TRANSITION FROM KINETIC THEORY TO MACROSCOPIC FLUID EQUATIONS: A PROBLEM FOR DOMAIN DECOMPOSITION AND A SOURCE FOR NEW ALGORITHMS

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ABSTRACT

In the paper we discuss the transition from kinetic theory to macroscopic fluid equations, where the macroscopic equations are defined as asymptotic limits of a kinetic equation. This relation can be used to derive computationally efficient domain decomposition schemes for the simulation of rarefied gas flows close to the continuum limit. Moreover, we present some basic ideas for the derivation of kinetic induced numerical schemes for macroscopic equations, namely kinetic schemes for general conservation laws as well as Lattice–Boltzmann methods for the incompressible Navier–Stokes equations.

1 Introduction

In the kinetic theory of gases one works with a time–dependent density function $f(t,x,v)$ on the phase space $\Omega \times I\!R^3$ to describe non–equilibrium effects, where $x \in \Omega$ denotes the space variable and $v \in I\!R^3$ the individual velocity of a gas particle. This density function evolves according to a kinetic transport equation, the Boltzmann equation, given by

$$\frac{\partial f}{\partial t} + \frac{1}{\varepsilon^j} v \nabla f = \frac{1}{\varepsilon^{j+1}} Q(f), \tag{1.1}$$

where the small parameter $\varepsilon \ll 1$ acts as a scaling parameter and $Q(f)$ denotes the collision operator describing binary collisions among the gas. In the limit when $\varepsilon \to 0$, the kinetic function $f(t,x,v)$ tends to a certain local "equilibrium" state and in this case it seems to be sufficient to describe the fluid motion in terms of the macroscopic variables, which are defined as the moments of the kinetic function $f(t,x,v)$,

like the macroscopic density $\rho(t,x)$, which is given by $\rho(t,x) = \int f(t,x,v)\,\mathrm{d}v$.
The resulting macroscopic fluid equations connected with the asymptotic limits of (1.1) are the classical equations from fluid dynamics, like the compressible Euler equations stated in macroscopic variables, namely the density $\rho(t,x)$, the mean flow velocity $u(t,x)$ as well as the temperature $T(t,x)$ (or the corresponding conserved quantities). Another asymptotic limit of (1.1) is given by the incompressible Navier–Stokes equation formulated in terms of the fluid velocity $u(t,x)$ and the pressure $P(t,x)$ as well as an energy equation, typically in the form of the Boussinesq approximation. The two different macroscopic fluid models are obtained from two different scaling limits, here expressed in terms of the integer j in the kinetic equation (1.1).
The so–called **hydrodynamic limit** of (1.1) is obtained taking $j = 0$ and the well–known Hilbert expansion yields formally the compressible Euler equation: with $j = 0$, the parameter ε scales the time between two collisions of a gas particle with the unperturbed free flow according to the particle velocity v. Taking the asymptotic limit $\varepsilon \to 0$ means, that the mean collision time (or the mean free path) in the gas tends to zero, i.e. the gas ensemble will instantaneouslu relax to an local equilibrium state governed by the equation $Q(f) = 0$. Moreover, the dynamic behaviour is completely described by the macroscopic variables ρ, u and T and these variables are solutions of the compressible Euler equations. Formally, the compressible Euler equations are derived applying an asymptotic expansion of the density function $f(t,x,v)$ in the form

$$f(t,x,v) = \sum_{n=0}^{N} \varepsilon^n f_n(t,x,v)$$

and substituting the expansion into the scaled Boltzmann equation (1.1) with $j = 0$. Then a solvability condition on the first order term $f_1(t,x,v)$ gives the compressible Euler equations for the moments of the zeroth order approximation $f_0(t,x,v)$.
One may derive the compressible Navier–Stokes from the hydrodynamic scaling applying the so–called Chapman–Enskog expansion or using a two–scale expansion in the time variable t, where the second time scale τ is given by $\tau = \varepsilon t$, i.e. we take into account changes running on a diffusion time scale, see the discussion given below.
Taking $j = 1$ defines the so–called **diffusion limit** and applying an asymptotic expansion of $f(t,x,v)$ in the form

