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Towards an ultra efficient kinetic scheme. Part II: The high order case ☆

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ABSTRACT

In a recent paper we presented a new ultra efficient numerical method for solving kinetic equations of the Boltzmann type (Dimarco and Loubere, 2013) [17]. The key idea, on which the method relies, is to solve the collision part on a grid and then to solve exactly the transport part by following the characteristics backward in time. On the contrary to classical semi-Lagrangian methods one does not need to reconstruct the distribution function at each time step. This allows to tremendously reduce the computational cost and to perform efficient numerical simulations of kinetic equations up to the six-dimensional case without parallelization. However, the main drawback of the method developed was the loss of spatial accuracy close to the fluid limit. In the present work, we modify the scheme in such a way that it is able to preserve the high order spatial accuracy for extremely rarefied and fluid regimes. In particular, in the fluid limit, the method automatically degenerates into a high order method for the compressible Euler equations. Numerical examples are presented which validate the method, show the higher accuracy with respect to the previous approach and measure its efficiency with respect to well-known schemes (Direct Simulation Monte Carlo, Finite Volume, MUSCL, WENO).

1. Introduction

The kinetic equations provide a description of non-equilibrium gases and more generally of particle systems [2,8]. The distribution function, which describes the evolution of the system, depends, in the most general case, on seven independent variables: the time, the physical and the velocity space. It turns out that the numerical simulation of these kind of equations with deterministic techniques presents several drawbacks due to the large dimension of the problem. On the other side of the spectrum of the numerical techniques used to approximate kinetic equations, there are the probabilistic methods [2,6,7,33]. These methods and in particular Monte Carlo methods (DSMC) are extensively used due to their very low computational cost especially in the multi-dimensional cases, compared to finite volume, finite difference or spectral methods [20,21,31,32,34,39,37,38]. However, DSMC furnishes only poorly accurate and fluctuating solutions which cannot be easily ameliorated. This is especially true in non-stationary situations in which time averages techniques turn to be useless.

Many different works have been dedicated to reduce some of the disadvantages of Monte Carlo methods. We quote [6] for an overview on efficient and low variance Monte Carlo methods. Let us remind to the works of Homolle and Hadjiconstantinou [25] and [26] and of Dimarco, Pareschi and Degond [18,19,15,16] for some applications of variance reduction techniques to kinetic equations in transitional and general regimes. We recall also the works of Burt and Boyd [5] and of Pullin [40] who developed a low diffusion particle methods for simulating compressible inviscid flows.

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In this work, we continue the development of a new deterministic ultra fast method which permits to solve kinetic equations of the Boltzmann type [17]. The scheme is based on the classical discrete velocity models (DVM) approach [3,34,37,38]. The DVM models are obtained by discretizing the velocity space into a set of fixed discrete velocities [3,31,34,35]. As a result of this discretization, the original kinetic equation is then represented as a set of linear transport equations plus a source term. The source term describes the collisions or the interactions between the particles and couples all the equations of the resulting system. In order to solve the transport part of the DVM model, many different techniques can be employed like finite difference, finite volume or fast methods [4,21,20,27,32,31,24,44,45]. One of the most common strategies for solving this kind of problems is the semi-Lagrangian approach [9,10,21,41] which will be also the basis of the method here developed. Unfortunately, for each of the method cited, we recall that, the computational effort needed for solving the full six-dimensional equation, prevents still nowadays realistic simulations even with parallel machines.

