High-fidelity phonon transport simulation in graphene devices using efficient, variance-reduced Monte Carlo methods

COLIN LANDON, NICOLAS HADJICONSTANTINOU, Mechanical Engineering, MIT — In this talk we consider thermal transport in graphene at sufficiently small scales that diffusive transport (Fourier’s law) is no longer valid. In this regime, the Boltzmann transport equation may be used to describe thermal transport, and Monte Carlo is the typical solution method, especially in the context of device simulation. Unfortunately, due to the slow rate of convergence of Monte Carlo solutions with the number of samples, such simulations can be prohibitively costly. By employing a recently developed variance-reduced Monte Carlo method, we are able to efficiently simulate the Boltzmann equation for phonon transport without resorting to approximations for reducing the problem complexity or dimensionality, such as neglecting phonon-phonon scattering events, or modeling boundary scattering as a homogeneous relaxation (scattering) process. We use our simulations to characterize the error associated with these approximations in the context of thermal transport in graphene devices, but also to study thermal transport in novel two-dimensional geometries.

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