

# Fluid-kinetic coupling of the BGK and lattice Boltzmann equations

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## Abstract

The present paper deals with the boundary problems for rarefied gas dynamics which are solved using the splitting of the spatial domain in two parts and solving the lattice Boltzmann equations and Bhatnagar-Gross-Krook equations (BGK) in corresponding domains. The mapping procedures are performed at the intersections of the domains. The results of the numerical study are presented. It was shown that the values of the bulk velocity and the hybrid method is in excellent agreement with the tabulated data.

## 1. Introduction

A recent interest in describing of multi-scale flows with the connection of micro- and macro-scales has resulting in construction of hybrid methods. In direct solving the kinetic equations discrete velocity models (DVM) as a rule is used. There is an obvious relation between the number of the discrete velocities and the number of the appropriate moments for the distribution function. For instance, as the Vandermonde determinant does not equal zero one can deal with DVM or with the equal number of the moment equations. For the realization of the mentioned connection it is convenient to use the orthogonal polynomials. Moreover, using the Gauss Hermite quadratures one can match the moments with some set of weights and lattice velocities which constitute the Lattice Boltzmann method. For the near-continuum zones where the Navier-Stokes equations are valid it is sufficient in principle to apply only a small finite set of velocities since 13 moments appear in the Navier-Stokes equations. These crude approximation by DVM could be fit the need accuracy for the moments in these regions. The LBE approach is based on the same idea of the discrete velocities. But the apparatus of LBE is developed and therefore it is natural to elaborate a hybrid method of the BE+LBE type.

In the present paper we deal with the flow between the two parallel planes which have non-zero relative velocity (the plane Couette flow) for small Knudsen numbers. For solving of this problem we develop a hybrid BGK and LBGK coupling method. The gas dynamics in Knudsen layers is considered using the full nonlinear BGK equation while the internal zone is handled by the application of the LBGK model. At the boundaries of the BGK and LBGK domains the coupling method is applied. We show that the results of the hybrid method with very close to the well-known tabulated solutions of the Couette flow.

## 2. The main kinetic equations

In the present paper we will use two kinetic models based on the nonlinear Boltzmann equation. The first is the Bhatnagar-Gross-Krook kinetic model<sup>1</sup> which reads in the dimensionless variables as

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{1}{\tau Kn} (\Phi - f), \quad \Phi \equiv \frac{\rho}{(2\pi T)^{3/2}} e^{-(\mathbf{v}-\mathbf{u})^2/2T}, \quad (1)$$

where  $f(t, \mathbf{x}, \mathbf{v})$  is distribution function of a dilute gas,  $\tau$  is dimensionless relaxation time ( which equals to average number of collisions until relaxation per particle) assumed to be constant in the present study,  $\rho, \mathbf{u}, T$  is density, bulk velocity and temperature and  $Kn$  is Knudsen number. This model is derived from the full Boltzmann equation substituting the collision integral term by the local Maxwell distribution  $\Phi$ . Formally the nonlinearity in  $\Phi$  is more severe than in the full Boltzmann equation since  $\Phi$  depends on  $f$  via the first moments  $\rho, \mathbf{u}, T$  but the BGK model (1) is simpler for the numerical study and can adequately describe strongly non-equilibrium effects in a dilute gas.

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The second approach is called the Lattice Boltzmann method which is the further simplification of the BGK model.<sup>2</sup> We assume that the considered flow is slow, i.e the Mach number is close to zero and isothermal, then we can expand the local Maxwell term  $\Phi$  in the Taylor series on the bulk velocity  $\mathbf{u}$  up to the terms of the second order. Moreover, we assume that the particle can travel with the velocities  $\mathbf{c}_i$  from a finite discrete set of possible velocities. Finally the general LBGK model is obtained by the finite difference integration of the BGK equations on the characteristics jointly with the aforementioned assumptions

$$f(t + \delta t, \mathbf{x} + \mathbf{c}_j \delta t) - f(t, \mathbf{x}) = \frac{1}{\left(\frac{1}{2} + \frac{\tau Kn}{\delta t}\right)} \left\{ \rho w_j \left( 1 + \frac{\mathbf{c}_j \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_j \mathbf{u})^2 - c_s^2 u^2}{2c_s^4} \right) - f(t, \mathbf{x}) \right\}, \quad j = 1 \dots N, \quad (2)$$

