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o Further numerical and theoretical studies of the coupling of Boltzmann equation and its hydrodynamic limits.

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COUPLING OF KINETIC EQUATIONS AND THEIR HYDRODYNAMIC LIMITS

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Objectives

- Development of alternative approaches to the full Boltzmann model in transition regimes.
- Applications to the numerical simulation of flight at high altitudes particularly the computation of flows around full airplanes at high altitudes.

Status of effort

During the last two years, the author continued his efforts to reach the above objectives. In particular he focused on the following:

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- Numerical and theoretical analysis of the coupling of kinetic equations and their hydrodynamic limits for particular kinetic models. (This gives more insight into the coupling method for the full Boltzmann model)
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Accomplishments/New Findings

1 Introduction

The main problem of kinetic theory consists in deriving an evolution equation for the one-particle distribution function and in solving mathematical problems related to this equation, so that the moments of the solution can enable the calculation of the relevant macroscopic variables.

The celebrated Boltzmann equation is certainly the most famous and successful mathematical model to describe the time and space evolution, at a statistical level, of the position and velocity distribution function of particles in a dilute gas. This equation is a powerful instrument both in the analysis of thermodynamical properties of fluids and in the solution of fluid dynamical problems in rarefied gas dynamics, which are often relevant in modern technology. The range of problems of rarefied gas dynamics includes, for example, problems of flow past aircraft flying at high altitudes, motion of gases in a vacuum apparatus, ultrasonic vibrations in gases, structure of shock waves, nonequilibrium flows, etc... A survey of several applications to typical fluid dynamics flows, such as shock waves, Couette and Poiseuille flows, etc... can be found in the book by Kogan [36]. The ideas of kinetic theory also find applications in other fields, such as radiative transfer, the theory of ionized gases, the theory of neutron transport and the study of quantum effects in gases [10, 20]

The Boltzmann equation is a mathematical model of the phenomenological kinetic theory of gases which defines the evolution, in time and space, of the one particle distribution function for a simple monoatomic gas. The evolution equation for the distribution function

$$f = f(x, v, t) : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \to \mathbb{R}_+,$$

is obtained equating the total derivate of f to the gain and loss terms due to the collisions of the particles which at the time $t \in [0, T]$ are in a neighbourhood of the phase point x, v, where $x \in D \subset \mathbb{R}^3$ is the position and $v \in \mathbb{R}^3$ is the velocity. The Boltzmann equation, for a large class of pair-particles interaction potentials, is [20, 16]

$$\begin{aligned} \frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f &= Q(f, f) \\ &= Q_+(f, f) - Q_-(f, f) \end{aligned} \tag{1}$$

where Q_+ and Q_- denote, respectively, the gain and loss terms, respectively are given by

$$\begin{cases} Q_+(f, f) &= \int_{\mathbb{R}^3 \times S^2_+} B(z, q) f(x, v', t) f(x, v'_\star, t) dz dv'_\star \\ Q_-(f, f) &= f(x, v, t) \int_{\mathbb{R}^3 \times S^2_+} B(z, q) f(x, v_\star, t) dz dv_\star \end{cases}$$

Above

- F is the external force field acting on the particles;
- z is the unit vector in the direction of the apse-line bisecting velocities $q = v_\star - v$ and $q' = v'_\star - v'$;
- v and $v_\star$ are the pre-collision velocities of the test and field particles, respectively, and v', $v\star'$ are the post-collision velocities. Since for binary interactions, collisions conserve momentum and energy, these velocities are related to v and $v_\star$ by the relations $v' = v + z(z.q)$, $v'_\star = v_\star - z(z.q)$;
- S^2_+ is the integration domain of z, $S^2_+ = \left\{ z \in \mathbb{R}^3 : |z| = 1, < z, q > \geq 0 \right\}$
- B is a collision kernel which depends upon the interaction potential [20, 16].

The Boltzmann equation is a difficult model to deal with both at an analytical and computational level. This difficulty has been an important challenge for numerous applied mathematicians also engaged by the demand of aerodynamicists and engineers to solve fluid dynamics problems in molecular flow conditions; namely in physical conditions such that the models of continuum hydrodynamics cannot be any longer considered valid for the applications. A great effort has been devoted to solve mathematical and computational problems related to the Boltzmann equation. Some of them, as we shall see, have been (or partially) solved by several authors among them the author. These problems deal with the following fundamental topics

(i) the existence and uniqueness theory,

(ii) the hydrodynamic limit,

(iii) the boundary conditions,

(iv) the intermediate regimes,

(v) finding models alternative to the one of the classic Boltzmann equation.

Here, the intermediate regimes refer to the cases where the Knudsen (K_n) number which measures the ratio between the average time separating two successive collisions of a given particle and a characteristic time of the flow satisfies either:

(a) $K_n \leq 0.510^{-1}$ or

(b) $0.510^{-1} \leq K_n \leq 10$.

In the first case it is assumed that the Knudsen number is not extremely small ($K_n << 0.510^{-1}$), because otherwise the standard continuous model is valid. In both cases the direct Boltzmann simulation is very expensive and may be impossible in case **(a)** because the computational method requires one cell per mean free path. The hydrodynamic limit refers to the study of the asymptotic trends of the kinetic equations as the Knudsen number tends to zero.

These problems have been and still (some of them) are today a challenging objective and a hard obstacle for applied and computational mathematicians with interest in this field of mathematical physics. Some of them are solved recently by the author, as we shall see. A further development of his solution will be considered in the proposed research.

Consider for instance the physically interesting problems: the interior domain problem which is such that the gas is contained in a volume with a solid surface on the boundary and the exterior domain problem, which is such that the gas occupies the whole space $\mathbb{R}^3$ and contains an obstacle. The surface of the solid wall is defined in both cases by $\partial\Gamma_w$, the normal to the surface directed towards the gas is ν.

Let f^+ and f^- denote the partial incoming and outgoing traces on the boundary $\partial\Gamma_w$. For f continuous, they can be defined as follows

$$\begin{cases} f^+(x,v) &= f(x,v), \ x \in \partial\Gamma_w, \ v \cdot n(x) > 0 \\ f^+(x,v) &= 0, \ x \in \partial\Gamma_w, \ v \cdot n(x) < 0 \end{cases}$$

and

$$\begin{cases} f^-(x,v) &= f(x,v), \ x \in \partial\Gamma_w, \ v \cdot n(x) < 0 \\ f^-(x,v) &= 0, \ x \in \partial\Gamma_w, \ v \cdot n(x) > 0 \end{cases}$$

Then the boundary conditions are formally defined by

$$f^+(x,v,t) = Rf^-(x,v,t) \tag{2}$$

where the operator R is characterized, for a broad range of physical problems, by the following properties:

1) R is linear, of local type with respect to x and is positive, i.e. $f^- \geq 0 \Rightarrow Rf^-(x,v,t)$.

2) R preserves mass, i.e. the flux of the incoming particles equals the one of the particles which leave the surface.

3) R preserves local equilibrium at the boundary, i.e. $M_w^+ = RM_w^-$, where M_w is the Maxwellian distribution at the wall temperature.

4) R is dissipative, i.e. satisfies the Darrozes and Guiraud [21] inequality at the wall

$$\int_{\mathbb{R}^3}(v\cdot z)(f^- + Rf^-)(logf + \frac{|v|^2}{\theta})dv \leq 0.$$

More details about the operator R and the mathematical aspects on the formulation of the boundary conditions can be found in [14, 21, 33, 16]. The experimental activity on the gas-surface interaction addressed to validate the mathematical models for the applications is documented in [49, 50]. The formulation of the initial-boundary value problem, in the case of the interior domain problem, consists in linking the evolution equation (1) to the boundary conditions (2) on the wall $\partial\Gamma_w$. In the case of the exterior domain problems, in addition to the boundary conditions on the wall, generally suitable Maxwellian equilibrium conditions at infinity are assumed.

