

# SPARC

Simulation Package for Ab-initio Real-space Calculations

User guide

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[Contributors](#)

[Citation](#)

[Acknowledgements](#)

# Introduction

SPARC is an open-source software package for the accurate, efficient, and scalable solution of the Kohn-Sham density functional theory (DFT) problem. The main features of SPARC currently include

- Applicable to isolated systems such as molecules as well as extended systems such as crystals, surfaces, and wires.
- Local, semilocal, and nonlocal (including hybrid) exchange-correlation functionals.
- Standard ONCV pseudopotentials, including nonlinear core corrections.
- Calculation of ground state energy, atomic forces, and stress tensor.
- Structural relaxation and ab initio molecular dynamics (NVE, NVT, and NPT).
- Spin polarized and unpolarized calculations.
- Spin-orbit coupling.
- Dispersion interactions through DFT-D3, vdW-DF1, and vdW-DF2.

# Introduction

- Symmetry-adaption for cyclic and/or helical symmetries.
- Linear-scaling Spectral Quadrature (SQ) method.
- Soft and transferable table of SPMS pseudopotentials.
- On-the-fly machine-learned force field (MLFF) molecular dynamics (MD) simulations.

# Contributors

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  - **Xin Jing**: Code infrastructure, Hybrid functionals, SOC
  - **Abhiraj Sharma**: Code infrastructure, k-points, PBE, Stress, Non-orthogonal, Relaxation, NLCC
  - **Boqin Zhang**: vdW-DF, DFT-D3, meta-GGA (SCAN)
  - **Shashikant Kumar**: Testing framework, NLCC, MLFF
  - **Mostafa Faghieh Shojaei**: SPMS table of pseudopotentials
  - **Sayan Bhowmik**<sup>1</sup>: Atom code, DFT+U (Dudarev)
  - **Swarnava Ghosh**: Preliminary development
  - **Deepa Phanish**: Initial development
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# Contributors

- **Benjamin Comer**: Code testing, Initial testing framework
- **Sushree Jagriti Sahoo**: Code testing
- **Tian Tian**: Socket communication layer, code testing, Python API
- **Lucas R Timmerman**: Socket communication layer, code testing, Python API
- **Sayan Bhowmik**<sup>1</sup>: Atom code, DFT+U (Dudarev)

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<sup>1</sup>co-advised

# Citation

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

- General: <https://doi.org/10.1016/j.simpa.2024.100649> (v2),  
<https://doi.org/10.1016/j.softx.2021.100709> (v1),  
<https://doi.org/10.1016/j.cpc.2016.09.020> (initial developments, isolated systems),  
<https://doi.org/10.1016/j.cpc.2017.02.019> (initial developments, extended systems)
- 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>

# Citation

- Atomic forces: <https://doi.org/10.1016/j.cpc.2016.09.020> (isolated systems), <https://doi.org/10.1016/j.cpc.2017.02.019> (extended systems)
- Mixing: <https://doi.org/10.1016/j.cplett.2016.01.033>, <https://doi.org/10.1016/j.cplett.2015.06.029> (restarting), <https://doi.org/10.1016/j.cplett.2019.136983> (preconditioning)
- SPMS pseudopotentials: <https://doi.org/10.1016/j.cpc.2022.108594>
- Cyclic and/or helical symmetry: <https://doi.org/10.1103/PhysRevB.103.035101>, <https://doi.org/10.1103/PhysRevB.100.125143> (initial developments, extended systems), <https://doi.org/10.1016/j.jmps.2016.08.007> (initial developments, isolated systems)

# Citation

- O(N) Spectral Quadrature method:  
<https://doi.org/10.1016/j.cpc.2015.11.005> (initial implementation),  
<https://doi.org/10.1016/j.cplett.2013.08.035> (formulation),  
[https://doi.org/10.1007/978-3-031-22340-2\\_12](https://doi.org/10.1007/978-3-031-22340-2_12) (detailed mathematical formulation)
- On-the-fly MLFF: <https://doi.org/10.1063/5.0180541>,  
<https://doi.org/10.1063/5.0204229> (SQ),  
<https://doi.org/10.48550/arXiv.2408.07554> (Cyclix),  
<https://doi.org/10.48550/arXiv.2407.15290> (internal energy)



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# Installation - Option 1

Prerequisite: C compiler, MPI.

There are several options to compile SPARC, depending on the available external libraries.