where  $\mathbf{c}_j$  are lattice velocities,  $c_s$  is sound velocity defined by  $\sum_j w_j \mathbf{c}_j^2 = c_s^2$ ,  $w_j$  are lattice weights (or discrete analogs of the Maxwell state) obeying  $\sum_j w_j = 1$ ,  $\tau$  is relaxation time,  $\delta t$  is lattice time step and  $N$  is number of lattice velocities. The lattice weights and velocities should be evaluated in a such way that at the  $Kn \rightarrow 0$  limit the resulting Navier-Stokes equations are reproduced with negligible error terms (commonly of the order  $Ma^3$ ). The integration on the characteristics using the trapezium rule adds the small error terms of the order  $\delta t^2$ . Several approaches can be applied for the construction of the such models like Gauss-Hermite<sup>6</sup> quadratures method or entropic method,<sup>7,8,9</sup> We also mention that the lattice Boltzmann model leads to the Navier-Stokes equations with the shear viscosity  $\mu$  equals

$$\mu = c_s^2 \frac{\tau Kn}{\delta t}.$$

We adopt the spatial domain splitting procedure for solving the boundary problems for rarefied gas dynamics. Commonly the non-equilibrium effects in flows appear near boundaries, therefore the boundary domains are modeled with the BGK model while the internal zone which is modeled with the Lattice BGK. Previously, the approach based on solving the gas dynamics with DSMC method and LBGK models using domain splitting was presented in papers<sup>3-4</sup> where the Couette and Poiseuille flow was considered. Nevertheless, LBGK and DSMC coupling leads to appearance of some noise<sup>10</sup> therefore the introduction of the LBGK and BGK coupling method is very desirable.

### 3. The mapping method

We will discuss the matching procedure at the boundary between the domains. This procedure is presented schematically in Fig. 1 and Fig. 2. First of all, we assume that in the intersection of the domains the gas real distribution function is close to Maxwell state with zero bulk velocity, unit temperature and can be casted in the form of the truncated Grad expansion

$$f_{Grad}(\mathbf{x}, \mathbf{v}) = \frac{1}{\sqrt{(2\pi)^3}} \exp\left(-\frac{\mathbf{v}^2}{2}\right) \left( a(\mathbf{x}) + \sum_j a_j(\mathbf{x}) H_j + \frac{1}{2} \sum_{jk} a_{jk}(\mathbf{x}) H_{jk} \right), \quad (3)$$

where  $H_j, H_{jk}$  are the Hermite polynomials of the first and second order defined by

$$H_j = \frac{(-1)^j}{w(\mathbf{v})} \frac{\partial^j}{\partial v_j} w(\mathbf{v}), \quad H_{jk} = \frac{1}{w} \frac{\partial^2}{\partial v_j \partial v_k} w(\mathbf{v})$$

where we have introduced

$$w(\mathbf{v}) \equiv \frac{1}{\sqrt{(2\pi)^3}} \exp\left(-\frac{\mathbf{v}^2}{2}\right).$$

The terms  $a, a_j, a_{jk}$  are coefficients depending on  $x$  (the point on the intersection plane). We suppose that the truncation of the Grad expansion at the second order is minimal possible but sufficient variant since the Navier-Stokes equations can be reproduced for this case when Knudsen number tends to zero. We will use the function (3) for the transfer of the boundary data between the lattice Boltzmann and the BGK models. We will discuss this procedure in turn.

At the first step we update the BGK distribution function  $f_{BGK}(x_\alpha, v_\beta)$  (where we define  $x_\alpha, v_\beta$ ) as the difference scheme's spatial points and velocities) for the velocities with positive  $v_x$  component in the whole BGK domain using the boundary data on the wall. At the intersection plane we map the BGK scheme distribution on the Grad distribution function by calculating the coefficients  $a, a_j, a_{jk}$  using the formulas below

$$a(x_\beta) = \sum_\beta f_{BGK}(x_\alpha, v_\beta), \quad a_j(x_\beta) = \sum_\beta f_{BGK}(x_\alpha, v_\beta) H_j(v_\beta), \quad a_{jk}(x_\beta) = \sum_\beta f_{BGK}(x_\alpha, v_\beta) H_{jk}(v_\beta). \quad (4)$$

Once this summation is performed we are able to recover the Grad distribution function (3) in the intersection domain.

