M-SPARC

User guide

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Introduction

Matlab-Simulation Package for Ab-initio Real-space Calculations (M-SPARC) is a real-space code for performing electronic structure calculations based on Kohn-Sham Density Functional Theory (DFT). Its primary purpose is the rapid development and testing of new algorithms and methods within DFT. The main features of M-SPARC include

- Applicable to isolated systems such as molecules as well as extended systems such as crystals, surfaces, and wires.
- Local (LDA), semilocal (GGA/meta-GGA), and nonlocal (hybrid) exchange-correlation functionals.
- Standard ONCV pseudopotentials, including nonlinear core corrections (NLCC).
- Calculation of ground state energy, atomic forces, and stress tensor.
- Structural relaxation and ab initio molecular dynamics (NVE).
- Spin polarized and unpolarized calculations.

Introduction

- Spin-orbit coupling (SOC).
- Dispersion interactions through DFT-D3, vdW-DF1, and vdW-DF2.
- Soft and transferable table of SPMS pseudopotentials

Contributors

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  - **Xin Jing**: Hybrid functionals, SOC
  - **Shashikant Kumar**: Testing framework, NLCC

Citation

If you publish work using/regarding M-SPARC, please cite some of the following articles, particularly those that are most relevant to your work:

- General:
  https://doi.org/10.1016/j.softx.2022.101295(v2.0.0),
  https://doi.org/10.1016/j.softx.2020.100423(v1.0.0)
- Non-orthogonal systems:
  https://doi.org/10.1016/j.cplett.2018.04.018
- Linear solvers: https://doi.org/10.1016/j.cpc.2018.07.007,
  https://doi.org/10.1016/j.jcp.2015.11.018
- Stress tensor/pressure: https://doi.org/10.1063/1.5057355
- Atomic forces: https://doi.org/10.1016/j.cpc.2016.09.020,
  https://doi.org/10.1016/j.cpc.2017.02.019

Citation

- Mixing: https://doi.org/10.1016/j.cplett.2016.01.033, https://doi.org/10.1016/j.cplett.2015.06.029, https://doi.org/10.1016/j.cplett.2019.136983
- SPMS pseudopotentials: https://doi.org/10.1016/j.cpc.2022.108594

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Installation

Prerequisite: Matlab
No installation required.

Input files

The required input files to run a simulation with M-SPARC are

- ".inpt" file – User options and parameters.
- ".ion" file – Atomic information.

It is required that the ".inpt" and ".ion" files are located in the same directory and share the same name. A detailed description of the input options is provided in this document. Examples of input files can be found in the directory `M-SPARC/tests`.
In addition, M-SPARC requires pseudopotential files of psp8 format which can be generated by D. R. Hamann's open-source pseudopotential code ONCVPSP. A large number of accurate and efficient pseudopotentials are already provided within the package. For access to more pseudopotentials, the user is referred to the SG15 ONCV potentials. Using the ONCVPSP input files included in the SG15 ONCV potentials, one can easily convert the SG15 ONCV potentials from upf format to psp8 format. Paths to the pseudopotential files are specified in the ".ion" file.

Execution

M-SPARC can be executed in MATLAB by calling the `msparc` function (which is located under `src/` directory). It is required that the ".inpt" and ".ion" files are located in the same directory and share the same name. For example, to run a simulation with input files as "filename.inpt" and "filename.ion" in the `src/` directory, use the following command:

```
S = msparc('filename');
```

In many cases, we would not want to put the input files inside the `src/` directory. In such cases, we need to provide the path to the input file name, without any extension. As an example, one can run a test located in `M-SPARC/tests/Example_tests/`. First go to `src/` directory. Run a DC silicon system by:

```
S = msparc('../tests/Example_tests/Si8_kpt');
```

Execution

The result is printed to output file "Si8_kpt.out", located in the same directory as the input files. If the file "Si8_kpt.out" is already present, the result will be printed to "Si8_kpt.out_1" instead. The max number of ".out" files allowed with the same name is 100. Once this number is reached, the result will instead overwrite the "Si8_kpt.out" file. One can compare the result with the reference out file named "Si8_kpt.refout".

In the `tests/` directory, we also provide a sample script file `run_examples.m`, which launches four example tests one by one. To run these examples, simply change directory to `tests/examples/` directory, and run:

```
run_examples
```

Execution

Note that in this case, we're trying to call the `msparc` function from a different directory. This is achieved by using the MATLAB function `addpath` to add the `src/` directory to search path.
One can also run M-SPARC using the MATLAB parallel pool over k-points/spin by providing a second argument, `parallel_switch`, when running M-SPARC:

```
S = msparc('filename',parallel_switch);
```

Execution

If `parallel_switch = 1`, M-SPARC will start using the parallel pool, and if `parallel_switch = 0`, M-SPARC will not use the parallel pool, which is the default.
A suite of test systems is provided in the `tests/` directory. The test systems are arranged in a hierarchal systems of directories. Input and reference output files for each test system is stored in separate folders with the same name. A python script named `'test.py'` is also provided to launch the tests on a cluster. Details on how to use the Python script can be found in `Readme` file in the `tests/` folder.

