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A fast iterative model for discrete velocity calculations on triangular grids

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ABSTRACT

A fast synthetic type iterative model is proposed to speed up the slow convergence of discrete velocity algorithms for solving linear kinetic equations on triangular lattices. The efficiency of the scheme is verified both theoretically by a discrete Fourier stability analysis and computationally by solving a rarefied gas flow problem. The stability analysis of the discrete kinetic equations yields the spectral radius of the typical and the proposed iterative algorithms and reveal the drastically improved performance of the latter one for any grid resolution. This is the first time that stability analysis of the full discrete kinetic equations related to rarefied gas theory is formulated, providing the detailed dependency of the iteration scheme on the discretization parameters in the phase space. The corresponding characteristics of the model deduced by solving numerically the rarefied gas flow through a duct with triangular cross section are in complete agreement with the theoretical findings. The proposed approach may open a way for fast computation of rarefied gas flows on complex geometries in the whole range of gas rarefaction including the hydrodynamic regime.

1. Introduction

Fully deterministic discrete velocity (or ordinates) algorithms have been extensively used in the direct numerical solution of the Boltzmann equation or alternatively of kinetic model equations [1–4]. Of course, the involved computational effort is significant since solving for the unknown distribution function, in a general-geometry problem, would require a six-dimensional phase space grid (three variables in the physical space and three variables in the molecular velocity space), which imposes severe demands on computer resources (time and memory). In spite of this, the discrete velocity (DV) method is considered as an efficient approach for solving problems in rarefied gas dynamics [5]. Even more, in certain physical systems where, due to the flow conditions and parameters, linearization of the governing kinetic equations and reduction of the number of spatial and velocity coordinates are permitted, the DV method has shown to be probably the most powerful computational scheme for providing reliable results in the whole range of the Knudsen number [6,7]. Such problems commonly appear in several technological fields including the emerging field of nano and microfluidics [8].

The direct differencing of kinetic equations implementing the discrete velocity approach yields a discretized coupled integro–differential system, which is solved in an iterative manner. The convergence speed of this iterative algorithm is satisfactory in highly rarefied atmospheres (large Knudsen numbers) but it slows down significantly as the atmosphere becomes less rarefied and finally, it becomes very slow at intermediate and small Knudsen numbers (part of the transition as well as in the slip regimes). This slow convergence has been recently circumvented by introducing a synthetic acceleration methodology to speed up the DV convergence rate in dense atmospheres [9–11]. That is an important advancement of the DV algorithm since it upgrades its overall performance and it allows its efficient implementation in all flow regimes. The

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discretized version of this rapidly convergent iteration scheme has been applied so far to flow configurations, which can be adequately described on standard orthogonal grids.

It is important to note that fast iterative algorithms for discrete ordinates particle calculations have been originated and then extensively developed and efficiently implemented in the field of neutron and radiative transfer [12,13]. However, corresponding work in rarefied gas dynamics is very limited.

In the present work a fast iterative algorithm is proposed for the efficient computational solution of linear kinetic equations on triangular lattices. This non-regular lattice consisting of triangular grid elements has been recently introduced [14] and it is very useful for generalizing kinetic type solutions to rarefied flows in domains with complex boundaries. The discretization of the accelerated scheme on such non-standard grids is not trivial. Also, the convergence rates of both the typical and accelerated discrete algorithms are estimated by a discrete Fourier stability analysis. As far as the authors are aware of, this is the first time that a stability analysis of discrete kinetic equations in the field of rarefied gas dynamics is presented. It is found theoretically that the accelerated method performs significantly faster than the typical one. It is also shown that the discrete models with increasing resolution rapidly reach the convergence rate of the continuous equations. The theoretical findings are verified computationally be solving, as a benchmark problem, the flow of a gas through a triangular channel, described by the linearized two-dimensional Bhatnagar–Gross–Krook (BGK) kinetic equation [14]. The dependency of the iteration scheme on the discretization parameters in the phase space is investigated. The simulation results are in agreement with the theoretical findings.