$$f = M[\rho, 0, T]\Big(1 + \varepsilon g\Big)$$

where $M[\rho, 0, T]$ denotes a global Maxwellian with zero velocity and uniform density and temperature, yields the incompressible Navier–Stokes equations. The assumption of a vanishing flow velocity is appropriate in the diffusion limit, because incompressible fluids are low Mach number flows.
If only the asymptotic limits of the kinetic equation, i.e. the macroscopic fluid equations itself, are of interest, one may choose the most simple collision term, which still gives the correct limit, e.g, the BGK collision model: there exists an “equilibrium distribution” $f_{eq}(t,x,v)$ depending on the state variables U, e.g., in the case of the

compressible Euler equation the macroscopic variables ρ, u and T,

$$f_{eq}(t,x,v) = F[U(t,x)](v)$$

and the BGK collision operator reads

$$Q_{BGK}[f](t,x,v) = \frac{1}{\tau}\Big(f_{eq} - f\Big)(t,x,v)$$

There are several possibilities to choose the equilibrium distribution in the BGK model: the most natural choice is to use a local Maxwellian given

$$f_{eq}(t,x,v) = M[\rho,u,T](v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left\{-\frac{\|v-u\|^2}{2T}\right\}$$

because the local Maxwellian belongs to the kernel of the full collision operator $Q(f)$ and therefore defines the the asymptotic form of the distribution function $f(t,x,v)$ of the full Boltzmann equation in the limit when $\varepsilon \to 0$. From a numerical point a view, it is a special interest to investigate distribution functions with compact support in the velocity space, because then the computation of moments of f_{eq} is reduced to integrals over bounded domains. Kaniel [1] proposed a distribution function of the form

$$f_{eq}(t,x,v) = A[\rho, \|v-u\|] \infty_{[0,c[\rho]]}\Big(\|v-u\|\Big) \tag{1.2}$$

and constructed kinetic schemes for the 2D–isentropic Euler equations on the basis of the equilibrium function (1.2).
Let us consider the scaled BGK model, which is given by

$$\frac{\partial f}{\partial t} + \frac{1}{\varepsilon^j} v \frac{\partial f}{\partial x} = \frac{1}{\varepsilon^{j+1}\tau}\big(f_{eq} - f\big)$$

where, in general, the relaxation time τ depends on the space variable x and the time t, i.e. $\tau = \tau(t,x)$. Now, if $\varepsilon^{j+1}\tau(t,x) \ll 1$, we know from the discussion given above, that we are close to the corresponding macroscopic fluid equation and therefore the kinetic equation may by substituted by the macroscopic one. In particular, we may define a macroscopic region Ω_{macro} as

$$\Omega_{macro}(t) = \{x \, : \, \tau(t,x) \text{ sufficiently small}\}$$

Then, if $\Omega_{macro} \neq \Omega$, we will have to different flow regions: a kinetic region, where the flow is described by a kinetic equation including non–equilibrium effects, and a macroscopic region, where it suffices to describe the flow by its macroscopic variables. Hence, we are concerned with domain decomposition techniques for kinetic and macroscopic fluid equations and hope to find computationally efficient numerical schemes in this transition regime.
Besides domain decomposition techniques, the transition from kinetic to macroscopic fluid equations offers a further interesting aspect: one may use kinetic fluid

models to develop new and efficient numerical schemes for macroscopic fluid equation itself, without having in mind to construct domain decomposition methods. We will discuss two of these schemes in Section 3, namely kinetic schemes for general conservation laws as well as the so–called Lattice–Boltzmann methods to simulate incompressible Navier–Stokes equations. Both schemes are based on the simplified BGK collision model as underlying kinetic transport equation.

2 Domain Decomposition for Kinetic and Macroscopic Fluid Equations

In this section we discuss domain decomposition techniques for kinetic and macroscopic fluid equations in order to build computationally efficient numerical schemes for flows close to the continuum limit. As we saw in the introduction, one may define a macroscopic flow region, if the local relaxation time to a local equilibrium distribution is sufficiently small.

