COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

PHOEBE: A NEW OPEN-SOURCE PACKAGE FOR ELECTRICAL AND THERMAL MATERIALS TRANSPORT PREDICTIONS FROM FIRST-PRINCIPLES

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ABSTRACT:

Understanding the electrical and thermal transport properties of materials is critical to the design of all kinds of devices. The theoretical prediction of these quantities relies on an accurate description of the electron and phonon properties of each material. Additionally, a number of different quasiparticle interactions must be considered to accurately predict transport behavior. While first-principles methods based on density functional theory can describe these material-specific quasiparticle properties, using this information to calculate transport coefficients can be computationally demanding and memory intensive.

To address this challenge, we present a recently developed software package, Phoebe (https://github.com/mir-group/phoebe), which includes the effects of electron-phonon, phonon-phonon, boundary, and isotope scattering to predict the electron and phonon transport properties of materials by solving the Boltzmann transport equation (BTE) using a scattering matrix formalism. This open source C++ code utilizes MPI-OpenMP hybrid parallelization as well as GPU acceleration and distributed memory structures to manage computational cost and take advantage of modern HPC systems. Using this new framework, we are able to accurately and efficiently predict a wide range of material transport properties such as the electrical and thermal conductivity and thermoelectric performance.

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https://math.mit.edu/sites/crib/

ZOOM MEETING info:

https://mit.zoom.us/j/96155042770
Meeting ID: 961 5504 2770

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