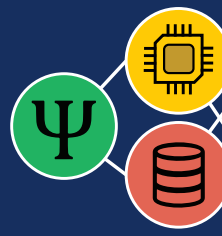
Phoebe

A collection of Phonon and Electron Boltzmann Equation solvers

CSGF Program Review

Jenny Coulter
Harvard University

Harvard John A. Paulson School of Engineering and Applied Sciences



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Motivation

- Goal: Predict what happens when an electric field or thermal gradient is applied to a material
- On a macroscopic scale: electrical or thermal conductivity observed
- On a microscopic scale: electrons and phonons (“particles” representing vibrations of the atomic lattice) are influenced by the applied potential
- We want to use this microscopic information to predict the macroscopic scale effects for new materials

Boltzmann Transport Equation

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We describe influence of a field as changes in particle distribution
(f, where f is ~ concentration of particles with a given energy and momenta)

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{\text{forces}} + \left(\frac{\partial f}{\partial t}\right)_{\text{diffusion}} + \left(\frac{\partial f}{\partial t}\right)_{\text{scattering}}$$

Due to some external force (such as E field)

Due to thermal gradient

Inter-particle collisions slow forward flow

This is the BTE — an integro-differential equation we want to solve numerically

Boltzmann Transport Equation

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- We can approximate and "linearize" the BTE — then write it as a matrix problem

$$A_{\nu,\nu'} f_{\nu}^{\mathrm{EX}} = b_{\nu'}$$

Scattering matrix: contains interaction information

Solution vector: distribution of particles

Collected single-particle terms

- If we solve for f, we know transport coeffs:

$$Q \propto (\boldsymbol{b} \cdot \boldsymbol{f}^{\mathrm{EX}}) \nabla T \longrightarrow \kappa \propto \boldsymbol{b} \cdot \boldsymbol{f}^{\mathrm{EX}}$$

Solution: Phoebe

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- This is a computationally challenging problem to solve!
  - Calculating interactions is complicated
  - The scattering matrix is a huge, dense matrix

- A collection of phonon and electron Boltzmann equation solvers
- Can predict a wide range of transport effects (taking into account both phonon and electron interactions)

Workflow Overview

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In general, we calculate these transport properties by:

Calculate coupling matrix elements → Calculate scattering rates → Solve BTE to find transport coefficients

This is a very broad view of Phoebe workflow.

For the sake of brevity, we'll consider this process for phonons.

(However, we have the ability to do electrons as well.)

Phonon-Phonon Coupling

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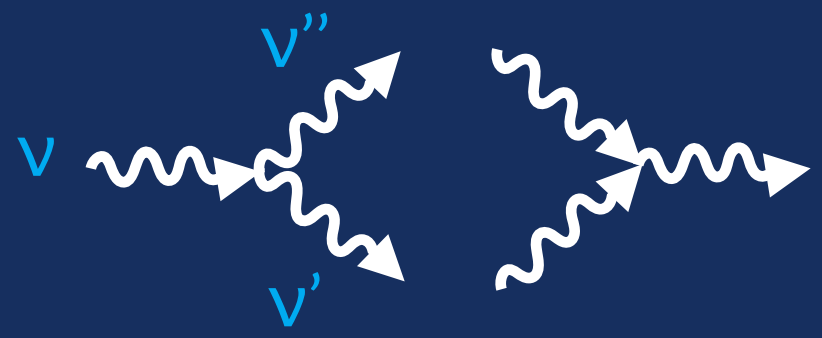
- Ph-ph coupling is needed to understand how phonons scatter
- Calculate (real space) force constants using an external code (phono3py or ShengBTE) using forces from DFT
- Fourier transform them onto a dense mesh of particle states (ν)

$$V^{(3)}(R, R', R'') \longrightarrow \begin{matrix}\text{Fourier} \\ \text{Interpolation}\end{matrix} \longrightarrow V^{(3)}(\nu, \nu', \nu'')$$