Mathematical problems related to the applications may involve additional difficulties. For instance it may be necessary to deal with non regular or concave geometries. In addition, it may be useful or even necessary, to decompose the domain occupied by the gas into domains where one can apply the equations of the continuum fluids and into domains where one has to apply the Boltzmann equation. Such decomposition has been introduced by the author [73]. It has several computational advantages, as we shall see, but involves additional mathematical and physical difficulties related to the matching of the two models.

Since the existence theory involves rather restrictive assumptions, it is only partially useful for the applications. The most important existence results are obtained by DiPerna and Lions [23, 24] who considered the solutions for large L^1 initial data. This type of results exploit the averaging Lemma by Golse, Lions, Perthame and Sentis [28] to obtain existence of weak renormalized solutions. A further important developments are obtained in [34, 2, 37, 40]. For a complete survey on the recent development on the existence theory the reader is refered to [3].

The other topics (ii)-(v) were (and are still) covered to some extent by the author [73]-[88],[11]-[12] ,[51]-[56]. The program proposed here is a continuation of the prior and current research of the author. Since it will use mainly the methods developed by the author, his prior and current research are included with a little more detail and the rest of this proposal will refer mainly to the work by the author [73]-[88], [11]-[12],[51]-[56].

2 Current and prior research of the author related to (ii)-(v)

The Boltzmann equation is one of the most important tools in gas dynamics calculations when physical phenomena of a molecular scale cannot be neglected. In this case the model of continuum hydrodynamics cannot be any-longer considered valid for the applications. But, when the mean free path gets too small, the numerical solution of Boltzmann equations becomes impossible because the discretization step of the associated grids must be smaller than the mean free path. The classical solution consists then in replacing the Boltzmann equation by its fluid limit obtained when the mean free path goes to zero.

The hydrodynamical limit theory aims to find the connection between the Boltzmann equation and the hydrodynamical equations (Euler and Navier-Stokes equations). This can be formulated as the search of asymptotic relationships between solutions of these equations. This connection results from two types of properties of the collision operator:

1) Conservation properties and an entropy relation that implies that the equilibrium distribution corresponds to a Maxwellian for the limit at the order zero.

2) The derivative of the collision operator satisfies a formal Fredholm alternative with a kernel related to the conservation properties of 1).

The compressible Euler equations are obtained formally using the conservation properties and the entropy dissipation which are consequences of the properties of the collision operator. In the Chapman-Enskog or Hilbert expansion [20] of f in $\epsilon = K_n$ the compressible Euler equations are the leading-order dynamics.

Since the compressible Euler equations generally become singular after a finite time [71], any global in time convergence proof cannot rely on uniform regularity estimates. In [7] assumptions are made on the kinetic level. The authors assume a formally consistent convergence for the fluid dynamical moments and entropy of the solution of the kinetic equations (1). A more detailed knowledge of the collision operator is needed in order to obtain the compressible Navier-Stokes equations. These equations arise as corrections to those of Euler at the next order in the Chapman-Enskog expansion. Strong hypothesis are needed on the regularity of solutions of the compressible Navier-Stokes equations in order to make sens of these expressions. The results available up to now consider only the case of the full space or periodic domain [7, 8, 15, 60].

In presence of obstacles boundary conditions must be specified. When the Knudsen number is extremely small (very dense gas), the classical hypothesis of no-slip boundary conditions give accurate boundary conditions. However, when the Knudsen number lies in the range of values of the case **(a)** and **(b) (iv)**, a breakdown of the aerodynamic theory in the region neighboring the obstacle (the so-called Knudsen layer) is observed and boundary conditions of slip type must be specified. The Chapman-Enskog expansion (or any other method based on the use of a finite number of moments) does not in general satisfy the kinetic boundary conditions. Therefore, this expansion is not valid in the Knudsen layer which is of width of the order of the mean free path.

The standard solution is to use analytical slip boundary conditions as described in [36, 13, 16]. But the constants which are involved are hard to identify and their validity is questionable. On the other hand, the direct simulation of the kinetic problem is rapidly too expensive, because it requires one computational cell per mean free path. To overcome such difficulties many authors have recently tried to use intermediate asymptotic models such as Burnett equations [89]. However, in [18] the authors have shown that the Burnett equations are in violation of the second law of thermodynamics thus explaining their long history of numerical difficulties.

On the other hand when the mean free path is roughly one thousand times smaller than the length of the obstacle these asymptotic models are no-longer valid.

In [73], the author proposed a fundamental strategy that permits the coupling of differents models and/or different approximations to compute the solution of the exterior domain problem. This strategy is very general and can be applied to many different physical systems [73]-[88], [51]-[56],[11]-[12]. The application of this strategy to the solution of intermediate regimes (as defined in **(iv)**) consists of coupling the hydrodynamics equations (Euler or Navier-Stokes equations) with the Boltzmann equation. The resulting method involves additional mathematical and physical difficulties related to the matching of equations of the two models. However, this approach has several computational advantages. One of the great advantages is the use of the correct model related to the physical features of the flow.

The application of this approach to the solution of Boltzmann equation for external domain problem consists of the following steps

(1) Domain decomposition of the external field into the domains, possibly overlapped, of validity of the Boltzmann Equation and of the equations of hydrodynamics.

(2) Solution of the kinetic equations in the domain of validity of the Boltzmann equation.

(3) Solution of the hydrodynamics equations in their domain of validity.

(4) Coupling of the solution to the two models, the continuous and kinetic ones.

These steps are documented in the next paragraphs. The first paragraph deals with the asymptotic models at the fluid limit. The description of the geometry and the coupling of these asymptotic models with the original Boltzmann equation is then discussed in the second paragraph. The third paragraph presents a brief description of the different discretization methods employed for the kinetic model and the hydrodynamic one. In the last paragraph some comments are presented.

2.1 Asymptotic models

The Boltzmann equation, in dimensionless form, can be written as follows [16]

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\epsilon} Q(f, f). \tag{3}$$

The number $\epsilon = Kn$ is the Knudsen number defined in the previous section. The fluid regime corresponds to very small values of ϵ ($\epsilon < 0.01$). In such regimes, the governing equations can be obtained by a formal expansion of Boltzmann equation in power of ϵ. At first order, the Chapman-Enskog expansion assumes that f is as follows

$$f = f_0(1 + \epsilon\phi). \tag{4}$$

By writing the Boltzmann equation at first-order in ϵ yields

$$\frac{1}{\epsilon} Q(f_0, f_0) = 0. \tag{5}$$

The distribution f_0 is therefore a collision invariant, that is a Maxwellian

$$f_0(x, v, t) = n\omega_\epsilon(u(x, t)). \tag{6}$$

Plugging this value of f_0 into the Boltzmann equation yields

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f_0, f_0\phi) + Q(f_0\phi, f_0) + \mathcal{O}(\epsilon), \tag{7}$$

and introducing the linear operator $L\phi = Q(f_0, f_0\phi) + Q(f_0\phi, f_0)$, yields

$$L\phi = \frac{\partial f_0}{\partial t} + v\nabla_x f_0 = \frac{df_0}{dt} + \mathcal{O}(\epsilon), \tag{8}$$

that is (assuming L to be invertible)

$$\phi = L^{-1}(\frac{df_0}{dt} + \mathcal{O}(\epsilon)). \tag{9}$$

The dependence of f_0 in x is obtained by solving the conservation laws, that follows from the Boltzmann equation multiplied by $U = (1, v, |v|^2)$ and integrated in the velocity domain. This integration cancels the collision terms (since mass, momentum and energy are conserved during collision) and yields

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^3} f_0(1 + \epsilon\phi) U dv + \nabla_x \int_{\mathbb{R}^3} v f_0(1 + \epsilon\phi) U dv = 0. \tag{10}$$

Up to now, all equations are exact. Three simplifications are then made in the explicit calculation of ϕ. In particular

i) The left hand side term in Eq. (9) is computed at first order by writing the conservation laws (10) at order 0 in ϵ.

ii) The correction term ϕ is normalized by means of the condition

$$\int f_0 \phi \begin{bmatrix} 1 \\ v \\ \frac{1}{2}m(v-u)^2 \end{bmatrix} dv = 0. \tag{11}$$

In other words, the parameters ρ, u and T of the Maxwellian f_0 correspond to the fluid macroscopic density, velocity and temperature.

iii) The perturbation equation

$$L\phi = \frac{df_0}{dt} + O(\epsilon) \tag{12}$$

is only solved within the subspace generated by the first Laguerre-Sonine polynomials.

