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DIRECT COUPLING OF FLUID AND KINETIC EQUATIONS: I

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1 Introduction

In the past few years a growing interest has been brought on coupling approaches in rarefied gas dynamics [3, 4, 7, 12, 14, 18, 20]. An important parameter -the mean free path- rules numerical computations. Mesh refinements are proportional to it and when it is too small, cost of simulations becomes prohibitive if not impossible. A typical example is the reentry of space shuttle in atmosphere. At high altitude stochastic methods for solving the Boltzmann equation (BE) give satisfaying results (see e.g [5, 13]) while they fail for lower altitudes provided the mean free path decreases. It turns out that rarefied gas phenomena occur principally in certain regions of the flow and that aerodynamics equations (Euler or Navier-Stokes) may be enough to describe the reminding regions. Attempts to define properly these regions are essentially based on the Chapman-Enskog expansion which gives the link between kinetic and continuum description. For this question we refer to [2, 6] for theoretical investigations and to [4, 7, 12] for numerics.

In this paper we do not address this problem and the computational domain is decomposed a priori into two regions: kinetic and aerodynamic. A particular attention is payed on the following questions: how to link codes solving different equations and what to do at the interface between kinetic and aerodynamic descriptions?

Our starting point is the method developped by A. Lukschin&all [12]. In this paper, the authors proposed a domain decomposition method based on a Schwarz algorithm. This method can be described in 4 steps:
1- solve Euler equation until stationary solution,

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2- calculate boundary conditions for Boltzmann region,
3- compute the stationary solution in Boltzmann domain,
4- calculate the incoming flux in Euler domain by using Boltzmann values. Go back to step 1.
This method has shown good results and it is of interest to improve some points. In particular, steps 1 and 3 involve inner loops and one may ask the question whether it is possible to avoid these loops in order to reduce CPU time. It was shown in [8] that it is in principle possible to solve one equation after another only during a fixed time Δt (and not until stationary solution). Nevertheless numerical issues of this direct approach are uncertain since solutions of BE have high frequency fluctuations and it is not obvious how the Euler domain would react to fluctuating boundary conditions.

Our paper is constructed as follows: firstly we recall the link between Boltzmann and Euler equations and numerical methods for solving them (sections 2 and 3). Then the problem of boundary conditions at the interface is addressed (section 4). Simple conditions are proposed under assumption of local equilibrium. We continue by studying the influence of fluctuating boundary conditions and show that fluctuations are not penalizing when the Euler solver is "robust" enough (section 5). Solutions are proposed to stabilize these fluctuations at stationary states. Finally numerical results are shown for a flow around an ellipse at Mach 12 and various Knudsen numbers.

2 Generalities

Let us recall the equations that are solved in each domain and the connection between them. We first consider the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f = \frac{1}{Kn} Q(f,f) \tag{1}$$

where $f = f(t, \mathbf{x}, \mathbf{v})$ is the distribution function, Kn the knudsen number and $Q(f,f)$ the collision integral (for more details see [6]). If we multiply (1) by 1, $\mathbf{v}$ and $1/2\mathbf{v}^2$ and integrate over velocity space, we obtain the following system of equations:

$$\begin{cases} \partial_t \rho + \nabla_{\mathbf{x}} \rho \mathbf{u} = 0 \\ \partial_t \rho \mathbf{u} + \nabla_{\mathbf{x}} (\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{p}) = 0 \\ \partial_t \rho E + \nabla_{\mathbf{x}} \mathbf{u} (\rho E + \mathbf{p}) = 0 \end{cases} \tag{2}$$

where

$$\rho = \int f d\mathbf{v}, \quad \rho \mathbf{u} = \int f \mathbf{v} d\mathbf{v}, \quad \rho E = \frac{1}{2} \int f \mathbf{v}^2 d\mathbf{v},$$

and $\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{p}$ is the tensor: $(\rho u_i u_j + \int f (v_i - u_i)(v_j - u_j) d\mathbf{v})_{ij}$.

Non-diagonal terms of the pressure tensor $\mathbf{p}$ vanish when the distribution function is symmetric around the mean velocity $\mathbf{u}$. In particular, at local equilibrium f is of the form:

$$f_M(\rho, \mathbf{u}, T)|_{\mathbf{v}} = \frac{\rho}{(2\pi RT)^{\frac{3}{2}}} \exp(-\frac{(\mathbf{v}-\mathbf{u})^2}{2RT}) \tag{3}$$

and the following closure relation holds:

$$\bigoplus \; p = \frac{1}{3} tr\mathbf{p} = \frac{2}{3}\rho(E - 1/2\mathbf{u}^2) = \rho RT. \tag{4}$$

This last equation together with (2) is the Euler system of equations for monoatomic gases.

Inversely if $\rho(t,\mathbf{x}), \mathbf{u}(t,\mathbf{x}), T(t,\mathbf{x})$ is a solution of (2,4), one can construct an approximate solution of the Boltzmann equation by using f_M [2]. More precisely, there exists a function ϕ orthogonal to the mass, momentum and energy for the measure $< \phi, \psi >= \int f_M \phi\psi d\mathbf{v}$ such that $f = f_M(1 + K_n\phi)$ is a solution of BE at the first order:

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f = Kn^{-1} Q(f,f) + O(K_n),$$

and therefore the Euler solution is enough to describe gas behavior when $Kn \to 0$.

Remark 1 *The coefficient* $2/3(= \gamma - 1)$ *appearing in closure relation (4) corresponds to the case where particles have 3 degrees of freedom i.e* $\gamma = 5/3$.

3 Methods for solving Boltzmann and Euler equations

3.1 The Finite Poinset Method (FPM)

The FPM is a particle method for solving the Boltzmann equation derived from a mathematical interpretation of Nanbu's simulation scheme [1]. Numerical improvements were brought later on in [13].

