



Fast Computational Techniques for Sub-continuum Transport

Tuesday,
October 15, 2013,
3:30P.M.

Lower Level
Auditorium,

Geddes Hall

Refreshments served
at 3:00 p.m. in the
Geddes Hall
Coffee House

In recent explosion of interest in exploring micro- and nanoscale physics has driven a concomitant interest in efficient computational methods to aid in the design and interpretation of experiments, and to understand the behavior of microscale devices and systems. In our group, we have been developing finite volume methods for sub-continuum transport which recognize the commonality of the theory underlying phonon and gas-phase transport at small scales. In the particle limit, when coherence effects can be neglected, phonon transport may be described by the phonon Boltzmann transport equation. In contrast to previously published "gray" phonon transport models, recent work has begun to resolve the wave-vector space in detail; this is essential for understanding the physics underlying strongly non-equilibrium transport, such as that encountered in ultra-scaled transistors. However, phonon relaxation times in materials such as silicon span 4-5 orders of magnitude and the resulting spread in Knudsen number causes conventional computational algorithms to perform very poorly or even fail completely. Similar problems are encountered in rarefied gas dynamics, for example, in the Bhatnagar-Gross-Krook (BGK) model and its variants. We have developed fast convergent finite volume schemes which address this range of Knudsen number and which are 2-200 times faster than existing schemes and which scale extremely well on large-scale parallel platforms. Recent applications of these methods to the simulation of realistic particle composites and to microsystem simulation are discussed.



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