- Option 1: Compile with BLAS and LAPACK.
  - Step 1: Install/Load OpenBLAS/BLAS and LAPACK.
  - Step 2: Go to `src/` directory, there is an available `makefile`.
  - Step 3 (optional): Edit `makefile`. If the BLAS library path and LAPACK library path are not in the search path, edit the `BLASROOT` and `LAPACKROOT` variables, and add them to `LDFLAGS`. If you are using BLAS instead of OpenBLAS, replace all `-lopenblas` flags with `-lblas`.
  - Step 4 (optional): To turn on `DEBUG` mode, set `DEBUG_MODE` to 1 in the `makefile`.
  - Step 5: Within the `src/` directory, compile the code by  
`$ make clean; make`

# Installation - Option 2

- Option 2 (default): Compile with MKL.
  - Step 1: Install/Load MKL.
  - Step 2: Go to `src/` directory, there is an available `makefile`.
  - Step 3: Edit `makefile`. Set `USE_MKL` to 1 to enable compilation with MKL. If the MKL library path is not in the search path, edit the `MKLROOT` variable to manually set the MKL path.
  - Step 4 (optional): For the projection/subspace rotation step, to use SPARC routines for matrix data distribution rather than ScaLAPACK (through MKL), set `USE_DP_SUBEIG` to 1. We found on some machines this option is faster.
  - Step 5 (optional): To turn on `DEBUG` mode, set `DEBUG_MODE` to 1 in the `makefile`.
  - Step 6: Within the `src/` directory, compile the code by  
`$ make clean; make`

# Installation - Option 3

- Option 3: Compile with BLAS, LAPACK, and ScaLAPACK.
  - Step 1: Install/Load OpenBLAS/BLAS, LAPACK, and ScaLAPACK.
  - Step 2: Go to `src/` directory, there is an available makefile.
  - Step 3: Edit makefile. Set `USE_SCALAPACK` to 1 to enable compilation with ScaLAPACK. If the BLAS library path, LAPACK library path, and/or ScaLAPACK library path are not in the search path, edit the `BLASROOT`, `LAPACKROOT`, and/or `SCALAPACKROOT` variables accordingly, and add them to `LD_FLAGS`. If you are using BLAS instead of OpenBLAS, replace all `-lopenblas` flags with `-lblas`.
  - Step 4 (optional): For the projection/subspace rotation step, to use SPARC routines for matrix data distribution rather than ScaLAPACK, set `USE_DP_SUBEIG` to 1. We found on some machines this option is faster.
  - Step 5 (optional): To turn on DEBUG mode, set `DEBUG_MODE` to 1 in the makefile.
  - Step 6: Within the `src/` directory, compile the code by  
`$ make clean; make`

# Installation - lib

Once compilation is done, a binary named `sparc` will be created in the `lib/` directory.

# Installation - Option 4

- Option 4: Install pre-compiled sparc binaries distributed by conda-forge

Pre-compiled sparc package can be installed on x86\_64 or aarch64 Linux platforms with anaconda or miniconda installed. The binary is compiled with OpenBLAS and OpenMPI using flags `USE_MKL=0` `USE_SCALAPACK=1` `USE_FFTW=1`.

- Step 1 (optional): create a conda environment (e.g. `sparc-env`)  
\$ `conda create -n sparc-env`  
\$ `conda activate sparc-env`
- Step 2: install conda package `sparc-x`  
\$ `conda install -c conda-forge sparc-x`  
\$ `echo sparc binary is located at: $(which sparc)`  
\$ `echo .psp files installed at: $SPARC_PSP_PATH`  
\$ `echo SPARC doc files installed at: $SPARC_DOC_PATH`

# Input files

The required input files to run a simulation with 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 SPARC/tests.

In addition, SPARC requires pseudopotential files of psp8 format which can be generated by D. R. Hamann’s open-source pseudopotential code **ONCVSP**. 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 **ONCVSP** 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

SPARC can be executed in parallel using the `mpirun` command. Sample PBS script files are available in "SPARC/tests" folder. 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 8 processes with input files as "filename.inpt" and "filename.ion" in the root directory (SPARC/), use the following command:

```
$ mpirun -np 8 ./lib/sparc -name filename
```

As an example, one can run one of the tests located in 'SPARC/tests/'. First go to 'SPARC/tests/Example\_tests/' directory:

```
$ cd tests/Example_tests/
```

There are a few input files available. Run a DC silicon system by



# Execution

```
$ mpirun -np 24 ../../lib/sparc -name Si8_kpt
```

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 suite of tests which are arranged in a hierarchy of folders. Each test system has its own directory. A python script is also provided which launches the suite of test systems. To run a set of four quick tests locally on the CPU, simply run:

```
$ python test.py quick_run
```

# Execution

The result is stored in the corresponding directory of the tests. A message is also printed in the terminal showing if the tests passed or failed. The tests can also be launched in parallel on a cluster by using the Python script. Detailed information on using the python script can be found in the 'ReadMe' file in the 'tests/' directory.

# Output

Upon successful execution of the `sparc` code, depending on the calculations performed, some output files will be created in the same location as the input files.

## Single point calculations

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

## Structural relaxation calculations

- “.out” file – See above.

# Output

- “.geopt” file – Atomic positions and atomic forces for atomic relaxation, cell lengths and stress tensor for volume relaxation, and atomic positions, atomic forces, cell dimensions, and stress tensor for full relaxation.
- “.restart” file – Information necessary to perform a restarted structural relaxation calculation. Only created if atomic relaxation is performed.

