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Hydrodynamic Regimes, Knudsen Layer, Numerical Schemes: Definition of Boundary Fluxes

Christophe Besse[1], Saja Borghol[1], Thierry Goudon[1,*], Ingrid Lacroix-Violet[1] and Jean-Paul Dudon[2]

[1] *Project-Team SIMPAF, INRIA Lille Nord Europe Research Centre, Park Plazza, 40 av. Halley, 59650 Villeneuve d'Ascq France*
& Labo P. Painlevé UMR 8524 CNRS–Université des Sciences et Technologies Lille
[2] *Thales Alenia Space, Cannes La Bocca*

Abstract. We propose a numerical solution to incorporate in the simulation of a system of conservation laws boundary conditions that come from a microscopic modeling in the small mean free path regime. The typical example we discuss is the derivation of the Euler system from the BGK equation. The boundary condition relies on the analysis of boundary layers formation that accounts from the fact that the incoming kinetic flux might be far from the thermodynamic equilibrium.

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1 Introduction

A statistical picture of a cloud of particles leads to the following PDE

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{\tau} Q(F) \tag{1.1}$$

satisfied by the particles distribution function $F(t,x,v) \geq 0$. Here, N being a positive integer, $t \geq 0$, $x \in \Omega \subset \mathbb{R}^N$ and $v \in \mathbb{R}^N$ are the time, space and velocity variables respectively. The left hand side of the equation describes the transport of particles, that is the simple motion on straight line with velocity v, and the interactions process the particles are subject to is embodied in the right hand side $Q(F)$, for instance interparticles collisions. The parameter $\tau > 0$ is related to the mean free path which is the average distance travelled by the particles without being affected by any interaction.[†] As τ becomes small, the distribution F tends to an equilibrium $F_{\rm eq}$ that is a function which makes the collision operator vanish $Q(F_{\rm eq}) = 0$. By considering conservation laws associated to the collision dynamics, we can then derive macroscopic equations satisfied by moments with respect to the velocity variable

*Corresponding author.
Email: Christophe.Besse@math.univ-lille1.fr (Christophe Besse), saja.borghol@math.univ-lille1.fr (Saja Borghol), thierry.goudon@inria.fr (Thierry Goudon), ingrid.violet@math.univ-lille1.fr (Ingrid Lacroix-Violet), jean-paul.dudon@thalesaleniaspace.com (Jean-Paul Dudon)

[†]Precisely, throughout the paper we shall implicitly work with dimensionless equations so that τ is actually the Knudsen number that is the ratio of a typical (macroscopic) length scale of the flow over the mean free path.

v. A difficulty arises when the boundary conditions are not compatible with the equilibrium state. In such a case boundary layers appear, whose analysis is quite delicate. The questions we address are related to the numerical treatment of the boundary layer: considering a system of conservation laws obtained as a small mean free path limit of a kinetic model, what are the associated boundary conditions for the hydrodynamic fields? How the boundary fluxes can be evaluated in numerical procedures?

The paper is organized as follows. First we need to set up a few definition and notation. Our framework will be the Euler system, obtained as the limit of the BGK equation (but the method can be extended to more intricate collision operators like the Boltzmann operator or the Landau-Fokker-Planck operator). The necessary material is recalled in Section 2. In particular entropy dissipation has a central role. A difficulty for hyperbolic equations set on a bounded domain relies on the fact that the number of necessary boundary conditions for the problem to be well–posed usually depends on the solution itself. The entropy provides a natural way to determine the incoming fluxes, with a direct analogy with the microscopic picture. The discussion is strongly inspired by the analysis of the Knudsen layer for the linearized Boltzmann equation by F. Coron-F. Golse-C. Sulem [20], see also the lecture notes of F. Golse [32], and their result is the cornerstone of the definition of numerical fluxes we propose in this paper. Section 3 is the main part of the paper: we discuss how we can take into account the boundary layer in a Finite Volume scheme for the conservation laws. The point is precisely to define a suitable numerical flux on the boundary cells. The definition that we design relies on a decomposition of the numerical solution, according to the nature of the flow (sub or supersonic) combined with an approximation of the half-space problem which defines the matching condition. Finally Section 4 comments the numerical experiments with comparison to direct simulations of the kinetic model.