One starts with a particle discretization of the distribution function f at time $t = 0$:

$$f(0,\mathbf{x},\mathbf{v}) \approx f^0 = \sum_i \delta(\mathbf{x} - \mathbf{x}_i^0)\delta(\mathbf{v} - \mathbf{v}_i^0)\,, \tag{5}$$

and with a spacial discretization of computational domain: $\Omega = \cup_l \Omega_l$. The solution is supposed to be piecewise constant and macroscopic parameters in a cell Ω_l are defined as:

$$\rho_l = \sum_{\mathbf{x}_i \in \Omega_l} 1, \quad \rho_l \mathbf{u}_l = \sum_{\mathbf{x}_i \in \Omega_l} \mathbf{v}_i, \quad \rho_l E_l = \sum_{\mathbf{x}_i \in \Omega_l} |\mathbf{v}_i|^2 \tag{6}$$

The numerical method is based on a splitting of (1). A first step consists in solving the transport equation:

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{x}} f = 0 \tag{7}$$

during a time step Δt. In our case far field boundary conditions are coupling conditions while specular reflexion is used at body surface $\delta\Gamma$:

$$f(t,\mathbf{x},\mathbf{v}) = f(t,\mathbf{x},\mathbf{v} - 2\mathbf{n} < \mathbf{v},\mathbf{n} >) \ \ \forall \mathbf{v} \in \mathbf{R}^3, \ \ \forall \mathbf{x} \in \delta\Gamma \tag{8}$$

($\mathbf{n}$ is the outward normal at $\mathbf{x}$).

The exact solution of (7) with initial value data (5) and boundary condition (8) is given by the method of characteristics.

The second step amounts to solve the space homogeneous BE:

$$\frac{\partial f}{\partial t} = \frac{1}{Kn} Q(f,f) \tag{9}$$

in each cell Ω_l of Ω with initial condition:

$$f(\mathbf{v}) = \sum_{\mathbf{v}_i \in V_l} \delta(\mathbf{v} - \mathbf{v}_i), \ \ V_l = \{\mathbf{v}_i / \ \mathbf{x}_i \in \Omega_l\}.$$

The collision procedure is as follows:

1. Divide randomly V_l into two disjoint sets $(\mathbf{v}_i{}^1)_{i=1,...,\frac{N}{2}}$ and $(\mathbf{v}_i{}^2)_{i=1,...,\frac{N}{2}}$ and choose a permutation Π onto $\{1,...,\frac{N}{2}\}$. Then collision pairs are:

$$(\mathbf{v}_i{}^1, \mathbf{v}^2_{\Pi(i)}) \ \ , i = 1,...,\frac{N}{2}$$

2. Select randomly $\frac{N}{2}$ parameters $x_i \in B(0, 1/\sqrt{\pi})$ associated to each collision. These parameters can be considered as impact parameters though they have got a more general meaning (dummy collisions are possible).

3. Calculate post-collision velocities:

$$(\mathbf{v}_i{}'^1, \mathbf{v}'^2_{\Pi(i)}) = \psi(\mathbf{v}_i{}^1, \mathbf{v}^2_{\Pi(i)}, x_i)$$

where the operator ψ depends on time step Δt and on collision kernel (see [13]).

Then,

$$f(\mathbf{v}) = \sum_{\mathbf{v}_i \in V_l'} \delta(\mathbf{v} - \mathbf{v}_i') \ \text{ with } V_l' = \{\mathbf{v}_i' / \ \mathbf{x}_i \in \Omega_l\},$$

is the solution of (9) in Ω_l after time Δt and one can repeat the transport phase (7).

Spacial discretization and time step: Mesh steps are chosen so as "to capture" phenomena occuring on a characteristic length of the order of the mean free path. The mean free path is a local parameter but it is generally enough to use its value at infinity. Then a global time step Δt is given by

$$\Delta t = \frac{\Delta x}{|\mathbf{u}_\infty|} \tag{10}$$

where $\mathbf{u}_\infty$ is the velocity of the incoming flow. This means that particle do not cross in average more than one cell during the transport phase.

Remark 2 *The computation of solution of homogeneous BE is based on an explicit discretization in time of (9). The corresponding stability condition may be stronger than (10) and one has to repeat the collision procedure (1-3) until one gets the correct time.*

3.2 The Van Leer flux splitting scheme

This well-known scheme [17] is chosen for its robustness. A complete description of this scheme is given in [11]. Here, we restrict ourselves to a rough description in the 2D case. A finite volume formulation of the Euler system (2) onto a mesh with tetrahedrical cells of control volume $V_{i,j}$ is:

$$V_{i,j}.\frac{\partial \mathbf{W}_{i,j}}{\partial t} = -\mathbf{R}_{i+\frac{1}{2},j} + \mathbf{R}_{i-\frac{1}{2},j} - \mathbf{R}_{i,j+\frac{1}{2}} + \mathbf{R}_{i,j-\frac{1}{2}}, \tag{11}$$

where

$$\mathbf{W}_{i,j} \approx \frac{1}{|V_{i,j}|}\int_{V_{i,j}} (\rho, \rho u_x, \rho u_y, \rho E)^T d\mathbf{x},$$

and $R_{i\pm\frac{1}{2},j}$ and $R_{i,j\pm\frac{1}{2}}$ are the fluxes through the cell interfaces $(i \pm \frac{1}{2}, j)$ and $(i, j \pm \frac{1}{2})$. Let $\mathbf{S}_{i+\frac{1}{2},j} = [s_x, s_y]^T$ be the surface vector normal to the cell face $i+\frac{1}{2}, j$, c the sound velocity and $H = E + p/\rho$ the enthalpy. Then fluxes $\mathbf{R}$ at the cell interfaces are calculated as follows:

$$\mathbf{R}_{i+\frac{1}{2},j} = |\mathbf{S}_{i+\frac{1}{2},j}| \left(\frac{1}{2} M_{i+\frac{1}{2},j} \left(\begin{bmatrix} \rho c \\ \rho c u_x \\ \rho c u_y \\ \rho c H \end{bmatrix}_R + \begin{bmatrix} \rho c \\ \rho c u_x \\ \rho c u_y \\ \rho c H \end{bmatrix}_L \right) \right.$$
$$\left. - \frac{1}{2}\phi_{i+\frac{1}{2},j} \left(\begin{bmatrix} \rho c \\ \rho c u_x \\ \rho c u_y \\ \rho c H \end{bmatrix}_R - \begin{bmatrix} \rho c \\ \rho c u_x \\ \rho c u_y \\ \rho c H \end{bmatrix}_L \right) \right) + \begin{bmatrix} 0 \\ s_x p \\ s_y p \\ 0 \end{bmatrix}_{i+\frac{1}{2},j} \tag{12}$$

where L and R hold for left and right and $M_{i+\frac{1}{2},j}$ is a combination of both left and right Mach numbers:

$$M_{i+\frac{1}{2},j} = M_L^+ + M_R^-, \quad M^\pm = \begin{cases} \frac{p}{4}(M \pm 1)^2(2 \pm M) & \text{if } |M| \leq 1, \\ \frac{p}{2}(M \pm |M|)/M & \text{otherwise.} \end{cases}$$

In a same spirit:

$$p_{i+\frac{1}{2},j} = p_L^+ + p_R^-, \quad p^\pm = \begin{cases} \pm\frac{1}{4}(M \pm 1)^2 & \text{if } |M| \leq 1, \\ \frac{1}{2}(M \pm |M|) & \text{otherwise.} \end{cases}$$

Finally, the dissipative term $\phi_{i+\frac{1}{2},j}$ is defined as:

$$\phi_{i+\frac{1}{2},j} = \begin{cases} |M_{i+\frac{1}{2},j}| & \text{if } |M| \leq 1, \\ |M_{i+\frac{1}{2},j}| + \frac{1}{2}(M_R - 1)^2 & \text{if } 0 \leq M_{i+\frac{1}{2},j} < 1, \\ |M_{i+\frac{1}{2},j}| + \frac{1}{2}(M_L + 1)^2 & \text{if } -1 < M_{i+\frac{1}{2},j} \leq 0. \end{cases}$$

Time-step

In view of a coupling with the Boltzmann equation, it is easier to use an explicit Euler scheme for approaching the solution of (11). Δt has again to satisfy to a stability condition:

$$\Delta t_{eul} \leq \frac{|V_{i,j}|}{\delta x \lambda_y(i,j) + \delta y \lambda_x(i,j)} \quad \forall i,j \tag{13}$$

where δx and δy are the mesh steps in the $x-$ and $y-$directions and $\lambda_x(i,j)$, $\lambda_y(i,j)$ are the largest eigenvalues of flux matrix in each direction i.e:

$$\lambda_x(i,j) = u_x + c|_{(i,j)}, \quad \lambda_y(i,j) = u_y + c|_{(i,j)}.$$

When this condition is stronger than (10), it is preferable to repeat the Euler phase until one reaches the same time step since computations are more expensive for BE than for EE.

4 Coupling conditions

Let Γ_{BE} be the boundary between the Boltzmann and Euler domains and $\mathbf{n}(\mathbf{x})$ be the outward normal of Boltzmann domain at a point $\mathbf{x}$ of this boundary.

Let us first look for boundary conditions for the Boltzmann equation. The Euler solution gives only macroscopic parameters and we say for want of anything better that particles coming from the Euler domain are distributed according to a Maxwellian distribution $f_M(\rho, \mathbf{u}, T)$ (3). If we think in the same way as for determination of far field boundary conditions for the Euler equation, we should distinguish between subsonic or hypersonic ingoing or outgoing flows [10]. In this vein, the number of parameters $(\rho, \mathbf{u}, T)$ given by the Euler solution should

be directly proportional to the number of characteristics entering the Boltzmann domain.

We now look for conditions at the Euler boundary. A natural one is the continuity of fluxes. For $\mathbf{v}.\mathbf{n}(\mathbf{x}) > 0$ ($\mathbf{x} \in \Gamma_{BE}$), f is given by BE and is not necessarily a Maxwellian. On the Euler side this function should be a Maxwellian since it is at equilibrium (see section 2). Therefore continuity of fluxes writes:

$$\int_{\mathbf{v}.\mathbf{n}>0} < \mathbf{v}.\mathbf{n} > \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} f(\mathbf{v})d\mathbf{v} = \int_{\mathbf{v}.\mathbf{n}>0} < \mathbf{v}.\mathbf{n} > \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} f_M(\rho, \mathbf{u}, T)|_{\mathbf{v}} d\mathbf{v} \quad (14)$$

This relation is called Marshak condition and parameters $\rho, \mathbf{u}, T$ are the boundary conditions for the Euler equation (for theoretical investigations see [9]). One should again count the number of characteristics entering the domain to determine the right number of conditions. Besides, system (14) is very difficult to solve when $\mathbf{u} \neq 0$ and it is of interest to try to simplify these boundary conditions.