## Quantum molecular dynamics (QMD) calculations

- “.out” file – See above.
- “.aimd” file – Atomic positions, atomic velocities, atomic forces, electronic temperature, ionic temperature and total energy for each QMD step.
- “.restart” file – Information necessary to perform a restarted QMD 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 | EXX\_RANGE\_FOCK | EXX\_RANGE\_PBE |  
ATOM\_TYPE | PSEUDO\_POT | N\_TYPE\_ATOM | COORD | COORD\_FRAC | RELAX |  
SPIN | HUBBARD\_FLAG | HUBBARD | U\_ATOM\_TYPE | U\_VAL

# Input file options

## SCF

CHEB\_DEGREE | CHEFSI\_BOUND\_FLAG | RHO\_TRIGGER | NUM\_CHEFSI |  
MAXIT\_SCF | MINIT\_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 | FIX\_RAND | TOL\_FOCK | MAXIT\_FOCK |  
MINIT\_FOCK | TOL\_SCF\_INIT | EXX\_ACC | EXX\_METHOD | EXX\_MEM |  
EXX\_FRAC | EXX\_ACE VALENCE\_STATES | EXX\_DOWNSAMPLING |  
EXX\_DIVERGENCE | READ\_INIT\_DENS

# Input file options

## Electrostatics

TOL\_POISSON | MAXIT\_POISSON | TOL\_PSEUDOCARGE |  
REFERENCE\_CUTOFF

## Stress calculation

CALC\_STRESS | CALC\_PRES

## QMD

MD\_FLAG | MD\_METHOD | MD\_NSTEP | MD\_TIMESTEP | ION\_TEMP |  
ION\_TEMP\_END | ION\_VEL\_DSTR | ION\_VEL\_DSTR\_RAND | QMASS |  
NPT\_NH\_QMASS | NPT\_NH\_BMASS | NPT\_NP\_QMASS | NPT\_NP\_BMASS |  
NPT\_SCALE\_VECS | NPT\_SCALE\_CONSTRAINTS | TARGET\_PRESSURE |  
RESTART\_FLAG | TWTIME

# Input file options

## Structural relaxation

RELAX\_FLAG | RELAX\_METHOD | RELAX\_NITER | TOL\_RELAX |  
TOL\_RELAX\_CELL | RELAX\_MAXDILAT | NLCG\_SIGMA | L\_HISTORY |  
L\_FINIT\_STP | L\_MAXMOV | L\_AUTOSCALE | L\_LINEOPT | L\_ICURV |  
FIRE\_DT | FIRE\_MASS | FIRE\_MAXMOV | RESTART\_FLAG

## Band structure

BAND\_STRUCTURE | KPT\_PATHS | KPT\_PER\_LINE | INPUT\_DENS\_FILE



# Input file options

## Print options

PRINT\_ATOMS | PRINT\_FORCES | PRINT\_MDOUT | PRINT\_RELAXOUT |  
PRINT\_RESTART | PRINT\_RESTART\_FQ | PRINT\_VELS | OUTPUT\_FILE |  
PRINT\_EIGEN | PRINT\_DENSITY | PRINT\_ORBITAL |  
PRINT\_ENERGY\_DENSITY

## Parallelization options

NP\_SPIN\_PARAL | NP\_KPOINT\_PARAL | NP\_BAND\_PARAL |  
NP\_DOMAIN\_PARAL | NP\_DOMAIN\_PHI\_PARAL | EIG\_SERIAL\_MAXNS |  
EIG\_PARAL\_BLKSZ | EIG\_PARAL\_ORFAC | EIG\_PARAL\_MAXNP

## Orbital Free DFT

OFDFT\_FLAG | TOL\_OFDFT | OFDFT\_LAMBDA

# Input file options

## Socket communication

`SOCKET_FLAG` | `SOCKET_HOST` | `SOCKET_PORT` | `SOCKET_INET` |  
`SOCKET_MAX_NITER` |

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 (revised PBE GGA), and GGA\_PBEsol (PBE GGA revised for solids), PBE0, HF (Hartree-Fock), HSE, 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. Currently SCAN, RSCAN 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.



### 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 pseudopotential 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 for odd k-point mesh  
0.5 for even k-point mesh

## Example

KPOINT\_SHIFT: 0.5 0.5 0.5

## Description

Shift of k-points with respect to k-point grid containing  $\Gamma$ -point.

## Remark

The shift is in reduced coordinates.

## 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

2320.904 for gaussian

1160.452 for fermi-dirac

Example

ELEC\_TEMP: 315.775

Description

Electronic temperature.

Remark

This is equivalent to setting **SMEARING** (0.001 Ha = 315.775 Kelvin).

# SMEARING

Type

Double

Unit

Ha

Default

0.007350 for gaussian

0.003675 for fermi-dirac

Example

SMEARING: 0.001

Description

Value of smearing.

Remark

Equivalent to setting [ELEC\\_TEMP](#) ( $0.001 \text{ Ha} = 315.775 \text{ Kelvin}$ ).

# 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\_RTHR should be larger or equal to cutoff radius of CN coefficient, [D3\\_CN\\_THR](#).

