[Cwan]] [GridN_Atom[Gc_AN]]. Type_Orbs_Grid is defined as float.

Listing 2.10: DFT: Set_Orbitals_Grid()

```
1  ||    0.3% |   0.242072 |DFT:DFT.c:line.810
2  |||------------------------------
3  3||    0.0% |   0.000014 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.34
4  3||    0.0% |   0.000005 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.58
5  ||||-----------------------------
6  4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
8  4|||    0.0% |   0.000001 |dtime:dtime.c:line.15
9  ||||=============================
10 3||    0.0% |   0.000003 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.77
11 4||         |            | dtime:dtime.c:line.15
12 3||    0.0% |   0.015241 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.90
13 |||============================
14 3||    0.1% |   0.065867 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.102
15 4||         |            | Get_Grid_XYZ:openmx_common.c:
       line.866
16 3||    0.2% |   0.160924 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.118
17 ||||-----------------------------
18 4|||    0.1% |   0.091499 |Get_Orbitals:Get_Orbitals.c:
       line.18
19 4|||    0.1% |   0.069425 |Get_Orbitals:Get_Orbitals.c:
       line.51
20 5|||         |            | xyz2spherical:xyz2spherical.c
       :line.20
21 ||||=============================
22 3||    0.0% |   0.000005 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.138
23 4||         |            | dtime:dtime.c:line.15
24 3||    0.0% |   0.000012 |Set_Orbitals_Grid:
       Set_Orbitals_Grid.c:line.198
25 ||||-----------------------------
26 4|||    0.0% |   0.000008 |MPI_Allreduce:...:line.0
27 4|||    0.0% |   0.000004 |MPI_Allreduce(sync):...:line.0
28 ||||=============================
29 3||    0.0% |   0.000002 |Set_Orbitals_Grid:
```

```
    Set_Orbitals_Grid.c:line.286
4||          |              | dtime:dtime.c:line.15
```

- Set_Hamiltonian() (in Set_Hamiltonian.c): a subroutine to make Hamiltonian matrix within LDA or GGA. This one is called when the number of iterations SCF = 1.
  - double *****H0; matrix elements of basis orbitals for T+VNL. size: H0[4] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - double *****HNL; real matrix elements of basis orbitals for non-local VPS. size: HNL[List_YOUSO[5]] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - double *****H; Kohn-Sham matrix elements of basis orbitals. size: H[SpinP_switch+1] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - double ******DM; current and old density matrices. size: DM[List_YOUSO[16]] [SpinP_switch+1] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - Set_Vpot() (in Set_Vpot.c): a subroutine to calculate the value of local potential on each grid point.
  - Set_XC_Grid() (in Set_XC_Grid.c):
  - XC_Ceperly_Alder() in (XC_Ceperly_Alder.c): a subroutine to calculate an exchange- correlation potential for a given density "den" by the local density approximation.
  - double **Vxc_Grid; exchange-correlation potentials on grids. size: Vxc_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
  - double **Vpot_Grid; Kohn-Sham effective potentials on grids. size: Vpot_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].

Listing 2.11: DFT: Set_Hamiltonian() when the number of iterations SCF = 1

```
1 ||    0.3% |   0.309241 |DFT:DFT.c:line.929
2 |||-------------------------------
3 3||    0.0% |   0.000031 |Set_Hamiltonian:Set_Hamiltonian
      .c:line.46
4 3||    0.0% |   0.000008 |Set_Hamiltonian:Set_Hamiltonian
      .c:line.100
5 ||||-----------------------------
6 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
7 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
8 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
9 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
```

```
 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
 ||||==========================================
 3||    0.0% |   0.000001 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.167
 4||         |            | dtime:dtime.c:line.15
 3||    0.0% |   0.000002 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.198
 4||         |            | dtime:dtime.c:line.15
 3||    0.3% |   0.307711 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.215
 ||||------------------------------
 4|||    0.0% |   0.001555 |__ipai_Set_Vpot:Set_Vpot.c:
    line.34
 4|||    0.0% |   0.000003 |__ipai_Set_Vpot:Set_Vpot.c:
    line.53
 |||||-----------------------------
 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
 |||||==============================
 4|||    0.3% |   0.306145 |__ipai_Set_Vpot:Set_Vpot.c:
    line.92
 |||||-----------------------------
 5||||    0.0% |   0.000007 |Set_XC_Grid:Set_XC_Grid.c:
    line.29
 5||||    0.0% |   0.000003 |Set_XC_Grid:Set_XC_Grid.c:
    line.72
 ||||||---------------------------
 6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
 6|||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
 |||||==============================
 5||||    0.0% |   0.032888 |Set_XC_Grid:Set_XC_Grid.c:
    line.290
 5||||    0.3% |   0.273247 |Set_XC_Grid:Set_XC_Grid.c:
    line.322
 6||||         |            | XC_Ceperly_Alder:
    XC_Ceperly_Alder.c:line.20
 4|||    0.0% |   0.000007 |dtime:dtime.c:line.15
 ||||==========================================
 3||    0.0% |   0.001479 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.257
 3||    0.0% |   0.000010 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.569
 ||||------------------------------
 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
 4|||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
 4|||    0.0% |   0.000004 |dtime:dtime.c:line.15
 |||==========================================
```

- Poisson() (in Poisson.c): a subroutine to solve Poisson's equation using

fast Fourier transformation.

- FFT_Density()
- double **Density_Grid; electron densities on grids. size: Density_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
- FFT_Poisson()
- Get_Value_inReal()

Listing 2.12: DFT: Poisson()

```
1  ||    0.1% |   0.097813 |DFT:DFT.c:line.956
2  |||-------------------------------
3  3||    0.1% |   0.097705 |Poisson:Poisson.c:line.37
4  3||    0.0% |   0.000006 |Poisson:Poisson.c:line.53
5  ||||-----------------------------
6  4|||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000004 |MPI_Comm_size:...:line.0
8  ||||=============================
9  3||    0.0% |   0.000010 |Poisson:Poisson.c:line.60
10 ||||-----------------------------
11 4|||    0.0% |   0.000003 |MPI_Barrier:...:line.0
12 4|||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
13 4|||    0.0% |   0.000004 |dtime:dtime.c:line.15
14 ||||=============================
15 3||    0.0% |   0.000026 |Poisson:Poisson.c:line.67
16 ||||-----------------------------
17 4|||    0.0% |   0.000006 |FFT_Density:Poisson.c:line.498
18 |||||---------------------------
19 5||||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
20 5||||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
21 |||||===========================
22 4|||    0.0% |   0.000021 |FFT_Density:Poisson.c:line.717
23 5|||         |            | FFT_Poisson:Poisson.c:line
       .137
24 ||||||-------------------------
25 6|||||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
26 6|||||    0.0% |   0.000018 |MPI_Comm_size:...:line.0
27 |||=============================
28 3||    0.0% |   0.000065 |Poisson:Poisson.c:line.105
29 ||||-----------------------------
30 4|||    0.0% |   0.000027 |Get_Value_inReal:Poisson.c:
       line.761
31 |||||---------------------------
32 5||||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
33 5||||    0.0% |   0.000023 |MPI_Comm_size:...:line.0
34 |||||===========================
35 4|||    0.0% |   0.000006 |Get_Value_inReal:Poisson.c:
       line.776
```

```
5|||          |              | FFT_Poisson:Poisson.c:line
    .137
||||||-------------------------------
6|||||    0.0%  |   0.000003  |MPI_Comm_rank:...:line.0
6|||||    0.0%  |   0.000003  |MPI_Comm_size:...:line.0
||||||===============================
4|||    0.0%  |   0.000004  |MPI_Barrier:...:line.0
4|||    0.0%  |   0.000025  |MPI_Barrier(sync):...:line.0
4|||    0.0%  |   0.000004  |dtime:dtime.c:line.15
||||=================================
```

- Set_Hamiltonian() (in Set_Hamiltonian.c): a subroutine to make Hamiltonian matrix within LDA or GGA. This one is called when the number of iterations $SCF > 1$.

Listing 2.13: DFT: Set_Hamiltonian() when the number of iterations $SCF > 1$

```
||    0.7%  |   0.619556  |DFT:DFT.c:line.970
|||-----------------------------
3||    0.0%  |   0.000065  |Set_Hamiltonian:Set_Hamiltonian
    .c:line.46
3||    0.0%  |   0.000015  |Set_Hamiltonian:Set_Hamiltonian
    .c:line.100
||||----------------------------
4|||    0.0%  |   0.000003  |MPI_Comm_rank:...:line.0
4|||    0.0%  |   0.000004  |MPI_Comm_size:...:line.0
4|||    0.0%  |   0.000003  |MPI_Barrier:...:line.0
4|||    0.0%  |   0.000003  |MPI_Barrier(sync):...:line.0
4|||    0.0%  |   0.000003  |dtime:dtime.c:line.15
||||================================
3||    0.0%  |   0.000004  |Set_Hamiltonian:Set_Hamiltonian
    .c:line.167
4||          |             | dtime:dtime.c:line.15
3||    0.0%  |   0.000003  |Set_Hamiltonian:Set_Hamiltonian
    .c:line.198
4||          |             | dtime:dtime.c:line.15
3||    0.7%  |   0.616535  |Set_Hamiltonian:Set_Hamiltonian
    .c:line.215
||||----------------------------
4|||    0.0%  |   0.001957  |__ipai_Set_Vpot:Set_Vpot.c:
    line.34
4|||    0.0%  |   0.000006  |__ipai_Set_Vpot:Set_Vpot.c:
    line.53
|||||--------------------------
5||||    0.0%  |   0.000003  |MPI_Comm_rank:...:line.0
5||||    0.0%  |   0.000003  |MPI_Comm_size:...:line.0
|||||===============================
4|||    0.7%  |   0.614560  |__ipai_Set_Vpot:Set_Vpot.c:
    line.92
```

```
|||||----------------------------
 5||||    0.0% |   0.000011 |Set_XC_Grid:Set_XC_Grid.c:
    line.29
 5||||    0.0% |   0.000005 |Set_XC_Grid:Set_XC_Grid.c:
    line.72
||||||----------------------------
 6|||||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
 6|||||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
|||||============================
 5||||    0.1% |   0.062264 |Set_XC_Grid:Set_XC_Grid.c:
    line.290
 5||||    0.6% |   0.552280 |Set_XC_Grid:Set_XC_Grid.c:
    line.322
 6||||          |            | XC_Ceperly_Alder:
    XC_Ceperly_Alder.c:line.20
 4|||    0.0% |   0.000012 |dtime:dtime.c:line.15
||||==================================
 3||    0.0% |   0.002915 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.257
 3||    0.0% |   0.000019 |Set_Hamiltonian:Set_Hamiltonian
    .c:line.569
||||----------------------------
 4|||    0.0% |   0.000003 |MPI_Barrier:...:line.0
 4|||    0.0% |   0.000008 |MPI_Barrier(sync):...:line.0
 4|||    0.0% |   0.000009 |dtime:dtime.c:line.15
||==================================
```

- Cluster_DFT("scf") (in Cluster_DFT.c): a subroutine to perform cluster calculations.
  - Cluster_collinear(): collinear without spin-orbit coupling.
  - Overlap_Cluster() (in Overlap_Cluster.c): a subroutine to make an overlap matrix for cluster or molecular systems. This one is called only when the number of iterations SCF = 1.
  - double **S; a full overlap matrix. size: S[Size_Total_Matrix+2][Size_Total_Matrix+2].
  - double *****OLP; overlap matrix elements of basis orbitals. size: OLP[4] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - Hamiltonian_Cluster() (in Hamiltonian_Cluster.c): a subroutine to make a Hamiltonian matrix for cluster or molecular systems.
  - double **H;
  - Eigen_PReHH() (in Eigen_PReHH.c): a MPI parallelized subroutine to solve a standard eigenvalue problem with a real symmetric matrix using Householder method and lapack's dstevx_(), dstegr_(), or dstedc_().

- Eigen_Improved_PReHH()
- myHH(): Householder method.
- BroadCast_ReMatrix() (in BroadCast_ReMatrix.c): a subroutine to broadcast a matrix "Mat" which is distributed by row in each processor.
- double *****EDM; current energy density matrices. size: EDM[SpinP_switch+1] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
- dcomplex *****HOMOs_Coef; LCAO coefficients of HOMOs. size: HOMOs_Coef[List_YOUSO[33]] [2] [List_YOUSO[31]] [List_YOUSO[1]] [List_YOUSO[7]].
- dcomplex *****LUMOs_Coef; LCAO coefficients of HOMOs. size: HOMOs_Coef[List_YOUSO[33]] [2] [List_YOUSO[32]] [List_YOUSO[1]] [List_YOUSO[7]].
- double *****Partial_DM; partial density matrix to calculate partial density in an energy window specified by a keyword, scf.energy.window.partial.charge. size: Partial_DM [2] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].

