MOVING BOUNDARY PROBLEMS FOR THE BGK MODEL OF RAREFIED GAS DYNAMICS

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Abstract

A new semilagrangian method is presented for the numerical solution of the BGK model of the Boltzmann equation in a domain with moving boundary. The method is based on discretization of the equation on a fixed grid in space and velocity. The equation is discretized in characteristic form, and the distribution function is reconstructed at the foot of the characteristics by a third order piecewise Hermite interpolation. Reflecting moving boundary at the piston are suitably described by assigning the value of the distribution function at ghost cells. A comparison with Euler equation of gas dynamics for the piston problem has been performed in the case of small Knudsen number.

Key words

Rarefied gas dynamics, semilagrangian methods, moving boundary problems.

1 Introduction

This work is motivated by the computation of rarefiled flow in MEMS (Micro Electro Mechanical Systems) [5]. The size of such devices is small enough that gas flow requires a kinetic treatment even at normal pressure and temperature conditions. Micro accelerators are often composed of several elements, each of which consists of a moving part, the *shuttle*, which is free to oscillate inside a fixed part, the *stator*. Although under certain conditions one can obtain an accurate description of the flow by quasi-static approximation [4], more general flow conditions inside the element require the treatment of a domain whose boundaries are not fixed. As a warm up problem, we consider the evolution of a gas in a one dimensional piston. Since we are interested in description of the moving boundary, we choose the simple BGK model to describe the gas [1], which is a simple relaxation approximation of the Boltzmann equation of rarefied gas dynamics. The numerical method that we use is a deterministic semilagrangian method on a fixed grid in space and velocity. Such a method is illustrated in detail in paper [7].

2 Description of the method

First let us assume that the integration domain in space is $[0, L]$, with a fixed L. The initial-boundary problem can be written as

$$\begin{aligned} \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} &= \frac{1}{\tau}(M[f] - f), \\ f(t, x, v) &= f_0(x, v) \end{aligned} \tag{1}$$

where $v \in \mathbb{R}$, $x \in [0, L]$, and $t > 0$, and $M[f]$ represents the local Maxwellian that has the same conservative moments of f.

Suppose we want to integrate the equation up to a fixed time $t = t_f$. For simplicity we assume constant time step $\Delta t = t_f/N_t$ and uniform grid in physical and velocity space, with mesh spacing Δx and Δv, respectively, and denote the grid points by $t_n = n\Delta t$, $x_i = i\Delta x, i = 0, \ldots, N_x$, $v_j = j\Delta v, j = -N_v, \ldots, N_v$, where N_x+1 and $2N_v+1$ are the number of grid nodes in space and velocity, respectively. We assume that the distribution function is negligible for $|v| > v_{\max} = N_v\Delta v$.

Let f_{ij}^n denote the approximation of the solution $f(t_n, x_i, v_j)$ of the problem (1) at time t_n in each spatial and velocity node, and assume that it is given.

Integration of Eq. (1) along the characteritsics by implicit Euler scheme gives

$$\begin{aligned} f_{ij}^{n+1} &= \tilde{f}_{ij}^n + \frac{\Delta t}{\tau}(M_{ij}^{n+1} - f_{ij}^{n+1}), \\ x_i &= \tilde{x}_{ij} + v_j\Delta t, \quad i = 0, \ldots, N_x, \\ j &= -N_v, \ldots, N_v. \end{aligned} \tag{2}$$

The value of the function $\tilde{f}_{ij}^n$ is reconstructed at position $\tilde{x}_{ij} = x_i - v_j\Delta t$ by a suitable high order reconstruction. In particular, here we use a piecewise cubic

polynomial, which is obtained by Hermite interpolation in each interval $[x_i, x_{i+1}]$. The first derivatives of the function at location x_i, $(\partial f_j/\partial x)_{x_i}$, are computed by second order central difference. The reconstruction is linear, without limiters. This guarantees that the scheme is conservative [3].

2.1 Implicit calculation

The implicit term can be explicitly computed by multiplying Eq. (2) by $1, v, |v|^2$ and summing over the velocities. This procedure allows the computation of the moments, because $M_{i,\cdot}^{n+1}$ and $f_{i,\cdot}^{n+1}$ have the same moments. Therefore one obtains

$$\begin{aligned} \rho_i^{n+1} = \sum_j \tilde{f}_{ij}^n, \quad (\rho u)_i^{n+1} = \sum_j v_j \tilde{f}_{ij}^n, \\ E_i^{n+1} = \frac{1}{2}\sum_j |v_j|^2 \tilde{f}_{ij}^n. \end{aligned} \tag{3}$$

Once the moments have been computed, the Maxwellian can be calculated from the moments, and the density function can be explicitly computed as

$$f_{ij}^{n+1} = \frac{\tau \tilde{f}_{ij}^n + \Delta t M_{ij}^{n+1}}{\tau + \Delta t}. \tag{4}$$

Notice that as $\tau \to 0$ the distribution function f_{ij}^{n+1} is projected onto the Maxwellian. Furthermore, in this limit the whole scheme becomes a relaxation scheme for the Euler equations. We say that the scheme is *Asymptotic Preserving* [6].

3 The piston problem

The system consists in a gas inside a one dimensional slab, which is driven by a moving piston (see Figure 1). On the left boundary of the domain there is a fixed wall (the origin of our coordinate system), at the right end there is a piston, whose position is an assigned function of time $x_p : t \in \mathbb{R} \to x_p(t) \in [0, L]$. We assume that the gas inside the slab is governed by the BGK equation. The system is discretized on a uniform grid in the computational domain $[0, L]$ by $N_x + 1$ grid points of coordinates $x_i = ih$, $i = 0, \ldots, N_x$, $h = L/N_x$. As the piston moves, the domain occupied by the gas changes, while the position of the grid points remains fixed. As a consequence, only a certain number $N_x(t)$ of grid points is actually used (*active points*) while other points lie outside of the domain (*ghost points*).