## 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.  
D3\_CN\_THR should be smaller or equal to cutoff radius of DFT-D3 correction cutoff radius, [D3\\_RTHR](#).

## EXX\_RANGE\_FOCK

Type

Double

Unit

1/Bohr

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 HSE03 value. Different code has different parameters. Be careful with the results.

## EXX\_RANGE\_PBE

Type

Double

Unit

1/Bohr

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 HSE03 value. Different code has different parameters. Be careful with the results.

# HUBBARD\_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

HUBBARD\_FLAG: 1

Description

Flag for adding hubbard correction on top of the [EXCHANGE\\_CORRELATION](#).

Remark

Usually used along with LDA, GGA or SCAN type functionals.

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/QMD.

# 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.

# HUBBARD

Type

None

Unit

No unit

Default

None

Example

HUBBARD:

Description

Start of the DFT+U parameter block. Must be followed by specifying the atoms on which a U correction is desired along with value of U as per Dudarev's scheme.

Remark

**HUBBARD\_FLAG** must be specified to 1 in .inpt file.



## U\_ATOM\_TYPE

Type

String

Unit

No unit

Default

None

Example

U\_ATOM\_TYPE: Ni

### Description

Atomic type symbol for which a U correction is desired. Must be specified within the [HUBBARD](#) block. The atomic type should already have been specified above in the `.ion` file.

## U\_VAL

Type

Double

Unit

Hartree

Default

None

Example

U\_VAL: 0 0 0.1 0

### Description

Value of effective  $U$  for every azimuthal quantum number (s, p, d, and f orbitals) of the atom on which the correction is applied per Dudarev's scheme. The corrections will only be applied to the outermost states available in the corresponding [PSEUDO\\_POT](#). Must be specified after specifying the [U\\_ATOM\\_TYPE](#).

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.

## CHEFSI\_BOUND\_FLAG

Type

Integer

Unit

No unit

Default

0

Example

CHEFSI\_BOUND\_FLAG: 1

### Description

Flag to recalculate the bounds for Chebyshev filtering. If set to 0, then only for the very first SCF will the upper bound be evaluated based on the maximum eigenvalue using Lanczos algorithm, and the upper bound will be the same for the rest steps. If set to 1, the upper bound will be reevaluated for every SCF.

## RHO\_TRIGGER

### Type

Integer

### Unit

No unit

### Default

4, 6, or 10

### 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. For non-collinear spin calculation, default is 6 otherwise 4. For band structure calculations, default is 10.

# 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.

# MINIT\_SCF

Type

Integer

Unit

No unit

Default

3

Example

MAXIT\_SCF: 5

Description

Minimum number of SCF iterations.

## 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.

### 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

density

Example

```
MIXING_VARIABLE:  
potential
```

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

kerker

Example

MIXING\_PRECOND: none

Description

This specifies the preconditioner used in the SCF iteration. Available options are: none, 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 preconditioner ([MIXING\\_PRECOND](#)).

## PRECOND\_KERKER\_THRESH

Type

Double

Unit

No unit

Default

0.1

Example

PRECOND\_KERKER\_THRESH: 0.0

Description

The threshold for the kerker preconditioner ([MIXING\\_PRECOND](#)).

Remark

This threshold will be scaled by the [MIXING\\_PARAMETER](#). If the threshold is set to 0, the original 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.

# FIX\_RAND

Type

Integer

Unit

No unit

Default

0

Example

FIX\_RAND: 1

## Description

Flag to fix the random seeds for setting initial guesses. Once set to 1, the random seeds will be fixed for different runs and for different numbers of processors. This option will make sure the answers will be exactly the same (up to machine precision) when SPARC is executed with different numbers of processors.



# TOL\_FOCK

## Type

Double

## Unit

No unit

## Default

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

## Example

TOL\_FOCK: 1e-6

## Description

The tolerance on the Hartree-Fock outer loop, measured by the difference between the band energy 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

1

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.

## EXX\_ACC

Type

Integer

Unit

No unit

Default

1

Example

EXX\_ACC: 0

Description

Use accelerated method for exact exchange. For low-T, use ACE operator to accelerate the hybrid calculation, while in high-T, use the local projection method.

Remark

Without acceleration, the hybrid functional will be extremely slow.

## EXX\_METHOD

Type

String

Unit

No unit

Default

KRON

Example

EXX\_METHOD: FFT

### Description

Method to solve the Poisson's equations in exact exchange. Options include KRON (Laplacian using kronecker product) and FFT (FFT to solve in Fourier space). Now, KRON is only available for orthogonal periodic cell on gamma point and dirichlet molecule using PBE0. Generally, KRON way is faster than FFT, while FFT is faster on certain type of grid with even number of grid points each direction etc.

## EXX\_MEM

Type

Integer

Unit

No unit

Default

20

Example

EXX\_MEM: 0

### Description

Number of Poisson's equations to be solved in each process at a time when creating exact exchange operator or ACE operator. Typically, when EXX\_MEM is larger than 20, the speed of code is barely affected. When it is 0, all Poisson's equations are solved together and it hits the fastest speed but largest memory requirement. Only effective on low-T calculation.