Next we will map the distribution (3) on the lattice Boltzmann distribution using the Gauss-Hermite quadrature method. The method is based on the fact that the expansion of the distribution function in the Grad form around the absolute Maxwell state is equivalent to the to a lattice Boltzmann method<sup>5-6</sup>. Following the ideas from<sup>5-6</sup> we consider the first moments  $a, a_j, a_{jk}$  represented in the integral form and calculate them via Gauss-Hermite quadratures

$$\{a, a_j, a_{jk}\} = \int f_{Grad}(\mathbf{v})\{1, H_j(\mathbf{v}), H_{jk}(\mathbf{v})\}d\mathbf{v} = \sum_s w_s \frac{f_{Grad}(\mathbf{v}_s)}{w(\mathbf{v}_s)}\{1, H_j(\mathbf{v}_s), H_{jk}(\mathbf{v}_s)\},$$

where  $w_s, v_s$  are the weights and the nodes of the Gauss-Hermite quadratures. The nodes  $v_s$  can be considered as the lattice Boltzmann velocities while  $w_s \frac{f_{Grad}(\mathbf{v}_s)}{w(\mathbf{v}_s)}$  is the lattice Boltzmann distribution function values and  $w_s$  are the lattice analog of the total Maxwell distribution. Then the formula

$$f_{latt,s} \equiv w_s \frac{f_{Grad}(\mathbf{v}_s)}{w(\mathbf{v}_s)} \quad (5)$$

gives the mapping from the Grad truncated distribution function  $f_{Grad}$  to the lattice Boltzmann distribution function  $f_{latt,s}$  for the correspondent speeds  $v_s$ . Now having the boundary values we update the lattice Boltzmann distribution function  $f_{latt,s}$  for the velocities  $v_s$  with positive  $x$  component. This calculations finishes the first step, see Fig. 1.

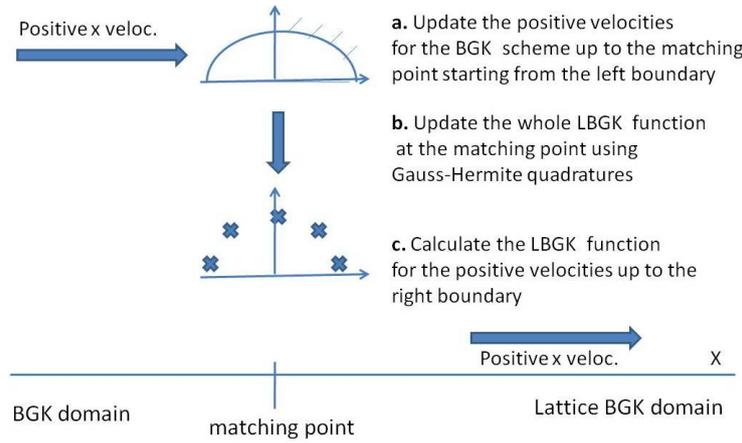


Figure 1: Step 1 of the mapping scheme.

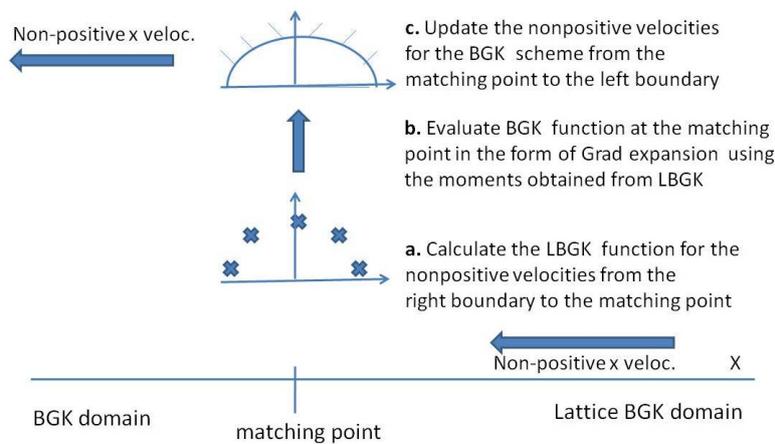


Figure 2: Step 2 of the mapping scheme.