Listing 2.14: DFT: Cluster_DFT(scf)

```
1  ||    0.0% |   0.007623 |DFT:DFT.c:line.1012
2  |||-------------------------------
3  3||    0.0% |   0.005772 |_ipas_Cluster_DFT:Cluster_DFT.c
       :line.93
4  |||===============================
5  3||    0.0% |   0.001851 |__ipas_Cluster_DFT:Cluster_DFT.
       c:line.103
6  ||||----------------------------
7  4|||    0.0% |   0.000406 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.158
8  |||||--------------------------
9  5||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
10 5||||    0.0% |   0.000007 |MPI_Barrier(sync):...:line.0
11 5||||    0.0% |   0.000009 |MPI_Comm_rank:...:line.0
12 5||||    0.0% |   0.000009 |MPI_Comm_size:...:line.0
13 5||||    0.0% |   0.000028 |Make_Comm_Worlds:
       Make_Comm_Worlds.c:line.35
14 5||||    0.0% |   0.000344 |Make_Comm_Worlds:
       Make_Comm_Worlds.c:line.88
15 ||||||------------------------
16 6|||||    0.0% |   0.000309 |MPI_Comm_create:...:line.0
17 6|||||    0.0% |   0.000007 |MPI_Comm_group:...:line.0
18 6|||||    0.0% |   0.000005 |MPI_Group_free:...:line.0
19 6|||||    0.0% |   0.000023 |MPI_Group_incl:...:line.0
20 ||||||========================
21 5||||    0.0% |   0.000005 |dtime:dtime.c:line.15
```

```
22 |||||==============================
23  4|||    0.0% |   0.000375 |__ipas_Cluster_collinear:
        Cluster_DFT.c:line.270
24  5|||         |            | PrintMemory:PrintMemory.c:
        line.19
25  4|||    0.0% |   0.000013 |__ipas_Cluster_collinear:
        Cluster_DFT.c:line.340
26 |||||------------------------------
27  5||||    0.0% |   0.000008 |MPI_Barrier:...:line.0
28  5||||    0.0% |   0.000005 |MPI_Barrier(sync):...:line.0
29 |||||==============================
30  4|||    0.0% |   0.000039 |__ipas_Cluster_collinear:
        Cluster_DFT.c:line.343
31 |||||------------------------------
32  5||||    0.0% |   0.000009 |Overlap_Cluster:
        Overlap_Cluster.c:line.25
33  5||||    0.0% |   0.000006 |Overlap_Cluster:
        Overlap_Cluster.c:line.30
34 ||||||-----------------------------
35  6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
36  6|||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
37  6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
38  6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
39 ||||||==============================
40  5||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.63
41 ||||||-----------------------------
42  6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
43  6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
44 |||||==============================
45  5||||    0.0% |   0.000005 |Overlap_Cluster:
        Overlap_Cluster.c:line.74
46 ||||||-----------------------------
47  6|||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
48  6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
49 |||||==============================
50  5||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.86
51 ||||||-----------------------------
52  6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
53  6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
54 |||||==============================
55  5||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.95
56 ||||||-----------------------------
57  6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
58  6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
59 |||||==============================
60  5||||    0.0% |   0.000003 |Overlap_Cluster:
```

```
    Overlap_Cluster.c:line.106
||||||---------------------------
 6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
 6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
||||||===========================
 5||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.109
||||||---------------------------
 6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
||||||===========================
 5||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.143
||||||---------------------------
 6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
 6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
||||||===========================
 5||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.149
||||||---------------------------
 6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
||||||===========================
 4|||    0.0% |   0.000070 |__ipas_Cluster_collinear:
    Cluster_DFT.c:line.346
|||||---------------------------
 5||||    0.0% |   0.000016 |Hamiltonian_Cluster:
    Hamiltonian_Cluster.c:line.27
 5||||    0.0% |   0.000016 |Hamiltonian_Cluster:
    Hamiltonian_Cluster.c:line.32
||||||---------------------------
 6|||||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
 6|||||    0.0% |   0.000004 |MPI_Comm_size:...:line.0
 6|||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
 6|||||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
|||||===========================
 5||||    0.0% |   0.000013 |Hamiltonian_Cluster:
    Hamiltonian_Cluster.c:line.75
||||||---------------------------
 6|||||    0.0% |   0.000009 |MPI_Bcast:...:line.0
 6|||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
||||||===========================
 5||||    0.0% |   0.000008 |Hamiltonian_Cluster:
    Hamiltonian_Cluster.c:line.95
||||||---------------------------
 6|||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
 6|||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
|||||===========================
 5||||    0.0% |   0.000008 |Hamiltonian_Cluster:
```

```
    |     Hamiltonian_Cluster.c:line.108
101 ||||||---------------------------
102 6|||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
103 6|||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
104 ||||||===========================
105 5||||    0.0% |   0.000008 |Hamiltonian_Cluster:
    |     Hamiltonian_Cluster.c:line.146
106 ||||||---------------------------
107 6|||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
108 6|||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
109 ||||||===========================
110 4|||    0.0% |   0.000361 |__ipas_Cluster_collinear:
    |     Cluster_DFT.c:line.377
111 |||||---------------------------
112 5||||    0.0% |   0.000015 |Eigen_PReHH:Eigen_PReHH.c:
    |     line.58
113 5||||    0.0% |   0.000346 |Eigen_PReHH:Eigen_PReHH.c:
    |     line.59
114 ||||||---------------------------
115 6|||||    0.0% |   0.000003 |Eigen_Improved_PReHH:
    |     Eigen_PReHH.c:line.73
116 |||||||-------------------------
117 7||||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
118 7||||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
119 |||||===========================
120 6|||||    0.0% |   0.000198 |Eigen_Improved_PReHH:
    |     Eigen_PReHH.c:line.158
121 7|||||         |            | myHH:Eigen_PReHH.c:line.723
122 |||||||-------------------------
123 8|||||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
124 8|||||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
    |     .0
125 8|||||||    0.0% |   0.000003 |MPI_Bcast:...:line.0
126 8|||||||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
127 8|||||||    0.0% |   0.000009 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.29
128 8|||||||    0.0% |   0.000164 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.57
129 9|||||||         |            | MPI_Isend:...:line.0
130 8|||||||    0.0% |   0.000004 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.63
131 9|||||||         |            | MPI_Irecv:...:line.0
132 8|||||||    0.0% |   0.000012 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.69
133 9|||||||         |            | MPI_Waitall:...:line.0
134 |||||||===========================
135 6|||||    0.0% |   0.000133 |Eigen_Improved_PReHH:
    |     Eigen_PReHH.c:line.191
136 7|||||         |            | lapack_dstevx1:
```

```
    |    lapack_dstevx1.c:line.27
137 | 6|||||    0.0% |   0.000012 |Eigen_Improved_PReHH:
    |    Eigen_PReHH.c:line.298
138 | |||||||-------------------------
139 | 7||||||    0.0% |   0.000004 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.29
140 | 7||||||    0.0% |   0.000003 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.57
141 | 8||||||         |            | MPI_Isend:...:line.0
142 | 7||||||    0.0% |   0.000002 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.63
143 | 8||||||         |            | MPI_Irecv:...:line.0
144 | 7||||||    0.0% |   0.000004 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.69
145 | 8||||||         |            | MPI_Waitall:...:line.0
146 | |||||||=========================
147 | 4|||    0.0% |   0.000008 |__ipas_Cluster_collinear:
    |    Cluster_DFT.c:line.447
148 | |||||-------------------------
149 | 5||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
150 | 5||||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
151 | |||||=========================
152 | 4|||    0.0% |   0.000063 |__ipas_Cluster_collinear:
    |    Cluster_DFT.c:line.565
153 | |||||-------------------------
154 | 5||||    0.0% |   0.000016 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.29
155 | 5||||    0.0% |   0.000015 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.57
156 | 6||||         |            | MPI_Isend:...:line.0
157 | 5||||    0.0% |   0.000010 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.63
158 | 6||||         |            | MPI_Irecv:...:line.0
159 | 5||||    0.0% |   0.000022 |BroadCast_ReMatrix:
    |    BroadCast_ReMatrix.c:line.69
160 | 6||||         |            | MPI_Waitall:...:line.0
161 | |||||=========================
162 | 4|||    0.0% |   0.000189 |__ipas_Cluster_collinear:
    |    Cluster_DFT.c:line.659
163 | |||||-------------------------
164 | 5||||    0.0% |   0.000022 |Eigen_PReHH:Eigen_PReHH.c:
    |    line.58
165 | 5||||    0.0% |   0.000166 |Eigen_PReHH:Eigen_PReHH.c:
    |    line.59
166 | 6|||||    0.0% |   0.000009 |Eigen_Improved_PReHH:
    |    Eigen_PReHH.c:line.73
167 | |||||||-------------------------
168 | 7||||||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
169 | 7||||||    0.0% |   0.000005 |MPI_Comm_size:...:line.0
```

```
170 ||||||---------------------------
171  6|||||    0.0% |   0.000065 |Eigen_Improved_PReHH:
         Eigen_PReHH.c:line.158
172  7|||||         |            | myHH:Eigen_PReHH.c:line.723
173 |||||||-------------------------
174  8|||||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
175  8|||||||    0.0% |   0.000005 |MPI_Barrier(sync):...:line
         .0
176  8|||||||    0.0% |   0.000009 |MPI_Bcast:...:line.0
177  8|||||||    0.0% |   0.000011 |MPI_Bcast(sync):...:line.0
178  8|||||||    0.0% |   0.000007 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.29
179  8|||||||    0.0% |   0.000006 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.57
180  9|||||||         |            | MPI_Isend:...:line.0
181  8|||||||    0.0% |   0.000005 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.63
182  9|||||||         |            | MPI_Irecv:...:line.0
183  8|||||||    0.0% |   0.000018 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.69
184  9|||||||         |            | MPI_Waitall:...:line.0
185 |||||||=========================
186  6|||||    0.0% |   0.000092 |Eigen_Improved_PReHH:
         Eigen_PReHH.c:line.191
187  7|||||         |            | lapack_dstevx1:
         lapack_dstevx1.c:line.27
188 |||||=============================
189  4|||    0.0% |   0.000028 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.736
190 |||||---------------------------
191  5||||    0.0% |   0.000007 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.29
192  5||||    0.0% |   0.000006 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.57
193  6||||         |            | MPI_Isend:...:line.0
194  5||||    0.0% |   0.000005 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.63
195  6||||         |            | MPI_Irecv:...:line.0
196  5||||    0.0% |   0.000010 |BroadCast_ReMatrix:
         BroadCast_ReMatrix.c:line.69
197  6||||         |            | MPI_Waitall:...:line.0
198 |||||=============================
199  4|||    0.0% |   0.000017 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.794
200 |||||---------------------------
201  5||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
202  5||||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
203  5||||    0.0% |   0.000005 |MPI_Bcast:...:line.0
204  5||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
```

```
205 |||||==================================
206  4|||    0.0% |   0.000008 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.815
207 |||||----------------------------------
208  5||||    0.0% |   0.000004 |MPI_Bcast:...:line.0
209  5||||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
210 ||||==================================
211  4|||    0.0% |   0.000216 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.1017
212  4|||    0.0% |   0.000020 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.1134
213 |||||----------------------------------
214  5||||    0.0% |   0.000014 |MPI_Allreduce:...:line.0
215  5||||    0.0% |   0.000006 |MPI_Allreduce(sync):...:line
         .0
216 |||||==================================
217  4|||    0.0% |   0.000006 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.1158
218  5|||         |            | __ipap_fnjoint:openmx_common.
         c:line.358
219  4|||    0.0% |   0.000015 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.1364
220  5|||         |            | MPI_Comm_free:...:line.0
221  4|||    0.0% |   0.000016 |__ipas_Cluster_collinear:
         Cluster_DFT.c:line.1367
222 |||||----------------------------------
223  5||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
224  5||||    0.0% |   0.000005 |MPI_Barrier(sync):...:line.0
225  5||||    0.0% |   0.000007 |dtime:dtime.c:line.15
226 |||||==================================
```

- Mulliken_Charge() (in Mulliken_Charge.c): a subroutine to calculate Mulliken charge.
  - double *InitN_USpin; the number of the upspin electon of initial atoms. size: InitN_USpin[atomnum+1].
  - double *InitN_DSpin; the number of the upspin electon of initial atoms. size: InitN_DSpin[atomnum+1].

