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# 1 What is "STATE"?

## 1.1 Introduction

"STATE" is an abbreviation for "Simulation Tool for Atom Technology" and it is a standard first-

## 1.2 Caution

Right now STATE is becoming an important and powerful tool not only for the theoretical group in JRCAT but also for many other groups in Japan. We are planning to develop STATE and trying to implement more functions into STATE in near future. Therefore, STATE is updated frequently and the input and output files explained in this manual might be inconsistent with the latest version of the code.

## 1.3 Main features

STATE was designed to perform band structure, total energy and molecular dynamics calculations on parallel supercomputers. The Main features include:

- Norm-conserving pseudopotentials (Troullier & Martins type) and ultra-soft pseudopotentials (Vanderbilt type) are available.
- Local (spin) density approximation (LSDA) and the generalized gradient approximation (PBE version) are available.
- LDA+U method for strongly correlated systems.
- The Davidson and RMM methods with real-space technique can be used for the electronic structure calculations.
- Total energy and force calculations for determining the equilibrium structure and for molecular dynamic simulations.
- Automatic  $K$ -points generation with corrected linear tetrahedral method for the  $K$ -space integration.
- Parallelized FFT.
- Parallelization by MPI so that the code can run across many computers.

The parallelization of STATE is done mainly based on the G-points distribution for most of the subroutines, and the code is particularly optimized for Vector machines. Therefore, it is efficient to run STATE on vector supercomputers with limited number of PEs, like VPP500~700 and Fujitsu SR8000, rather than on massively parallel computers with many PEs. However, there is one exception. The RMM method in the code is parallelized across bands, so that it can be used efficiently on massive computers like IBM SP.

## 2 Structure of “STATE”

The source of STATE consists of many subroutines, which are all included in one directory with suffix “.f90”. The main structure of STATE is illustrated in following diagram. You can follow the main structure from the file named “main.f90”

```
USE MPI
USE parameters
:
Initialization
:
DO MD steps
    :
    Optimization of Wave Functions for fixed atom position
    :
    Molecular Dynamics for atoms
    :
END DO
:
Output
:
END program MAIN
```

### 2.1 Modules

Only two modules are defined in the code. They include the definitions for all the common variables and arrays, and are used by most of the subroutines.

- MODULE MPI (my\_mpi.f90)

This module includes all common variables, arrays, and subroutines related to MPI. It should be used in every subroutine which has parallelization.

- MODULE parameters (m\_para.f90)

This module includes all common variables and arrays related to calculations. It can be used in the following way.

```
USE parameters, only : kngpm keg, zaj_l, ...
```

## 2.2 Parallelization

A typical Do loop with parallelization by G-points is show below. First the Do loop is distributed to different PEs. After finishing the DO loop, the 'Call my\_allreduce' will sum up all the results calculated in different PEs. Please remember that the initialization of arrays should be done carefully.

```
DO ig=kngp_start,kngp_end
  :
END DO
CALL my_allreduce(...)
```

- MPI subroutine my\_allreduce

```
CALL my_allreduce(Length, r_in=..., i_in=...,)
```

- MPI subroutine my\_bcast

```
CALL my_bcast(Length,
```

```
r1_size=..., r1=..., r2_size=..., r2=..., ..., r10_size=..., r10_size=...,
```

```
i1_size=..., i1=..., i2_size=..., i2=..., ..., i10_size=..., i10_size=...,
```

```
c1_size=..., c1=..., c2_si...., i10
```

## 3 Running “STATE”

### 3.1 Getting “STATE” source files

Source files of ”STATE” are obtained from gzipped file STATE.tar.gz. Please ungzip and untar the file:

```
gzip -d STATE.tar.gz
tar xvf STATE.tar . (Please do not forget the last period!)
```

Then you will have the following directories.

STATE/outs/	Execute directory. Input files, Output files, Executables.
STATE/src/	Source files and makefile
STATE/src/CPPSRC	Working directory for compiling
STATE/gncpp/	Pseudopotential files for various atoms
STATE/sample/	sample input and output files

### 3.2 Compiling source files

To produce the executable module of “STATE”, you just do ’make’ at directory where you copied the source files. Working directory, CPPSRC, must be prepared under src before compiling.

```
(You are at STATE/src/.)
make
```

### 3.3 Constructing the necessary files

Create the input file “nfnp.data” in the HOME directory where you run “STATE”. (See the section ?? to set the parameters.) You can tentatively prepare the input file in another directory and link to the nfnp.data in the running directory.

