APPLIED MATHEMATICS COLLOQUIUM

On the fundamentals and simulation of nanoscale kinetic transport

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Abstract: As characteristic lengthscales become on the order of or smaller than carrier free paths in dilute systems, the traditional continuum transport laws fail. In this talk we discuss recent developments in the fundamentals and simulation of such phenomena in the context of nanoscale kinetic transport, and in particular, phonon-mediated (solid state) heat transport.
Using asymptotic analysis of the Boltzmann equation, we show how the differential equations and boundary conditions governing heat transfer in the limit of finite but small mean free path can be derived. This analysis shows that the first kinetic effects that appear as lengthscales decrease (from the macroscopic) are in the vicinity of the boundaries and can be captured by imposing modified boundary conditions to the heat conduction equation. The modified boundary conditions, typically of the jump type, can be rigorously and systematically derived by solving a boundary layer problem, matching the outer (Fourier solution) with an inner, kinetic-Boltzmann, problem. A well-known example of such behavior is the Kapitza resistance associated with the interface between two materials. We show how our asymptotic solution procedure can be used to calculate this resistance from first principles.
Problems featuring even smaller lengthscales (on the order of the mean free path or smaller) can be simulated using the recently developed deviational Monte Carlo method for solving the Boltzmann transport equation. By solving only for the deviation from equilibrium (and providing the equilibrium part of the solution analytically), deviational Monte Carlo methods use significantly fewer computational particles for the same resolution, or alternatively, they provide significantly improved resolution, compared to traditional Monte Carlo methods for the same computational cost. These benefits are particularly prominent in multiscale problems where the ability to focus computational resources only in regions where deviations from equilibrium are large is key to computational efficiency.

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