

SHENGBTE: a solver for the Boltzmann transport equation for phonons

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1 How to download, compile and use SHENGBTE

Development of SHENGBTE is hosted at [Bitbucket](https://bitbucket.org/sousaw/shengbte). The latest version can be downloaded using the “download” link at <https://bitbucket.org/sousaw/shengbte>. Alternatively, it is possible to clone its [GIT](#) repository from the command line with

```
git clone git@bitbucket.org:sousaw/shengbte.git ShengBTE
```

or from one of the many graphical frontends available.

To compile the code it is enough to run `make` in the `Src` subdirectory of the distribution, but a suitable `arch.make` must be present in that directory. An example is provided as `Src/arch.make.example`. As a minimum, `$MPIFC` must contain a valid command to compile Fortran 90 code with MPI directives, while the combination of `$LDFLAGS` and `$LIBS` must contain any linker flags required in order to link against an implementation of LAPACK and against Atsushi Togo’s [spglib](#). ShengBTE uses some Fortran 2003 extensions, most notably its new syntax for array initialization, and a recent Fortran compiler is required that supports them; `gfortran 4.8.2` and `ifort 12.0.0` are known to work.

After compilation succeeds, a ShengBTE binary will be created in the root directory of the distribution. This executable takes no command-line options and accepts no input from the terminal. It can be invoked simply as

```
./ShengBTE
```

for serial mode, but most often it will be run using a command like

```
mpirun -n 32 ./ShengBTE 2>BTE.err >BTE.out
```

often as part of a script to be submitted to a batch system.

2 Input files

Exactly three files are required for a SHENGBTE run: `CONTROL`, one of `FORCE_CONSTANTS_2ND` or `espresso.ifc2`, and `FORCE_CONSTANTS_3RD`. Their contents are detailed below; for a complete example, the reader is referred to the `Test` subdirectory of the distribution.

2.1 The `CONTROL` file

The contents of this file describe the system to be studied and specify a set of parameters and flags controlling execution. Its format is merely a sequence of four Fortran [namelists](#), with a reasonably flexible syntax that should become apparent after looking at the example `Test/CONTROL` for zincblende InAs. Some parameters and flags are mandatory, whereas others are optional and take a default value when unspecified.

&allocations namelist:

- `nelements` (integer, mandatory): number of different elements in the compound
- `natoms` (integer, mandatory): number of atoms in the unit cell
- `ngrid` (integer, 3, mandatory): number of grid planes along each axis in reciprocal space
- `norientations` (integer, default=0): number of orientations along which to study nanowires

&crystal namelist:

- `lfactor` (real, nm, default=1.0): unit of measurement for lattice vectors
- `lattvec` (real, 3×3 , mandatory): real-space lattice vectors, in units of `lfactor`
- `types` (integer, `natoms`, mandatory): a vector of `natom` integers, ranging from 1 to `nelements`, assigning an element to each atom in the system
- `elements` (string, `nelements`, mandatory): a vector of element names
- `positions` (real, $3 \times \text{natoms}$, mandatory): atomic positions in lattice coordinates

- **masses** (real, **nelements**, g/mol, default=automatic): atomic masses corresponding to each element. If they are omitted and **autoisotopes** is true and the element names are known, they are computed automatically.
- **gfactors** (real, **nelements**, default=automatic): g factors for isotopic scattering associated to each element. If they are omitted and **autoisotopes** is true and the element names are known, they are computed automatically.
- **epsilon** (real, 3×3 , ϵ_0 , default=1): dielectric tensor of the system in the Cartesian basis
- **born** (real, $3 \times 3 \times \text{natoms}$, e , default=0): Born effective charge tensor of each atom in the Cartesian basis
- **scell** (integer, 3, mandatory): supercell sizes along each crystal axis used for the 2nd-order force constant calculation
- **orientations** (integer, $3 \times \text{norientations}$, mandatory unless **nororientations** = 0): terns of integer indices defining the crystallographic directions along which to study nanowires

¶meters namelist:

- **T** (real, K, mandatory): temperature to be used in all calculations
- **scalebroad** (real, default=1.0): scale parameter for Gaussian smearing. The default is theoretically guaranteed to work, but significant speedups can sometimes be achieved by reducing it, with negligible loss of precision.
- **rmin** (real, nm, default=5.0): minimum radius of nanowires whose thermal conductivity will be computed
- **rmax** (real, nm, default=505.0): maximum radius of nanowires whose thermal conductivity will be computed
- **dr** (real, nm, default=100.0): radius increment to be used when simulating nanowires from **rmin** to **rmax**
- **maxiter** (integer, default=1000): maximum number of iterations allowed in the BTE convergence process
- **nticks** (integer, default=100): number of different values of the mean free path at which to compute the cumulative thermal conductivity
- **eps** (real, default= 10^{-5}): the iterative solver of the BTE will stop when the relative change in the thermal conductivity tensor is less than **eps**. Such change between steps $n - 1$ and n is measured as $||\kappa_n - \kappa_{n-1}|| / ||\kappa_{n-1}||$, where $||\cdot||$ denotes a matrix 2-norm.

&flags namelist:

- **nonanalytic** (logical, default=.true.): compute and use the nonanalytic part of the dynamical matrix
- **convergence** (logical, default=.true.): if true, iterate the BTE solver until convergence is achieved. If false, compute thermal conductivities in the relaxation time approximation.
- **isotopes** (logical, default=.true.): include isotopic scattering in the relaxation times
- **autoisotopes** (logical, default=.true.): compute atomic masses and g factors automatically
- **nanowires** (logical, default=.false.): study the thermal conductivity of nanowires in addition to that of the bulk
- **onlyharmonic** (logical, default=.false.): stop the program after computing the specific heat and small-grain thermal conductivity
- **espresso** (logical, default=.false.): read second-order force constants from **espresso.ifc2** (Quantum Espresso format) instead of the default **FORCE_CONSTANTS_2ND** (Phonopy format)

2.2 The **FORCE_CONSTANTS_2ND** file

This file contains the second derivatives of the system's energy with respect to the Cartesian coordinates of the nuclei, *i.e.* the interatomic force constant matrix. Its format is precisely that chosen in [Phonopy](#) for the **FORCE_CONSTANTS** file, so that the result of a Phonopy calculation can be used directly. The first line of the file declares the total number of atoms in the supercell, `npairs`, which must be equal to `scell(1) × scell(2) × scell(3) × natoms`, and is followed by `npairs` blocks of four lines each. The first line of each of those blocks contains two integers with the 1-based indices of the atoms forming the pair; the remaining three lines contain the 3×3 matrix of second-order interatomic force constants linking those two atoms, in $\text{eV}/\text{\AA}^2$.

2.3 The **espresso.ifc2** file

The information contained in this file is equivalent to that in **FORCE_CONSTANTS_2ND**, but the format is different. For details, consult the [Quantum Espresso](#) documentation. Please note that although this file's header contains information about lattice vectors, atomic positions, Born effective charges and so forth, it is ignored by **SHENGBTE**. It is the user's responsibility to ensure that **espresso.ifc2** and **CONTROL** are compatible.

2.4 The **FORCE_CONSTANTS_3RD** file

Similarly, this file contains the third-order interatomic force constant matrix, but uses a sparse description to save space. All constants are implicitly referred to a central unit cell i taken as the origin of coordinates. The first line again contains a single integer, `nb`, which is followed by `nb` blocks with the following structure:

- A blank line
- A 1-based sequential index
- A line with the Cartesian coordinates of the second unit cell in \AA .
- A line with the Cartesian coordinates of the third unit cell in \AA .
- A line with the 1-based indices of the three atoms involved, each from 1 to `natoms`.
- 27 lines, each of which starts with a tern of integers specifying three Cartesian axes and is completed by a force constant in $\text{eV}/\text{\AA}^3$. The last element of the tern changes first.

