

**STATE-senri**  
(**S**imulation **T**ool for **A**tom **T**Echnology)

*USER's MANUAL*

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# 1 What is "STATE"?

## 1.1 Introduction

"STATE" is an abbreviation of "Simulation Tool for Atom Technology" and it is a standard first-principles molecular dynamics code based on the density functional theory with pseudo-potentials and plane wave basis set, developed mainly in the Joint Research Center for Atom Technology (JRCAT) of the National Institute for Advanced Interdisciplinary Research (NAIR), with helps from many colleagues in Japan. The development of STATE dates back to middle of 1980's and summarized briefly below.

~1985 H. Ishida (Nihon Univ.): A norm-conserving pseudopotential and plane wave code was developed from scratch at the Institute for Solid State Physics, University of Tokyo.

~1990 K. Kobayashi (National Institute for Research on Inorganic Materials): Modified steepest descent algorithm and Kleinman-Bylander type separable pseudopotential scheme.

~1993 Y. Morikawa (JRCAT-NAIR): Ultrasoft-pseudopotential scheme of Vanderbilt.

~1994 T. Yamasaki (Fujitsu Lab.), K. Kato (Toshiba Co. LTD), and Y. Morikawa: Parallelized on the Fujitsu vector parallel computer VPP500 using VPP FORTRAN, Generalized Gradient Correction, and Spin polarization.

~1995 T. Miyazaki (National Research Institute for Metals): Linear tetrahedron.

~1997 H. Sawada (Nippon Steel), J. Lee (Sogang Univ.), and Y. Morikawa: LDA+U scheme.

~1998 Y. Morikawa: Davidson iterative diagonalization scheme for wave function optimization, Blügel method for charge density mixing, generalized direct inversion for iterative diagonalization (GDIIS) scheme for geometry optimization, and Perdew-Wang-Ernzerhof (PBE96) exchange-correlation functional.

~1999 Z. Fang (JRCAT-ATP): Conversion from FORTRAN77 to Fortran 90 for dynamic memory allocation and from VPP FORTRAN to MPI for parallelization.

~1999 T. Sanada (Thinking Machines), Z. Fang, and Y. Morikawa: Residual vector Minimization Method (RMM) and Real space implementation.

~2000 T. Ikeda (JRCAT-ATP) and T. Uchiyama (Matsushita Co. LTD): Nose-Hoover thermostat and blue moon algorithm.

2004~ Y. Morikawa, I. Hamada, and S. Yanagisawa (ISIR, Osaka Univ.): STATE-senri launched. Parallelization on the Earth Simulator, Electric Field Effect and more.

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

## 1.2 Main features

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

- Norm-conserving pseudopotential (Troullier & Martins type) and the ultra-soft pseudopotential (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 the molecular dynamic simulations.
- Automatic  $K$ -points generation with corrected linear tetrahedral method for the  $K$ -space integration.
- Parallelized FFT.
- Parallelization by the MPI so that the code can run on many different parallel 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 the STATE on vector supercomputer 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 by band, so that it can be used efficiently on massive computer like IBM SP.

## 2 Structure of “STATE”

The source of STATE consists of many subroutines, which are all included in one directory with affix “.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 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_size=..., c2=...,....., c10_size=..., c10_size=...)
```

## 3 Running “STATE”

### 3.1 Getting “STATE” source files

Source files of ”STATE” are obtained from tar-zgipped file STATE.tar.gz. Please unzigip 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 directoryy. 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 do just ‘make’ at directory where you copied the source files. Working directory, CPPSRS, 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 attentively prepare the input file in another directories 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 elements 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 input file has a key-word style as follows.