(This part of Phoebe is GPU accelerated)

Phonon-Phonon Scattering



A phonon splits into two, or two phonons combine into one

- Use "Fermi's golden rule" to calculate scattering rates

$$P_{\nu}^{\nu',\nu''} = \frac{2\pi}{N_0\hbar^2}\left|V^{(3)}\right|^2 \bar{n}_{\nu}\left(\bar{n}_{\nu'}+1\right)\left(\bar{n}_{\nu''}+1\right)\delta\left(q-q'-q''\right)\delta\left(\omega_{\nu}-\omega_{\nu'}-\omega_{\nu''}\right)$$

Coupling matrix elements

Occupation factors

Energy/momentum conservation via delta fns

Transport Coefficients

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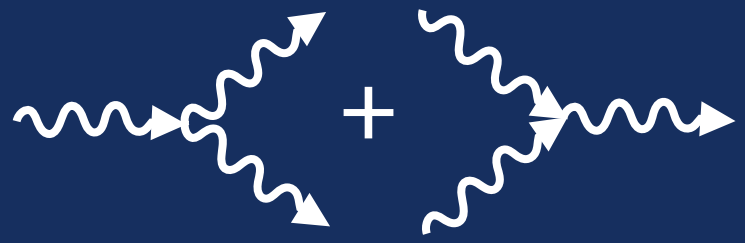
- We build the scattering matrix, A from our scattering rates

