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Hierarchical Boltzmann simulations and model error estimation

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ABSTRACT

An hierarchical simulation approach for Boltzmann's equation should provide single numerical framework in which a coarse representation can be used to compute gas flows as accurately and efficiently as in computational fluid dynamics, but a subsequent refinement allows to successively improve the result to the complete Boltzmann result. We use Hermite discretization, or moment equations, for the steady linearized Boltzmann equation for a proof-of-concept of such a framework. All representations of the hierarchy are rotationally invariant and the numerical method is formulated on fully unstructured triangular and quadrilateral meshes using a implicit discontinuous Galerkin formulation. We demonstrate the performance of the numerical method on model problems which in particular highlights the relevance of stability of boundary conditions on curved domains.
The hierarchical nature of the method allows also to provide model error estimates by comparing subsequent representations. We present various model errors for a flow through a curved channel with obstacles.

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1. Introduction

From the point of view of non-equilibrium thermodynamics there are two fundamentally different approaches to flow computations. The vast majority are based on fluid dynamic equations using the classical closure relations of Navier–Stokes and Fourier [17]. Sometimes these relations maybe refined or extended [28,34], but those models still remain in the context of macroscopic field theories [27]. On the other hand, if one is interested in precise non-equilibrium predictions, typically the Boltzmann equation is solved for the velocity distribution function of the particles [7].

The differences of the approaches are evident both mathematically and numerically. There is the use of continuum fields, like flow velocity and temperature in fluid dynamics on the one side and the microscopic probability function of the particle velocities on the other. Often, the distribution function is considered the cost to pay for increased non-equilibrium accuracy. Still, engineering fields are the preferred variables in applications and only obtained indirectly by averaging the distribution function. Numerically, there exists a very rich literature on different methods how to solve partial differential equations of fluid dynamics, from Finite-Volume (FV) to Finite-Element (FE) methods [20,14], which are still further developed. These often deal with accurate representation of the fields and the handling of nonlinearities in the equations. The Boltzmann equation, on the other hand, is frequently solved by particle methods, like the direct simulation Monte-Carlo method [3],

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where a central issue is given by speed-up [15] and noise reduction [2]. Direct discretizations use basic ingredients of the FV- or FE-approaches [8], but most effort goes into the efficient computation of the collision integral [23,12].

It is interesting to note, that any numerical approach to solve the Boltzmann equation necessarily contains a numerical method for fluid dynamic equations in the asymptotic limit of small mean free paths (small Knudsen number). While this limit may not be the focus of a Boltzmann solution, it is reasonable to expect that a serious implementation of the Boltzmann equation for flow computations should at least exhibit the capability of a fluid dynamic flow solver. On the other hand computing flow based on fluid dynamic equations is usually challenged by model errors when applied to non-equilibrium flows. In many cases model errors dominate numerical discretization errors and estimating these errors in an efficient way becomes essential when judging the results for flow applications.

This paper aims at a *hierarchical simulation* approach for the Boltzmann equation with the properties:

- The discretization of the Boltzmann equation ranges from coarse to fine representations in a cascading hierarchy using a *single numerical framework*.
- The coarse representation should result in an *accurate and efficient* numerical method to solve the classical fluid dynamic equations within the single framework.
- The finer representations give a *valid and successively better* numerical discretization of the Boltzmann equation which allows high accuracy.
- All representations are *rotationally invariant* such that the numerical method can handle unstructured meshes and possibly complex geometries easily.
- The framework should provide a systematic for *model error estimation* between the different representations and allow model-refinement local in space.

To present a proof of concept for such a framework this paper will consider steady and slow processes (low Mach number) and thus linear equations. The main challenge is to find a formulation that can include both the hyperbolic nature of the Boltzmann transport process in the fine representation as well as the elliptic nature of the Stokes problem in the coarse representation. We use a Hermite-discretization which results in hyperbolic relaxation systems, known as moment equations [21,5], that are solved with a discontinuous Galerkin method [18]. The Hermite-discretization yields the classical fluid dynamic equations in a reformulated way which fit into the framework. Additionally, stable boundary conditions are an essential ingredient. The entropy estimate for the hyperbolic systems provides simple conditions to guarantee stability of boundary conditions [29,24] and we demonstrate and discuss the numerical impact of these conditions for several simplified model systems. We also show that the coarsest representation in the framework gives an accurate discretization to fluid dynamic equations.

The hierarchy of representations allows to quickly obtain model error estimates by comparing a result with the solution on the next finer level. To demonstrate this approach we will consider the flow through a curved channel with obstacles and efficiently estimate the local model error of a classical fluid dynamic simulation within the hierarchical Boltzmann framework. The local errors of finer representations can be estimated in an analogous way and an example is also given. Local model refinement and using different representations in different domains is left for future work.

The original idea of using moment equations for hierarchical simulations was formulated by Müller in the context of extended thermodynamics, see the text book [21]. The moment systems were introduced as 'theory of theories' in which the convergence behavior of subsequent systems was used to predict their validity. Both well-posed boundary conditions and suitable computational methods were not available so that the examples of extended thermodynamics were mostly simple cases.

Note that the requirement to have a valid discretization for fluid dynamic equations on the coarsest level is similar to asymptotic preserving schemes [10]. However, in this paper no smallness parameter is involved, instead we demand that when reducing the numerical degrees of freedom for the Boltzmann discretization we literally arrive at a fluid dynamics implementation. The approach in [9] is similar in spirit, but lacks the cascading hierarchical setup.

The implementation of the methods presented in this paper is freely available at the website GitHub [36]. This code not only is capable to produce the simulation results presented, but also contain the explicit details of the large system matrices and analytical solutions used. In this way the code complements the information of this paper.

2. Hermite-discretization for the Boltzmann equation

We consider the Boltzmann equation for monatomic ideal gases in the form

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = S(f) \tag{1}$$

where $S(f)$ is the collision operator. The Maxwell distribution

$$f_M(\mathbf{c}; \rho, \mathbf{v}, \theta) = \rho/m(2\pi\theta)^{-3/2} \exp\left(-\frac{(c_i - v_i)(c_i - v_i)}{2\theta}\right) \tag{2}$$

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