### 3.4 Linking pseudo potentials and STATE to the running directory

Choose the pseudopotential for each type of element from the directory where pseudopotentials are stored (typically, HOME/pseudo/), and link the chosen pseudopotentials to the files “fort.37”, “fort.38”, and so on in the source directory, e.g., “src/”. The following is an example with three elements for CH<sub>3</sub>OH.

```
(You are at at STATE/outs)
ln -fs ../gncpp/pot.C_pbe3 fort.37
ln -fs ../gncpp/pot.H_lda3 fort.38
```

The executable file ”STATE” is linked to the directory where you want to run, say HOME, as follows.

```
(You are at at STATE/outs )
ln -fs ../src/STATE STATE
```

### 3.5 Running STATE

- Move to the HOME directory.
- Submit nqs job. The following is an example to run on Compaq.

```
cd /STATE/outs/  
mpirun -np 1 ./STATE < nfinp_25Ry > nfout_25Ry &
```



## 4 Constructing input files

### 4.1 “nfnp.data” to run “STATE”

There are several input files used by “STATE”. The most important one is “nfnp.data”. It is necessary to know the meaning of each parameter in the input file, ”nfnp.data”. The following is the typical input file to calculate an isolated C<sub>2</sub>H<sub>4</sub> molecule.

```

01. 0 0 0 0 0 0 : Ictrl
02. 5.0000 15.0000 2 3 6 : GMAX, GMAXP, NTYP, NATM, NATM2
03. 47 0 : number of space group, type of bravis lattice
04. 22.0000 21.0000 20.0000 90.0 90.0 90.0 : a,b,c,alpha,beta,gamma
05. 1 1 1 1 1 1 : knx,kny,knz, k-point shift
06. 1 1 : NCORD, NINV, : IWEI, IMDTYP, ITYP
07. 1.2627229833 0.0000000000 0.0000000000 2 1 1
08. 2.3483288468 1.7534586685 0.0000000000 2 1 2
09. 2.3483288468 -1.7534586685 0.0000000000 2 1 2
10. 6 0.1500 12.01115 3 1 0.d0 : TYPE 1IATOMN,ALFA,AMION,ILOC,IVAN
11. 1 0.1500 1.00797 3 1 0.d0 : TYPE 2IATOMN,ALFA,AMION,ILOC,IVAN
12. 0 0 0 0 0 : icond, inipos, inivel, ininos, iniacc
13. 0 1 : IPRE, IPRI
14. 200 200 0 7200.00 0 : NMD1, NMD2, iter_last, CPUMAX,ifstop
15. 6 1 : Simple=1,Broyd2=3,Blugel=6, 1:charge, 2:potential mix.
16. 0 8 0.8 : starting mixing, kbxmix,alpha
17. 0.60 0.50 0.60 0.70 1.00 : DTIM1, DTIM2, DTIM3, DTIM4, dtim_last
18. 300.00 4 1 0.10D-07 1.d-06 : DTIO ,IMDALG, IEXPL, EDELTA
19. 0.0010 0.05D-02 0 : WIDTH,FORCCR,ISTRESS
20. ggapbe 1 : XCTYPE, nspin
21. 1.00 3 : destm, n_stm
22. 102 : NBZTYP 0-SF, 1-BK, 2-SC, 3-BCC, 4-FCC, 5-DIA, 6-HEX
23. 0 0 0 : NKX, NKY, NKZ
24. 0 0 0 : NKX2,NKY2,NKZ2
25. 10 : NEG
26. 1 : NonLocalProjection
27. 0 : 0; random numbers, 1; matrix diagon
28. 2 0 0 0(MB) : imsd, i_2lm, i_sd2another, wksz for phase
29. 0 : evaluation of eko difference.0 = no ,1 = yes
30. 0
31. 0 0.0
32. 10 : mvelsc
33. 300.0D0 50.0D0 30 1.0D0 : tempw,tolp,nroll,anneal
34. 500.0D0 8 15 1 : wnosep,nhc,nosy,ndrt
35. 5.0D-8 : frict
36. 0 : mcnstr
37. DIST 1 3 1.83401
38. DIST 2 3 1.83401
39. BEND 1 3 2 104.23195

```

The above input parameters for “STATE” are explained below. The following explanations are in the order of appearance in the input file “nfinp.data”.

