

DOMAIN DECOMPOSITION: LINKING KINETIC AND AERODYNAMIC DESCRIPTIONS

by

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ABSTRACT

We discuss how kinetic and aerodynamic descriptions of a gas can be matched at some prescribed boundary. The boundary (matching) conditions arise from the requirement that the relevant moments (ρ, u, \dots) of the particle density function be continuous at the boundary, and from the requirement that the closure relation, by which the aerodynamic equations (holding on one side of the boundary) arise from the kinetic equation (holding on the other side), be satisfied at the boundary. We do a case study involving the Knudsen gas equation on one side and a system involving the Burgers equation on the other side in section 2, and a discussion for the coupling of the full Boltzmann equation with the compressible Navier-Stokes equations in section 3.

1. **INTRODUCTION.** The problems we are concerned with in this paper arise naturally if one wants to predict, by computation, the flow around a space vehicle (shuttle) reentering the atmosphere. The varying atmospheric conditions at different heights lead to specific problems: At heights above 120 km the air is so thin that collisions between its molecules can safely be neglected (Knudsen gas); between 70 and 120 km, collisions become significant, so we cannot use a Knudsen gas model anymore. On the other hand, we are (in regions of significant size, which decrease as we lose altitude) too far from thermodynamic

equilibrium to use exclusively classical aerodynamic equations- the latter only become a reasonably accurate model at heights under 70 km, except in a kinetic boundary layer around the shuttle, which remains in principle at every altitude.

The implications for numerical simulation are that we have to solve the Knudsen gas equation

$$\partial_t f + v \cdot \nabla_x f = 0 \quad (1.1)$$

in the first regime. As easy as it is to solve (1), its solutions are very sensitive to the boundary conditions on the shuttle- we have to pay careful attention to modelling the gas-surface interaction correctly [3].

The middle domain is where we have to use the Boltzmann equation, whose numerical solution requires large effort in spite of the typically smooth flow patterns — the Reynolds number, being inversely proportional to the Knudsen number, is relatively small. Boundary effects become less significant as we lose altitude.

Why at all is it necessary to use the Boltzmann equation in this regime? There are in fact two reasons. First, observe that we are still in a regime of low density, and the Boltzmann collision term contains a factor $\frac{1}{Kn}$, where Kn is the Knudsen number, which goes to zero as the density grows. In other words, small density means slow thermalization from collisions, i.e. we cannot assume to be (or remain) near thermal equilibrium. Second, the space vehicle itself, via boundary effects, will cause significant deviations from the equilibrium distribution. For example, in the "bow shock" in front of the shuttle, one expects nonequilibrium in spite of high densities, because the bow shock is caused by the encounter with and reflection from the front end of the shuttle by molecules. Strictly speaking, the whole Knudsen layer around the vehicle requires a kinetic treatment. Worse, high density means large computation times, because large numbers of particles are needed for the simulation.

The Euler or Navier-Stokes equations which are used in the third (lowest) domain can (in principle) be solved by existing and tested algorithms, where, however, more and more complex structures emerge at lower altitudes near the surface of the shuttle. These complexities lead to significant numerical difficulties. The boundary conditions, on the other hand, become simple (e.g., for the Navier-Stokes equations, after some complicated slip conditions, ultimately "no slip").

In a transition regime between the Boltzmann equation and the aerodynamic equations, the latter, wherever they are justified, are usually solved with less effort.

These considerations lead to the general task of coupling codes for the simulation of the Boltzmann equation on the one hand and the aerodynamic equations on the other hand. The following problems arise:

(I) At every height, identify the domains in position space which allow aerodynamic modeling, and identify those where a Boltzmann simulation is required or not more time-consuming

than an aerodynamic calculation.

(II) Once these domains are known (we will label them as (A) for aerodynamics and (B) for Boltzmann), one has to address the problem of coupling the solution procedures.

Problem (I) is the validity problem, problem (II) is the "matching" problem; (I) and (II) together are the domain decomposition problem.

The validity problem is intimately related to the question under what conditions, and how well, solutions of aerodynamic equations approximate solutions of the Boltzmann equation. This question is typically addressed in the context of Hilbert or Chapman-Enskog expansions, which yield aerodynamics as an approximation of Boltzmann equations. For example, an extremely difficult question arising here is how the approximation errors in the equations influence the approximation errors in the solutions. Only preliminary results for this exist ([5], [6]). Gropengiesser [4] has suggested an approach which is applicable to the space shuttle simulation.

Here, we are concerned with the matching problem (II) for the time-dependent case. Suppose that our domain decomposes at time 0 into two subdomains A and B, where we know initial data for the aerodynamic and kinetic descriptions respectively. The whole domain $\Omega = A \cup B$ will partly be bounded by the spacecraft, partly by an artificial exterior boundary. Problem (II) is then to find appropriate "transfer" boundary conditions on $\partial\bar{A} \cap \partial\bar{B}$.

We sketch a method which, to our knowledge, is the only one being used so far ([7], [10], [11]). A solution to the aerodynamic equations is computed in the whole domain and then used as "zeroth" approximation for the kinetic equation. This gives macroscopic quantities ρ^0, u^0 and T^0 (density, bulk velocity and temperature) everywhere, in particular at the boundary between A and B. If one now wants to "improve" this solution by solving the Boltzmann equation, one uses for the ingoing particle density at the boundary a suitable kinetic density based on the macroscopic quantities ρ^0, u^0 and T^0 . For the Euler equations, the Maxwellian

$$\frac{\rho^0}{(2\pi RT^0)^{3/2}} M\left(\frac{v - u^0}{\sqrt{2RT^0}}\right) = \frac{\rho^0}{(2\pi RT^0)^{3/2}} \exp\left\{-\frac{\|v - u^0\|^2}{2RT^0}\right\}$$

is a natural choice. For the Navier-Stokes equations, the so-called Navier-Stokes density

$$f_{NS}[\rho^0, u^0, T^0](v) = \sum_i a_i(\rho^0, u^0, T^0, \nabla\rho^0, \nabla u^0, \nabla T^0) b_i\left(\frac{v - u^0}{\sqrt{2RT^0}}\right) M\left(\frac{v - u^0}{\sqrt{2RT^0}}\right) \quad (1.2)$$

is suggested by the formal derivation of the compressible Euler equations via the Chapman-Enskog expansion. Here, the b_i are certain Sonine polynomials. We mention the problem that f_{NS} is, in the usual form, not necessarily nonnegative. Lukschin [11] has suggested a simple modification to avoid this difficulty.

Given these densities at the boundary, we know in particular the incoming density there, and can therefore solve the Boltzmann equation (in principle) in B. This solution will then determine the distribution density of the gas leaving B, and, unfortunately, this density will in general *not* be of the form prescribed above (i.e. Maxwellian or f_{NS} associated with ρ^0, u^0 etc.). Recall that we are specifically interested in the case where solving the Boltzmann equation in B is essential, i.e. where the density deviates significantly from equilibrium.