To overcome the problem of the excessive computational cost, we recently proposed in [17] to use a splitting method to separate the transport from the collision step [12,43]. Then, we used a Lagrangian technique which exactly solves the transport step on the entire domain and we projected the solution on a grid to compute the contribution of the collision operator. The resulting scheme (Fast Kinetic Scheme, FKS) shares many analogies with semi-Lagrangian methods [9–11,21,41] and with Monte Carlo schemes [29], but on the contrary to them, the method is as fast as a particle method while the numerical solution remains fully deterministic, which means that there is no source of statistical error. When used to solve the limiting fluid model, the FKS method shares also some analogies with the so-called Lattice Boltzmann methods [1], but on the contrary to them its application is not limited to dense flows, all the regimes from rarefied to dense can be studied with such approach. Thanks to this new scheme, we were able to compute the solution of the full six-dimensional kinetic equation on a laptop for acceptable mesh sizes and in a reasonable amount of time (about ten hours for 100^3 space $\times$ 12^3 velocity space mesh points for 110 time steps up to $t = 0.1$ on the spherical Sod-like problem). However, the method developed, exhibited some limitations in term of spatial accuracy. In fact, it was only poorly accurate when used to compute solutions close to the fluid limit. We showed in [17] that, in these cases, the computed solutions laid between a first order and a second order MUSCL scheme. In the present work, we developed a strategy which permits to preserve a desired high order of accuracy in space for all the different regimes from the extremely rarefied to the high dense cases. In particular, it permits to recover the solution of the compressible Euler equations, when the number of collisions tends to infinity, with an high order shock capturing scheme. The modification introduced consists in coupling the fast kinetic scheme (FKS) to a solver for the compressible Euler equations, then to match the moments obtained from the solution of the macroscopic equations with those obtained from the solution of the equilibrium part of the kinetic equation. Finally, the solution, in term of the moments, is recovered as a convex combination of the two contributions: the macroscopic and the microscopic parts. We will show that the introduction of a macroscopic solver will not increase dramatically the computational cost, instead this modification will represent only a fraction of the time employed for computing the solution. In this work, the interaction term between the particles is the BGK collision operator [23]. However, the high order version of the Fast Kinetic Scheme can in principle be extended to other collisional operators as the Boltzmann one.

The article is organized as follows. In Section 2, we introduce the Boltzmann–BGK equation and its properties. In Section 3, we present the discrete velocity model (DVM). Then, in Section 4, we present the fast kinetic scheme (FKS) and the High Order Fast Kinetic Scheme (HOFKS). Several test problems which demonstrate the accuracy and the strong efficiency of the new method are presented and discussed in Section 5. Some final considerations and future developments are finally drawn in the last section.

2. Boltzmann–BGK equation

The equation to be solved is the following:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}(M_f - f), \tag{1}$$

with the initial condition $f(x, v, t = 0) = f_0(x, v)$. The non-negative function $f = f(x, v, t)$ describes the time evolution of the distribution of particles which move with velocity $v \in \mathcal{R}^d$ in the space $x \in \Omega \subset \mathcal{R}^d$ at time $t > 0$. For simplicity, in the description of the method we will do the hypothesis that the dimension of the physical space is the same of the dimension of the velocity space d. However, the method is not restricted to this particular choice and it is possible to consider different dimensions between the space and the velocity in order to obtain different simplified models. The type of interactions term which characterizes the kinetic equation in (1) is the so-called BGK relaxation operator. With this choice the collisions are modeled by a relaxation towards the local thermodynamical equilibrium defined by the Maxwellian distribution function M_f

$$M_f = M_f[\rho, u, T](v) = \frac{\rho}{(2\pi\theta)^{d/2}} \exp\left(\frac{-|u - v|^2}{2\theta}\right), \tag{2}$$

where $\rho \in \mathcal{R}$, $\rho > 0$ and $u \in \mathcal{R}^d$ are respectively the density and mean velocity while $\theta = RT$ with T the temperature of the gas and R the gas constant. The macroscopic values ρ, u and T are related to f by:

$$\rho = \int_{\mathcal{R}^d} f\,dv, \qquad u = \frac{1}{\rho}\int_{\mathcal{R}^d} vf\,dv, \qquad \theta = \frac{1}{\rho d}\int_{\mathcal{R}^d} |v - u|^2 f\,dv, \tag{3}$$