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Kinetic schemes and initial boundary value problems for the Euler system

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Abstract

We study kinetic solutions, including shocks, of initial and boundary value problems for the EULER equations of gases. In particular we consider moving adiabatic boundaries, which may be driven either by a given path or because they are subjected to forces.

In the latter case we consider a gas contained in a cylinder which is closed by a piston. Here the boundary represents the piston that suffers forces by the incoming and outgoing gas particles. Moreover, we will study periodic boundary conditions.

A kinetic scheme consists of three ingredients: (i) There are periods of free flight of duration τ_M , where the gas particles move according to the free transport equation. (ii) It is assumed that the distribution of the gas particles at the beginning of each of these periods is given by a MAXWELLian. (iii) The interaction of gas particles with a boundary is described by a so called extension law, that determines the phase density at the boundary, and provides additionally continuity conditions for the the fields at the boundary in order to achieve convergence.

The Euler equations result in the limit $\tau_M \to 0$.

We prove rigorous results for these kinetic schemes concerning (i) regularity, (ii) weak conservation laws, (iii) entropy inequality and (iv) continuity conditions for the fields at the boundaries. The study is supplemented by some numerical examples.

This approach is by no mean restricted to the EULER equations or to adiabatic boundaries, but it holds also for other hyperbolic systems, namely those that rely on a kinetic formulation.

1 Introduction

In this paper we study initial and boundary value problems for the EULER system of gases which rely on the evolution of the phase density of the gas atoms. The phase density is determined by a kinetic transport equation, the Maximum Entropy Principle and appropriate boundary conditions. The methods that we will discuss here are more general than those which are presented in the papers [7] and [8] by DREYER and KUNIK, where the pure initial value problem and the initial- and boundary value problem with moving adiabatic boundaries were also studied for the EULER system.

It is important to note that the basic ideas of this study can also be applied to other hyperbolic systems and to more general boundary data. For example, we mention the evolution of temperature and heat flux in a BOSE gas of phonons. At low temperature the corresponding field equations constitute a hyperbolic system which was solved by DREYER and KUNIK in [10] and [11]. The hyperbolic systems that can be treated by the kinetic method are those which may be generated from kinetic transfer equations and the Maximum Entropy Principle, see [2], [6] and [15]. Since these systems lead to a convex entropy function, they enable several rigorous mathematical results, see for example [12], [5].

Kinetic schemes for the EULER system were already studied by PERTHAME in [16] and [17]. Some interesting links between the EULER system and the so called kinetic BGK-model, which is introduced in [1], are discussed in the textbooks by CERCIG-NANI [3] and by GODLEWSKI & RAVIART [13].

The most important feature of the current paper is the consistent incorporation of boundary conditions for the EULER system as well as for its kinetic schemes. The EULER system constitutes a hyperbolic system for the five variables ρ - mass density, \boldsymbol{v} - velocity, T - temperatue. For simplicity we consider often only one space dimension, and the vector \boldsymbol{v} reduces to one variable v. In case of a non-moving impermeable wall at x = 0 the only possible boundary condition for the EULER system is

$$v(t,0) = 0$$
. (1)

Since mass flux, energy flux and entropy flux are all proportional to v, such a wall is adiabatic too. In particular we conclude that boundary data for the temperature cannot be prescribed in this case, see [8]. However, from the viewpoint of the kinetic regime, the equation 1 does not imply an adiabatic wall, because here there are many kinetic realization of the condition (1). Even boundary data for the temperature are possible in the kinetic range. In other words, (1) is not equivalent to the adiabatic boundary condition in the kinetic regime. Therefore it is not suprising that we shall present two different approaches in order to realize the boundary condition (1), and both approaches reduce to the same EULERian limit.

Next we describe the characteristic features of a kinetic scheme. Kinetic schemes rely on the fact that all macroscopic quantities that appear in the EULER system can be represented by integrals over the atomic velocity space of the gas particles. The central quality under the integrals is the phase denisty f(t, x, c) which gives the number density of particles with atomic speed c at (t, x). A kinetic scheme determines the phase density so that the resulting macroscopic fields solve the given initial and boundary value problem of the EULER system. The details are discussed in section 2.1.

This approach confronts us with the problem to relate the given initial and boundary data for the EULER system to the corresponding initial and boundary data for the phase density. The establishment of these relations for the pure initial value problem is an easy task that will be resumed in section 2.2.

The formulation of appropriate boundary data is not an easy task and this is the main objective of the current study. For the determination of the phase density $f(t, 0, c) = f^B(t, c)$ at the boundary x = 0, it is useful to split the boundary phase density into two parts, one for the incoming particles with c < 0, which turns out to be completely determined by the phase density at the preceding times, and one for the outgoing particles with c > 0 according to

$$f^{B}(t, c) = \begin{cases} f^{in}(t, c) & \text{for } c < 0, \\ f^{out}(t, c) & \text{for } c > 0. \end{cases}$$
(2)

In contrast to the known incoming part f^{in} we must determine f^{out} by an extra condition that we will call an *extension law* in section 2.3. We will show in this study, that there are different extension laws that all imply the same macroscopic boundary conditions. This feature is related to the already mentioned fact that the macroscopic boundary condition (1) has many kinetic realizations.

In section 2.4 we will derive two extension laws for an adiabatic wall at rest. The first extension law was already studied in [8] and expresses a simple reflection law of the gas atoms. In order to formulate the second extension law we assume in section 2.4 that the phase density at the boundary for the outgoing particles is given by a MAXWELLian with respect to three *auxiliary fields* $\rho^A(t)$, $v^A(t)$ and $T^A(t)$, where continuity and boundary conditions yield algebraic equations for the auxiliary fields.

In section 2.5 we consider a single wall at rest and formulate the corresponding kinetic scheme. We derive its mathematical properties in section 3, including conservation laws, the entropy inequality, regularity and continuity conditions at the boundary.

The sections 4 and 5 are devoted to moving boundaries. In particular, we are interested in free moving boundaries whose path is not given explicitly, but is part of the solution of the problem. Moreover, we discuss periodic boundary conditions. To illustrate the main results we study some numerical examples in section 6.

2 Kinetic solutions for initial and boundary value problems

2.1 The EULER system and moment definitions

We consider a mon-atomic ideal gas, and we describe its state at a space time point (t, x) by the variables

$$\rho > 0$$
 — mass density, v — velocity, $T > 0$ — temperature.

Sometimes it is useful to replace the temperature T by the pressure p of the gas as a variable. T and p are related by the ideal gas law $p = \rho T$. We assume that the variables evolve according to the EULER equations. For one space dimension, a case that we will consider exclusively, the EULER equations read in regular points

$$\partial_t \rho + \partial_x (\rho v) = 0,$$

$$\partial_t (\rho v) + \partial_x (\rho v^2 + p) = 0,$$

$$\partial_t (\frac{1}{2}\rho v^2 + \frac{d}{2}p) + \partial_x (\frac{1}{2}\rho v^3 + \frac{d+2}{2}pv) = 0.$$
(3)

On singular surfaces that move with the normal speed V_S there are the well known jump conditions, see [4] and [18],

$$\begin{aligned} &-V_s[\![\rho]\!] &+ [\![\rho v]\!] &= 0, \\ &-V_s[\![\rho v]\!] &+ [\![\rho v^2 + p]\!] &= 0, \\ &-V_s[\![(\frac{1}{2}\rho v^2 + \frac{d}{2}p)]\!] &+ [\![(\frac{1}{2}\rho v^3 + \frac{d+2}{2}pv)]\!] &= 0. \end{aligned}$$

Here, d may assume the values 1, 2 or 3. The objective of this study is the solution of initial and boundary value problems for the EULER system. In order to establish uniqueness for discontinuous solutions we use the second law of thermodynamics as a selection criterion. To this end we introduce the entropy density h and the entropy flux ϕ according to

$$h(\rho, T) := \frac{d}{2}\rho \ln(T) - \rho \ln\rho + \frac{d}{2}\rho + \frac{d}{2}\rho \ln(2\pi), \quad \phi(\rho, v, T) = vh(\rho, T), \quad (5)$$

and the second law reads

$$\partial_t h + \partial_x \phi = 0 \quad \text{and} \quad -V_s \llbracket h \rrbracket + \llbracket \phi \rrbracket \ge 0,$$
(6)

respectively.

To simplify the notation we introduce the vectors of densities $\mathbf{u} = (u_0, u_1, u_2)^T$ and of fluxes $\mathbf{F} = (F_0, F_1, F_2)^T$ by

$$\mathbf{u}(\rho, v, T) := \left(\rho, \rho v, \frac{1}{2}\rho v^2 + \frac{d}{2}\rho T\right)^T \quad \text{and} \quad \mathbf{F}(\mathbf{u}) := \left(\rho, \rho v, \frac{1}{2}\rho v^3 + \frac{d+2}{2}\rho T v\right)^T (\mathbf{u})$$
(7)

Since the vector of densities \mathbf{u} as function of ρ , v and T is invertible we can express the entropy h and the entropy flux ϕ as function of \mathbf{u} . Thus the abbreviated EULER system with entropy condition reads

$$\begin{aligned} \partial_t \mathbf{u} &+ \partial_x \mathbf{F}(\mathbf{u}) &= 0, \quad -V_s \llbracket \mathbf{u} \rrbracket &+ \llbracket \mathbf{F}(\mathbf{u}) \rrbracket &= 0, \\ \partial_t h(\mathbf{u}) &+ \partial_x \phi(\mathbf{u}) 7 &= 0, \quad -V_s \llbracket h(\mathbf{u}) \rrbracket &+ \llbracket \phi(\mathbf{u}) \rrbracket &\geq 0. \end{aligned}$$

Our strategy to solve the EULER system relies on the kinetic representation of all quantities appearing here. The kinetic representation reduces the evolution of these quantities to the evolution of the phase density f(t, x, c) which gives at any space time point (t, x) the number density of gas atoms with the atomic speed c. For simplicity regarding the notation we consider in the following sections only the one-dimensional case, i.e. $\mathbf{c} = (c, 0, 0)^T$ which implies d = 1. However, the numerical calculations are carried out for the general case with $\mathbf{c} = (c_1, c_2, c_3)^T$ and d = 3.

