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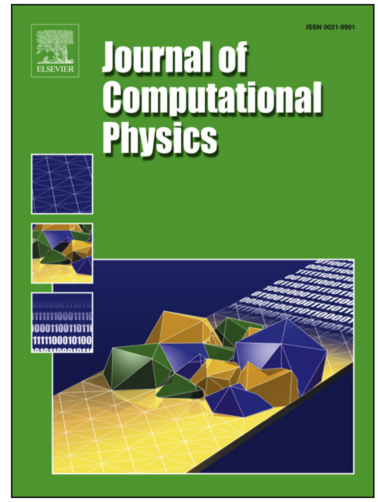

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Efficient Algorithms and Implementations of Entropy-based Moment Closures for Rarefied Gases

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Abstract

We present efficient algorithms and implementations for the 35-moment system equipped with the maximum-entropy closure in the context of rarefied gases. While closures based on the principle of entropy maximization have been shown to yield very promising results for non-equilibrium gas processes, such as shock-structure problems, the computational cost of these closures is in general much higher than for closure theories with explicit closed-form expressions of the closing fluxes, such as Grad's classical closure. Following a similar approach as Garrett et al. (J. Comput. Phys., 2015), we investigate efficient implementations of the computationally expensive numerical quadrature to compute moments of the maximum-entropy distribution by exploiting its inherent fine-grained parallelism with the parallelism offered by multi-core processors and graphics cards. We show that using a single graphics card as an accelerator allows speed-ups of two orders of magnitude compared to a serial CPU implementation. In order to accelerate the time-to-solution for steady-state problems, we propose a new semi-implicit time discretization scheme. For the semi-implicit time discretization the resulting nonlinear system of equations is solved with a Newton type method in the Lagrange multipliers of the dual optimization problem in order to reduce the computational cost. Additionally, fully explicit Lax-Wendroff type schemes of first and second order accuracy are presented. We investigate the accuracy and efficiency of the proposed methods for several numerical test cases, including a steady-state shock-structure problem.

Keywords: non-equilibrium, maximum-entropy, semi-implicit, hyperbolic, roofline, shock-structure, AVX, GPU
PACS: 47.10.Ab, 47.11.Df, 47.40.Ki, 47.45.Ab
2000 MSC: 35L45, 35L60, 35L65, 35L67, 68W10, 76J20, 82C40

1. Introduction

In this paper we consider moderately rarefied gas flows in the transition regime, for which the mean-free-path of the particles can approach the order of magnitude of the macroscopic reference length scale. Processes in rarefied gases can lead to strong deviations from the local equilibrium distribution function, which invalidate the model assumptions of Navier-Stokes-Fourier. Therefore, more detailed models are necessary for an accurate description of moderately rarefied gas flows.

Moment equations are derived directly from Boltzmann's equation by a projection of the one-particle distribution function on a finite polynomial basis in velocity space, yielding evolution equations for macroscopic quantities of the gas. Thus moment equations are lower dimensional approximations of Boltzmann's equation, which depends on up to 7 independent variables. For gas dynamics, the most fundamental moment system are the Euler equations, consisting of conservation laws for mass, momentum and energy density. The validity of the Euler equations can be extended to non-equilibrium processes by including higher-order moment equations into the system.

The mathematical and computational properties of moment systems crucially depend on the closure theory. While Grad's classical closure [1, 2] has a low computational complexity, the resulting moment system is ill-posed for strong deviations from the local equilibrium state, see e.g. [3, 4, 5]. Furthermore, Grad's closure does not ensure non-negativity of the model distribution in velocity space.

Entropy-based closures [6, 7, 8] lead to symmetric hyperbolic systems equipped with a convex entropy law. In contrast to Grad's closure, the resulting velocity distribution is non-negative. Here we consider closures maximiz-