

SPARC

Simulation Package for Ab-initio Real-space Calculations

User guide

Material Physics & Mechanics Group

PI: Phanish Suryanarayana

Main Developers: Qimen Xu, Abhiraj Sharma

Collaborators: J.E. Pask (LLNL), A.J. Medford (GT), E. Chow (GT)

Georgia Institute of Technology

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

- Isolated systems such as molecules and clusters as well as extended systems such as crystals, surfaces, and wires.
- Calculation of ground state energy, atomic forces, and stress tensor.
- Unconstrained collinear magnetization via spin polarized calculations.
- Structural relaxation and quantum molecular dynamics (QMD).
- Local and semilocal exchange correlation functionals.
- ONCV and TM pseudopotentials in psp8 (ABINIT) format.

Additional details regarding the formulation and implementation of SPARC can be found in the accompanying paper. Please direct any questions and report any bugs to Prof. Phanish Suryanarayana.

Acknowledgments

- U.S. Department of Energy, Office of Science: DE-SC0019410
- U.S. National Science Foundation: 1553212, 1663244, and 1333500

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>
- 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>

Installation - Option 1

Prerequisite: C compiler, MPI.

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

- Option 1 (default): 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 (recommended): 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.

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

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

Execution

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

In the tests/ directory, we also provide a 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 | VDWDF_GEN_KERNEL
ATOM_TYPE | PSEUDO_POT | N_TYPE_ATOM | COORD | COORD_FRAC | RELAX |
SPIN

Input file options

SCF

CHEB_DEGREE | CHEFSI_BOUND_FLAG | RHO_TRIGGER | 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

Electrostatics

TOL_POISSON | MAXIT_POISSON | TOL_PSEUDOCARGE |
REFERENCE_CUTOFF

Input file options

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 | TARGET_PRESSURE | RESTART_FLAG | TWTIME

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

Input file options

Print options

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

Parallelization options

NP_SPIN_PARAL | NP_KPOINT_PARAL | NP_BAND_PARAL | NP_DOMAIN_PARAL
| NP_DOMAIN_PHI_PARAL | EIG_SERIAL_MAXNS | EIG_PARAL_BLKSZ

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_PBEso1 (PBE GGA revised for solids), vdWDF1 (van der Waals Density Functional developed by Dion et al.), vdWDF2 (vdW Density Functional modified by Lee et al).

Remark

For spin-polarized calculation ([SPIN_TYP](#) = 1), LDA_PZ, vdWDF1, vdWDF2 are not available. Before using vdWDF1 or vdWDF2, please read the description and remark of [VDWDF_GEN_KERNEL](#) to see the requirements.

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.

Remark

SPIN_TYP can only take values 0 and 1.

KPOINT_GRID

Type

Integer array

Unit

No unit

Default

1 1 1

Example

KPOINT_GRID: 2 3 4

Description

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

Remark

Time-reversal symmetry is assumed to hold.

KPOINT_SHIFT

Type

Double array

Unit

No unit

Default

0.0 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** ($0.001 \text{ Ha} = 315.775 \text{ Kelvin}$).

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

Bohr²

Default

1600

Example

D3_RTHR: 9000

Description

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

Remark

Only applicable when DFT-D3 correction [D3_FLAG](#) is used.

D3_CN_THR

Type

Double

Unit

Bohr²

Default

625

Example

D3_CN_THR: 1600

Description

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

Remark

Only applicable when DFT-D3 correction [D3_FLAG](#) is used.

VDWDF_GEN_KERNEL

Type

0 or 1

Unit

No Unit

Default

1

Example

VDWDF_GEN_KERNEL: 1

Description

Flag for computing the kernel functions, its 2nd derivatives and the 2nd derivative of spline functions. If 0 is set, the program will read the files (kernel_d2.txt; spline_d2.txt in the folder saving input files) directly; if 1 is set, the program will generate these files before computation.