In order the establish the kinetic representation we define at first the integrals

$$\mathbf{u}_f(t, x) := - + \int_{-\infty}^{+\infty} \mathbf{m}(c) f(t, x, c) dc$$
(9)

$$\mathbf{F}_f(t, x) := - + \int_{-\infty}^{+\infty} c \mathbf{m}(c) f(t, x, c) dc$$
(10)

$$h_f(t, x) := -\int_{-\infty}^{+\infty} (f \ln f)(t, x, c) dc$$
(11)

$$\phi_f(t, x) := -\int_{-\infty}^{+\infty} c(f \ln f)(t, x, c) \, dc.$$
(12)

as functions of x, t and f, where **m** denotes the function

$$\mathbf{m}(c) := \left(1, c, \frac{c^2}{2}\right)^T.$$
(13)

In general the evolution of the phase density is described by the BOLTZMANN equation. However, this aspect does not interest us here. Instead, we pose the question whether it is possible to use the kinetic representation (9) - (12) in order to approach a solution of the EULER system.

To this end we recall that the phase density f, that maximizes the entropy density h_f under the constraint of a prescribed vector \mathbf{u}_f , is given by the MAXWELLian phase density

$$f(t, x, c) = w_M(\mathbf{u}, c) = \frac{\rho(\mathbf{u})}{\sqrt{2\pi T(\mathbf{u})}} \exp\left(\frac{-(c - v(\mathbf{u}))^2}{2T(\mathbf{u})}\right).$$
(14)

The MAXWELLian reflects the local equilibrium of the gas. If we insert the MAXWELLian phase density into the kinetic integrals (9) - (12) we obtain for any vector $\mathbf{u} = (u_0, u_1, u_2)^T \in \mathbb{R}^3$ with $u_0 > 0$ and $u_1^2 < 2u_0u_2$ the identities

$$\mathbf{u} = + \int_{-\infty}^{+\infty} \mathbf{m}(c) w_M(\mathbf{u}, c) dc,$$

$$\mathbf{F}(\mathbf{u}) = + \int_{-\infty}^{+\infty} c \mathbf{m}(c) w_M(\mathbf{u}, c) dc,$$

$$h(\mathbf{u}) = - \int_{-\infty}^{+\infty} \mathbf{m}(c) (w_M \ln w_M)(\mathbf{u}, c) dc,$$

$$\phi(\mathbf{u}) = - \int_{-\infty}^{+\infty} c \mathbf{m}(c) (w_M \ln w_M)(\mathbf{u}, c) dc.$$
(15)

2.2 The kinetic scheme for the pure initial value problem

The kinetic solution of the EULER system is best illustrated for the pure initial value problem.

- **Scheme 2.2.1** 1. We choose a constant $\tau_M > 0$ and we consider the equidistant times $t_n = n\tau_M$, for n = 0, 1, 2, ...
 - 2. At $t_0 = 0$ we start with initial data $\mathbf{u}_0(x)$ and we define $f(0, x, c) = w_M(\mathbf{u}_0(x), c)$.
 - 3. For $0 < \tau \leq \tau_M$ and $t = t_n + \tau$ the gas particles move according to the collision free kinetic transport equation

$$\frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = 0. \tag{16}$$

We choose the initial phase density $f(t_n, x, c) = w_M(\mathbf{u}(t_n, x), c)$, and we obtain the solution

$$f(t_n + \tau, x, c) = f(t_n, x - c\tau, c) = w_M(\mathbf{u}(t_n, x - c\tau), c).$$
(17)

Then we calculate \mathbf{u}_f , \mathbf{F}_f , h_f , ϕ_f for $0 < \tau \leq \tau_M$ and $t = t_n + \tau$.

4. We proceed with step 3 for n + 1.

For small τ_M the resulting densities and fluxes can regarded as a good approximation of the solution of the EULER system. For more details we refer the reader to [7] and [8]. In the following subsection we will generalize the scheme to initial and boundary value problems.

2.3 Discussion of initial and boundary value problems

For a first illustration of the initial and boundary value problem we consider a half space with a non-moving boundary at x = 0. More precisely we consider the space time region

$$\Omega := \{ (t, x) : t \ge 0, x \ge 0 \}.$$
(18)

The kinetic solution of the EULER system consists of several pieces: We choose a constant $\tau_M > 0$ and consider the equidistant times $t_n = n\tau_M$, for n = 0, 1, 2, ... Within the intervals $t_n < t \leq t_n + \tau_M$ the gas particles move according to the collision free transport equation

$$\frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = 0, \tag{19}$$

except when they interact with the boundary at x = 0. Since there are no interactions between gas particles in this interval we call the full time interval $t_n < t \leq t_n + \tau_M$ a period of free flight. The explicit procedure of determining the phase density will be explained in detail later on. If this problem is solved we can use the phase density to calculate the thermodynamic fields \mathbf{u}_f . At the times $t_n = n\tau_M$ we stop and use $u_f(t_n + \tau_M, x)$ as constrains for the maximization of the entropy. The resulting phase density is obviously the MAXWELLian

$$w_M\left(u_f\left(t_n+\tau_M,\,x\right),\,c\right)\tag{20}$$

which in turn is used as the initial value for the next period of free flight. The times t_n are called maximization times. Next we study the periods of free flight seriously. The equation (19) gives rise to micro characteristics that relate for given c any point (t, x) either to the initial axes t = 0 or to the boundary at x = 0 by straight lines along which every solution of (19) is a constant. The micro characteristics have the generic form

$$t' \rightsquigarrow x' = x - c(t - t'), \tag{21}$$

and we thus may write

$$f(t, x, c) = f(t', x', c).$$
(22)



Figure 1: micro characteristics relating the initial- or boundary line

Figure 1 shows three micro characteristics for three different values of c which all start in the point $(t_n + \bar{\tau}, \bar{x})$. If $c < \bar{x}/\bar{\tau}$, the micro characteristic intersects the initial axes at $(t', x') = (t_n, \bar{x} - c\bar{\tau})$, and we obtain

$$f(t_n + \tau, x, c) = f(t_n, x - \tau c, c) = w_M(\mathbf{u}(t_n, x), c).$$
(23)

In this case the phase density can be calculated at time $t_n + \tau$ from the fields **u** at the former time t_n . If $c > \bar{x}/\bar{\tau}$, the micro characteristic intersects the boundary at $(t', x') = (t_n + \bar{\tau} - \bar{x}/c, 0)$. Here we obtain

$$f(t_n + \tau, x, c) = f(t_n + \tau - \frac{x}{c}, 0, c).$$
(24)

On the right hand side of (24) there appears the phase density of the boundary. Its determination will be discussed next. We call the phase density of the boundary simply *boundary density* and we write

$$f^B(t, c) = f(t, 0, c).$$
 (25)

We observe that there are two different types of micro characteristics which may end in given point of the boundary. A characteristic with c < 0 corresponds to *incoming* particles. For c < 0 the boundary density can be calculated at time $t_n + \bar{\tau}$ from the data at the former maximization time t_n , viz.

$$f^{B}(t_{n}+\tau, c) = f(t_{n}, -\tau c, c) = w_{M}(\mathbf{u}(t_{n}, -\tau c), c) \qquad \forall c < 0.$$
(26)

However, the part of the boundary density that corresponds to *outgoing* particles, i.e. c > 0, can not be calculated from data at former times. In order to exhibit the

fundamental difference between the two cases c > 0 and c < 0 we write

$$f^{B}(t, c) = \begin{cases} f^{in}(t, c) & \text{for } c < 0, \\ f^{out}(t, c) & \text{for } c > 0. \end{cases}$$
(27)

As it is indicated by the upper indices, f^{in} and f^{out} correspond to the incoming and outgoing particles, respectively. The determination of f^{out} require the prescription of boundary conditions. The problem of reasonable initial and boundary conditions that guarantee existence and uniqueness of a solution of the EULER system is a complicate problem that will not be discussed here. Rather we start from the assumption that this problem has already been solved, and we pose the question how the boundary data can be realized by the microscopic motion of the gas particles in order to determine f^{out} . This realization can be done in several ways and it is called *extension law*, because it leads to an extension of f^{in} to the complete boundary density f^B .