With these assumptions, the approximate solution of the Boltzmann equation (written at first order level) becomes

$$\begin{aligned} f \simeq f_{CE} &= \frac{n}{(2\pi r\theta)^{\frac{3}{2}}}\exp(-\frac{|c|^2}{2})[1 - \frac{2}{5}\frac{\lambda}{\rho(r\theta)^2}(\frac{|c|^2}{2r\theta} - \frac{5}{2})c\cdot\nabla\theta - \frac{\mu}{\rho(r\theta)^2}(c\otimes c - \frac{1}{3}c^2 Id) : \nabla u] \\ &= \frac{n}{(2\pi r\theta)^{\frac{3}{2}}}\exp(-\frac{|c|^2}{2})[1 + \frac{2}{5}\frac{\mathcal{T}\cdot c}{\rho(r\theta)^2}(\frac{c^2}{2r\theta} - \frac{5}{2}) - \frac{1}{2}\frac{\Lambda : c\otimes c}{\rho(r\theta)^2}], \end{aligned} \tag{13}$$

where

$$\Lambda = -\int m f_0 \epsilon\phi c\otimes c dc = \mu[\nabla u + \nabla\theta - \nabla u Id], \tag{14}$$

$$\mathcal{T} = \int f_0 \epsilon\phi mc^2 c dc = -\lambda\nabla\theta, \tag{15}$$

$$c = \frac{v-u}{\sqrt{r\theta}}, \tag{16}$$

λ and μ are viscosity coefficients depending of the form on the collision kernel and on the degree of the Sonine plynomials used in the calculation of ϕ, and Id denotes the indentity tensor and $\Lambda : H$ the quantity $Tr(\Lambda H)$.

Plugging this expression of f back in the conservation laws, finally gives the Navier-Stokes equations

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix} + \nabla\cdot\begin{bmatrix} \rho u \\ \rho u\otimes u + pId \\ ((\rho E + p)Id - \Lambda).u + q \end{bmatrix} = 0 \tag{17}$$

The conservation laws Eq. (10) are quite natural from the physical point of view and are justified on the mathematical level. Indeed, by writing the Boltzmann equation for

$$f = f_{CE} + \epsilon^2 f_2 = f_0(1+\epsilon\phi) + \epsilon^2 f_2, \tag{18}$$

one gets, at order 2 in ϵ

$$\begin{aligned}\frac{df_{CE}}{dt} &= Q(f_0, f_0\phi + \epsilon f_2) + Q(f_0\phi + \epsilon f_2, f_0) + \epsilon Q(f_0\phi, f_0\phi) \\ &= L(\phi + \epsilon\frac{f_2}{f_0}) + \epsilon Q(f_0\phi, f_0\phi). \end{aligned} \tag{19}$$

This equation has a solution of the type $\phi + \epsilon\dfrac{f_2}{f_0}$ if and only if the term

$$\frac{df_{CE}}{dt} - \epsilon Q(f_0\phi, f_0\phi) \tag{20}$$

belongs to the image of L, i.e.

$$\langle \frac{df_{CE}}{dt} - \epsilon Q(f_0\phi, f_0\phi), \psi \rangle = 0, \quad \forall \psi \in (\mathrm{Im}L)^\top, \tag{21}$$

with $(\mathrm{Im}L)^\top$ of the form

$$(\mathrm{Im}L)^\top = \left\{ \psi, \quad \psi = \alpha + \beta v + \gamma \frac{1}{2}|v|^2 \right\} \tag{22}$$

Because of the invariance properties of the collision operator Q, this solvability condition reduces exactly to the conservation laws (10).

2.2 Coupling

Consider the flow of rarefied gas in a global domain Ω around a solid body of boundary Γ_w. This domain is splitt into two (possibly overlapped) subdomains Ω_e and Ω_b. The domain Ω_b will be used for the Boltzmann equations. This is a local domain which contains the obstacle, with internal boundary Γ_w and external boundary $\Gamma_b \subset \bar{\Omega}_e$. The domain Ω_e will be used for the Euler or Navier-Stokes equations. This is a large domain, with an internal boundary $\Gamma_{int} \subset \bar{\Omega}_b$, which surrounds the body and an external boundary Γ_{ext} which is the external boundary of the computational domain Ω. Depending of the gas density, either the Boltzmann domain Ω_b or the fluid domain Ω_e can be suppressed.

We shall now describe a numerical method for the simultaneous solution of the Navier-Stokes and Boltzmann equations when these equations are used together but on two different domains. For this purpose, we first introduce compatibility conditions to be imposed at the interfaces, and we then propose an algorithm for the numerical solution of the resulting coupled problem.

In a first case where $\Gamma_{int} = \Gamma_w$ ($\Omega_b \subset \Omega_e$: full overlapping), we must specify boundary conditions for the Navier-Stokes equations on the wall Γ_w. These boundary conditions cannot be obtained from the asymptotic model since the latter is based on the Chapman-Enskog model which is not valid in the kinetic layer. These are obtained by considering boundary fluxes calculated using their discrete kinetic definition

$$\begin{cases} \sigma_B \cdot \nu = \frac{m}{d\Gamma K\Delta t} \sum_{i\in I}(v_i^+ - v_i^-) \\ q_B \cdot \nu = -\frac{m}{2d\Gamma K\Delta t} \sum_{i\in I}(|v_i^+|^2 - |v_i^-|^2), \end{cases} \tag{23}$$

which correspond, respectively to momentum and energy fluxes. Here, I denotes the set of particles which collide with the subset $d\Gamma$ of the wall during the time $K\Delta t$, and v_i^- (respectively v_i^+) denotes the pre-(respectively post-) collision velocity of the individual particle i of mass m.

In the second case where $\Gamma_{int} \neq \Gamma_w$ the compatibility conditions are simpler to obtain and are based on the above kinetic derivation of the Navier-Stokes equations. Therefore, on each domain,

we only need to impose as boundary conditions the kinetic distribution of the incoming particles. For the fluid domain, this ditribution is taken to be equal to the distribution f_B of particles leaving the Boltzmann domain at the same point. Similarly, for the Boltzmann domain, the distribution of incoming particles is taken to be equal to the distribution of particles f_{CE} leaving the fluid domain at this point, where f_{CE} is computed from the Navier-Stokes macroscopic quantities, by the relation (13). Thus, in the Boltzmann domain Ω_b, the Boltzmann equation (1) is solved with the boundary conditions (2) at the wall and

$$f(x,v,t) = f_{CE}(x,v,t), \ \ \forall v \cdot \nu_B < 0, \tag{24}$$

on the Navier-Stokes interface Γ_b. In the fluid domain Ω_e, the Navier-Stokes equations (17) are solved. In these equations, the kinetic boundary condition $f_{CE}(x,v,t) = f_B(x,v,t), \ \ \forall v \cdot \nu_E < 0$ cannot be imposed pointwise and must therefore be integrated in v, yielding the Neumann type of boundary condition

$$\begin{aligned} \begin{bmatrix} \rho u \\ \rho u \otimes u + pId - \Lambda \\ ((\rho E + p)u + q - \Lambda : \nabla_u \end{bmatrix} \nu &= F^+ + F^- \\ &= \int_{v\cdot\nu\geq 0} (v\cdot\nu) \begin{bmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{bmatrix} f_{CE} + \int_{v\cdot\nu\leq 0} (v\cdot\nu) \begin{bmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{bmatrix} f_B. \end{aligned} \tag{25}$$

The coupling algorithm is the transmission time marching algorithm introduced and studied by the author in [73]. It successively solves the Boltzmann equations on the Boltzmann domain with imposed boundary conditions deduced from the previous solution, and the Navier-Stokes equations on the fluid domain with imposed boundary conditions deduced from the Boltzmann solution.