Remark

If this is the first time to use vdWDF1 or vdWDF2 as [EXCHANGE_CORRELATION](#), setting the flag as 1 is necessary, which is also the default setting. After the two files are generated, you can use the two generated files by copying them into the folders saving input files of other vdWDF tasks, and VDWDF_GEN_KERNEL flag can be closed to save the time of generating the two files.

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^{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.

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:

1.0

-1.0

Description

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

SCF

CHEB_DEGREE

Type

Integer

Unit

No unit

Default

Automatically set.

Example

CHEB_DEGREE: 25

Description

Degree of polynomial used for Chebyshev filtering.

Remark

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

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

Example

RHO_TRIGGER: 5

Description

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

Remark

Values smaller than the default value of 4 can result in a significant increase in the number of SCF iterations. Larger values can sometimes reduce the number of SCF iterations.

MAXIT_SCF

Type

Integer

Unit

No unit

Default

100

Example

MAXIT_SCF: 50

Description

Maximum number of SCF iterations.

Remark

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

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

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

Example

TOL_SCF: 1e-5

Description

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

Remark

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

SCF_FORCE_ACC

Type

Double

Unit

Ha/Bohr

Default

None

Example

SCF_FORCE_ACC: 1e-4

Description

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

Remark

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

SCF_ENERGY_ACC

Type

Double

Unit

Ha/atom

Default

None

Example

SCF_ENERGY_ACC: 1e-5

Description

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

Remark

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

TOL_LANCZOS

Type

Double

Unit

No unit

Default

1e-2

Example

TOL_LANCZOS: 1e-3

Description

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

Remark

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

MIXING_VARIABLE

Type

String

Unit

No unit

Default

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⁻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.

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` × 0.01

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

Permutation of 1, 2, 3

Unit

No unit

Default

1 2 3

Example

NPT_SCALE_VECS: 2

Description

Specify which lattice vectors can be rescaled in NPT-NH

Remark

Only 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. Only NPT-NH can specify the rescaled vector

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_FINISH_STP

Type

Double

Unit

Bohr

Default

5e-3

Example

L_FINISH_STP: 0.01

Description

Step length for line optimizer in LBFGS ([RELAX_METHOD](#)).

Remark

Default value works well in most cases.

L_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

L_MAXMOV: 1.0

Description

The maximum allowed step size in LBFGS ([RELAX_METHOD](#)).

Remark

Default value works well in most cases.

L_AUTOSCALE

Type

Integer

Unit

No unit

Default

1

Example

L_AUTOSCALE: 0

Description

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

Remark

Default works well in most cases.

L_LINEOPT

Type

Integer

Unit

No unit

Default

1

Example

L_LINEOPT: 0

Description

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

Remark

Required only if [L_AUTOSCALE](#) is 0.

L_ICURV

Type

Double

Unit

No unit

Default

1.0

Example

L_ICURV: 0.1

Description

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

Remark

Needed only if [L_AUTOSCALE](#) is 0. Default value works well in most cases.

FIRE_DT

Type

Double

Unit

Femto second

Default

1

Example

FIRE_DT: 0.1

Description

Time step used in FIRE ([RELAX_METHOD](#)).

Remark

Default value works well in most cases.

FIRE_MASS

Type

Double

Unit

Atomic mass unit

Default

1.0

Example

FIRE_MASS: 2.5

Description

Pseudomass used in FIRE ([RELAX_METHOD](#)).

Remark

Default value works well in most cases.

FIRE_MAXMOV

Type

Double

Unit

Bohr

Default

0.2

Example

FIRE_MAXMOV: 1.0

Description

Maximum movement for any atom in FIRE ([RELAX_METHOD](#)).

Remark

Default value works well in most cases.

Print options

PRINT_ATOMS

Type

0 or 1

Unit

No unit

Default

0

Example

PRINT_ATOMS: 1

Description

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

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.