We conclude this section with an important remark concerning the maximization times $t_n > 0$. At first we consider an inner space time point (t_n, x) with x > 0. If we approach t_n from the left, the phase density $f(t_n, x, c)$ is given by

$$\lim_{\tau \to 0^+} f(t_n - \tau, x, c) = \begin{cases} f(t_n - \tau_M, x - \tau_M c, c) & \text{for } c < x/\tau_M, \\ f(t_n - \frac{x}{c}, 0, c) & \text{for } c > x/\tau_M. \end{cases}$$
(28)

If we approach t_n from the right, the phase density approaches a MAXWELLian and we write

$$\lim_{\tau \to 0^+} f(t_n + \tau, x, c) = w_M(\mathbf{u}(t_n, x), c).$$
(29)

Note that we define $f(t_n, x, c)$ by the equation (28). This definition interprets the maximization times t_n as the end points of the periods of free flight. Corresponding to (28) and (29) there are also two limits of the boundary density $f^B(t_n, cc)$ at the maximization times. For f^{in} we obtain for any c < 0

$$f^{in}(t_n, c) = \lim_{\tau \to 0^+} f^{in}(t_n - \tau, c) = f(t_n - \tau_M, -\tau_M c, c), \qquad (30)$$

$$\lim_{\tau \to 0^+} f^{in}(t_n + \tau, c) = w_M(\mathbf{u}(t_n, 0), c) \,. \tag{31}$$

2.4 Extension laws for the EULER system with an adiabatic wall at rest

For a first and simple discussion of reasonable extension laws we consider a lower adiabatic wall at x = 0. From the point of view of the EULER system, an impermeable wall at rest, i.e. v(t, 0) = 0, implies that the mass flux, the energy flux and the

entropy flux vanish simultaneously at the boundary, see (5) and (7). In particular, this means that an impermeable wall at rest is adiabatic. In the kinetic range this can be realized by the extension law

$$f^{out}(t_n + \tau, c) = f^{in}(t_n + \tau, -c) \qquad \forall \ c > 0.$$
(32)

This law expresses a simple reflection law, i.e. an incoming gas particle with speed c will be reflected at the adiabatic wall so that after the encounter it has the speed -c. This extension law was investigated by DREYER and KUNIK in [8]. The extension law (32) implies that the conditions for an adiabatic wall at rest, namely

$$\int_{-\infty}^{+\infty} c f^B(t, c) \ dc = 0, \\ \int_{-\infty}^{+\infty} \frac{1}{2} c^3 f^B(t, c) \ dc = 0, \\ \int_{-\infty}^{+\infty} c \left(f^B \ln f^B \right)(t, c) \ dc = 0,$$
(33)

are identically satisfied. Note that the extension law (32) implies that the conditions (33) are satisfied during the total periods of free flight. This is not a necessary property in order to obtain a solution of the EULER system. We illustrate this fact by studying another extension law that is also used to solve the same boundary value problem. For this purpose we assume, that the boundary density of the outgoing particles is given by a MAXWELLian with respect to three *auxiliary fields* ρ^A , v^A and T^A , in other words

$$f^{out}(t, c) = w_M(\mathbf{u}^A(t), c) \qquad \forall \ c > 0,$$
(34)

where \mathbf{u}^A is related to ρ^A , v^A and T^A as \mathbf{u} is related to ρ , v and T. The three auxiliary fields are determined by the requirements

$$\int_{-\infty}^{+\infty} c f^B(t, c) \ dc = 0, \\ \int_{-\infty}^{+\infty} \frac{1}{2} c^3 f^B(t, c) \ dc = 0 \quad \text{and} \quad v^A(t) = 0.$$
(35)

The conditions $(35)_1$ and $(35)_2$ are identical to the conditions $(33)_1$ and $(33)_2$ of the first extension law. However, the condition $(35)_3$ does not imply a vanishing entropy flux at the wall. If we were to replace $v^A(t) = 0$ by the condition $(33)_3$, then we end up with a highly nonlinear algebraic system for the auxiliary fields $\mathbf{u}^A(t)$ which cannot be resolved easily. For that reason we have used the condition $v^A(t) = 0$. But it is important to note that (33) and (35) both satisfy the boundary condition $\lim_{x\to 0^+} v(t,x) = 0$ in the kinetic range, and numerical studies will lead us to the conjecture that both conditions yield the same EULERian limit $\tau_M \to 0$, which satisfies the adiabatic boundary condition. For the exploitation of the extension law (34), (35) we write explicitly

$$\int_{0}^{+\infty} c w_M(\mathbf{u}^A(t), c) \, dc = -\int_{0}^{0} c f^{in}(t, c) \, dc =: -I_1(t)$$

$$\int_{0}^{+\infty} \frac{1}{2} c^3 w_M(\mathbf{u}^A(t), c) \, dc = -\int_{-\infty}^{0} \frac{1}{2} c^3 f^{in}(t, c) \, dc =: -I_3(t).$$
(36)

Note that the left hand sides of these equations represent algebraic expressions for the auxiliary fields ρ^A and T^A at time $t = t_n + \tau$, while the right hand sides are known from the densities at the former time t_n . A straight forward calculation leads to

$$T^{A}(t) = \frac{I_{3}(t)}{I_{1}(t)}$$
 and $\rho^{A}(t) = -I_{1}(t)\sqrt{\frac{2\pi}{T^{A}(t)}}$. (37)

The definitions of $I_1(t)$ and $I_3(t)$ imply immediately $I_1(t) < 0$ and $I_3(t) < 0$, so that $\rho^A(t)$ and $T^A(t)$ result as positive quantities. Note, that the auxiliary fields $\rho^A(t)$ and $T^A(t)$ do not coincide with the boundary values $\rho^B(t)$ and $T^B(t)$ which result from the kinetic scheme.

We conclude this section with some general remarks regarding the differences of the two considered extension laws. While the first extension law relies on the kind of reflection of the individual gas particles at the adiabatic wall, the second extension law takes only care for the prescribed boundary condition v(t,0) = 0, but do not have such a suggestive physical interpretation. In particular, both laws are not equivalent in the kinetic range, but they coincide in the EULER range. In other words, the boundary condition v(t,0) = 0 is equivalent to the reflection at the adiabatic boundary only in the EULER range, but not in the kinetic range.

Regarding the initial and boundary value problem of an ideal gas of material particles, the second extension law using the auxiliary fields at the boundaries seems to be somehow artificial. However, for other kinetic initial and boundary value problems there is in general no reflection law, whereas extension laws which rely on auxiliary fields may still be used. This situation is met in the phonon gas, a case which has extensively been studied by DREYER and KUNIK in [10] and [11].

2.5 Kinetic schemes for a lower adiabatic wall at rest

We proceed with the half space problem and the boundary condition

$$v(t,0) = 0$$
 (38)

for the velocity at x = 0. We introduce the abbreviations

$$f_n^I(x, c) := w_M(u(t_n, x), c), \quad f_n^B(\tau, c) := f^B(t_n + \tau, c).$$
(39)

The functions f_n^I and f_n^B are the initial phase density and the boundary density for the *n*-th period of free flight, respectively. The initialization of the kinetic scheme is given by

- 1. We start with bounded and integrable initial values $\mathbf{u}_0(x)$ satisfying $\rho_0(x) \ge \varepsilon > 0$, $T_0(x) \ge \varepsilon > 0$ where ε is a constant.
- 2. We choose a fixed time τ_M of free flight, so that the entropy will be maximized at the equidistant times $t_n := n\tau_M$, $n \in \mathbb{N}$.
- 3. We choose one of the two extension laws from the above or any other one that implies (38).

Scheme 2.5.1

1. At $t_0 = 0$ we define

$$f(0, x, c) = w_M(\mathbf{u}_0(x), c).$$
(40)

- 2. We solve the n-th free flight problem for $t = t_n + \tau$, $0 < \tau \leq \tau_M$ in three steps
 - (a) We calculate the boundary density for the incoming particles (c < 0) by means of free flight

$$f_n^{in}(\tau, c) = f_n^I(-\tau c, c).$$
(41)

- (b) We use the extension law to determine the boundary density for the outgoing particles (c > 0).
- (c) Every macroscopic field results as a sum of two integrals, which contain the initial phase density and the boundary density, respectively:

$$\begin{aligned}
\mathbf{u}(t_{n} + \tau, x) &:= \mathbf{u}_{n}^{I}(\tau, x) + \mathbf{u}_{n}^{B}(\tau, x) \\
\mathbf{F}(t_{n} + \tau, x) &:= \mathbf{F}_{n}^{I}(\tau, x) + \mathbf{F}_{n}^{B}(\tau, x) \\
h(t_{n} + \tau, x) &:= h_{n}^{I}(\tau, x) + h_{n}^{B}(\tau, x) \\
\phi(t_{n} + \tau, x) &:= \phi_{n}^{I}(\tau, x) + \phi_{n}^{B}(\tau, x)
\end{aligned} \tag{42}$$

with

$$\begin{aligned} \mathbf{u}_{n}^{I}(\tau, x) &:= + \int_{-\infty}^{x/\tau} \mathbf{m}(c) f_{n}^{I}(x - \tau c, c) \, dc, \\ \mathbf{u}_{n}^{B}(\tau, x) &:= + \int_{x/\tau}^{+\infty} \mathbf{m}(c) f_{n}^{B}(\tau - x/c, c) \, dc, \\ \mathbf{F}_{n}^{I}(\tau, x) &:= + \int_{-\infty}^{x/\tau} c \mathbf{m}(c) f_{n}^{I}(x - \tau c, c) \, dc, \\ \mathbf{F}_{n}^{B}(\tau, x) &:= + \int_{x/\tau}^{-\infty} c \mathbf{m}(c) f_{n}^{B}(\tau - x/c, c) \, dc, \\ h_{n}^{I}(\tau, x) &:= - \int_{-\infty}^{x/\tau} (f_{n}^{I} \ln f_{n}^{I})(x - \tau c, c) \, dc, \\ h_{n}^{B}(\tau, x) &:= - \int_{x/\tau}^{+\infty} (f_{n}^{B} \ln f_{n}^{B})(\tau - x/c, c) \, dc, \\ \phi_{n}^{I}(\tau, x) &:= - \int_{-\infty}^{-\infty} c(f_{n}^{I} \ln f_{n}^{I})(x - \tau c, c) \, dc, \\ \phi_{n}^{B}(\tau, x) &:= - \int_{x/\tau}^{-\infty} c(f_{n}^{I} \ln f_{n}^{I})(x - \tau c, c) \, dc, \\ \phi_{n}^{B}(\tau, x) &:= - \int_{x/\tau}^{-\infty} c(f_{n}^{B} \ln f_{n}^{B})(\tau - x/c, c) \, dc. \end{aligned}$$

