Domain decomposition techniques and hybrid multiscale methods for kinetic equations

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Summary. In this note we consider the development of a domain decomposition scheme directly obtained from the multiscale hybrid scheme described in [7]. The basic idea is to couple macroscopic and microscopic models in all cases in which the macroscopic model does not provide correct results. We will show that it's possible to view a Boltzmann-Euler domain decomposition method as a subset of the hybrid scheme if we impose the value of the relaxation parameter equal to zero in some regions of the computational domain. Applications to the two-dimensional BGK equation is presented to show the performance of the method.

1 Introduction

In this note we afford the problem of developing efficient numerical methods for multiscale phenomena in Rarefied Gas Dynamic (RGD). In some fluid dynamic simulations the Navier-Stokes or the Euler equations do not give a satisfactory descriptions of the physical system and a kinetic description through the Boltzmann equation is often required. For regions not too far from thermodynamic equilibrium the BGK approximation is known to be accurate in describing the physics of the problem. However, the computational cost of a direct discretization of the BGK equation is still high and the use of particle simulation methods is preferable. The price to pay for the reduction of computational cost is the presence of fluctuations in the solution. As a consequence particle methods loose their competitiveness in continuum regions where a finite volume solver for the Euler or Navier-Stokes equations can be used. Domain decomposition techniques are then used in order to better treat these difficulties and to design suitable numerical schemes. In many situation in fact we don't need to solve the kinetic equations in the whole computational domain but it's sufficient to solve the hydrodynamical equations except in small zones where departure from thermodynamical equilibrium like shock waves are present. To this aim we developed a numerical scheme derived from

the multiscale hybrid scheme [7], which can be used to obtain a decomposition of the domain, artificially imposing the value of the Knudsen number ε equal to zero, where the thermodynamic profiles provided by Euler equations are sufficiently accurate.

2 The BGK Equation

We will consider the BGK equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon}(M_f - f), \tag{1}$$

with the initial condition

$$f(x, v, t = 0) = f_0(x, v), \tag{2}$$

where $f = f(x, v, t)$ is a non negative function describing the time evolution of the distribution of particles which move with velocity $v \in \mathbb{R}^3$ in the position $x \in \Omega \subset \mathbb{R}^3$ at time $t > 0$. The parameter $\varepsilon > 0$ is the Knudsen number and is proportional to the mean free path between collison. In the BGK equation the collision are modelled with a relaxation towards the Maxwellian equilibrium M_f. The local Maxwellian function is defined by

$$M_f(\varrho, u, T)(v) = \frac{\varrho}{(2\pi T)^{3/2}} \exp\left(\frac{-|u - v|^2}{2T}\right), \tag{3}$$

where ϱ, u, T are the density, mean velocity and temperature of the gas

$$\varrho = \int_{\mathbb{R}^3} f dv,\ u = \int_{\mathbb{R}^3} v f dv,\ T = \frac{1}{3\varrho}\int_{\mathbb{R}^3} [v - u]^2 f dv. \tag{4}$$

In addition we define the energy E as

$$E = \frac{1}{2}\int_{\mathbb{R}^3} v^2 f dv, \tag{5}$$

and the kinetic entropy H_f by

$$H_f = \int_{\mathbb{R}^3} f \log f dv. \tag{6}$$

It is easy to show the entropy dissipation inequality

$$\partial_t \int_{\mathbb{R}^3} f \log f dv + \nabla_x \int_{\mathbb{R}^3} v f \log f dv \leq 0. \tag{7}$$

Now, if we consider the BGK equation (1) and multiply it for the collision invariants 1, v, $\frac{1}{2}|v^2|$ by integrating in v we obtain the evolution of the first three moments of the distribution function f

$$\partial_t \int_{\mathbb{R}^3} f\phi(v)dv + \nabla_x \int_{\mathbb{R}^3} vf\phi(v)dv = 0,\ \phi(v) = 1, v_1, v_2, v_3, |v|^2. \quad (8)$$