We obtain a new density distribution for the particles leaving B and therefore new macroscopic quantities ρ^1, u^1 and T^1 . The next step is to solve the aerodynamic equations in A with ρ^1, u^1 and T^1 as boundary conditions — whether this is possible depends on the type of aerodynamic equation (for the compressible Navier-Stokes equations, u^1 and T^1 can indeed be prescribed at the boundary) and also on the flow conditions (e.g., if u^1 is directed from A into B, we cannot prescribe ρ^1 , which solves the continuity equation, on the boundary. See the case study in section 2 for a discussion of this phenomenon). In any case, we possibly get new boundary values ρ^2, u^2, T^2 by solving the aerodynamics equations in A, or we keep ρ^1, u^1 and T^1 . Forming the Maxwellian or Navier-Stokes densities with these macroscopic quantities, we solve the Boltzmann equation again in B, etc.

This procedure implies an iteration between Boltzmann and aerodynamic equations, a very lengthy and expensive proposition. If this procedure converges (and there is so far no convergence proof), we would obtain conditions for the flow at the boundary separating A and B which would guarantee continuity of ρ, u and T there. The isolines for density, Mach number and temperature would then be without jumps—the final objective of such an iteration. Further smoothing of the isolines can be achieved by adding an intermediate layer between A and B. This is better from a computational point of view, but hardly different conceptually [10].

We must ask whether continuity of ρ, u and T across the boundary is really the right thing to ask for. This question has been investigated in the context of a Knudsen boundary layer, inside which a linearized Boltzmann equation has to be solved [9]. However, the generalization of Golse's theory to our case of interior boundaries leads to additional problems, as pointed out by A. Klar (personal communication).

The idea is to visualize in A, near the boundary, a boundary layer of width ϵ . This boundary layer is rescaled by a transformation $y = \frac{x}{\epsilon}$; after taking the limit $\epsilon \rightarrow 0$, one obtains a half-space problem for the linearized Boltzmann equation, which forms a natural interpolating problem between our two descriptions. For this linearized half-space problem, the inflow from B is given by the solution of the full Boltzmann equation. Under some restrictions, it is shown that the solution of the linearized problem at infinity (i.e. at the other end of the boundary layer) is an aerodynamic density distribution with specific values for ρ, u and T , which differ in general from the values at the boundary of B. If these new macroscopic quantities are used as boundary values for the aerodynamic equations, there

will therefore be "jumps", i.e. significant changes in the aerodynamic quantities over the width of the boundary layer.

We should not be surprised: Why should continuity give the best global result?

However, even if we neglect these unresolved theoretical questions of the approach, there remain almost unsurmountable computational difficulties. It is exceedingly hard to calculate the new ρ , u and T ; and once they are there, we have to resolve the question of how to match the solution in A and B such that the "right" jumps will emerge. The last question is the one we are really interested in; it is independent from the continuity requirement, and we will therefore simply assume continuity in the sequel.

We approach the problem from a formal mathematical point of view. Different equations do govern the evolution of the system in (A) and (B), but the equations in (A) follow from the equation in (B) as moment equations plus a closure relation. Hence we can summarize: A transport equation (β) holds in region (B), and the equations (α) holding in (A) are simply moment equations of (β), complemented by a closure relation. The solution of (β) is a density function $f(t, x, v)$, which yields in particular the relevant moments $\rho|_B$, $u|_B$ and $T|_B$; in (A), the equations (α) will typically directly yield $\rho|_A$, $u|_A$ and $T|_A$ (but as we shall see, this may not be true for some choices of the decomposition and some examples of aerodynamic equations).

On the boundary we insist on a match, i.e. the moments calculated from both sides must define continuous or even differentiable functions.

2. A SIMPLE CASE STUDY. Our objective in this section is a coupling of the simplest kinetic equation, the equation for a Knudsen gas in one dimension, with simple aerodynamic equations. Let $A = \{x; x < 0\}$, $B = \{x; x > 0\}$,

$$\partial_t f + v \partial_x f = 0, \quad f(0, x, v) = f_0(x, v) \text{ in } B \quad (2.1)$$

(2.1) yields equations for the moments $N_j(t, x) = \int v^j f(t, x) dv$, $j = 0, 1, 2, \dots$,

$$\partial_t N_j + \partial_x N_{j+1} = 0, \quad j = 0, 1, 2, \dots \quad (2.2)$$

If all moments of f make sense, then (2.2) follows from (2.1). Conversely, (2.1) can be reconstructed from (2.2) under certain assumptions on f . In this sense, we call (2.1) and (2.2) equivalent.

In the domain (A), we now close the infinite system (2.2) by choosing a closure relation. To be consistent with standard notation, let $\rho = N_0$, $\rho u = N_1$ and set

$$p(t, x) := \int (v - u)^2 f(t, x, v) dv$$

(the notation p is here chosen because of the relation to pressure). The closure relation we discuss is

$$p(t, x) = N_2 - 2uN_1 + u^2 N_0 = p(t)$$

in A , or

$$\partial_x p = 0 \quad (2.3)$$

in A , i.e. we assume that p does not depend on x there. Alternatively, we could assume the validity of a state equation

$$p_x = p'(\rho)\rho_x$$

in A , and the subsequent calculations would change slightly (but not significantly). We confine our attention to (2.3) for simplicity.

By using the definition of N_0 , N_1 , ρ and u , we see that the closure relation (2.3) can also be written as

$$\partial_x N_2 = \partial_x (u^2 \rho). \quad (2.4)$$

The first two equations in (2.2) then form a closed system and read

$$\begin{aligned} \partial_t \rho + \partial_x (\rho u) &= 0 \\ \partial_t (\rho u) + \partial_x N_2 &= 0 \\ \partial_x N_2 &= \partial_x (u^2 \rho) \end{aligned} \quad (2.5)$$

or, assuming enough regularity,

$$\begin{aligned} \partial_t \rho + \partial_x (\rho u) &= 0 \\ \partial_t u + u \partial_x u &= 0 \end{aligned} \quad (2.6)$$

i.e. we have the continuity equation coupled with Burgers' equation. Equation (2.1) is uniquely solvable in (B) , provided that the incoming flow is given at the boundary, i.e.

$$f(t, 0, v) = F(t, v) \text{ for } v > 0. \quad (2.6a)$$

The solution of (2.1) in $x > 0$ is then

$$f(t, x, v) = \begin{cases} f_0(x - vt, v) & \text{for } x - vt > 0, \text{ i.e. } v < \frac{x}{t} \\ F(t - \frac{x}{v}, v) & \text{for } t - \frac{x}{v} > 0, \text{ i.e. } v > \frac{x}{t} \end{cases}$$

For $x = 0$ we get

$$f(t, 0, v) = f_0(-vt, v)$$

for $v < 0$, and

$$\partial_x f(t, 0, v) = \begin{cases} f_{0x}(-vt, v) & \text{for } v < 0 \\ F_t(t, v) \cdot \left(-\frac{1}{v}\right) & \text{for } v > 0 \end{cases} \quad (2.7)$$

We need this later.