3. We proceed with step 3 for n + 1.

Note that f^B and f_n^B enter the momentum integrals only for c > 0, i.e. only their part f^{out} is used. In the case of the second extension law from the last section, step 2b reduces to the calculation of the auxiliary fields ρ^A and T^A by means of the equations (37).

We call a pentupel $(\tau_M, u_f, F_f, h_f, \phi_f)$ a kinetic approximation. If there is no confusion we omit the index f.

To complete this section we discuss briefly the case d = 3, where the one dimensional atomic speed c and the space variable x must be replaced by the vectors $\mathbf{c} = (c_1, c_2, c_3)$ and $\mathbf{x} = (x_1, x_2, x_3)$, respectively. However, also in this case we consider all macroscopic fields as one dimensional. Certainly, we have to suppose translational symmetry of the phase density (with respect to x_2, x_3, c_2 and c_3) and therefore translational symmetry of all macroscopic fields (with respect to x_2, x_3). These symmetries allow us to formulate kinetic schemes, including the extension law, analogously to the case d = 1. Next we list the necessary changes in scheme 2.5.1 under the assumption that we use an extension law with auxiliary fields. We write x and c instead of x_1 and c_1 , respectively. Furthermore we use the abbreviation

$$\mathbf{M}(\mathbf{u}, c) = \mathbf{m}(c)w(\mathbf{u}, c) + \left(0, 0, T(\mathbf{u})\right)^T w(\mathbf{u}, c)$$
(44)

in order to replace the equations $(43)_1$ - $(43)_4$ by

$$\mathbf{u}_{n}^{I}(\tau, x) := \int_{-\infty}^{x/\tau} \mathbf{M}\left(\mathbf{u}(t_{n}, x - \tau c), c\right) dc,
\mathbf{u}_{n}^{B}(\tau, x) := \int_{x/\tau}^{+\infty} \mathbf{M}\left(\mathbf{u}^{A}(t_{n} + \tau - \frac{x}{c}), c\right) dc,
\mathbf{F}_{n}^{I}(\tau, x) := \int_{-\infty}^{x/\tau} c \mathbf{M}\left(\mathbf{u}(t_{n}, x - \tau c), c\right) dc,
\mathbf{F}_{n}^{B}(\tau, x) := \int_{x/\tau}^{+\infty} c \mathbf{M}\left(\mathbf{u}^{A}(t_{n} + \tau - \frac{x}{c}), c\right) dc.$$
(45)

At first glance the equations (45) and $(43)_1$ -(43)₄ look totally different. The simple reason is that, while (43) is valid for any extension law, whereas a special extension law has already been used in the equations (45). The steps 2a and 2b of the scheme 2.5.1 reduce to the calculation of the auxiliary fields $\mathbf{u}^A(t)$, which we determine also in the case d = 3 by the requirement, that the fluxes of mass and energy and the auxiliary velocity $v^A(t)$ vanish. We obtain after a straight forward calculation the expressions

$$v^{A}(t) = 0, \quad T^{A}(t) = \frac{1}{2} \frac{I_{3}(t)}{I_{1}(t)}, \quad \rho^{A} = -I_{1}(t) \sqrt{\frac{2\pi}{T^{A}(t)}},$$
 (46)

where $I_1(t)$ and $I_3(t)$ are components of the vector $\mathbf{I}(t) = (I_1, I_2, I_3)^T(t)$ which is given by

$$\mathbf{I}(t_n + \tau) = \int_{-\infty}^{0} \mathbf{M} \Big(\mathbf{u}(t_n, -\tau c), c \Big) \, dc.$$
(47)

3 Analytical properties of the kinetic scheme

In this section we derive analytical properties of the scheme 2.5.1. To this end we restrict the class of admissible extension laws. We only consider so called *normal* extension laws and these have the following two properties

- 1. $f^{out}(t_n + \tau, c)$ is smooth with respect to c,
- 2. $c^i f^{out}(t_n + \tau, c)$ is integrable with respect to c for $i \in \{0, 1, 2, 3\}$.

3.1 The periods of free flight

Up to now we have defined the periods of free flight by the intervals $t_n < t_n + \tau \leq t_n + \tau_M$. In order to remind the reader that the maximization times must be

studied separately, we consider in this section only the *open* intervals $(t_n, t_n + \tau_M)$. Furthermore, for shortness we omit the lower index n at u_n^I , u_n^B and at the other appearing fields.

Lemma 3.1.1 Within a period of free flight the densities \mathbf{u} , h and their fluxes \mathbf{F} , ϕ are smooth in space and time and here they satisfy the conservation laws

$$\partial_t \mathbf{u} + \partial_x \mathbf{F} = 0 \quad and \quad \partial_t h + \partial_x \phi = 0.$$
 (48)

Proof: We replace in (43) the integration variable c by $y = x - \tau c$ and $s = \tau - x/c$, respectively. There follows

$$\mathbf{u}^{I}(\tau, x) = \frac{1}{\tau} \int_{-\infty}^{0} \mathbf{m}(\frac{x-y}{\tau}) f^{I}(y, \frac{x-y}{\tau}) \, dy, \qquad (49)$$

$$u^{B}(\tau, x) = \frac{x}{(\tau - s)^{2}} \int_{0}^{+\infty} \mathbf{m}(\frac{x}{\tau - s}) f^{B}(s, \frac{x}{\tau - s}) \, ds.$$
(50)

The smoothness of the phase densities f^I and f^B with respect to the atomic speed *c* implies the smoothness of **u** with respect to *x* and *t*. The smoothness of *h*, **F** and ϕ follow by a similar argument. In order to prove the equation (48)₁ we differentiate formally the fields **u** and **F** with respect to τ and *x* and apply the chain rule to obtain

$$egin{aligned} \partial_{ au} \mathbf{u}^I(t_n+ au,\,x) &= &+ \int\limits_{-\infty}^{x/ au} \mathbf{m}(c) \partial_{ au} f^I_n(x- au c,\,c) \,\, dc - rac{x}{ au^2} \mathbf{m}(rac{x}{ au}) f^I_n(0,\,rac{x}{t}) \ &= &- \int\limits_{-\infty}^{x/ au} c \mathbf{m}(c) \partial_x f^I_n(x- au c,\,c) \,\, dc - rac{x}{ au^2} \mathbf{m}(rac{x}{ au}) f^I_n(0,\,rac{x}{t}), \end{aligned}$$

$$\partial_ au {}^B(t_n+ au,\,x) \quad = \quad + \int\limits_{x/ au}^{+\infty} {f m}(c) \partial_ au f^B_n(au-x/c,\,c) \,\, dc + rac{x}{ au^2} {f m}(rac{x}{ au}) f^B_n(0,\,rac{x}{ au}),$$

$$\partial_x \mathbf{F}^I(t_n+ au,\,x) \quad = \quad + \int\limits_{-\infty}^{x/ au} c \mathbf{m}(c) \partial_x f^I_n(x- au c,\,c) \,\, dc + rac{x}{ au^2} \mathbf{m}(rac{x}{ au}) f^I_n(0,\,rac{x}{ au}),$$

$$egin{aligned} \partial_x \mathbf{F}^B(t_n+ au,\,x) &= &+ \int\limits_{x/ au}^{+\infty} c \mathbf{m}(c) \partial_x f^B_n(au-x/c,\,c) \,\,dc - rac{x}{ au^2} \mathbf{m}(rac{x}{ au}) f^B_n(0,\,rac{x}{ au}) \ &= &- \int\limits_{x/ au}^{+\infty} \mathbf{m}(c) \partial_ au f^B_n(au-x/c,\,c) \,\,dc - rac{x}{ au^2} \mathbf{m}(rac{x}{ au}) f^B_n(0,\,rac{x}{ au}) \,. \end{aligned}$$

There follow the two systems of conservation laws

$$\partial_{\tau} \mathbf{u}^{I} + \partial_{x} \mathbf{F}^{I} = 0 \quad \text{and} \quad \partial_{\tau} \mathbf{u}^{B} + \partial_{x} \mathbf{F}^{B} = 0.$$
 (51)

The summation of both systems yields $(48)_1$. The proof of equation $(48)_2$ can be carried out analogously. Note that the differentiations can also be applied rigorously to the transformed integrals (49) and (50).