Output

Upon successful execution of the "`S = msparc('filename');`" command, an output structure is returned and stored in `S`. The structure `S` contains detailed information that can be useful for post-processing and debugging. Information such as the input parameters, densities, wavefunctions, eigenvalues, and all electronic ground-state properties calculated are stored in the output structure.
Apart from the output structure returned, depending on the calculations performed, some output files will be created in the same location as the input files too.

Single point calculations

- ".out" file – Contains general information about the test, including input parameters, SCF convergence progress, ground state properties and timing information.
- ".static" file – Contains the atomic positions and atomic forces if the user chooses to print these information..

Output

Structrual relaxation calculations

- ".out" file – See above.
- ".geopt" file – Contains the atomic positions and atomic forces for each relaxation step. This file is created only when the unit cell is fixed. For cell relaxation a '.cellopt' file is created instead.
- ".cellopt" file – Contains the cell information (lattice vectors, cell lengths, volume) and stresses for each relaxation step. Only created for cell relaxation.
- ".restart" file – Contains information necessary to perform a restarted structural relaxation calculation.

Molecular dynamics (MD) calculations

- ".out" file – See above.

Output

- “.aimd" file – Contains the atomic positions, atomic velocities, atomic forces, electronic temperature, ionic temperature and total energy for each MD step.
- “.restart" file – Contains information necessary to perform a restarted MD calculation.

Input file options

System

CELL | LATVEC_SCALE | LATVEC | FD_GRID | MESH_SPACING | ECUT | BC | FD_ORDER | EXCHANGE_CORRELATION | SPIN_TYP | KPOINT_GRID | KPOINT_SHIFT | ELEC_TEMP_TYPE | ELEC_TEMP | SMEARING | NSTATES | D3_FLAG | D3_RTHR | D3_CN_THR| VDWDF_GEN_KERNEL | EXX_RANGE_FOCK | EXX_RANGE_PBE | ATOM_TYPE | PSEUDO_POT | N_TYPE_ATOM | COORD | COORD_FRAC | RELAX | SPIN

Input file options

SCF

CHEB_DEGREE | RHO_TRIGGER | NUM_CHEFSI | MAXIT_SCF | TOL_SCF | SCF_FORCE_ACC | SCF_ENERGY_ACC | TOL_LANCZOS | MIXING_VARIABLE | MIXING_HISTORY | MIXING_PARAMETER | MIXING_PARAMETER_SIMPLE | MIXING_PARAMETER_MAG | MIXING_PARAMETER_SIMPLE_MAG | PULAY_FREQUENCY | PULAY_RESTART | MIXING_PRECOND | MIXING_PRECOND_MAG | TOL_PRECOND | PRECOND_KERKER_KTF | PRECOND_KERKER_THRESH | PRECOND_KERKER_KTF_MAG | PRECOND_KERKER_THRESH_MAG | TOL_FOCK | MAXIT_FOCK | MINIT_FOCK | TOL_SCF_INIT | ACE_FLAG | EXX_METHOD | EXX_ACE_VALENCE_STATES | EXX_DOWNSAMPLING | EXX_DIVERGENCE

Input file options

Electrostatics

TOL_POISSON | TOL_PSEUDOCHARGE | REFERENCE_CUTOFF

Stress calculation

CALC_STRESS | CALC_PRES

MD

MD_FLAG | MD_METHOD | MD_NSTEP | MD_TIMESTEP | ION_TEMP | ION_ELEC_EQT | RESTART_FLAG

Input file options

Structural relaxation

RELAX_FLAG | RELAX_METHOD | RELAX_NITER | TOL_RELAX | TOL_RELAX_CELL | RELAX_MAXDIAL | NLCG_SIGMA | L_HISTORY | L_FINIT_STP | L_MAXMOV | L_AUTOSCALE | L_LINEOPT | L_ICURV | FIRE_DT | FIRE_MASS | FIRE_MAXMOV | RESTART_FLAG

Print options

PRINT_ATOMS | PRINT_FORCES | PRINT_MDOUT | PRINT_RELAXOUT | PRINT_RESTART | PRINT_RESTART_FQ | PRINT_VELS | OUTPUT_FILE

System: .inpt file

CELL

Type

Double

Unit

Bohr

Default

None

Example

CELL: 10.20 11.21 7.58

Description

A set of three whitespace delimited values specifying the cell lengths in the lattice vector (LATVEC) directions, respectively.

Remark

Note that CELL ignores the lengths of the lattice vectors specified in the .inpt file and only treats them as unit vectors. LATVEC_SCALE and CELL cannot be specified simultaneously.

LATVEC_SCALE

Type

Double

Unit

Bohr

Default

None

Example

LATVEC_SCALE: 10.20 11.21 7.58

Description

A set of three whitespace delimited values specifying the scaling factors in the lattice vectors (LATVEC), respectively.

LATVEC_SCALE

Remark

The difference between LATVEC_SCALE and CELL is that CELL treats the lattice vectors as unit vectors, whereas LATVEC_SCALE scales the lattice vectors directly as specified by the user. LATVEC_SCALE and CELL cannot be specified simultaneously.

LATVEC

Type

Double array

Unit

No unit

Default

1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0

Example

LATVEC:
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5

Description

A set of three vectors in row major order specifying the lattice vectors of the simulation domain (CELL).

