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# Local Discrete Velocity Grids for Multi-Species Rarefied Flow Simulations

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**Abstract.** This article deals with the derivation of an adaptive numerical method for mono-dimensional kinetic equations for gas mixtures. For classical deterministic kinetic methods, the velocity domain is chosen accordingly to the initial condition. In such methods, this velocity domain is the same for all time, all space points and all species. The idea developed in this article relies on defining velocity domains that depend on space, time and species. This allows the method to locally adapt to the support of the distribution functions. The method consists in computing macroscopic quantities by the use of conservation laws, which enables the definition of such local grids. Then, an interpolation procedure along with a upwind scheme is performed in order to treat the advection term, and an implicit treatment of the BGK operator allows for the derivation of an AP scheme, where the stability condition is independent of the relaxation rate. The method is then applied to a series of test case and compared to the classical DVM method.

**AMS subject classifications**: 76P05, 82B40

**Key words**: Discrete velocity model, BGK model for mixtures, local grids, rarefied gases.

## 1 Introduction

In the process of designing vehicles such as aircrafts, it is necessary to study gas mixture dynamics in rarefied configurations. In such cases, systems of PDEs such as Euler or Navier-Stokes equations may not be suitable when the Knudsen number, describing the level of rarefaction of a gas, becomes important. To this end, kinetic models, involving distribution functions defined over the phase space — a space with a larger dimension than the physical one —, need to be used. These equations, much more general and more

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accurate than the so-called fluid models, allow for the modelling of any level of rarefied gas.

However, in the context of numerical simulations, accuracy is obtained in exchange for computational cost. More specifically, in a general $d$-dimensional configuration, the kinetic variable, denoted $v$, ranges over all $\mathbb{R}^d$. Hence, in order to perform numerical approximations, the definition domain of $v$ needs to be replaced by a bounded subset of $\mathbb{R}^d$ which contains most of the information. Close to thermodynamical equilibrium, macroscopic quantities (velocities and temperatures) can be used to determine the bounds of such a subset. However, since the bounds depend on the macroscopic quantities, that themselves depend on the physical point $x \in \mathbb{R}^d$ considered, the suitable subset can vary greatly from one physical point to the other, especially through shock waves. Besides, from one species to the other, the disparities of particle masses lead to different bounds, even in the case of equivalent velocities and temperatures. Finally, quantities at a point can also vary importantly over time.

In classical numerical methods, one grid is usually taken for all physical points and all species, for all time, based on the initial data. This implies that this grid has large enough bounds to encompass the broadest distribution, and that it is precise enough in order to "see" the narrowest one.

In this article, an adaptive numerical method is proposed for multi-species kinetic equations. Such a method is able to use a different velocity grid for each physical point and each gas species, and is also adaptive in time. The idea is to use conservation laws, at each time step, in order to compute macroscopic quantities beforehand. These quantities, depending on space, time and species, are then used to define a velocity grid suitable at the subsequent discrete time. Moreover, the computation of these macroscopic quantities allows for the implicit treatment of the relaxation operator modelling collisions, which gives an asymptotic-preserving scheme for Euler in the case of a Knudsen number tending to zero. Once local velocity grids are computed, in order to apply a upwind scheme to the distribution functions, since every quantity is defined on its own grid, it is necessary to perform an interpolation procedure. This is done by using a ENO4 interpolation method, which consists in choosing an interpolation stencil with the smallest variation rate of the solution. This method prevents the interpolation through discontinuities, which can degrade the quality of the method. A second version of the method is proposed, where velocity grids are chosen in order to avoid interpolations. This is done by choosing grids with steps that are all multiple of the same quantity, so that they possess an important amount of common velocities, where interpolating is then not required. This allows for a decrease of computational cost when the number of prevented interpolations is great.

Collisions in a multi-species gas are modeled by the multi-species Boltzmann operator, presented for example in [2, 13, 27]. However, for numerical purposes, it is more interesting to replace the Boltzmann operator by a simpler relaxation term. In the case of mono-species gas, the well-known Bhatnagar-Gross-Krook model [5] ensures all the fundamental properties of the mono-species Boltzmann operator (positivity of the solu-