1. **Ictrl** 6 digits in the first line are obsolete.
2. **GMAX** Wave number cutoff for pseudowave function (soft part).

$$E_{\text{cut}}^{\text{soft}}(\text{Ry}) = \text{GMAX}^2$$

**2. GMAXP** Wave number cutoff for localized charge density (hard mode).

$$E_{\text{cut}}^{\text{hard}}(\text{Ry}) = \text{GMAXP}^2$$

(See Vanderbilt representation of the real charge density)

**2. NTYP** Number of atom types regardless of point group symmetry. But, types are also distinguished by spin polarization.

**2. NATM** Total reduced number of atoms under the inversion symmetry.

**2. NATM2** Total number of atoms.

**3. Space Group Number** C1  $\rightarrow$ 1\*, S2  $\rightarrow$ 2\*, C2v $\rightarrow$ 25, C4  $\rightarrow$ 75, C4v $\rightarrow$ 99\*, D4h $\rightarrow$ 123\*, C3  $\rightarrow$ 143, C3v $\rightarrow$ 156, C6  $\rightarrow$ 168, D6h $\rightarrow$ 191\*, Oh  $\rightarrow$ 221\*  
(\* tested; others, not tested).

**3. Type of Bravis Lasttice** Simple  $\rightarrow$ 0, Body center  $\rightarrow$ 1, Face center  $\rightarrow$ 2, A center  $\rightarrow$ 3, B center  $\rightarrow$ 4, C center  $\rightarrow$ 5, Rhombohedral center $\rightarrow$ 6.

**4. a, b, c, alpha, beta, gamma** Lattice parameters and the angles between axes

**5. n1, n2, n3** number of  $K$ -point meshes along each axes

**5. m1, m2, m3** shift; no shift $\rightarrow$ 1, shifted $\rightarrow$ 2.

**6. NCORD** Unit of coordinates; primitive cell units  $\rightarrow$ 0, Cartesian units  $\rightarrow$ 1, conventional cell units  $\rightarrow$ 2.

**6. NINV** Inversion symmetry; counted  $\rightarrow$ 1, otherwise $\rightarrow$ 0.

Atom coordinates are given here in the NCORD units. IWEI, IMDTYP, and ITYP follow them for each atom (NATM should be equal to the number of atoms of which coordinates are listed here.).

**7-9. x, y, z** x-, y-, z-coordinates of atom

**7-9. IWEI** Number of equivalent atoms under inversion symmetry (must be 1 or 2).

**7-9. IMDTYP** Relaxing the atom in MD; yes  $\rightarrow$ 1, not relaxing  $\rightarrow$ 0, attaching to the thermostat  $>$ 1000.

**10-11. ITYP** Atom type number.

Here are presented some information for each atom type following ITYP.

**10-11. IATOMN** Atomic number.

**10-11. ALFA** Obsolete

**10-11. AMION** Nucleus mass for MD in the unit of electronic mass (which could be larger than real value).

**10-11. ILOC**  $l_{max} + 1$  for local PP.

**10-11. IVAN** Pseudopotential; ultrasoft PP  $\rightarrow 1$ , otherwise  $\rightarrow 0$ .

**10-11. zeta1** Initial spin polarization for each type of element

**12. ICOND** : describes whether continuing the calculations; Start the calculation from beginning  $\rightarrow 0$ , Continue the calculations from last iteration  $\rightarrow 1$ , Fixed-charge calculations  $\rightarrow 2$ , Fixed-Charge-Continuation  $\rightarrow 3$ , CHARGE-FFT  $\rightarrow 10$ , DOS-calculations  $\rightarrow 12$ , ALDOS  $\rightarrow 13$ , PDOS  $\rightarrow 14$ .

**12. INIPOS** Specify the atom positions actually used; read from nfinp.data  $\rightarrow 0$ , read from restart file  $\rightarrow 1$ , read from GEOMETRY file  $\rightarrow 2$ .