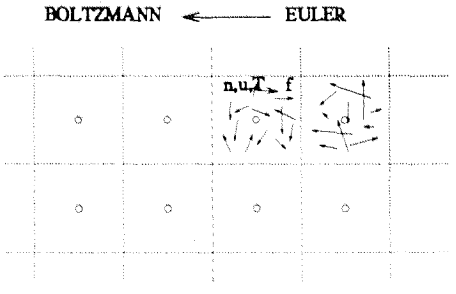
The interface between the two domains is supposed to be in a region where Euler solution is the same (or nearly the same) as Boltzmann solution. Therefore f should be at local equilibrium. In this case, continuity of fluxes is equivalent to continuity of moments:

$$\int_{\mathbf{v}\in\mathbf{R}^3} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} f(\mathbf{v})d\mathbf{v} = \begin{pmatrix} \rho \\ \rho\mathbf{u} \\ \rho E \end{pmatrix} \quad (15)$$

Moreover, additional condition(s) should be transparent when the number of ingoing characteristics is lower than the number of prescribed parameters at boundary. Therefore it is enough to impose at Boltzmann boundary:

$$f(t, \mathbf{x}, \mathbf{v}) = f_M(\rho, \mathbf{u}, T)(t, \mathbf{x}, \mathbf{v}) \ \ \forall \mathbf{x} \in \Gamma_{BE}, \ \ \mathbf{v}.\mathbf{n}(\mathbf{x}) < 0, \quad (16)$$

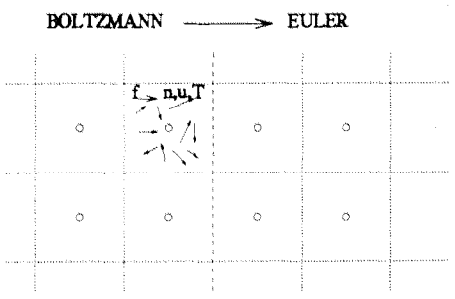
where the parameters $\rho, \mathbf{u}, T$ are solutions of the Euler system. It corresponds numerically to create a set of particles approaching the Maxwellian distribution $f_M(\rho, \mathbf{u}, T)$ in cells nearby the boundary (with possible use of distant cells depending on the mean velocity):



Likewise, conditions at Euler boundary are:

$$\begin{pmatrix} \rho \\ \rho\mathbf{u} \\ \rho E \end{pmatrix} = \int_{\mathbf{v}\in\mathbf{R}^3} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}|\mathbf{v}|^2 \end{pmatrix} f(t,\mathbf{x},\mathbf{v})d\mathbf{v}, \quad \forall \mathbf{x} \in \Gamma_{BE} \tag{17}$$

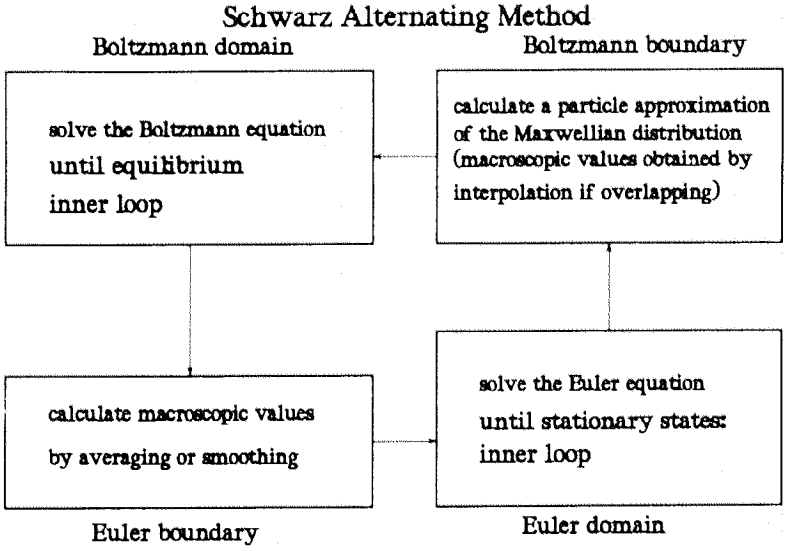
where f is solution of BE for $\mathbf{v}.\mathbf{n} > 0$ and Maxwellian for $\mathbf{v}.\mathbf{n} < 0$. Practically it is easier to compute them by taking f in a Boltzmann cell nearby the boundary (i.e for all $\mathbf{v} \in \mathbf{R}^3$):



Remark 3 *When the assumption that Euler solution behaves as Boltzmann solution is not fulfilled, conditions (16,17) are not valid and they amount to force the continuity at interface. It is proved that those conditions produce false results in certain cases (see [9]). Numerical examples of such cases are given in section 6.*

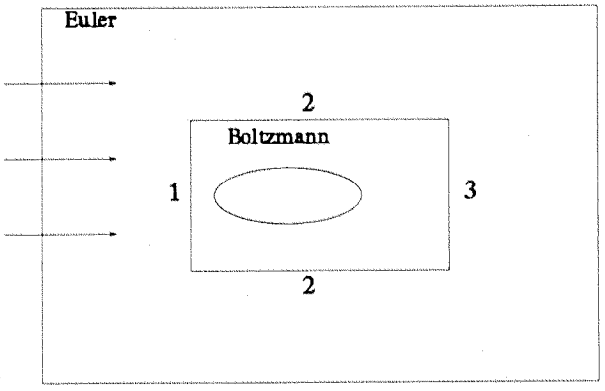
5 Fluctuations at the Euler boundary and stabilization

Macroscopic values $\rho_l, \mathbf{u}_l, E_l$ in Boltzmann cells nearby the interface fluctuate with high frequency due to the stochastic treatment of collision phase (see section 3.1). A way to smoothen these fluctuations is to average the solution in time. This has lead many authors [3, 12, 14] to use the following algorithm (Schwarz algorithm):



Here, the fact that one computes the solution until stationary state during each phase allows to average the Boltzmann solution at interface. It should be theoretically possible to solve each equation just during a fixed time T (see [8]) and then go to the other. But this idea is based on the assumption that solutions behave well at the boundary, i.e are in a certain sense monotonic which is not the case for the Boltzmann numerical solution.

We now want to analyse more precisely what happens at the boundary. There exist actually three different cases:



1. Upstream: boundary conditions for the Euler domain are transparent (in the sense of the previous section) since all characteristics go out of the Euler domain. From the numerical point of view fluctuations are cancelled by upwind schemes.