Listing 2.15: DFT: Mulliken_Charge()

```
1  ||    0.0% |   0.000163 |DFT:DFT.c:line.1261
2  |||----------------------------------
3  3||    0.0% |   0.000076 |Mulliken_Charge:Mulliken_Charge
       .c:line.29
4  3||    0.0% |   0.000009 |Mulliken_Charge:Mulliken_Charge
       .c:line.79
5  ||||----------------------------------
6  4|||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
```

```
 4|||    0.0%  |   0.000005  |MPI_Comm_size:...:line.0
||||=================================
 3||    0.0%  |   0.000008  |Mulliken_Charge:Mulliken_Charge
    .c:line.99
 4||          |             | dtime:dtime.c:line.15
|||=================================
 3||    0.0%  |   0.000008  |Mulliken_Charge:Mulliken_Charge
    .c:line.255
 4||          |             | dtime:dtime.c:line.15
 3||    0.0%  |   0.000012  |Mulliken_Charge:Mulliken_Charge
    .c:line.288
||||-----------------------------
 4|||    0.0%  |   0.000008  |MPI_Allreduce:...:line.0
 4|||    0.0%  |   0.000004  |MPI_Allreduce(sync):...:line.0
||||=================================
 3||    0.0%  |   0.000033  |Mulliken_Charge:Mulliken_Charge
    .c:line.291
||||-----------------------------
 4|||    0.0%  |   0.000018  |MPI_Bcast:...:line.0
 4|||    0.0%  |   0.000015  |MPI_Bcast(sync):...:line.0
||||=================================
 3||    0.0%  |   0.000016  |Mulliken_Charge:Mulliken_Charge
    .c:line.309
||||-----------------------------
 4|||    0.0%  |   0.000008  |MPI_Bcast:...:line.0
 4|||    0.0%  |   0.000008  |MPI_Bcast(sync):...:line.0
||||=================================
```

- Mixing_DM() (in Mixing_DM.c): simple, RMM-DIIS, or GR-Pulay mixing for density matrix.
  - DIIS_Mixing_DM() (in DIIS_Mixing_DM.c): a subroutine to achieve self-consistent field using the direct inversion in the iterative subspace.
  - double ******ResidualDM; current and old residual real density matrices, which are defined as the difference between input and output density matrices. size: ResidualDM[List_YOUSO[16]] [SpinP_switch+1] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - double ******iResidualDM; current and old residual imaginary density matrices, which are defined as the difference between input and output density matrices. size: iResidualDM[List_YOUSO[16]] [2] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - Simple_Mixing_DM() (in Simple_Mixing_DM.c): a subroutine to achieve self-consistent field using the simple mixing method.

Listing 2.16: DFT: Mixing_DM()

```
1  ||    0.0% |   0.006797 |DFT:DFT.c:line.1387
2  |||-------------------------------
3  3||    0.0% |   0.000017 |__ipai_Mixing_DM:Mixing_DM.c:
       line.33
4  3||    0.0% |   0.000021 |__ipai_Mixing_DM:Mixing_DM.c:
       line.45
5  ||||-----------------------------
6  4|||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000005 |MPI_Comm_size:...:line.0
8  4|||    0.0% |   0.000004 |MPI_Barrier:...:line.0
9  4|||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
10 4|||    0.0% |   0.000004 |dtime:dtime.c:line.15
11 |||=============================
12 3||    0.0% |   0.000284 |__ipai_Mixing_DM:Mixing_DM.c:
       line.108
13 ||||-----------------------------
14 4|||    0.0% |   0.000015 |DIIS_Mixing_DM:DIIS_Mixing_DM.
       c:line.31
15 4|||    0.0% |   0.000003 |DIIS_Mixing_DM:DIIS_Mixing_DM.
       c:line.58
16 |||||----------------------------
17 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
18 5||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
19 ||||===============================
20 4|||    0.0% |   0.000253 |DIIS_Mixing_DM:DIIS_Mixing_DM.
       c:line.194
21 5|||         |            | PrintMemory:PrintMemory.c:
       line.19
22 4|||    0.0% |   0.000013 |DIIS_Mixing_DM:DIIS_Mixing_DM.
       c:line.214
23 |||||----------------------------
24 5||||    0.0% |   0.000005 |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.41
25 5||||    0.0% |   0.000003 |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.50
26 ||||||---------------------------
27 6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
28 6|||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
29 |||||============================
30 5||||    0.0% |   0.000004 |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.109
31 ||||||---------------------------
32 6|||||    0.0% |   0.000003 |MPI_Allreduce:...:line.0
33 6|||||    0.0% |   0.000002 |MPI_Allreduce(sync):...:line
       .0
34 ||||||===========================
35 3||    0.0% |   0.000067 |__ipai_Mixing_DM:Mixing_DM.c:
       line.121
```

```
36 ||||----------------------------
37  4|||    0.0%  |   0.000018  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.41
38  4|||    0.0%  |   0.000006  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.50
39 |||||----------------------------
40  5||||    0.0%  |   0.000003  |MPI_Comm_rank:...:line.0
41  5||||    0.0%  |   0.000003  |MPI_Comm_size:...:line.0
42 ||||==================================
43  4|||    0.0%  |   0.000011  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.109
44 |||||----------------------------
45  5||||    0.0%  |   0.000008  |MPI_Allreduce:...:line.0
46  5||||    0.0%  |   0.000003  |MPI_Allreduce(sync):...:line
       .0
47 |||||================================
48  4|||    0.0%  |   0.000006  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.134
49  5|||          |             | sgn:openmx_common.c:line.338
50  4|||    0.0%  |   0.000010  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.156
51  5|||          |             | sgn:openmx_common.c:line.338
52  4|||    0.0%  |   0.000005  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.176
53  5|||          |             | sgn:openmx_common.c:line.338
54  4|||    0.0%  |   0.000001  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.180
55  5|||          |             | largest:openmx_common.c:line
       .487
56  4|||    0.0%  |   0.000008  |Simple_Mixing_DM:
       Simple_Mixing_DM.c:line.196
57  5|||          |             | sgn:openmx_common.c:line.338
58  3||    0.0%  |   0.000012  |__ipai_Mixing_DM:Mixing_DM.c:
       line.244
59 ||||----------------------------
60  4|||    0.0%  |   0.000004  |MPI_Barrier:...:line.0
61  4|||    0.0%  |   0.000004  |MPI_Barrier(sync):...:line.0
62  4|||    0.0%  |   0.000004  |dtime:dtime.c:line.15
63 ||||==================================
```

- Set_Density_Grid() (in Set_Density_Grid.c): a subroutine to calculate a charge density on grid by one-particle wave functions.
  - double **Density_Grid; electron densities on grids. size: Density_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
  - Type_Orbs_Grid ***COrbs_Grid; values of contrated basis orbitals on grids. size: COrbs_Grid[Matomnum+MatomnumF+1] [Spe_Total_NO[Cwan]] [GridN_Atom[Gc_AN]]. Type_Orbs_Grid is

defined as float.

Listing 2.17: DFT: Set_Density_Grid()

```
1  ||    0.0% |   0.006797 |DFT:DFT.c:line.1387
2  |||-------------------------------
3  3||    0.0% |   0.003426 |Set_Density_Grid:
       Set_Density_Grid.c:line.37
4  3||    0.0% |   0.000013 |Set_Density_Grid:
       Set_Density_Grid.c:line.80
5  ||||------------------------------
6  4|||    0.0% |   0.000004 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000005 |MPI_Comm_size:...:line.0
8  4|||    0.0% |   0.000004 |dtime:dtime.c:line.15
9  ||||==============================
10 3||    0.0% |   0.000005 |Set_Density_Grid:
       Set_Density_Grid.c:line.274
11 4||         |            | dtime:dtime.c:line.15
12 3||    0.0% |   0.002870 |Set_Density_Grid:
       Set_Density_Grid.c:line.289
13 3||    0.0% |   0.000012 |Set_Density_Grid:
       Set_Density_Grid.c:line.317
14 4||         |            | dtime:dtime.c:line.15
15 3||    0.0% |   0.000013 |Set_Density_Grid:
       Set_Density_Grid.c:line.481
16 4||         |            | dtime:dtime.c:line.15
17 3||    0.0% |   0.000004 |Set_Density_Grid:
       Set_Density_Grid.c:line.514
18 4||         |            | dtime:dtime.c:line.15
19 3||    0.0% |   0.000017 |Set_Density_Grid:
       Set_Density_Grid.c:line.570
20 ||||------------------------------
21 4|||    0.0% |   0.000011 |MPI_Allreduce:...:line.0
22 4|||    0.0% |   0.000006 |MPI_Allreduce(sync):...:line.0
23 ||||==============================
24 3||    0.0% |   0.000004 |Set_Density_Grid:
       Set_Density_Grid.c:line.637
25 4||         |            | dtime:dtime.c:line.15
26 3||    0.0% |   0.000008 |Set_Density_Grid:
       Set_Density_Grid.c:line.653
27 4||         |            | dtime:dtime.c:line.15
28 3||    0.0% |   0.000013 |Set_Density_Grid:
       Set_Density_Grid.c:line.666
29 4||         |            | dtime:dtime.c:line.15
30 3||    0.0% |   0.000004 |Set_Density_Grid:
       Set_Density_Grid.c:line.674
31 4||         |            | dtime:dtime.c:line.15
32 3||    0.0% |   0.000006 |Set_Density_Grid:
       Set_Density_Grid.c:line.822
33 4||         |            | dtime:dtime.c:line.15
```

```
34 ||    0.0% |   0.001607 |DFT:DFT.c:line.1568
35 |||-------------------------------
36 3||    0.0% |   0.001603 |__ipas_outputfile1:outputfile1.
       c:line.16
37 3||    0.0% |   0.000005 |__ipas_outputfile1:outputfile1.
       c:line.23
38 4||         |            | MPI_Comm_rank:...:line.0
39 |||===============================
```

- TRAN_Output_Trans_HS() (in TRAN_Output_Trans_HS.c): a subroutine to save the SCF result by the NEGF for calculation of transmission and current by the TranMain.
- Mulliken_Charge() (in Mulliken_Charge.c)

Listing 2.18: DFT: Mulliken_Charge()

```
1  ||    0.0% |   0.000005 |DFT:DFT.c:line.1599
2  3|         |            | __ipap_TRAN_Output_Trans_HS:
       TRAN_Output_Trans_HS.c:line.106
3  ||    0.0% |   0.000426 |DFT:DFT.c:line.1617
4  |||-------------------------------
5  3||    0.0% |   0.000396 |Mulliken_Charge:Mulliken_Charge
       .c:line.29
6  3||    0.0% |   0.000003 |Mulliken_Charge:Mulliken_Charge
       .c:line.79
7  ||||-------------------------------
8  4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
9  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
10 ||||===============================
11 3||    0.0% |   0.000003 |Mulliken_Charge:Mulliken_Charge
       .c:line.99
12 4||         |            | dtime:dtime.c:line.15
13 |||===============================
14 3||    0.0% |   0.000003 |Mulliken_Charge:Mulliken_Charge
       .c:line.255
15 4||         |            | dtime:dtime.c:line.15
16 3||    0.0% |   0.000005 |Mulliken_Charge:Mulliken_Charge
       .c:line.288
17 ||||-------------------------------
18 4|||    0.0% |   0.000003 |MPI_Allreduce:...:line.0
19 4|||    0.0% |   0.000002 |MPI_Allreduce(sync):...:line.0
20 ||||===============================
21 3||    0.0% |   0.000011 |Mulliken_Charge:Mulliken_Charge
       .c:line.291
22 ||||-------------------------------
23 4|||    0.0% |   0.000006 |MPI_Bcast:...:line.0
24 4|||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
25 ||||===============================
```

```
26 | 3||    0.0% |   0.000005 |Mulliken_Charge:Mulliken_Charge
       .c:line.309
27 ||||----------------------------
28 | 4|||    0.0% |   0.000003 |MPI_Bcast:...:line.0
29 | 4|||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
30 ||||============================
```

- Cluster_DFT("dos") (in Cluster_DFT.c): a subroutine to perform cluster calculations.
  - Cluster_collinear(): collinear without spin-orbit coupling.
  - Hamiltonian_Cluster() (in Hamiltonian_Cluster.c): a subroutine to make a Hamiltonian matrix for cluster or molecular systems.
  - BroadCast_ReMatrix() (in BroadCast_ReMatrix.c): a subroutine to broadcast a matrix "Mat" which is distributed by row in each processor.
  - Eigen_PReHH() (in Eigen_PReHH.c): a MPI parallelized subroutine to solve a standard eigenvalue problem with a real symmetric matrix using Householder method and lapack's dstevx_(), dstegr_(), or dstedc_().
  - Eigen_Improved_PReHH()
  - myHH(): Householder method.
  - Save_DOS_Col(): to save density of states to the .Dos.vec file
  - Overlap_Cluster() (in Overlap_Cluster.c): a subroutine to make an overlap matrix for cluster or molecular systems. This one is called only when the number of iterations SCF = 1.

