

COMPUTATIONAL MATERIAL PHYSICS GROUP

DFT-FE

Density Functional Theory With Finite-Elements

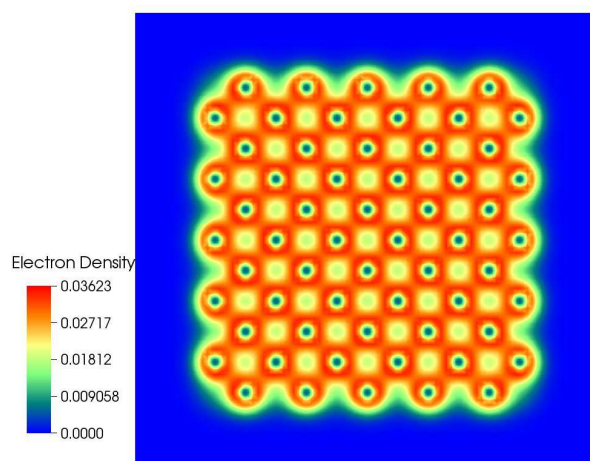
User Manual

Version 0.9.0-pre

(generated April 16, 2018)

Sambit Das

Phani Motamarri



with contributions by:
Shiva Rudraraju

dftfe.org

Contents

1	Introduction	2
2	Contributing to dftfe's development	2
3	Future plans for dftfe	2
4	Finding answers to more questions	2
A	Run-time input parameters	2
A.1	Global parameters	2
A.2	Parameters in section Boundary conditions	2
A.3	Parameters in section Brillouin zone k point sampling options	3
A.4	Parameters in section Brillouin zone k point sampling options/Monkhorst-Pack (MP) grid generation	3
A.5	Parameters in section Checkpointing and Restart	4
A.6	Parameters in section DFT functional related parameters	4
A.7	Parameters in section Eigen-solver/Chebyshev solver related parameters	5
A.8	Parameters in section Finite element mesh parameters	6
A.9	Parameters in section Finite element mesh parameters/Auto mesh generation parameters	6
A.10	Parameters in section Geometry	7
A.11	Parameters in section Geometry/Optimization	7
	Index of run-time parameters with section names	8

- 1 Introduction
- 2 Contributing to dftfe's development
- 3 Future plans for dftfe
- 4 Finding answers to more questions

A Run-time input parameters

A.1 Global parameters

- *Parameter name:* REPRODUCIBLE OUTPUT
Default: false
Description: Limit output to that which is reproducible, i.e. don't print timing or absolute paths.
Possible values: A boolean value (true or false)
- *Parameter name:* VERBOSITY
Default: 1
Description: Parameter to control verbosity of terminal output. 0 for low, 1 for medium, and 2 for high.
Possible values: An integer n such that $0 \leq n \leq 2$

A.2 Parameters in section Boundary conditions

- *Parameter name:* PERIODIC1
Default: false
Description: Periodicity along domain bounding vector, v1.
Possible values: A boolean value (true or false)
- *Parameter name:* PERIODIC2
Default: false
Description: Periodicity along domain bounding vector, v2.
Possible values: A boolean value (true or false)
- *Parameter name:* PERIODIC3
Default: false
Description: Periodicity along domain bounding vector, v3.
Possible values: A boolean value (true or false)
- *Parameter name:* SELF POTENTIAL ATOM BALL RADIUS
Default: 3.0
Description: The radius (in a.u) of the ball around an atom on which self-potential of the associated nuclear charge is solved
Possible values: A floating point number v such that $1.5 \leq v \leq 10$

A.3 Parameters in section Brillouin zone k point sampling options

- *Parameter name:* NUMBER OF POOLS

Default: 1

Description: Number of pools the irreducible k-points to be split on should be a divisor of total number of procs and be less than or equal to the number of irreducible k-points

Possible values: An integer n such that $1 \leq n \leq 2147483647$

- *Parameter name:* USE GROUP SYMMETRY

Default: false

Description: Flag to control whether to use point group symmetries (set to false for relaxation calculation)

Possible values: A boolean value (true or false)

- *Parameter name:* USE TIME REVERSAL SYMMETRY

Default: false

Description: Flag to control usage of time reversal symmetry

Possible values: A boolean value (true or false)

- *Parameter name:* kPOINT RULE FILE

Default:

Description: File specifying the k-Point quadrature rule to sample Brillouin zone. CAUTION: This option is only used for postprocessing, for example band structure calculation. To set k point rule for DFT solve use the Monkhorst-Pack (MP) grid generation.

Possible values: Any string

A.4 Parameters in section Brillouin zone k point sampling options/Monkhorst-Pack (MP) grid generation

- *Parameter name:* SAMPLING POINTS 1

Default: 2

Description: Number of Monkhorst-Pack grid points to be used along reciprocal lattice vector 1.

Possible values: An integer n such that $1 \leq n \leq 100$

- *Parameter name:* SAMPLING POINTS 2

Default: 2

Description: Number of Monkhorst-Pack grid points to be used along reciprocal lattice vector 2.