It is important to note that the equations $(48)_1$ do not constitute a local hyperbolic system for the fields **u**, because the fluxes **F** at $(t_n + \tau, x)$ depend globally on the functions $\mathbf{u}(t_n, \cdot)$.

Remark 3.1.2 Within a period of free flight the fields \mathbf{u} , h, \mathbf{F} and ϕ can be extended continuously to the boundary x = 0. We obtain in the limit $x \to 0$

$$\mathbf{u}(\tau, 0) = \int_{-\infty}^{0} \mathbf{m}(c) f^{I}(-\tau c, c) \, dc + \int_{0}^{+\infty} \mathbf{m}(c) f^{B}(\tau, c) \, dc, \qquad (52)$$

and analogous results follow for \mathbf{F} , h and ϕ .

3.2 The maximization times

In this section we consider an arbitrary but fixed maximization time $t_n > 0$. At first we investigate the properties of the fields at the *inner* points (t_n, x) with x > 0.

Lemma 3.2.1 Let be x > 0. Then the densities **u** are continuous at (t_n, x) and the entropy h increases with time, in other words

$$\lim_{\tau \to 0^+} \mathbf{u}(t_n + \tau, x) = \lim_{\tau \to 0^+} \mathbf{u}(t_n - \tau, x), \quad \lim_{\tau \to 0^+} h(t_n + \tau, x) \ge \lim_{\tau \to 0^+} h(t_n - \tau, x).$$
(53)

Proof: We use the equations (15) and the definitions (42) and (43), and we obtain

$$\lim_{\tau \to 0^+} \mathbf{u}(t_n + \tau, x) = \int_{-\infty}^{+\infty} \mathbf{m}(c) w_M(\mathbf{u}(t_n, x), c) \, dc = \mathbf{u}(t_n, x),$$
$$\lim_{\tau \to 0^+} \mathbf{u}(t_n - \tau, x) = \int_{-\infty}^{+\infty} \mathbf{m}(c) f(t_n, x, c) \, dc = \mathbf{u}(t_n, x).$$

Analogously we obtain for the entropy density h the limits

$$\lim_{\tau \to 0^+} h(t_n + \tau, x) = -\int_{-\infty}^{+\infty} (w_M \ln w_M) (\mathbf{u}(t_n, x), c) \, dc,$$
$$\lim_{\tau \to 0^+} h(t_n - \tau, x) = -\int_{-\infty}^{+\infty} (f \ln f) (t_n, x, c) \, dc.$$

Next we define for an arbitrary c the expressions

$$a = a(c) := w_M(\mathbf{u}(t_n, x), c) \text{ and } b = b(c) := f(t_n, x, c).$$
 (54)

If we apply TAYLORs formula to the function $x \ln x$ at the point x = a(c), we obtain

$$b\ln b - a\ln a = (1 + \ln a)(b - a) + \frac{1}{2\xi}(b - a)^2 \ge (1 + \ln a)(b - a),$$
 (55)

where $\xi(c) > 0$ is between a(c) and b(c). Since a(c) is a MAXWELLian with respect to c, the function $1 + \ln a(c)$ is a quadratic polynomial with respect to c, i.e.

$$\alpha(c) = \alpha_0 + \alpha_1 c + \frac{1}{2} \alpha_2 c^2.$$
(56)

.

The coefficients of $\alpha(c)$ depend only on $\mathbf{u}(t_n, x)$ and we conclude

$$\begin{split} \lim_{\tau \to 0^+} \left(h(t_n + \tau, x) - h(t_n - \tau, x) \right) &= \int_{-\infty}^{+\infty} \left(b(c) \ln b(c) - a(c) \ln a(c) \right) dc \\ &\geq \int_{-\infty}^{+\infty} \left(1 + \ln a(c) \right) \left(b(c) - a(c) \right) dc \\ &= \left(\alpha_0, \, \alpha_1, \, \alpha_2 \right)^T \cdot \int_{-\infty}^{+\infty} \mathbf{m}(c) \left(b(c) - a(c) \right) dc \\ &= \left(\alpha_0, \, \alpha_1, \, \alpha_2 \right)^T \cdot \lim_{\tau \to 0^+} \left(\mathbf{u}(t_n + \tau, \, x) - \mathbf{u}(t_n - \tau, \, x) \right) \end{split}$$

We have thus established $(53)_2$.

The lemma verbally reads: Across the maximization times the densities \mathbf{u} are conserved while the entropy increases. The continuity of the fluxes can obviously not be expected in general.

Remark 3.2.2 At the maximization times the entropy h as well as the fluxes \mathbf{F} and ϕ become functions of the variables \mathbf{u} , e.q.

$$\mathbf{F}(t_n, x) = (\mathbf{F} \circ \mathbf{u})(t_n, x), \quad h(t_n, x) = (h \circ \mathbf{u})(t_n, x), \quad \phi(t_n, x) = (\phi \circ \mathbf{u})(t_n, x).$$
(57)

The functions F, h and ϕ on the right hand sides are defined in (5) and (7).

Proof: The proposition follows immediately from the equations (15). \Box

Next we shall discuss the behavior of the fields **u** at the boundary points $(t_n, 0)$. For given $n \in \mathbb{N}_+$ we consider the following three limits

$$\mathbf{u}_{n}^{\downarrow} := \lim_{\varepsilon \to 0^{+}} \mathbf{u}(t_{n}, \varepsilon), \quad \mathbf{u}_{n}^{\leftarrow} := \lim_{\tau \to 0^{+}} \mathbf{u}(t_{n} + \tau, 0), \quad \mathbf{u}_{n}^{\rightarrow} := \lim_{\tau \to 0^{+}} \mathbf{u}(t_{n} - \tau, 0).$$
(58)

The definitions (42) and (43) imply immediately the equality

$$\mathbf{u}_n^{\downarrow} = \mathbf{u}_n^{\rightarrow}. \tag{59}$$

In order to establish a relation between $\mathbf{u}_n^{\downarrow}$ and $\mathbf{u}_n^{\leftarrow}$ we regard the beginning of a period of free flight, starting with the maximation time t_n , see also section 2.3. We can express $\mathbf{u}_n^{\downarrow}$ and $\mathbf{u}_n^{\leftarrow}$ as follows

$$\mathbf{u}_{n}^{\downarrow} = \int_{-\infty}^{+\infty} \mathbf{m}(c) w_{M}(\mathbf{u}_{n}^{\downarrow}(0), c) dc, \qquad (60)$$

$$\leftarrow \int_{-\infty}^{0} (c) \psi_{M}(\mathbf{u}_{n}^{\downarrow}(0), c) dc, \qquad (61)$$

$$\mathbf{u}_{n}^{\leftarrow} = \int_{-\infty} \mathbf{m}(c) \lim_{\tau \to 0^{+}} f^{in}(t_{n} + \tau, c) \ dc + \int_{0} \mathbf{m}(c) \lim_{\tau \to 0^{+}} f^{out}(t_{n} + \tau, c) \ dc.$$
(61)

The evaluation of these equations, where we take care for the obvious relation

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$$\lim_{\tau \to 0^+} f^{in}(t_n + \tau, c) = w_M(\mathbf{u}_{\mathbf{n}}^{\downarrow}(0), c) \qquad \forall \ c < 0,$$

$$\tag{62}$$

reveals that the equality $\mathbf{u}_n^{\downarrow} = \mathbf{u}_n^{\leftarrow}$ cannot be expected in general. However, if we assume the continuity condition

$$\lim_{\tau \to 0^+} f^{out}(t_n + \tau, 0, c) = w_M(\mathbf{u}_{\mathbf{n}}^{\downarrow}(0), c) \qquad \forall \ c > 0$$
(63)

at each maximization time, we obtain

$$\mathbf{u}_{n}^{\downarrow} = \mathbf{u}_{n}^{\rightarrow} = \mathbf{u}_{n}^{\leftarrow}. \tag{64}$$

Recall that in the current approach, the phase density f^{out} is given by an extension law. For example, in section 2.4 we discussed the extension law

$$f^{out}\left(t_n+\tau,\,c\right) = w_M(\mathbf{u}^{\mathbf{A}}(t_n+\tau),\,c) \qquad \forall \,c>0.$$
(65)

Thus the necessary assumption (63) is very natural and identically satisfied if

$$\lim_{\tau \to 0^+} \mathbf{u}^A(t_n + \tau) = \mathbf{u}_n^{\downarrow} \tag{66}$$

holds. This condition implies, that the auxiliary fields and the boundary fields coincide at the maximization times $t_n > 0$.

The condition (63) cannot be guaranteed for any extension law, and we can only check its validity for each case separately. It is easy to prove, that the extension law (32) satisfy this condition. In the case of the extension law with auxiliary fields $\mathbf{u}^{\mathbf{A}}$ this condition can be established by using the algebraic equations (35)₃ and (37). This check will be carried out in section 5.1. Extension laws are called *regular*, if they are normal and if they satisfy additionally the condition (63).