2. Perpendicular to the shock: when the normal velocity through boundary is lower than sound speed c, characteristics are going in and out of Euler domain.

3. Downstream: all characteristics enter the Euler domain and it seems to be the worse case.

Let us discuss formally about cases 2 and 3. A model problem would be to analyse the case of a stationary and constant solution with small perturbation at the boundary. Linearization around the equilibrium reduces Euler equations to the wave equation: $\partial_{tt}\phi - \gamma\partial_{xx}\phi = 0$ ($\gamma > 0$) and fluctuations propagate with constant velocity and amplitude.

Large perturbations do not allow to do this simplification and one has to study the propagation of fluctuations in nonlinear hyperbolic system. We may say as a first approach that fluctuations propagate along characteristics (see for example the book of G.B. Whitham [19]).

So let us now suppose that fluctuations are in some way not a "fatal cause of disorder", the question is: how to recover the right solution in the Euler domain when the stationary solution is reached in the Boltzmann domain? For the sake of simplicity we consider a half space problem for the Burger equation:

$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0, \quad u(0,x) = u_0 \; \forall x \geq 0, \tag{18}$$

with perturbation at the boundary:

$$u(t,0) = u_0 + \epsilon(t) > 0$$

The solution without fluctuation is constant $u(t,x) = u_0$ ($\forall t, x > 0$). Let us discretize (18) over time and space by a simple first order upwind scheme (i.e the Van Leer scheme in this simple case):

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}[(u_i^n)^2 - (u_{i-1}^n)^2] \tag{19}$$

where Δt and Δx are discretization steps in time and space and u_i^n is the approximate solution at time $n\Delta t$ in the cell $[(i-1/2)\Delta x, (i+1/2)\Delta x]$.

For this scheme, a maximum principle holds under the stability (CFL) condition $\frac{\Delta t}{\Delta x}(u_0 + M) \leq 1$:

$$|u_0^n - u_0| \leq M \Rightarrow |u_i^n - u_0| \leq M \quad \forall i, n \tag{20}$$

with $u_0^n = u_0 + \epsilon(n\Delta t) = u_0 + \epsilon^n$.

We assume that fluctuations (ϵ^n) are bounded along time ($|\epsilon^n| \leq M \quad \forall n$) and distributed around 0:

$$\frac{1}{N}\sum_{n=1}^{N} \epsilon^n \to 0 \text{ as } N \to \infty. \tag{21}$$

This assumption means that one can obtain the right solution at the boundary by averaging in time; this is the case for solutions of BE once the stationary state

is reached. Can we obtain the solution of Burger equation by doing so? That is to say, does

$$\frac{1}{N}\sum_{n=1}^{N} u_i^n \to u_0 \ ?$$

The answer is negative but one can nevertheless prove that:

$$\begin{aligned} \frac{1}{N}\sum_{n=1}^{N}(u_j^n)^2 &= \frac{1}{N}\sum_{n=1}^{N}(u_0^n)^2 + O(\frac{j}{N}) \\ &= {u_0}^2 + \frac{1}{N}\sum_{n=1}^{N}(\epsilon^n)^2 + o(N) \ \ \forall j \geq 0 \end{aligned} \tag{22}$$

Indeed, by summation of (19) over time and space one has:

$$\begin{aligned} \sum_{i=1}^{j}(u_i^{N+1} - u_i^1) &= -\frac{\Delta t}{\Delta x}\sum_{n=1}^{N}\sum_{i=1}^{j}[(u_i^n)^2 - (u_{i-1}^n)^2] \\ &= -\frac{\Delta t}{\Delta x}\sum_{n=1}^{N}[(u_j^n)^2 - (u_0^n)^2] \end{aligned}$$

which gives (22) by using the maximum principle (20) and property (21). This shows two things: on one hand (u_i^N) is in average not too far from u_0 and on the other hand one cannot obtain the right solution by averaging in time. In fact, this is essentially due to the non-linearity of the equation.

A way to recover the right solution is to replace ϵ^n by the series:

$$\sigma^N = \frac{1}{N}\sum_{n=1}^{N}\epsilon^n = \frac{1}{N}[(N-1)\sigma^{N-1} + \epsilon^N]. \tag{23}$$

σ^n tends to 0 as $n \to \infty$ and one can prove that $u_i^n \to u_0$ uniformly on a finite set of points for such boundary conditions.

Remarks 1

1. *There are two different ways to obtain the stationary solution: in Boltzmann domain by averaging over time and in Euler domain by using a condition like (23).*

2. *The numerical success of this direct coupling approach seems to lean principally on the robustness of the Euler solver. Here we have formally proved that any monotonic or TVD scheme should be adapted to such calculation.*

6 Numerical results

We present numerical results for hypersonic flows around an ellipse. Different angles of attack and Mach numbers lead to the same conclusions as concerns the influence of both decomposition of the domain and Knudsen number. Therefore results are shown only in the case where these parameters are fixed: the angle of attack $\theta = 30°$ and the Mach number is 12.

On every graphics, the small rectangle in the domain is the interface between kinetic region (inside) and aerodynamic region (outside). When there is no rectangle, the computation is done completely with BE. Knudsen number is defined as:

$$Kn = \frac{\text{mean free path}}{L},$$

where L is the length of the ellipse projected on a straight-line perpendicular to the incoming flux:

$$L = R\sqrt{\cos^2\theta + 4\sin^2\theta} \quad (\text{great axis} = 2 \times \text{small axis} = 2R).$$

The meshing is global. This means that meshes for kinetic and aerodynamic regions fit together and that there is no need to use an overlapping domain (as in [12]). Moreover for simplicity we choose to use a regular rectangular mesh so that locating particles is an easy task. Such a mesh is of course not adapted to real calculation but it is more convenient to study the influence of the decomposition. Cell sizes are defined so as to capture phenomena occuring on a mean free path length (see table 1).