$$A_{\nu,\nu'} = \left[\quad + \quad + \ldots \right]$$

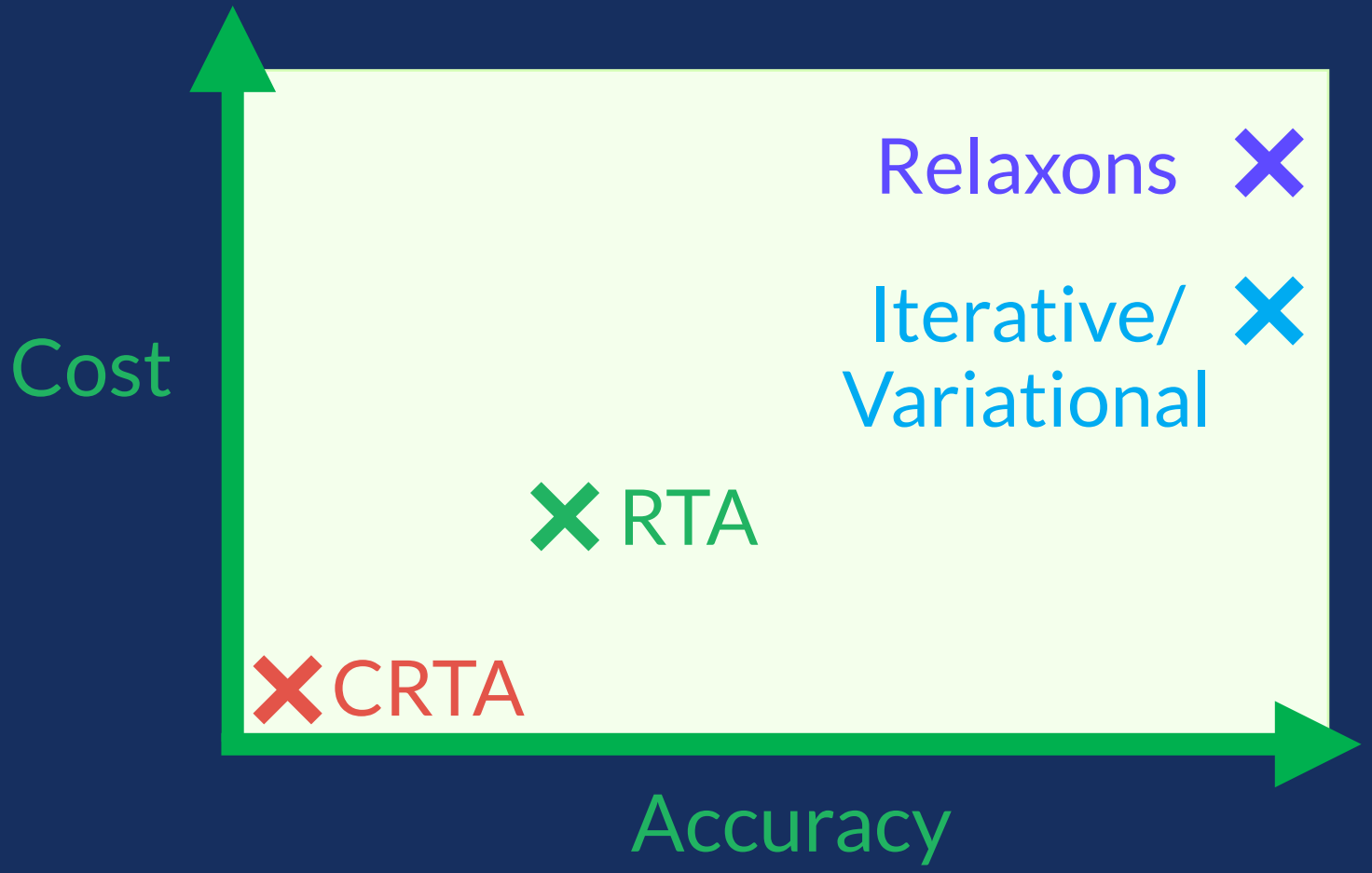


Scattering rate from ν -> ν',
summed over all states ν''