```
! comments
Keyword1      value1      ! comment1
Keyword2      value2      ! comment2
&Keyword3
                Keyword4   value4      ! comment4
                Keyword5   value5      ! comment5
&END_Keyword5
.....
INPUT_END
```

“!” indicates that any words right of it are comments. The meaning of each keyword is explained in the following.

**ENERGY\_CUTOFF\_FOR\_WAVEFUNCTION** Cutoff energy of a plane wave basis set for pseudo-wavefunctions in Ry.

$E_{\text{cut}}^{\text{soft}}$  (Ry) =  $\text{GMAX}^2$ , where GMAX is the cutoff wave number for pseudo-wavefunctions. Wave functions are expanded in a plane wave basis set.

$$\phi_{\vec{k},i} = \sum_{\vec{G}}^{|\vec{k}+\vec{G}| \leq \text{GMAX}} \exp\left(i(\vec{k} + \vec{G}) \cdot \vec{r}\right) \quad (1)$$

$E_{\text{cut}}$  corresponds to the maximum kinetic energy of the basis set.

**ENERGY\_CUTOFF\_FOR\_CHARGE** Cutoff energy of a plane wave basis set for localized charge density in Ry.

$E_{\text{cut}}^{\text{hard}}$  (Ry) =  $\text{GMAXP}^2$ , where GMAXP is the cutoff wave number for localized charge. The charge density is expanded also in a basis set. (See Vanderbilt representation of the real charge density)

**INITIAL\_CONDITION** : Describes initial conditions of calculations. Choose one of the following conditions.

**SCRATCH** Start calculations from scratch.

**RESTART** Restart calculations using previous calculated results.

**CHARGE\_FFT** Calculate partial charge density for STM simulation.

**ALDOS\_CALCULATION** Calculate atom resolved density of states.

The following options are not available now.

**CHARGE\_MAP**

**CHARGE\_CONTINUE**

**DOS\_CALCULATION**

**INITIAL\_POSITIONS** Positions of atoms are read from the following files.

**INPUTS** Input files.

**RESTART** Restart file "restart.data", which is provided by preceding calculations.

**GEOMETRY\_FILE** "GEOMETRY" file which is provided by preceding calculations or modified by users.

**INITIAL\_VELOCITY** Velocities of atoms are read from the following files. At present, this key word does not work.

**INPUTS** Input files.

**RESTART** Restart file "restart.data".

**GEOMETRY\_FILE** "GEOMETRY" file.

**INITIAL\_NOSE\_THERMOSTAT** Specify how to prepare parameters of Nose thermostat.

**INITIALIZE** Initialize.

**RESTART** Read from restart file "restart.data".

**INITIAL\_ACCUMULATOR** Specify accumulation of thermostat average.

**INITIALIZE** Initialize.

**RESTART** Read from restart file "restart.data".

**LEVEL\_OF\_DEBUG\_PRINT** Specify print-out level.

**0** Lower level.

**2** Higher level.

**NUMBER\_OF\_ITERATION\_ELECTRON** Number of iterations for electronic structure optimization.

**TOTAL\_STEP** Total number molecular dynamics steps for ionic degrees of freedom.

**MAX\_CPU\_TIME** Maximum cpu time in seconds.

**WAVEFUNCTION\_OPTIMIZE** Choose one of the following scheme for wavefunction optimization.

**DAVIDSON** Davidson scheme.

**RMM** Residual vector minimization method.

The RMM scheme is fast for nearly converged wavefunctions while it is quite unstable for poorly converged wave functions. Therefore, the Davidson scheme should be chosen for first few iterations if you start calculations from scratch and switch to the RMM scheme.

**NON\_LOCAL\_PSEUDO\_PROJECT** Non-local pseudopotential projection is done in either real-space or fourier space.

**REAL-SPACE** Real space.

**G-SPACE** Fourier space.

**ENERGY\_CRITERIA\_CONVERGENCE\_ELECTRON** Energy criteria for wave-function convergence [in Hartree/atom]. 1.0D-7~1.D-8 is recommended.

**POTENTIAL\_CRITERIA\_CONVERGENCE\_ELECTRON** Energy criteria for wave-function convergence [in Hartree/atom]. It is obsolete.

**MIXING\_WAY** Choose one of the following scheme for charge density or potential mixing.

**SIMPLE** Simple mixing.

**BROYDEN** Broyden scheme.

**BLUGEL** Blügel scheme.

Broyden or Blügel scheme is recommended.

