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

- 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.

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

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    - U.S. National Science Foundation: 1553212, 1663244, and 1333500

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.

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 | VDWDF_GEN_KERNEL | EXX_RANGE_FOCK | EXX_RANGE_PBE | ATOM_TYPE | PSEUDO_POT | N_TYPE_ATOM | COORD | COORD_FRAC | RELAX | SPIN

Input file options

SCF

CHEB_DEGREE | 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 | 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` | `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

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

Input file options

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`

Spectral Quadrature

`SQ_FLAG` | `SQ_TYPE_DM` | `SQ_GAUSS_MEM` | `SQ_NPL_C` | `SQ_NPL_G` |
`SQ_RCUT` | `SQ_FAC_G2C` | `SQ_TOL_OCC` | `SQ_EIGSHIFT_FLAG`| `SQ_EIGSHIFT`
| `NP_DOMAIN_SQ_PARAL`

System: .inpt file

CELL

Type	Unit
Double	Bohr

Default	Example
None	`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	Unit
Integer	No unit

Default	Example
None	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	Unit
Double	Bohr

Default	Example
None	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	Unit
Double	Ha

Default	Example
None	`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	Unit
Integer	No unit

Default	Example
12	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	Unit
String	No unit

Default	Example
No Default	`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), and `SCAN` (SCAN metaGGA).

EXCHANGE_CORRELATION

Remark

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

SPIN_TYP

Type	Unit
Integer	No unit

Default	Example
0	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 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	Unit
Integer	No unit

Default	Example
$N_e/2 \times 1.2 + 5$	`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	Unit
0 or 1	No unit

Default	Example
0	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	Unit
Double	Bohr^2

Default	Example
1600	`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	Unit
Double	Bohr^2

Default	Example
625	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`.

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.

VDWDF_GEN_KERNEL

> **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.

EXX_RANGE_FOCK

Type	Unit
Double	1/Bohr

Default	Example
0.1587	`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	Unit
Double	1/Bohr

Default	Example
0.1587	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	Unit
String	No unit

Default	Example
None	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	Unit
String	No unit

Default	Example
None	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	Unit
Integer	No unit

Default	Example
None	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	Unit
Double	Bohr

Default	Example
None	`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	Unit
Double	None

Default	Example
None	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) × CELL(j), $(j = 1, 2, 3)$ gives the coordinate of the ith atom along the jth 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	Unit
Integer	No unit

Default	Example
1 1 1	RELAX: 1 0 1 0 1 0

Description

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

SPIN

Type	Unit
Double	No unit

Default	Example
0.0	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_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	Unit
Integer	No unit

Default	Example
4	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	Unit
Integer	No unit

Default	Example
100	`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.

TOL_SCF

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

SCF_FORCE_ACC

Type	Unit
Double	Ha/Bohr

Default	Example
None	`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	Unit
Double	Ha/atom

Default	Example
None	`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	Unit
Double	No unit

Default	Example
1e-2	`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	Unit
Integer	No unit

Default	Example
7	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	Unit
Double	No unit

Default	Example
0.3	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

Default

Automatically set to the same
as MIXING_PARAMETER

Unit

No unit

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	Unit
Integer	No unit

Default	Example
1	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	Unit
Integer	No unit

Default	Example
0	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	Unit
String	No unit

Default	Example
kerker	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

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	Unit
Double	No unit

Default	Example
$h^2 \times 0.001$	`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	Unit
Double	Bohr^{-1}

Default	Example
1.0	`PRECOND_KERKER_KTF: 0.8`

Description

The Thomas-Fermi screening length appearing in the `kerker` preconditioner (`MIXING_PRECOND`).

PRECOND_KERKER_THRESH

Type	Unit
Double	No unit

Default	Example
0.1	`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	Unit
Double	Bohr^{-1}

Default	Example
1.0	`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	Unit
Double	No unit

Default	Example
0.1	`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	Unit
Integer	No unit

Default	Example
0	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	Unit
Double	No unit

Default	Example
0.2*TOL_SCF	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	Unit
Integer	No unit

Default	Example
2	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$\times$10, 0.001)

Example
TOL_SCF_INIT: 1e-6

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

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

ACE_FLAG

Type	Unit
Integer	No unit

Default	Example
1	`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	Unit
Integer	No unit

Default	Example
20	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	Unit
Integer	No unit

Default	Example
3000	MAXIT_POISSON: 1000

Description

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

TOL_PSEUDOCHARGE

Type	Unit
Double	No unit

Default	Example
TOL_SCF×0.001	TOL_PSEUDOCHARGE: 1e-6

Description

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

REFERENCE_CUTOFF

Type	Unit
Double	Bohr

Default	Example
0.5	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	Unit
Integer	No unit

Default	Example
0	CALC_STRESS: 1

Description

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

CALC_PRES

Type	Unit
Integer	No unit

Default	Example
0	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	Unit
String	No unit

Default	Example
NVT_NH	`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	Unit
Integer	No unit

Default	Example
1e7	`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	Unit
Double	Femtosecond

Default	Example
1	MD_TIMESTEP: 0.1

Description

QMD time step.

Remark

Total QMD time is given by: MD_TIMESTEP $\times$ (MD_NSTEP - 1).