FD_GRID

Type

Integer

Unit

No unit

Default

None

Example

`FD_GRID: 26 26 30`

Description

A set of three whitespace delimited values specifying the number of finite-difference intervals in the lattice vector (LATVEC) directions, respectively.

FD_GRID

Remark

The convergence of results with respect to spatial discretization needs to be verified. ECUT, MESH_SPACING, FD_GRID cannot be specified simultaneously.

MESH_SPACING

Type

Double

Unit

Bohr

Default

None

Example

```
MESH_SPACING: 0.4
```

Description

Mesh spacing of the finite-difference grid.

Remark

The exact mesh-size will be determined by the size of the domain.
MESH_SPACING, FD_GRID, ECUT cannot be specified simultaneously.

ECUT

Type

Double

Unit

Ha

Default

None

Example

ECUT: 30

Description

Equivalent plane-wave energy cutoff, based on which MESH_SPACING will be automatically calculated.

Remark

This is not exact, but rather an estimate. ECUT, MESH_SPACING, FD_GRID cannot be specified simultaneously.

BC

Type

Character

Unit

No unit

Default

None

Example

```
BC: P D D
```

Description

A set of three whitespace delimited characters specifying the boundary conditions in the lattice vector directions, respectively. `P` represents periodic boundary conditions and `D` represents Dirichlet boundary conditions.

FD_ORDER

Type

Integer

Unit

No unit

Default

12

Example

`FD_ORDER: 12`

Description

Order of the finite-difference approximation.

Remark

Restricted to even integers since central finite-differences are employed. The default value of 12 has been found to be an efficient choice for most systems.

EXCHANGE_CORRELATION

Type

String

Unit

No unit

Default

No Default

Example

```
EXCHANGE_CORRELATION: LDA_PW
```

Description

Choice of exchange-correlation functional. Options are `LDA_PW` (Perdew-Wang LDA), `LDA_PZ` (Purdew-Zunger LDA), `GGA_PBE` (PBE GGA), `GGA_RPBE` (PBE RGGA), `GGA_PBEsol` (PBE GGAsol), `vdWDF1` (van der Waals Density Functional developed by Dion et al.), `vdWDF2` (vdW Density Functional modified by Lee et al), `SCAN` (SCAN metaGGA), `RSCAN` (rSCAN metaGGA) and `R2SCAN` (r2SCAN metaGGA).

Remark

For spin-polarized calculation (SPIN_TYP = 1), LDA_PZ is not available.
Before using vdWDF1 or vdWDF2, please read the description and remark of VDWDF_GEN_KERNEL.
Currently SCAN and R2SCAN does not support nonlinear core correction pseudopotential.

SPIN_TYP

Type

Integer

Unit

No unit

Default

0

Example

SPIN_TYP: 1

Description

SPIN_TYP: 0 performs spin unpolarized calculation.
SPIN_TYP: 1 performs unconstrained collinear spin-polarized calculation.
SPIN_TYP: 1 performs unconstrained noncollinear spin-polarized calculation.

SPIN_TYP

Remark

SPIN_TYP can only take values 0, 1, 2. For collinear calculation, non-relativistic pseudopotential need to be used. For noncollinear calculation, fully relativistic pseudopotentiail need to be used.

KPOINT_GRID

Type

Integer array

Unit

No unit

Default

1 1 1

Example

KPOINT_GRID: 2 3 4

Description

Number of k-points in each direction of the Monkhorst-Pack grid for Brillouin zone integration.

Remark

Time-reversal symmetry is assumed to hold.

KPOINT_SHIFT

Type

Double array

Unit

No unit

Default

0.0 0.0 0.0

Example

KPOINT_SHIFT: 0.5 0.5 0.5

Description

Shift of k-points in each direction of the k-point lattice.

Remark

The shift is in reduced coordinates. The default zero shift corresponds to the Monkhorst-Pack grid.

ELEC_TEMP_TYPE

Type

String

Unit

No unit

Default

`gaussian`

Example

```
ELEC_TEMP_TYPE: fd
```

Description

Function used for the smearing (electronic temperature). Options are: `fermi-dirac` (or `fd`), `gaussian`.

Remark

Use ELEC_TEMP or SMEARING to set smearing value.

ELEC_TEMP

Type

Double

Unit

Kelvin

Default

1160.452

Example

```
ELEC_TEMP: 315.773
```

Description

Electronic temperature.

Remark

This is equivalent to setting SMEARING (0.001 Ha = 315.773 Kelvin).

SMEARING

Type

Double

Unit

Ha

Default

0.003675 for `gaussian`
0.007350 for `fermi-dirac`

Example

`SMEARING`: 0.001

Description

Value of smearing.

Remark

Equivalent to setting `ELEC_TEMP` (0.001 Ha = 315.773 Kelvin).

NSTATES

Type

Integer

Unit

No unit

Default

$N_e/2 \times 1.2 + 5$

Example

```
NSTATES: 24
```

Description

The number of Kohn-Sham states/orbitals.

Remark

This number should not be smaller than half of the total number of valence electrons (N_e) in the system. Note that the number of additional states required increases with increasing values of ELEC_TEMP/SMEARING.

D3_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

```
D3_FLAG: 1
```

Description

Flag for adding Grimme's DFT-D3 correction on the result

Remark

Only active when using GGA-PBE, GGA-RPBE and GGA-PBEsol.