6.1 Good agreement

We firstly present a comparison between a full Boltzmann calculation and the direct coupling method for a relatively small Knudsen number: $Kn = 0.023$. In this case theoretical expectation is that the two solutions should be roughly the same. Regardless of numerical noises, the comparison between the two approaches is excellent (figures 1, 2, 3). A comparison on drag and lift coefficients draws the same conclusion: $C_d(B) = 1.14$, $C_d(B/E) = 1.15$, $C_l(B) = 0.555$, $C_l(B/E) = 0.550$. This means on one hand that Euler equation is valid far enough from the body for such Knudsen numbers. On the other hand this result corroborates theoretical investigations concerning fluctuations at the boundary of Euler domain.

An artificial shock spreading is observed in the Euler domain (figure 1). It is due to the diffusivity of the Van Leer scheme at the first order. This artificial dissipation is somehow of help for higher Knudsen numbers since the shock thickness increases with mean free path but it would be preferable to use an higher order scheme and a physical dissipative term (Navier-Stokes equation).

6.2 What should not be done

Let us now increase the Knudsen number. Figures 4 and 5 show a typical effect of rarefied gas dynamics: as the Knudsen number increases the shock widens in the Boltzmann region while it keeps the same shape in the Euler region. The continuity at interface is still ensured by condition (15) but the result has no physical meaning. Nevertheless the shape of the solution within the Boltzmann domain is the right one and a comparison between lift and drag coefficients gives good agreement: $C_d(B) = 1.18$, $C_d(B/E) = 1.18$, $C_l(B) = 0.567$, $C_l(B/E) = 0.564$ for $Kn = 0.076$ and $C_d(B) = 1.29$, $C_d(B/E) = 1.29$, $C_l(B) = 0.582$, $C_l(B/E) = 0.577$ for $Kn = 0.227$.

Another non physical solution is shown in figure 6. The interface is too close to the body so that it creates an artificial shock. The relative velocity between kinetic and aerodynamic domains is indeed too large. This is a case where neither continuity conditions (15) nor aerodynamic approach are valid.

The last and most difficult situation is encountered in the wake of the ellipse. In this low density region, a standard particle code is unable to describe properly the distribution function provided the number of particles is proportional to the density. It happens that there is one or even no particle in some cells at the interface. Since characteristics are going out of Boltzmann domain in this region, one faces the following difficulties:

1. with 0 or 1 particle, one cannot define a temperature or a Mach number.
2. fluctuations are extremely large since the density varies with the number of particles (from 0 to 1 or 2).

One may argue that this is a false problem since there is no evidence of the validity of Euler equation in this region and Boltzmann domain should be prolonged. The other possible answer is to use a method giving a uniform representation of the solution in the Boltzmann domain (for example weighted particle method [16] or discrete velocity models [15]). In the present case fluctuations at the boundary are smoothed by averaging in time:

$$\mathbf{W}^n_{aver} = \frac{1}{T} \sum_{i=n-T+1}^{n} \mu_i \mathbf{W}^i_{bound}$$

Average is done over T time steps and coefficients (μ_i) conserve the positivity of the density, energy and pressure ($\sum \mu_i = 1$ and $\mu_i \geq 0$).

6.3 Performance

The following array gives CPU times on a IBM6000 for the previous tests. In each case the number of iterations is 200 and the runs start with 30 particles per cell in Boltzmann domain. The second column gives the size of the mesh. The third

and fourth ones are CPU times respectively for full BE and coupling approach. In the fourth column the number which appears in bracket is the number of cells in Boltzmann domain.

Table 1: Computational time on an IBM6000

Kn	*Cells*	*Boltzmann*	*Boltzmann-Euler*
0.076	2501	14 mn	7 mn (1056)
0.076	3710	20 mn	5 mn (390)
0.0223	4455	25 mn	12 mn (1711)

The second test case gives an idea of performances: 20 minutes are necessary to compute the solution with BE while 5 minutes are sufficient for the aerodynamic solution.

7 Conclusion

We have shown that direct coupling of a stochastic method for a kinetic equation and a "deterministic" method for aerodynamic description is possible in the context of rarefied gas dynamics. Under suitable physical parameters, the agreement between full kinetic solution and coupled solution is excellent. Moreover the coupled approach allows to save significant CPU time.

In order to be valid, the method has to be applied with a correct decomposition of the computational domain. It is therefore important to continue this research with a determination of a switching criteria between kinetic and aerodynamic regions [4].

Other improvements can be brought to the present algorithm: higher order schemes for the aerodynamic region and possible use of Navier-Stokes equation.

The following paper will address these issues.