3.3 The complete scheme

In this section we derive properties of the kinetic procedure during a time period that contains several maximization times. In particular we summarize the complete scheme for the half space problem with the non-moving wall at x = 0.

Lemma 3.3.1 Let Ω be a bounded domain in $\mathbb{R}_+ \times \mathbb{R}_+$ with a smooth boundary $\partial \Omega$. We denote the positive oriented surface element of $\partial \Omega$ by $d\sigma$. Then there hold the weak conservation law and the weak entropy inequality

$$\int_{\partial\Omega} (\mathbf{u}, \mathbf{F}) \, d\sigma = 0, \quad \int_{\partial\Omega} (h, \phi) \, d\sigma \ge 0.$$
(67)

Sketch of the proof: We divide Ω into subdomains

$$\Omega_n := \left\{ (t, x) \in \Omega : t_n < t \le t_{n+1} \right\}, \qquad n = 0, 1, \dots$$
(68)

Since Ω is bounded, only a finite number of these subdomains are not empty. Without any restriction we consider only the first two subdomains, viz. $\Omega = \Omega_0 \cup \Omega_1$. Furthermore we define

$$\Gamma := \left\{ (t_1, x) \in \Omega \right\},\tag{69}$$

and we define for positive $\varepsilon < \frac{1}{2}\tau_M$ the substructure

$$\Omega_M^{\varepsilon} := \Big\{ (t, x) \in \Omega : t_1 - \varepsilon \le t < t_1 + \varepsilon \Big\}, \quad \Omega_L^{\varepsilon} := \Omega_0 \setminus \Omega^{\varepsilon}, \quad \Omega_R^{\varepsilon} := \Omega_1 \setminus \Omega^{\varepsilon}.$$
(70)

This decomposition of Ω is visualized in the following figure.



Figure 2: The decomposition of Ω

Recall lemma 3.1.1, which states the conservation law $(48)_1$ in Ω_L^{ε} and in Ω_R^{ε} and implies here

$$\int_{\partial\Omega} (\mathbf{u}, \mathbf{F}) \, d\sigma = \int_{\partial\Omega_L^{\varepsilon}} (\mathbf{u}, \mathbf{F}) \, d\sigma + \int_{\partial\Omega_M^{\varepsilon}} (\mathbf{u}, \mathbf{F}) \, d\sigma + \int_{\partial\Omega_R^{\varepsilon}} (\mathbf{u}, \mathbf{F}) \, d\sigma = \int_{\partial\Omega_M^{\varepsilon}} (\mathbf{u}, \mathbf{F}) \, d\sigma.$$
(71)

We conclude that

$$\int_{\partial\Omega} (\mathbf{u}, \mathbf{F}) \, d\sigma = \lim_{\varepsilon \to 0} \int_{\partial\Omega_M^\varepsilon} (\mathbf{u}, \mathbf{F}) \, d\sigma = \int_{\Gamma} \lim_{\varepsilon \to 0} \left(\mathbf{u}(t_1 + \varepsilon, x) - \mathbf{u}(t_1 - \varepsilon, x) \right) dx.$$

The last integral vanishes due to the continuity of **u** in the points (t_1, \cdot) and this proves $(67)_1$. By similar arguments we obtain

$$\int_{\partial\Omega} (h, \phi) \, d\sigma = \int_{\Gamma} \lim_{\varepsilon \to 0} \left(h(t_1 + \varepsilon, x) - h(t_1 - \varepsilon, x) \right) \, dx. \tag{73}$$

Lemma 3.2.1 yields the positivity of the right hand side as it is stated in $(67)_2$. \Box

3.4 The limit $\tau_M \to 0$

Up to now we are not able to give a rigorous mathematical proof of the convergence of the kinetic scheme 2.5.1 in the limit $\tau_M \to 0$. However, we have observed the convergence in various numerical tests, at least for reasonable initial data, boundary values and extension laws. On the other hand, if we assume convergence, then we can prove that the limit functions establish solutions of the EULER system. In other words:

Lemma 3.4.1 Let $(\tau_M^n, \mathbf{u}^n, \mathbf{F}^n, h^n, \phi^n)$ be a sequence of kinetic approximations with $\tau_M^n \to 0$ and let $(\mathbf{u}, \mathbf{F}, h, \phi)$ be limit functions, such that

$$\mathbf{u}^n \to \mathbf{u}, \quad \mathbf{F}^n \to \mathbf{F}, \quad h^n \to h, \quad \phi^n \to \phi$$

$$\tag{74}$$

for $n \to \infty$ in $L^1_{loc}(\mathbb{R}_+ \times \mathbb{R}_+; \mathbb{R}^3)$. Then there holds:

1. The entropy h and the fluxes \mathbf{F} , ψ become local function of \mathbf{u} , i.e.

$$\mathbf{F} = \mathbf{F} \circ \mathbf{u}, \quad h = h \circ \mathbf{u}, \quad \phi = \phi \circ \mathbf{u}. \tag{75}$$

2. The following weak conservation law and the weak entropy condition are satisfied:

$$\int_{\mathbb{R}_{+}\times\mathbb{R}_{+}} \mathbf{u}\partial_{t}\psi + \mathbf{u}\partial_{x}\psi = 0, \int_{\mathbb{R}_{+}\times\mathbb{R}_{+}} h\partial_{t}\psi + \psi\partial_{x}\psi \leq 0,$$
(76)

where ψ denotes any smooth function with compact support in $\mathbb{R}_+ \times \mathbb{R}_+$. Regarding the entropy inequality we have to require that the test function ψ satisfies in addition $\psi \geq 0$.

It is important to note that the convergence at the boundary is a crucial point which is intimately related to the choice of appropriate continuity conditions for the extension law. Numerical tests have lead We state the conjecture, that only regular extension laws will lead to convergent schemes. This is supported by several numerical tests.

4 Discussion of two moving boundaries

In this section we generalize the kinetic scheme 2.5.1 to two moving boundaries. In particular we will demonstrate that moving boundaries, a case that was already



Figure 3: micro characteristics related to inner points and to points at the boundary

described in [8] by means of reflection laws, can also be described by extension laws. In what follows we consider a lower and an upper boundary given by the piecewice smooth paths $x_L^B(t)$ and $x_U^B(t)$, respectively. Thus we are seeking for solutions of the EULER system in the domain

$$\Omega := \left\{ (t, x) : t \ge 0, x_L^B(t) \le x \le x_U^B(t) \right\}.$$
(77)

Since there are now at every time t two boundary points, $(t, x_L^B(t))$ and $(t, x_U^B(t))$, there are also two boundary densities $f_L^B(t)$ and $f_U^B(t)$. Both functions will be decomposed into parts indicating incoming and outgoing particles. The boundary speeds $\dot{x}_L^B(t)$ and $\dot{x}_U^B(t)$ determine whether any particle with atomic speed c is incoming or outgoing. Especially there are the obvious indications

$$f_{L}^{B}(t, c) = \begin{cases} f_{L}^{in}(t, c) & \text{for } c < \dot{x}_{L}^{B}(t), \\ f_{L}^{out}(t, c) & \text{for } c > \dot{x}_{L}^{B}(t), \end{cases}$$
(78)

$$f_{U}^{B}(t, c) = \begin{cases} f_{U}^{in}(t, c) & \text{for } c > \dot{x}_{U}^{B}(t), \\ f_{U}^{out}(t, c) & \text{for } c < \dot{x}_{U}^{B}(t). \end{cases}$$
(79)

Next we discuss the free flight problem in Ω . It is sufficient to consider the first period of free flight. At first we fix an inner point (τ, x) . According to the reasoning from the above we can express the phase density $f(\tau, x, c)$ by means of the initial phase density f^{I} and the by the boundary densities f_{L}^{B} and f_{U}^{B} at former times (see the non-dashed micro characteristics in Figure 3). Let us consider a micro characteristic with atomic speed c which starts in (τ, x) and intersects the boundary point (τ', x') with $\tau' < \tau$ which might belong to the upper or to the lower boundary.

We read off from equations (78) and (79) that c is the atomic speed of an outgoing particle with respect to (τ', x') .

We consider now a point $(\tau, x_U^B(\tau))$ of the upper boundary. For incoming particles with atomic speed c we can determine the boundary density $f_U^B(\tau, c) = f_U^{in}(\tau, c)$ by means of free flight (see the dashed lines in Figure 3). The boundary density for outgoing particles cannot be determined by means of free flight, obviously it must again be determined by an extension law. In the next section we will study some extension laws for moving boundaries.

Note that the case of two walls which additionally might move is in some aspects much more difficult as the former case of a single non-moving wall. For a given extension law, the boundary density of the former case is completely given by the initial phase density. Here, however, in the case of two walls, a boundary density is determined by the initial phase density and by two boundary densities at former times.

Nevertheless, a kinetic scheme can be formulated in an analogous manner as in 2.5.1, although a rigorous formulation becomes more complicate. We mention that every lemmas in section 5 can be generalized to the case of two moving boundaries.

Fortunately, for the practical application to solve a hyperbolic system with initial and boundary data, the study a single boundary does not mean a restriction, because for a sufficiently small time step in the kinetic scheme there is only a local influence from each boundary, and the boundaries may be treated separately. For many applications boundaries is described by polygons, which is linear between two subsequent maximization times.