Possible values: An integer n such that $1 \leq n \leq 100$

- *Parameter name:* SAMPLING POINTS 3

Default: 2

Description: Number of Monkhorst-Pack grid points to be used along reciprocal lattice vector 3.

Possible values: An integer n such that $1 \leq n \leq 100$

- *Parameter name:* SAMPLING SHIFT 1

Default: 0.0

Description: Fractional shifting to be used along reciprocal lattice vector 1.

Possible values: A floating point number v such that $0 \leq v \leq 1$

- *Parameter name:* SAMPLING SHIFT 2

Default: 0.0

Description: Fractional shifting to be used along reciprocal lattice vector 2.

Possible values: A floating point number v such that $0 \leq v \leq 1$

- *Parameter name:* SAMPLING SHIFT 3

Default: 0.0

Description: Fractional shifting to be used along reciprocal lattice vector 3.

Possible values: A floating point number v such that $0 \leq v \leq 1$

A.5 Parameters in section Checkpointing and Restart

- *Parameter name:* CHK TYPE

Default: 0

Description: Checkpoint type, 0(dont create any checkpoint), 1(create checkpoint only for ion optimization restart if ION OPT is set to true. This option writes the current atomic coordinates and the cg ion relaxation solver state to checkpoint files. This option assumes CELL OPT is set to false. The checkpoint is created at the end of the last ground state solve.), 2(create checkpoint for scf restart. This option also creates checkpoint for ion optimization restart if ION OPT is set to true.)

Possible values: An integer n such that $0 \leq n \leq 2$

- *Parameter name:* RESTART FROM CHK

Default: false

Description: Boolean parameter specifying if the current job reads from a checkpoint. The nature of the restart corresponds to the CHK TYPE parameter. Hence, the checkpoint being read must have been created using the same value of the CHK TYPE parameter. RESTART FROM CHK is always false for CHK TYPE 0.

Possible values: A boolean value (true or false)

A.6 Parameters in section DFT functional related parameters

- *Parameter name:* EXCHANGE CORRELATION TYPE

Default: 1

Description: Parameter specifying the type of exchange-correlation to be used: 1(LDA: Perdew Zunger Ceperley Alder correlation with Slater Exchange[PRB. 23, 5048 (1981)]), 2(LDA: Perdew-Wang 92 functional with Slater Exchange [PRB. 45, 13244 (1992)]), 3(LDA: Vosko, Wilk & Nusair with Slater Exchange[Can. J. Phys. 58, 1200 (1980)]), 4(GGA: Perdew-Burke-Ernzerhof functional [PRL. 77, 3865 (1996)])

Possible values: An integer n such that $1 \leq n \leq 4$

- *Parameter name:* PSEUDOPOTENTIAL CALCULATION

Default: true

Description: Boolean Parameter specifying whether pseudopotential DFT calculation needs to be performed

Possible values: A boolean value (true or false)

- *Parameter name:* PSEUDOPOTENTIAL TYPE

Default: 1

Description: Type of nonlocal projector to be used: 1 for KB, 2 for ONCV, default is KB

Possible values: An integer n such that $1 \leq n \leq 2$

- *Parameter name:* SPIN POLARIZATION

Default: 0

Description: Spin polarization: 0 for no spin polarization and 1 for spin polarization

Possible values: An integer n such that $0 \leq n \leq 1$

- *Parameter name:* START MAGNETIZATION

Default: 0.0

Description: Magnetization to start with (must be between -0.5 and +0.5)

Possible values: A floating point number v such that $-\text{MAX_DOUBLE} \leq v \leq \text{MAX_DOUBLE}$

A.7 Parameters in section Eigen-solver/Chebyshev solver related parameters

- *Parameter name:* CHEBYSHEV FILTER PASSES

Default: 1

Description: The number of the Chebyshev filter passes per SCF (Default value is used when the input parameter is not specified)

Possible values: An integer n such that $1 \leq n \leq 20$

- *Parameter name:* CHEBYSHEV POLYNOMIAL DEGREE

Default: 0

Description: The degree of the Chebyshev polynomial to be employed for filtering out the unwanted spectrum (Default value is used when the input parameter value is 0)

Possible values: An integer n such that $0 \leq n \leq 2000$

- *Parameter name:* LOWER BOUND WANTED SPECTRUM

Default: -10.0

Description: The lower bound of the wanted eigen spectrum

Possible values: A floating point number v such that $-\text{MAX_DOUBLE} \leq v \leq \text{MAX_DOUBLE}$

- *Parameter name:* NUMBER OF KOHN-SHAM WAVEFUNCTIONS

Default: 10

Description: Number of Kohn-Sham wavefunctions to be computed. For insulators use $N/2+(10-20)$ and for metals use 20 percent more than $N/2$ (atleast 10 more). N is the total number of electrons

Possible values: An integer n such that $0 \leq n \leq 2147483647$

A.8 Parameters in section Finite element mesh parameters

- *Parameter name:* MESH FILE

Default:

Description: External mesh file path. If nothing is given auto mesh generation is performed

Possible values: Any string

- *Parameter name:* POLYNOMIAL ORDER

Default: 4

Description: The degree of the finite-element interpolating polynomial

Possible values: An integer n such that $1 \leq n \leq 12$

A.9 Parameters in section Finite element mesh parameters/Auto mesh generation parameters

- *Parameter name:* ATOM BALL RADIUS

Default: 2.0

Description: Radius of ball enclosing atom

Possible values: A floating point number v such that $0 \leq v \leq 10$

- *Parameter name:* BASE MESH SIZE

Default: 2.0

Description: Mesh size of the base mesh on which refinement is performed.