For $n \geq 0$, and knowing estimates $(\rho^n, \rho u^n, E^n)$ and f_B^n of the Navier-Stokes and Boltzmann solutions on Ω_e and Ω_b, new estimates f_B^{n+1} and $(\rho^{n+1}, \rho u^{n+1}, E^{n+1})$ are therefore computed by:

i) solving the Boltzmann equation (1) on Ω_b with initial condition $f(.,0) = f_B^n$ and boundary conditions (2). At the end of this step, we obtain an improved estimate f_B^{n+1} of the Boltzmann solution on Ω_e and an updated value

$$(F^{n+1})^- = \int_{v\cdot\nu\leq 0} (v\cdot\nu) \begin{bmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{bmatrix} f_B^{n+1}(x,v,\epsilon) dv \tag{26}$$

of the half-flux entering Ω_e through Γ_{int};

ii) solving The Navier-Stokes equations (17) on Ω_e with boundary conditions (25), where the value of the half-flux entering Ω_e through Γ_{int} is replaced by the value $(F^{n+1})^-$ computed in Eq. (26) if $\Gamma_{int} \neq \Gamma_w$, and boundary conditions (23) if $\Gamma_{int} = \Gamma_w$.

In the sequel the coupling with $\Gamma_{int} = \Gamma_w$ will be refereed to as the coupling (α) and the coupling with $\Gamma_{int} \neq \Gamma_w$ will be refereed to as the coupling (β).

2.3 Discretization

For the Boltzmann domain the discretization method is based on splitting the physical processes into a free transport phase and a collision phase. This splitting converges, as the time step tends to zero [22] to the DiPerna-Lions [23, 24] renormalized solution of the Boltzmann equation. The collision phase is solved by so-called random particle methods which are more closely related to

the Boltzmann equation [4]-[6],[46]-[48]. The analysis of convergence of the particle method can be found in [4]-[6],[66]. For the fluid domain three methods have been used: the hybrid finite element/finite volume methods [68, 79], the streamline upwind Petrov-Galerkin methods [44, 69] and the hybrid upwind splitting [19]. The coupled approach introduced new boundary conditions and geometry and their treatment constitutes an important step in the discretization process [73, 12].

2.4 Comments

Compared with the coupling strategy (β) which uses very little overlapping between the kinetic and hydrodynamic region, the coupling (α) is:

-simpler because the Navier-Stokes equations are used in the whole physical domain,

-less sensitive to the choice of the interface Γ_{int}, which makes it more robust at dense regimes especially in the case where the direct Boltzmann simulation is not possible because it requires one computational cell per mean free path.

-but restricted to rather dense situations (case **(a)** of Section 1) because it integrates the hydrodynamic model up to the wall.

-gives, without changing the global Navier-Stokes solver, an easy way of supplementing and testing a large variety of kinetic boundary conditions. These kinetic boundary conditions are first imposed on the Boltzmann model, and the resulting fluxes σ_B and q_B are then plugged in the Navier-Stokes equations. They correspond to the losses in tangential momentum and energy of particles colliding into the wall [76].

By contrast, the coupled approach (β) is used mainly for rarefied regimes, and faces difficulties for denser cases.

Therefore, the solution procedure described herein provides a fundamental contribution to the solution of the problem of intermediate regimes **(iv)**, the problem of boundary conditions for hydrodynamic limits **(iii)** and to some extent the problem **(v)**. Moreover, this solution procedure has been successfully developed not only for a simple gas, but also for particles with internal degrees of freedom. In particular, the coupling strategy allowed the treatment of experimental situations in the intermediate regimes. The results obtained are compatibles with available experimental results [51]-[52],[12]. Hence, they provide a major contribution to the solution of transitional regimes. More details about the different aspects of the solution procedure presented here, including its mathematical, numerical and physical validity, can be found in the series of papers by the author [73]-[88],[51]-[56],[11]-[12].

Although the solution procedure described above is very flexible, the author is currently investigating the possibility of making it even more flexible. For instance the determination of a suitable simple criterion in order to choose an optimal Boltzmann domain. Also, certain difficulties met in the study of these methods need to be removed. For instance, if we compare the CPU time of the coupling approach and the asymptotic model (in the range of its validity: $K_n \leq 10^{-4}$), the coupling strategy requires more than twice the CPU time of a direct asymptotic model simulation. However, the latter (within its range of validity:$K_n \leq 10^{-4}$) fails for more complex physical situations, while the coupled strategy works well. Also the Navier-Stokes calculations performed within the coupling approach required robust solvers and adequate meshes. This led the author to pursue further investigation of the solution procedure. For instance, the developement of new coupling models is considered. This has to be done in connection with the problem **(v)**. In the solution procedures developed above one has to deal with a singular perturbed problem, where the small parameter is the mean free path. In [7, 8], the different incompressible limits of the Boltzmann equations are obtained using a very interesting scaling of both the initial data and the equation. The small

parameter they use is the ratio between the Mach number and the Reynolds number. It would be interesting to develop the coupling techniques according to different scaling. Finally, there is no theoretical estimate of the number of time steps within each model calculation for each coupling iteration. This motivates further mathematical development related to these coupling methods. Some of these constitute part of the proposed research as documented in the next sections.

3 Development of new coupling models

The objective here is to develop new coupling models. From the previous section it is clear that the most difficult part to solve in the intermediate regime corresponds to case (a) of Section 1. The direct Boltzmann simulation becomes impossible near the limit range of validity of the direct asymptotic approach. The solution procedure described above provides an efficient solution to this problem, but, becomes expensive in the limit range of validity of the direct asymptotic approach. The objective is then to find a model that would replace the Boltzmann equation. This model should retain the pertinent physical properties of the gas while having simpler mathematical form. The BGK model introduced by Bhatnager, Gross and Krook [10] satisfies these requirements. Hence, this is the model that will be considered here. The main difficulty in handling the Boltzmann equations arises from the complicated nature of the collision terms. The BGK model consists precisely in replacing the collision integrals by mathematically simpler terms; these however, are chosen so as to conform to the conservation laws for mass, momentum, and energy and at the same time to represent certain essential features of collisions. It corresponds to the following set of equations

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{P}{\mu}(f_0 - f). \tag{27}$$

where P is the pressure, μ is the Navier-Stokes viscosity and

$$f_0 = \frac{\rho}{(2\pi RT)^{3/2}} \exp(-\frac{|v-u|^2}{2RT})$$

is the local Maxwellian. The macroscopic quantities are related to f through the moments:

$$\rho(x,t) = < f >, \quad u(x,t) = \frac{1}{\rho} < vf >, \quad RT = \frac{1}{3\rho(x,t)} < |c|^2 f >,$$
$$c = v - u, \quad < f >= \int_{\mathbb{R}^3} f(x,t,v)dv.$$

The appearance of the local Maxwellian f_0 means that the equation remains a nonlinear integro-differential equation. The existence of a solution to this nonlinear equation has been established by Perthame[62]. This approach makes possible a survey of the whole range from low density to high density, including the intermediate regime. Moreover, it satisfies the correct microscopic boundary conditions. This is fundamental for the objective of the actual proposed research. The model leads also to the correct asymptotic behavior in the two limiting cases: $K_n \to 0$ and $K_n \to \infty$. Moreover, this method is capable of considerable extension and generalization to include physically complex problems.