## EXX\_FRAC

Type

Double

Unit

No unit

Default

0.25 for PBE0 and HSE

Example

EXX\_FRAC: 0.3

Description

Fraction of exact exchange in hybrid functional, e.g. PBE0 and HSE, while the fraction of PBE is 1-EXX\_FRAC



## 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.  
Only effective on low-T calculation.

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. Only effective on low-T calculation.

### Remark

One could only do downsampling on directions of periodic boundary condition.

## 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). Only effective on low-T calculation.

### 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.

## READ\_INIT\_DENS

Type

Integer

Unit

No unit

Default

0

Example

READ\_INIT\_DENS: 1

Description

Flag for reading initial density guess for SCF calculation.

Remark

Please use it together with [INPUT\\_DENS\\_FILE](#)

# 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.



# MAXIT\_POISSON

Type

Integer

Unit

No unit

Default

3000

Example

MAXIT\_POISSON: 1000

Description

The maximum number of iterations for solving the Poisson equation using an iterative linear solver.

## TOL\_PSEUDOCHARGE

Type

Double

Unit

No unit

Default

`TOL_SCF` × 0.001

Example

TOL\_PSEUDOCHARGE: 1e-6

Description

The 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

Integer

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

Integer

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.

QMD

## MD\_FLAG

Type

Integer

Unit

No unit

Default

0

Example

MD\_FLAG: 1

Description

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

Remark

`MD_FLAG` and `RELAX_FLAG` both cannot be set to a value greater than 0.



## MD\_METHOD

Type

String

Unit

No unit

Default

NVT\_NH

Example

MD\_METHOD: NVE

### Description

Type of QMD to be performed. Currently, NVE (microcanonical ensemble), NVT\_NH (canonical ensemble with Nose-Hoover thermostat), NVK\_G (isokinetic ensemble with Gaussian thermostat), NPT\_NH (isothermal-isobaric ensemble with Nose-Hoover thermostat) and NPT\_NP (isothermal-isobaric ensemble with Nose-Poincare thermostat) are supported.

## MD\_NSTEP

Type

Integer

Unit

No unit

Default

1e7

Example

MD\_NSTEP: 100

Description

Specifies the number of QMD steps.

Remark

If  $\text{MD\_NSTEP} = N$ , the QMD 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

QMD time step.

Remark

Total QMD time is given by:  $\text{MD\_TIMESTEP} \times (\text{MD\_NSTEP} - 1)$ .

## ION\_TEMP

Type

Double

Unit

Kelvin

Default

No Default

Example

ION\_TEMP: 315

Description

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

Remark

Must be specified if [MD\\_FLAG](#) is set to 1. It is also the target temperature in [MD\\_METHOD](#) NPT\_NH and NPT\_NP.

## ION\_TEMP\_END

Type

Double

Unit

Kelvin

Default

ION\_TEMP

Example

ION\_TEMP\_END: 100

Description

Specifies the final temperature of the thermostat. Thermostat temperature is varied linearly from [ION\\_TEMP](#) to [ION\\_TEMP\\_END](#) with respect to time.

Remark

Available for NVT\_NH quantum molecular dynamics only. Not supported in NPT\_NH and NPT\_NP.

## ION\_VEL\_DSTR

Type

Integer

Unit

No unit

Default

2

Example

ION\_VEL\_DSTR: 1

Description

Specifies the type of distribution for the initial velocity of atoms based on their initial temperature. Choose 1 for uniform velocity distribution and 2 for Maxwell-Boltzmann distribution.

Remark

Currently, the code supports only two options for the variable.

## ION\_VEL\_DSTR\_RAND

Type

Integer

Unit

No unit

Default

0

Example

ION\_VEL\_DSTR\_RAND: 1

Description

Flag to reseed the initial velocities of atoms in a QMD simulation. Set this flag to 1 to shuffle (change the random seed for) the initial velocities for different runs. Set this flag to 0 to maintain the same initial velocities.

Remark

This option is convenient for parallel statistics calculations.

# QMASS

Type

Double

Unit

atomic unit

Default

1653.654933459720

Example

QMASS: 100000

Description

Gives the inertia factor for Nose Hoover thermostat.

Remark

Applicable to NVT\_NH [MD\\_METHOD](#) only.



# NPT\_NH\_QMASS

## Type

1st number int; others double

## Unit

atomic unit

## Default

No default value

## Example

NPT\_NH\_QMASS: 2 700.0 700.0

## Description

Gives the amount (first number) and inertia masses (others) of thermostats in NPT\_NH. The maximum amount of thermostat variables of the Nose-Hoover chain is 60

## Remark

Applicable to NPT\_NH [MD\\_METHOD](#) only. Program will exit if NPT\_NH is selected but NPT\_NH\_QMASS is not input

# NPT\_NH\_BMASS

Type

Double

Unit

atomic unit

Default

No default value

Example

NPT\_NH\_BMASS: 5000

Description

Gives the inertia mass for the barostat variable in NPT\_NH.