5 Further examples of extension laws

In this section we continue the discussion of those extension laws that rely on auxiliary fields.

5.1 Moving adiabatic walls

We consider a single adiabatic wall. Its motion is given by a smooth path $x^B(t)$ and the gas is located above the wall. For the following purposes it is not important whether there is a second wall. Thus we are looking for solutions in the domain

$$\Omega = \left\{ (t, x) : t \ge 0, x \ge x^B(t) \right\}.$$
(80)

We choose the macroscopic boundary condition

$$v(t, x^B(t)) = \dot{x}^B(t).$$
 (81)

There are two interesting cases of moving adiabatic walls

- 1. Driven adiabatic walls with a given path $x^{B}(t)$.
- 2. Free adiabatic walls which are subjected to an external force F(t) and to the gas pressure. In this case the path $x_B(t)$ is also unknown.

The gas pressure gives rise to a force on the wall which we denote by -K(t). A simple calculation of the temporal development of the total mass, the total moment and the total energy yields the equations

$$\int_{-\infty}^{+\infty} \left(c - \dot{x}^B(t)\right) f^B(t, c) \ dc = 0, \tag{82}$$

$$\int_{-\infty}^{+\infty} c\left(c - \dot{x}^B(t)\right) f^B(t, c) \ dc = K(t), \tag{83}$$

$$\int_{-\infty}^{+\infty} \frac{1}{2} c^2 \left(c - \dot{x}^B(t) \right) f^B(t, c) \ dc = K(t) \dot{x}^B(t).$$
(84)

Note that these equations hold for any EULER-solution which satisfy (81). However, here these equations serve as conditions for the auxiliary fields.

At time t the micro characteristics with atomic speed $c < \dot{x}^B(t)$ and $c > \dot{x}^B(t)$ correspond to incoming and outgoing particles, respectively. Recall that the parts of the integrals that correspond to incoming particles are known and we abbreviate these, as before, by $\mathbf{I}(t) = (I_1, I_2, I_3)^T(t)$ with

$$\mathbf{I}(t) = \int_{-\infty}^{\dot{x}^B(t)} \left(c - \dot{x}^B(t)\right) \mathbf{m} \left(c - \dot{x}^B(t)\right) f^I(t, c) \ dc.$$
(85)

Thus we can rewrite the equations (82)-(84) as

$$\int_{\dot{x}^{B}(t)}^{+\infty} \left(c - \dot{x}^{B}(t)\right) f^{out}(t, c) \ dc = -I_{1}(t), \tag{86}$$

$$\int_{\dot{x}^{B}(t)}^{+\infty} \left(c - \dot{x}^{B}(t)\right)^{2} f^{out}(t, c) \ dc = K(t) - I_{2}(t), \tag{87}$$

$$\int_{\dot{x}^{B}(t)}^{+\infty} \frac{1}{2} \left(c - \dot{x}^{B}(t) \right)^{3} f^{out}(t, c) \ dc = -I_{3}(t).$$
(88)

We can interpret the centered moments in the equations (82)-(84) as moments measured by an observer which moves with the wall. The fluxes of mass and energy are zero for this observer. Thus he meets the same situation as in the case of non-moving walls. For this reason it is obvious to choose

$$v^A(t) = \dot{x}^B(t). \tag{89}$$

The resulting algebraic equations for the other auxiliary fields are the same as before, and they read

$$T^{A}(t) = \frac{I_{3}(t)}{I_{1}(t)}, \quad \rho^{A}(t) = -I_{1}(t)\sqrt{\frac{2\pi}{T^{A}(t)}}.$$
(90)

These equations guarantee again the positivity of $T^A(t)$ and $\rho^A(t)$. However, there is an important difference between (90) and (37). If the wall is at rest (or moves with constant velocity) the integrals I_i at time t depend only on the fields **u** calculated at the previous maximization time. For time dependent velocities $\dot{x}^B(t)$ the integrals I_i depend in addition on the auxiliary fields at former times. Nevertheless, the formulas (90) become explicit if we assume that all data for times t' < t are given.

In the case of a free adiabatic wall, there remains the determination of the path $x^{B}(t)$, which follows from NEWTONS law for the wall with the mass M

$$M\ddot{x}^{B}(t) = F(t) - K(t).$$
(91)

Here we replace the gas force K(t) by (87) and obtain

$$M\ddot{x}(t) = F(t) - I_2(t) - \int_{\dot{x}^B(t)}^{+\infty} \left(c - \dot{x}^B(t)\right)^2 f^{out}(t, c) \ dc = F(t) - I_2(t) - \frac{1}{2}\rho^A(t)T^A(t).$$
(92)

There remains to prove that the extension law (89), (90) guarantees the continuity of the boundary fields $\mathbf{u}(t, x^B(t))$ across the maximization times. In section 3.2 we have called an extension law with this property a regular extension law. In an analogous manner to the procedure in section 3.2, we consider at the time $t_n > 0$ the one-sided limits

$$\mathbf{u}_{n}^{\downarrow} := \lim_{\varepsilon \to 0^{+}} \mathbf{u}(t_{n}, x^{B}(t_{n}) + \varepsilon), \qquad \mathbf{u}_{n}^{\leftarrow} := \lim_{\tau \to 0^{+}} \mathbf{u}(t_{n} + \tau, x^{B}(t_{n} + \tau)), \mathbf{u}_{n}^{\rightarrow} := \lim_{\tau \to 0^{+}} \mathbf{u}(t_{n} - \tau, x^{B}(t_{n} + \tau)).$$

$$(93)$$

As before it can be shown that $\mathbf{u}_n^{\rightarrow} = \mathbf{u}_n^{\downarrow}$. Furthermore we find by means of (89) the equality $v_n^{\leftarrow} = v_n^{\rightarrow} = \dot{x}^B(t_n)$ and we conclude $v_n^{\downarrow} = \dot{x}^B(t_n)$. Next we use the identity $\lim_{\tau \to 0^+} f^{in}(t_n + \tau, c) = w_M(\mathbf{u}_n^{\downarrow}, c)$ and definition (85) in order to calculate $\lim_{\tau \to 0^+} \mathbf{I}(t_n + \tau)$. We obtain

$$\lim_{\tau \to 0^+} I_1(t_n + \tau) = \rho_n^{\downarrow} \sqrt{\frac{T_n^{\downarrow}}{2\pi}}, \qquad \lim_{\tau \to 0^+} I_3(t_n + \tau) = \rho_n^{\downarrow} T_n^{\downarrow} \sqrt{\frac{T_n^{\downarrow}}{2\pi}}, \tag{94}$$

which implies

$$\lim_{\tau \to 0^+} \rho^A(t_n + \tau) = \rho_n^{\downarrow}, \qquad \lim_{\tau \to 0^+} T^A(t_n + \tau) = T_n^{\downarrow}.$$
(95)

Finally there follows

$$\mathbf{u}^{\leftarrow} = \int_{-\infty}^{\infty} \mathbf{m}(c) w_M(\mathbf{u}_n^{\downarrow}, c) \ dc = \mathbf{u}_n^{\downarrow} = \mathbf{u}_n^{\rightarrow}.$$
(96)

Similar formulas for the auxiliary fields and the force K can be derived in the case d = 3. Analogously to the equations (46) and (47) we find for a lower adiabatic wall that moves with speed $\dot{x}^{B}(t)$ the expressions

$$v^{A}(t) = \dot{x}^{B}(t), \quad T^{A}(t) = \frac{1}{2} \frac{I_{3}(t)}{I_{1}(t)}, \quad \rho^{A}(t) = -I_{1}(t) \sqrt{\frac{2\pi}{T^{A}(t)}}$$
 (97)

and

$$K(T) = I_2(t) - \frac{1}{2}\rho^A(t)T^A(t),$$
(98)

where $\mathbf{I}(t) = (I_1, I_2, I_3)^T(t)$ are the corresponding centered moment integrals of $f^{in}(t, x^B(t))$. It can be shown again, that this extension law guarantees the continuity of the boundary fields across the maximization times.

An upper adiabatic wall can be treated analogously to the case of a lower adiabatic wall.

