SPARC

Simulation Package for Ab-initio Real-space Calculations

User guide

Material Physics & Mechanics Group, Georgia Tech
PI: Phanish Suryanarayana

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.

Contributors

- **Phanish Suryanarayana** (PI)
  - **Qimen Xu**: Code infrastructure, SCF, Energy, Force, LDA
  - **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
  - **Mostafa Faghih Shojaei**: SPMS table of pseudopotentials
  - **Swarnava Ghosh**: Preliminary development
  - **Deepa Phanish**: Initial development
- **John E. Pask** (co-PI)
- **Edmond Chow** (co-PI)
  - **Hua Huang**: Subspace eigensolver, DP
  - **Lucas Erlandson**: Subspace eigensolver, DP
- **Andrew J. Medford** (co-PI)
  - **Benjamin Comer**: Code testing, Initial testing framework
  - **Sushree Jagriti Sahoo**: Code testing

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.softx.2021.100709, https://doi.org/10.1016/j.cpc.2016.09.020, https://doi.org/10.1016/j.cpc.2017.02.019
- Non-orthogonal systems: https://doi.org/10.1016/j.cplett.2018.04.018
- Linear solvers: https://doi.org/10.1016/j.cpc.2018.07.007, https://doi.org/10.1016/j.jcp.2015.11.018
- Stress tensor/pressure: https://doi.org/10.1063/1.5057355
- Atomic forces: https://doi.org/10.1016/j.cpc.2016.09.020, https://doi.org/10.1016/j.cpc.2017.02.019

Citation

- Mixing: https://doi.org/10.1016/j.cplett.2016.01.033, https://doi.org/10.1016/j.cplett.2015.06.029, https://doi.org/10.1016/j.cplett.2019.136983
- SPMS pseudopotentials: https://doi.org/10.1016/j.cpc.2022.108594
- Cyclic and/or helical symmetry: https://doi.org/10.1103/PhysRevB.103.035101, https://doi.org/10.1103/PhysRevB.100.125143
- O(N) Spectral Quadrature method: https://doi.org/10.1016/j.cpc.2015.11.005, https://doi.org/10.1016/j.cplett.2013.08.035, https://doi.org/10.1007/978-3-031-22340-2_12

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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 `LDFLAGS`. 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 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

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

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 | ACE_FLAG | EXX_METHOD | EXX_MEM | EXX_FRAC | EXX_ACE_VALENCE_STATES | EXX_DOWNSAMPLING | EXX_DIVERGENCE

Input file options

Electrostatics

TOL_POISSON | MAXIT_POISSON | TOL_PSEUDOCHARGE | 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

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	Unit
Double	Bohr

Default	Example
None	LATVEC_SCALE: 10.20 11.21 7.58

Description

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

LATVEC_SCALE

Remark

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

LATVEC

Type

Double array

Unit

No unit

Default

1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0

Example

LATVEC:
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5

Description

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

FD_GRID

Type

Integer

Unit

No unit

Default

None

Example

`FD_GRID: 26 26 30`

Description

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

FD_GRID

Remark

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

MESH_SPACING

Type

Double

Unit

Bohr

Default

None

Example

```
MESH_SPACING: 0.4
```

Description

Mesh spacing of the finite-difference grid.

Remark

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

ECUT

Type

Double

Unit

Ha

Default

None

Example

ECUT: 30

Description

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

Remark

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

BC

Type

Character

Unit

No unit

Default

None

Example

```
BC: P D D
```

Description

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

FD_ORDER

Type

Integer

Unit

No unit

Default

12

Example

```
FD_ORDER: 12
```

Description

Order of the finite-difference approximation.

Remark

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

EXCHANGE_CORRELATION

Type

String

Unit

No unit

Default

No Default

Example

```
EXCHANGE_CORRELATION: LDA_PW
```

Description

Choice of exchange-correlation functional. Options are `LDA_PW` (Perdew-Wang LDA), `LDA_PZ` (Purdew-Zunger LDA), `GGA_PBE` (PBE GGA), `GGA_RPBE` (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.

