Journal of Computational Physics 257 (2014) 572–593

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

# Locally refined discrete velocity grids for stationary rarefied flow simulations

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ARTICLE INFO

*Article history:*
Received 19 April 2013
Received in revised form 4 October 2013
Accepted 7 October 2013
Available online 15 October 2013

*Keywords:*
Rarefied flow simulation
Hypersonic flows
Re-entry problem
Transition regime
BGK model
Discrete velocity model

ABSTRACT

Most of deterministic solvers for rarefied gas dynamics use discrete velocity (or discrete ordinate) approximations of the distribution function on a Cartesian grid. This grid must be sufficiently large and fine to describe the distribution functions at every space position in the computational domain. For 3-dimensional hypersonic flows, like in re-entry problems, this induces much too dense velocity grids that cannot be practically used, for memory storage requirements. In this article, we present an approach to generate automatically a locally refined velocity grid adapted to a given simulation. This grid contains much less points than a standard Cartesian grid and allows us to make realistic 3-dimensional simulations at a reduced cost, with a comparable accuracy.



## 1. Introduction

The description of a flow surrounding a flying object at hypersonic speed in the rarefied atmosphere (more than 60 km altitude) is still a challenge in the atmospheric Re-Entry community [2]. When this flow is in a rarefied state, that is to say when the Knudsen number (which is the ratio $Kn = \frac{\lambda}{L}$ between the mean free path $\lambda$ of particle and a characteristic macroscopic length $L$) is larger than 0.01, the flow cannot be accurately described by the compressible Navier–Stokes equations of gas dynamics. In this case, the kinetic theory has to be used. The evolution of the molecules of the gas is then described by a mass density distribution in phase space, which is a solution of the Boltzmann equation. In the transitional regime, this equation can be replaced by the simpler Bhatnagar–Gross–Krook (BGK) model.

In order to be able to compute parietal heat flux and aerodynamic coefficients in the range of 60–120 km, a kinetic description of the stationary flow is necessary.

The most popular numerical method to simulate rarefied flows is the Direct Simulation Monte Carlo method (DSMC) [9]. However, it is well known that this method is very expensive in transitional regimes, in particular for flows in the range of altitude we are interested in. The efficiency of DSMC can be improved by using coupling strategies (see [12,14]) or implicit schemes (see [24,15]), but these methods are still not very well suited for stationary computations. In contrast, deterministic methods (based on a numerical discretization of the stationary kinetic model) can be more efficient in transitional regimes. Up to our knowledge, there are few deterministic simulation codes specifically designed for steady flows. One of the most advanced ones is the 3D code of Titarev [25] developed for unstructured meshes. Another 3D code has been developed by

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0021-9991/$ – see front matter 
http://dx.doi.org/10.1016/j.jcp.2013.10.014

G. Brook [10]. Other codes exist, but they are rather designed for unsteady problems, see for instance [20,1] or the recent UGKS scheme developed by K. Xu and his collaborators [27,18], which is an asymptotic preserving scheme for unsteady flows.

In our team, we developed several years ago a code to make 2D plane and axisymmetric simulations of rarefied flows based on the BGK model (see a description in [22,23,4]). This code has recently been extended to 3D computations, for polyatomic gases. Due to the physical model (polyatomic gases), the space discretization (block structured mesh), and the parallelization (space domain decomposition with MPI and inner parallelization with OpenMP), this code is rather different from the other existing 3D codes recently presented in the literature for the same kind of problems (the 3D code of Titarev [25] for example), even if space domain decompositions have already been used for unsteady simulations (see [20]).

All the codes designed for steady flows have a common feature: they are based on a "discrete ordinate" like approach, and use a global velocity grid. This grid is generally a Cartesian grid with a constant step size. The number of points of this grid is roughly proportional to the Mach number of the flow in each direction, and hence can be prohibitively large for hypersonic flows, even with parallel computers. To compute realistic cases (3D configurations with Mach number larger than 20), the velocity space discretization has to be modified in order to decrease CPU time and memory storage requirements. It has already been noticed that a refinement of the grid around small velocities can improve the accuracy and reduce the cost of the computation (especially for large Knudsen numbers in flows close to solid boundaries, see [25]). However, up to our knowledge, there is no general strategy in the literature that helps us to reduce the number of discrete velocities of a velocity grid for any rarefied steady flow, even if some works on adaptive velocity grids have already been presented: the first attempt seems to be [5] for a 1D shock wave problem, and recently, more general adaptive grid techniques designed for unsteady flows have been presented in [21,13,19,11].