D3_RTHR

Type

Double

Unit

$Bohr^2$

Default

1600

Example

```
D3_RTHR: 9000
```

Description

Square of cut-off radius for calculating DFT-D3 correction between two atoms

Remark

Only applicable when DFT-D3 correction D3_FLAG is used.

D3_CN_THR

Type

Double

Unit

Bohr^2

Default

625

Example

```
D3_CN_THR: 1600
```

Description

Square of cut-off radius for calculating CN value of every atom and DFT-D3 correction between three atoms

Remark

Only applicable when DFT-D3 correction D3_FLAG is used.

VDWDF_GEN_KERNEL

Type

0 or 1

Unit

No Unit

Default

0

Example

```
VDWDF_GEN_KERNEL: 1
```

Description

Flag for computing the kernel functions, its 2nd derivatives and the 2nd derivative of spline functions. If 0 is set, the program will read the functions (vdWDF_kernel.mat, vdWDF_d2Phidk2.mat and vdWDF_D2yDx2.mat in \vdW\vdWDF folder) directly; if 1 is set, the program will generate these functions before computation.

EXX_RANGE_FOCK

Type

Double

Unit

No unit

Default

0.1587

Example

```
EXX_RANGE_FOCK: 0.106
```

Description

Short range screen parameter of hartree-fock operator in HSE functional.

Remark

Default is using VASP's value. Different code has different parameters. Be careful with the results.

EXX_RANGE_PBE

Type

Double

Unit

No unit

Default

0.1587

Example

```
EXX_RANGE_PBE: 0.106
```

Description

Short range screen parameter of PBE in HSE functional.

Remark

Default is using VASP's value. Different code has different parameters. Be careful with the results.

System: .ion file

ATOM_TYPE

Type

String

Unit

No unit

Default

None

Example

```
ATOM_TYPE: Fe
```

Description

Atomic type symbol.

Remark

The atomic type symbol can be attached with a number, e.g., Fe1 and Fe2. This feature is useful if one needs to provide two different pseudopotential files (PSEUDO_POT) for the same element.

PSEUDO_POT

Type

String

Unit

No unit

Default

None

Example

```
PSEUDO_POT: ../psp/Fe.psp8
```

Description

Path to the pseudopotential file.

Remark

The default directory for the pseudopotential files is the same as the input files. For example, if a pseudopotential Fe.psp8 is put in the same directory as the input files, one can simply specify `PSEUDO_POT: Fe.psp8`.

N_TYPE_ATOM

Type

Integer

Unit

No unit

Default

None

Example

```
N_TYPE_ATOM: 2
```

Description

The number of atoms of a ATOM_TYPE specified immediately before this variable.

Remark

For a system with different types of atoms, one has to specify the number of atoms for every type.

COORD

Type

Double

Unit

Bohr

Default

None

Example

```
COORD:
0.0 0.0 0.0
2.5 2.5 2.5
```

Description

The Cartesian coordinates of atoms of a ATOM_TYPE specified before this variable. If the coordinates are outside the fundamental domain (see CELL and LATVEC) in the periodic directions (see BC), it will be automatically mapped back to the domain.

COORD

Remark

For a system with different types of atoms, one has to specify the coordinates for every ATOM_TYPE. One can also specify the coordinates of the atoms using COORD_FRAC.

COORD_FRAC

Type

Double

Unit

None

Default

None

Example

```
COORD_FRAC:
0.5 0.5 0.0
0.0 0.5 0.5
```

Description

The fractional coordinates of atoms of a ATOM_TYPE specified before this variable. COORD_FRAC(i, j) $\times$ CELL(j), $(j = 1, 2, 3)$ gives the coordinate of the i^{th} atom along the j^{th} LATVEC direction. If the coordinates are outside the fundamental domain (see CELL and LATVEC) in the periodic directions (see BC), it will be automatically mapped back to the domain.

COORD_FRAC

Remark

For a system with different types of atoms, one has to specify the coordinates for every ATOM_TYPE. One can also specify the coordinates of the atoms using COORD.

RELAX

Type

Integer

Unit

No unit

Default

1 1 1

Example

```
RELAX:
1 0 1
0 1 0
```

Description

Atomic coordinate with the corresponding RELAX value 0 is held fixed during relaxation/MD.

SPIN

Type

Double

Unit

No unit

Default

0.0

Example

```
SPIN:
0 0 1.0
0 0 -1.0
```

Description

Specifies the net initial spin on each atom for a spin-polarized calculation. If collinear spin used, user could use either 1 column of data for z-direction of each atom, or 3 columns of data with 0 on the first 2 columns (x,y-directions). For noncollinear spin, use need to use 3 columns of data for all directions.

SCF

CHEB_DEGREE

Type

Integer

Unit

No unit

Default

Automatically set.

Example

CHEB_DEGEE: 25

Description

Degree of polynomial used for Chebyshev filtering.

Remark

For larger mesh-sizes, smaller values of CHEB_DEGREE are generally more efficient, and vice-versa.

RHO_TRIGGER

Type

Integer

Unit

No unit

Default

4 or 6

Example

```
RHO_TRIGGER: 5
```

Description

The number of times Chebyshev filtering is repeated before updating the electron density in the very first SCF iteration.