- Now we return to our matrix problem, where we want f^{EX}

$$A_{\nu,\nu'} f_{\nu}^{\mathrm{EX}} = b_{\nu'}$$

Transport Coefficients



- Phoebe offers a number of ways to solve this problem

Transport Coefficients

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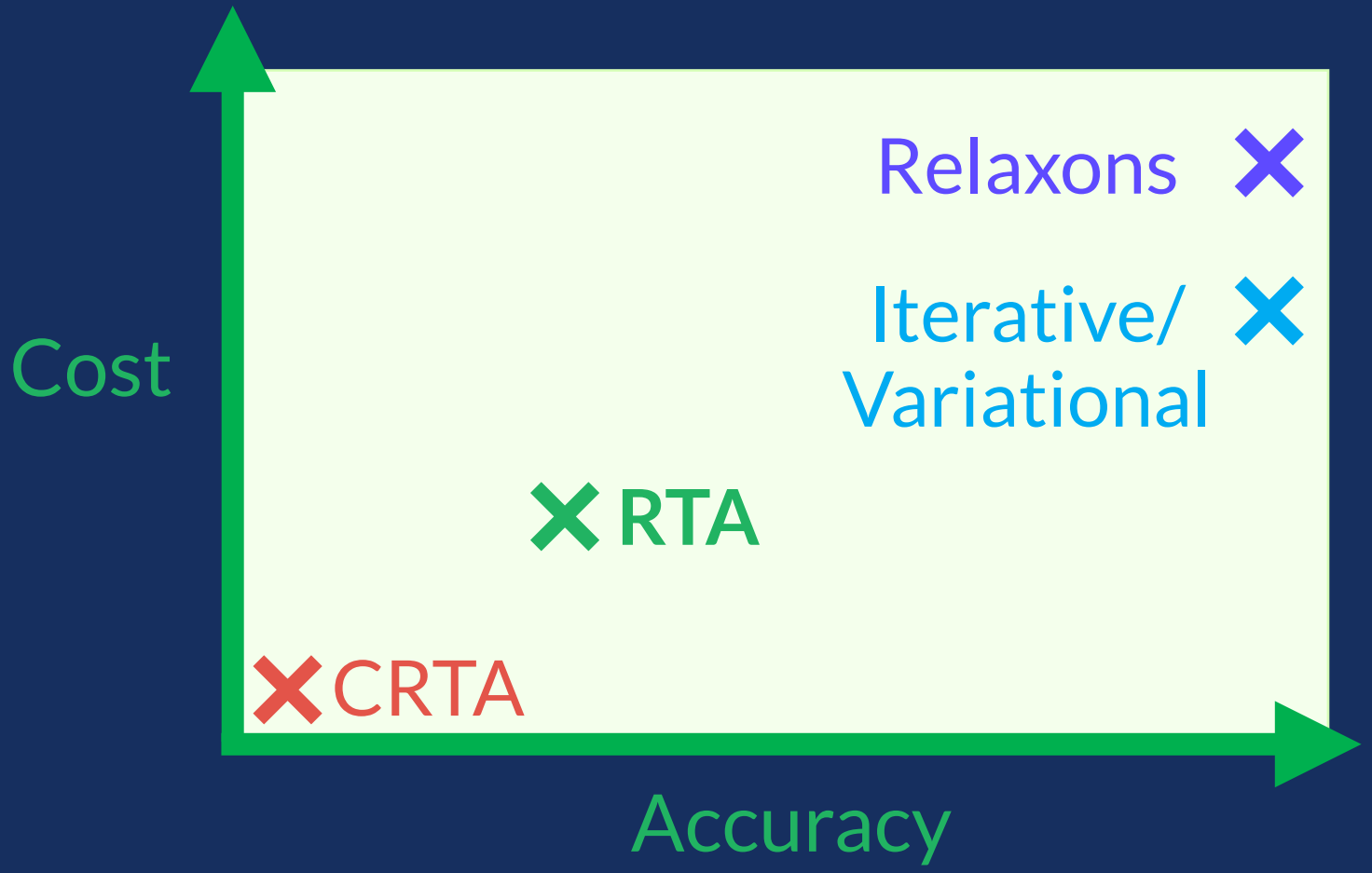
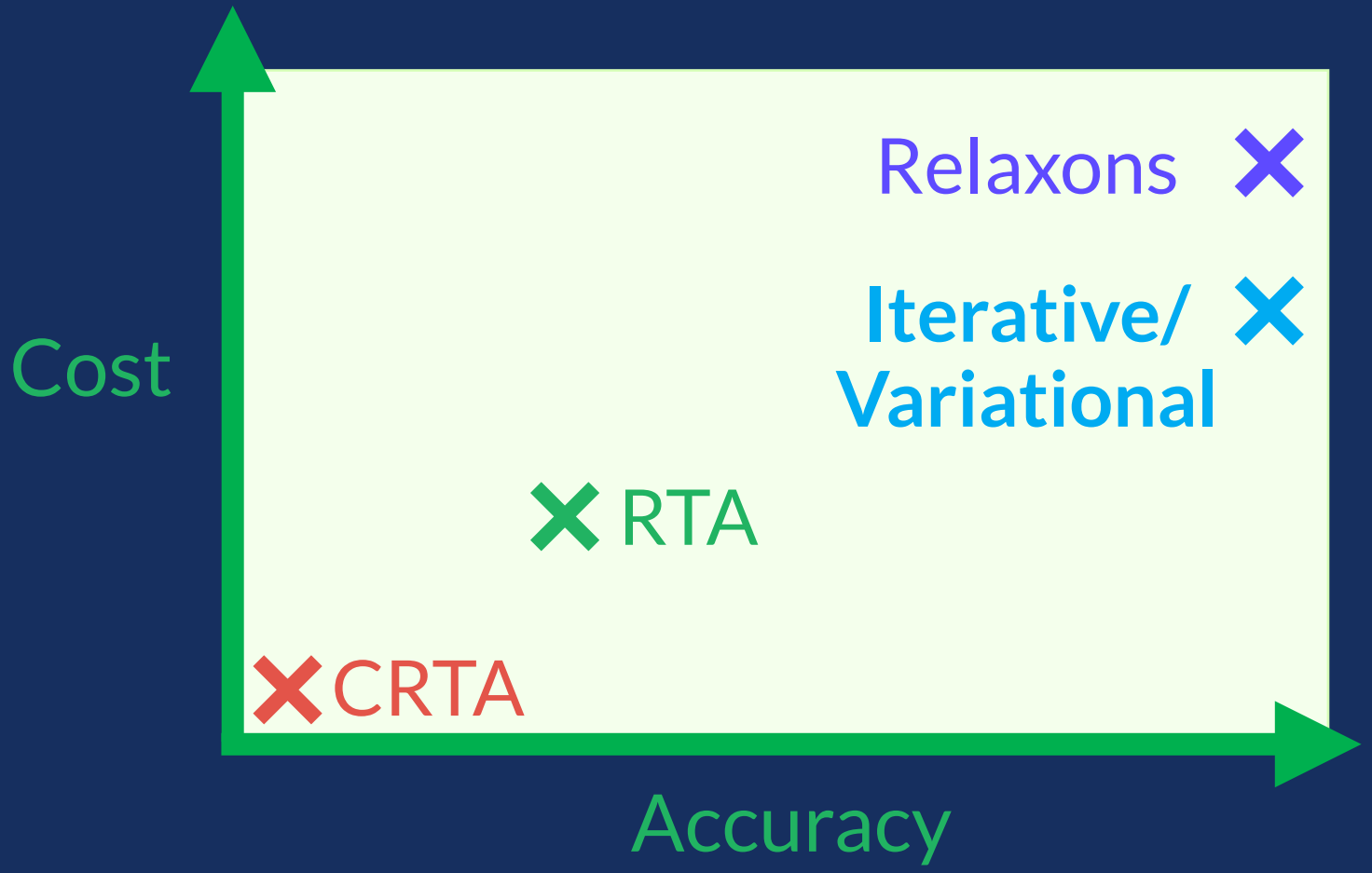