SPIN_TYP

Remark

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

KPOINT_GRID

Type

Integer array

Unit

No unit

Default

1 1 1

Example

KPOINT_GRID: 2 3 4

Description

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

Remark

Time-reversal symmetry is assumed to hold.

KPOINT_SHIFT

Type

Double array

Unit

No unit

Default

0.0 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 Γ-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 Ha = 315.775 Kelvin).

NSTATES

Type

Integer

Unit

No unit

Default

$N_e/2 \times 1.2 + 5$

Example

```
NSTATES: 24
```

Description

The number of Kohn-Sham states/orbitals.

Remark

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

D3_FLAG

Type

0 or 1

Unit

No unit

Default

0

Example

```
D3_FLAG: 1
```

Description

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

Remark

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

D3_RTHR

Type

Double

Unit

Bohr^2

Default

1600

Example

```
D3_RTHR: 9000
```

Description

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

Remark

Only applicable when DFT-D3 correction D3_FLAG is used.
D3_RTHR should be larger or equal to cutoff radius of CN coefficient, D3_CN_THR.

D3_CN_THR

Type

Double

Unit

Bohr^2

Default

625

Example

```
D3_CN_THR: 1600
```

Description

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

Remark

Only applicable when DFT-D3 correction D3_FLAG is used.
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.

System: .ion file

ATOM_TYPE

Type

String

Unit

No unit

Default

None

Example

```
ATOM_TYPE: Fe
```

Description

Atomic type symbol.

Remark

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

PSEUDO_POT

Type

String

Unit

No unit

Default

None

Example

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

Description

Path to the pseudopotential file.

Remark

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

N_TYPE_ATOM

Type

Integer

Unit

No unit

Default

None

Example

```
N_TYPE_ATOM: 2
```

Description

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

Remark

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

COORD

Type

Double

Unit

Bohr

Default

None

Example

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

Description

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

COORD

Remark

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

COORD_FRAC

Type

Double

Unit

None

Default

None

Example

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

Description

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

COORD_FRAC

Remark

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

RELAX

Type

Integer

Unit

No unit

Default

1 1 1

Example

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

Description

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

SCF

CHEB_DEGREE

Type

Integer

Unit

No unit

Default

Automatically set.

Example

CHEB_DEGEE: 25

Description

Degree of polynomial used for Chebyshev filtering.

Remark

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

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.

RHO_TRIGGER

Remark

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

TOL_SCF

Remark

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

SCF_FORCE_ACC

Type

Double

Unit

Ha/Bohr

Default

None

Example

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

Description

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

Remark

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

SCF_ENERGY_ACC

Type

Double

Unit

Ha/atom

Default

None

Example

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

Description

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

Remark

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

TOL_LANCZOS

Type

Double

Unit

No unit

Default

1e-2

Example

`TOL_LANCZOS: 1e-3`

Description

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

Remark

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

MIXING_VARIABLE

Type

String

Unit

No unit

Default

`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.

MIXING_PARAMETER_MAG

Remark

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

MIXING_PARAMETER_SIMPLE_MAG

Type

Double

Unit

No unit

Default

Automatically set to the same as MIXING_PARAMETER_MAG

Example

```
MIXING_PARAMETER_SIMPLE_MAG:
4.0
```

Description

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

PULAY_FREQUENCY

Type

Integer

Unit

No unit

Default

1

Example

```
PULAY_FREQUENCY: 4
```

Description

The frequency of Pulay mixing in Periodic Pulay.

Remark

The default value of 1 corresponds to Pulay mixing.