To derive such domain decomposition schemes, we have to answer the following three questions: first of all, we need appropriate detection criteria to detect those regions, where we are able to switch from kinetic to the macroscopic fluid equations. Then we have to discuss, how we may match (or patch) the different fluid models at the interface between the two flow domains. And finally, we should decide which codes are the proper ones to be matched. The first two questions will be discussed in the following two subsections, whereas the last one is postponed to the next section.

2.1 Automatic Detection Criteria

As mentioned in the introduction given above, one may define appropriate macroscopic flow regions as those parts of the computational domain, where the local relaxation time $\tau(t,x)$ is sufficiently small. This condition needs to be transformed into a detection criterion, which is handable from a numerical point of view.

One possibility is to use the fact, that the kinetic distribution function will be close to a local Maxwellian $M[\rho,u,T]$, where the macroscopic variables are computed via the given distribution. Hence, one may use the distance between $f(t,x,v)$ and the local Maxwellian $M[\rho,u,T]$ in terms of a certain norm, like the L^p or the H^{-s} norm: Tiwari and Rjasanow [2] presented some numerical results based on the H^{-2} norm as a criterion of local thermal equilibrium, but it turned out to be computational too expensive. In a subsequent work, Tiwari [3] proposed to use the following norm based on Grads 13–moment method, see also Tiwari and Klar [4]: if the kinetic density $f(t,x,v)$ is close to an equilibrium distribution, we may write

$$f \approx M[\rho,u,T]\Big(1+\Phi\Big),$$

where the perturbation Φ is expressed in terms of the first 13 moments of f, i.e. we have

$$\Phi = a + \langle b, v-u\rangle + \langle C(v-u), v-u\rangle + \langle d, v-u\rangle \|v-u\|^2$$

Now we choose the 13 parameters a, b, C and d such that the 13 moments u, T, q and τ of f are correct. Then, we introduce the norm

$$\|\Phi\| = \left(\int |\Phi|^2 \frac{M}{\rho} \, \mathrm{d}v \right)^{\frac{1}{2}}$$

and use $\|\Phi\|$ to qualify the distance between the kinectic distribution f and its corresponding local Maxwellian $M[\rho, u, T]$. In particular this yields the expression

$$\|\Phi\| = \frac{1}{\rho RT} \left[\frac{2}{5} \frac{\|q\|^2}{RT} + \frac{1}{2} \|\tau\|^2 \right]^{\frac{1}{2}} \tag{2.1}$$

and the macroscopic flow regions Ω_{macro} is defined by

$$\Omega_{macro} = \{x \ : \ \|\Phi\| < \delta\},$$

where δ denotes an appropriate constant. An example showing Boltzmann and Euler domains for the rarefied gas flow around an ellipse is given in Fig. 1. One should notice, that the criterion given in (2.1) is actually a generalization of some previous work by Boyd et al. [5], Kreuzer [6], Liepmann et al. [7] and Meixner [8], because it combines the deviation in terms of the shear stress tensor and the heat flux vector.

2.2 Coupling Conditions at the Interface

After defining the different flow regions for kinetic and macroscopic fluid equations, one needs to determine appropriate coupling conditions at the interface between the two regions. On the kinetic level, we know that the inflow boundary condition $f_+(t, x, v) = f(t, x, v)\Big|_{(v,n)>0}$ defines via the solution of the Boltzmann equation the corresponding outflux $f_((t, x, v)$, i.e.

$$f_-(t, x, v) = Af_+(t, x, v),$$

where A denotes the so–called Albedo operator. Both densities f_- and f_+ together define the macroscopic moments at the interface Γ and therefore the macrocospic moments ρ, u and T,

$$\int\limits_{(v,n)>0} f_+ v^\alpha \, \mathrm{d}v + \int\limits_{(v,n)<0} Af_+ v^\alpha \, \mathrm{d}v = M^\alpha \tag{2.2}$$

Hence, to define appropriate coupling conditions we need approximations for Af_+, which means appropriate approximations for the Albedo operator A.