**12. INIVEL** Specify the atom velocities actually used; initialized  $\rightarrow 0$ , read from restart file  $\rightarrow 1$ , read from GEOMETRY file  $\rightarrow 2$ .

**12. ININOS** Specify the thermostat variables actually used; initialized  $\rightarrow 0$ , read from restart file  $\rightarrow 1$ .

**12. INIACC** Reset accumulators and the counter of MD steps  $\rightarrow 0$ , read from restart file and continue accumulating  $\rightarrow 1$ .

**13. IPRE** Obsolete.

**13. IPRI** The level of printing message for debugging.

**14. NMD1** Number of iterations for electronic structure optimization.

**14. NMD2** Number of total iterations including molecular dynamics of the ionic system.

**14. ITER\_LAST** Last iteration number to continue.

- 14. **CPUMAX** Maximum cpu time in seconds.
- 14. **ifstop** The number of iterations where the program should stop.
- 15. **Way-of-Mix** 1=SIMPLE, 2=BROYD1, 3=BROYD2, 4=DFP, 5=PULAY, 6=BLÜGEL
- 15. **mix-what** change mixing →1, potential mixing →2.
- 16. **mix-start** The number of iterations when the mixture should start
- 16. **kbxmix** The total number of iterations. in which the charge information was used for mixture
- 16. **alpha** The mixture parameter
- 17. **DTIM1~DTIM4** Obsolete
- 17. **DTIM\_LAST** Fictitious-time increment after continuing the last iteration.
- 18. **DTIO** Fictitious-time increment of ions in MD.
- 18. **IMDALG** Algorithms of MD; Newtonian equations of motion→1, quenched MD →2, DIIS MD →4, finite temperature MD →-1, Langevin MD →-2.
- 18. **IEXPL** Extrapolating to predict the wave function with respect to changed ionic positions→1, otherwise→0.
- 18. **EDELTA** Energy criteria for convergence [in Hartree/atom].
- 19. **WIDTH** Tetrahedral scheme used to generate  $k$ -points in BZ if  $WIDTH < -10.0$   
Special  $k$ -points scheme is used and  $|WIDTH|$  means the energy broadening around  $k$ -points if  $-10.0 < WIDTH < 10.0$ .
- 19. **FORCCR** Criterion for force in MD.  
If the maximum force is smaller than FORCCR, the molecular dynamics is terminated.
- 19. **STRESS** Calculating stress tensor→1, otherwise→0 (Now obsolete).
- 20. **XCTYPE** Name of exchange-correlation type {ggapbe, ldapw91 or lda+u}.
- 20. **NSPIN** No spin polarization →1, Spin polarization →2.
- 21. **DESTM** Energy width for STM-imaging.

- 21. NBZTYP** This item works only if  $WIDTH < -10.0$  (Tetrahedral method).  
 100=tetrahedral method with reduced G vectors  
 101=linear corrected tetrahedral method with extended G vectors (Recommended)  
 102=linear corrected tetrahedral method with reduced G vectors
- 23. NKX, NKY, NKZ** Obsolete
- 24. NKX2, NKY2, NKZ2** Obsolete
- 25. KEG** : Number of eigenvalues (a little larger than number of valence electrons/spin).
- 26. NonLocalProjection** Non-local Pseudopotential Projection 1= in real-space, 2= in G-space
- 27. Scheme to generate the trial wave function** Random number scheme  $\rightarrow 0$ .
- 28. IMSD** 1=RMM, 2=Davidson
- 30. npdosao** without pdos calculations  $\rightarrow 0$ , with pdos calculation  $\rightarrow$ larger than 0
- 32. MVELSC** Method of velocity control for finite temperature MD; microcanonical  $\rightarrow 0$ , simulated annealing  $\rightarrow 1$ , simple velocity scaling  $\rightarrow 2$ , rolling average method  $\rightarrow 3$ , Gaussian dynamics  $\rightarrow 4$ , Nosé-Hoover chain (NHC) method  $\rightarrow 10$ , Generalized Gaussian Moment Thermostatting (GGMT) method  $\rightarrow 11$ .
- 33. TEMPW** Target temperature [K].
- 33. ANNEAL** Annealing factor. Square root of this factor is multiplied by ionic velocities every MD step when a keyword `SIMULATED_ANNEALING` is activated.
- 34. TOLP** Tolerance of temperature [K]. This variable is used when simple velocity scaling or rolling average method are activated.
- 34. WNOSEP** Characteristic vibrational frequency [ $\text{cm}^{-1}$ ]. This quantity is used to generate the thermostat variables. The vibrational frequency depends on the system but the typical value is  $\sim 300 \text{ cm}^{-1}$ .
- 34. NHC** Length of thermostat chains. This also means that up to the order of  $2 \times \text{NHC}$  Gaussian moments are controlled when a keyword `GGMT_METHOD` is specified. The recommended value is 4 and 2 for the NHC and GGMT method, respectively.
- 34. NOSY** The order of Suzuki-Yoshida integrator which is used to integrate thermostat variables. The available order is 1, 3, 5, 7, 15, 25, 125, and 625, however, 15 is recommended.

