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DEVIATIONAL METHODS FOR MULTISCALE KINETIC SIMULATION

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We discuss a class of recently-developed [1] variance reduction methods for Monte Carlo simulation methods based on the principle of control variates. We show that this principle becomes particularly useful for a number of kinetic phenomena of interest exhibiting small deviations from equilibrium, because the control can be chosen as the nearby equilibrium state. By removing the statistical uncertainty associated with equilibrium fluctuations, such approaches can capture arbitrarily small deviations from equilibrium at a cost that is independent of the deviation from equilibrium. This results in speedups (compared to traditional Monte Carlo methods) which scale as Ma^{-2}; here Ma denotes the deviation from equilibrium.

Moreover, by algebraically decomposing the distribution function into an analytical part that is known and a part described by particles, deviational methods represent a seamless and powerful approach towards multiscale simulation, because they automatically and adaptively focus the computational effort on the regions where kinetic effects are important [2,3].

We will conclude with a discussion of recent results from application of these methods to problems involving small-scale transport described by Boltzmann-type transport equations; examples include nanoscale gas flows [4] as well as phonon transport in the context of nanoscale heat transfer in semiconducting materials [2]. For these applications, deviational simulation methods provide speedups of several orders of magnitude (typically 3-4, but depending on the problem, as large as 8 [2]), enabling us to simulate problems that are out of reach of other state-of-the-art solution methods.

REFERENCES

[1] L.L.Baker and N.G. Hadjiconstantinou, Variance Reduction for Monte Carlo Solutions of the Boltzmann Equation. *Phys. Fluids*, Vol. **17**, 051703, 2005.

[2] J-P. M. Peraud and N. G. Hadjiconstantinou, Efficient Simulation of Multidimensional Phonon Transport Using Energy-based Variance-reduced Monte Carlo Formulations. *Phys. Rev. B*, Vol. **84**, 205331, 2011.

[3] G.A. Radtke, J-P. M. Peraud and N. G. Hadjiconstantinou, On Efficient Simulations of Multiscale Kinetic Transport. *Phil. Trans. R. Soc. A*, Vol. **371**, 2012182, 2013.

[4] G.A. Radtke, N.G. Hadjiconstantinou, and W. Wagner, "Low-Noise Monte Carlo Simulation of the Variable Hard-Sphere Gas. *Phys. Fluids*, Vol. **23**, 030606, 2011.