Now, the idea is the following: in the macroscopic flow regions Ω_{macro} we may assume, that the density function f is close to an equilibrium distribution $M[\rho, u, T]$, therefore we use the Ansatz

$$Af_+ \approx M[\rho, u, T] \tag{2.3}$$

Subsituting (2.3) into (2.2) yields the so–called Marshak conditions given by

$$(2.4) \qquad \int\limits_{(v,n)>0} (v,n) \begin{pmatrix} 1 \\ v \\ \frac{\|v\|^2}{2} \end{pmatrix} f_+ \, \mathrm{d}v + \int\limits_{(v,n)<0} (v,n) \begin{pmatrix} 1 \\ v \\ \frac{\|v\|^2}{2} \end{pmatrix} M \, \mathrm{d}v$$

$$= \text{ Euler fluxes } = \begin{pmatrix} \rho u \\ \rho u \otimes u + pI \\ (\rho e + p)u \end{pmatrix}$$

Eq. (2.4) gives five nonlinear equations for five fluxes at the interface Γ. Arnold and Giering [9] showed, that in one dimension, this system determines exactly as many fluxes as needed for Euler boundary conditions.
Other attempts to derive appropriate coupling conditions where given, e.g., by Klar [10] and Giering [11]: the first author introduced a small kinetic layer at the interface between to the flow regions, where the flow in the layer is described by a linearized Boltzmann equation. Then, the problem to define coupling conditions is reduced to a half space problem for the linearized equation, which can be solved explicitly and therefore yields appropriate coupling conditions at the interface. Giering proposed to approximate the nonlinear Albedo operator using the well–known splitting method for the Boltzmann equation, which is used to separate the collision operator from the free flow part in the Boltzmann equation.

3 Kinetic Induced Schemes for Macroscopic Fluid Equations

In the previous section we discussed domain decomposition techniques for rarefied gas flows close to the continuum regime as one aspect for the transition from kinetic to macroscopic fluid models. In the following two subsections we will concentrate on numerical schemes for macroscopic fluid equations, which are obatined from the underlying kinetic equation.
Kinetic schemes can be formulated for general conservation laws and the main point in this schemes is an appropriate definition of the equilibrium distribution used in the BGK collision model. On the other, the Lattice–Boltzmann method uses the BGK model, but the whole system is discretized in space, in the velocity and the time variable and the relaxation parameter τ is used to relate the numerical solution of the model to the (incompressible) Navier–Stokes equations. Hence, Lattice–Boltzmann schemes are often referred to as “digital physics”.

3.1 Kinetic Schemes for General Conservation Laws

Let us consider a general conservation in the form

$$(3.1) \qquad \frac{\partial U}{\partial t} + \sum_{i=1}^{d} \frac{\partial G_i(U)}{\partial x_i} = 0, \quad U \in I\!R^m$$

Applying a kinetic scheme for (3.1) means to define a m–dimensional equilibrium function $F[U(t,x)](v)$ in combination with a m–dimensional BGK–model, i.e. the kinetic equation

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{d} v_i \frac{\partial f}{\partial x_i} = \frac{1}{\varepsilon}\Big[F[U] - f\Big]$$

In the limit $\varepsilon \to 0$, we obtain – at least formally – the equation $f = F[U]$ and the moments U of the equilibrium function F satisfy the macroscopic equation

$$\frac{\partial}{\partial t}\int F[U]\,\mathrm{d}v + \sum_{i=1}^{d} \frac{\partial}{\partial x_i}\int v_i F[U]\,\mathrm{d}v = 0$$

Hence, a function $F[U]$ is called equilibrium function, if the moment equations (3.2) coincide with given conservation laws (3.1), i.e. if

$$\int F[U]\,\mathrm{d}v = U \tag{3.2}$$

$$\int v_i F[U]\,\mathrm{d}v = G_i(U) \tag{3.3}$$

Now the idea to construct a numerical scheme, i.e. a kinetic scheme, for the conservation laws (3.1) is straightforward: we use the equation $f = F[U]$ with $U = \int f\,\mathrm{d}v$ as constraint for the free transport equation