Relaxation Time Approximation:

- Approximate A using only its diagonal.
- Solve is now trivial, but approx is inaccurate in some situations.

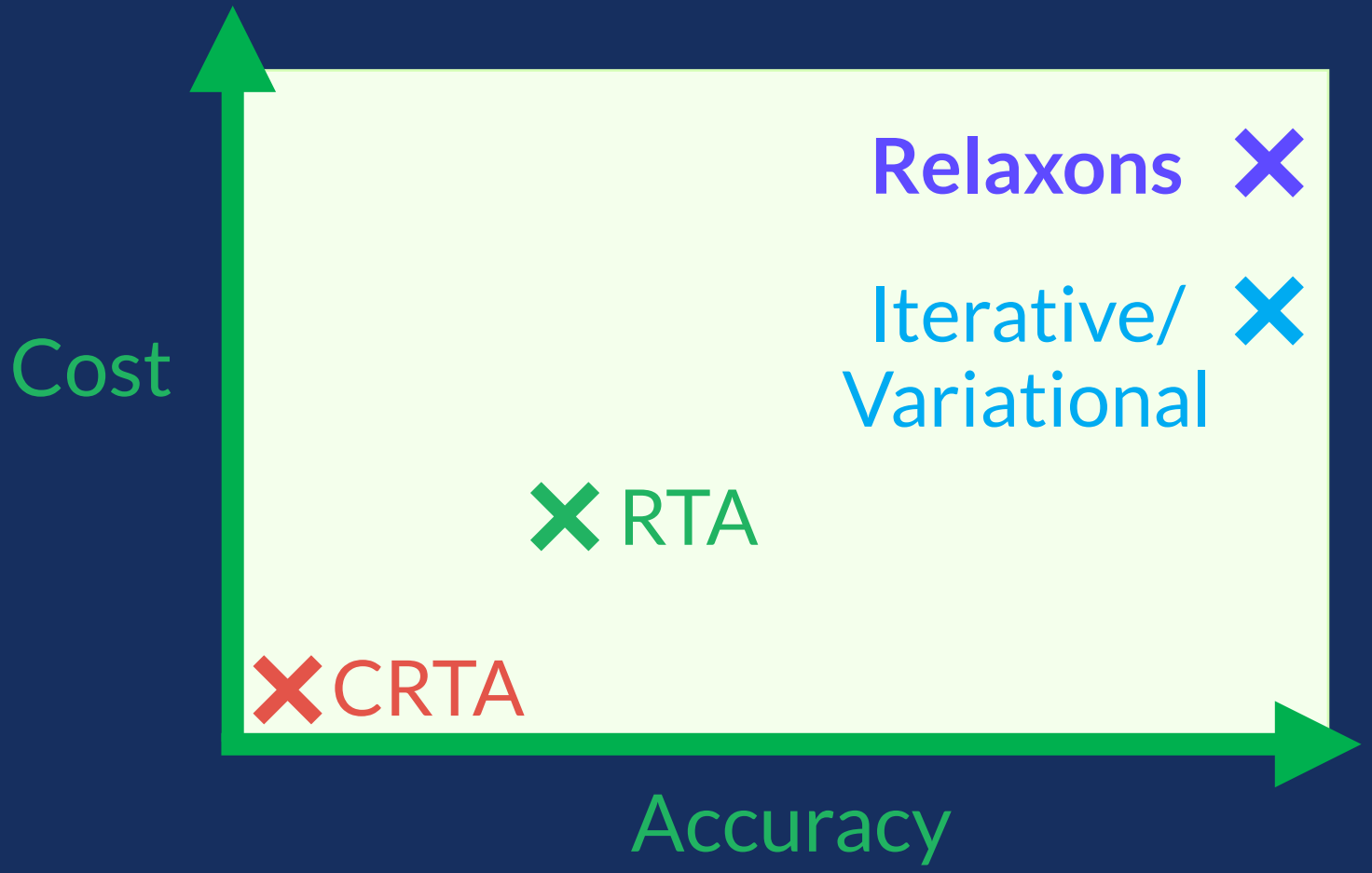
Transport Coefficients



Iterative/Variational Solvers:

- Iterative: iterate on f as a geometric series, until convergence
- Variational: iterate using CG method to find f which maximizes κ[f]