Listing 2.19: DFT: Cluster_DFT(dos)

```
1  ||    0.0% |   0.002414 |DFT:DFT.c:line.1673
2  |||---------------------------
3  | 3||    0.0% |   0.002124 |__ipas_Cluster_DFT:Cluster_DFT.
       c:line.93
4  |||===========================
5  | 3||    0.0% |   0.000290 |__ipas_Cluster_DFT:Cluster_DFT.
       c:line.103
6  ||||--------------------------
7  | 4|||    0.0% |   0.000066 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.158
8  |||||-------------------------
9  | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
10 | 5||||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
11 | 5||||    0.0% |   0.000003 |MPI_Comm_rank:...:line.0
12 | 5||||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
```

```
13 | 5||||    0.0% |   0.000003 |Make_Comm_Worlds:
       Make_Comm_Worlds.c:line.35
14 | 5||||    0.0% |   0.000053 |Make_Comm_Worlds:
       Make_Comm_Worlds.c:line.88
15 | ||||||---------------------------
16 | 6|||||    0.0% |   0.000048 |MPI_Comm_create:...:line.0
17 | 6|||||    0.0% |   0.000002 |MPI_Comm_group:...:line.0
18 | 6|||||    0.0% |   0.000001 |MPI_Group_free:...:line.0
19 | 6|||||    0.0% |   0.000002 |MPI_Group_incl:...:line.0
20 | ||||||===========================
21 | 5||||    0.0% |   0.000002 |dtime:dtime.c:line.15
22 | |||||=============================
23 | 4|||    0.0% |   0.000003 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.340
24 | |||||---------------------------
25 | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
26 | 5||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
27 | |||||=============================
28 | 4|||    0.0% |   0.000021 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.346
29 | |||||---------------------------
30 | 5||||    0.0% |   0.000004 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.27
31 | 5||||    0.0% |   0.000005 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.32
32 | ||||||---------------------------
33 | 6|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
34 | 6|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
35 | 6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
36 | 6|||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
37 | ||||||===========================
38 | 5||||    0.0% |   0.000003 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.75
39 | ||||||---------------------------
40 | 6|||||    0.0% |   0.000002 |MPI_Bcast:...:line.0
41 | 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
42 | ||||||===========================
43 | 5||||    0.0% |   0.000003 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.95
44 | ||||||---------------------------
45 | 6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
46 | 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
47 | |||||=============================
48 | 5||||    0.0% |   0.000003 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.108
49 | ||||||---------------------------
50 | 6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
51 | 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
52 | ||||||===========================
```

```
53 | 5||||    0.0% |   0.000003 |Hamiltonian_Cluster:
       Hamiltonian_Cluster.c:line.146
54 ||||||----------------------------
55 | 6|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
56 | 6|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
57 ||||||============================
58 | 4|||    0.0% |   0.000003 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.447
59 |||||----------------------------
60 | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
61 | 5||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
62 |||||============================
63 | 4|||    0.0% |   0.000014 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.565
64 |||||----------------------------
65 | 5||||    0.0% |   0.000003 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.29
66 | 5||||    0.0% |   0.000003 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.57
67 | 6||||         |            | MPI_Isend:...:line.0
68 | 5||||    0.0% |   0.000002 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.63
69 | 6||||         |            | MPI_Irecv:...:line.0
70 | 5||||    0.0% |   0.000005 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.69
71 | 6||||         |            | MPI_Waitall:...:line.0
72 |||||============================
73 | 4|||    0.0% |   0.000047 |__ipas_Cluster_collinear:
       Cluster_DFT.c:line.659
74 |||||----------------------------
75 | 5||||    0.0% |   0.000006 |Eigen_PReHH:Eigen_PReHH.c:
       line.58
76 | 5||||    0.0% |   0.000041 |Eigen_PReHH:Eigen_PReHH.c:
       line.59
77 ||||||----------------------------
78 | 6|||||    0.0% |   0.000003 |Eigen_Improved_PReHH:
       Eigen_PReHH.c:line.73
79 |||||||----------------------------
80 | 7||||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
81 | 7||||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
82 |||||============================
83 | 6|||||    0.0% |   0.000018 |Eigen_Improved_PReHH:
       Eigen_PReHH.c:line.158
84 | 7|||||         |            | myHH:Eigen_PReHH.c:line.723
85 |||||||----------------------------
86 | 8|||||||    0.0% |   0.000002 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.29
87 | 8|||||||    0.0% |   0.000002 |BroadCast_ReMatrix:
       BroadCast_ReMatrix.c:line.57
```

```
 88 | 9|||||||          |              | MPI_Isend:...:line.0
 89 | 8|||||||    0.0% |   0.000002 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.63
 90 | 9|||||||          |              | MPI_Irecv:...:line.0
 91 | 8|||||||    0.0% |   0.000003 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.69
 92 | 9|||||||          |              | MPI_Waitall:...:line.0
 93 | 8|||||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
 94 | 8|||||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
    |     .0
 95 | 8|||||||    0.0% |   0.000003 |MPI_Bcast:...:line.0
 96 | 8|||||||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
 97 | |||||||============================
 98 | 6|||||    0.0% |   0.000020 |Eigen_Improved_PReHH:
    |     Eigen_PReHH.c:line.191
 99 | 7|||||          |              | lapack_dstevx1:
    |     lapack_dstevx1.c:line.27
100 | 4|||    0.0% |   0.000009 |__ipas_Cluster_collinear:
    |     Cluster_DFT.c:line.736
101 | |||||----------------------------
102 | 5||||    0.0% |   0.000002 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.29
103 | 5||||    0.0% |   0.000002 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.57
104 | 6||||          |              | MPI_Isend:...:line.0
105 | 5||||    0.0% |   0.000002 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.63
106 | 6||||          |              | MPI_Irecv:...:line.0
107 | 5||||    0.0% |   0.000004 |BroadCast_ReMatrix:
    |     BroadCast_ReMatrix.c:line.69
108 | 6||||          |              | MPI_Waitall:...:line.0
109 | |||||==============================
110 | 4|||    0.0% |   0.000006 |__ipas_Cluster_collinear:
    |     Cluster_DFT.c:line.794
111 | |||||----------------------------
112 | 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
113 | 5||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
114 | 5||||    0.0% |   0.000002 |MPI_Bcast:...:line.0
115 | 5||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
116 | |||||==============================
117 | 4|||    0.0% |   0.000003 |__ipas_Cluster_collinear:
    |     Cluster_DFT.c:line.815
118 | |||||----------------------------
119 | 5||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
120 | 5||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
121 | ||||==============================
122 | 4|||    0.0% |   0.000109 |__ipas_Cluster_collinear:
    |     Cluster_DFT.c:line.1329
123 | |||||----------------------------
```

```
124 | 5||||    0.0% |   0.000003 |Save_DOS_Col:Cluster_DFT.c:
        line.2545
125 ||||||---------------------------
126 | 6|||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
127 | 6|||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
128 ||||||===========================
129 | 5||||    0.0% |   0.000002 |Save_DOS_Col:Cluster_DFT.c:
        line.2554
130 | 6||||         |            | __ipap_fnjoint:openmx_common
        .c:line.358
131 | 5||||    0.0% |   0.000003 |Save_DOS_Col:Cluster_DFT.c:
        line.2560
132 | 6||||         |            | __ipap_fnjoint:openmx_common
        .c:line.358
133 | 5||||    0.0% |   0.000036 |Save_DOS_Col:Cluster_DFT.c:
        line.2594
134 ||||||---------------------------
135 | 6|||||    0.0% |   0.000008 |Overlap_Cluster:
        Overlap_Cluster.c:line.25
136 | 6|||||    0.0% |   0.000006 |Overlap_Cluster:
        Overlap_Cluster.c:line.30
137 |||||||--------------------------
138 | 7||||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
139 | 7||||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
140 | 7||||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
141 | 7||||||    0.0% |   0.000002 |MPI_Barrier(sync):...:line
        .0
142 |||||||==========================
143 | 6|||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.63
144 |||||||--------------------------
145 | 7||||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
146 | 7||||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
        .0
147 |||||||==========================
148 | 6|||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.74
149 |||||||--------------------------
150 | 7||||||    0.0% |   0.000002 |MPI_Bcast:...:line.0
151 | 7||||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
152 |||||||==========================
153 | 6|||||    0.0% |   0.000003 |Overlap_Cluster:
        Overlap_Cluster.c:line.86
154 |||||||--------------------------
155 | 7||||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
156 | 7||||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
        .0
157 |||||||==========================
158 | 6|||||    0.0% |   0.000003 |Overlap_Cluster:
```

```
    Overlap_Cluster.c:line.95
159 |||||||--------------------------
160 7|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
161 7|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
162 ||||||============================
163 6|||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.106
164 |||||||--------------------------
165 7|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
166 7|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
    .0
167 |||||||============================
168 6|||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.109
169 |||||||--------------------------
170 7|||||    0.0% |   0.000001 |MPI_Bcast:...:line.0
171 7|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
172 |||||||============================
173 6|||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.143
174 |||||||--------------------------
175 7|||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
176 7|||||    0.0% |   0.000001 |MPI_Barrier(sync):...:line
    .0
177 |||||||============================
178 6|||||    0.0% |   0.000003 |Overlap_Cluster:
    Overlap_Cluster.c:line.149
179 |||||||--------------------------
180 7|||||    0.0% |   0.000002 |MPI_Bcast:...:line.0
181 7|||||    0.0% |   0.000001 |MPI_Bcast(sync):...:line.0
182 ||||||============================
183 5||||    0.0% |   0.000065 |Save_DOS_Col:Cluster_DFT.c:
    line.2623
184 |||||============================
185 4|||    0.0% |   0.000005 |__ipas_Cluster_collinear:
    Cluster_DFT.c:line.1364
186 5|||         |            | MPI_Comm_free:...:line.0
187 4|||    0.0% |   0.000005 |__ipas_Cluster_collinear:
    Cluster_DFT.c:line.1367
188 |||||--------------------------
189 5||||    0.0% |   0.000001 |MPI_Barrier:...:line.0
190 5||||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
191 5||||    0.0% |   0.000002 |dtime:dtime.c:line.15
192 |||||============================
```

- RestartFileDFT() (in RestartFileDFT.c): a subroutine to make the .rst restart file.
  - double *****H; Kohn-Sham matrix elements of basis orbitals.

size: H[SpinP_switch+1] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].

- double *****CntH; Kohn-Sham matrix elements of contracted basis orbitals. size: CntH[SpinP_switch+1] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_CNO[Cwan]] [Spe_Total_CNO[Hwan]].
- Output_HKS()

Listing 2.20: DFT: RestartFileDFT()

```
1  ||    0.1% |   0.080956 |DFT:DFT.c:line.1768
2  |||-------------------------------
3  3||    0.1% |   0.080928 |__ipap_RestartFileDFT:
       RestartFileDFT.c:line.43
4  3||    0.0% |   0.000003 |__ipap_RestartFileDFT:
       RestartFileDFT.c:line.50
5  ||||------------------------------
6  4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
8  ||||==============================
9  3||    0.0% |   0.000003 |__ipap_RestartFileDFT:
       RestartFileDFT.c:line.60
10 ||||------------------------------
11 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
12 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
13 ||||==============================
14 3||    0.0% |   0.000007 |__ipap_RestartFileDFT:
       RestartFileDFT.c:line.62
15 ||||------------------------------
16 4|||    0.0% |   0.000003 |__ipap_Output_HKS:
       RestartFileDFT.c:line.543
17 |||||-----------------------------
18 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
19 5||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
20 |||||============================
21 4|||    0.0% |   0.000004 |__ipap_Output_HKS:
       RestartFileDFT.c:line.561
22 |||||-----------------------------
23 5||||    0.0% |   0.000002 |MPI_Barrier:...:line.0
24 5||||    0.0% |   0.000003 |MPI_Barrier(sync):...:line.0
25 ||||==============================
26 3||    0.0% |   0.000007 |__ipap_RestartFileDFT:
       RestartFileDFT.c:line.65
27 ||||------------------------------
28 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
29 4|||    0.0% |   0.000003 |MPI_Barrier(sync):...:line.0
30 4|||    0.0% |   0.000003 |Output_Charge_Density:
       RestartFileDFT.c:line.687
31 |||||-----------------------------
32 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
```

```
33 | 5||||     0.0% |    0.000001 |MPI_Comm_size:...:line.0
34 | 3||     0.0% |    0.000002 |MPI_Barrier:...:line.0
35 | 3||     0.0% |    0.000006 |MPI_Barrier(sync):...:line.0
36 |||=================================
```

- Set_Density_Grid() (in Set_Density_Grid.c): a subroutine to calculate a charge density on grid by one-particle wave functions.
  - double **Density_Grid; electron densities on grids. size: Density_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
  - Type_Orbs_Grid ***COrbs_Grid; values of contrated basis orbitals on grids. size: COrbs_Grid[Matomnum+MatomnumF+1] [Spe_Total_NO[Cwan]] [GridN_Atom[Gc_AN]]. Type_Orbs_Grid is defined as float.