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{d} v_i \frac{\partial f}{\partial x_i} = 0 \tag{3.4}$$

The numerical realization of a kinetic scheme runs as follows: given a discrete time step Δt, one solves Eq. (3.4) simply using the method of characteristics, which yields the solution

$$f(\Delta, x, v) = f_0(0, x - \Delta v, v),$$

where f_0 defines the initial condition of (3.4) at time $t = 0$. This solution does obviously not fulfill the constraint $fi(\Delta t) = F[U](\Delta t)$. Hence after the time increment Δt, one projects the function $f(\Delta t)$ back to the equilibrium distribution with moments $U(\delta t)$ calculated via $f(\Delta)$.
An geometric interpretation for a kinetic scheme is shown in Fig. 2: solving the free transport equation (3.4) with the constraint $f = F[U]$ means to compute a trajectory which lies in the manifold of distribution functions $f = F[U]$. If we compute the solution of (3.4) over a small time increment Δt, we will in general leave this manifold. Hence we should stop after Δt and perform a projection down to the given equilibrium distribution in order to return back the given constraint on f. One should notice, that kinetic schemes are due to (3.2), (3.3) equivalent to solutions of moment problems, see, e.g., Junk [12].
Kinetic schemes may be used in combination with classical discretization techniques for conservation laws, like finite–differences or finite–volume schemes: one may use the kinetic formulation for the derivation of appropriate numerical flux functions.

But, kinetic schemes may even be realized as pure particle codes, which is in particular useful when combing kinetic schemes with domain decomposition techniques for the full Boltzmann equation: assume, that our computational domain Ω is divided into a macroscopic regions Ω_{macro}, where it suffices to solve the compressible Euler equations, and a kinetic region, where we need to solve the full Boltzmann equation in order to take care for non–equilibrium effects. Moreover, both flow domains are connected through an interface Γ, see Fig. 3. Then we use in both domains a finite number of particles to approximate the kinetic distribution f, where $f = F[U]$ in Ω_{macro}. In a first part of the time evolution, we move all particles with their velocity over a small time increment Δt and resample the resulting particle ensemble to the given cell structure. Then, in each Euler cell we recompute the new macroscopic moments and project the distribution function back to the equilibrium form, whereas in Boltzmann cells, one performs a standard collision process based on the full Boltzmann equation.
This mixed particle code was investigated by Tiwari in [3]. In Tiwari and Klar [4] an adaptive procedure using appropriate grid sizes and time steps has been suggested, a typical grid structure is shown in Fig. 4. It turned out, that one can use very large time steps in the macroscopic flow domain compared to the one in the Boltzmann cells and this yields a computational accerelaration of the complete simulation by a factor between 10 and 15. Moreover, this kind of numerical scheme to realize a domain decomposition does not show any problem at the interface between the kinetic and macroscopic flow regions: the correct information transport at the interface is guaranteed automatically by the particles crossing the interface during the free flow step. Some results showing contour plots of the density and temperature for a flow around an ellipse are given in Fig. 6.

3.2 Lattice–Boltzmann Schemes for the Incompressible Navier–Stokes Equations

The derivation of Lattice–Boltzmann Schemes is again based on the kinetic BGK model, i.e. we consider the transport equation

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \frac{1}{\tau}\big[F - f\big], \tag{3.5}$$

but now we do not perform the asymptotic limit $\tau \to 0$. Instead of this, we introduce some other simplifications for (3.5), namely we use a discretized spatial domain, discretized velocites and time variable, like indicated in Fig. 5. If we denote the discrete velocities by $c_i, i = 1, \ldots, n$, the discrete analogon of (3.5) reads

$$\frac{\partial f_i}{\partial t} + c_i\frac{\partial f}{\partial x} = \frac{1}{\tau}\Big[F_i - f_i\Big], \tag{3.6}$$

where $f_i(t, x)$ denote the density functions for the ith discrete velocity c_i. Now we introduce a spatial grid, like the hexagonal grid shown in Fig. 5 and discretize (3.6) further on in space and time,

$$f_i(t + \Delta t, x_j + \Delta t c_i) - f_i(t, x_j) = \frac{1}{\tau}\Big(F_i - f_i\Big)(t, x_j) \tag{3.7}$$

