EFFICIENT SIMULATION OF MULTISCALE NON-CONTINUUM TRANSPORT

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Summary We propose a new class of simulation methods for kinetic problems based on a decomposition of the governing description into an equilibrium part that is described deterministically (analytically or numerically), and a small remainder, which is described using a particle simulation method. By deriving evolution equations for these parts from the governing equation, a dynamically and automatically adaptive decomposition is obtained, resulting in a multiscale method that seamlessly bridges the two descriptions without introducing any approximation. Such decompositions can also be thought of as variance reduction techniques with the equilibrium state serving as the control. The resulting computational benefits are substantial and can be realized in a broad spectrum of applications, because typical transport processes and phenomena of practical interest correspond to small perturbations from nearby equilibrium distributions. In many cases, the computational cost reduction enables otherwise intractable simulations.

INTRODUCTION

The advent of micro- and nanoscale science and technology has led to increased interest in efficient simulation methods of microelectromechanical processes and phenomena. The work presented here focuses on problems involving kinetic transport and described by the Boltzmann transport equation, governing the single-particle distribution function. Applications include micro- and nanoscale gas dynamics [1,2], plasma physics [3], micro- and nanoscale solid-state heat transfer as mediated by phonon transport [4], electron transport [5] and neutron transport [6].

The most prevalent method for solving the Boltzmann equation is a stochastic particle method known as direct simulation Monte Carlo (DSMC) [7]. DSMC (and its variants) are considerably more efficient than molecular dynamics simulations, because rather than numerically solving the equations of motion of all particles in the system, it instead exploits the weakly interacting nature of carriers to stochastically generate particle trajectories that are consistent with the Boltzmann dynamics (collisionless advection interrupted by binary collisions). Despite this, it still suffers from the basic limitations associated with atomistic simulations, namely, high statistical uncertainty [8] and increased computational cost as the continuum limit is approached. The present paper describes a new methodology which alleviates these limitations without introducing any new approximations.

ALGEBRAIC DECOMPOSITION

In contrast to traditional multiscale formulations which apply different descriptions based on a domain spatial decomposition, here we discuss methods based on a decomposition of the distribution function into an equilibrium part and a non-equilibrium part. For problems close to equilibrium (small temperature differences, small flow velocities), the non-equilibrium part will be small; by choosing to describe only the non-equilibrium part using a particle method, the number of simulation particles required can be reduced significantly.

As remarked above, deviation from equilibrium is defined with respect to a *uniform* global equilibrium state, in contrast to the deviation from the local equilibrium distribution, which is a measure of the breakdown of the Navier-Stokes description [2]. The difference between the two can be highlighted by considering a high speed (Mach number, Ma) flow which can be described by the Euler system of equations: although in this flow local equilibrium conditions prevail, the deviation from a uniform equilibrium at rest are large. In more technical terms, given Ma=Re.Kn, where Kn is the Knudsen number defined as the ratio of the molecular mean free path to the characteristic flow lengthscale, small deviations from (global) equilibrium (Ma<<1) do *not* require, nor imply, Kn<<1.

Variance reduction

Due to the prevalence of small deviations from equilibrium in micro- and nanoscale science and engineering, simulating the deviation from equilibrium was recently proposed as a variance-reduction methodology [9], namely a control-variate approach with the equilibrium serving as the control. The resulting deviational methods [10,11,12,13], achieve large speedups in the limit of small deviation from equilibrium for *all* Kn. An example can be seen in the figure below, which shows a deviational simulation of phonon transport in response to impulsive laser heating. Due to the small temperature differences involved, this (essentially noise-free) simulation is impossible using traditional simulation methods [11].

Remarkably, the statistical uncertainty of deviational methods is proportional to the deviation from equilibrium; as a result, for a fixed signal-to-noise ratio, they can be used to simulate arbitrarily small deviations from equilibrium (signals) at a cost that does not scale with the signal. This is in stark contrast with molecular simulation methods (including DSMC) whose cost, for a fixed signal-to-noise ratio, diverges quadratically as the signal goes to zero.

Deviation from local equilibrium and multiscale implications

Use of a spatially and temporally variable equilibrium distribution as a control would be expected to provide improved variance reduction, because, in principle, it can be chosen such that it minimizes the non-equilibrium component of the

distribution function. This has been verified by developing a deviational method which uses a spatially variable equilibrium as a control [13]; in this case, computational results show [13] that the variance reduction improves as the Knudsen number decreases, since local equilibrium conditions become an increasingly better approximation.
The latter observation highlights the utility of algebraic decomposition as a powerful multiscale method: in contrast to standard particle simulation methods, which become increasingly more expensive as the limit Kn<<1 is approached, a formulation utilizing algebraic decomposition becomes more efficient in this limit, because it is able to relegate increasingly more of the description to the *local* equilibrium part, thus reducing the number of particles required for the simulation. Although the deviational simulation that generated the result in the figure below was based on a uniform global equilibrium, this example still highlights the benefits of a decomposition that allows the use of a deterministic solution to describe the far-field region, thus reducing the number of simulation particles by orders of magnitude.
Simulating the deviation from the local equilibrium is challenging both because the latter needs to be tracked as function of time, but also because particle advection does not preserve equilibrium and thus, unless special measures are taken, the algebraic decomposition is not preserved in time [14]. Computationally tractable algorithms which preserve the algebraic decomposition can be found in Refs 10 and 13.

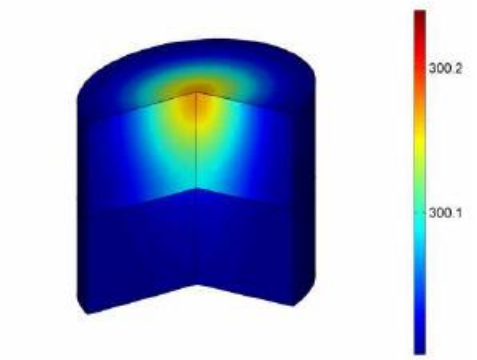

Figure: Snapshot of deviational simulation of phonon transport in a thin aluminium film resting on a semi-infinite substrate following impulsive heating by a laser pulse.

DISCUSSION

By capturing the governing kinetic equation where necessary while requiring only a small number of particles to describe (large) regions where continuum conditions apply, algebraic decomposition provides a seamless and dynamically adaptive approach for coupling microscopic and macroscopic descriptions. Of particular interest is the extension of algebraic decomposition methods to more complex systems (e.g. dense fluids) where governing equations for the distribution function reside in higher-dimensional spaces. Such systems are more challenging to treat because the governing equation is typically more complex, making it harder to derive explicit expressions for the dynamics of the equilibrium part and the deviation therefrom.

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