RHO_TRIGGER

Remark

Values smaller than the default value of 4 can result in a significant increase in the number of SCF iterations. Larger values can sometimes reduce the number of SCF iterations. For non-collinear spin calculation, default is 6 otherwise 4.

NUM_CHEFSI

Type

Integer

Unit

No unit

Default

1

Example

```
NUM_CHEFSI: 2
```

Description

The number of times ChefSI algorithm is repeated in SCF iteration except the first one, which is controlled by `RHO_TRIGGER`.

Remark

For non-collinear spin calculation, it might helped SCF convergence in some cases.

MAXIT_SCF

Type

Integer

Unit

No unit

Default

100

Example

MAXIT_SCF: 50

Description

Maximum number of SCF iterations.

Remark

Larger values than the default of 100 may be required for highly inhomogeneous systems, particularly when small values of SMEARING/ELEC_TEMP are chosen.

TOL_SCF

Type

Double

Unit

No unit

Default

see description

Example

TOL_SCF: 1e-5

Description

In case of single point calculation, TOL_SCF is set for 10^{-5} Ha/atom energy accuracy. In case of MD, TOL_SCF is set for 10^{-3} Ha/Bohr force accuracy. In case of relaxation, TOL_SCF is set for TOL_RELAX/5 Ha/Bohr force accuracy.
The tolerance on the normalized residual of the effective potential or the electron density for convergence of the SCF iteration.

TOL_SCF

Remark

Only one of TOL_SCF, SCF_ENERGY_ACC, or SCF_FORCE_ACC can be specified.

SCF_FORCE_ACC

Type

Double

Unit

Ha/Bohr

Default

None

Example

```
SCF_FORCE_ACC: 1e-4
```

Description

The tolerance on the atomic forces for convergence of the SCF iteration.

Remark

Only one of SCF_FORCE_ACC, TOL_SCF or SCF_ENERGY_ACC can be specified.

SCF_ENERGY_ACC

Type

Double

Unit

Ha/atom

Default

None

Example

```
SCF_ENERGY_ACC: 1e-5
```

Description

The tolerance on the free energy for the convergence of the SCF iteration.

Remark

Only one of SCF_ENERGY_ACC, SCF_FORCE_ACC, or TOL_SCF can be specified.

TOL_LANCZOS

Type

Double

Unit

No unit

Default

1e-2

Example

`TOL_LANCZOS: 1e-3`

Description

The tolerance within the Lanczos algorithm for calculating the extremal eigenvalues of the Hamiltonian, required as part of the CheFSI method.

Remark

Typically, the Lanczos tolerance does not need to be very strict.

MIXING_VARIABLE

Type

String

Unit

No unit

Default

`potential`

Example

`MIXING_VARIABLE: density`

Description

This specifies whether potential or density mixing is performed in the SCF iteration. Available options are: `potential` and `density`.

MIXING_HISTORY

Type

Integer

Unit

No unit

Default

7

Example

```
MIXING_HISTORY: 40
```

Description

The mixing history used in Pulay mixing.

Remark

Too small values of MIXING_HISTORY can result in poor SCF convergence.

MIXING_PARAMETER

Type

Double

Unit

No unit

Default

0.3

Example

```
MIXING_PARAMETER: 0.1
```

Description

The value of the relaxation parameter used in Pulay/simple mixing.

Remark

Values larger than the default value of 0.3 can be used for insulating systems, whereas smaller values are generally required for metallic systems, particularly at small values of SMEARING or ELEC_TEMP.

MIXING_PARAMETER_SIMPLE

Type

Double

Unit

No unit

Default

Automatically set to the same as MIXING_PARAMETER

Example

```
MIXING_PARAMETER_SIMPLE:
0.1
```

Description

The value of the relaxation parameter used in the simple mixing step in the periodic Pulay scheme.

MIXING_PARAMETER_MAG

Type

Double

Unit

No unit

Default

Automatically set to the same as MIXING_PARAMETER.

Example

```
MIXING_PARAMETER_MAG: 4.0
```

Description

The mixing parameter for the magnetization density in Pulay mixing for spin-polarized calculations.

MIXING_PARAMETER_MAG

Remark

For spin-polarized calculations, when SCF has difficulty to converge, increasing the mixing parameter to magnetization density might help. For example, setting it to 4.0, while turning off the preconditioner applied to the magnetization density (by setting MIXING_PRECOND_MAG to 'none') is a good choice.

MIXING_PARAMETER_SIMPLE_MAG

Type

Double

Unit

No unit

Default

Automatically set to the same as MIXING_PARAMETER_MAG

Example

```
MIXING_PARAMETER_SIMPLE_MAG:
4.0
```

Description

The value of the relaxation parameter for the magnetization density used in the simple mixing step in the periodic Pulay scheme for spin-polarized calculations.

PULAY_FREQUENCY

Type

Integer

Unit

No unit

Default

1

Example

```
PULAY_FREQUENCY: 4
```

Description

The frequency of Pulay mixing in Periodic Pulay.

Remark

The default value of 1 corresponds to Pulay mixing.

PULAY_RESTART

Type

Integer

Unit

No unit

Default

0

Example

```
PULAY_RESTART: 1
```

Description

The flag for restarting the 'Periodic Pulay' mixing. If set to 0, the restarted Pulay method is turned off.

