shengBTE接口

- 简介
- 安装
- 示例
- 结果文件说明

简介

ShengBTE solves the full linearized Boltzmann transport equation for phonons using an iterative method. This goes far beyond the widely used relaxation-time approximation (RTA); the difference can be important in materials where "normal" (quasimomentum-conserving) three-phonon processes play a relevant role. By using inputs coming from ab-initio calculations, ShengBTE yields results with predictive power without the need for fitting to experiment.

Two kinds of system can currently be studied: bulk crystalline materials and nanowires thereof. The dominant phonon scattering mechanism in the former are three-phonon processes and isotopic disorder. Both are implemented in ShengBTE:

- Isotopic scattering: Implemented using Tamura's formula. The projected vibrational density of states appearing in the formula is computed using a locally adaptive broadening algorithm.
- Three-phonon processes: Three-phonon scattering amplitudes are computed from a set of 3rd-order derivatives of the energy. A crucial point is enforcing conservation of energy so that only allowed processes are considered. In contrast with other approaches to the problem, in ShengBTE this problem is solved using a locally adaptive, parameter-free method.

As regards nanowires, an efficient and accurate approximation developed by some of the authors is implemented to solve the Boltzmann transport equation in the presence of boundaries.

Thanks to a general implementation of symmetries based on spglib, ShengBTE is able to deal with arbitrary three-dimensional lattices. Symmetry is used to dramatically reduce the complexity of the calculation.

In addition to the thermal conductivity tensor, ShengBTE outputs the following quantities:

- Phonon frequencies at the sampled q-points.
- Phonon group velocities.
- Lattice specific heat.
- Nanograined thermal-conductivity per unit mean free path.

- Fraction of three-phonon processed allowed by conservation of energy, sometimes called three-phonon phase space.
- Mode contributions to the three-phonon phase space.
- Vibrational density of states: total and projected.
- Per-mode contributions to the thermal conductivity.
- Cumulative thermal conductivity: contribution to this quantity by phonons with mean free paths smaller than a threshold.
- Scattering rates: total, RTA values, isotopic and anharmonic contributions.
- Thermal conductivity of nanowires cut along arbitrary crystallographic directions of the bulk.
- Total and mode Grüneisen parameters.

The number of 3rd-order derivatives of the energy needed to accurately describe three-phonon scattering can easily run into the hundreds of thousands. Their direct calculation using a real-space supercell approach can thus be prohibitively expensive. By harnessing the symmetries of the system, thirdorder.py can typically reduce the problem to a few hundreds of DFT runs. This means third-order calculations will still be the most computationally-expensive part of the process, but it becomes tractable for single compounds or even for moderately-sized libraries.

安装

> (1)利用git克隆shengBTE库:

```
git clone https://bitbucket.org/sousaw/shengbte.git
```

或者在网站下载代码包

```
https://bitbucket.org/sousaw/shengbte
```

> (2)编译shengBTE:

以**arch.make.example**为例准备一个**arch.make**文件并移至**Src**文件夹下(安装需要Atsushi Togo的spglib库，若没有安装可参考（3）)。进入**Src**文件夹后使用**make**编译代码，成功编译后可执行文件为**./shengBTE**
arch.make示例

```
export FFLAGS= -O2 -static-intel -qopenmp
export LDFLAGS=-L/data/home/hxj/software/spglib/spglib-1.9.7/build/lib -lsymspg
export MPIFC=mpiifort
MKL=$(MKLROOT)/lib/intel64/libmkl_lapack95_lp64.a -Wl,--start-group     \
$(MKLROOT)/lib/intel64/libmkl_intel_lp64.a                              \
 $(MKLROOT)/lib/intel64/libmkl_sequential.a                             \
 $(MKLROOT)/lib/intel64/libmkl_core.a -Wl,--end-group -lpthread -lm
export LAPACK=$(MKL)
export LIBS=$(LAPACK)
```

> (3)若未安装spglib

- 下载spglib-1.9.7.tar.gz,并解压 **$tar -zxvf spglib-1.9.7.tar.gz**
- **$cd spglib-1.9.7/**
- 建立安装文件夹，输出并复制安装目录路径 **$mkdir build && cd build && pwd && cd ../**
- 在安装目录中生成Makefile文件 **$./configure –prefix=/path/to/spglib-1.9.7/build**,注意这里需要将这个地址替换为上一步复制的安装目录路径
- **$make && make install**等待编译成功