Listing 2.21: DFT: Set_Density_Grid()

```
 1 ||     0.0% |    0.002218 |DFT:DFT.c:line.1783
 2 |||-------------------------------
 3 | 3||     0.0% |    0.001174 |Set_Density_Grid:
       Set_Density_Grid.c:line.37
 4 | 3||     0.0% |    0.000006 |Set_Density_Grid:
       Set_Density_Grid.c:line.80
 5 ||||------------------------------
 6 | 4|||     0.0% |    0.000002 |MPI_Comm_rank:...:line.0
 7 | 4|||     0.0% |    0.000002 |MPI_Comm_size:...:line.0
 8 | 4|||     0.0% |    0.000003 |dtime:dtime.c:line.15
 9 ||||==============================
10 | 3||     0.0% |    0.000002 |Set_Density_Grid:
       Set_Density_Grid.c:line.274
11 | 4||          |             | dtime:dtime.c:line.15
12 | 3||     0.0% |    0.001001 |Set_Density_Grid:
       Set_Density_Grid.c:line.289
13 | 3||     0.0% |    0.000004 |Set_Density_Grid:
       Set_Density_Grid.c:line.317
14 | 4||          |             | dtime:dtime.c:line.15
15 | 3||     0.0% |    0.000005 |Set_Density_Grid:
       Set_Density_Grid.c:line.481
16 | 4||          |             | dtime:dtime.c:line.15
17 | 3||     0.0% |    0.000001 |Set_Density_Grid:
       Set_Density_Grid.c:line.514
18 | 4||          |             | dtime:dtime.c:line.15
19 | 3||     0.0% |    0.000011 |Set_Density_Grid:
       Set_Density_Grid.c:line.570
20 ||||------------------------------
21 | 4|||     0.0% |    0.000009 |MPI_Allreduce:...:line.0
22 | 4|||     0.0% |    0.000002 |MPI_Allreduce(sync):...:line.0
23 ||||==============================
```

```
24 | 3||    0.0% |   0.000002 |Set_Density_Grid:
       Set_Density_Grid.c:line.637
25 | 4||         |            | dtime:dtime.c:line.15
26 | 3||    0.0% |   0.000003 |Set_Density_Grid:
       Set_Density_Grid.c:line.653
27 | 4||         |            | dtime:dtime.c:line.15
28 | 3||    0.0% |   0.000005 |Set_Density_Grid:
       Set_Density_Grid.c:line.666
29 | 4||         |            | dtime:dtime.c:line.15
30 | 3||    0.0% |   0.000001 |Set_Density_Grid:
       Set_Density_Grid.c:line.674
31 | 4||         |            | dtime:dtime.c:line.15
32 | 3||    0.0% |   0.000002 |Set_Density_Grid:
       Set_Density_Grid.c:line.822
33 | 4||         |            | dtime:dtime.c:line.15
34 |=============================================
```

- Force() (in Force.c): a subroutine to calculate force on atoms.
  - double **Gxyz; atomic global coordinates, velocities, and gradients of the total energy with respect to the atomic coordinates. size: Gxyz[atomnum+1][YOUSO26].
  - double *****H0; matrix elements of basis orbitals for T+VNL. size: H0[4] [Matomnum+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - double ******DS_NL; overlap matrix elements between projectors, of non-local potentials, and basis orbitals. size: DS_NL[SO_switch+1] [4] [Matomnum+MatomnumF+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_VPS_Pro[Hwan]+2].
  - double *****OLP; overlap matrix elements of basis orbitals. size: OLP[4] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]].
  - Set_XC_Grid() (in Set_XC_Grid.c):
  - XC_Ceperly_Alder() in (XC_Ceperly_Alder.c): a subroutine to calculate an exchange- correlation potential for a given density "den" by the local density approximation.
  - double **Vxc_Grid; exchange-correlation potentials on grids. size: Vxc_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3].
  - Dr_AtomicDenF() (in Dr_AtomicDenF.c): a subroutine to calculate the derivative, with respect to R, of atomic charge density of one atom specified "Gensi".
  - dHNL(): to calculate the contributions from non-local parts.

- dampingF() (in dampingF.c): a subroutine to calculate a damping function which is used for calculation of nonlocal projector matrices.
- deri_dampingF() (in deri_dampingF.c): a subroutine to calculate the derivative of a damping function which is used for calculation of nonlocal projector matrices.
- Force3(): to calculate the 3rd contribution of the force; dn/dx * (VNA + dVH + Vxc) or dn/dx * (dVH + Vxc).
- Get_dOrbitals() (in Get_dOrbital.c): a subroutine to calculate derivatives of basis orbitals.
- Force4B(): to calculate the 4th contribution of the force from separable VNA projectors.

Listing 2.22: DFT: Force()

```
1  ||    0.9% |   0.797156 |DFT:DFT.c:line.1867
2  |||-------------------------------
3  3||    0.0% |   0.000148 |Force:Force.c:line.95
4  3||    0.0% |   0.000007 |Force:Force.c:line.137
5  ||||-----------------------------
6  4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
7  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
8  4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
9  4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
10 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
11 ||||=============================
12 3||    0.0% |   0.000966 |Force:Force.c:line.270
13 4||         |            | PrintMemory:PrintMemory.c:line
       .19
14 3||    0.3% |   0.294952 |Force:Force.c:line.689
15 ||||-----------------------------
16 4|||    0.0% |   0.000003 |dtime:dtime.c:line.15
17 4|||    0.0% |   0.000005 |Set_XC_Grid:Set_XC_Grid.c:line
       .29
18 4|||    0.0% |   0.000003 |Set_XC_Grid:Set_XC_Grid.c:line
       .72
19 |||||---------------------------
20 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
21 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
22 |||||===========================
23 4|||    0.0% |   0.030587 |Set_XC_Grid:Set_XC_Grid.c:line
       .290
24 4|||    0.3% |   0.264354 |Set_XC_Grid:Set_XC_Grid.c:line
       .322
25 5|||         |            | XC_Ceperly_Alder:
       XC_Ceperly_Alder.c:line.20
26 ||||=============================
```

```
27 | 3||    0.0% |   0.037489 |Force:Force.c:line.704
28 | 3||    0.0% |   0.000005 |Force:Force.c:line.712
29 | 4||         |            | dtime:dtime.c:line.15
30 | 3||    0.1% |   0.049398 |Force:Force.c:line.723
31 | 4||         |            | Get_Grid_XYZ:openmx_common.c:
   |     line.866
32 | 3||    0.1% |   0.067210 |Force:Force.c:line.744
33 | 4||         |            | Dr_AtomicDenF:Dr_AtomicDenF.c:
   |     line.19
34 | 3||    0.1% |   0.054730 |Force:Force.c:line.761
35 | 4||         |            | Dr_AtomicPCCF:Dr_AtomicPCCF.c:
   |     line.19
36 | 3||    0.0% |   0.000005 |Force:Force.c:line.792
37 | 4||         |            | dtime:dtime.c:line.15
38 | 3||    0.0% |   0.000002 |Force:Force.c:line.798
39 | 4||         |            | dtime:dtime.c:line.15
40 | 3||    0.0% |   0.000006 |Force:Force.c:line.857
41 |||+-----------------------------
42 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
43 | 4|||    0.0% |   0.000004 |MPI_Barrier(sync):...:line.0
44 |||=============================
45 | 3||    0.0% |   0.000004 |Force:Force.c:line.885
46 |||+-----------------------------
47 | 4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
48 | 4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
49 | 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
50 |||=============================
51 | 3||    0.0% |   0.000206 |Force:Force.c:line.900
52 ||==============================
53 | 3||    0.0% |   0.000005 |Force:Force.c:line.1001
54 | 4||         |            | dtime:dtime.c:line.15
55 | 3||    0.0% |   0.000072 |Force:Force.c:line.1037
56 | 4||         |            | Complex:openmx_common.c:line
   |     .91
57 | 3||    0.0% |   0.000017 |Force:Force.c:line.1052
58 |||+-----------------------------
59 | 4|||    0.0% |   0.000012 |dHNL:Force.c:line.3726
60 | 5|||         |            | dampingF:dampingF.c:line.21
61 | 4|||    0.0% |   0.000005 |dHNL:Force.c:line.4578
62 | 5|||         |            | deri_dampingF:deri_dampingF.c
   |     :line.22
63 |||=============================
64 | 3||    0.0% |   0.000004 |Force:Force.c:line.1341
65 | 4||         |            | dtime:dtime.c:line.15
66 | 3||    0.0% |   0.000003 |Force:Force.c:line.1445
67 | 4||         |            | dtime:dtime.c:line.15
68 | 3||    0.3% |   0.290785 |Force:Force.c:line.1464
69 |||+-----------------------------
70 | 4|||    0.0% |   0.000004 |Force3:Force.c:line.2177
```

```
71 |||||----------------------------
72  5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
73  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
74 |||||============================
75  4|||    0.0% |   0.020396 |Force3:Force.c:line.2190
76  4|||    0.1% |   0.050627 |Force3:Force.c:line.2233
77  5|||         |            | Get_Grid_XYZ:openmx_common.c:
       line.866
78  4|||    0.2% |   0.219753 |Force3:Force.c:line.2248
79 |||||----------------------------
80  5||||    0.2% |   0.163663 |Get_dOrbitals:Get_dOrbitals.c
       :line.19
81  5||||    0.1% |   0.056090 |Get_dOrbitals:Get_dOrbitals.c
       :line.75
82  6||||         |            | xyz2spherical:xyz2spherical.
       c:line.20
83 |||||============================
84  4|||    0.0% |   0.000005 |dtime:dtime.c:line.15
85 ||||===============================
86  3||    0.0% |   0.001065 |Force:Force.c:line.1488
87 ||||-------------------------------
88  4|||    0.0% |   0.000006 |Force4B:Force.c:line.2640
89 |||||----------------------------
90  5||||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
91  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
92  5||||    0.0% |   0.000002 |dtime:dtime.c:line.15
93 |||||============================
94  4|||    0.0% |   0.000002 |Force4B:Force.c:line.2735
95  5|||         |            | dtime:dtime.c:line.15
96  4|||    0.0% |   0.000005 |Force4B:Force.c:line.2783
97  5|||         |            | dtime:dtime.c:line.15
98  4|||    0.0% |   0.000279 |Force4B:Force.c:line.2793
99  4|||    0.0% |   0.000021 |Force4B:Force.c:line.2844
100 |||||----------------------------
101  5||||    0.0% |   0.000004 |MPI_Barrier:...:line.0
102  5||||    0.0% |   0.000007 |MPI_Barrier(sync):...:line.0
103  5||||    0.0% |   0.000010 |dtime:dtime.c:line.15
104 |||||============================
105  4|||    0.0% |   0.000008 |Force4B:Force.c:line.3161
106  5|||         |            | dtime:dtime.c:line.15
107  4|||    0.0% |   0.000214 |Force4B:Force.c:line.3176
108  4|||    0.0% |   0.000011 |Force4B:Force.c:line.3191
109  5|||         |            | dtime:dtime.c:line.15
110  4|||    0.0% |   0.000033 |Force4B:Force.c:line.3216
111 |||||----------------------------
112  5||||    0.0% |   0.000022 |dHVNA:Force.c:line.4710
113  6||||         |            | dampingF:dampingF.c:line.21
114  5||||    0.0% |   0.000011 |dHVNA:Force.c:line.5018
115  6||||         |            | deri_dampingF:deri_dampingF.
```

```
    c:line.22
|||||==============================
 4|||    0.0%  |   0.000009  |Force4B:Force.c:line.3254
 5|||          |             |  dtime:dtime.c:line.15
 4|||    0.0%  |   0.000017  |Force4B:Force.c:line.3275
|||||------------------------------
 5||||   0.0%  |   0.000004  |MPI_Barrier:...:line.0
 5||||   0.0%  |   0.000005  |MPI_Barrier(sync):...:line.0
 5||||   0.0%  |   0.000008  |dtime:dtime.c:line.15
|||||==============================
 4|||    0.0%  |   0.000016  |Force4B:Force.c:line.3296
 5|||          |             |  dtime:dtime.c:line.15
 4|||    0.0%  |   0.000018  |Force4B:Force.c:line.3496
 5|||          |             |  dtime:dtime.c:line.15
 4|||    0.0%  |   0.000017  |Force4B:Force.c:line.3509
 4|||    0.0%  |   0.000341  |Force4B:Force.c:line.3537
 4|||    0.0%  |   0.000046  |Force4B:Force.c:line.3577
|||||------------------------------
 5||||   0.0%  |   0.000035  |dHVNA:Force.c:line.4710
 6||||         |             |  dampingF:dampingF.c:line.21
 5||||   0.0%  |   0.000011  |dHVNA:Force.c:line.5018
 6||||         |             |  deri_dampingF:deri_dampingF.
    c:line.22
|||||==============================
 4|||    0.0%  |   0.000010  |Force4B:Force.c:line.3633
 5|||          |             |  dtime:dtime.c:line.15
 4|||    0.0%  |   0.000008  |Force4B:Force.c:line.3652
 5|||          |             |  dtime:dtime.c:line.15
 4|||    0.0%  |   0.000004  |Force4B:Force.c:line.3657
 5|||          |             |  dtime:dtime.c:line.15
||||============================
 3||    0.0%  |   0.000003  |Force:Force.c:line.1491
 4||          |             |  dtime:dtime.c:line.15
 3||    0.0%  |   0.000059  |Force:Force.c:line.1515
 3||    0.0%  |   0.000004  |Force:Force.c:line.1523
 4||          |             |  dtime:dtime.c:line.15
 3||    0.0%  |   0.000003  |Force:Force.c:line.1562
 4||          |             |  dtime:dtime.c:line.15
 3||    0.0%  |   0.000002  |Force:Force.c:line.1570
 4||          |             |  dtime:dtime.c:line.15
 3||    0.0%  |   0.000006  |Force:Force.c:line.2149
||||----------------------------
 4|||    0.0%  |   0.000001  |MPI_Barrier:...:line.0
 4|||    0.0%  |   0.000002  |MPI_Barrier(sync):...:line.0
 4|||    0.0%  |   0.000003  |dtime:dtime.c:line.15
||||============================
```

- Total_Energy() (in Total_Energy.c): a subroutine to calculate the total energy.