The second step consists of the evaluation of the distribution functions for the non-positive velocities. Now we start from the right boundary and using the boundary conditions at the right plane we calculate the Lattice Boltzmann distribution for the velocities with non-positive  $x$ -component down to the matching point. Next we evaluate the

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moments  $a, a_j, a_{jk}$  and finally recover the Grad distribution function. We have

$$a = \sum_s f_{latt,s}, \quad a_j = \sum_s f_{latt,s} H_j(v_s), \quad a_{jk} = \sum_s f_{latt,s} H_{jk}(v_s).$$

Now we are ready derive the BGK distribution function in the domain intersecting plane. This can be made by a simple discretization of the Grad distribution functions at the nodes of the BGK difference scheme. Finally, we evaluate the BGK distribution function for the all velocities with non-positive  $x$ -component in the left domain, see Fig. 2.

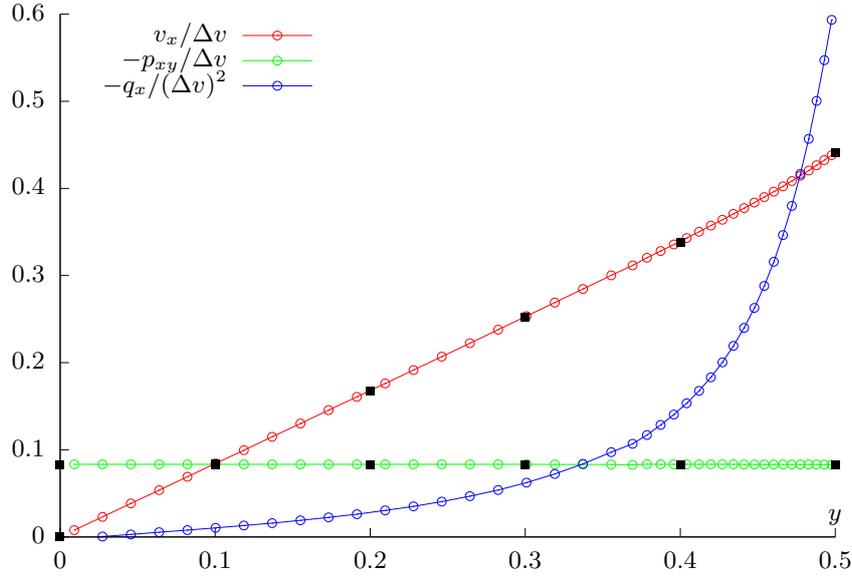


Figure 3: The results of the numerical study for the BGK nonlinear model  $\Delta v = 0.02, Kn = 0.1$ . The black boxes correspond to the tabulated theoretical solutions.<sup>11</sup> The point  $y = 0.5$  corresponds to the position of the right plane, the point  $y = 0$  lies in the middle between the moving planes.

#### 4. Discrete-velocity method and numerical example

Equation (1) is solved by the second-order splitting scheme into the transport equation

$$\frac{\partial f}{\partial t} + \zeta_i \frac{\partial f}{\partial x_i} = 0, \quad (6)$$

for which a finite-volume method with an explicit second-order TVD scheme is used, and the space-homogeneous BGK equation

$$\frac{\partial f}{\partial t} = \nu(\Phi - f), \quad (7)$$

which has the exact solution

$$f = \Phi + (f - \Phi) \exp(-\nu t). \quad (8)$$

The three-dimensional velocity space is discretized by the uniform lattice confined with the sphere of radius  $\zeta_{\max} = 4$ .  $M = 16$  nodes are placed along each axis. The total amount of nodes is equal to 6528.

The proposed hybrid method is tested on the linearized Couette-flow problem. The gas is placed between two infinite parallel plates at  $y = \pm 1/2$  with constant temperature  $T = 1$  and velocities  $(v = \pm \Delta v/2, 0, 0)$ . Complete diffuse reflection are assumed at the plates. The average density is equal to unity:

$$\int_{-1/2}^{1/2} \rho dy = 1. \quad (9)$$

The physical space  $0 < y < 1/2$  is divided into  $N = 40$  nonuniform cells refined near  $y = 1/2$ . The obtained results for  $Kn = 0.1$  and  $\Delta v = 0.02$  are presented in Fig.3-5. The buffer layer is located at a distance of 1.2 mean free path from the plate.