2 Hydrodynamic limits, entropy dissipation and boundary layer analysis

2.1 BGK equation and Euler system

For the sake of concreteness we consider the BGK collision operator:

$$Q(F) = M[F] - F \tag{2.1}$$

where

$$M[F](v) = \frac{\rho}{(2\pi\theta)^{N/2}} \exp\Big(-\frac{|v-u|^2}{2\theta}\Big) \tag{2.2}$$

and the macroscopic quantities (ρ, u, θ) are defined by

$$\begin{aligned} &\text{density:} && \rho = \int_{\mathbb{R}^N} F \,\mathrm{d}v, \\ &\text{velocity:} && \rho u = \int_{\mathbb{R}^N} vF \,\mathrm{d}v, \\ &\text{temperature:} && \rho u^2 + N\rho\theta = \int_{\mathbb{R}^N} |v|^2 F \,\mathrm{d}v. \end{aligned} \tag{2.3}$$

This non linear operator can be seen as a caricature of the Boltzmann or the Landau-Fokker-Planck collision operators that arise in gas dynamics and plasma physics, see [11]. It allows the derivation of rather simple formulae, but our discussion can be extended to more complex collision operators.

As a matter of fact, we remark that $(1, v, |v|^2)$ are collision invariants: it means that

$$\int_{\mathbb{R}^N} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} Q(F)\,\mathrm{d}v = 0$$

holds. In turn, integration of (1.1)–(2.2) yields the following (local) conservation laws

$$\partial_t \int_{\mathbb{R}^N} \begin{pmatrix} 1 \\ v \\ \dfrac{|v|^2}{2} \end{pmatrix} F\,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^N} v \begin{pmatrix} 1 \\ v \\ \dfrac{|v|^2}{2} \end{pmatrix} F\,\mathrm{d}v = 0. \tag{2.4}$$

The system is not closed since the higher order moments cannot be expressed by means of the macroscopic quantities (2.3). Next, it is clear that the equilibria are the Maxwellian functions

$$Q(F_{\mathrm{eq}}) = 0 \text{ iff } F_{\mathrm{eq}}(v) = \frac{\rho}{(2\pi\theta)^{N/2}} \exp\Big(-\frac{|v-u|^2}{2\theta}\Big) = M_U(v),$$

where U stands for the triple (ρ, u, θ) that parametrizes the Maxwellian. Therefore, as $\tau \to 0$ we expect that F, solution of (1.1)–(2.2), resembles a Maxwellian, whose macroscopic parameters ρ, u, θ are still functions of t and x. Inserting this information into the moment system (2.4) we obtain

$$\partial_t \int_{\mathbb{R}^N} \begin{pmatrix} 1 \\ v \\ \dfrac{|v|^2}{2} \end{pmatrix} M_U(v)\,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^N} v \begin{pmatrix} 1 \\ v \\ \dfrac{|v|^2}{2} \end{pmatrix} M_U(v)\,\mathrm{d}v = 0$$

which is now a closed system since it can be recast as the Euler system[‡]

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u) + \nabla_x (\rho\theta) = 0 \\ \partial_t \dfrac{\rho u^2 + N\rho\theta}{2} + \nabla_x \cdot \dfrac{(\rho u^2 + (N+2)\rho\theta)u}{2} = 0. \end{cases} \tag{2.5}$$

However, when x lies in a domain Ω of $\mathbb{R}^N$, equation (1.1) has to be completed with boundary conditions which prescribe the incoming distribution function. We assume that $\partial\Omega$ is smooth and we denote $\nu(x)$ to be the outward normal unit vector at point $x \in \partial\Omega$. We set

$$\Gamma^{\mathrm{out}} = \big\{(t,x,v) \in (0,\infty) \times \partial\Omega \times \mathbb{R}^N,\ v \cdot \nu(x) > 0\big\}$$

and

$$\Gamma^{\mathrm{inc}} = \big\{(t,x,v) \in (0,\infty) \times \partial\Omega \times \mathbb{R}^N,\ v \cdot \nu(x) < 0\big\}.$$

The theory of traces on $\Gamma^{\mathrm{inc/out}}$ for solutions of transport equations has been developped in [10, 17, 18, 46] after the seminal work [5]; we denote $\gamma^{\mathrm{inc/out}}$ the trace operators. The boundary condition for (1.1) has the following expression

$$\gamma^{\mathrm{inc}} F(t,x,v) = \Phi^{\mathrm{data}}(t,x,v), \qquad \text{for } (t,x,v) \in \Gamma^{\mathrm{inc}}, \tag{2.6}$$

[‡]Here and below for given vectors a, b in $\mathbb{R}^N$, $a \otimes b$ is the $N \times N$ matrix with components $a_i b_j$ and, given a matrix valued field A, $\nabla_x \cdot A$ stands for the vector in $\mathbb{R}^N$ with components $\sum_{j=1}^N \partial_j A_{ij}$.