- double **Gxyz; atomic global coordinates, velocities, and gradients of the total energy with respect to the atomic coordinates. size: Gxyz[atomnum+1][YOUSO26].
- Calc_Ecore(): to calculate the core-core repulsion energy (the 6th contribution of force).
- Calc_EH0(): $EH0 = -1/2 \int n^a(r) V_H^a dr$.
- AtomicDenF() (in AtomicDenF.c): a subroutine to calculate the atomic charge density of one atom specified "Gensi" at R.
- EH0_TwoCenter_at_Cutoff()
- VH_AtomF() (in VH_AtomF.c): a subroutine to calculate the Hartree potential potential of a free atom specified by "Gensi".
- EH0_TwoCenter()
- Dr_VH_AtomF() (in Dr_VH_AtomF.c): a subroutine to calculate the derivative, with respect to R, of neutral atom potential of one atom specified by "Gensi".
- Calc_Ekin(): to calculate the kinetic energy.
- Calc_Ena(): to calculate the neutral atom potential energy.
- Calc_Enl(): to calculate the non-local pseudo potential energy.
- Calc_EXC_EH1(): to calculate $EXC = \sum_\sigma n_\sigma(\epsilon_{xc} - \mu_{xc,\sigma})$ and $EH1 = -1/2 \int n(r) + n^a(r) \delta V_H dr$.
- Set_XC_Grid()
- XC_Ceperly_Alder()
- AtomicPCCF() (in AtomicPCCF.c): a subroutine to calculate the atomic partial core charge density of one atom specified "Gensi" at R.
- Dr_AtomicDenF() (in Dr_AtomicDenF.c): a subroutine to calculate the derivative, with respect to R, of atomic charge density of one atom specified "Gensi".
- Dr_AtomicPCCF() (in Dr_AtomicPCCF.c): a subroutine to calculate the derivative, with respect to R, of partial core charge density of one atom specified "Gensi".

Listing 2.23: DFT: Total_Energy()

```
1 ||    6.7% |   6.217427 |DFT:DFT.c:line.1885
2 |||-----------------------------
3 3||    0.0% |   0.016337 |__ipas_Total_Energy:
      Total_Energy.c:line.51
4 3||    0.0% |   0.000005 |__ipas_Total_Energy:
      Total_Energy.c:line.59
5 ||||-----------------------------
```

```
 6 | 4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
 7 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
 8 | 4|||    0.0% |   0.000002 |dtime:dtime.c:line.15
 9 | ||||==========================================
10 | 3||    0.5% |   0.494115 |__ipas_Total_Energy:
   |     Total_Energy.c:line.83
11 | ||||------------------------------
12 | 4|||    0.0% |   0.000003 |Calc_Ecore:Total_Energy.c:line
   |     .708
13 | |||||------------------------------
14 | 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
15 | 5||||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
16 | |||||==================================
17 | 4|||    0.0% |   0.000003 |Calc_Ecore:Total_Energy.c:line
   |     .717
18 | 4|||    0.0% |   0.000072 |Calc_Ecore:Total_Energy.c:line
   |     .726
19 | 4|||    0.0% |   0.000004 |Calc_Ecore:Total_Energy.c:line
   |     .734
20 | 5|||         |            | dtime:dtime.c:line.15
21 | 4|||    0.0% |   0.000003 |Calc_Ecore:Total_Energy.c:line
   |     .781
22 | 5|||         |            | dtime:dtime.c:line.15
23 | 4|||    0.0% |   0.000010 |Calc_Ecore:Total_Energy.c:line
   |     .790
24 | |||||------------------------------
25 | 5||||    0.0% |   0.000008 |MPI_Allreduce:...:line.0
26 | 5||||    0.0% |   0.000002 |MPI_Allreduce(sync):...:line
   |     .0
27 | |||||==================================
28 | 4|||    0.0% |   0.000012 |dtime:dtime.c:line.15
29 | ||==========================================
30 | 4|||    0.0% |   0.000003 |Calc_EH0:Total_Energy.c:line
   |     .832
31 | |||||------------------------------
32 | 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
33 | 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
34 | |||||==================================
35 | 4|||    0.0% |   0.000001 |Calc_EH0:Total_Energy.c:line
   |     .853
36 | 5|||         |            | dtime:dtime.c:line.15
37 | 4|||    0.0% |   0.000003 |Calc_EH0:Total_Energy.c:line
   |     .885
38 | 5|||         |            | Allocate_Arrays:
   |     Allocate_Arrays.c:line.7
39 | 4|||    0.0% |   0.003704 |Calc_EH0:Total_Energy.c:line
   |     .895
40 | 4|||    0.0% |   0.027863 |Calc_EH0:Total_Energy.c:line
   |     .931
```

```
41 | 5|||          |              | AtomicDenF:AtomicDenF.c:line
       .18
42 | 4|||    0.0% |   0.000002 |Calc_EH0:Total_Energy.c:line
       .962
43 | 5|||          |              | dtime:dtime.c:line.15
44 | 4|||    0.0% |   0.043304 |Calc_EH0:Total_Energy.c:line
       .980
45 | |||||---------------------------
46 | 5||||    0.0% |   0.000004 |
       __ipas_EH0_TwoCenter_at_Cutoff:Total_Energy.c:line
       .2185
47 | 5||||    0.0% |   0.003954 |
       __ipas_EH0_TwoCenter_at_Cutoff:Total_Energy.c:line
       .2197
48 | 5||||    0.0% |   0.039347 |
       __ipas_EH0_TwoCenter_at_Cutoff:Total_Energy.c:line
       .2204
49 | 6||||          |              | VH_AtomF:VH_AtomF.c:line.18
50 | |||||===============================
51 | 4|||    0.0% |   0.000003 |Calc_EH0:Total_Energy.c:line
       .1005
52 | 5|||          |              | dtime:dtime.c:line.15
53 | 4|||    0.0% |   0.000004 |Calc_EH0:Total_Energy.c:line
       .1015
54 | 4|||    0.1% |   0.058230 |Calc_EH0:Total_Energy.c:line
       .1024
55 | 4|||    0.0% |   0.000005 |Calc_EH0:Total_Energy.c:line
       .1032
56 | 5|||          |              | dtime:dtime.c:line.15
57 | 4|||    0.2% |   0.173608 |Calc_EH0:Total_Energy.c:line
       .1047
58 | |||||---------------------------
59 | 5||||    0.1% |   0.120548 |EH0_TwoCenter:Total_Energy.c:
       line.2107
60 | 6||||          |              | VH_AtomF:VH_AtomF.c:line.18
61 | 5||||    0.1% |   0.053060 |EH0_TwoCenter:Total_Energy.c:
       line.2123
62 | 6||||          |              | Dr_VH_AtomF:Dr_VH_AtomF.c:
       line.19
63 | |||||===============================
64 | 4|||    0.2% |   0.187241 |Calc_EH0:Total_Energy.c:line
       .1057
65 | |||||---------------------------
66 | 5||||    0.1% |   0.134068 |EH0_TwoCenter:Total_Energy.c:
       line.2107
67 | 6||||          |              | VH_AtomF:VH_AtomF.c:line.18
68 | 5||||    0.1% |   0.053173 |EH0_TwoCenter:Total_Energy.c:
       line.2123
69 | 6||||          |              | Dr_VH_AtomF:Dr_VH_AtomF.c:
```

```
    line.19
70  |||||==================================
71  4|||    0.0%  |   0.000005  |Calc_EH0:Total_Energy.c:line
    .1064
72  5|||          |             | dtime:dtime.c:line.15
73  4|||    0.0%  |   0.000016  |Calc_EH0:Total_Energy.c:line
    .1074
74  |||||--------------------------
75  5||||    0.0%  |   0.000010  |MPI_Allreduce:...:line.0
76  5||||    0.0%  |   0.000004  |MPI_Allreduce(sync):...:line
    .0
77  5||||    0.0%  |   0.000002  |dtime:dtime.c:line.15
78  |||||==================================
79  4|||    0.0%  |   0.000013  |Calc_EH0:Total_Energy.c:line
    .1116
80  |||||--------------------------
81  5||||    0.0%  |   0.000010  |MPI_Bcast:...:line.0
82  5||||    0.0%  |   0.000003  |MPI_Bcast(sync):...:line.0
83  |||||==================================
84  3||    0.0%  |   0.000142  |__ipas_Total_Energy:
    Total_Energy.c:line.122
85  ||||-------------------------
86  4|||    0.0%  |   0.000004  |Calc_Ekin:Total_Energy.c:line
    .226
87  |||||--------------------------
88  5||||    0.0%  |   0.000002  |MPI_Comm_rank:...:line.0
89  5||||    0.0%  |   0.000002  |MPI_Comm_size:...:line.0
90  |||||==================================
91  4|||    0.0%  |   0.000004  |Calc_Ekin:Total_Energy.c:line
    .231
92  4|||    0.0%  |   0.000117  |Calc_Ekin:Total_Energy.c:line
    .244
93  4|||    0.0%  |   0.000007  |Calc_Ekin:Total_Energy.c:line
    .254
94  5|||          |             | dtime:dtime.c:line.15
95  4|||    0.0%  |   0.000006  |Calc_Ekin:Total_Energy.c:line
    .290
96  5|||          |             | dtime:dtime.c:line.15
97  4|||    0.0%  |   0.000004  |Calc_Ekin:Total_Energy.c:line
    .347
98  |||||--------------------------
99  5||||    0.0%  |   0.000003  |MPI_Allreduce:...:line.0
100 5||||    0.0%  |   0.000002  |MPI_Allreduce(sync):...:line
    .0
101 ||||==================================
102 3||    0.0%  |   0.000003  |__ipas_Total_Energy:
    Total_Energy.c:line.124
103 4||          |             | dtime:dtime.c:line.15
104 3||    0.0%  |   0.000077  |__ipas_Total_Energy:
```

```
    Total_Energy.c:line.135
|||+-------------------------------
4|||    0.0%  |   0.000003  |Calc_Ena:Total_Energy.c:line
    .380
|||||-----------------------------
5||||    0.0%  |   0.000001  |MPI_Comm_rank:...:line.0
5||||    0.0%  |   0.000001  |MPI_Comm_size:...:line.0
|||||=============================
4|||    0.0%  |   0.000003  |Calc_Ena:Total_Energy.c:line
    .385
4|||    0.0%  |   0.000056  |Calc_Ena:Total_Energy.c:line
    .403
4|||    0.0%  |   0.000007  |Calc_Ena:Total_Energy.c:line
    .413
5|||          |             | dtime:dtime.c:line.15
4|||    0.0%  |   0.000006  |Calc_Ena:Total_Energy.c:line
    .449
5|||          |             | dtime:dtime.c:line.15
4|||    0.0%  |   0.000004  |Calc_Ena:Total_Energy.c:line
    .507
|||||-----------------------------
5||||    0.0%  |   0.000002  |MPI_Allreduce:...:line.0
5||||    0.0%  |   0.000002  |MPI_Allreduce(sync):...:line
    .0
|||+================================
3||    0.0%  |   0.000003  |__ipas_Total_Energy:
    Total_Energy.c:line.137
4||          |             | dtime:dtime.c:line.15
3||    0.0%  |   0.000071  |__ipas_Total_Energy:
    Total_Energy.c:line.148
|||+-------------------------------
4|||    0.0%  |   0.000003  |Calc_Enl:Total_Energy.c:line
    .540
|||||-----------------------------
5||||    0.0%  |   0.000001  |MPI_Comm_rank:...:line.0
5||||    0.0%  |   0.000001  |MPI_Comm_size:...:line.0
|||||=============================
4|||    0.0%  |   0.000003  |Calc_Enl:Total_Energy.c:line
    .545
4|||    0.0%  |   0.000050  |Calc_Enl:Total_Energy.c:line
    .563
4|||    0.0%  |   0.000007  |Calc_Enl:Total_Energy.c:line
    .573
5|||          |             | dtime:dtime.c:line.15
4|||    0.0%  |   0.000005  |Calc_Enl:Total_Energy.c:line
    .608
5|||          |             | dtime:dtime.c:line.15
4|||    0.0%  |   0.000004  |Calc_Enl:Total_Energy.c:line
    .674
```

```
138 |||||----------------------------
139  5||||    0.0%  |   0.000002  |MPI_Allreduce:...:line.0
140  5||||    0.0%  |   0.000002  |MPI_Allreduce(sync):...:line
         .0
141 ||||================================
142  3||    6.1%  |   5.706673  |__ipas_Total_Energy:
         Total_Energy.c:line.150
143 ||||----------------------------
144  4|||    0.7%  |   0.606127  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1161
145 |||||----------------------------
146  5||||    0.0%  |   0.000001  |MPI_Comm_rank:...:line.0
147  5||||    0.0%  |   0.000001  |MPI_Comm_size:...:line.0
148  5||||    0.0%  |   0.000012  |Set_XC_Grid:Set_XC_Grid.c:
         line.29
149  5||||    0.0%  |   0.000007  |Set_XC_Grid:Set_XC_Grid.c:
         line.72
150 ||||||----------------------------
151  6|||||    0.0%  |   0.000003  |MPI_Comm_rank:...:line.0
152  6|||||    0.0%  |   0.000004  |MPI_Comm_size:...:line.0
153 |||||==============================
154  5||||    0.1%  |   0.060357  |Set_XC_Grid:Set_XC_Grid.c:
         line.290
155  5||||    0.6%  |   0.545748  |Set_XC_Grid:Set_XC_Grid.c:
         line.322
156  6||||          |             | XC_Ceperly_Alder:
         XC_Ceperly_Alder.c:line.20
157  4|||    0.0%  |   0.000011  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1471
158  4|||    0.0%  |   0.002135  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1480
159  4|||    0.0%  |   0.000006  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1575
160  4|||    0.0%  |   0.002357  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1587
161  4|||    0.0%  |   0.000006  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1621
162  4|||    0.6%  |   0.517802  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1663
163  4|||    2.4%  |   2.268153  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1699
164 |||||----------------------------
165  5||||    1.4%  |   1.335328  |AtomicDenF:AtomicDenF.c:line
         .18
166  5||||    1.0%  |   0.932826  |AtomicPCCF:AtomicPCCF.c:line
         .18
167 |||||==============================
168  4|||    1.2%  |   1.132379  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1721
```

```
169 |||||----------------------------
170  5||||    0.7%  |   0.647810  |Dr_AtomicDenF:Dr_AtomicDenF.c
         :line.19
171  5||||    0.5%  |   0.484569  |Dr_AtomicPCCF:Dr_AtomicPCCF.c
         :line.19
172 |||||============================
173  4|||    1.3%  |   1.165313  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1727
174  5|||          |             | XC_Ceperly_Alder:
         XC_Ceperly_Alder.c:line.20
175  4|||    0.0%  |   0.000013  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1805
176 |||||----------------------------
177  5||||    0.0%  |   0.000006  |MPI_Bcast:...:line.0
178  5||||    0.0%  |   0.000006  |MPI_Bcast(sync):...:line.0
179 |||||============================
180  4|||    0.0%  |   0.000017  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1813
181 |||||----------------------------
182  5||||    0.0%  |   0.000013  |MPI_Allreduce:...:line.0
183  5||||    0.0%  |   0.000001  |MPI_Allreduce(sync):...:line
         .0
184  5||||    0.0%  |   0.000001  |MPI_Barrier:...:line.0
185  5||||    0.0%  |   0.000001  |MPI_Barrier(sync):...:line.0
186 |||||============================
187  4|||    0.0%  |   0.000003  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1823
188 |||||----------------------------
189  5||||    0.0%  |   0.000002  |MPI_Allreduce:...:line.0
190  5||||    0.0%  |   0.000001  |MPI_Allreduce(sync):...:line
         .0
191 |||||============================
192  4|||    0.0%  |   0.000018  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1855
193  4|||    0.0%  |   0.012289  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1877
194  4|||    0.0%  |   0.000024  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1921
195 |||||----------------------------
196  5||||    0.0%  |   0.000013  |MPI_Allreduce:...:line.0
197  5||||    0.0%  |   0.000011  |MPI_Allreduce(sync):...:line
         .0
198 |||||============================
199  4|||    0.0%  |   0.000008  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.1962
200 |||||----------------------------
201  5||||    0.0%  |   0.000005  |MPI_Allreduce:...:line.0
202  5||||    0.0%  |   0.000004  |MPI_Allreduce(sync):...:line
         .0
```

```
203 |||||=================================
204  4|||    0.0%  |   0.000002  |__ipas_Calc_EXC_EH1:
         Total_Energy.c:line.2024
205  5|||          |             | __ipap_fnjoint:openmx_common.
         c:line.358
206  4|||    0.0%  |   0.000009  |dtime:dtime.c:line.15
207 ||||===============================
208  3||    0.0%  |   0.000001  |__ipas_Total_Energy:
         Total_Energy.c:line.193
209  4||          |             | dtime:dtime.c:line.15
```