The following is an example of one such block:

```
1
0.000  0.000  0.000
0.000  0.000  0.000
1 1 1
1 1 1      0.0000000000E+00
1 1 2      0.0000000000E+00
1 1 3      0.0000000000E+00
1 2 1      0.0000000000E+00
1 2 2      0.0000000000E+00
1 2 3      0.2346653425E+02
1 3 1      0.0000000000E+00
1 3 2      0.2346653425E+02
1 3 3      0.0000000000E+00
2 1 1      0.0000000000E+00
2 1 2      0.0000000000E+00
2 1 3      0.2346653425E+02
2 2 1      0.0000000000E+00
2 2 2      0.0000000000E+00
```

2	2	3	0.0000000000E+00
2	3	1	0.2346653425E+02
2	3	2	0.0000000000E+00
2	3	3	0.0000000000E+00
3	1	1	0.0000000000E+00
3	1	2	0.2346653425E+02
3	1	3	0.0000000000E+00
3	2	1	0.2346653425E+02
3	2	2	0.0000000000E+00
3	2	3	0.0000000000E+00
3	3	1	0.0000000000E+00
3	3	2	0.0000000000E+00
3	3	3	0.0000000000E+00

3 Output files

Many files are created during a successful run of SHENGBTE. They contain not only the thermal conductivity and related quantities, but also a set of intermediate results that may be useful to diagnose problems. This section includes a brief description of their contents.

BTE.qpoints: the first column in this file contains the indices of a set of irreducible q -points in the Brillouin zone obtained starting with an $\text{ngrid}(1) \times \text{ngrid}(2) \times \text{ngrid}(3)$ Monkhorst-Pack grid. The second column lists the corresponding degeneracies. The remaining three columns are the Cartesian coordinates of a representative q -point in each equivalence class.

BTE.omega: phonon angular frequencies at each of those q -points, in rad/ps

BTE.v: group velocities of those modes, in km/s (or nm THz)

BTE.cv: specific heat of the system, in J/($\text{m}^3 \text{K}$)

BTE.kappa_sg: thermal conductivity per unit of mean free path in the small-grain limit, in W/(m K nm)

BTE.dos: the second column of this file contains the phonon density of states evaluated at the angular frequencies (in rad/ps) specified by its first column

BTE.pdos: the second and further column of this file contains the phonon density of states evaluated at the angular frequencies (in rad/ps) specified by its first column and projected over each atom in the unit cell

BTE.P3 : volume in phase space available for three-phonon processes, for each irreducible q -point and phonon band

BTE.P3_total: sum of all the contributions in BTE.P3, total volume in phase space available for three-phonon processes.

BTE.gruneisen : Grüneisen parameter for each irreducible q -point and phonon band

BTE.gruneisen_total: total Grüneisen parameter obtained as a weighted sum of the mode contributions

BTE.w_isotopic: isotopic contribution to the scattering rate, for each q -point and each band, in ps^{-1}

BTE.w_anharmonic: contribution of three-phonon processes to the scattering rate, for each q -point and each band, in ps^{-1}

BTE.w: total zeroth-order scattering rate for each q -point and each band, in ps^{-1}

BTE.w_final: total converged scattering rate for each q -point and each band, in ps^{-1}

BTE.kappa: tensorial contribution to the thermal conductivity from each band, in W/(m K). The last line contains converged values, the rest show the convergence process.

BTE.kappa_tensor: total thermal conductivity, a 3×3 tensor expressed in W/(m K). The last line contains converged values, the rest show the convergence process.

BTE.kappa_scalar: average of diagonal elements of the thermal conductivity tensor, in W/(m K). The last line contains converged values, the rest show the convergence process.

BTE.kappa_nw_*: thermal conductivities of nanowires built along different directions of the bulk material, for different radii. The first column in each file is a diameter, the following $3 \times \text{natoms}$ contain the contributions of each band and the last column contains the total thermal conductivity. Diameters are expressed in nm and conductivities in W/(m K)

BTE.kappa_nw_*_lower: lower bounds to the thermal conductivities of nanowires built along different directions of the bulk material, for different radii. The first column in each file is a diameter, the following $3 \times \text{natoms}$ contain the contributions of each band and the last column contains the total thermal conductivity. Diameters are expressed in nm and conductivities in W/(m K). Each lower bound is estimated by using the set of zeroth-order bulk relaxation times.

BTE.cumulative_kappa_*: this set of files is analogous to **BTE.kappa_***, except in that their first column specifies a cutoff mean free path for phonons.