

# M-SPARC

User guide

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[Contributors](#)

[Citation](#)

[Acknowledgements](#)

# 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, 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

- **Phanish Suryanarayana (PI)**
  - **Qimen Xu**: Code infrastructure, SCF, Energy, Force, LDA
  - **Abhiraj Sharma**: Code infrastructure, k-points, PBE, Stress, Non-orthogonal, Relaxation, NLCC
  - **Boqin Zhang**: vdW-DF, DFT-D3, meta-GGA (SCAN)
  - **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.2020.100423>
- 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>
- 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 `msharc` 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 = msharc('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 = msharc('../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 hierarchical 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

## Structural 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 | 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.

## 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.

### 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.

**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), and SCAN (SCAN 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`.



# SPIN\_TYP

Type

0 or 1

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.

Remark

SPIN\_TYP can only take values 0 and 1.

# 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** ( $0.001 \text{ Ha} = 315.773 \text{ Kelvin}$ ).

# 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<sup>2</sup>

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<sup>2</sup>

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.

### 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.  $\text{COORD\_FRAC}(i, j) \times \text{CELL}(j)$ , ( $j = 1, 2, 3$ ) gives the coordinate of the  $i^{\text{th}}$  atom along the  $j^{\text{th}}$  [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.

### 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:

1.0

-1.0

Description

Specifies the net initial spin on each atom for a spin-polarized calculation.

SCF



# CHEB\_DEGREE

Type

Integer

Unit

No unit

Default

Automatically set.

Example

CHEB\_DEGREE: 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

Example

RHO\_TRIGGER: 5

## Description

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

## 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.

# 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

Automatically set for  $10^{-3}$   
Ha/Bohr accuracy in force

### Example

TOL\_SCF: 1e-5

### Description

The tolerance on the normalized residual of the effective potential or the electron density for convergence of the SCF iteration.

### 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.

### 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<sup>-1</sup>

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<sup>-1</sup>

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

$\max(\text{TOL\_FOCK} \times 10, 0.001)$

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.

### 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).

### 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` × 0.01

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  $\text{MD\_NSTEP} = N$ , the MD runs from 0 to  $(N - 1) \times \text{MD\_TIMESTEP}$  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:  $\text{MD\_TIMESTEP} \times \text{MD\_NSTEP}$ .

## 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\_FINISH\_STP

Type

Double

Unit

Bohr

Default

5e-3

Example

L\_FINISH\_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').

### 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.