MIXING_PRECOND

Type

String

Unit

No unit

Default

none

Example

`MIXING_PRECOND: kerker`

Description

This specifies the preconditioner used in the SCF iteration. Available options are: `none`, `kerker`, `resta` and `truncated_kerker`.

MIXING_PRECOND_MAG

Type

String

Unit

No unit

Default

none

Example

MIXING_PRECOND_MAG: kerker

Description

This specifies the preconditioner used for the magnetization density in the SCF iteration for spin-polarized calculations. Available options are: none, kerker.

TOL_PRECOND

Type

Double

Unit

No unit

Default

$h^2 \times 0.001$

Example

```
TOL_PRECOND: 1e-4
```

Description

The tolerance on the relative residual for the linear systems arising during the real-space preconditioning of the SCF.

Remark

The linear systems do not need to be solved very accurately. h is the mesh spacing.

PRECOND_KERKER_KTF

Type

Double

Unit

Bohr^{-1}

Default

1.0

Example

```
PRECOND_KERKER_KTF: 0.8
```

Description

The Thomas-Fermi screening length appearing in the `kerker` and `truncated_kerker` preconditioners (MIXING_PRECOND).

PRECOND_KERKER_THRESH

Type

Double

Unit

No unit

Default

0.25

Example

```
PRECOND_KERKER_THRESH: 0.1
```

Description

The threshold for the `truncated_kerker` preconditioner (`MIXING_PRECOND`).

Remark

This threshold will be scaled by the `MIXING_PARAMETER`. If the threshold is set to 0, the `kerker` preconditioner is recovered.

PRECOND_KERKER_KTF_MAG

Type

Double

Unit

Bohr^{-1}

Default

1.0

Example

```
PRECOND_KERKER_KTF_MAG: 0.8
```

Description

The Thomas-Fermi screening length appearing in the `kerker` preconditioner for the magnetization density (MIXING_PRECOND_MAG).

PRECOND_KERKER_THRESH_MAG

Type

Double

Unit

No unit

Default

0.1

Example

```
PRECOND_KERKER_THRESH_MAG: 0.0
```

Description

The threshold for the `kerker` preconditioner the magnetization density (MIXING_PRECOND_MAG).

Remark

This threshold will be scaled by the MIXING_PARAMETER_MAG. If the threshold is set to 0, the original `kerker` preconditioner is recovered.

TOL_FOCK

Type

Double

Unit

No unit

Default

0.2*TOL_SCF

Example

```
TOL_FOCK: 1e-6
```

Description

The tolerance on the Hartree-Fock outer loop, measured by the exact exchange energy difference per atom in 2 consecutive outer loops.

Remark

Only active when using hybrid functionals, like PBE0 and HSE.

MAXIT_FOCK

Type

Integer

Unit

No unit

Default

20

Example

```
MAXIT_FOCK: 50
```

Description

The maximum number of iterations for Hartree-Fock outer loop.

Remark

Only active when using hybrid functionals, like PBE0 and HSE.

MINIT_FOCK

Type

Integer

Unit

No unit

Default

2

Example

```
MINIT_FOCK: 3
```

Description

The minimum number of iterations for Hartree-Fock outer loop.

Remark

Only active when using hybrid functionals, like PBE0 and HSE.

TOL_SCF_INIT

Type

Double

Unit

No unit

Default

max(TOL_FOCK×10, 0.001)

Example

TOL_SCF_INIT: 1e-6

Description

The initial SCF tolerance for PBE iteration when using hybrid functionals.

Remark

Only active when using hybrid functionals, like PBE0 and HSE. Change the TOL_SCF_INIT to change the initial guess for Hartree Fock outer loop.

ACE_FLAG

Type

Integer

Unit

No unit

Default

1

Example

```
ACE_FLAG: 0
```

Description

Use ACE operator to accelarte the hybrid calculation.

Remark

Without ACE operator, the hybrid calculation will be way slower than with it on depending on the system size.

EXX_METHOD

Type

String

Unit

No unit

Default

`FOURIER_SPACE`

Example

`EXX_METHOD: REAL_SPACE`

Description

Methods to solve Poisson's equation in Exact Exchange part. Options include using FFT to solve it in Fourier space and using linear solver, like CG, to solve in Real space.

EXX_METHOD

Remark

Only active when using hybrid functionals for molecule simulation, like PBE0 and HSE. `FOURIER_SPACE` method is much faster than `REAL_SPACE` method.

EXX_MEM

Type

Integer

Unit

No unit

Default

0

Example

```
EXX_MEM: 1
```

Description

Number of Poisson's equations to be solved in each process at a time when creating exact exchange operator or ACE operator. It could be any non negative integer.

Remark

If set to 0, user could get fastest speed but with highest memory requirement. If set to positive integer, user could run large systems with relatively small memory but slower speed.

EXX_ACE_VALENCE_STATES

Type

Integer

Unit

No unit

Default

3

Example

```
EXX_ACE_VALENCE_STATES: 1
```

Description

Control of number of unoccupied states used to construct ACE operator.

Remark

Only active when using hybrid functionals with ACE operator.

EXX_DOWNSAMPLING

Type

Integer

Unit

No unit

Default

1 1 1

Example

```
EXX_DOWNSAMPLING: 1 2 3
```

Description

Down-sampling of k-points grids. There should be 3 nonnegative integers. 0 means using 0 k-point in that direction, requiring 0 is one of the k-point after time-reversal symmetry in that direction. Positive value should be a factor of the number of grid points in that direction.