The system (2.6) is uniquely solvable in (A) if we have initial data $\rho(0, x) = \rho_0(x)$, $u(0, x) = u_0(x)$ and if we assume that $u_0(x) > 0$.

Remark. Here, "uniquely solvable" is meant in a local sense. We shall assume that there is a time $T > 0$ such that the initial value problem for (2.6) is classically solvable, via the method of characteristics, in $A \times [0, T]$. If $u_0 > 0$ in A , the characteristics starting at $t = 0$ have positive slope and therefore "cover" the region $\{x \leq 0\} \times [0, T]$. In particular, this defines the boundary values $U(t) := u(t, 0)$ and $P(t) := \rho(t, 0)$.

See Figure 1.

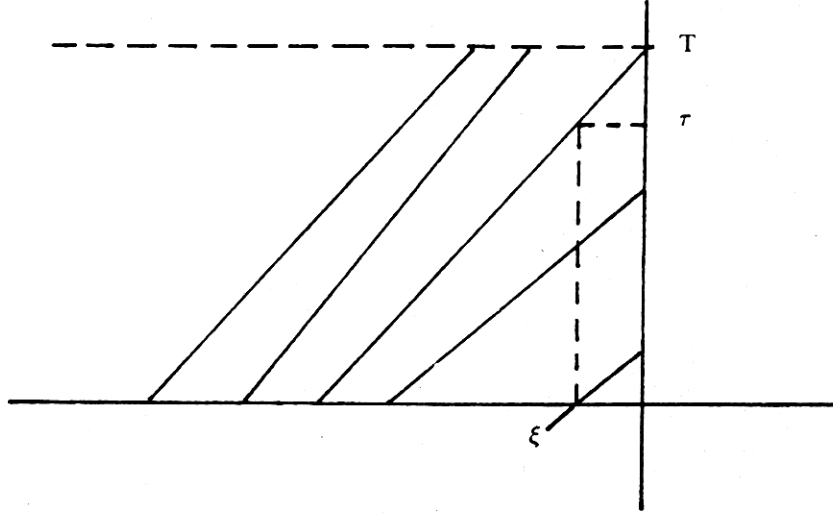


Figure 1

A characteristic for $\partial_t u + u \partial_x u = 0$ passing through (ξ, τ) satisfies an equation $\alpha = \frac{x-\xi}{t-\tau}$, and it therefore must have left the line $t = 0$ from $x(\xi, \tau) = \xi - \alpha\tau < 0$. Here, the slope α is given by the initial value and the equation, as

$$\alpha = u_0(\xi - \alpha\tau).$$

We will assume that for every (ξ, τ) with $\xi < 0$ and $0 \leq \tau \leq T$ this equation has a unique solution $\alpha = \alpha(\xi, \tau) > 0$. Thus

$$u(\xi, \tau) = u_0(\xi - \alpha(\xi, \tau)\tau) = \alpha(\xi, \tau).$$

The equation for ρ can be solved over the same characteristic base lines $x = \xi + \alpha(t - \tau)$, but ρ is not constant along these lines, because

$$\partial_t \rho + u \partial_x \rho = -\rho \partial_x u$$

and so

$$\rho(\xi, \tau) = \rho_0(\xi - \alpha\tau) \exp \left\{ - \int_0^\tau \partial_x u(\xi + \alpha(\sigma - \tau), \sigma) d\sigma \right\}.$$

The boundary values $U(t)$ and $P(t)$ on $x = 0$ are given by solving

$$\alpha = u_0(-\alpha t).$$

This equation will determine $\alpha = \alpha(t)$, and we can then calculate

$$\begin{aligned} U(t) &= u_0(-\alpha t) = \alpha(t) \\ P(t) &= \rho_0(-\alpha t) \exp \left\{ \int_0^t u_x(\alpha(\sigma - t), \sigma) d\sigma \right\}. \end{aligned}$$

If $u_0(x)$ is negative and in particular $u_0(0) < 0$, this method of characteristics will not determine u and ρ in $A \times [0, T]$; the method only works for $x \leq u_0(0)t$ (see Figure 2). In fact, we can prescribe U and P on $x = 0$, and they will then determine the solution of (2.6) in $u_0(0)t \leq x \leq 0$ as

$$u(x, t) = U \left(t - \frac{x}{\alpha(x, t)} \right) = \alpha(x, t),$$

where α is the solution of the last equation.

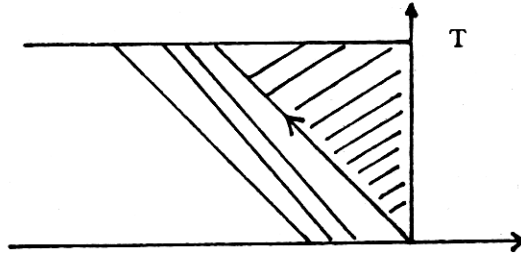


Figure 2

The difference between the two cases $u_0 > 0$ and $u_0 < 0$ is that in the first case, the macroscopic flow is from the aerodynamic into the kinetic regime, and the initial condition alone suffices to obtain a unique continuation of ρ and u onto the boundary, whereas in the second case, no such continuation is given — we have additional degrees of freedom.

The closure relation (2.4) should hold at the boundary if the transition from kinetic to aerodynamic is to be meaningful there. A first glance at (2.4) suggests that in order to discuss (2.4), we need methods to calculate u_x and ρ_x at $x = 0$. However, we shall later see that the special closure relation which we consider here is such that we can actually satisfy it *without knowing* u_x and ρ_x beforehand at $x = 0$.

However, their values there can actually be easily determined, as follows. If we assume for the moment that the equations (2.6) still hold at $x = 0$, we can easily calculate $u_x(t, 0)$ and $\rho_x(t, 0)$ in terms of U and P : Solving $u_t + uu_x = 0$ for u_x yields

$$u_x(t, 0) = -\frac{U'(t)}{U(t)} \quad (2.8)$$

and from $\rho u_x + u \rho_x = -\rho_t$ it follows that

$$\begin{aligned} \rho_x|_{x=0} &= -\frac{\rho_t + \rho u_x}{u} \Big|_{x=0} = \frac{-P_t + P \frac{U'}{U}}{U} \\ &= \frac{-U' P' + P U''}{U^2} = -\left(\frac{P}{U}\right)' \end{aligned} \quad (2.9)$$

The validity of the representations (2.8-9) actually follows also from the solution representation given earlier and thus implies that our equation remain valid at $x = 0$. We formulate this as a Lemma:

Lemma. $u_x(t, 0) = -\frac{U'(t)}{U(t)}$, $\rho_x(t, 0) = -\left(\frac{P}{U}\right)'$.