Possible values: A floating point number v such that $0 \leq v \leq 20$

- *Parameter name:* MAX REFINEMENT STEPS

Default: 10

Description: Maximum number of refinement steps to be used. The default value is good enough in most cases.

Possible values: An integer n such that $1 \leq n \leq 10$

- *Parameter name:* MESH SIZE ATOM BALL

Default: 0.5

Description: Mesh size in a ball around atom

Possible values: A floating point number v such that $0 \leq v \leq 10$

- *Parameter name:* MESH SIZE NEAR ATOM

Default: 0.5

Description: Mesh size near atom. Useful for all-electron case.

Possible values: A floating point number v such that $0 \leq v \leq 10$

A.10 Parameters in section Geometry

- *Parameter name:* ATOMIC COORDINATES FILE

Default:

Description: Atomic-coordinates file. For fully non-periodic domain give cartesian coordinates of the atoms (in a.u) with respect to origin at the center of the domain. For periodic and semi-periodic give fractional coordinates of atoms. File format (example for two atoms): x1 y1 z1 (row1), x2 y2 z2 (row2).

Possible values: Any string

- *Parameter name:* DOMAIN BOUNDING VECTORS FILE

Default:

Description: Set file specifying the domain bounding vectors v1, v2 and v3 in a.u. with the following format: v1x v1y v1z (row1), v2x v2y v2z (row2), v3x v3y v3z (row3). Domain bounding vectors are the typical lattice vectors in a fully periodic calculation.

Possible values: Any string

A.11 Parameters in section Geometry/Optimization

- *Parameter name:* CELL CONSTRAINT TYPE

Default: 12

Description: Cell relaxation constraint type, 1(isotropic shape-fixed volume optimization), 2(volume-fixed shape optimization), 3(relax only cell component v1x), 4(relax only cell component v2x), 5(relax only cell component v3x), 6(relax only cell components v2x and v3x), 7(relax only cell components v1x and v3x), 8(relax only cell components v1x and v2x), 9(volume optimization- relax only v1x, v2x and v3x), 10(2D- relax only x and y components relaxed), 11(2D- relax only x and y shape components- in-plane area fixed), 12(relax all cell components), 13 automatically decides the constraints based boundary conditions. CAUTION: A majority of these options only make sense in an orthorhombic cell geometry.

Index of run-time parameters with section names

The following is a listing of all run-time parameters, sorted by the section in which they appear.

Boundary conditions

PERIODIC1, [2](#)
PERIODIC2, [2](#)
PERIODIC3, [2](#)
SELF POTENTIAL ATOM BALL
RADIUS, [2](#)

Brillouin zone k point sampling options

kPOINT RULE FILE, [3](#)
Monkhorst-Pack (MP) grid generation
SAMPLING POINTS 1, [3](#)
SAMPLING POINTS 2, [3](#)
SAMPLING POINTS 3, [3](#)
SAMPLING SHIFT 1, [3](#)
SAMPLING SHIFT 2, [4](#)
SAMPLING SHIFT 3, [4](#)
NUMBER OF POOLS, [3](#)
USE GROUP SYMMETRY, [3](#)
USE TIME REVERSAL SYMMETRY, [3](#)

Checkpointing and Restart

CHK TYPE, [4](#)
RESTART FROM CHK, [4](#)

DFT functional related parameters

EXCHANGE CORRELATION TYPE, [4](#)
PSEUDOPOTENTIAL CALCULATION,
[4](#)
PSEUDOPOTENTIAL TYPE, [5](#)
SPIN POLARIZATION, [5](#)
START MAGNETIZATION, [5](#)

Eigen-solver/Chebyshev solver related parameters

CHEBYSHEV FILTER PASSES, [5](#)
CHEBYSHEV POLYNOMIAL
DEGREE, [5](#)
LOWER BOUND WANTED
SPECTRUM, [5](#)
NUMBER OF KOHN-SHAM
WAVEFUNCTIONS, [5](#)

Finite element mesh parameters

Auto mesh generation parameters
ATOM BALL RADIUS, [6](#)
BASE MESH SIZE, [6](#)
MAX REFINEMENT STEPS, [6](#)
MESH SIZE ATOM BALL, [6](#)
MESH SIZE NEAR ATOM, [6](#)
MESH FILE, [6](#)
POLYNOMIAL ORDER, [6](#)

Geometry

ATOMIC COORDINATES FILE, [7](#)
DOMAIN BOUNDING VECTORS FILE,
[7](#)

Optimization

CELL CONSTRAINT TYPE, [7](#)

REPRODUCIBLE OUTPUT, [2](#)

VERBOSITY, [2](#)