- 34. NDRT** The number of integration cycles for thermostat variables. Usually  $\text{NDRT} = 1$  is enough to integrate thermostat variables stably.
- 34. NROLL** Rolling average is taken every `nroll` MD steps. This short time average of temperature is used to determine a rescaling factor for velocities when `ROLLING_AVERAGE_METHOD` is specified. The typical value is 10.
- 35. FRICT** Friction coefficient used to generate random forces for Langevin MD.
- 36. MCNSTR** The number of constraints achieved using SHAKE and RATTLE algorithms. The available constraints are atom-atom distance (`DISTANCE`), bond angle (`BEND`), difference of distances between three atoms (`DIFF`), and dihedral angle (`DIHEDRAL`).

## 5 Output files

Output files are created in the same directory where the program ran.

nfout.data	Log file
zaj.data	Wave function
potential.data	Electron density
nfinp_new.data	New input file to be used to continue the run. Atomic positions are renewed.



## 6 Examples

In this section, several examples of input and output files are explained.

### 6.1 C2H4

In the directory

STATE/sample/c2h4/

isolated ethylene molecule is calculated. The input file is

```

0 0 0 0 0 0 : Ictrl
5.0000 15.0000 2 3 6 : GMAX, GMAXP, NTYP, NATM, NATM2
47 0 : number of space group, type of bravis lattice
22.0000 21.0000 20.0000 90.0 90.0 90.0 : a,b,c,alpha,beta,gamma
1 1 1 1 1 1 : knx,kny,knz, k-point shift
1 1 : NCORD, NINV, : IWEI, IMDTYP, ITYP
1.2627229833 0.0000000000 0.0000000000 2 1 1
2.3483288468 1.7534586685 0.0000000000 2 1 2
2.3483288468 -1.7534586685 0.0000000000 2 1 2
6 0.1500 12.01115 3 1 0.d0 : TYPE 1IATOMN,ALFA,AMION,ILOC,IVAN
1 0.1500 1.00797 3 1 0.d0 : TYPE 2IATOMN,ALFA,AMION,ILOC,IVAN
0 0 0 0 0 : icond, inipos, inivel, ininos, iniacc
0 1 : IPRE, IPRI
200 200 0 7200.00 0 : NMD1, NMD2, iter_last, CPUMAX,ifstop
6 1 : Simple=1,Broyd2=3,Blugel=6, 1:charge, 2:potential mix.
0 8 0.8 : starting mixing, kbxmix,alpha
0.60 0.50 0.60 0.70 1.00 : DTIM1, DTIM2, DTIM3, DTIM4, dtim_last
300.00 4 1 0.10D-07 1.d-06 : DTIO ,IMDALG, IEXPL, EDELTA
0.0010 0.05D-02 0 : WIDTH,FORCCR,ISTRESS
ggapbe 1 : XCTYPE, nspin
1.00 3 : destm, n_stm
102 : NBZTYP 0-SF, 1-BK, 2-SC, 3-BCC, 4-FCC, 5-DIA, 6-HEX
0 0 0 : NKX, NKY, NKZ
0 0 0 : NKX2,NKY2,NKZ2
10 : NEG
1 : NonLocalProjection
0 : 0; random numbers, 1; matrix diagon
2 0 0 0(MB) : imsd, i_2lm, i_sd2another, wksz for phase
0 : evaluation of eko difference.0 = no ,1 = yes
0
0 0.0
10 : mvelsc
300.0D0 50.0D0 30 1.0D0 : tempw,tolp,nroll,anneal
500.0D0 8 15 1 : wnosep,nhc,nosy,ndrt
5.0D-8 : frict
0 : mcnstr
DIST 1 3 1.83401
DIST 2 3 1.83401
BEND 1 3 2 104.23195