The results of our study shows that the Hybrid method based on the LBGK and BGK coupling has very good correspondence with the extremely accurate data from.<sup>11</sup>

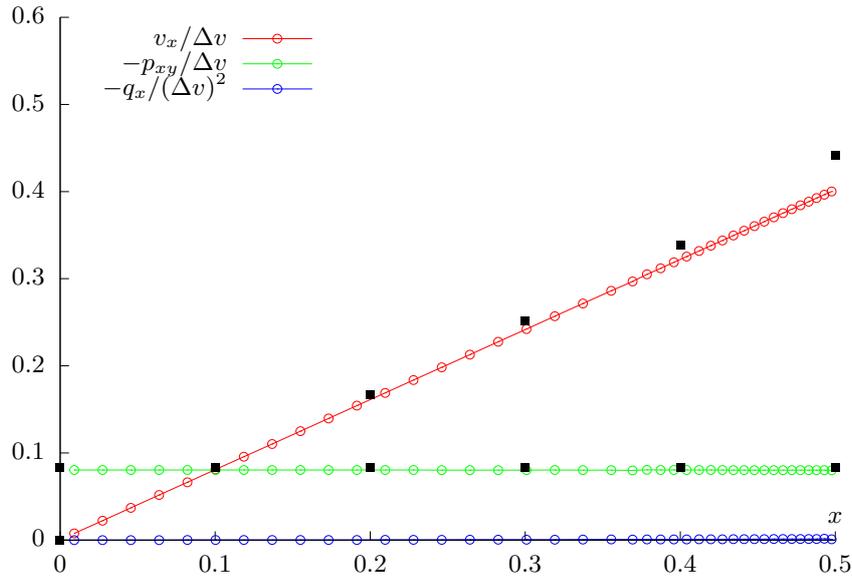


Figure 4: The results of the numerical study for the Lattice Boltzmann D3Q19 model  $\Delta v = 0.02$ ,  $Kn = 0.1$ . The black boxes correspond to the tabulated theoretical solutions.<sup>11</sup> The departure of the LBGK bulk velocity from the theoretical values is observed in the Knudsen layer. The point  $y = 0.5$  corresponds to the position of the right plane, the point  $y = 0$  lies in the middle between the moving planes.

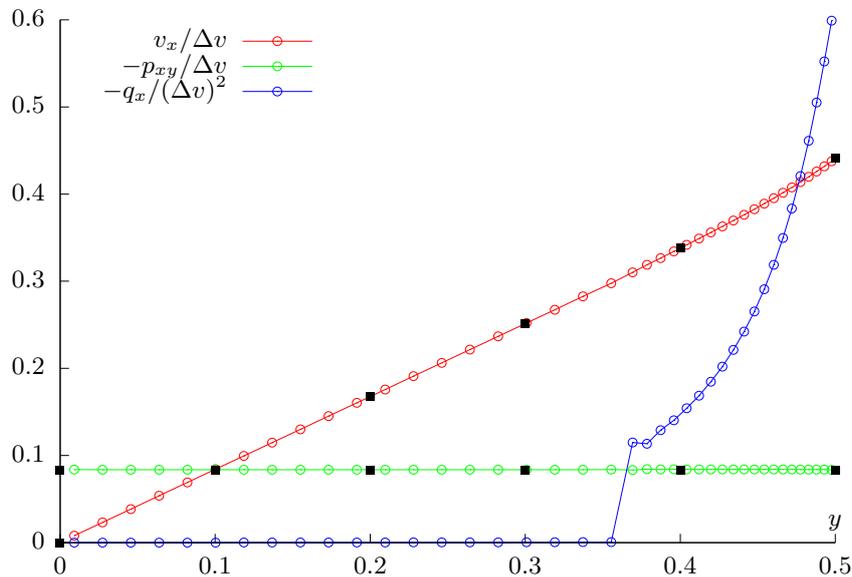


Figure 5: The results of the numerical study for the hybrid BGK and LBGK models  $\Delta v = 0.02$ ,  $Kn = 0.1$ . The black boxes correspond to the tabulated theoretical solutions.<sup>11</sup> The matching point is located at  $y = 0.38$ . The point  $y = 0.5$  corresponds to the position of the right plane, the point  $y = 0$  lies in the middle between the moving planes.

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