The number of equations to be solved changes with time. We choose the time step in such a way that the piston can move by at most one grid point in one step, and denote by $u_p(t) \equiv \dot{x}_p(t)$ the assigned piston velocity.

Different boundary conditions may be assigned to the boundary. Here we consider the case of specular reflection.

3.1 Specular reflection

At the wall, at each time t, the distribution function, for positive velocities, is given by

$$f(t, 0, v) = f(t, 0, -v),$$

which is discretized as

$$f_{-i,j}^n = f_{i,-j}^n, \quad i \le 0, j > 0,$$

keeping in mind that $v_j = j\Delta v$.

A similar condition can be used to treat reflecting boundary conditions near the piston:

$$f(t, x_p, v) = f(t, x_p, v^*), \quad v^* = 2u_p - v.$$

We convert the condition into an initial value for the ghost point using the following argument. We approximate the motion of the piston by a piecewise linear function of time, i.e. we assume that in time interval $[t_n, t_{n+1}]$ the velocity of the piston is unchanged. Then the value of the density function $f(t_n, \tilde{x}_{ij}, v_j)$, at the foot of the characteristics corresponding to the velocity $v_j < u_p$, is set to $f^n(x^*, v^*)$, where $x_{ij} + x^* = 2x_p(t_n)$ and $v_j + v^* = 2u_p(t_n)$ (see Figure 2).

The simplest way to implement such condition is to precompute the values of the distribution function at ghost points $x_i > x_p(t_n)$, for $v_j < u_p$, as $f^n(x_i, v_j) = f^n(x^*, v^*)$, with $x_i + x^* = 2x_p(t_n)$ and $v_j + v^* = 2u_p(t_n)$, and then use the standard piecewise Hermite interpolation from grid points (active or ghost) at time level t_n. In general point (x^*, v^*) is not on a grid in phase space, therefore interpolation in x and v has to be used. In some cases, point (x^*, v^*) is in a cell whose values of the function is known at the vertices, and bilinear interpolation can be used. In other cases, the function at the vertices is itself not known, and an iterative procedure has to be used.

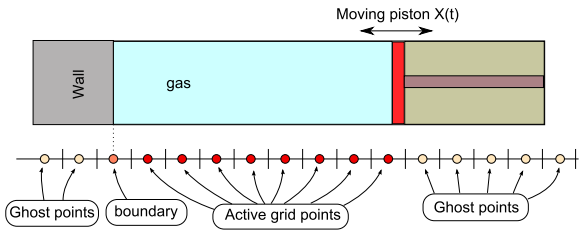

Figure 1. Setup of the piston problem. The equations are solved for the values of the distribution function in the active grid points. The values outside of the computational domain (*ghost points*) are computed by making use of the boundary conditions

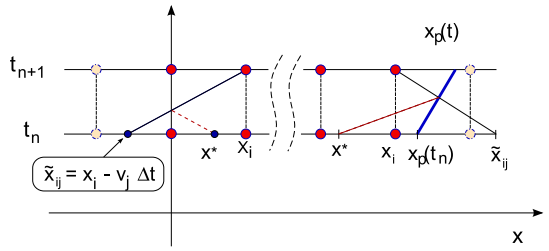

Figure 2. Definition of the specular boundary conditions at the wall (left) and at the piston (right)

4 Numerical tests

As numerical test we solve the BGK equation with Maxwellian initial condition, and reflecting boundary conditions at the wall and at the piston. We impose the motion of the piston with a given velocity $u_p(t) = 0.25\sin(t)$. The piston induces waves that move back and forth into the slab. For small Knudsen number the behavior of the gas should be well described by the Euler equations of gas dynamics. To validate this expectation, a comparison is performed between solution of the BGK equation and the solution of the Euler equations of gas dynamics. The latter is obtained by writing the equations in Lagrangian form, so that the domain in Lagrangian coordinates becomes fixed, and then applying a finite volume central scheme to solve the equations numerically (see [2] for details).

The pressure at the piston and at the wall for the BGK model and for the Euler equations are shown in Figure 3. During the talk, the time evolution of the distribution function $f(x, v, t)$ is shown.

Implementation of Maxwell boundary conditions and extension to two space dimensions will allow a realistic simulation of the oscillation of the shuttle in MEMS.

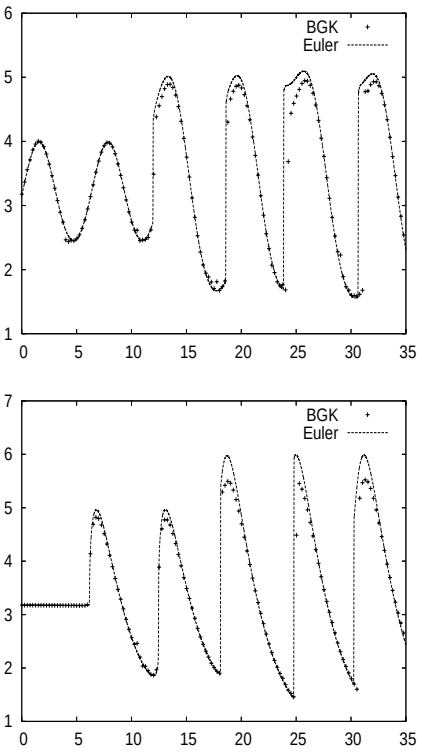

Figure 3. $\tau = 10^{-3}$: the pressure at the boundary $x = x_p(t)$ (top) and $x = L$ (bottom) obtained by the semi-Lagrangian method for BGK equations and a Lagrangian scheme for Euler equations.

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