where $\Phi^{\rm data} \geq 0$ is a given function in $L^1(\Gamma^{\rm inc}, |v\cdot\nu(x)|\,\mathrm{d}v\,\mathrm{d}\sigma(x)\,\mathrm{d}t)$. Here and below $\mathrm{d}\sigma(x)$ stands for the Lebesgue measure on $\partial\Omega$. Of course, the problem is also completed by an initial condition

$$F(0,x,v) = F^{\rm Init}(x,v) \in L^1(\Omega\times\mathbb{R}^N). \tag{2.7}$$

Remark 2.1. *Prescribing the incoming data as in* (2.6) *might be unsatisfactory on a physical viewpoint. More realistic boundary conditions are intended to describe the interaction of the particles with the boundary. This is a complicated issue, which requires subsequent modeling efforts, see [16, 42]. Simple and classical reflection laws are, for* $(t,x,v)\in\Gamma^{\rm inc}$

$$\textit{Specular reflection law:}\quad \gamma^{\rm inc}F(t,x,v) = \alpha\,\gamma^{\rm out}F\big(t,x,v-2(v\cdot\nu(x))\nu(x)\big),$$

$$\textit{Maxwell diffusive law:}\quad \gamma^{\rm inc}F(t,x,v) = \alpha\,\frac{\displaystyle\int_{v_\star\cdot\nu(x)>0} v_\star\cdot\nu(x)\gamma^{\rm out}F(t,x,v_\star)\,\mathrm{d}v_\star}{\displaystyle\int_{v_\star\cdot\nu(x)<0}|v_\star\cdot\nu(x)|\,e^{-|v_\star|^2/(2\theta_{\rm w}(x))}\,\mathrm{d}v_\star}\,e^{-|v|^2/(2\theta_{\rm w}(x))},$$

where $0\leq\alpha\leq 1$ *is an accomodation parameter that gives the fraction of reflected particles and* $\theta_{\rm w}$ *is the temperature of the wall* $\partial\Omega$*. We refer to [36, 37] for further comments and references on boundary conditions.*

2.2 Entropy

The collision operator verifies a dissipation property that will be crucial to our discussion. We introduce the entropy functional

$$\mathcal{H}(F) = \int_{\mathbb{R}^N} F\ln(F)\,\mathrm{d}v.$$

As a consequence of the definition of the collisional invariants, we observe that

$$\int_{\mathbb{R}^N}(M[F]-F)\ln(M[F])\,\mathrm{d}v = 0.$$

Then, by using integration by parts and the boundary condition (2.6) we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega\mathcal{H}(F)\,\mathrm{d}x + \int_{\partial\Omega}\int_{v\cdot\nu(x)>0}\gamma^{\rm out}F\ln(\gamma^{\rm out}F)v\cdot\nu(x)\,\mathrm{d}v\,\mathrm{d}\sigma(x) + \frac{1}{\tau}\int_\Omega\int_{\mathbb{R}^N}D(F)\,\mathrm{d}v\,\mathrm{d}x\\ = \int_{\partial\Omega}\int_{v\cdot\nu(x)<0}\Phi^{\rm data}\ln(\Phi^{\rm data})|v\cdot\nu(x)|\,\mathrm{d}v\,\mathrm{d}\sigma(x),\end{aligned}$$

with

$$D(F) = (M[F]-F)\ln\Big(\frac{M[F]}{F}\Big)\geq 0.$$

Thus the entropy is dissipated and we deduce the following estimate of the solution by means of the data

$$\begin{aligned}\int_\Omega\mathcal{H}(F)(t,x)\,\mathrm{d}x + \int_0^t\int_{\partial\Omega}\int_{v\cdot\nu(x)>0}\gamma^{\rm out}F\ln(\gamma^{\rm out}F)v\cdot\nu(x)\,\mathrm{d}v\,\mathrm{d}\sigma(x)\,\mathrm{d}s\\ \leq\int_\Omega\mathcal{H}(F^{\rm Init})\,\mathrm{d}x + \int_0^t\int_{\partial\Omega}\int_{v\cdot\nu(x)<0}\Phi^{\rm data}\ln(\Phi^{\rm data})|v\cdot\nu(x)|\,\mathrm{d}v\,\mathrm{d}\sigma(x).\end{aligned}$$

This remarkable relation is referred to as the H-Theorem. In what follows, we will work with the relative entropy between two particles distribution functions F and $F_\star$

$$\mathcal{H}(F|F_\star) := \int_{\mathbb{R}^N}\Big[F\ln\Big(\frac{F}{F_\star}\Big) - F + F_\star\Big]\,\mathrm{d}v = \int_{\mathbb{R}^N}\Big[\frac{F}{F_\star}\ln\Big(\frac{F}{F_\star}\Big) - \frac{F}{F_\star} + 1\Big]\,F_\star\,\mathrm{d}v \geq 0.$$

This quantity is non negative and vanishes iff $F = F_\star$. It has been shown to be very useful in kinetic theory to evaluate how far a solution F of (1.1) is from a reference state $F_\star$ (see e. g. [57] and the references therein).