- outputfile1() (in outputfile1.c)

Listing 2.24: DFT: outputfile1()

```
1  ||    0.0%  |   0.000002  |DFT:DFT.c:line.1911
2  3|          |             | dtime:dtime.c:line.15
3  ||    0.0%  |   0.000289  |DFT:DFT.c:line.1990
4  |||--------------------------------
5  3||    0.0%  |   0.000287  |__ipas_outputfile1:outputfile1.c:
       line.16
6  3||    0.0%  |   0.000002  |__ipas_outputfile1:outputfile1.c:
       line.23
7  4||          |             | MPI_Comm_rank:...:line.0
8  |||================================
9  ||    0.0%  |   0.000006  |DFT:DFT.c:line.2388
10 |||--------------------------------
11 3||    0.0%  |   0.000002  |MPI_Barrier:...:line.0
12 3||    0.0%  |   0.000004  |MPI_Barrier(sync):...:line.0
13 |||================================
```

2.2.3 iterout and MD_pac

- iterout() (in iterout.c): a subroutine to output xyz-coordinates at each MD step to filename.md and filename.md2.
- MD_pac() (in MD_pac.c): a subroutine to perform molecular dynamics simulations and geometry optimization.
- Make_InputFile_with_FinalCoord() (in Make_InputFile_with_FinalCoord.c): a subroutine to make an input file with the final coordinate of the system.
- Steepest_Descent():
- iterout_md() (in iterout_md.c): to write information to the .ene file.

Listing 2.25: DFT: iterout() and MD_pac()

```
1  |    0.0% |   0.020461 |main:openmx.c:line.475
2  |         |            |  iterout:iterout.c:line.18
3  |    0.0% |   0.018146 |main:openmx.c:line.479
4  ||-----------------------------------
5  ||   0.0% |   0.001226 |MD_pac:MD_pac.c:line.53
6  ||   0.0% |   0.000002 |MD_pac:MD_pac.c:line.58
7  3|         |            |  dtime:dtime.c:line.15
8  ||   0.0% |   0.000003 |MD_pac:MD_pac.c:line.63
9  |||----------------------------------
10 3||   0.0% |   0.000001 |MPI_Comm_rank:...:line.0
11 3||   0.0% |   0.000002 |MPI_Comm_size:...:line.0
12 |||==================================
13 ||   0.0% |   0.001476 |MD_pac:MD_pac.c:line.74
14 |||----------------------------------
15 3||   0.0% |   0.001282 |Make_InputFile_with_FinalCoord:
       Make_InputFile_with_FinalCoord.c:line.40
16 3||   0.0% |   0.000193 |Make_InputFile_with_FinalCoord:
       Make_InputFile_with_FinalCoord.c:line.43
17 ||||--------------------------------
18 4|||   0.0% |   0.000003 |
       Make_InputFile_with_FinalCoord_Normal:
       Make_InputFile_with_FinalCoord.c:line.106
19 5|||        |            | string_tolower:openmx_common.c:
       line.893
20 4|||   0.0% |   0.000003 |
       Make_InputFile_with_FinalCoord_Normal:
       Make_InputFile_with_FinalCoord.c:line.71
21 |||||------------------------------
22 5||||   0.0% |   0.000001 |MPI_Comm_rank:...:line.0
23 5||||   0.0% |   0.000002 |MPI_Comm_size:...:line.0
24 ||||==============================
25 4|||   0.0% |   0.000187 |
       Make_InputFile_with_FinalCoord_Normal:
       Make_InputFile_with_FinalCoord.c:line.94
26 5|||        |            | string_tolower:openmx_common.c:
       line.893
27 |||==================================
28 ||   0.0% |   0.015432 |MD_pac:MD_pac.c:line.81
29 |||----------------------------------
30 3||   0.0% |   0.000007 |Steepest_Descent:MD_pac.c:line.648
31 ||||--------------------------------
32 4|||   0.0% |   0.000001 |MPI_Barrier:...:line.0
33 4|||   0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
34 4|||   0.0% |   0.000001 |MPI_Comm_rank:...:line.0
35 4|||   0.0% |   0.000002 |MPI_Comm_size:...:line.0
36 ||||==============================
37 3||   0.0% |   0.000006 |Steepest_Descent:MD_pac.c:line.671
38 ||||--------------------------------
```

```
39 | 4|||    0.0% |   0.000005 |MPI_Allreduce:...:line.0
40 | 4|||    0.0% |   0.000001 |MPI_Allreduce(sync):...:line.0
41 ||||=================================
42 | 3||    0.0% |   0.015400 |Steepest_Descent:MD_pac.c:line.726
43 | 4||         |            | iterout_md:iterout_md.c:line.17
44 | 3||    0.0% |   0.000014 |Steepest_Descent:MD_pac.c:line.759
45 ||||---------------------------------
46 | 4|||    0.0% |   0.000008 |MPI_Bcast:...:line.0
47 | 4|||    0.0% |   0.000006 |MPI_Bcast(sync):...:line.0
48 ||||=================================
49 | 3||    0.0% |   0.000002 |Steepest_Descent:MD_pac.c:line.782
50 | 4||         |            | __ipap_fnjoint:openmx_common.c:
       line.358
51 | 3||    0.0% |   0.000003 |Steepest_Descent:MD_pac.c:line.814
52 | 4||         |            | __ipap_fnjoint:openmx_common.c:
       line.358
53 |||================================
54 | ||    0.0% |   0.000007 |MD_pac:MD_pac.c:line.109
55 | |||--------------------------------
56 | 3||    0.0% |   0.000002 |MPI_Bcast:...:line.0
57 | 3||    0.0% |   0.000003 |MPI_Bcast(sync):...:line.0
58 | 3||    0.0% |   0.000002 |dtime:dtime.c:line.15
59 | |||================================
```

2.3 Output

2.3.1 Make_FracCoord

Make_FracCoord.c: to generate the .frac file containing the fractional coordinates of the system. The zero coordinates are taken as the origin of the unit cell, and the fractional coordinates are kept within 0 to 1.

- Subroutine: Make_FracCoord()
- Input: double **Cell_Gxyz (atomic global coordinates spanned by the unit cell vectors, size: Cell_Gxyz[atomnum+1][4])
- Output: double **Cell_Gxyz (atomic global coordinates spanned by the unit cell vectors, size: Cell_Gxyz[atomnum+1][4]) written to the file .frac)
- MPI process: only the host/master process.

2.3.2 OutData

OutData.c: to output values of electron densities (out_density()), potentials, wave functions on the grids in the Gaussian cube format, and atomic Cartesian coordinates.

- Subroutine: out_atomxyz(), out_density(), out_Veff(), out_Vhart(), out_grid(), out_Vna(), out_Vxc(), out_Cluster_NC_MO(), etc.
- Input:
  - double **Gxyz (atomic global coordinates, velocities, and gradients of the total energy with respect to the atomic coordinates, size: Gxyz[atomnum+1][YOUSO26])
  - double **Density_Grid (electron densities on grids, size: Density_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3])
  - double **Vpot_Grid (Kohn-Sham effective potentials on grids, size: Vpot_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3])
  - double *dVHart_Grid (Hartree potential of the differential electron density on grids, size: dVHart_Grid[Num_Cells0*Ngrid2*Ngrid3])
  - double **Vxc_Grid (exchange-correlation potentials on grids, size: Vxc_Grid[2 or 4][Num_Cells0*Ngrid2*Ngrid3])
  - etc.
- Output:
  - double **Gxyz written to the .xyz file, double *ADensity_Grid (electron densities by the superposition of atomic densities on grids, size: ADensity_Grid[Num_Cells0*Ngrid2*Ngrid3])) written to the .dden file.
  - double **Density_Grid written to the .tden file, up-spin, down-spin, and spin electron densities written to the .den0, .den1, and sden files, respectively.
  - double **Vpot_Grid written to the .v0 and .v1 files.
  - double *dVHart_Grid written to the .vhart file.
  - The real space grids written to the .grid file.
  - double **Vxc_Grid written to the .vxc0 and .vxc1 files.
  - Cluster MOs (HOMOs and LUMOs) written to homo*.cube and lumo*.cube files.
  - etc.
- MPI process: each process is responsible for its own local data, then the host/master process merges them.