This model has the advantage of describing the right fluid limit. However, the transport coefficients obtained at the Navier-Stokes level through Chapman-Enskog expansion are not satisfactory. For instance the Prandtl number $Pr = \frac{\gamma}{\gamma-1}\frac{R\mu}{\kappa}$ relating the viscosity ν to the heat conduction κ

is equal to 1. For most gases $Pr < 1$. Using Boltzmann equation the hard-sphere model for a monoatomic gas yields a Prandtl number = 2/3. Several modification to the BGK model have been proposed [13, 16]. These however do not satisfy simultaneously the requirements of yielding a nonegative distributions, predicting a Prandtl number less than 1, and satisfying the celebrated Boltzmann theorem: $\int Q(f)\ln f dv \leq 0$. A model satisfying the first two requirements was proposed by Holway [31]. The third requirement was proved to be true for the Holway model, also known as the Gaussian or ellipsoidal (ES-BGK) model, only very recently [1]. The Gaussian BGK model corresponds to

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{P}{\mu(1-\nu)}(\tilde{f}_0 - f). \tag{28}$$

where

$$\tilde{f}_0 = \frac{\rho}{\sqrt{\det(2\pi\Lambda)}}\exp(-\frac{1}{2}(v-u)\cdot\Lambda^{-1}\cdot(v-u)),$$
$$\Lambda = (1-\nu)RT\mathrm{Id} + \nu\Theta,$$
$$T = \frac{1}{3R}\mathrm{tr}\Theta, \quad \Theta = \frac{1}{\rho} < c\otimes cf >,$$

and the parameter $-\frac{1}{2} \leq \nu < 1$ is introduced to give the right Prandtl number through the formula: $\frac{2}{3} \leq Pr = \frac{1}{1-\nu} \leq +\infty$.

The new proposed coupling model is therefore to use the Gaussian BGK (ES-BGK) model in place of the Boltzmann model in the coupling strategy introduced in the previous sections. Since the Chapman-Enskog method may be applied to the ES-BGK model, the compatibility conditions and the coupling (α) and (β) for the Gaussian BGK are derived in a similar fashion as in Section 2. The study of the resulting algorithms includes the analysis of the coupling algorithms, and the numerical study of the solution procedures.

3.1 Numerical studies of the coupling (α) and (β) for the Gaussian BGK

A first step in the numerical study of our strategies for the Gaussian BGK model consists in validating this model by performing comparison tests with experiments and against the results obtained using the Boltzmann model. To do this, we first used a variant of the Direct Simulation Monte Carlo method, which we have already developed and studied for the full Boltzmann model [12]. We have also studied the Gaussian BGK model for polyatomic gases. The detail of this study is given in [88]. As an illustration of this we present the numerical results for the following test cases. The first case corresponds to a computation of a flow around an ellipse for a semi-rarefied gas with the following data

Monoatomic case with $R = 287$
Mean free path $\lambda_\infty = 8.310^{-4}$
Characteristic length $L = 0.1m$, which yields $Kn_\infty = 8.310^{-3}$
$\rho_\infty = 5.1910^{-5}kg/m^3$
$T_\infty = 14.5K$
$V_\infty = 1663m/s$, which yields $\mathrm{Mach}_\infty = 20$
At the wall $T_w = 290K$ and we use total accomodation

Viscosity law: $\mu = \mu_\infty(\frac{T}{T_\infty})^\omega$ with $\omega = 0.657$ and $\mu_\infty = 0.24910^{-5}Pa.s$. At the wall $\mu_w = 0.17810^{-4}Pa.s$. This yields $Re_\infty = 3469$ and $Re_w = 484$.
Computational domain: $0.12m \times 0.08m$.
Rectangular mesh: $h_x = 10^{-3}m$, $h_y = 2.510^{-4}m$
Time step: $\Delta t = 0.20410^{-6}s$
Number of particles in a cell at infinity: 25

The numerical results for this case are presented in Figures 1-5. The second test case corresponds to a flow around an ellipse in the transitional regime case. This corresponds to

Mean free path $\lambda_\infty = 1.010^{-4}$
Characteristic length $L = 0.1m$, which yields $Kn_\infty = 1.010^{-3}$.
Computational domain: $0.12m \times 0.08m$.
Rectangular mesh: $h_x = 8.010^{-4}m$, $h_y = 2.010^{-4}m$
Time step: $\Delta t = 0.1610^{-6}s$

The remaining data are the same as in the first test case. The numerical results for this case are presented in Figures 6-10. The third test case corresponds to a flow around an ellipse in the transitional regime case for a polyatomic gas. The data are the same as in the second test case. The numerical results are shown in Figures 11-15.

These results together with our study [88] show that in the transitional regime the Gaussian BGK model gives results that are in good agreements with those given by the Boltzmann model. This clearly justifies the study of our coupling strategies in which the Boltzmann model is replaced by the Gaussian BGK model. We are currently performing a numerical study of our coupling (α) and (β) for the Gaussian BGK model. In these coupling, we are using DSMC method for the discretisation of the Gaussian BGK, while for the Navier Stokes computation we are using the same numerical methods used already for the discretisation of the Navier-Stokes equations in the coupling (α) and (β) for Boltzmann model described in section 2.3. We are considering several test cases where experimental data are available. We shall also apply our methods to experimental situations where the direct and classical methods are not feasible. This will show the fundamental importance and contribution of our strategies.

In order to simplify further the numerical procedure and cut down the cost in terms of computer time and memory, we are investigating deterministic approaches for the Gaussian BGK. The polyatomic Gaussian BGK model was obtained using an internal energy parameter I which takes into account the degrees of freedom in a general way just like the Boltzmann case [12] (and the references therein). Numerically this is expensive. For BGK models, the introduction of an internal energy variable is not necessary. In fact all macroscopic variables can be equivalently obtained by a simpler procedure. It consists of introducing two density distributions, one for mass and one for internal energy. We obtain a BGK system governing the evolution of the two distributions [88] (and the references therein). We shall perform a thorough numerical study for this new BGK system. We shall first extend the Direct Simulation Monte Carlo (DSMC) method mentioned above (for the case of polyatomic gase using an internal energy variable). We shall then compare the results to a DSMC computation for the (polyatomic) Gaussian BGK using an internal energy variable. We shall also extend the deterministic approach we are intending to develop for the monoatomic Gaussian BGK model to the polyatomic case. Another numerical investigation that we are planning to accomplish is the numerical study of the Gaussian BGK for mixtures.

3.2 Theoretical study of the methodologies (α) and (β)

To establish the mathematical foundations of the proposed models (α) and (β), we shall look, in particular, at the following topics:
(i) Hydrodynamic limits and the rigorous derivation of the models (α) and (β).
(ii) Existence, stability, regularity, and positivity of the solutions of the models (α) and (β).
(iii) Asymptotic analysis and trend to equilibrium for the models (α) and (β).
(iv) Convergence analysis of the approximations of the models (α) and (β) by the transmission time marching algorithm and error estimates.

We shall present below our recent accomplishments together with our future plans concerning each of the above points **(i)**-**(iv)**.

(i): The hydrodynamical limit is of fundamental importance; it is at the heart of the development of our models. The foundations of the hydrodynamic limit has been established by Hilbert for kinetic models of rarefied gases in his famous paper [35]. This method has been later improved by Chapman [17] and Enskog [26] to account for dissipative terms. A mathematical framework has been provided by Grad [29]. Most of the existing results in this direction are obtained for simple models and periodic or full space problems. In our case, we want to solve problems in general domains and with general boundary conditions. The first simplified Boltzmann model we studied is a Carleman model. For this model we proved the global convergence of Chapman-Enskog on a bounded domain [80]. This is the first result of hydrodynamic limit on bounded domain. Using this result we have been able to derive rigorously the coupling (α) and (β) for the Carleman model. We have proved similar results for the linearized Boltzmann model [81]. In a very recent work we have performed a rigorous derivation of the coupling (α) and (β) for a (nonlinear) BGK type model [87]. We expect these results to have an impact in other areas of applied analysis.