The main contribution of this article is to propose an algorithm for an automatic construction of a locally refined velocity grid that allows a dramatic reduction of the number of discrete velocities, with the same accuracy as a standard Cartesian grid. This algorithm uses a compressible Navier–Stokes pre-simulation to obtain a rough estimation of the macroscopic fields of the flow. These fields are used to refine the grid wherever it is necessary by using some indicators of the width of the distribution functions in all the computational domain. This strategy allows us to simulate hypersonic flows that can hardly be simulated by standard methods, since we are indeed able to apply our method to our kinetic code to simulate a re-entry flow at Mach 25 and for temperature and pressure conditions of an altitude of 90 km. In this example, the CPU time and memory storage can be decreased up to a factor 24, as compared to a method with a standard Cartesian velocity grid. Note that preliminary results have already been presented in [6] and [7].

The outline of this article is the following. In Section 2, we briefly present the kinetic description of a rarefied gas. In Section 3, we discuss the problems induced by the use of a global velocity grid, and our algorithm is presented. Our approach is illustrated in Section 4 with several numerical tests. To simplify the reading of the paper, the presentation of our simulation code is made in the appendix.

## 2. Boltzmann equation and Cartesian velocity grid

### 2.1. Kinetic description of rarefied gases

In kinetic theory, a monoatomic gas is described by the distribution function $f(t,\mathbf{x},\mathbf{v})$ defined such that $f(t,\mathbf{x},\mathbf{v})\,d\mathbf{x}\,d\mathbf{v}$ is the mass of molecules that at time $t$ are located in an elementary space volume $d\mathbf{x}$ centered in $\mathbf{x}=(x,y,z)$ and have a velocity in an elementary volume $d\mathbf{v}$ centered in $\mathbf{v}=(v_x,v_y,v_z)$.

Consequently, the macroscopic quantities as mass density $\rho$, momentum $\rho\mathbf{u}$ and total energy $E$ are defined as the five first moments of $f$ with respect to the velocity variable, namely:

$$\left(\rho(t,\mathbf{x}),\rho\mathbf{u}(t,\mathbf{x}),E(t,\mathbf{x})\right)=\int_{\mathbb{R}^3}\left(1,\mathbf{v},\frac{1}{2}|\mathbf{v}|^2\right)f(t,\mathbf{x},\mathbf{v})\,d\mathbf{v}. \tag{1}$$

The temperature $T$ of the gas is defined by the relation $E=\frac{1}{2}\rho|\mathbf{u}|^2+\frac{3}{2}\rho RT$, where $R$ is the gas constant defined as the ratio between the Boltzmann constant and the molecular mass of the gas.

When the gas is in a thermodynamical equilibrium state, it is well known that the distribution function $f$ is a Gaussian function $M[\rho,\mathbf{u},T]$ of $\mathbf{v}$, called Maxwellian distribution, that depends only on the macroscopic quantities:

$$M[\rho,\mathbf{u},T]=\frac{\rho}{(2\pi RT)^{\frac{3}{2}}}\exp\left(-\frac{|\mathbf{v}-\mathbf{u}|^2}{2RT}\right). \tag{2}$$

It can easily be checked that $M$ satisfies relations (1).

If the gas is not in a thermodynamical equilibrium state, its evolution is described by the following kinetic equation

$$\partial_t f+\mathbf{v}\cdot\nabla_{\mathbf{x}}f=Q(f), \tag{3}$$

which means that the total variation of $f$ (described by the left-hand side) is due to the collisions between molecules (described by the right-hand side). The most realistic collision model is the Boltzmann operator but it is still very computationally expensive to use. In this paper, we use the simpler BGK model [8,26]