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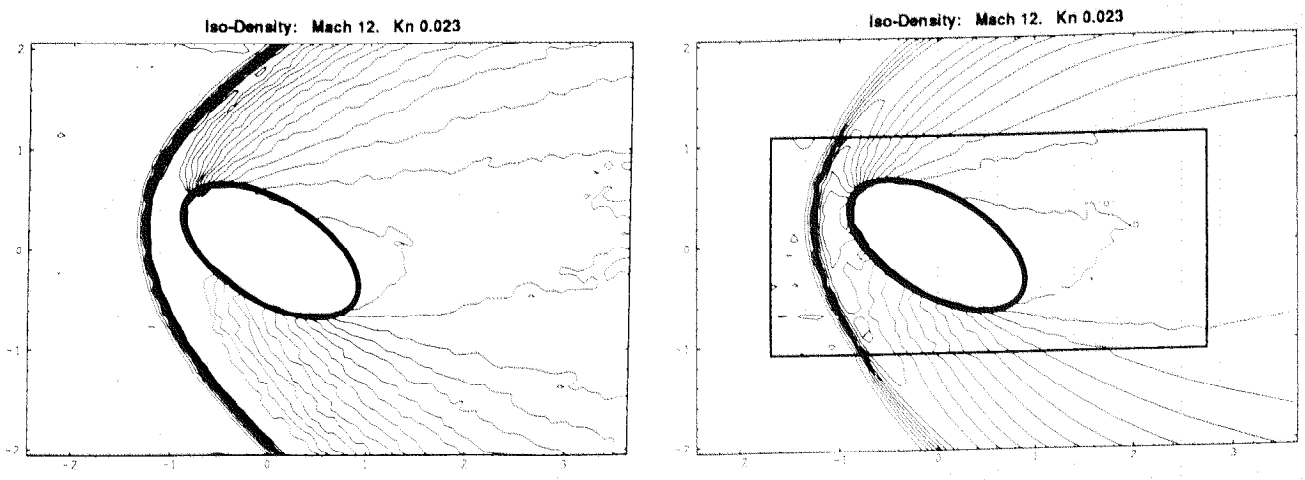

Figure 1: Isolines of density (BE and B/E) at low Knudsen number ($Kn = 0.0223$).