ION_TEMP

Type	Unit
Double	Kelvin

Default	Example
No Default	`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	Unit
Double	Kelvin

Default	Example
ION_TEMP	`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	Unit
Integer	No unit

Default	Example
2	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	Unit
Integer	No unit

Default	Example
0	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	Unit
Double	atomic unit

Default	Example
No default value	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	Unit
Double	atomic unit

Default	Example
No default value	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	Unit
Double	GPa

Default	Example
0.0	`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	Unit
Integer	No unit

Default	Example
0	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	Unit
Double	min

Default	Example
1e9	`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	Unit
String	No unit

Default	Example
LBFGS	`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	Unit
Double	Ha/Bohr

Default	Example
5e-4	`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	Unit
Double	GPa

Default	Example
1e-2	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	Unit
Double	No unit

Default	Example
1.06	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	Unit
Double	No unit

Default	Example
0.5	`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	Unit
Double	Bohr

Default	Example
5e-3	`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	Unit
Double	Bohr

Default	Example
0.2	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	Unit
Double	No unit

Default	Example
1.0	`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	Unit
Double	Atomic mass unit

Default	Example
1.0	`FIRE_MASS: 2.5`

Description

Pseudomass used in FIRE (`RELAX_METHOD`).

Remark

Default value works well in most cases.

FIRE_MAXMOV

Type	Unit
Double	Bohr

Default	Example
0.2	`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	Unit
0 or 1	No unit

Default	Example
0	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	Unit
0 or 1	No unit

Default	Example
0	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	Unit
0 or 1	No unit

Default	Example
1	PRINT_MDOUT: 0

Description

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

PRINT_RELAXOUT

Type	Unit
0 or 1	No unit

Default	Example
1	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	Unit
0 or 1	No unit

Default	Example
1	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	Unit
Integer	No unit

Default	Example
1	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	Unit
0 or 1	No unit

Default	Example
1	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	Unit
int	No unit

Default	Example
0	PRINT_EIGEN: 1

Description

Flag for writing eigenvalues and occupations into .eigen file.

PRINT_DENSITY

Type	Unit
int	No unit

Default	Example
0	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
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
nband	int, 1	Number of bands printed

PRINT_ORBITAL

Remark – cont.

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, isReal, nspin, nkpt, nband, followed by the data for real or complex Kohn-sham orbital. Below is the pseudo-code to read orbitals after reading variables in headers.

PRINT_ORBITAL

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	Unit
int	No unit

Default	Example
0	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 paralllization parameters in practice.

EIG_SERIAL_MAXNS

Type	Unit
Integer	No unit

Default	Example
2000	`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	Unit
Double	No unit

Default	Example
0.0	`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.

Spectral Quadrature

Comments

The code will fail with the following options and the related input options are listed.

- Polarized calculation: SPIN_TYP.
- K-point calculation: KPOINT_GRID, KPOINT_SHIFT.
- Dirichlet boundary condition in any direction: BC
- Define number of states/orbitals: NSTATES
- CS and SQ3 method: CS_FLAG, SQ3_FLAG
- Hybrid functionals: EXCHANGE_CORRELATION
- Print eigenvalues into file: PRINT_EIGEN

SQ_FLAG

Type	Unit
Integer	No unit

Default	Example
0	SQ_FLAG: 1

Description

Flag to turn on SQ method

Remark

SQ method can not be turned on simultaneously with CS, SQ3, hybrid functionals.

SQ_TYPE_DM

Type	Unit
String	No unit

Default	Example
GAUSS	SQ_TYPE_DM: CC

Description

Flag to choose type of quadrature for density matrix. Available options are Gauss (GAUSS) and Clenshaw-Curtis (CC).

SQ_GAUSS_MEM

Type
String

Unit
No unit

Default
LOW

Example
SQ_GAUSS_MEM: HIGH

Description
Flag for memory option when using Gauss quadrature for density matrix.

SQ_NPL_C

Type
Integer

Unit
No unit

Default
SQ_NPL_G $\times$ SQ_FAC_G2C

Example
SQ_NPL_C: 24

Description
Degree of polynomial for Clenshaw Curtis in forces and stress.

SQ_NPL_G

Type
Integer

Unit
No unit

Default
None

Example
SQ_NPL_G: 24

Description

Degree of polynomial for Gauss Quadrature.

Remark

SQ_NPL_G must be specified if SQ is turned on.

SQ_RCUT

Type	Unit
Double	Bohr

Default	Example
None	SQ_RCUT: 2.0

Description

Truncation or localization radius

Remark

SQ_RCUT must be specified if SQ is turned on.

SQ_FAC_G2C

Type
Double

Unit
No unit

Default
2.0

Example
`SQ_FAC_G2C: 3.0`

Description

`SQ_NPL_C` = `SQ_FAC_G2C` $\times$ `SQ_NPL_G`. Used if `SQ_NPL_C` is not specified.

SQ_TOL_OCC

Type
Double

Unit
No unit

Default
10^{-6}

Example
SQ_TOL_OCC: 1E-5

Description

Tolerance for occupation corresponding to maximum eigenvalue.

SQ_EIGSHIFT_FLAG

Type

Integer

Unit

No unit

Default

0

Example

SQ_EIGSHIFT_FLAG: 1

Description

Flag for choosing to use minmax eigenvalues of Gauss for Clenshaw Curtis in forces/stress after shifting by eigshift.

SQ_EIGSHIFT

Type

Double

Unit

Percent

Default

5

Example

SQ_EIGSHIFT: 10

Description

Percentage shift in eigenspectrum.

NP_DOMAIN_SQ_PARAL

Type	Unit
Integer	No unit

Default	Example
Automatically optimized	NP_DOMAIN_SQ_PARAL: 3 3 2

Description

Dimensions of the 3D Cartesian topology for SQ method.

Remark

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