Proof. From $u(x, t) = U\left(t - \frac{x}{\alpha(x, t)}\right) = \alpha(x, t)$ we conclude that $u_x = \alpha_x$. If we set $G(t, x, \alpha) := U\left(t - \frac{x}{\alpha}\right) - \alpha$, the function $\alpha(t, x)$ is implicitly defined from $G(t, x, \alpha) = 0$. The implicit function theorem guarantees differentiability of α , and from $G_x + G_\alpha \cdot \alpha_x = 0$ it follows that

$$\alpha_x = -\frac{G_x}{G_\alpha}.$$

By using the definition of G , it follows that $G_x(t, x, \alpha) = U'\left(t - \frac{x}{\alpha}\right)\left(\frac{1}{\alpha}\right)$, that $G_\alpha(t, x, \alpha) = U'\left(t - \frac{x}{\alpha}\right) \cdot \frac{x}{\alpha^2} - 1$ and finally that

$$\alpha_x(x, t) = \frac{\alpha U'\left(t - \frac{x}{\alpha}\right)}{x U'\left(t - \frac{x}{\alpha}\right) - \alpha^2}.$$

For $x = 0$, the identity $\alpha(0, t) = U(t)$ implies

$$u_x(0, t) = \alpha_x(0, t) = -\frac{U'(t)}{U(t)}.$$

Furthermore, from

$$\rho(x, t) = \rho\left(0, t - \frac{x}{\alpha}\right) \exp\left(-\int_{t-\frac{x}{\alpha}}^t u_x\left(\alpha\left(\tau - t + \frac{x}{\alpha}\right), \tau\right) d\tau\right)$$

we find

$$\partial_x \rho(0, t) = \dot{P}(t) \partial_x \left(-\frac{x}{\alpha(x, t)}\right) \Big|_{x=0} + P(t) \cdot \partial_x \left(-\int_{t-\frac{x}{\alpha}}^t u_x\left(\alpha\left(\tau - t + \frac{x}{\alpha}\right), \tau\right) d\tau\right).$$

Now use that

$$\partial_x \left(-\frac{x}{\alpha(x, t)}\right) \Big|_{x=0} = \frac{-\alpha + x\alpha_x}{\alpha^2} \Big|_{x=0} = -\frac{1}{\alpha} + x\alpha_x \Big|_{x=0} = -\frac{1}{U(t)}.$$

The remaining derivative also simplifies at $x = 0$. We obtain

$$\begin{aligned} \rho_x(0, t) &= -\frac{\dot{P}}{U} + P u_x(0, t) \left(-\frac{1}{U}\right) \\ &= -\frac{\dot{P}}{U} + \frac{P}{U} \cdot \frac{\dot{U}}{U} \\ &= -\left(\frac{P}{U}\right)'. \end{aligned}$$

A brief way to summarize this result is to state that the Poincaré–Steklov operator for our problem, defined as

$$\begin{pmatrix} P \\ U \end{pmatrix} \mapsto \begin{pmatrix} \rho_x(0, t) \\ u_x(0, t) \end{pmatrix}.$$

is given explicitly as

$$PS \left(\frac{\rho}{u} \right) = - \frac{d}{dt} \left(\frac{\frac{\rho}{u}}{\ln u} \right).$$

We have now solved problems (α) and (β) separately in the regions (A) and (B) and finally face the "matching" problem. The situation is as follows. In (A) we have equations (2.5), whereas in (B) we have only the first two equations of (2.5), and N_2 is given via the solution of a kinetic equation. At $x = 0$, we require the "matching" conditions

$$\rho|_A = \rho|_B \quad (2.10)$$

$$u|_A = u|_B, \quad (2.11)$$

and, most important, that the boundary values at $x = 0$ of the solution in (B) will satisfy the same closure relation as the solution of the equations in (A), i.e.

$$\lim_{x \searrow 0} (\partial_x N_2 - \partial_x (N_0 N_1)) = 0 \quad (2.12)$$

(compare this with (2.4)). Please note that (2.12) can well be violated if

$$\lim_{x \searrow 0} (N_2 - N_0 N_1) = 0. \quad (2.13)$$

The closure relation is (2.12), not (2.13)!

Now note that

$$N_2 - N_0 N_1 = \int_{-\infty}^{\infty} (v - u)^2 f \, dv,$$

hence

$$\partial_x (N_2 - N_0 N_1) = -2u_x \int (v - u) f \, dv + \int (v - u)^2 f_x \, dv.$$

The first term on the right is zero by the definition of u (this is the reason why we do not need the value of u_x at $x = 0$), and our closure relation therefore reduces to

$$\int (v - u)^2 f_x(t, x, v) \, dv = 0 \quad (2.14)$$

with

$$u = u|_A = u|_B = U$$

by (2.11).

The equations (2.10), (2.11) and (2.14) yield the following conditions for P , U and F from (2.6a):

$$P(t) = \int_{-\infty}^0 f_0(-vt, v) \, dv + \int_0^{\infty} F(t, v) \, dv \quad (2.15)$$

$$P(t)U'(t) = \int_{-\infty}^0 v f_0(-vt, v) \, dv + \int_0^{\infty} v F(t, v) \, dv \quad (2.16)$$

$$\int_0^\infty (v - U(t))^2 \frac{F_i(t, v)}{v} dv = \int_{-\infty}^0 (v - U(t))^2 \partial_x f_0(-vt, v) dv. \quad (2.17)$$

Let $G(t, v) = \frac{1}{v} F(t, v)$ and $G_i(t) = \int_0^\infty v^i G(t, v) dv$. Then (2.15-17) read as

$$G_1(t) = P(t) - \int_0^\infty f_0(-vt, v) dv \quad (2.18)$$

$$G_2(t) = P(t)U(t) - \int_{-\infty}^0 v f_0(-vt, v) dv \quad (2.19)$$

$$\begin{aligned} \partial_t G_2 - 2U \partial_t G_1 + U^2 \partial_t G_0 &= \int_{-\infty}^0 v^2 \partial_x f_0(-vt, v) dv \\ &- 2U \int_{-\infty}^0 v \partial_x f_0(-vt, v) dv + U^2 \int_{-\infty}^0 \partial_x f_0(-vt, v) dv. \end{aligned} \quad (2.20)$$

Obviously $\partial_x f_0(-vt, v) = \partial_t f_0(-vt, v) \cdot (-\frac{1}{v})$. By substituting this in the right hand side of (2.20), we get

$$\begin{aligned} \frac{d}{dt} \left(G_2 + \int_{-\infty}^0 v f_0(-vt, v) dv \right) - 2U \frac{d}{dt} \left(G_1 + \int_{-\infty}^0 f_0(-vt, v) dv \right) \\ + U^2 \frac{d}{dt} \left(G_0 + \int_{-\infty}^0 f_0(-vt, v) \frac{dv}{v} \right) = 0, \end{aligned}$$

and by using (2.18) and (2.19) here this simplifies to

$$\frac{d}{dt}(PU) - 2U\dot{P} + U^2 \frac{d}{dt} \left(G_0 + \int_{-\infty}^0 f_0(-vt, v) \frac{dv}{v} \right) = 0,$$

or

$$\frac{d}{dt} \left(G_0 + \int_{-\infty}^0 f_0(-vt, v) \frac{dv}{v} \right) = \frac{d}{dt} \left(\frac{P}{U} \right). \quad (2.21)$$

Please note that in order to justify these calculations, we have to make the assumption that $\frac{1}{v} f_0(-vt, v)$ is integrable over $(-\infty, 0)$, an assumption which is, for example, violated for $f_0(x, v) = e^{-v^2}$. Integrability of $\frac{1}{v} \partial_t f_0(-vt, v)$ holds provided that $\partial_x f_0(-vt, v)$ is integrable (clearly, $v = 0$ is the critical value).