> (4) thirdorder安装

解压后进入目录，填写setup.py中的INCLUDE_DIRS和LIBRARY_DIRS。进入或创建一个python2.7的环境，运行compile.sh，等待编译成功。

示例

> (1)运行thirdorder_pwmat.py,获取FORCE_CONSTANTS_3RD

a. 产生一系列扰动后的结构 **$python /path/to/thirdorder_pwmat.py sow na nb nc cutoff[nm/-integer]**

其中**na nb nc**为超胞的维度，必须为正整数。**cutoff**参数决定力截止的距离，距离超过此参数的原子之间的相互作用将被忽略。如果cutoff是正实数，则将其解释为以nm为单位的距离；另一方面，如果是负整数-n，则表示为超胞中第n个近邻之间的最大距离，并相应地设置截止距离。

```
[hxj@login si]$ python /data/home/hxj/software/shengBTE/thirdorder/thirdorder_pwmat.py sow 2 2 2 -2
Reading atom.config
Analyzing the symmetries
- Symmetry group Fd-3m detected
- 48 symmetry operations
Creating the supercell
Computing all distances in the supercell
- Automatic cutoff: 4.17172211886 nm
Looking for an irreducible set of third-order IFCs
- 5 triplet equivalence classes found
- 48 DFT runs are needed

.d88888b    .88888.  dP   dP   dP
88.     "' d8'   `8b 88   88   88
`Y88888b. 88     88 88  .8P  .8P
      `8b 88     88 88  d8'  d8'
d8'   .8P Y8.    .8P 88.d8P8.d8P
 Y88888P   `8888P'  8888' Y88'
oooooooooooooooooooooooooooooooo

Writing undisplaced coordinates to 3RD.atom.config
Writing displaced coordinates to 3RD.atom.config

PWmat input files moved to FC-3RD successfully
48 PWmat jobs are prepared for submission

888888ba    .88888.  888888ba   88888888b
88    `8b d8'   `8b 88    `8b  88
88     88 88     88 88     88 a88aaaa
88     88 88     88 88     88  88
88    .8P Y8.   .8P 88     88  88
8888888P   `8888P'  dP     dP  88888888P
oooooooooooooooooooooooooooooooooooooooooo
```

如上图产生了48个计算任务在文件夹FC-3RD下

```
[hxj@login si]$ ls FC-3RD
job-01  job-04  job-07  job-10  job-13  job-16  job-19  job-22  job-25  job-28  job-31  job-34  job-37  job-40  job-43  job-46
job-02  job-05  job-08  job-11  job-14  job-17  job-20  job-23  job-26  job-29  job-32  job-35  job-38  job-41  job-44  job-47
job-03  job-06  job-09  job-12  job-15  job-18  job-21  job-24  job-27  job-30  job-33  job-36  job-39  job-42  job-45  job-48
```

b.将产生的结构做DFT计算，并收集结果产生FORCE_CONSTANTS_3RD

下图为示例，注意修改图中的路径以及最后一行命令的na nb nc cutoff[nm/-integer]等值

```
#!/bin/sh
#SBATCH --partition=3080ti
#SBATCH --job-name=shengBTE
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4
#SBATCH --gres=gpu:4
#SBATCH --gpus-per-task=1

module load compiler/2022.0.2
module load mkl/2022.0.2
module load mpi/2021.5.1
module load cuda/11.6
module load pwmat --lastest
module load conda/2-5.2.0

for ((i=1; i<=48; i++)); do
  folder=$(printf "job-%02d" $i)
  cd /path/to/workdir/FC-3RD/${folder}
  mpirun -np $SLURM_NPROCS  PWmat | tee output
  cd -
done
cd ..
find FC-3RD/job* -name OUT.FORCE| sort -n| python /path/to/thirdorder_pwmat.py reap 2 2 2 -2
```

其中module load conda/2-5.2.0是安装thirdoder时调用的环境，用户在实际使用时需要根据自身安装情况增加删改环境。
计算结束后可以在当前文件夹下看到FORCE_CONSTANTS_3RD