Remark

Applicable to NPT\_NH [MD\\_METHOD](#) only. Program will exit if NPT\_NH is selected but NPT\_NH\_BMASS is not input

## NPT\_NP\_QMASS

Type

Double

Unit

atomic unit

Default

No default value

Example

NPT\_NP\_QMASS: 100

Description

Gives the inertia mass for the thermostat variable in NPT\_NP.

Remark

Applicable to NPT\_NP [MD\\_METHOD](#) only. Program will exit if NPT\_NP is selected but NPT\_NP\_BMASS is not input

## NPT\_NP\_BMASS

Type

Double

Unit

atomic unit

Default

No default value

Example

NPT\_NP\_BMASS: 20

Description

Gives the inertia mass for the barostat variable in NPT\_NP.

Remark

Applicable to NPT\_NP [MD\\_METHOD](#) only. Program will exit if NPT\_NP is selected but NPT\_NP\_BMASS is not input

## NPT\_SCALE\_VECS

Type

Int

Unit

No unit

Default

1 2 3

Example

NPT\_SCALE\_VECS: 2

### Description

Specify which lattice vectors can be rescaled in NPT\_NH and NPT\_NP. The cell will only expand or shrink in the specified directions. Rescaled vectors can be specified for orthogonal systems if NPT\_NP thermostat is used.

### Remark

Only three numbers 1, 2 and 3 can be accepted. For example, if “2 3” is the input, the cell will only expand or shrink in the directions of lattice vector 2 and lattice vector 3.

If it is set in NPT\_NH, the expansion or shrinkage on designated lattice vector will try to keep the total pressure to oscillate near the target pressure.

If it is set in NPT\_NP, the expansion or shrinkage on designated lattice vector will only try to keep the normal stress at their direction to oscillate near the target pressure.

# NPT\_SCALE\_CONSTRAINTS

Type

Double

Unit

No unit

Default

none

Example

NPT\_SCALE\_CONSTRAINTS: 12

## Description

Set the scale constraint for lattice vectors in NPT\_NP. The length ratio between the designated lattice vector keeps constant in NPT\_NP thermostat. For example, if "12" is set, then the length ratio between 1st and 2nd lattice vectors will keep constant.

### Remark

Applicable to orthogonal system using NPT\_NP MD\_METHOD only.

There are 4 types of available constraints. "12" or "21"; "13" or "31"; "23" or "32"; "123" or "132" or "213" or "231" or "312" or "321".



## TARGET\_PRESSURE

Type

Double

Unit

GPa

Default

0.0

Example

TARGET\_PRESSURE: 40.9611

Description

Gives the outer pressure in NPT\_NH and NPT\_NP.

Remark

Applicable to NPT\_NH and NPT\_NP **MD\_METHOD** only.

# RESTART\_FLAG

Type

Integer

Unit

No unit

Default

0

Example

RESTART\_FLAG: 0

Description

Flag for restarting quantum molecular dynamics and structural relaxation. Stores last three histories for quantum molecular dynamics simulations in .restart, .restart-0 and .restart-1 files, respectively.

### Remark

Restarts from the previous configuration which is stored in a .restart file. Currently, code provides restart feature for atomic relaxation and QMD only.

# TWTIME

Type

Double

Unit

min

Default

1e9

Example

TWTIME: 1000

Description

Gives the upper bound on the wall time for quantum molecular dynamics.

# Structural relaxation

## RELAX\_FLAG

Type

Integer

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. 3 represents full optimization of the cell i.e., both atoms and cell volume are relaxed

### 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

300

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\_MAXDILAT

Type

Double

Unit

No unit

Default

1.06

Example

RELAX\_MAXDILAT: 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.

# Band structure

## BAND\_STRUCTURE

Type

Integer

Unit

No unit

Default

0

Example

BAND\_STRUCTURE: 1

Description

Flag for calculation of the band structure.

# KPT\_PATHS

Type

Double

Unit

No unit

Default

None

Example

```
KPT_PATHS: 2  
0.0 0.0 0.0 # Gamma  
0.5 0.5 0.5 # A  
0.5 0.5 0.5 # A  
0.5 0.5 0.0 # M
```

Description

The k-point paths (high-symmetry lines) for band structure calculations. It starts with the total number of high-symmetry lines, followed by fractional coordinates indicating the start and end points of each line.



## KPT\_PER\_LINE

Type

Integer

Unit

No unit

Default

10

Example

KPT\_PER\_LINE: 15

Description

The number of k-points on each high-symmetry line.

Remark

This value accounts for both endpoints of the high-symmetry line.

# INPUT\_DENS\_FILE

Type

String

Unit

No unit

Default

None

Example

INPUT\_DENS\_FILE: Si.dens  
Si.densUp Si.densDwn

Description

The name of the input density file(s) in cube format.

Remark

For spin-unpolarized systems, only the total density file is required. For spin-polarized systems, three density files are required, which are the total electron density, spin-up density, and spin-down density, respectively.