We will work either under the assumption that $\frac{1}{v} f_0(-vt, v)$ is actually integrable over v (by truncating f_0 in a neighborhood of $v = 0$, this can always be enforced), or that f_0 be independent of x (as in the above example). In this latter case clearly $\frac{1}{v} \partial_t f_0(-vt, v) = 0$, and the problem terms disappear from the start.

Motivated by the definition of G_i , we now set

$$\tilde{G}_i(t) = \int_{-\infty}^0 v^{i-1} f_0(-vt, v) dv.$$

Then (2.18), (2.19) and (2.21) become

$$\begin{aligned} G_1(t) &= P(t) - \tilde{G}_1(t) \\ G_2(t) &= P(t)U(t) - \tilde{G}_2(t) \\ \frac{d}{dt} (G_0 + \tilde{G}_0) &= \frac{d}{dt} \left(\frac{P}{U} \right). \end{aligned} \quad (2.22)$$

Theorem. If the "matching conditions" (2.22) are satisfied, then even the derivatives of ρ and u are continuous at $x = 0$.

Proof. In domain (B) we have

$$\rho(t, x) = \int_{-\infty}^{x/t} f_0(x - vt, v) dv + \int_{x/t}^{\infty} F(t - \frac{x}{v}, v) dv,$$

and therefore, assuming the reasonable normalization

$$f_0(0, v) = f(0, 0, v) = F(0, v),$$

$$\begin{aligned} \rho_x(t, 0) &= \int_{-\infty}^0 f_{0x}(-vt, v) dv - \int_0^{\infty} F_t(t, v) \frac{dv}{v} \\ &= -\frac{d}{dt} \tilde{G}_0(t) - \frac{d}{dt} G_0(t) \\ &= -\frac{d}{dt} \left(\frac{P}{U} \right) \\ &= \rho_x(t, 0)|_A. \end{aligned}$$

Similarly, in the domain (B)

$$\rho u = \int_{-\infty}^{x/t} f_0(x - vt, v) v dv + \int_{x/t}^{\infty} v F(t - \frac{x}{v}, v) dv,$$

hence

$$\begin{aligned} (\rho u)_x|_{x=0} &= \int_{-\infty}^0 f_{0x}(-vt, v) v dv - \int_0^{\infty} F_t(t, v) dv \\ &= -\frac{d}{dt} P. \end{aligned}$$

On the other hand, in (A)

$$(\rho u)_x = \rho_x u + \rho u_x,$$

hence

$$\begin{aligned} (\rho u)_x|_0 &= -\frac{d}{dt} \left(\frac{P}{U} \right) U - P \frac{\dot{U}}{U} \\ &= -\dot{P}. \end{aligned}$$

The Theorem follows from this.

The assertion of this Theorem follows also from the simple observation that u_x and ρ_x at $x = 0$ can be calculated from U and P via $u_x = -\frac{\dot{U}}{U}$ and $\rho_x = -\frac{d}{dt} \left(\frac{P}{U} \right)$. These identities hold at $x = 0$ also from the kinetic domain, because by our closure relation

$$\begin{aligned} U_t + U u_x &= 0 \\ P_t + P u_x + U \rho_x &= 0 \end{aligned}$$

at $x = 0$.

The equations (2.22) are equations for the functions $U(t)$, $P(t)$ and $G(t, v) = \frac{1}{t} F(t, v)$. The \tilde{G}_i depend only on the initial value f_0 .

We briefly discuss the difference between the two cases $u_0 \leq 0$ and $u_0 \geq 0$ in the domain (A). If $u_0 \geq 0$, then the initial values determine the solution in domain (A) completely as far as the method of characteristics is applicable (the formations of shocks is a phenomenon which can be discussed, but which we will not consider here). In particular, our assumptions then imply that $U(t)$ and $P(t)$ will be given for $0 \leq t \leq T$, and $U(t) \geq 0$. Hence the system (2.22) is then a system of equations for F .

If $u_0 < 0$, this is not the case. U and P can be prescribed arbitrarily (smooth for $t = 0$ at best) on $x = 0$, and there are infinitely many ways to match the two equations. This seems unreasonable from a physical point of view: The reduction at $t = 0$ to ρ and u in the domain (A) means that we lose all information about the domain $u(0)t \leq x \leq 0$, $0 \leq t \leq T$. This is unacceptable for our concept of "matching".

The remedy we suggest is to choose a different boundary in this situation, e.g. the moving boundary given by $x = u(0)t$ instead of $x = 0$. The boundary moves then *with* the flow; from the point of view of the aerodynamic observer, we do not accept boundaries lagging behind the flow.

Specifically, if $u(0) = \alpha_0 < 0$, then $x = \alpha_0 t$ is the new boundary. If the macroscopic equation holds on this boundary in the sense of characteristics, we have

$$\tilde{U}(t) = u(\alpha_0 t, t) = u(0) = \alpha_0.$$

$\tilde{P}(t) = \rho(\alpha_0 t, t)$ is given similarly.

If \tilde{F} is given on the new boundary, the solution in domain $(B) = \{(x, t); \alpha_0 t \leq x, 0 \leq t \leq T\}$ is then

$$f(t, \alpha_0 t, v) = \tilde{F}(t, v)$$

for $v \geq \alpha_0$, and

$$f(t, x, v) = \begin{cases} f_0(x - vt, v) & \text{if } x - vt > 0, \text{ i.e. } v < \frac{x}{t} \\ \tilde{F}\left(\frac{x - vt}{\alpha_0 - v}, v\right) & \text{if } \frac{x - vt}{\alpha_0 - v} > 0, \text{ i.e. } v > \frac{x}{t} \geq \alpha_0. \end{cases}$$

Therefore,

$$\frac{\partial f}{\partial x}(t, \alpha_0 t, v) = \begin{cases} f_{0x}((\alpha_0 - v)t, v) & \text{if } v < \alpha_0 \\ \tilde{F}_t(t, v) \frac{1}{\alpha_0 - v} & \text{if } v > \alpha_0. \end{cases}$$