(ii): In general the existence theory is established for (a system of) partial (or integro-partial) differential equations given in the same domain. Our models (α) and (β) consist of kinetic equations and their hydrodynamic limits used on their respective domains of validity and coupled through their boundary conditions. We thus have new set of integro-differential equations with new types of boundary conditions. As far as we know no such types of problems appeared in the litterature before (by other authors). To see what difficulties we must face to handle the mathematical theory of these novel models, assume for example, that we apply a fixed point iterative method to uncouple the models. Then we observe that we must deal with the kinetic equations (resp. the hydrodynamic equations) in bounded domains with new types of boundary conditions. To prove the existence of a fixed point, we need to derive appropriate estimates (particularly at the interfaces and boundaries). It is not straightforward to combine the kinetic theory with the hydrodynamic theory to obtain such estimates. The Sobolev spaces used in these two theories, for instance, can be (and are indeed) very different. "Similar" difficulties arise when dealing with the regularity, positivity, and asymptotic behaviour of the solutions to these novel models. Therefore, it is clear that new methods and ideas have to be introduced and developed in order to study these models. Such methods have been introduced by the author in [77, 78, 82, 85, 80, 81]. Using these methods, the author was able to establish the existence theory for the models (α) and (β) for the case of Carleman model, linearized Boltzmann model, and a nonlinear BGK type model [80, 81, 87]. We are currently working on the extension of these results to more general models.

(iii): The asymptotic analysis and trend to equilibrium for microscopic models is in general very difficult topic. There are only very few results for realistic models. For the models (α) and (β), the situation is even more difficult since here we are dealing with coupled problems of two different nature: one is microscopic and the other is macroscopic. In [77, 78, 82, 85, 80, 81] we have introduced and developed a general method that led to the asymptotic analysis and trend

to equilibrium for coupled microscopic-microscopic models and for the models (α) and (β) for Carleman model and a linearized Boltzmann model. This method also allows the obtention of the rate of decay. We shall use these ideas to obtain further results on the asymptotic and trend to equilibrium models (α) and (β) for a (nonlinear) BGK type model.

(iv): This part is even more difficult since to obtain any analysis of the approximations of the models (α) and (β) by the transmission time marching algorithm, we need to know detailed information regarding Parts **(ii)** and **(iii)** (the continuous problems). Again the methods introduced and developed by the author [77, 78, 85, 82, 86, 80, 81] were shown to play central roles in the development of the mathematical foundations of the approximations of the models (α) and (β) by the transmission time marching algorithm. This theory is obtained for the case of Carleman and linearized Boltzmann models [78, 86, 80, 81]. Further developments are underway.

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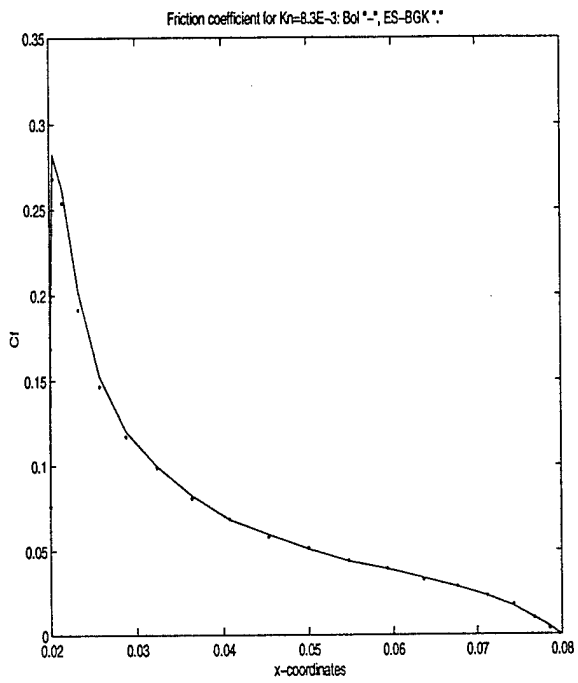