EXX_DIVERGENCE

Type

String

Unit

No unit

Default

SPHERICAL

Example

```
EXX_DIVERGENCE: AUXILIARY
```

Description

Treatment of divergence in exact exchange. Options are `SPHERICAL` (spherical truncation), `AUXILIARY` (auxiliary function method) and `ERFC` (erfc screening).

EXX_DIVERGENCE

Remark

For systems with cube-like geometry, both methods converge fast. For slab and wire, auxiliary function method is a better option. ERFC screening is the default option for HSE in bulk and molecule simulation.

Electrostatics

TOL_POISSON

Type

Integer

Unit

No unit

Default

TOL_SCF×0.01

Example

```
TOL_POISSON: 1e-6
```

Description

The tolerance on the norm of the relative residual for the Poisson equation.

Remark

The tolerance for poisson solver should not be worse than TOL_SCF, otherwise it might seriously affect the convergence of the SCF iteration.

TOL_PSEUDOCHARGE

Type

Double

Unit

No unit

Default

TOL_SCF×0.001

Example

```
TOL_PSEUDOCHARGE: 1e-6
```

Description

The normalized error in the net enclosed charge for the pseudocharge density of each atom.

REFERENCE_CUTOFF

Type

Double

Unit

Bohr

Default

0.5

Example

```
REFERENCE_CUTOFF: 1.0
```

Description

The cutoff radius of the reference potential used for evaluating the electrostatic correction arising from overlapping pseudocharge densities.

Remark

This number should be smaller than half the smallest interatomic distance.

Stress calculation

CALC_STRESS

Type

0 or 1

Unit

No unit

Default

0

Example

```
CALC_STRESS: 1
```

Description

Flag for calculation of the Hellmann-Feynman stress tensor (in cartesian coordinates).

CALC_PRES

Type

0 or 1

Unit

No unit

Default

0

Example

```
CALC_PRES: 1
```

Description

Flag for calculation of the pressure.

Remark

Pressure is directly calculated, without calculation of the stress tensor.

MD

MD_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

```
MD_FLAG: 1
```

Description

MD simulations are performed if the flag is set to 1.

Remark

MD_FLAG and RELAX_FLAG both cannot be set to 1.

MD_METHOD

Type

String

Unit

No unit

Default

NVE

Example

`MD_METHOD`: NVE

Description

Type of MD to be performed.

Remark

Only NVE (microcanonical ensemble) is supported.

MD_NSTEP

Type

Integer

Unit

No unit

Default

0

Example

MD_NSTEP: 100

Description

Specifies the number of MD steps.

Remark

If MD_NSTEP = N, the MD runs from 0 to $(N-1)\times$ MD_TIMESTEP fs.

MD_TIMESTEP

Type

Double

Unit

Femtosecond

Default

1

Example

```
MD_TIMESTEP: 0.1
```

Description

MD time step.

Remark

Total MD time is given by: MD_TIMESTEP × MD_NSTEP.

ION_TEMP

Type

Double

Unit

Kelvin

Default

No Default

Example

```
ION_TEMP: 315
```

Description

Starting ionic temperature in MD, used to generate initial velocity distribution.

Remark

Must be specified if MD_FLAG is set to 1.

ION_ELEC_EQT

Type

Integer

Unit

No unit

Default

1

Example

```
ION_ELEC_EQT: 0
```

Description

Flag that determines whether the ELEC_TEMP will be set equal to ION_TEMP during MD.

Remark

If the flag is set to 0, the values of ELEC_TEMP and ION_TEMP need to be identical.

RESTART_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

`RESTART_FLAG: 0`

Description

Flag for restarting molecular dynamics and structural relaxation.

Remark

Restarts from the previous configuration which is stored in a .restart file.

Structural relaxation

RELAX_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

```
RELAX_FLAG: 1
```

Description

Flag for performing structural relaxation. 0 means no structural relaxation. 1 represents relaxation of atom positions. 2 represents optimization of volume with the fractional coordinates of the atoms fixed.

Remark

This flag should not be specified if MD_FLAG is set to 1.

RELAX_METHOD

Type

String

Unit

No unit

Default

LBFGS

Example

`RELAX_METHOD`: NLCG

Description

Specifies the algorithm for structural relaxation. The choices are 'LBFGS' (limited-memory BFGS), 'NLCG' (Non-linear conjugate gradient), and 'FIRE' (Fast inertial relaxation engine).

Remark

LBFGS is typically the best choice.

RELAX_NITER

Type

Integer

Unit

No unit

Default

100

Example

```
RELAX_NITER: 25
```

Description

Specifies the maximum number of iterations for the structural relaxation (RELAX_FLAG).

Remark

If RESTART_FLAG is set to 1, then relaxation will restart from the last atomic configuration and run for maximum of RELAX_NITER iterations.

TOL_RELAX

Type

Double

Unit

Ha/Bohr

Default

5e-4

Example

```
TOL_RELAX: 1e-3
```

Description

Specifies the tolerance for termination of the structural relaxation. The tolerance is defined on the maximum force component (in absolute sense) over all atoms.