Finally, we have to define the discrete equilibrium distribution F_i for each discrete velocity $c_i, i = 1, \ldots, n$ and these functions are obtained from a Taylor expansion of a local Maxwellian distribution around $u = 0$. The actual form of the equilibrium function depends on the underlying discrete velocity model, e.g., in the case of a hexagonal grid as in Fig. 5 one has

$$F_i = \frac{1}{6}\rho + \frac{1}{3}\rho u_\alpha c_{i\alpha} + \frac{4}{3}\rho(c_{i\alpha}c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta})u_\alpha u_\beta$$

with $c_{i\alpha}, \alpha = 1, 2$ denoting the components of c_i and

$$\rho = \sum_{i=1}^{6} f_i, \; \rho u = \sum_{i=1}^{6} c_i f_i$$

From nonrigorous arguments, one can show, that the Lattice–Boltzmann schemes solve approximately the (incompressible) Navier–Stokes equations with a given Reynolds number Re, if the following relation between the Reynolds number and the relaxation time τ is choosen

$$Re = \frac{\sqrt{3}Ma}{\tau - \frac{1}{2}}$$

Formally, this relation is obtained from an asymptotic expansion method of the Lattice–Boltzmann scheme defined in (3.5), see, e.g., [14].
Hence, applying this kind of asymptotic expansion to the discrete Lattice–Boltzmann model gives the compressible Navier–Stokes equations with additional and wrong terms of the order

$$O\left(\tau^2\right) = O\left(\left(\frac{Ma}{Re}\right)^2\right),$$

where this error is independent of the choice of the grid. Moreover, the error against the incompressible Navier–Stokes is

$$O\left(\left(\frac{Ma}{Re}\right)^2\right) + O\left(Ma^k\right)$$

where k depends on the chosen grid. If $k > 2$, then this error does not count. If we choose, e.g., the hexagonal grid, we get $k = 3$. Hence, solving the kinetic transport equation (3.6) in the discrete space with $\Delta t \approx Ma$ and $\Delta x \approx \Delta t$ gives an approximation of the incompressible Navier–Stokes equation with an error of the order $O\left(\left(\frac{Ma}{Re}\right)^2\right)$.
The advantage of the Lattice–Boltzmann schemes certainly lies in the fact, that the dynamic is extremely fast when combing the scheme with a proper hardware. Hence, one may use very fine grids and this is in particular useful if requires very fine resolution or need to handle very complex geometries.

4 Conclusion

In the present paper we discussed domain decomposition techniques for the numerical coupling of kinetic and macroscopic fluid equations in order to derive computationally efficient flow solvers close to the continuum limit. Applying adaptive procedures for the spatial grids and time steps in the Euler domain, one is able to accelerate a full Boltzmann simulation close to the continuum limit by a factor of 10 to 15. Those schemes rely in particular on automatic detection criteria to define macroscopic and kinetic flow regions.
Moreover, we showed how kinetic induced numerical schemes for macroscopic fluid models may be derived from asymptotic limits of kinetic equations. Kinetic schemes as well as Lattice Boltzmann methods are certainly alternative numerical methods for macroscopic fluid models and may help in the development of general flow solvers, which are able to cover a wide range of flow problems from rarefied gases downto the incompressible Navier–Stokes equations.