These equations are the corresponding conservations laws for mass, momentum and energy. Unfortunately the differential system of equations (8) is not closed, since it involves higher order moments of the distribution function. As $\varepsilon \to 0$, from (1) we notice that $f \to M_f$. In this case the higher order moments of the distribution function can be computed as functions of ϱ, u, and T and we obtain the closed system of compressible Euler equations

$$\begin{aligned} &\frac{\partial \varrho}{\partial t} + \nabla_x \cdot (\varrho u) = 0, \\ &\frac{\partial \varrho u}{\partial t} + \nabla_x \cdot (\varrho u \otimes u + p) = 0, \\ &\frac{\partial E}{\partial t} + (Eu + pu) = 0, \\ &p = \varrho T, \quad E = \frac{3}{2}\varrho T + \frac{1}{2}\varrho |u|^2. \end{aligned} \quad (9)$$

3 Fluid Solver Indipendent Hybrid Method

In this section we introduce the Fluid Solver Indipendent (FSI) Hybrid Method, that will be used to compute our solution in the whole domain (see [7]). The domain decomposition will be achieved simply imposing the value of the Knudsen number equal to zero in some part of the domain. The FSI hybrid method is able to take advantage from the equilibrium part of the solution through a general fluid solver for the Euler equations instead of a kinetic scheme as in [6]. This represents an advantage in term of computational flexibility and cost. In this way the resulting scheme is faster and more accurate then a conventional Monte Carlo (MC) solver. In fact, since only the perturbation from equilibrium is solved by a MC scheme we have a reduction of the number of particles in the computational domain with respect to a full MC. In order to explain the algorithm we introduce the projection operator P. The projection operator computes from the microscopic variables f or M_f the macroscopic variables $U = (\varrho, u, T)$, thus $P(f) = U$ and $P(M_f) = U$, since the local Maxwellian has the same moments of the distribution function. If we split the BGK equation (1) into a relaxation step and in a transport step, from the exact solution of first step we have

$$f(x, v, t) = e^{-\Delta t/\varepsilon} f(x, v, t) + (1 - e^{-\Delta t/\varepsilon}) M_f(x, v, t), \quad (10)$$

Thus we can write

$$U(x, t) = (1 - \beta(x))P(f(x, v, t)) + \beta(x)P(M_f(x, v, t)) \quad (11)$$

Where $\beta(x)$ indicate the value of the equilibrium fraction at each time step in each cell. Now we set $f^p(x, v, t) = (1 - \beta(x))P(f(x, v, t))$ and solve the

transport step for f^p with Monte Carlo methods while for $\beta(x)P(M_f(x,v,t))$ we use any deterministic macroscopic scheme. Unfortunately the knowledge of f^p is linked to the solution of the entire distribution function f. Let us now introduce the relaxation and transport operators R and T. The solution of the microscopic problem for one time step can be written in the following way

$$R(f^{MC}(x,v,t)) = (1-\beta(x))f^{MC}(x,v,t) + \beta(x)M_f^{MC}(x,v,t) \tag{12}$$

$$T(R(f^{MC}(x,v,t))) = T((1-\beta(x))f^{MC}(x,v,t)) + T(\beta(x)M_f^{MC}(x,v,t)) \tag{13}$$

Where the apex MC , indicate that the solution is computed with MC scheme. After transport we loose the equilibrium structure of the solution, we define the quantity transported in the following way

$$\tilde{f}^p(x,v,t) = T((1-\beta(x))f^{MC}(x,v,t)) \tag{14}$$

$$\tilde{M}_f(x,v,t) = T(\beta(x)M_f^{MC}(x,v,t)) \tag{15}$$

On the other hand the solution of the macroscopic equations can be performed as

$$P(\beta(x)M_f^d(x,v,t)) = U^d(x,t) \tag{16}$$

$$T(U^d(x,t)) = \tilde{U}^d(x,t) \tag{17}$$

The final solution at each time step can be recovered by

$$U^h(x,t) = P(\tilde{f}^p(x,v,t)) + \tilde{U}^d(x,t) \tag{18}$$

At the next time step from relaxation we obtain

$$\begin{aligned} f(x,v,t+\Delta t) = (1-\beta(x))(\tilde{f}^p(x,v,t) + \tilde{M}_f(x,v,t)) \\ + \beta(x)M_f(x,v,t+\Delta t) \end{aligned} \tag{19}$$

The term $\tilde{f}^p + \tilde{M}_f$ represent the entire distribution function computed with MC algorithm, however, we need only $(1-\beta(x))$ of the latter quantity, thus instead of sampling from local Maxwellian a fraction of particle $\beta(x)U^h(x)$ we sample only $(1-\beta(x))\beta(x)U^h(x)$. This permits to avoid the effect of discarding and resampling particles at each time step.