**MIXING\_WHAT** Choose charge density mixing (**CHARGE\_MIXING**) or potential mixing (**POTENTIAL\_MIXING**). Charge mixing is recommended for systems which contain large empty space such as surfaces. Potential mixing is sometimes faster for bulk systems.

**CHARGE\_MIXING\_START** The number of iteration where the mixture should start. Generally, 0 is recommended.

**NUMBER\_OF\_CHARGE\_MIXING** Specify the maximum number of preceding charge or potential data used for mixing. 5 ~ 10 for isolated molecular systems. 20 ~ 30 for metallic systems. ~ 50 for spin-polarized transition metal systems.

**ALPHA\_MIXTURE** The mixture parameter. 0.3 ~ 0.8 for easy systems. 0.05 ~ 0.2 for difficult systems such as spin-polarized systems.

**ENERGY\_WIDTH\_STM** Energy window for STM-imaging in eV.

**EXCHANGE\_CORRELATION\_TYPE** Choose one of the following exchange-correlation energy functional.

**LDAPW91** Local density approximation.

**GGAPBE** Generalized gradient approximation proposed by Perdew, Burke, and Ernzerhof.

**RPBE** Revised version of PBE.

**&SPIN\_POLARIZATION** Choose one of the following spin states.

**PARA** Spin-non-polarized calculation.

**FERRO** Spin-polarized calculation.

**ANTIFERRO** Anti-ferro magnetic system.

For **ANTIFERRO**, specify symmetry operation matrix which transform spin-up charge density to spin-down charge density and vice versa.

**STRESS\_CALCULATION** At present, stress calculation is not available. Therefore, choose "OFF".

**&JOB\_TYPE** Choose one of the following options for ionic degrees of freedom.

**QUENCHING** Structure optimization by quenched molecular dynamics.

**GDIIS** Structure optimization by generalized direct inversion in iterative subspace scheme.

**NORMAL\_MODE** Vibrational normal mode analysis.

**NEB** Optimizing the minimum energy path by using the Nudged Elastic Band Method. Initial and the final states of reaction paths are required.

**FINITE\_TEMPERATURE\_MD** Finite temperature molecular dynamics simulation. For finite temperature md, the following key words should be also specified.

**TEMPERATURE\_CONTROL** Choose one of the following schemes for temperature control.

**NEV** Micro-Canonical Ensemble.

**SIMULATED\_ANNEALING**

**SIMPLE\_VELOCITY\_SCALING**

**NOSE-HOOVER\_CHAIN\_METHOD**

**ROLLING\_AVERAGE\_METHOD**

**GAUSSIAN\_THERMOSTAT**

**GGMT\_METHOD**

**FRICTION\_OF\_LANGEVIN\_EQUATION** Friction coefficient used to generate random forces for Langevin MD.

**TARGET\_TEMPERATURE** Target temperature [K].

**TOLERANCE\_TEMPERATURE** Tolerance of temperature [K]. This variable is used when simple velocity scaling or rolling average method are activated.

**NROLL** Rolling average is taken every nroll MD steps. This short time average of temperature is used to determine a rescaling factor of velocities when **ROLLING\_AVERAGE\_METHOD** is specified. The typical value is 10.

**ANNEAL** Annealing factor. Square root of this factor is multiplied by ionic velocities every MD step when a keyword **SIMULATED\_ANNEALING** is activated.

**CHARACTERISTIC\_FREQUENCY** 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  $\sim 300 \text{ cm}^{-1}$ .

**LENGTH\_OF\_THERMOSTAT\_CHAIN** 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.

**NUMBER\_OF\_YOSHIDA-SUZUKI\_STEPS** 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.

**NUMBER\_OF\_INTEGRATION\_CYCLES** The number of integration cycles for thermostat variables. Usually  $\text{NDRT} = 1$  is enough to integrate thermostat variables

stably.

**&CONSTRAINTS** Specify constraints imposed on ionic degrees of freedom.

**NUMBER\_OF\_CONSTRAINTS** 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).

**TIME\_STEP** Time increment of ions in atomic unit.

**TOLERANCE\_FORCE** Criterion for force in MD in hartree/ $a_B$ .

If the maximum force is smaller than TOLERANCE\_FORCE, the molecular dynamics is terminated.

**SPACE\_GROUP\_NUMBER** At present, the following space group numbers are implemented.

1 ~ 12, 25, 47, 75, 99, 123, 127, 136, 139, 141, 156, 191, 194, 195, 200, 221, 227, 229