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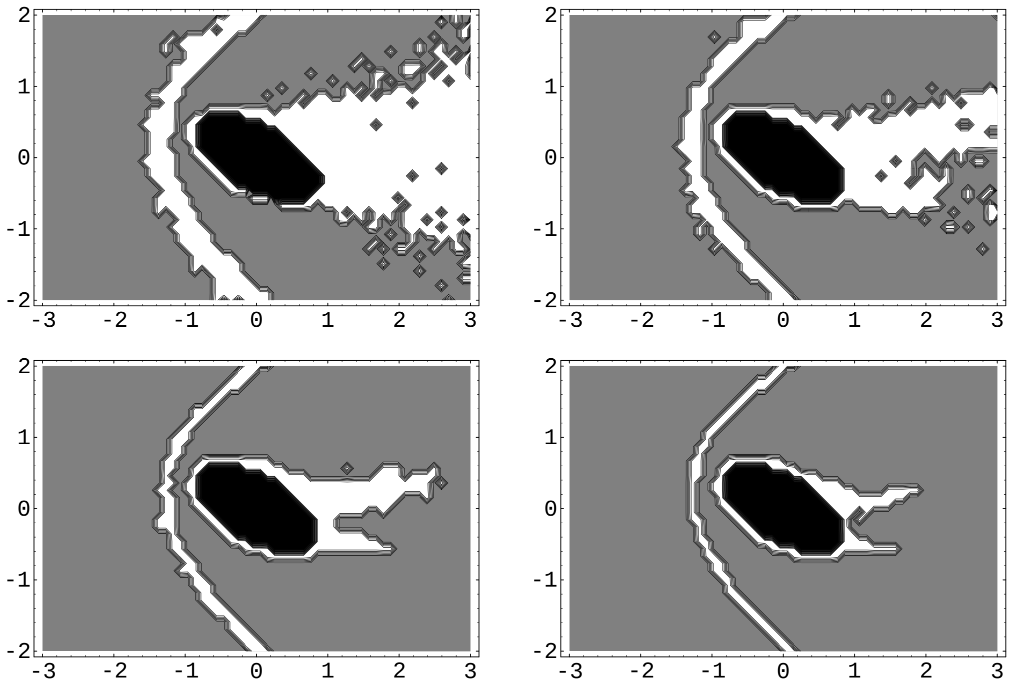

Figure 1: Boltzmann (white) and Euler domains for mean free paths $0.1, 0.05, 0.025$ and 0.0125 m.