The first two equations of (2.22) become

$$\begin{aligned} \tilde{P}(t) &= \int_{-\infty}^{\alpha_0} f_{0x}((\alpha_0 - v)t, v) dv + \int_{\alpha_0}^{\infty} \tilde{F}(t, v) dv \\ \tilde{P}(t)\tilde{U}(t) &= \int_{-\infty}^{\alpha_0} v f_{0x}((\alpha_0 - v)t, v) dv + \int_{\alpha_0}^{\infty} v \tilde{F}(t, v) dv \end{aligned} \quad (2.23)$$

and the third equation.

$$\partial_x \int_{-\infty}^{\infty} (v - u)^2 f(t, x, v) dv \Big|_{x=\alpha_0 t} = 0,$$

yields after substitutions

$$\int_{-\infty}^{\infty} (v - \tilde{U}(t))^2 \tilde{F}_t(t, v) \frac{dv}{v - \alpha_0} = \int_{-\infty}^{\alpha_0} (v - \tilde{U}(t))^2 f_{0x}((\alpha_0 - v)t, v) dv.$$

Setting $\tilde{U}(t) = \tilde{U}(t) - \alpha_0$ (the velocity relative to the boundary), $\hat{F}(t, w) = \tilde{F}(t, w + \alpha_0)$ and $\hat{G}_{0,k}(t) = \int_{-\infty}^0 f_0(-wt, \alpha_0 + w) w^{k-1} dw$ we arrive after some simplification at

$$\begin{aligned} \hat{G}_1(t) &= \int_0^{\infty} \hat{F}(t, w) dw = \tilde{P}(t) - \hat{G}_{0,1}(t) \\ \hat{G}_2(t) &= \int_0^{\infty} w \hat{F}(t, w) dw = \tilde{P}(t) \tilde{U}(t) - \hat{G}_{0,2}(t) \\ \hat{G}_0(t) &= \int_0^{\infty} \frac{\hat{F}(t, w)}{w} dw = \frac{\tilde{P}(t)}{\tilde{U}(t)} - \hat{G}_{0,0}(t), \end{aligned} \quad (2.24)$$

i.e. exactly the same equations as before, where we simply write $U - \alpha_0$ for \tilde{U} , $F(t, u + \alpha_0)$ for $\tilde{F}(t, u)$ and $f_0(x, w + \alpha_0)$ for $\tilde{f}_0(x, w)$. Note that after the transformation $\tilde{U}(t)$ and thus $\tilde{U}(t)$ will actually be constant.

We return to the equations (2.22). In the sequel, we will assume that U and P (\tilde{U} and \tilde{P} respectively) are given. Then the equations (2.22) are 3 equations for $F(t, v)$, equations which do of course *not* determine $F(t, v)$ uniquely. We have to restrict our attention to special classes of F 's such that (2.22) becomes uniquely solvable in each class. We suggest three possible such classes below.

(I) Assume that $G(t, v)$ is Maxwellian, i.e.

$$F(t, v) = v \cdot A e^{-\frac{(v-B)^2}{c}}.$$

Equations (2.22) become

$$\begin{aligned} A \int_0^{\infty} v e^{-\frac{(v-B)^2}{c}} dv &= P(t) - \tilde{G}_1(t) = H_1(t) \\ A \int_0^{\infty} v^2 e^{-\frac{(v-B)^2}{c}} dv &= P(t) U(t) - \tilde{G}_2(t) = H_2(t) \\ A \int_0^{\infty} e^{-\frac{(v-B)^2}{c}} dv &= \frac{P(t)}{\tilde{U}(t)} - \tilde{G}_0(t) + C_1 = H_0(t). \end{aligned}$$

Here, C_1 is an integration constant arising from an integration of the third equation of (2.22).

It is not immediately clear whether these three nonlinear equations have solutions $A(t)$, $B(t)$ and $C(t)$ with the necessary additional requirement $A \geq 0$, $C > 0$.

(II) A second class which we have investigated is of the form

$$F(t, v) = \alpha(t) e^{-\beta(t)v} \chi(v),$$

where α , β and χ are three functions to be determined. We have succeeded to formally solve the system (2.22) for this ansatz, by using Laplace transform methods and techniques from the theory of ordinary differential equations. We omit these details, because their practical significance is presently unclear.

(III) The third and for practical calculations promising class are discrete velocity models, defined by the form

$$F(t, v) = \sum_{j=1}^N \alpha_j(t) \delta_{v_j},$$

where the v_j , $j = 1, \dots, N$ are fixed velocities such that $0 < v_j$ for all j and such that $v_j \neq v_i$ for $i \neq j$. For this case

$$G_0(t) = \sum_{j=1}^N \frac{1}{v_j} \alpha_j(t), \quad G_1(t) = \sum_{j=1}^N \alpha_j(t), \quad G_2(t) = \sum_{j=1}^N v_j \alpha_j(t),$$

and defining $\beta_j = \frac{\alpha_j}{v_j}$, we obtain a system of 3 equations for the β_j :

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ v_1 & v_2 & \dots & v_N \\ v_1^2 & v_2^2 & \dots & v_N^2 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_N \end{pmatrix} = \begin{pmatrix} G_0 \\ G_1 \\ G_2 \end{pmatrix}.$$

For example, in the case $N = 3$ we have 3 equations for three unknowns, and as the determinant of the matrix is in this case

$$(v_2 - v_1)(v_3 - v_2)(v_3 - v_1) \neq 0,$$

the system is uniquely solvable. Please note, however, that we insist on nonnegative solutions! The velocities v_1, \dots, v_N must therefore be chosen such that nonnegativity of the α_j 's is true. For $N > 3$, there may well be more than one nonnegative solution, and we have the freedom to choose additional criteria to select one; this freedom is probably useful in practical calculations. Investigations to this end are planned for future work.

3. THE GENERAL CASE. We now consider the more realistic and more general situation of three dimensions, where $A = \{x \in \mathbb{R}^3; x_1 \leq 0\}$ and $B = \{x \in \mathbb{R}^3; x_1 \geq 0\}$. In B , we assume description of the gas by the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = Q(f, f) \quad (3.1)$$

where at $t = 0$ an initial density $f(0, x, v) = f_0(x, v)$ is given. In order to be able to solve (3.1) (even in principle), we need in addition data about the particles entering the domain B at $x_1 = 0$, i.e. about $f(0, x_2, x_3, v, t)$ for $v_1 > 0$. Setting $\tilde{x} = (x_2, x_3)$, we write

$$F(t, \tilde{x}, v) = f(t, 0, \tilde{x}, v) \text{ for } v_1 > 0.$$

The boundary density F may be coupled with the density of the particles leaving B via a boundary condition

$$v_1 F(t, \tilde{x}, v) = \int_{v'_1 < 0} R(v' \rightarrow v) v'_1 f(t, 0, \tilde{x}, v') dv'.$$

In the sequel, however, we will treat F as a boundary condition which is independent of the interior solution of the Boltzmann equation. This is consistent with the concept of an artificial "interior" boundary. As usual, we set

$$\begin{aligned} \rho(t, x) &= \int f(t, x, v) dv \\ u(t, x) &= \frac{1}{\rho} \int v f(t, x, v) dv \end{aligned}$$

and

$$p_{ij} = \int (v_i - u_i)(v_j - u_j) f(t, x, v) dv.$$

From the Boltzmann equation, we obtain by integration in the usual way and proper use of the collision invariants the moment equations

$$\begin{aligned} \partial_t \rho + \operatorname{div}(\rho u) &= 0 \\ \partial_t(\rho u_j) + \sum_{i=1}^3 \partial_{x_i}(\rho u_i u_j + p_{ij}) &= 0 \end{aligned} \quad (3.2)$$

$j = 1, 2, 3$. We will confine our attention to this system of 4 equations for more than 4 unknowns.