```

For output files, you will find

**nfout.data:** output file

**zaj.data:** wave function data

**potential.data:** charge density data.

First, please check the convergence of the total energy by

```
> grep ETOT nfout_25Ry
ETOT:  1      2.61793268  0.2618E+01  0.7542E-02
ETOT:  2     -8.63675635  0.1125E+02  0.5578E-02
ETOT:  3    -13.05601025  0.4419E+01  0.5501E-02
ETOT:  4    -13.70615311  0.6501E+00  0.3585E-02
.....
```

The second, third, fourth and the fifth columns indicate the number of self consistent iterations, the total energy in hartree unit, the total energy difference between two successive iterations, and the charge density difference between two successive iterations, respectively. If the total energy difference becomes smaller than  $\text{NATM2} \times \text{EDELTA}$ , the forces acting on atoms will be calculated and a molecular dynamics step will be taken. In the output file, you will find

```
.....
ETOT:  23    -13.90191343  0.7819E-08  0.1730E-06
ETOT:  24    -13.90191343  0.1423E-08  0.1628E-06
ETOT:  25    -13.90191343  0.3620E-09  0.6915E-07
  ETOT(Q) + SM_energy = -13.9019134295922      12.3567846487591
ETOT:  1    -13.90182603  0.8740E-04  0.1443E-03
ETOT:  2    -13.90176734  0.5870E-04  0.7264E-04
ETOT:  3    -13.90178410  0.1677E-04  0.7546E-04
.....
```

whenever a molecular dynamics step is taken. You can also check the molecular dynamics steps by

```
> grep CNVF nfout_25Ry
CNVF: iter_md, TotalEnergy,  f_max,    f_rms,    edel,    vdel,    fdel
CNVF:  1    -13.90191343  0.003702  0.002227
CNVF:  2    -13.90184480  0.010768  0.006397
CNVF:  3    -13.90193312  0.000609  0.000410
CNVF:  4    -13.90193422  0.000209  0.000171
```

The second, third, fourth, and the fifth columns show the number of molecular dynamics steps, the total energies, the maximum forces, and the root mean square of the forces, respectively. If the maximum force becomes smaller than the  $\text{FORCCR}$ , the program stops and the final position of the atoms, the wave functions, and the charge density will be stored. You can check the evolution of the atomic positions and forces at each molecular dynamics time step by

```

> grep MD nfout_25Ry
MD: 1
MD: 1 1.26272298 0.00000000 0.00000000 -0.00370 0.00000 0.00000
MD: 2 -1.26272298 0.00000000 0.00000000 0.00370 0.00000 0.00000
MD: 3 2.34832885 1.75345867 0.00000000 -0.00057 -0.00051 0.00000
MD: 4 2.34832885 -1.75345867 0.00000000 -0.00057 0.00051 0.00000
MD: 5 -2.34832885 1.75345867 0.00000000 0.00057 -0.00051 0.00000
MD: 6 -2.34832885 -1.75345867 0.00000000 0.00057 0.00051 0.00000
MD: 2
MD: 1 1.25161576 0.00000000 0.00000000 0.01077 0.00000 0.00000
MD: 2 -1.25161576 0.00000000 0.00000000 -0.01077 0.00000 0.00000
MD: 3 2.34662269 1.75192311 0.00000000 -0.00136 -0.00125 0.00000
MD: 4 2.34662269 -1.75192311 0.00000000 -0.00136 0.00125 0.00000
MD: 5 -2.34662269 1.75192311 0.00000000 0.00136 -0.00125 0.00000
MD: 6 -2.34662269 -1.75192311 0.00000000 0.00136 0.00125 0.00000
.....

```

The number in the first line is the molecular dynamics step and the number of each atom and their corresponding x, y, z coordinates and x, y, z forces follow.