# 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 QMD 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 QMD 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 QMD 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 greater than 0.

# 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 QMD 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 QMD 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 QMD 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.

# PRINT\_EIGEN

Type

int

Unit

No unit

Default

0

Example

PRINT\_EIGEN: 1

Description

Flag for writing eigenvalues and occupations into .eigen file.

# PRINT\_DENSITY

Type

int

Unit

No unit

Default

0

Example

PRINT\_DENSITY: 1

## Description

Flag for writing electron density into cube format. For spin-unpolarized calculation, electron density is printed into .dens file. For collinear spin calculation, total, spin-up and spin-down electron density are printed into .dens, .densUp and .densDwn file, respectively.

## PRINT\_ORBITAL

Type

int

Unit

No unit

Default

0

Example

PRINT\_ORBITAL: 1

Description

Flag for writing Kohn-Sham orbitals into a binary file.

## Remark

It consists of headers with system information and the orbitals. First define a few variables and their types.

name	type, length	description
Nx Ny Nz	int, 1	Number of FD nodes in x,y,z directions
Nd	int, 1	Total number of FD nodes
dx, dy,dz	double, 1	mesh size in x,y,z directions
dV	double, 1	unit Volume
Nspinor	int, 2	Number of spinor in orbitals
isReal	int, 1	Flag for orbitals being real or complex
nspin	int, 1	Number of spin channel printed
nkpt	int, 1	Number of k-point printed



## Remark – cont.

nband	int, 1	Number of bands printed
name	type, length	description
spin_index	int, 1	spin index of specific orbital
kpt_index	int, 1	k-point index of specific orbital
kpt_vec	double, 3	k-point in reduced coordinates
band_index	int, 1	band index of specific orbital
psi_real	double, Nd	real Kohn-Sham orbitals
psi_complex	double complex, Nd	complex Kohn-Sham orbitals

The header is organized as: Nx, Ny, Nz, Nd, dx, dy, dz, dV, Nspinor, isReal, nspin, nkpt, nband, followed by the data for Kohn-sham orbital. Below is the pseudo-code to read orbitals after reading variables in headers.

## Remark – cont.

```
for ispin = 1:nspin do
  for ikpt = 1:nkpt do
    for iband = 1:nband do
      spin_index, kpt_index, kpt_vec, band_index
      if isReal == 1 then
        psi_real
      else
        psi_complex
      end if
    end for
  end for
end for
```

# PRINT\_ENERGY\_DENSITY

Type

int

Unit

No unit

Default

0

Example

PRINT\_ENERGY\_DENSITY: 1

## Description

Flag for writing a few energy densities into cube format. Currently, only kinetic energy density, exchange correlation energy density (without exact exchange contribution) and exact exchange energy density (if any) are implemented.

### Remark

For spin-unpolarized calculation, kinetic energy density is written into .kedens, exchange correlation energy density is written into .xcedens, and exact exchange energy density is written into .exxedens. For collinear spin calculation, total, spin-up, spin-down kinetic energy density are written into .kedens, kedensUp, kedensDwn files, total, spin-up, spin-down exact exchange energy density are written into .exxedens, .exxedensUp, .exxedensDwn files, respectively.

# Parallelization options

## NP\_SPIN\_PARAL

Type

Integer

Unit

No unit

Default

Automatically optimized

Example

NP\_SPIN\_PARAL: 2

Description

Number of spin groups.

Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.

# NP\_KPOINT\_PARAL

Type

Integer

Unit

No unit

Default

Automatically optimized

Example

NP\_KPOINT\_PARAL: 5

Description

Number of k-point groups.

Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.

## NP\_BAND\_PARAL

Type

Integer

Unit

No unit

Default

Automatically optimized

Example

NP\_BAND\_PARAL: 5

Description

Number of band groups.

Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.



## NP\_DOMAIN\_PARAL

Type

Integer

Unit

No unit

Default

Automatically optimized

Example

NP\_DOMAIN\_PARAL: 3 3 2

Description

Dimensions of the 3D Cartesian topology embedded in each band group.

Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.

## NP\_DOMAIN\_PHI\_PARAL

### Type

Integer

### Unit

No unit

### Default

Automatically optimized

### Example

NP\_DOMAIN\_PHI\_PARAL: 1 1 2

### Description

Dimensions of the 3D Cartesian topology embedded in the global communicator.

### Remark

This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.

# EIG\_SERIAL\_MAXNS

Type

Integer

Unit

No unit

Default

2000

Example

EIG\_SERIAL\_MAXNS: 1000

## Description

Maximum **NSTATES** value up to which a serial algorithm will be used to solve the subspace eigenproblem.

## Remark

If one wants to use a parallel algorithm to solve the subspace eigenproblem for all cases, simply set EIG\_SERIAL\_MAXNS to 0. Alternatively, set EIG\_SERIAL\_MAXNS to a very large value to always use serial algorithm.

## EIG\_PARAL\_BLKSZ

Type

Integer

Unit

No unit

Default

128

Example

EIG\_PARAL\_BLKSZ: 64

Description

Block size for the distribution of matrix in block-cyclic format in a parallel algorithm for solving the subspace eigenproblem.