The presented work can be applied to more advanced kinetic model equations, such as the ES and the Shakhov models for single gases [15], as well as the McCormack model for gaseous mixtures [16,17], in a straightforward manner.

2. Iteration schemes of kinetic equations

A description of the typical and upgraded (acceleration) iteration schemes applied to the continuous form of the governing kinetic equations is provided. In addition, the model problem used as a benchmark to test the overall efficiency of the proposed scheme is introduced. All quantities are in dimensionless form.

2.1. Kinetic iteration

We base our discussion on the two-dimensional linearized BGK model equation

$$\boldsymbol{c}\cdot\nabla f^{(t+1/2)}(c,\theta,\boldsymbol{x})+\delta f^{(t+1/2)}(c,\theta,\boldsymbol{x})=\delta F_{0,0}^{(t)}(\boldsymbol{x})+S(\boldsymbol{x}), \tag{1}$$

with

$$F_{0,0}^{(t+1)}(\boldsymbol{x})=\frac{1}{\pi}\int_0^{2\pi}\int_0^{\infty} f^{(t+1/2)}(c,\theta,\boldsymbol{x})\exp(-c^2)c\,dc\,d\theta, \tag{2}$$

which describes the fully developed flow of a gas through a channel of arbitrary cross section [14,18]. In Eqs. (1) and (2), $f^{(t+1/2)}(c,\theta,\boldsymbol{x})$ is the unknown distribution function, $\boldsymbol{x}=(x_1,x_2)$ is the position vector, $\boldsymbol{c}\leftrightarrow(c,\theta)$ is the molecular velocity vector with c and θ denoting the magnitude and the polar angle respectively, $S(\boldsymbol{x})$ is an optional source term, $F_{0,0}^{(t)}(\boldsymbol{x})$ is the bulk velocity and t is the iteration index. It is noted that the bulk velocity corresponds to the zeroth-order Hermitian moment of the distribution function. Finally, δ, known as the rarefaction parameter, is a very important dimensionless flow quantity, which characterizes the rarefaction degree of the physical system. The rarefaction parameter is proportional to the inverse Knudsen number. Roughly speaking, the flow is in the free molecular regime for $\delta<0.1$, in the transition regime for $0.1\leqslant\delta\leqslant10$ and in the hydrodynamic regime for $\delta>10$.

Along the boundary of the flow domain, the Maxwell diffuse reflection model is implemented. Then, the distribution function representing particles departing from the wall is written by

$$f(\boldsymbol{c},\hat{\boldsymbol{x}})=0,\quad \text{for } \boldsymbol{c}\cdot\boldsymbol{n}>0, \tag{3}$$

where $\hat{\boldsymbol{x}}$ denotes the boundary position vector and $\boldsymbol{n}$ is the unit normal vector pointing towards the interior of the flow domain. A quantity of practical interest, used later on, is the dimensionless flow rate

$$G=\frac{2}{A}\int\int_A F_{0,0}(\boldsymbol{x})dx_1dx_2. \tag{4}$$

Here, A is the area of the cross section. It is assumed that the hydrodynamic diameter of the channel $D_h=4A/\Gamma$ is unity, where Γ denotes the perimeter of the channel.

The integro–differential system defined by Eqs. (1) and (2) is solved in an iterative manner as indicated by the iteration index t. In particular at the beginning of each iteration, one introduces an old estimate $F_{0,0}^{(t)}$ in the right hand side of Eq. (1). Using this estimate Eq. (1) is solved to obtain an estimate for $f^{(t+1/2)}$, which is introduced into Eq. (2) to obtain the new estimate $F_{0,0}^{(t+1)}$. This iteration process, which is named "kinetic iteration" is repeated until the difference between successive estimates of $F_{0,0}^{(t)}$ is less than a pre-assigned convergence criterion ϵ. It has been shown that the above described iteration process