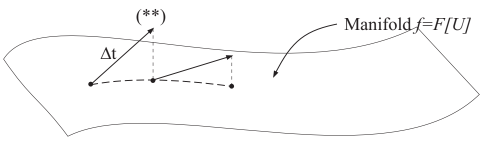

Figure 2: Equilibrium Manifold and Kinetic Schemes

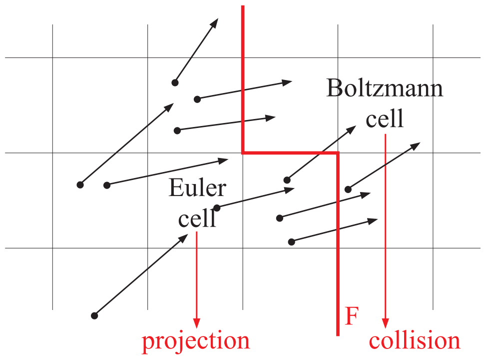

Figure 3: Kinetic Schemes as Particle Codes

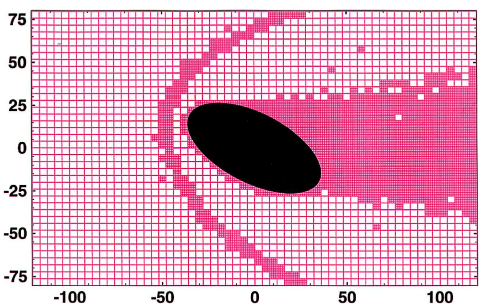

Figure 4: Adaptive Grid in Boltzmann Simulations

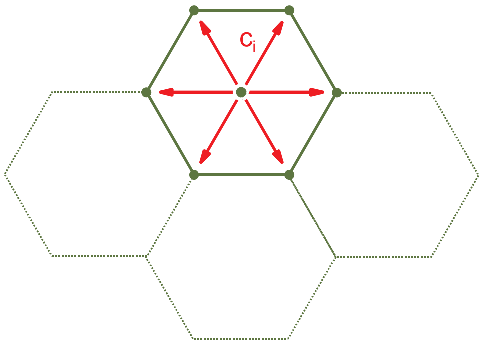

Figure 5: Discrete Velocities on a Hexagonal Grid

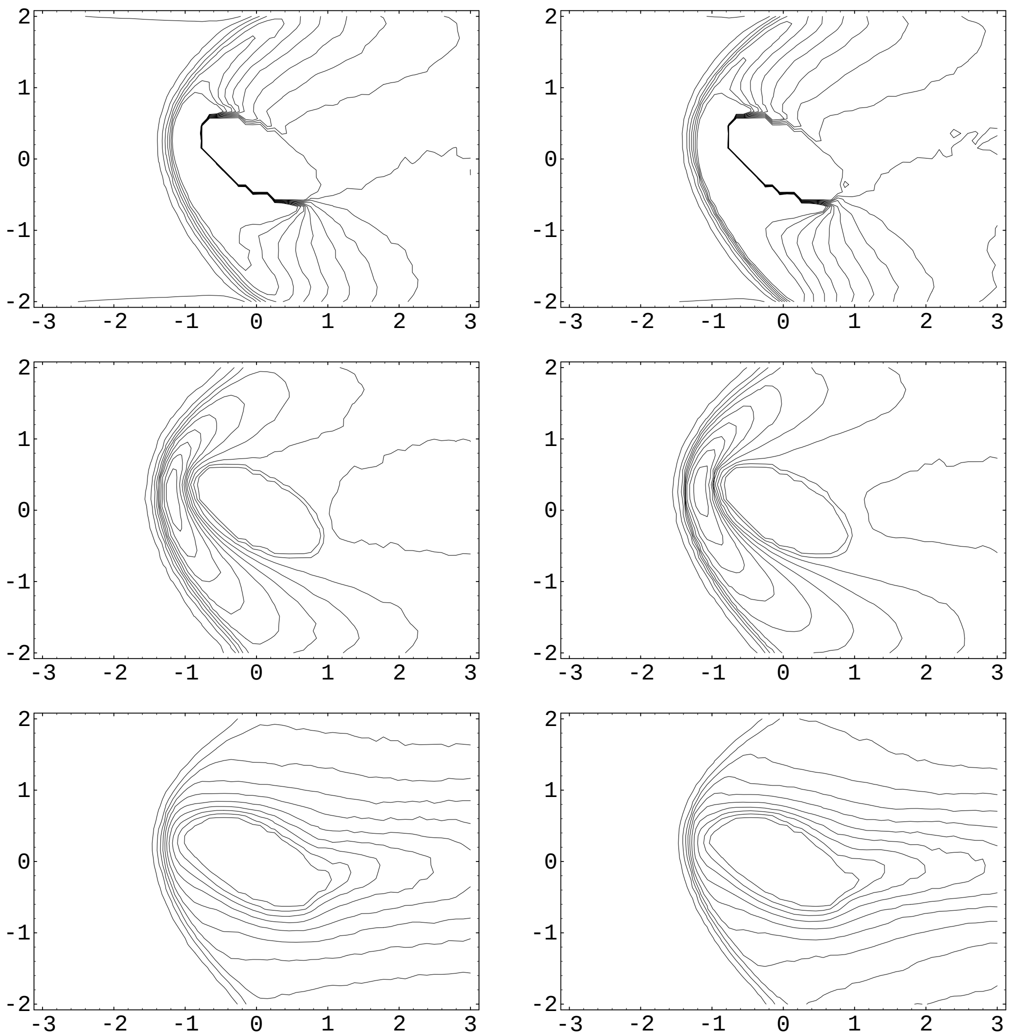

Figure 6: Contour plots of densities (row 1), temperatures (row 2) and Mach numbers (row 3) obtained from both the codes. Pictures on the left are from the pure Boltzmann code and those on the right are from coupling code