Figure 1: Skin Friction coefficient for $Kn = 8.310^{-3}$

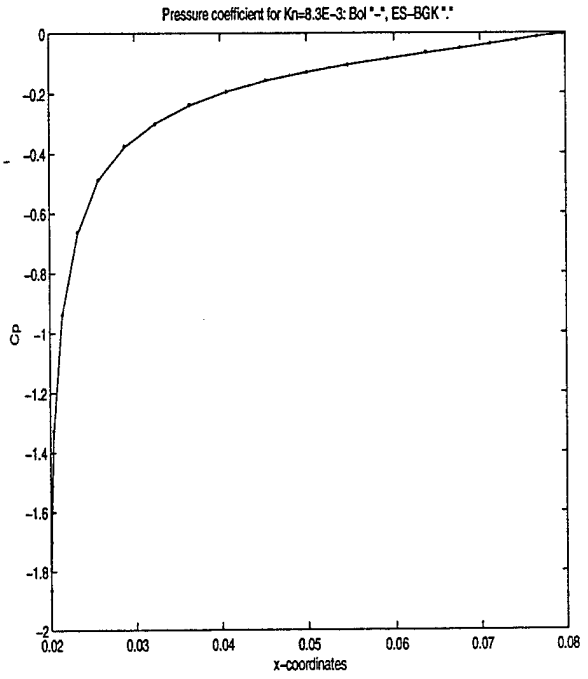

Figure 3: Pressure coefficient for $Kn = 8.310^{-3}$

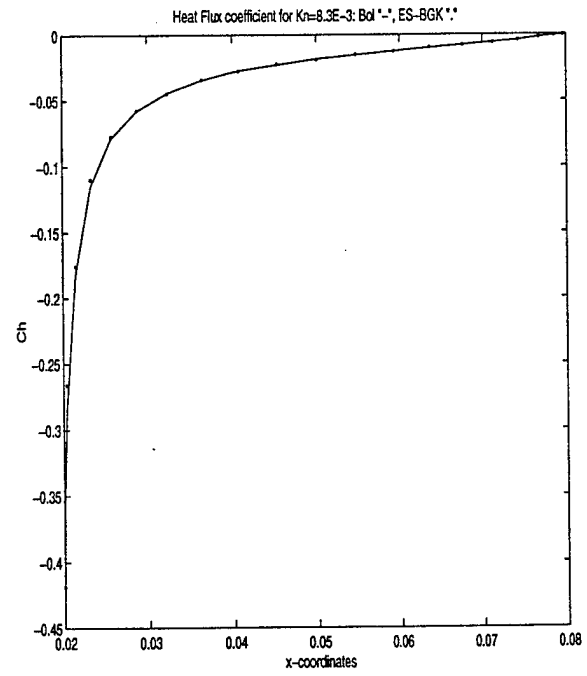

Figure 2: Heat Flux coefficient for $Kn = 8.310^{-3}$

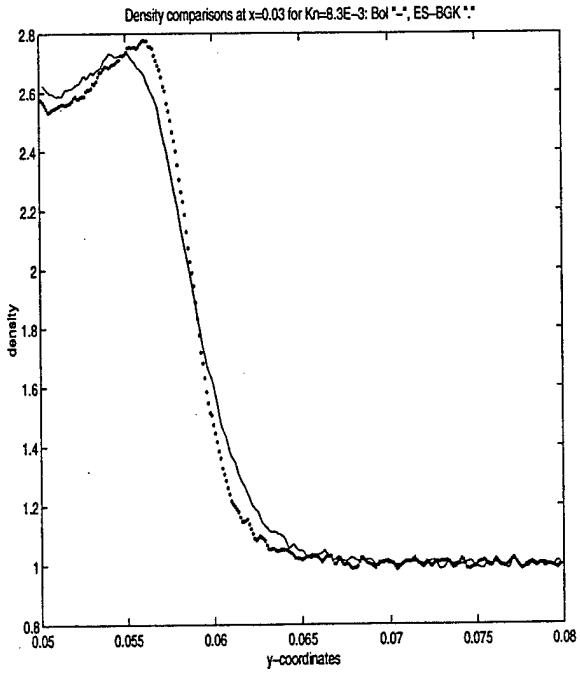

Figure 4: Density Cross Section for $Kn = 8.310^{-3}$

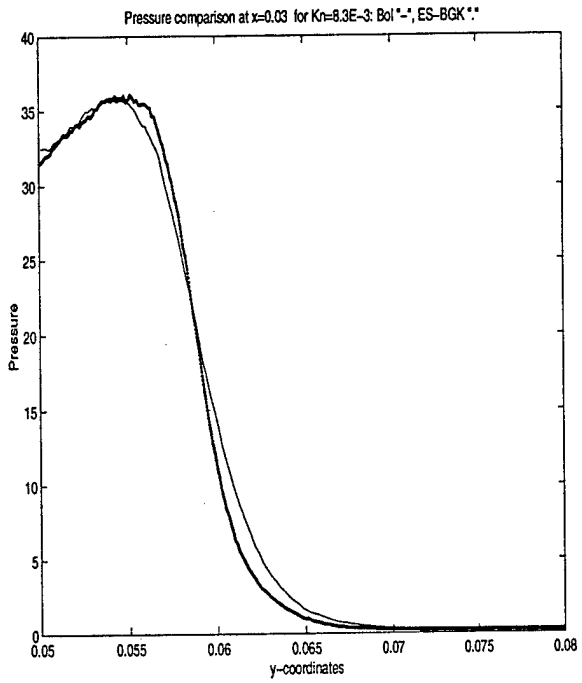

Figure 5: Pressure Cross Section for $Kn = 8.310^{-3}$

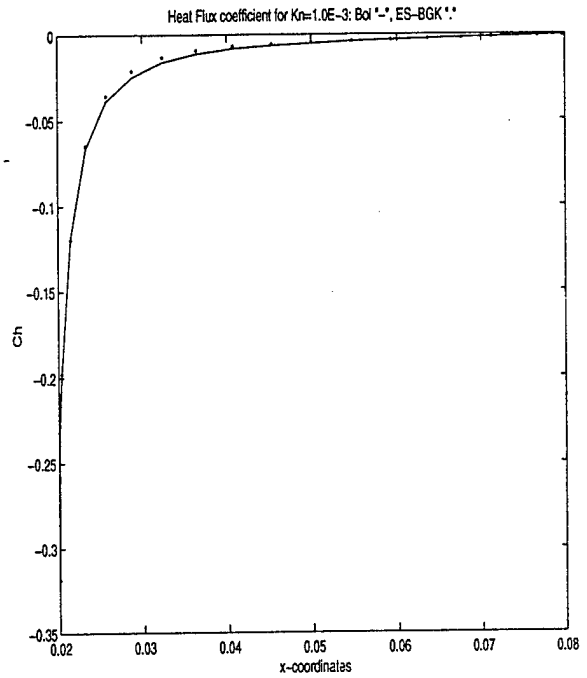

Figure 7: Heat Flux coefficient for $Kn = 1.010^{-3}$

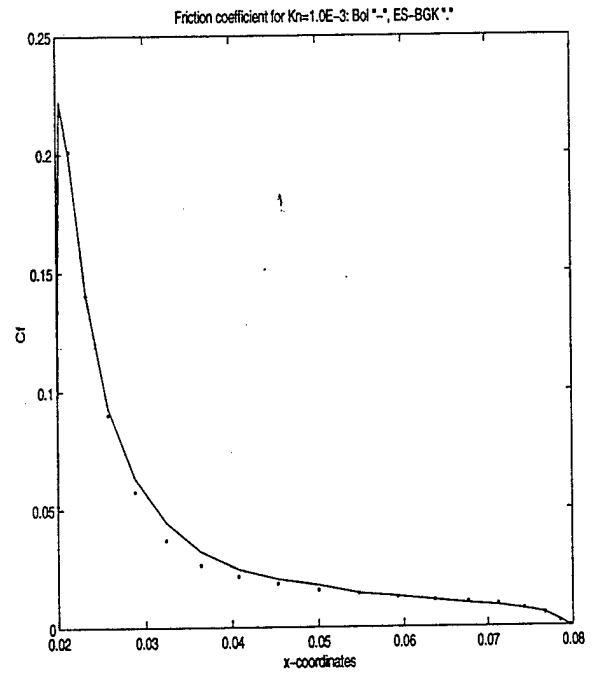

Figure 6: Skin Friction coefficient for $Kn = 1.010^{-3}$

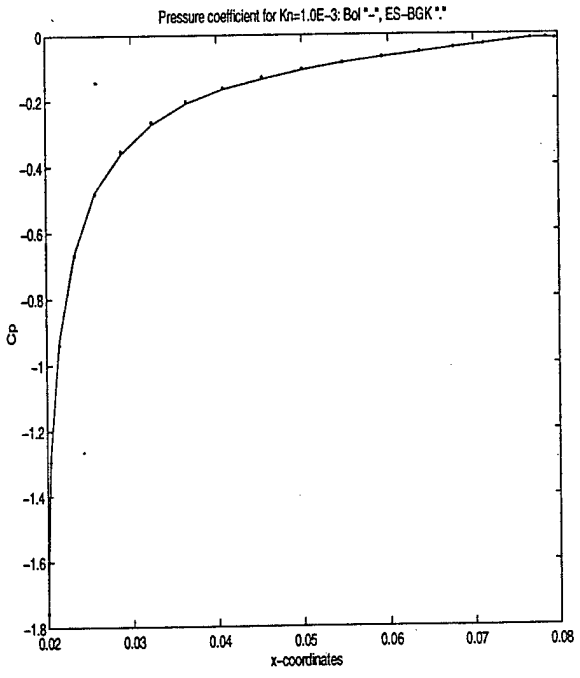

Figure 8: Pressure coefficient for $Kn = 1.010^{-3}$