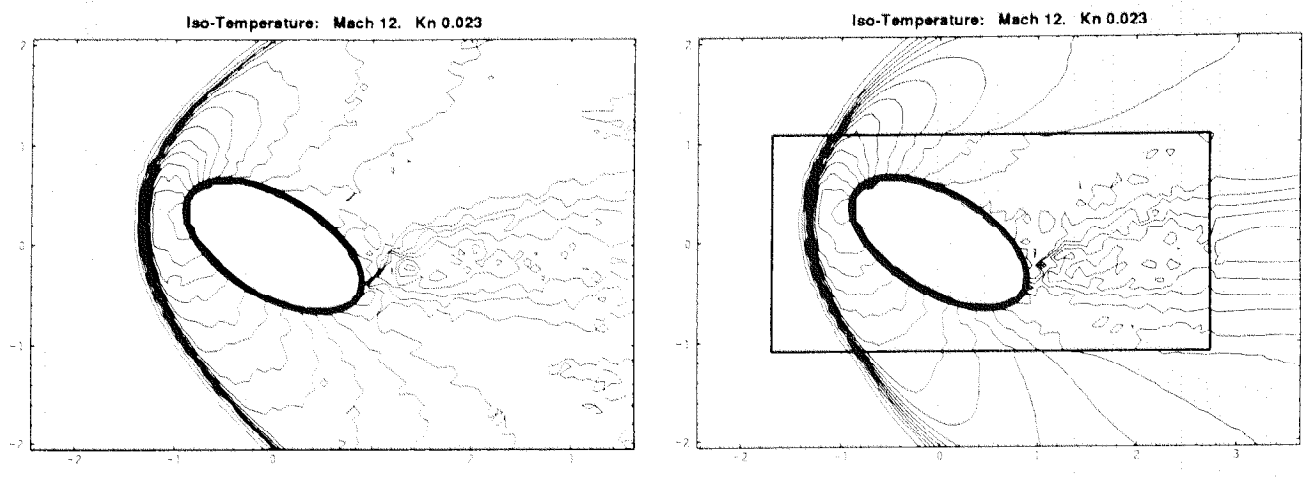

Figure 2: Isolines of temperature (BE and B/E), $Kn = 0.0223$

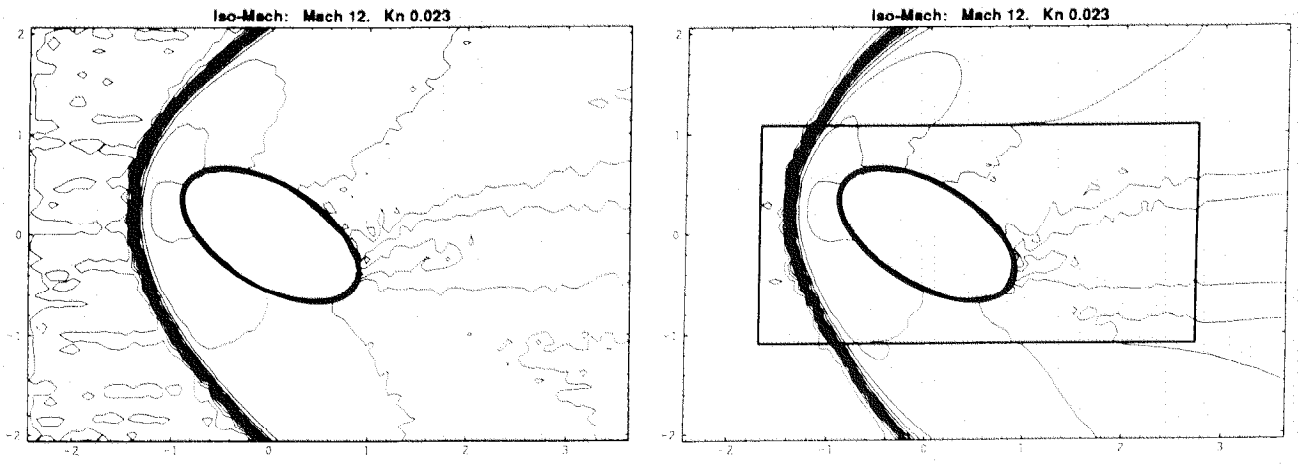

Figure 3: Isolines of Mach number (BE and B/E), $Kn = 0.0223$

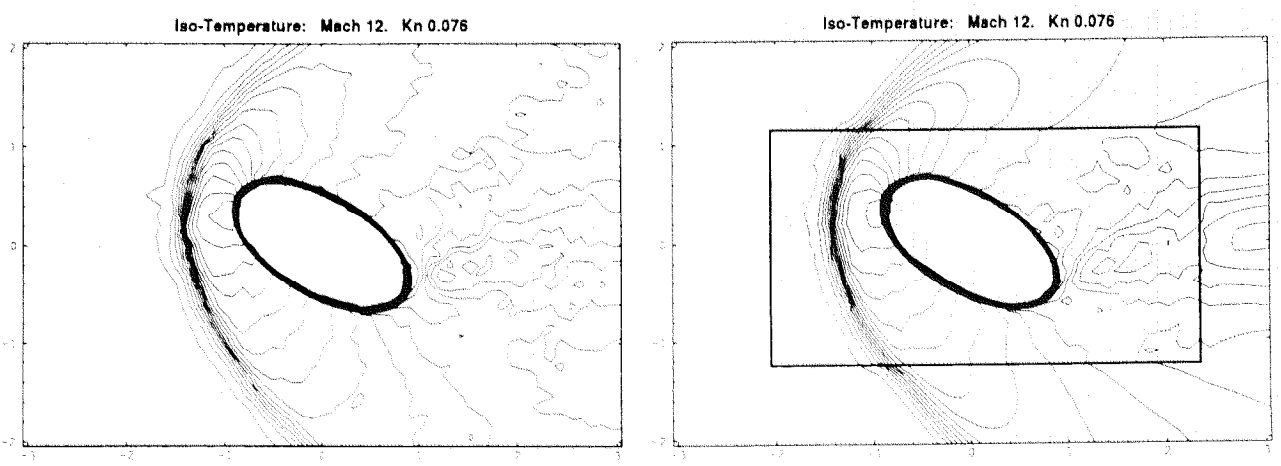

Figure 4: Temperature for increasing Knudsen number: $Kn = 0.076$.

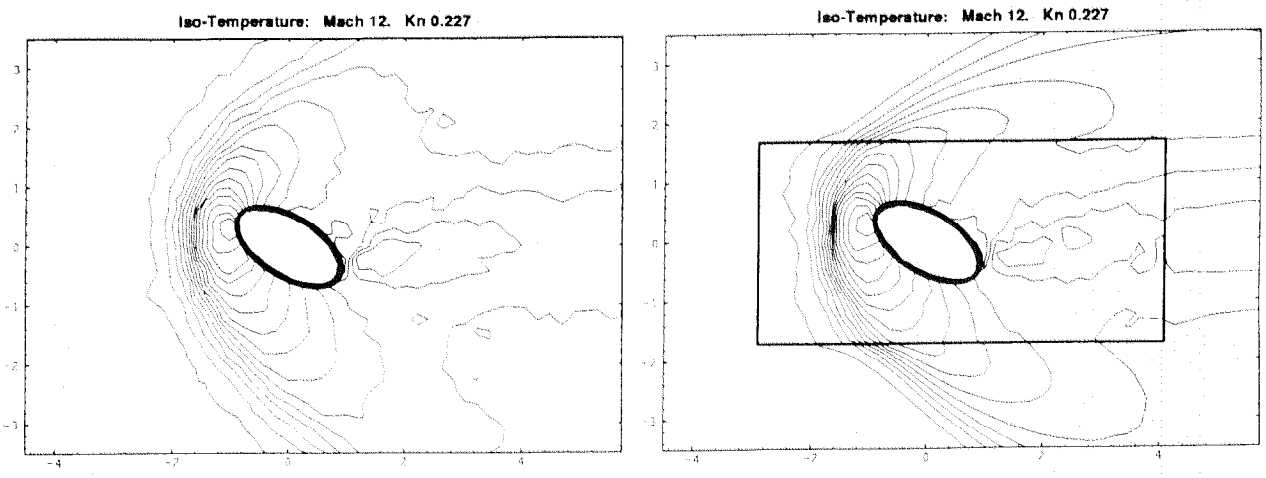

Figure 5: Temperature for increasing Knudsen number: $Kn = 0.227$.

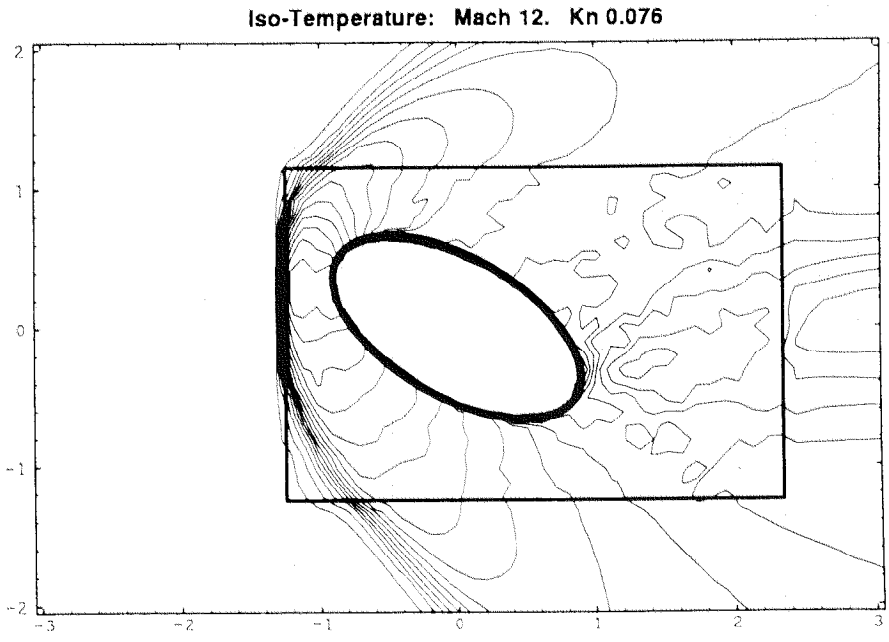

Figure 6: Deformation of the shock profile (temperature): $Kn = 0.076$.