As in the case study done in the previous section, we close these equations in the domain (A) by adding a closure relation. The closure relations leading to the compressible Navier-Stokes equations are

$$\sum_{i=1}^3 \partial_{x_i} p_{ij} = \sum_{i=1}^3 \partial_{x_i} \left(p \delta_{ij} - \mu (\partial_{x_i} u_j + \partial_{x_j} u_i) + \frac{2}{3} \mu \operatorname{div} u \delta_{ij} \right) \quad (3.3a)$$

(for $\mu = 0$, these closure relations lead to the compressible Euler equations), and we only consider the isentropic case by adding a state equation

$$p = p(\rho). \quad (3.3b)$$

We choose to write the closure relation in the differential form (3.3a), similarly to the way in which we chose a differential identity as closure relation in the case study.

Summarizing, we have equations (3.2) and (3.3) in domain (A), equation (3.1) and hence equation (3.2) in domain (B); in domain (B) the p_{ij} are not given by (3.3), but instead by solving the Boltzmann equation.

As before, we impose the following matching conditions at $x = 0$:

- continuity of ρ and u at $x = 0$
- validity of (3.3) at $x_1 = 0+$, i.e. for the kinetic equation at $x_1 = 0$.

We find as before

$$\int_{v_1 < 0} f(t, 0, \bar{x}, v) dv + \int_{v_1 \geq 0} F(t, \bar{x}, v) dv = \rho(t, 0, \bar{x}) \equiv P(t, \bar{x}). \quad (3.4)$$

However, the equation (3.4) is more subtle than the corresponding equation before, because now the density $f(t, 0, \bar{x}, v)$ for $v_1 < 0$ will in general depend on $F(t, \bar{x}, v)$. The mapping

$$F(t, \bar{x}, v)|_{v_1 \geq 0} \rightarrow f(t, 0, \bar{x}, v)|_{v_1 \leq 0},$$

where f_0 is given in (B), is called **albedo operator**. If $Q(f, f) = 0$, i.e. in the case of a Knudsen gas, the flux leaving the domain (B) is independent of the flux entering (B), and the albedo operator is trivial. If there is interaction, calculation of the albedo operator requires solving the Boltzmann equation, a formidable task. Hence even the equation (3.4) poses serious difficulties.

We suggest to overcome this problem by using the well-known procedure of "splitting", which allows us to decompose the Boltzmann equation for a short time interval into a free flow part (including the boundary conditions), modeled by the Knudsen gas equation, and into the spatially homogeneous equation, for which no boundary condition in space is needed. This procedure is standard in numerical approximation schemes for the Boltzmann equation and should in our case actually give an approximation of the albedo operator in question. Then, on short enough time intervals, we only need to study (3.4) for the case $Q(f, f) = 0$.

The second matching equation is

$$\int_{v_1 < 0} v_j f(t, 0, \bar{x}, v) dv + \int_{v_1 \geq 0} v_j F(t, \bar{x}, v) dv = \rho u_j(t, 0, \bar{x}) \equiv U_j P(t, \bar{x}) \quad (3.5)$$

(the same difficulty as in equation (3.4) arises, and we suggest the same remedy).

By using the obvious identity

$$\int (v_i - u_i) f(t, \bar{x}, v) dv = 0.$$

the validity of (3.3) at $0+$ transforms into

$$\begin{aligned}
\sum_{i=1}^3 \partial_{x_i} p_{ij} &= \sum_{i=1}^3 \partial_{x_i} \int_{\mathbb{R}^3} (v_i - u_i)(v_j - u_j) f(t, x, v) dv \\
&= \sum_{i=1}^3 \int (v_i - u_i)(v_j - u_j) \partial_{x_i} f(t, x, v) dv \\
&= \sum_{i=1}^3 \int v_i v_j \partial_{x_i} f dv - u_j \int \sum_{i=1}^3 v_i \partial_{x_i} f dv \\
&\quad - \sum_{i=1}^3 u_i \int v_j \partial_{x_i} f dv + \sum u_i u_j \int \partial_{x_i} f dv \\
&= \int v_j \langle v, \nabla_x f \rangle dv - u_j \int \langle v, \nabla_x f \rangle dv \\
&\quad - \sum_{i=1}^3 u_i \int v_j \partial_{x_i} f dv + u_j \int \langle u, \nabla_x f \rangle dv \\
&= - \int v_j \partial_t f dv + u_j \int \partial_t f dv - u_1 \int v_j \partial_{x_1} f dv \\
&\quad - \sum_{i=2}^3 u_i \int v_j \partial_{x_i} f dv + u_j u_1 \int \partial_{x_1} f dv + u_j \sum_{i=2}^3 u_i \int \partial_{x_i} f dv.
\end{aligned}$$

For the last identity, we have used that $\partial_t f + v \cdot \nabla_x f = 0$. Also, in the last terms, we have separated derivatives with respect to x_1 from others—the latter ones are “inner derivatives” at the boundary $x_1 = 0$ and can be expressed as derivatives of F . The former are derivatives transversal to $x_1 = 0$, and we have to eliminate them.

Every one of the integrals in the last chain of identities is over $v_1 \geq 0$ and $v_1 \leq 0$. On the boundary given by $x_1 = 0$, where the closure conditions are to apply, the integrals over $v_1 \geq 0$ can be written in terms of F if we take advantage of the representation

$$\partial_{x_1} f = -\frac{1}{v_1} (\partial_t f + v_2 \partial_{x_2} f + v_3 \partial_{x_3} f).$$

For $v_1 \geq 0$ this yields

$$\partial_{x_1} f|_{x_1=0, v_1>0} = -\frac{1}{v_1} (\partial_t F + v_2 \partial_{x_2} F + v_3 \partial_{x_3} F).$$

The other relevant derivatives, like, e.g. $\partial_{x_2} f$, are just given as $\partial_{x_2} F$ at $x_1 = 0$ and $v_1 > 0$.