**BRAVAIS\_LATTICE SIMPLE**

**BODY\_CENTER**

**FACE\_CENTER**

**A\_CENTER**

**B\_CENTER**

**C\_CENTER**

**RHOMBOHEDRAL\_CENTER**

**&UNIT\_CELL** Specify unit cell parameter.

**a, b, c, alpha, beta, gamma** Lattice parameters and the angles between axis

**&UNIT\_VECTOR** Specify unit vectors. Key word "**&UNIT\_CELL**" and "**&UNIT\_VECTOR**" both specify unit cell but in different way. You can choose one of the two ways. If both key-words are specified, program chooses one which appear earlier than the other.

**&DIPOLE\_CORRECTION** Dipole correction for non-symmetry slab calculations.

**&NUMBER\_K-POINT\_MESH\_XYZ** Specify k-point mesh and sampling scheme. Choose one from the following sampling schemes.

**BROADENING** Broadening. If "Width" is negative, then the Methfessel-Paxton scheme is used for the broadening. If "Width" is positive, parabolic function is used for the broadening.

**TETRAHEDRON** Linear tetrahedron method.

**knx, kny, knz** number of  $K$ -point meshes along each axis

**k-point shift** shift; no shift→1, shifted→2.

**NUMBER\_EIGENVALUES** Number of bands per one spin state.

**&ATOMIC\_TYPES** In this block of items, number of atomic types and their kinds are specified.

**NTYP** Number of types of atoms.

**IATOMN** Atomic number.

**AMION** Atomic mass in the atomic mass unit.

**ZETA** Spin polarization.  $\zeta = (\rho_{\uparrow} - \rho_{\downarrow}) / (\rho_{\uparrow} + \rho_{\downarrow})$ .

**&COORDINATES** In this block of items, number of atoms and their positions are specified.

**NATM, NATM2** Number of atoms in a unit cell.

**CARTESIAN** Atomic positions are given by Cartesian coordinates in Bohr radius unit.

**PRIMITIVE\_CELL** Atomic positions are given by coefficients of primitive cell vectors.

**CONVENTIONAL\_CELL** Atomic positions are given by coefficients of Bravais lattice vectors.

**ninv** Obsolete. Specify always "NO".

**x,y,z** x, y, and z coordinates of atoms.

**IWEI** Obsolete. Specify always "1"

**IMDTYP** If "0" is specified, this atom will be fixed. If "1" is specified, this atom will be moved. If "1000+i, i = 1, 2, ..." is specified, this atom will be attached to  $i$ -th thermostat.

**ITYP** Specify kind of atom.

**&PDOS\_CALCULATION** In this block of items, parameters for projected density of states (PDOS) are specified.

- In the first line, specify number of atoms for which you want to calculate their PDOS.

- In the next lines, specify which atoms you want calculate their PDOS by their numbers.
- Specify lower, and upper boundary of energy window, broadening width, and number of energy mesh.
- Specify cut-off radius and broadening width of atomic wave functions for each type of atoms.
- Specify mesh size and number of meshes.

**&VELOCITIES** Specify initial velocity of each atoms. At present, this item does not work.

## 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
restart.data	This file is necessary to restart the job.
GEOMETRY	The latest atomic coordinates and velocities are written
ENERGIES	Total energy and temperature of the system are written for each step of molecular dynamics simulations

## 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.

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 like

```
> 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 column indicate the number of self consistent iteration, the total energy in hartree unit, the total energy difference between the two successive iterations, and the charge density difference between the two successive iterations, respectively. If the total energy difference becomes smaller than  $NATM2 \times EDELTA$ , the forces acting on atoms will be calculated and the molecular dynamics step will be taken place. 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 the molecular dynamics steps are taken place. You can also check the molecular dynamics steps like

```
> 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 column 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 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

```
> 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 atom, the x, y, z coordinate, and x, y, z forces follow.