TOL_RELAX_CELL

Type

Double

Unit

GPa

Default

1e-2

Example

`TOL_RELAX: 1e-3`

Description

Specifies the tolerance for termination of the cell relaxation. The tolerance is defined on the maximum principle stress component.

RELAX_MAXDIAL

Type

Double

Unit

No unit

Default

1.2

Example

```
RELAX_MAXDIAL: 1.4
```

Description

The maximum scaling of the volume allowed with respect to the initial volume defined by CELL and LATVEC. This will determine the upper-bound and lower-bound in the bisection method (Brent's method) for the volume optimization.

NLCG_SIGMA

Type

Double

Unit

No unit

Default

0.5

Example

```
NLCG_SIGMA: 1
```

Description

Parameter in the secant method used to control the step length in NLCG (RELAX_METHOD).

Remark

Default value works well in most cases.

L_HISTORY

Type

Integer

Unit

No unit

Default

20

Example

```
L_HISTORY: 15
```

Description

Size of history in LBFGS (RELAX_METHOD).

Remark

Default value works well in most cases.

L_FINIT_STP

Type

Double

Unit

Bohr

Default

5e-3

Example

```
L_FINIT_STP: 0.01
```

Description

Step length for line optimizer in LBFGS (RELAX_METHOD).

Remark

Default value works well in most cases.

L_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

```
L_MAXMOV: 1.0
```

Description

The maximum allowed step size in LBFGS (RELAX_METHOD).

Remark

Default value works well in most cases.

L_AUTOSCALE

Type

Integer

Unit

No unit

Default

1

Example

```
L_AUTOSCALE: 0
```

Description

Flag for automatically determining the inverse curvature that is used to determine the direction for next iteration in LBFGS (RELAX_METHOD).

Remark

Default works well in most cases.

L_LINEOPT

Type

Integer

Unit

No unit

Default

1

Example

```
L_LINEOPT: 0
```

Description

Flag for atomic force based line minimization in LBFGS (RELAX_METHOD).

Remark

Required only if L_AUTOSCALE is 0.

L_ICURV

Type

Double

Unit

No unit

Default

1.0

Example

```
L_ICURV: 0.1
```

Description

Initial inverse curvature, used to construct the inverse Hessian matrix in LBFGS (RELAX_METHOD).

Remark

Needed only if L_AUTOSCALE is 0. Default value works well in most cases.

FIRE_DT

Type

Double

Unit

Femto second

Default

1

Example

```
FIRE_DT: 0.1
```

Description

Time step used in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

FIRE_MASS

Type

Double

Unit

Atomic mass unit

Default

1.0

Example

```
FIRE_MASS: 2.5
```

Description

Pseudomass used in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

FIRE_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

```
FIRE_MAXMOV: 1.0
```

Description

Maximum movement for any atom in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

Print options

PRINT_ATOMS

Type

0 or 1

Unit

No unit

Default

0

Example

```
PRINT_ATOMS: 1
```

Description

Flag for writing the atomic positions. For ground-state calculations, atom positions are printed to a '.static' output file. For structural relaxation calculations, atom positions are printed to a '.geopt' file. For MD calculations, atom positions are printed to a '.aimd' file.

PRINT_FORCES

Type

0 or 1

Unit

No unit

Default

0

Example

```
PRINT_FORCES: 1
```

Description

Flag for writing the atomic forces. For ground-state calculations, forces are printed to a '.static' output file. For structural relaxation calculations, forces are printed to a '.geopt' file. For MD calculations, forces are printed to a '.aimd' file.

PRINT_MDOUT

Type

0 or 1

Unit

No unit

Default

1

Example

```
PRINT_MDOUT: 0
```

Description

Flag for printing the the MD output into the .aimd file.

PRINT_RELAXOUT

Type

0 or 1

Unit

No unit

Default

1

Example

```
PRINT_RELAXOUT: 0
```

Description

Flag for printing the structural relaxation data in a .geopt file.

Remark

Required only if RELAX_FLAG is set to 1.

PRINT_RESTART

Type

0 or 1

Unit

No unit

Default

1

Example

```
PRINT_RESTART: 0
```

Description

Flag for writing the .restart file, used to restart MD and structural relaxation simulations.

Remark

Relevant only if either MD_FLAG is 1 or RELAX_FLAG is 1.

PRINT_RESTART_FQ

Type

Integer

Unit

No unit

Default

1

Example

PRINT_RESTART_FQ: 10

Description

Frequency at which .restart file is written in MD and structural optimization simulations.

Remark

Relevant only if either MD_FLAG is 1 or RELAX_FLAG is 1.

PRINT_VELS

Type

0 or 1

Unit

No unit

Default

1

Example

```
PRINT_VELS: 0
```

Description

Flag for printing the ion velocities in an MD simulation into the .aimd file.

Remark

Relevant only if MD_FLAG is set to 1.

OUTPUT_FILE

Type

String

Unit

No unit

Default

Same as the input file name

Example

OUTPUT_FILE: myfname

Description

The name of the output files. The output files are attached with a suffix (‘.out’,‘.static’,‘.geopt’ and ‘.aimd’).

OUTPUT_FILE

Remark

If an output file with the same name already exist, the results will be written to a file with a number attached, e.g., 'myfname.out_1'. The maximum number of output files with the same name allowed is 100. After that the output files will be overwritten in succession.