5.2 Periodic boundary conditions

In this section we will study a further example of an extension law with auxiliary fields that will be applied to spatial periodic boundary conditions. To this end we consider the domain

$$\Omega := \left\{ (t, x) : t \ge 0, \ -L \le x \le L \right\},$$
(99)

where L > 0 is a given constant. We consider the EULER system for the initial and boundary value problem

$$\mathbf{u}(0, x) = \mathbf{u}_0(x), \quad \mathbf{u}(t, +L) = \mathbf{u}(t, -L).$$
(100)

We denote the common boundary values by \mathbf{u}^B and ρ^B , v^B , T^B , respectively. In the following it is sufficient to consider only one single period of free flight, say the *n*-th period with fixed $n \in \mathbb{N}$. Regarding the initial and boundary phase densities, we introduce for $0 < \tau < \tau_M$ the abbreviations

$$f^{I}(x, c) := f(t_{n}, x, c), \quad f^{B}_{\pm}(\tau, c) := f(t_{n} + \tau, \pm L, c),$$
 (101)

where the lower index n has been omitted on the left hand sides. Thus we can rewrite the boundary condition (100) as

$$\mathbf{u}^{B}(t_{n}+\tau,-L) = \int_{-\infty}^{0} \mathbf{m}(c) f_{-}^{in}(\tau,c) \ dc + \int_{0}^{+\infty} \mathbf{m}(c) f_{-}^{out}(\tau,c) \ dc, \qquad (102)$$

$$\mathbf{u}^{B}(t_{n}+\tau, L) = \int_{-\infty}^{0} \mathbf{m}(c) f_{+}^{out}(\tau, c) \ dc + \int_{0}^{+\infty} \mathbf{m}(c) f_{+}^{in}(\tau, c) \ dc.$$
(103)

Next we will formulate the extension law at time $t_n + \tau$. To this end we assume that we already know the boundary densities f_{-}^{B} and f_{+}^{B} for all times $t_n + \tau'$ with $\tau' < \tau$. Thus we can calculate by means of free flight the integrals

$$\mathbf{I}_{-}(\tau) := \int_{-\infty}^{0} \mathbf{m}(c) f_{-}^{in}(\tau, c) \ dc, \quad \mathbf{I}_{+}(\tau) := \int_{0}^{+\infty} \mathbf{m}(c) f_{+}^{in}(\tau, c) \ dc.$$
(104)

We assume now that f_{-}^{out} and f_{+}^{out} at time τ are given by a MAXWELLian with respect to the auxiliary fields $\mathbf{u}^{A}(\tau)$ and put

$$\int_{-\infty}^{+\infty} \mathbf{m}(c) w_M(\mathbf{u}^A(\tau), c) \ dc = \mathbf{I}_-(\tau) + \mathbf{I}_+(\tau) =: \mathbf{I}(\tau), \tag{105}$$

where the components of the vector $\mathbf{I}(\tau)$ are denoted by $I_i(\tau)$ with i = 1, 2, 3. The evaluation of (105) yields the algebraic equations

$$\rho^{A}(\tau) = I_{1}(\tau), \quad v^{A}(\tau) = \frac{I_{2}(\tau)}{I_{1}(\tau)}, \quad T^{A}(\tau) = 2\frac{I_{3}(\tau)}{I_{1}(\tau)} - \frac{I_{2}(\tau)^{2}}{I_{1}(\tau)^{2}}.$$
 (106)

Note that, $f_{+}^{out}(\tau)$ as well as $f_{-}^{out}(\tau)$ are assumed to be MAXWELLians with respect to the same auxiliary fields $\mathbf{u}^{A}(\tau)$.

If we apply similar arguments to the case d = 3, we are led to the following extension law

$$\rho^{A}(\tau) = I_{1}(\tau), \quad v^{A}(\tau) = \frac{I_{2}(\tau)}{I_{1}(\tau)}, \quad T^{A}(\tau) = \frac{2}{3} \frac{I_{3}(\tau)}{I_{1}(\tau)} - \frac{1}{3} \frac{I_{2}(\tau)^{2}}{I_{1}(\tau)^{2}}.$$
 (107)

6 Numerical examples

For an illustration of the main result of this paper, we consider now some numerical examples. We choose d = 3. The applied extension laws were derived in the sections 2.4 and 5 and they all rely on auxiliary fields.

Since all kinetic schemes and extension laws from the latter sections are not discretized with respect to the space variable x and the atomic speed c, we shall resume briefly the numerical implementation. We mention that the construction of effective numerical algorithms is not among the objectives of this paper.

The initial data $\mathbf{u}_0(x)$ corresponding to $\rho_0(x)$, $v_0(x)$ and $T_0(x)$ of all examples are given in a space interval $[0, L_x]$. The number of entropy maximization within the total time interval L_t is denoted by N_M . The length of any period of free flight is thus L_t/N_M . For a given maximization time t_n we divide the space interval into N_x subintervals of equal length. The length of the space interval at time t_n depends in general on t_n according to the positions of the boundaries at time t_n . In order to calculate the auxiliary fields, every period of free flight will be decomposed into further N_A subintervals. To evaluate the moment integrals we apply the SIMPSON rule with respect to N_c integration nodes and a sufficient large domain of integration. The phase density at the current integration nodes is obtained by interpolation of the data from the proceeding maximization time and from the time grids at the boundaries. As a first example we consider a single shock which is reflected by an adiabatic wall at x = 0. The initial data are given by $\mathbf{u}_0(x) = \mathbf{u}_-$ for $x < \frac{3}{2}$ and $\mathbf{u}_0(x) = \mathbf{u}_+$ for $x > \frac{3}{2}$ with $\rho_- = \frac{2}{3}$, $v_- = 0$, $T_- = \frac{3}{4}$, $\rho_+ = 1$, $v_+ = -\frac{1}{2}$, $T_+ = 1$. This is a RIEMANN problem which can be solved analytically (see [18]). The discontinuity of the initial data creates a 1-shock that propagates with the speed $-\frac{3}{2}$. The shock will reach the wall at time t = 1, which leads to a reflection. After the reflection a 3-shock arises. It propagates with the speed $\frac{7}{6}$ and connects the state \mathbf{u}_+ to the state \mathbf{u}_* given by $\rho_* = \frac{10}{7}$, $v_* = 0$ and $T_* = \frac{77}{60}$. Figure 4 shows a numerical solution for the parameters $L_x = 2$, $L_t = \frac{13}{7}$, $N_x = 2000$, $N_M = 1000$, $N_A = 40$, $N_c = 3000$. There is a good agreement between the calculated values and the theoretical values for \mathbf{u}_* and the shock speeds, respectively. Note that for shocks the angle of incidence is not equal to the angle of reflection.

The evolution of a gas in a cylinder with two adiabatic walls is shown in Figure



Figure 4: Reflection of a shock wave on an adiabatic wall

5. Here the lower wall is at rest while the upper wall is driven along the given path $x^{U}(t) = \frac{3}{4}(t-2)^{2} + 1$. The parameters of the solution are $\rho_{0}(x) = 4$, $v_{0}(x) = 0$, $T_{0}(x) = 1$, $L_{x} = 4$, $L_{t} = 2$, $N_{x} = 800$, $N_{M} = 800$, $N_{A} = 20$, $N_{c} = 2000$.

Next we consider a gas in cylinder wich is closed by a free upper adiabatic wall and a lower adiabatic wall at rest. The upper wall has the mass M = 1, and it is subjected to the gas pressure and additionally to a constant external force F = 3. Figure 6 shows the solution for the parameters $\rho_0(x) = \frac{1}{4}$, $v_0(x) = 0$, $T_0(x) = 4$, $L_x = 4$, $L_t = 32$, $N_x = 800$, $N_M = 3200$, $N_A = 20$, $N_c = 2000$. We conclude from space time diagram of Figure 6 that the motion of the upper wall is irreversible. Irreversibility comes exclusively into to play due to the appearance of shocks.



Figure 5: Driven adiabatic walls

Finally we consider the case of periodic boundary conditions in a fixed spacial re-



Figure 6: A free adiabatic wall

gion with length $L_x = 4$. The RIEMANN initial data $\mathbf{u}_0(x) = \mathbf{u}_-$ for x < 2 and $\mathbf{u}_0(x) = \mathbf{u}_+$ for x > 2 are given by $\rho_- = 1$, $v_- = 0$, $T_- = 1$, $\rho_+ = \frac{3}{2}$, $v_+ = -\frac{1}{3}\sqrt{3}$, $T_+ = \frac{4}{3}$. The evolution of this fields, which is displayed in Figure 7, corresponds to the parameters $L_t = 4$, $N_x = 800$, $N_M = 800$, $N_A = 20$, $N_c = 2000$.

7 Conclusions and perspectives

The study of the EULER system has revealed that a kinetic solution of a hyperbolic initial and boundary value problem requires appropriate extension laws for the phase density at the boundaries. The incorporation of boundary data and extension laws leads to a generalization of the kinetic scheme presented in [7] for the pure initial value problem.

In this paper we have solved the EULER system for adiabatic boundary conditions,



Figure 7: Periodic boundary conditions

and to this end we have introduced two kinds of extension laws, namely the reflection law, that was already studied in [8], and a second method that uses auxiliary fields at the boundaries. While the second method may also work for some non-adiabatic boundary conditions, in this respect we refer the reader to the phonon BOSE gas studied in [10] and [11], the reflection method is only useful in order to simulate the reflection of particles at adiabatic boundaries.

For the further illustration of extension laws with auxiliary fields, we have solved the EULER system for periodic boundary conditions.

In this study we were lead to the conjecture that regular extension laws, which provide continuity for the fields at the boundaries, play an important role in order to achieve convergence of the kinetic schemes. Despite the fact that we could not prove convergence, we have rigorous results for the kinetic schemes itself, namely the weak form of the conservation laws and of the entropy inequality, regularity results and continuity conditions at the boundaries for the fields defined by the kinetic scheme. Numerical solutions with shock structures exhibit additionally the importance of regular extension laws.

In his textbook [3], CERCIGNANI discusses so called stochastical reflection laws. This might be an appropriate example for the construction of a further extension law. However, this task is left to the future.

Likewise important for future studies is the generalization to more than one space dimension, involving boundaries with a more complicated geometry. Regarding the evaluation of the integrals appearing in the kinitec scheme, the numerical efficiency should be improved. For example we mention here the grid refinement techniques, described by KRÖNER in [14], and the integration method that uses GAUSSian integration nodes, introduced in [9].

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