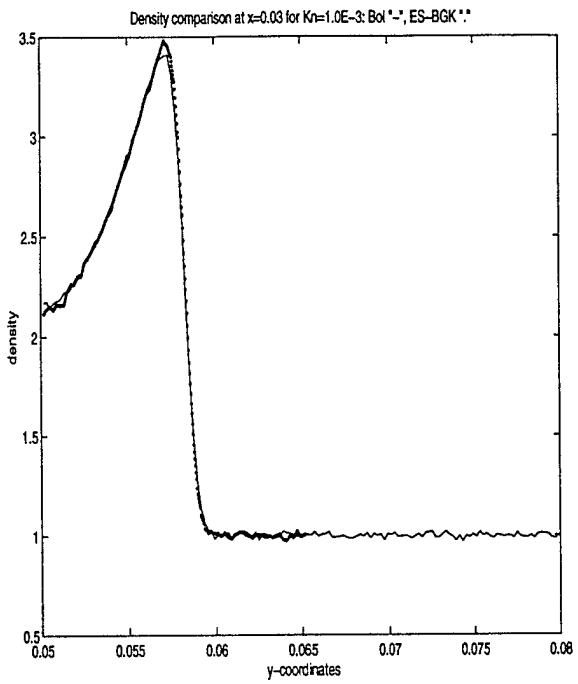

Figure 9: Density Cross Section for $Kn = 1.010^{-3}$

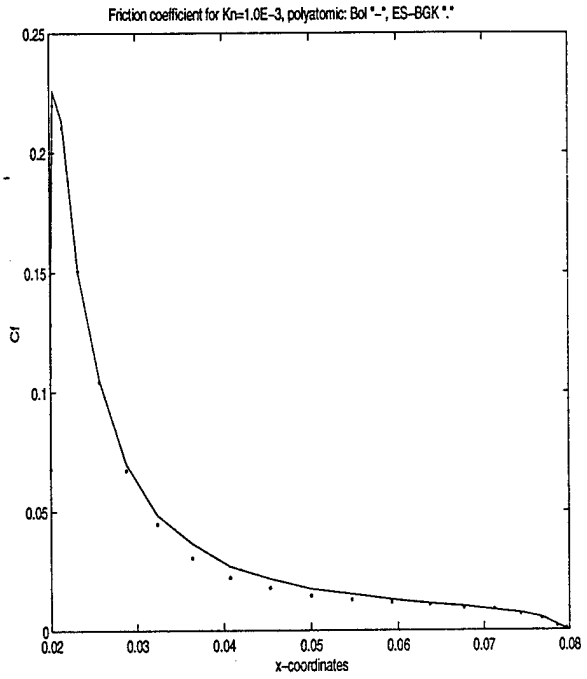

Figure 11: Skin Friction coefficient for $Kn = 1.010^{-3}$

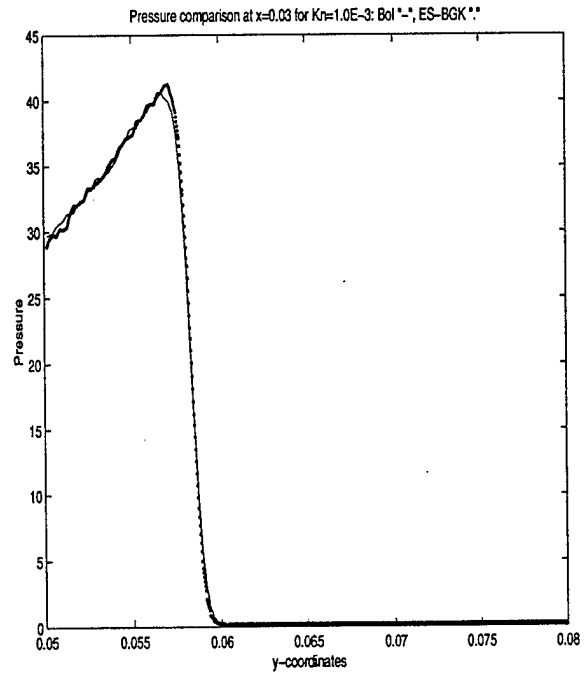

Figure 10: Pressure Cross Section for $Kn = 1.010^{-3}$

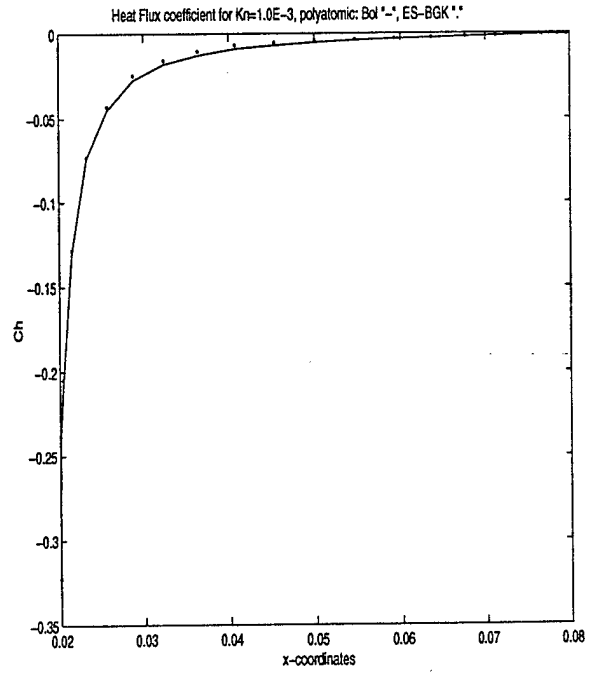

Figure 12: Heat Flux coefficient for $Kn = 1.010^{-3}$

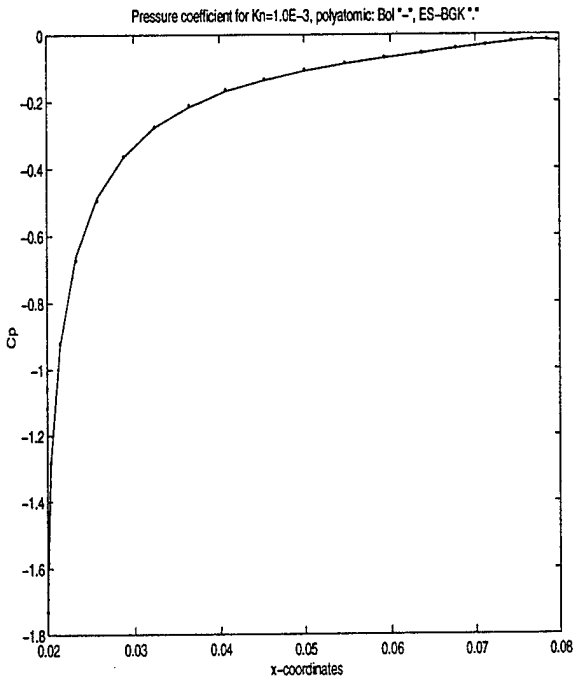

Figure 13: Pressure coefficient for $Kn = 1.010^{-3}$

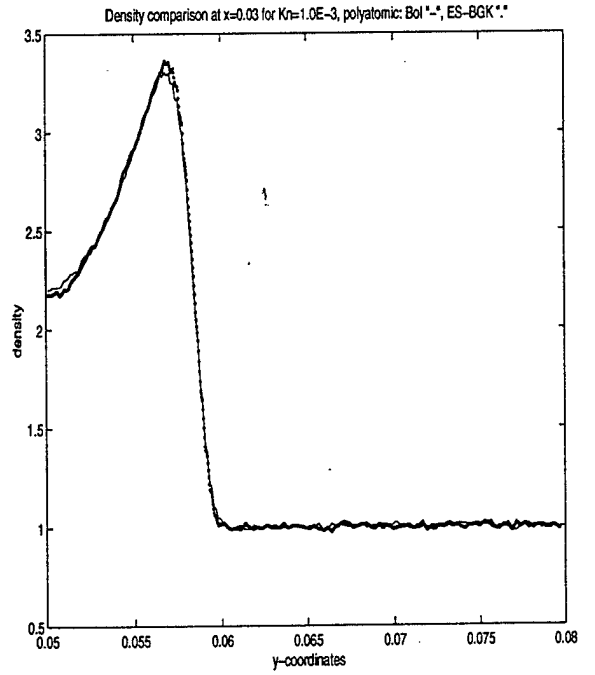

Figure 14: Density Cross Section for $Kn = 1.010^{-3}$

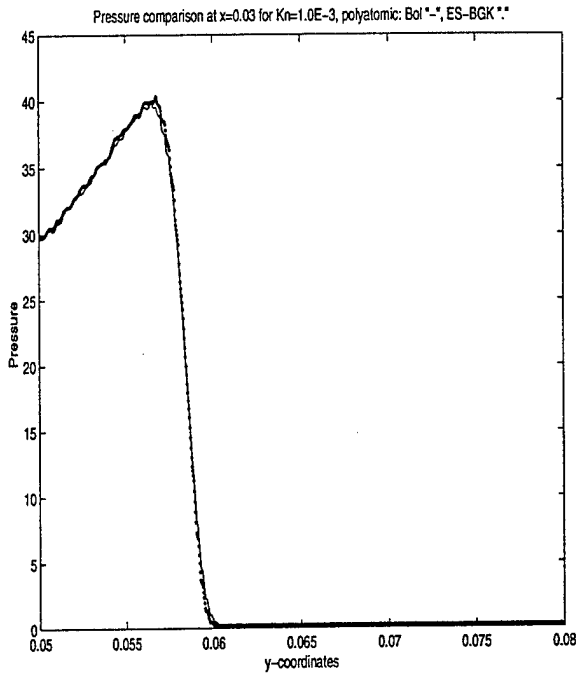

Figure 15: Pressure Cross Section for $Kn = 1.010^{-3}$