## EIG\_PARAL\_ORFAC

Type

Double

Unit

No unit

Default

0.0

Example

EIG\_PARAL\_ORFAC: 0.001

### Description

Specifies which eigenvectors should be reorthogonalized when using the parallel eigensolver `p?syevx` or `p?sygvx` for solving the subspace eigenproblem. The parallel eigensolvers can be turned on using the `EIG_SERIAL_MAXNS` flag. No reorthogonalization will be done if `EIG_PARAL_ORFAC` equals zero. A default value of 0.001 is used if `EIG_PARAL_ORFAC` is negative. Note that reorthogonalization of eigenvectors is extremely time-consuming.

## EIG\_PARAL\_MAXNP

### Type

Integer

### Unit

No unit

### Default

Generated by a linear model.

### Example

EIG\_PARAL\_MAXNP: 36

### Description

Maximum number of processors used in parallel eigensolver. The number is machine dependent. Users could provide their own value for best performance.

# Orbital Free DFT

# Comments

The code will fail with the following options if OFDFT is activated and the related input options are listed.

- Polarized calculation: `SPIN_TYP`.
- K-point calculation: `KPOINT_GRID`, `KPOINT_SHIFT`.
- Dirichlet boundary condition in any direction: `BC`
- Define number of states/orbitals: `NSTATES`
- Define SCF related variables: `TOL_SCF`, `CHEB_DEGREE`
- CS and SQ3 method: `CS_FLAG`, `SQ3_FLAG`
- Hybrid functionals: `EXCHANGE_CORRELATION`
- Stress and pressure calculation: `CALC_STRESS`, `CALC_PRES`
- Print eigenvalues into file: `PRINT_EIGEN`



## OFDFT\_FLAG

Type

Integer

Unit

No unit

Default

0

Example

OFDFT\_FLAG: 1

Description

Flag for Orbital-free DFT calculation.

## TOL\_OFDFT

Type

Double

Unit

No unit

Default

$10^{-3}$

Example

TOL\_OFDFT: 1E-6

Description

The tolerance on the normalized residual (l2-norm of residual/sqrt(N), N is number of nodes) for convergence of NLCG.

## OFDFT\_LAMBDA

Type

Double

Unit

No unit

Default

0.2

Example

OFDFT\_LAMBDA: 0.3

Description

The coefficient in front of Laplacian operator is  $-\lambda/2$ .

# Socket communication in SPARC

# Brief introduction

The socket communication layer allows SPARC to be controlled by a socket server that is compatible with **i-PI** protocol. The SPARC source code should be compiled with the `USE_SOCKET=1` option.

To start a SPARC program with socket interface, use either option:

- Option 1: Specify socket address in command line
  - To start an INET socket, use

```
$ mpirun -n 8 ./lib/sparc -socket localhost:12345 -name filename
```
  - To start a UNIX socket, use

```
$ mpirun -n 8 ./lib/sparc -socket /tmp/sparc.socket:unix -name filename
```
- Option 2: Provide `.inpt` parameters

Visit the following pages for parameter specifications. Any parameter `SPARC_*` in the `.inpt` file will overwrite the settings from command line.

# Output files

The following files will be generated in the socket mode and may slightly differ from standard SPARC outputs:

- `.out`: All the SCF steps will be written to `.out` file, similar to a relaxation / MD calculation.
- `.static`: It is concatenated from all single point steps. In addition to normal `.static` output, the lattice information are also recorded.

# SOCKET\_FLAG

## Type

Integer

## Unit

No unit

## Default

0

## Example

SOCKET\_FLAG: 1

## Description

Flag for starting the socket communication layer. It is equivalent to the `-socket` switch of command line.

Setting SOCKET\_FLAG: 1 will disable MD\_FLAG and RELAX\_FLAG.

## SOCKET\_HOST

Type

String

Unit

No unit

Default

localhost

Example

SOCKET\_HOST: 127.0.0.1

Description

Host name of the socket address that SPARC listens to. If it's an INET socket, it is the address of the interface. For a UNIX socket, it is the filename of the socket file (e.g. /tmp/sparc.socket).



# SOCKET\_PORT

## Type

Integer

## Unit

No unit

## Default

None

## Example

SOCKET\_PORT: 12345

## Description

When SPARC connects to an INET socket server, it is the port number. The SOCKET\_PORT has no effect for a UNIX socket.

# SOCKET\_INET

## Type

Integer

## Unit

No unit

## Default

None

## Example

SOCKET\_INET: 0

## Description

1 for INET socket, 0 for UNIX socket. If no set in `.inpt` file, its value is determined by the `-socket address:port` command line switch.

## SOCKET\_MAX\_NITER

Type

Integer

Unit

No unit

Default

10000

Example

SOCKET\_MAX\_NITER: 10000

Description

Maximum number of ionic SCF steps in the socket mode. As a socket client, SPARC will terminate after SOCKET\_MAX\_NITER steps are called.