Remark 2.2. *The dissipation property extends to the case of the specular or the Maxwell reflection law, and even to more general reflection laws: the dissipation due to the boundary condition essentially relies on a convexity argument and on a version of the Jensen lemma, referred to as the Darrozes-Guiraud lemma [21] (see also comments in [14]).*

Remark 2.3. *The entropy dissipation gives the basic a priori estimate that can be used for justifying the existence of weak (or renormalized) solutions. We refer to [24] for the Boltzmann equation, to [48, 51] for the BGK equation in the whole space, while the initial-boundary-value problem is investigated e. g. in [37, 39, 47]. Of course, entropy dissipation is also the basis for the analysis of hydrodynamic limits, according to the program addressed in [7, 8]: we refer to [35] and to the very complete survey [57] for detailed results and further references.*

Let us go back to the Euler system (2.5). We consider the mapping

$$U = (\rho, u, \theta) \in (0,\infty) \times \mathbb{R}^N \times (0,\infty) \longmapsto \mathscr{U} = (\rho, j, \mathscr{E}) = (\rho, \rho u, \rho u^2/2 + N\rho\theta/2), \tag{2.8}$$

which defines the conserved quantities. The Euler system recasts as

$$\partial_t \mathscr{U} + \nabla_x \cdot \mathscr{F}(\mathscr{U}) = 0,$$

with the matrix (with $N+2$ raws, N columns)

$$\mathscr{F}(\mathscr{U}) = \left(\begin{array}{c} j^T \\ \dfrac{j \otimes j}{\rho} + \Big(\dfrac{2}{N}\mathscr{E} - \dfrac{j^2}{N\rho} \Big) \mathbb{I}_N \\ \Big(\dfrac{N+2}{N}\mathscr{E} - \dfrac{j^2}{N\rho} \Big) \Big(\dfrac{j}{\rho} \Big)^T \end{array} \right).$$

An entropy for the Euler system is a convex function $\eta : \mathscr{U} \mapsto \eta(\mathscr{U}) \in \mathbb{R}$ such that there exists an entropy flux $q : \mathscr{U} \mapsto q(\mathscr{U}) \in \mathbb{R}^N$ verifying

$$\partial_t \eta(\mathscr{U}) + \nabla_x \cdot q(\mathscr{U}) = 0$$

for any smooth solution of (2.5). This definition[§] leads to a relation between the entropy η, the entropy flux q and the flux function $\mathscr{F}$; namely we have

$$\partial_{\mathscr{U}_k} q_j = \sum_{i=1}^{N+2} \partial_{\mathscr{U}_k} \mathscr{F}_{ij}\, \partial_{\mathscr{U}_i} \eta. \tag{2.9}$$

Given a reference (constant) state $\mathscr{U}_\star$, it is convenient to introduce the relative entropy

$$\eta(\mathscr{U}|\mathscr{U}_\star) = \eta(\mathscr{U}) - \eta(\mathscr{U}_\star) - \nabla_{\mathscr{U}} \eta(\mathscr{U}_\star) \cdot (\mathscr{U} - \mathscr{U}_\star).$$

Since η is convex, this quantity is non negative and it vanishes iff $\mathscr{U} = \mathscr{U}_\star$. As far as the solution $\mathscr{U}$ of (2.5) is smooth, we have

$$\partial_t \eta(\mathscr{U}|\mathscr{U}_\star) + \nabla_x \cdot q(\mathscr{U}|\mathscr{U}_\star) = 0 \tag{2.10}$$

[§]We refer for more details on this notion and its role for the analysis of hyperbolic systems e. g. to [52, Section 3.4 and ff.].

where the entropy flux is defined by

$$q(\mathscr{U}|\mathscr{U}_\star) = q(\mathscr{U}) - q(\mathscr{U}_\star) - \nabla_{\mathscr{U}}\eta(\mathscr{U}_\star)\cdot\big(\mathscr{F}(\mathscr{U}) - \mathscr{F}(\mathscr{U}_\star)\big).$$

A crucial remark is that the kinetic entropy defines an entropy for the Euler system. Indeed, let us set

$$\eta(\mathscr{U}) = \int_{\mathbb{R}^N} M_U \ln(M_U)\,\mathrm{d}v = \mathcal{H}(M_U)$$

with $U = (\rho, u, \theta)$ associated to $\mathscr{U}$ by (2.8).