The macroscopic scheme, for the compressible Euler equation, used is a MUSCL type (see [10], [7] for details), note however, that any numerical scheme is possible for the fluid equations to our purpose. The method deserves some remarks

Remark 1.

- We could try to compute the degree of equilibrium after transport of the distribution function, in that way it's possible to diminish particles and fluctuations similarly to [6]. Note however that this will cause an increase in the computational cost since we need the reconstruction of the distribution function f from samples. Moreover the evaluation of the equilibrium fraction will be rather difficult due to the probabilistic character of the component $\tilde{M}_f$ with respect to [5] and [6].
- It's possible to think to other strategies to compute the degree of equilibrium after transport. For example a strategy based on a best fitting of the higher order moments.

3.1 Domain decomposition method

We could view a domain decomposition technique as a subset of the FSI hybrid scheme just described. The method consist simply in setting artificially the value of the Knudsen number equal to zero where the Euler profiles are sufficiently accurate. Thus the scheme becomes a coupling of a Euler solver (by MUSCL scheme) in one part of the domain and a BGK solver in the rest of the domain (by FSI method). In fact if $\varepsilon \equiv 0$ from (10) we get

$$f(x, v, t) = M_f(x, v, t). \tag{20}$$

Thus after transport since we project the entire solution towards the equilibrium, we are no more interested to the form of the distribution function but only by their moments. As a consequence $P(\tilde{f}^p) \equiv 0$ and the hybrid solution is $U^h = \tilde{U}^d$. In order to divide the domain we need to decide some criteria which permit to detect the zones in thermodynamical equilibrium with respect to the others, this is still an open problem and it will not be addressed in the present work, we quote for instance [8] in which the question is considered in detail. Two consideration about the boundary conditions are necessary

- The deterministic scheme we use to solve the problem in regions where $\varepsilon = 0$, need a value which is supplied by the hybrid scheme. That value contains some statistical fluctuation that could be large, thus the full deterministic model could contain some boundary error given by the fluctuation which propagates in the rest of the domain. In order to avoid the problem a technique could be to make ε a smooth function of x which gently vary from some fixed value towards zero. For instance we could set ε as

$$\varepsilon(x) = \begin{cases} \varepsilon_F, & \text{for } x \leq a \\ 0, & \text{for } x \geq b \\ \dfrac{x-b}{a-b}\varepsilon_F, & \text{for } x \in [a, b] \end{cases} \tag{21}$$

  Where b represent the boundary of the equilibrium zones, a represent the boundary of the non equilibrium zones in which we use the full hybrid

scheme, while ε_F represent the value of the Knudsen number for the hybrid scheme.

- We need also the boundary value for the MC part of the FSI where $\varepsilon \neq 0$, thus at the boundary between $\varepsilon \equiv 0$ and $\varepsilon \neq 0$ we need to sample some particles from the Maxwellian. The number of samples we need is given by $(1-\beta(x))\beta(x)U^h(x)$, but they have to be taken from the local Maxwellian in the cell $(x-1)$, if we are considering the left boundary, the same of course it's true for the right boundary.

4 Numerical test

In this section we compare the performance of MC and of DD-FSI (Domain Decomposition-FSI). We consider an ellipse embedded in a flow with the following characteristic

$$\varrho = 1, \quad T = 5, \quad M = 10 \tag{22}$$

Where M indicates the Mach number, we choose full accommodation boundary condition with temperature $T_E = 10$. The Knudsen number is $\varepsilon = 10^{-4}$ that correspond to $\beta = 0.75$ if $((x-2)/1.8)^2 + (y-1)^2 < 0.8$ while $\varepsilon = 0$ if $((x-2)/1.9)^2 + (y-1)^2 > 0.8$ that correspond of course to $\beta = 1$. The value of the Knudsen number shift from the two reported value while we move from one region towards the other as shown in Figure 2. The number of space cell are 200×200, the number of particles are 40 for cell. Since we are computing a stationary solution we could after some fixed time strongly diminish the fluctuation by averaging in time the solution, however we want to stress the difference of fluctuations and computational time of our hybrid scheme with respect to Monte Carlo, for this reason the solution is not averaged. What we could see is the better accuracy and performance we obtain respect a Monte carlo scheme. In the test presented we have a computational gain of about 40% which clearly increases in simulations in which we approach the hydrodynamic limit. In fact if $\varepsilon \to 0$ particles and fluctuations completely disappear and the time we need to perform the solution is the same of a solver for the compressible gas dynamic equations.