> (2)计算声子谱，获取FORCE_CONSTANTS_2ND

参考 http://www.pwmat.com/modulefiles/pwmat-resource/moduledownload7/pdf/guide_PyPWmat2.0_20240507.pdf

重要的是在调用extract_phonon_data.sh之前需要在phonon_std文件夹内的**band_dos.conf**中加入**FORCE_CONSTANTS=WRITE**以及**FULL_FORCE_CONSTANTS = .TRUE.**，调用extract_phonon_data.sh后将得到的**FORCE_CONSTANTS**文件复制到shengBTE的工作目录下，并重命名为**FORCE_CONSTANTS_2ND**

> (3)准备shengBTE的输入文件CONTROL

再确认了二阶力常数和三阶力常数文件完整后，还需要准备shengBTE的输入文件CONTROL。

```
&allocations
        nelements=2,
        natoms=2,
        ngrid(:)=12 12 12
&end
&crystal
        lfactor=0.5715017844,
        lattvec(:,1)=0.0  0.5  0.5,
        lattvec(:,2)=0.5  0.0  0.5,
        lattvec(:,3)=0.5  0.5  0.0,
        elements="Ga" "As"
        types=1 2,
        positions(:,1)=0.00  0.00  0.00,
        positions(:,2)=0.25  0.25  0.25
        epsilon(:,1)=16.1676793 0.00000000 0.00000000,
        epsilon(:,2)=0.00000000 16.1676793 0.00000000,
        epsilon(:,3)=0.00000000 0.00000000 16.1676793,
        born(:,1,1)=2.1587779 0.0000000 0.0000000
        born(:,2,1)=0.0000000 2.1587779 0.0000000,
        born(:,3,1)=0.0000000 0.0000000 2.1587779,
        born(:,1,2)=-2.1587779  0.0000000  0.0000000,
        born(:,2,2)= 0.0000000 -2.1587779  0.0000000,
        born(:,3,2)= 0.0000000  0.0000000 -2.1587779,
        scell(:)=5 5 5
&end
&parameters
        T=300
        scalebroad=1.0
&end
&flags
        nonanalytic=.true.
        isotopes=.true.
&end
```

关于介电常数与波恩有效电荷的计算可以参考PWmat module：http://www.pwmat.com/module-download
其格式如下:

- &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 x 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 x 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 x 3, E0, default=1): dielectric tensor of the system in the Cartesian basis
    - born (real, 3 x 3 x 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 x norientations, mandatory unless norientations==0): terns of integer indices defining the crystallographic directions along which to study nanowires
- &parameters namelist:
    - T (real, K): temperature to be used in the case of single temperature calculation
    - T_min,T_max,T_step (real, K): the minimum temperature, the maximum temperature and the increment to be used for multiple-temperature calculation. T takes the priority if it is present.
    - omega_max (real, rad/ps, default=1.e100): the max angular frequency up to which the anharmonic scattering properties are calculated for limited purposes.
    - 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 ||Kn-Kn-1||, where ||·|| 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)
- nthreads (integer, default=1): number of OpenMP threads each MPI process in the program will use. If nthreads<0, the program will use the maximum number of threads available, which is usually the value of environment variable OMP_NUM_THREADS

> (4)运行shengBTE

通过 **$./ShengBTE**直接运行

通过 **$mpirun -n 32 ./ShengBTE 2>BTE.err >BTE.out** 并行的运行ShengBTE

也可以通过 **$OMP_NUM_THREADS=8 mpirun -n 16 -map-by numa:PE=8 ./ShengBTE 2>BTE.err >BTE.out**进行线程和进程的并行

如果在安装时未将spglib加入环境变量，此处会报错找不到对应的库。需要在提交计算前**export LD_LIBRARY_PATH=/path/to/spglib/spglib-1.9.7/build/lib:$LD_LIBRARY_PATH**将其加入环境变量。

详细可以参考shengBTE文档 https://bitbucket.org/sousaw/shengbte/src/master/README.md

结果文件说明

Many files including temperature-dependent directories 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. For some quantites, values only for the q points in the irreducible wedge are output, values for the rest can be recovered by looking into the equivilent points in the irreducible wedge. This section includes a brief description of their contents.