Listing 2.26: Make_FracCoord and OutData.

```
1 |    0.0% |    0.000649 |main:openmx.c:line.508
2 ||--------------------------------
```

```
3 | ||    0.0% |   0.000646 |Make_FracCoord:Make_FracCoord.c:line
      .31
4 | ||    0.0% |   0.000003 |Make_FracCoord:Make_FracCoord.c:line
      .34
5 | |||-----------------------------------
6 |  3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
7 |  3||    0.0% |   0.000001 |MPI_Comm_size:...:line.0
8 | ||===================================
9 | |    2.3% |   2.158985 |main:openmx.c:line.525
10| ||----------------------------------
11|  ||    1.9% |   1.772453 |OutData:OutData.c:line.61
12|  ||    0.0% |   0.000003 |OutData:OutData.c:line.73
13| |||-----------------------------------
14|  3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
15|  3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
16| |||===================================
17|  ||    0.0% |   0.000005 |OutData:OutData.c:line.78
18| |||-----------------------------------
19|  3||    0.0% |   0.000003 |out_atomxyz:OutData.c:line.705
20| ||||-----------------------------------
21|  4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
22|  4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
23| ||||===================================
24|  3||    0.0% |   0.000002 |out_atomxyz:OutData.c:line.720
25|  4||       |            |  __ipap_fnjoint:openmx_common.c:
      line.358
26| |||===================================
27|  ||    0.0% |   0.000117 |OutData:OutData.c:line.81
28| |||-----------------------------------
29|  3||    0.0% |   0.000014 |out_Veff:OutData.c:line.596
30| ||||-----------------------------------
31|  4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
32|  4|||    0.0% |   0.000012 |MPI_Comm_size:...:line.0
33| ||||===================================
34|  3||    0.0% |   0.000018 |out_Veff:OutData.c:line.621
35| ||||-----------------------------------
36|  4|||    0.0% |   0.000004 |Print_CubeData:OutData.c:line.1613
37| |||||-----------------------------------
38|  5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
39|  5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
40| |||||===================================
41|  4|||    0.0% |   0.000014 |Print_CubeData:OutData.c:line.1811
42| |||||-----------------------------------
43|  5||||    0.0% |   0.000002 |MPI_Barrier:...:line.0
44|  5||||    0.0% |   0.000012 |MPI_Barrier(sync):...:line.0
45| ||||===================================
46|  3||    0.0% |   0.000014 |out_Vhart:OutData.c:line.456
47| ||||-----------------------------------
48|  4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
```

```
 4|||    0.0%  |   0.000012  |MPI_Comm_size:...:line.0
||||==========================================
 3||    0.0%  |   0.000018  |out_Vhart:OutData.c:line.479
||||------------------------------
 4|||    0.0%  |   0.000004  |Print_CubeData:OutData.c:line.1613
|||||------------------------------
 5||||    0.0%  |   0.000001  |MPI_Comm_rank:...:line.0
 5||||    0.0%  |   0.000002  |MPI_Comm_size:...:line.0
||||==========================================
 4|||    0.0%  |   0.000014  |Print_CubeData:OutData.c:line.1811
|||||------------------------------
 5||||    0.0%  |   0.000002  |MPI_Barrier:...:line.0
 5||||    0.0%  |   0.000012  |MPI_Barrier(sync):...:line.0
||||==========================================
 3||    0.0%  |   0.000005  |out_density:OutData.c:line.191
||||------------------------------
 4|||    0.0%  |   0.000002  |MPI_Comm_rank:...:line.0
 4|||    0.0%  |   0.000003  |MPI_Comm_size:...:line.0
||||==========================================
 3||    0.0%  |   0.000021  |out_density:OutData.c:line.228
||||------------------------------
 4|||    0.0%  |   0.000007  |Print_CubeData:OutData.c:line.1613
|||||------------------------------
 5||||    0.0%  |   0.000002  |MPI_Comm_rank:...:line.0
 5||||    0.0%  |   0.000005  |MPI_Comm_size:...:line.0
||||==========================================
 4|||    0.0%  |   0.000014  |Print_CubeData:OutData.c:line.1811
|||||------------------------------
 5||||    0.0%  |   0.000002  |MPI_Barrier:...:line.0
 5||||    0.0%  |   0.000012  |MPI_Barrier(sync):...:line.0
||||==========================================
 3||    0.0%  |   0.000027  |out_density:OutData.c:line.255
||||------------------------------
 4|||    0.0%  |   0.000014  |Print_CubeData:OutData.c:line.1613
|||||------------------------------
 5||||    0.0%  |   0.000002  |MPI_Comm_rank:...:line.0
 5||||    0.0%  |   0.000012  |MPI_Comm_size:...:line.0
||||==========================================
 4|||    0.0%  |   0.000013  |Print_CubeData:OutData.c:line.1811
|||||------------------------------
 5||||    0.0%  |   0.000002  |MPI_Barrier:...:line.0
 5||||    0.0%  |   0.000012  |MPI_Barrier(sync):...:line.0
|||==========================================
 ||    0.4%  |   0.385263  |OutData:OutData.c:line.87
|||------------------------------
 3||    0.0%  |   0.000014  |out_grid:OutData.c:line.656
||||------------------------------
 4|||    0.0%  |   0.000002  |MPI_Comm_rank:...:line.0
 4|||    0.0%  |   0.000012  |MPI_Comm_size:...:line.0
```

```
 98 ||||==========================================
 99 3||    0.0% |   0.000002 |out_grid:OutData.c:line.673
100 4||         |            |  __ipap_fnjoint:openmx_common.c:
    line.358
101 3||    0.4% |   0.385247 |out_grid:OutData.c:line.681
102 4||         |            |  Get_Grid_XYZ:openmx_common.c:line
    .866
103 |||=========================================
104 ||    0.0% |   0.000024 |OutData:OutData.c:line.89
105 |||-----------------------------------------
106 3||    0.0% |   0.000006 |out_Vxc:OutData.c:line.533
107 ||||---------------------------------------
108 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
109 4|||    0.0% |   0.000004 |MPI_Comm_size:...:line.0
110 ||||=======================================
111 3||    0.0% |   0.000018 |out_Vxc:OutData.c:line.558
112 ||||---------------------------------------
113 4|||    0.0% |   0.000004 |Print_CubeData:OutData.c:line.1613
114 |||||-------------------------------------
115 5||||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
116 5||||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
117 ||||=======================================
118 4|||    0.0% |   0.000014 |Print_CubeData:OutData.c:line.1811
119 |||||-------------------------------------
120 5||||    0.0% |   0.000002 |MPI_Barrier:...:line.0
121 5||||    0.0% |   0.000012 |MPI_Barrier(sync):...:line.0
122 |=========================================
123 ||    0.0% |   0.001121 |OutData:OutData.c:line.101
124 |||-----------------------------------------
125 3||    0.0% |   0.000015 |out_Cluster_MO:OutData.c:line.872
126 ||||---------------------------------------
127 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
128 4|||    0.0% |   0.000013 |MPI_Comm_size:...:line.0
129 ||||=======================================
130 3||    0.0% |   0.000554 |out_Cluster_MO:OutData.c:line.922
131 ||||---------------------------------------
132 4|||    0.0% |   0.000549 |MPI_Reduce:...:line.0
133 4|||    0.0% |   0.000005 |MPI_Reduce(sync):...:line.0
134 |||=========================================
135 3||    0.0% |   0.000552 |out_Cluster_MO:OutData.c:line.1032
136 ||||---------------------------------------
137 4|||    0.0% |   0.000541 |MPI_Reduce:...:line.0
138 4|||    0.0% |   0.000012 |MPI_Reduce(sync):...:line.0
139 ||||=======================================
```

2.3.3 SCF2File

SCF2File.c: to output connectivity, Hamiltonian matrix, overlap matrix, density matrix, etc. to the .scfout binary file.

- Input:
  - double *****H (Kohn-Sham matrix elements of basis orbitals, size: H[SpinP_switch+1] [Matomnum+MatomnumF+MatomnumS+1] [FNAN[Gc_AN]+1][Spe_Total_NO[Cwan]][Spe_Total_NO[Hwan]])
  - double *****iHNL0 (imaginary matrix elements for non-local VPS, size: iHNL[List_YOUSO[5]][Matomnum+1][FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]])
  - double *****OLP (overlap matrix elements of basis orbitals, size: OLP[4][Matomnum+MatomnumF+MatomnumS+1][FNAN[Gc_AN]+1] [Spe_Total_NO[Cwan]][Spe_Total_NO[Hwan]])
  - Overlap matrices with position operator x, y, z.
  - double ******DM (current and old density matrices, size: DM[List_YOUSO[16]] [SpinP_switch+1][Matomnum+1][FNAN[Gc_AN]+1][Spe_Total_NO[Cwan]] [Spe_Total_NO[Hwan]])
- Output: the matrices written to the .scfout binary file.
- MPI process: each process is responsible for its own local data, then the host/master process merges them.

2.3.4 Output_CompTime

Output_CompTime.c: to output computational time to the .TRN file.

- Input: double **CompTime;
- Output: min and max computational times written to the file.
- MPI process: only the host/master process.

2.3.5 Merge_LogFile

Merge_LogFile.c: to merge several log files and write to the .out file.

- Input: other files.
- Output: the .out file.
- MPI process: only the host/master process.

2.3.6 Free_Arrays

Free_Arrays.c: to free all arrays used in the program.

2.3.7 PrintMemory

PrintMemory.c to save the memory size of each array.

Listing 2.27: SCF2File, Output_CompTime, Merge_LogFile, Free_Arrays, PrintMemory.

```
|    0.1% |   0.075020 |main:openmx.c:line.532
||---------------------------------
||    0.0% |   0.011836 |SCF2File:SCF2File.c:line.38
||    0.0% |   0.000004 |SCF2File:SCF2File.c:line.50
|||-------------------------------
3||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
||===============================
||    0.0% |   0.000010 |SCF2File:SCF2File.c:line.175
|||-------------------------------
3||    0.0% |   0.000005 |MPI_Bcast:...:line.0
3||    0.0% |   0.000005 |MPI_Bcast(sync):...:line.0
|||==============================
||    0.1% |   0.063170 |SCF2File:SCF2File.c:line.180
|||-------------------------------
3||    0.0% |   0.000006 |Calc_OLPpo:SCF2File.c:line.889
||||-----------------------------
4|||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
4|||    0.0% |   0.000001 |MPI_Barrier:...:line.0
4|||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
3||    0.0% |   0.000004 |Calc_OLPpo:SCF2File.c:line.940
4||         |            | dtime:dtime.c:line.15
3||    0.1% |   0.063149 |Calc_OLPpo:SCF2File.c:line.949
4||         |            | Get_Grid_XYZ:openmx_common.c:line
    .866
3||    0.0% |   0.000006 |Calc_OLPpo:SCF2File.c:line.1029
4||         |            | dtime:dtime.c:line.15
||||==============================
3||    0.0% |   0.000004 |Output:SCF2File.c:line.298
||||-----------------------------
4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
4|||    0.0% |   0.000003 |MPI_Comm_size:...:line.0
|||=============================
|    0.0% |   0.000922 |main:openmx.c:line.536
||---------------------------------
||    0.0% |   0.000904 |Output_CompTime:Output_CompTime.c:
    line.27
```

```
37 | ||    0.0% |   0.000003 |Output_CompTime:Output_CompTime.c:
       line.43
38 |||--------------------------------
39 | 3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
40 | 3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
41 |||================================
42 | ||    0.0% |   0.000008 |Output_CompTime:Output_CompTime.c:
       line.53
43 |||--------------------------------
44 | 3||    0.0% |   0.000005 |MPI_Bcast:...:line.0
45 | 3||    0.0% |   0.000004 |MPI_Bcast(sync):...:line.0
46 |||================================
47 | ||    0.0% |   0.000003 |Output_CompTime:Output_CompTime.c:
       line.55
48 |||--------------------------------
49 | 3||    0.0% |   0.000001 |MPI_Barrier:...:line.0
50 | 3||    0.0% |   0.000001 |MPI_Barrier(sync):...:line.0
51 |||================================
52 | ||    0.0% |   0.000002 |Output_CompTime:Output_CompTime.c:
       line.78
53 | 3|         |            | __ipap_fnjoint:openmx_common.c:line
       .358
54 | ||    0.0% |   0.000003 |dtime:dtime.c:line.15
55 ||================================
56 |    0.0% |   0.014513 |main:openmx.c:line.541
57 ||-------------------------------
58 | ||    0.0% |   0.014506 |Merge_LogFile:Merge_LogFile.c:line
       .30
59 | ||    0.0% |   0.000007 |Merge_LogFile:Merge_LogFile.c:line
       .43
60 |||--------------------------------
61 | 3||    0.0% |   0.000001 |MPI_Comm_rank:...:line.0
62 | 3||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
63 | 3||    0.0% |   0.000001 |MPI_Barrier:...:line.0
64 | 3||    0.0% |   0.000002 |MPI_Barrier(sync):...:line.0
65 ||================================
66 |    0.0% |   0.001054 |main:openmx.c:line.558
67 ||-------------------------------
68 | ||    0.0% |   0.000781 |__ipai_Free_Arrays:Free_Arrays.c:
       line.19
69 | ||    0.0% |   0.000003 |__ipai_Free_Arrays:Free_Arrays.c:
       line.21
70 | 3|         |            | array0:Free_Arrays.c:line.37
71 ||||-------------------------------
72 | 4|||    0.0% |   0.000002 |MPI_Comm_rank:...:line.0
73 | 4|||    0.0% |   0.000002 |MPI_Comm_size:...:line.0
74 ||================================
75 | ||    0.0% |   0.000269 |PrintMemory:PrintMemory.c:line.19
76 |    0.0% |   0.000003 |main:openmx.c:line.566
```

```
77 |  |          |              |  MPI_Finalize:...:line.0
78 |  |    0.0%  |   0.000111   | exit:...:line.0
79 |=================================
```