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Deviational formulations for efficient simulation of multiscale phonon transport JEAN-PHILIPPE PERAUD, NICOLAS HADJICONSTANTINOU, Mechanical Engineering, MIT — We show that by simulating only the deviation from equilibrium, considerable computational savings can be realized in Monte Carlo solutions of the Boltzmann equation describing phonon transport at small scales. The computational savings manifest themselves in the form of significantly smaller statistical uncertainty compared to standard Monte Carlo solution methods in the limit of small deviation from equilibrium (e.g. small temperature differences). Additional computational savings are realized in multiscale problems where the degree of deviation from equilibrium varies considerably over the simulation domain. By developing rigorous evolution equations for the deviation from equilibrium from the governing kinetic equation, the resulting algorithm seamlessly bridges the near- and far-equilibrium regions without introducing any approximation. We also show that considering an energy-based Boltzmann equation lends itself naturally to algorithms that conserve energy exactly, thus improving the simulation fidelity. Application of the proposed methods to practical problems of current interest, such as a transient thermoreflectance experiment used to extract information about the mean free path of heat carriers in various materials, will be presented and discussed.

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