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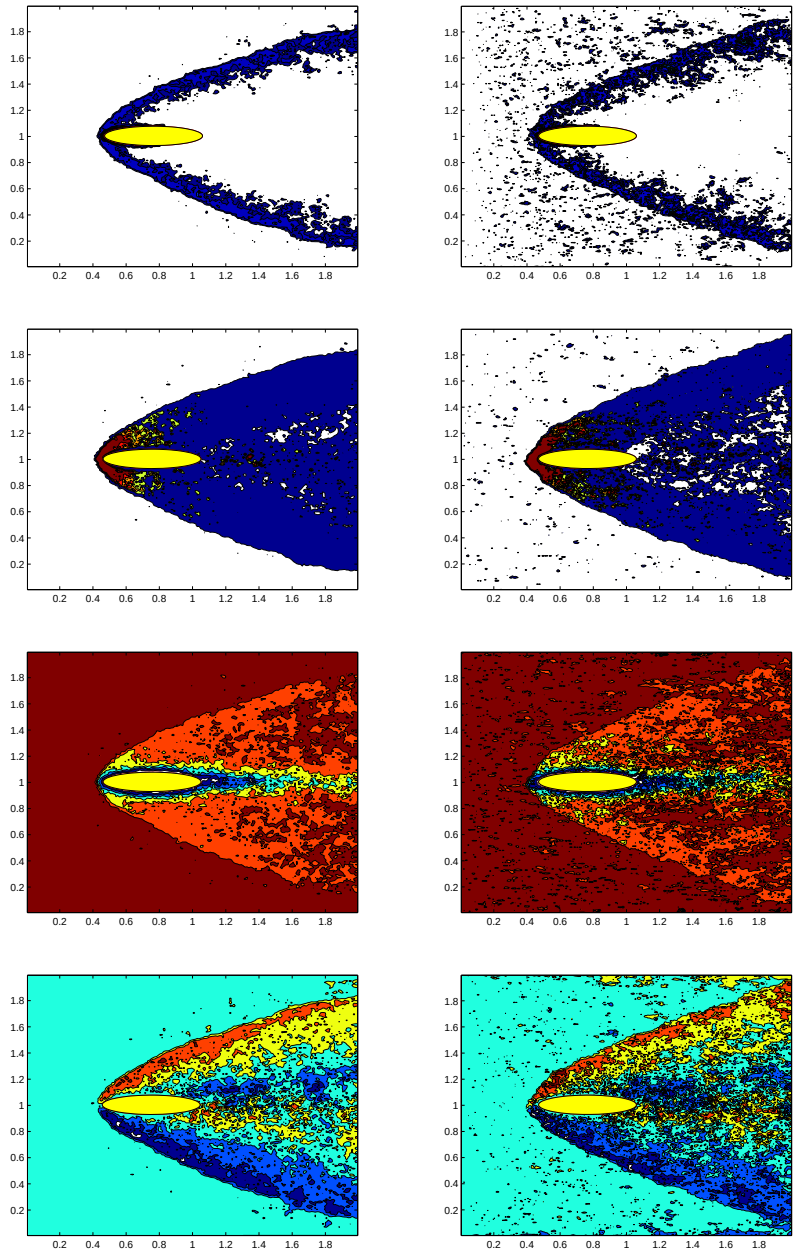

Fig. 1. 2D flow: Domain Decomposition Hybrid scheme(left) Monte Carlo (right) density (top), temperature (middle) velocity x- direction (middle) and velocity y-direction (bottom)

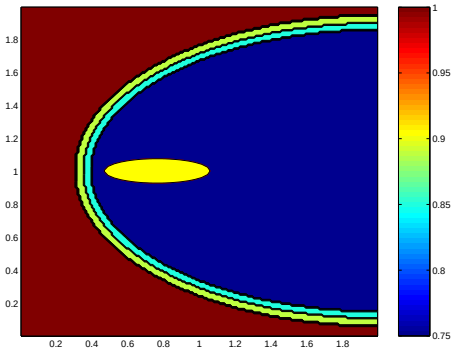

Fig. 2. Degree of equilibrium in different regions of the domain. β

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