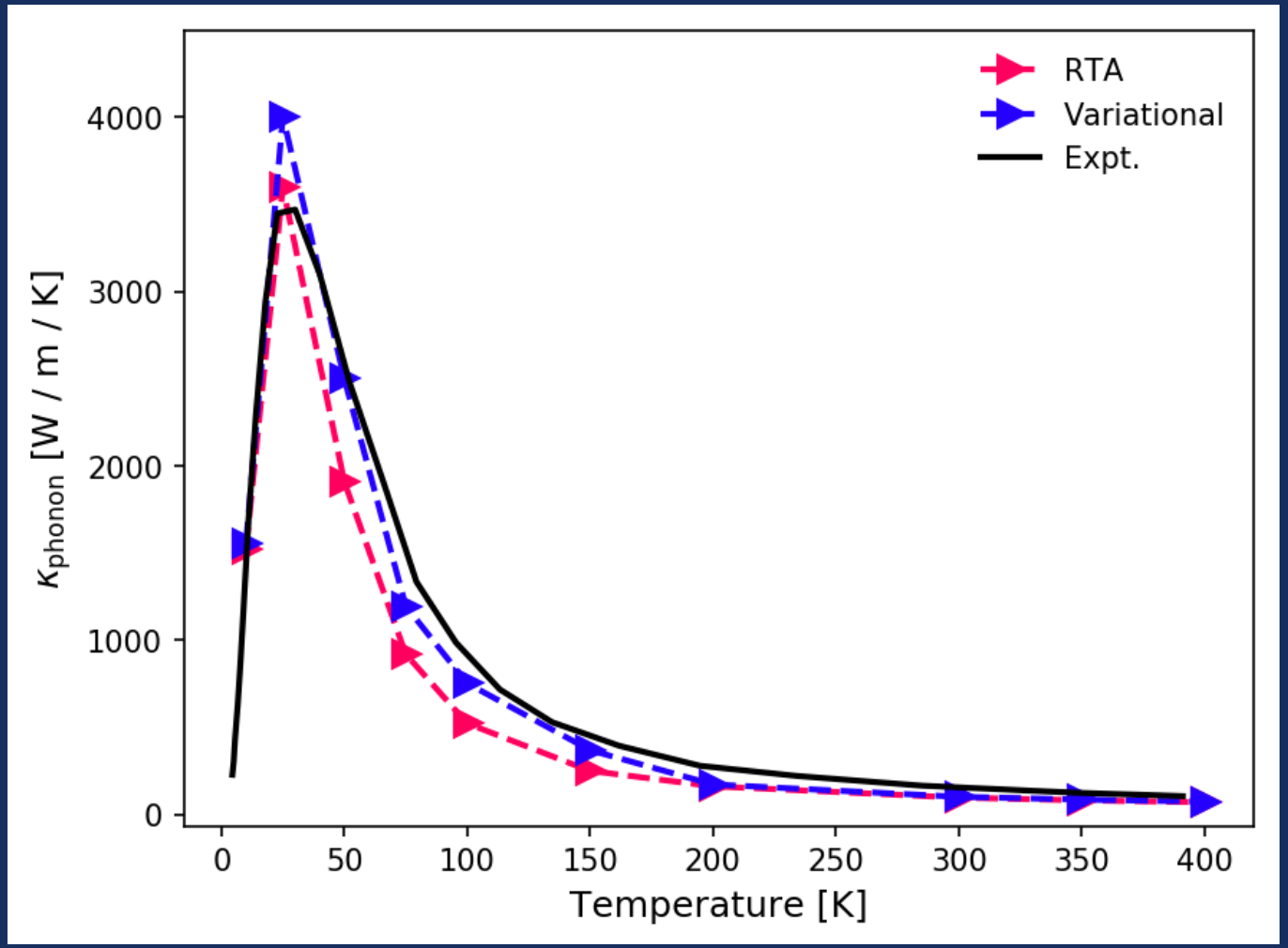
Transport Coefficients



Relaxons Solver:

- Direct diagonalization for solve
- Provides more microscopic information than iterative solvers

Transport Coefficients



Demonstration for bulk silicon. Experiment: *Phys. Rev. 134, A1058–A1069 (1964).*

Functionality Overview

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Phonon Transport

Input Codes: ShengBTE, phono3py

Scattering: Ph-ph, boundary, isotope

Solvers: RTA, iterative, variational, relaxons (+ Wigner correction)

Observables: $\kappa_{lattice}$, specific heat, phonon viscosity

Electronic Transport

Input Codes: QE

Scattering: El-ph (+polar), boundary

Solvers: CRTA, RTA, iterative, variational, relaxons (+ Wigner correction), EPA

Observables: σ, κ_{el}, S_d, specific heat, electron viscosity

Functionality Overview

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- An open-source code, written in object-oriented c++
- Designed for HPC systems:
  - MPI-OpenMP hybrid parallelism
  - Memory-distributed computing via ScaLAPACK
  - GPU (Kokkos) accelerated calculation of scattering rates
- (See the tutorials and documentation links on next page.)

Acknowledgements

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Phoebe

https://github.com/mir-group/phoebe

https://phoebe.readthedocs.io/

Check it out!