PULAY_RESTART

Type

Integer

Unit

No unit

Default

0

Example

```
PULAY_RESTART: 1
```

Description

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

MIXING_PRECOND

Type

String

Unit

No unit

Default

`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^{-1}

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^{-1}

Default

1.0

Example

```
PRECOND_KERKER_KTF_MAG: 0.8
```

Description

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

PRECOND_KERKER_THRESH_MAG

Type

Double

Unit

No unit

Default

0.1

Example

```
PRECOND_KERKER_THRESH_MAG: 0.0
```

Description

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

Remark

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

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

0.2*TOL_SCF

Example

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

Description

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

Remark

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

MAXIT_FOCK

Type

Integer

Unit

No unit

Default

20

Example

```
MAXIT_FOCK: 50
```

Description

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

Remark

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

MINIT_FOCK

Type

Integer

Unit

No unit

Default

2

Example

```
MINIT_FOCK: 3
```

Description

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

Remark

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

TOL_SCF_INIT

Type

Double

Unit

No unit

Default

max(TOL_FOCK×10, 0.001)

Example

TOL_SCF_INIT: 1e-6

Description

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

Remark

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

ACE_FLAG

Type

Integer

Unit

No unit

Default

1

Example

```
ACE_FLAG: 0
```

Description

Use ACE operator to accelarte the hybrid calculation.

Remark

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

EXX_METHOD

Type

String

Unit

No unit

Default

`FOURIER_SPACE`

Example

`EXX_METHOD: REAL_SPACE`

Description

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

EXX_METHOD

Remark

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

EXX_MEM

Type

Integer

Unit

No unit

Default

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.

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.

Remark

Only active when using hybrid functionals with ACE operator.

EXX_DOWNSAMPLING

Type

Integer

Unit

No unit

Default

1 1 1

Example

```
EXX_DOWNSAMPLING: 1 2 3
```

Description

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

EXX_DIVERGENCE

Type

String

Unit

No unit

Default

SPHERICAL

Example

```
EXX_DIVERGENCE: AUXILIARY
```

Description

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

EXX_DIVERGENCE

Remark

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

Electrostatics

TOL_POISSON

Type

Integer

Unit

No unit

Default

TOL_SCF×0.01

Example

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

Description

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

Remark

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

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 MD_NSTEP = N, the QMD runs from 0 to $(N-1)\times$ 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: MD_TIMESTEP × (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.

NPT_SCALE_VECS

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.

NPT_SCALE_CONSTRAINTS

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.

RESTART_FLAG

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_FINIT_STP

Type

Double

Unit

Bohr

Default

5e-3

Example

L_FINIT_STP: 0.01

Description

Step length for line optimizer in LBFGS (RELAX_METHOD).

Remark

Default value works well in most cases.

L_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

```
L_MAXMOV: 1.0
```

Description

The maximum allowed step size in LBFGS (RELAX_METHOD).

Remark

Default value works well in most cases.

L_AUTOSCALE

Type

Integer

Unit

No unit

Default

1

Example

```
L_AUTOSCALE: 0
```

Description

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

Remark

Default works well in most cases.

L_LINEOPT

Type

Integer

Unit

No unit

Default

1

Example

```
L_LINEOPT: 0
```

Description

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

Remark

Required only if L_AUTOSCALE is 0.

L_ICURV

Type

Double

Unit

No unit

Default

1.0

Example

```
L_ICURV: 0.1
```

Description

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

Remark

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

FIRE_DT

Type

Double

Unit

Femto second

Default

1

Example

```
FIRE_DT: 0.1
```

Description

Time step used in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

FIRE_MASS

Type

Double

Unit

Atomic mass unit

Default

1.0

Example

```
FIRE_MASS: 2.5
```

Description

Pseudomass used in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

FIRE_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

```
FIRE_MAXMOV: 1.0
```

Description

Maximum movement for any atom in FIRE (RELAX_METHOD).

Remark

Default value works well in most cases.

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’).

OUTPUT_FILE

Remark

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

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.

PRINT_ORBITAL

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.

PRINT_ENERGY_DENSITY

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 writted 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.