- BTE.ReciprocalLatticeVectors: three reciprocal lattice basis vectors b1, b2 and b3 in nm-1.
- BTE.qpoints: This file gives q points in the irreducible wedge of Brillouin zone (BZ), of which the relative coordinates with respect to the reciprocal lattice vectors are shown in the last 3 columns.

The 1st and 2nd columns correspond the indices of those q points numbered in the irreducible wedge and in the whole Brillouin zone, respectively. The 3rd column lists the corresponding degeneracies.

- BTE.qpoints_full: this file lists all q points in ngrid(1) x ngrid(2) x ngrid(3) Γ-centered regular grid. The 1st column is a sequentially increasing index, the 2nd column contains the index of the equivalent irreducible q point numbered in the irreducible wedge, and the 3 remaining columns are the relative coordinates with respect to the reciprocal lattice vectors for the q point.
- BTE.omega: phonon angular frequencies of those q points in the irreducible wedge, in rad/ps.
- BTE.v: group velocities of those modes (q index changes first, and then band index) in the irreducible wedge, in km/s (or nm THz)
- BTE.v_full: group velocities of all modes (q index changes first, and then band index)for all points listed in BTE.qpoints_full
- BTE.w_boundary: boundary scattering rate (in ps^{-1} , 2nd column) obtained for a characteristic length L=1 nm and a specularity parameter p=0 vs angular frequency (in rad/ps, 1st column) for those modes (q index changes first, and then band index) in the irreducible wedge.
- BTE.w_isotopic: isotopic scattering rate (in ps^{-1} , 2nd column) vs angular frequency (in rad/ps, 1st column) for those modes (q index changes first, and then band index) in the irreducible wedge.
- BTE.dos: the phonon density of states (2nd column) vs the angular frequencies (1st column, in rad/ps)
- BTE.pdos: the phonon density of states projected on each atom in the unit cell (from the 2nd column on) vs the angular frequencies (1st column, in rad/ps)
- 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.P3_plus*, BTE.P3_minus*: equivalents of BTE.P3 and BTE.P3_total, but including only contributions from emission (minus) or absorption (plus) processes
- BTE.gruneisen: Grüneisen parameter for each irreducible q point and phonon band
- BTE.cvVsT: specific heat of the system, in $J/(m^3K)$ as a function of T (1st column)
- BTE.gruneisenVsT_total: total Grüneisen parameter obtained as a weighted sum of the mode contributions as a function of T (1st column)
- BTE.KappaTensorVsT_sg: thermal conductivity tensor per unit of mean free path in the small-grain limit, in W/(m K nm) as a function of T (1st column).
- BTE.KappaTensorVsT_RTA: total thermal conductivity tensor in unit of W/(m K) in the Relaxation Time Approximation (zero-order) as a function of T (1st column).
- BTE.KappaTensorVsT_CONV: total CONVerged thermal conductivity tensor in unit of W/(m K) as a function of T (1st column). The last column gives the number of iterations reaching

convergence.

Under temperature-dependent directories:

- BTE.cv: specific heat of the system, in $J/(m^3K)$
- BTE.kappa_sg: thermal conductivity per unit of mean free path in the small-grain limit, in W/(m K nm)
- BTE.gruneisen_total: total Grüneisen parameter obtained as a weighted sum of the mode contributions
- BTE.WP3: weighted phase space available for three-phonon processes (in ps^4rad^{-4} , 2nd column) vs angular frequency (in rad/ps, 1st column) for those modes (q index changes first, and then band index) in the irreducible wedge. See [Phys. Rev. B 91, 144304 (2015)] for definition of weighted phase space.
- BTE.WP3_plus: WP3 contributed by phonon absorption processes alone
- BTE.WP3_minus: WP3 contributed by phonon emission processes alone
- 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 irreducible 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 x 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 x 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 x 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 1st column specifies a cutoff mean free path (in nm) when calculating the total contribution.
- BTE.cumulative_kappaVsOmega_tensor: this is analogous to BTE.cumulative_kappa_tensor, except in that the 1st column specifies a cutoff angular frequency (in rad/ps) when calculating the total contribution.