In the collisionless case, the integrals over $v_1 < 0$ depend only on f_0 and on U , and we write $\Phi(f_0, U)(t, \bar{x})$ for the result of all these integrations. Note that U enters quadratically

into Φ . After implementing all these changes and simplifications, we get

$$\begin{aligned}
\sum_{i=1}^3 \partial_{x_i} p_{ij} &= - \int_{v_1 > 0} v_j \partial_t F dv + U_j \int_{v_1 > 0} \partial_t F dv \\
&\quad + U_1 \int_{v_1 > 0} \frac{v_j}{v_1} (\partial_t F + v_2 \partial_{x_2} F + v_3 \partial_{x_3} F) dv \\
&\quad - \sum_{i=2}^3 \int_{v_1 > 0} u_i v_j \partial_{x_i} F dv - U_j U_1 \int_{v_1 \geq 0} \frac{1}{v_1} (\partial_t F + v_2 \partial_{x_2} F + v_3 \partial_{x_3} F) dv \\
&\quad + U_j \sum_{i=2}^3 U_i \int_{v_1 > 0} \partial_{x_i} F dv + \Phi(f_0, U)(t, \tilde{x}) \\
&= \sum_{i=1}^3 \partial_{x_i} \left(p(\rho) \delta_{ij} - \mu (\partial_{x_i} u_j + \partial_{x_j} u_i) + \frac{2}{3} \mu \operatorname{div} u \delta_{ij} \right) \Big|_{x_1=0} \\
&= NS[\rho, u](t, \tilde{x}).
\end{aligned} \tag{3.6}$$

Observe that this last expression does not only depend on P and U , but also on the derivatives $\partial_{x_i} \rho$, $\frac{\partial^2 u_i}{\partial x_i \partial x_j}$ at $x_1 = 0$.

If we introduce the convenient abbreviations

$$G(t, \tilde{x}, v) = \frac{1}{v_1} F(t, \tilde{x}, v),$$

and

$$\begin{aligned}
G^0(t, \tilde{x}) &= \int_{v_1 \geq 0} G dv, \\
G_j^1(t, \tilde{x}) &= \int_{v_1 \geq 0} v_j G(t, \tilde{x}, v) dv \\
G_{jk}^2(t, \tilde{x}) &= \int_{v_1 \geq 0} v_j v_k G(t, \tilde{x}, v) dv
\end{aligned}$$

the equations (3.6) become

$$\begin{aligned}
NS[\rho, u] - \Phi(f_0, U) &= - [\partial_t + U_2 \partial_{x_2} + U_3 \partial_{x_3}] G_{1j}^2 \\
&\quad + U_j [\partial_t + U_2 \partial_{x_2} + U_3 \partial_{x_3}] G_1^1 \\
&\quad + U_1 (\partial_{x_2} G_{j2}^2 + \partial_{x_3} G_{j3}^2) \\
&\quad - U_j U_1 (\partial_{x_2} G_2^1 + \partial_{x_3} G_3^1) \\
&\quad + U_1 (\partial_t G_j^1 - U_j \partial_t G^0)
\end{aligned} \tag{3.7}$$

In order to "solve" these equations, we have to do two more steps:

- express $NS[\rho, u](t, \tilde{x})$ in terms of f_0, P, U and their derivatives with respect to x_2, x_3 ("inner" derivatives)

choose a class of functions $G(t, \bar{x}, v)$ for which the resulting system of differential-algebraic equations is efficiently solvable.

The first step is straightforward. For the second one, we suggest again to try a discrete velocity approach, i.e.

$$G(t, \bar{x}, v) = \sum_{k=1}^K \alpha_k(t, \bar{x}) \delta_{v^k},$$

where $v^k = (v_1^k, v_2^k, v_3^k)$. By using the definitions of $G^0(t, \bar{x})$, $G_j^1(t, \bar{x})$ and $G_{jk}^2(t, \bar{x})$, (3.4) and (3.5) respectively turn into

$$\sum_{k=1}^K v_1^k \alpha_k(t, \bar{x}) = P(t, \bar{x}) + \Phi_1[f_0](t, \bar{x}) \quad (3.8)$$

$$\sum_{k=1}^K v_j^k v_1^k \alpha_k(t, \bar{x}) = P U_j(t, \bar{x}) + \Phi_2^j[f_0](t, \bar{x}) \quad (3.9)$$

where $\Phi_1[f_0]$ and $\Phi_2^j[f_0]$ are given in terms of f_0 (e.g., $\Phi_1[f_0](t, \bar{x}) = -\int_{v_1 < 0} f(t, 0, \bar{x}, v) dv$), see (3.4) and (3.5). Equation (3.7) becomes

$$\begin{aligned} & \sum_k U_j v_1^k [\partial_t + U_2 \partial_{x_2} + U_3 \partial_{x_3}] \alpha_k(t, \bar{x}) \\ & - \sum_k v_1^k v_j^k [\partial_t + U_2 \partial_{x_2} + U_3 \partial_{x_3}] \alpha_k(t, \bar{x}) \\ & + U_1 \left[\sum_k v_2^k (v_j^k - U_j) \partial_{x_2} \alpha_k + \sum_k v_3^k (v_j^k - U_j) \partial_{x_3} \alpha_k \right] \\ & + U_1 \sum_k (v_j^k - U_j) \partial_t \alpha_k \\ & = NS[\rho, u] - \Phi(f_0, U). \end{aligned} \quad (3.10)$$

We rewrite (3.10) as follows. Let \tilde{V} be the $3 \times K$ -matrix defined by

$$\tilde{V} = (v^1 - U, \dots, v^K - U).$$

After some calculation, (3.10) is seen to be equivalent to

$$\tilde{V} \begin{bmatrix} (U_1 - v_1^1) \partial_t \alpha_1 + (U_1 v_2^1 - U_2 v_1^1) \partial_{x_2} \alpha_1 + (U_1 v_3^1 - U_3 v_1^1) \partial_{x_3} \alpha_1 \\ \vdots \\ (U_1 - v_1^K) \partial_t \alpha_K + (U_1 v_2^K - U_2 v_1^K) \partial_{x_2} \alpha_K + (U_1 v_3^K - U_3 v_1^K) \partial_{x_3} \alpha_K \end{bmatrix} = E, \quad (3.11)$$

where $E := NS - \Phi$. The solution procedure for (3.10) is then clear: First solve the linear equations $\tilde{V} \beta = E$ (for $K = 3$, this is a quadratic system; otherwise it is underdetermined).

and we expect an infinity of solutions, one of which must be chosen by additional criteria). Once $\beta = (\beta_1(t, \hat{x}), \dots, \beta_K(t, \hat{x}))$ is given, one has to solve the first order partial differential equations

$$(U_1 - v_1^j) \partial_t \alpha_j + (U_1 v_2^j - U_2 v_1^j) \partial_{x_2} \alpha_j + (U_1 v_3^j - U_3 v_1^j) \partial_{x_3} \alpha_j = \beta_j.$$

$j = 1, \dots, K$, subject to algebraic side conditions given by (3.8) and (3.9).

Clearly, the solution of (3.11) with these side conditions is in itself a challenge, but, as we have demonstrated, it is a logical way to arrive at smooth isolines connecting the aerodynamic and the kinetic regimes. Numerical experiments will have to be made to investigate the practical feasibility of the boundary conditions which we have suggested here.

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