Lemma 2.1. *We have*

$$\eta(\mathscr{U}) = \rho\ln\Big(\frac{\rho}{\theta^{N/2}}\Big) - \frac{N}{2}(1+\ln(2\pi))\rho$$

and the function $\mathscr{U} \longmapsto \eta(\mathscr{U})$ is strictly convex. The associated flux is given by

$$q(\mathscr{U}) = \left[\ln\Big(\frac{\rho}{\theta^{N/2}}\Big) - \frac{N}{2}\big(1+\ln(2\pi)\big)\right]\times\rho u = \eta(\mathscr{U})\frac{j}{\rho} = \int_{\mathbb{R}^N} vM_U\ln(M_U)\,\mathrm{d}v.$$

The relative entropy is

$$\begin{aligned}\eta(\mathscr{U}|\mathscr{U}_\star) &= \eta(\mathscr{U}) - \rho\left[\ln\Big(\frac{\rho_\star}{\theta_\star^{N/2}}\Big) + 1 - \frac{N}{2} - \frac{N}{2}\ln(2\pi)\right] + \rho_\star + \frac{1}{2\theta_\star}\big(\rho|u-u_\star|^2 + \rho N(\theta-\theta_\star)\big)\\ &= \mathcal{H}(M_U|M_{U_\star}) \geq 0.\end{aligned} \tag{2.11}$$

Finally we have

$$q(\mathscr{U}|\mathscr{U}_\star) = \int_{\mathbb{R}^N} v\left[M_U\ln\Big(\frac{M_U}{M_{U_\star}}\Big) - M_U + M_{U_\star}\right]\mathrm{d}v.$$

The proof of this lemma is just a lengthy but straightforward computation and will be omitted here.

2.3 Linearization

We consider a given state, with fixed and constant density $\rho_\star > 0$, velocity $u_\star \in \mathbb{R}^N$ and temperature $\theta_\star > 0$; we thus set $U_\star = (\rho_\star, u_\star, \theta_\star)$. The Maxwellian

$$M_{U_\star}(v) = \frac{\rho_\star}{(2\pi\theta_\star)^{N/2}}\exp\Big(-\frac{|v-u_\star|^2}{2\theta_\star}\Big)$$

is a solution of (1.1)–(2.2). We set

$$F(t,x,v) = M_{U_\star}(v)\big(1+f(t,x,v)\big)$$

where the amplitude of the fluctuation is intended to be small. The fluctuation f satisfies

$$\partial_t f + v\cdot\nabla_x f = \frac{1}{\tau}L_{U_\star}(f) + \frac{1}{\tau}R(f, M_{U_\star}) \tag{2.12}$$

where $L_{U_\star}$ is the linearized BGK operator and R is the remainder, with at least a quadratic estimate with respect to the amplitude of the fluctuation, defined by the development

$$\frac{M[M_{U_\star} + M_{U_\star}f] - M_{U_\star} - M_{U_\star}f}{M_{U_\star}} = L_{U_\star}f + R(f, M_{U_\star}).$$

In other words, we have

$$L_{U_\star} f = \frac{1}{M_{U_\star}} \frac{\partial}{\partial F} \big(M[F] - F \big) \Big|_{F = M_{U_\star}} (M_{U_\star} f).$$

For the BGK operator, computing the linearized operator reduces to apply the chain rule to obtain the derivative of the composite function

$$F \mapsto (\rho, j, \mathscr{E}) = \int_{\mathbb{R}^N} (1, v, v^2/2) F \, \mathrm{d}v \mapsto U = (\rho, u, \theta) \mapsto M_U.$$

The first application is linear and its derivative is simply defined by moments. Introducing the fluctuation of the macroscopic quantities

$$U = U_\star + \widetilde{U}, \qquad \widetilde{U} = \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u} \\ \widetilde{\theta} \end{pmatrix},$$

we are led to the linearization of the relation (2.8) which in turn defines the following linear relation

$$\widetilde{\mathscr{U}} = \begin{pmatrix} \widetilde{\rho} \\ \widetilde{j} \\ \widetilde{\mathscr{E}} \end{pmatrix} = \begin{pmatrix} 1 & 0^T & 0 \\ u_\star & \rho_\star \mathbb{I}_N & 0 \\ \dfrac{u_\star^2 + N\theta_\star}{2} & \rho_\star u_\star^T & N\rho_\star/2 \end{pmatrix} \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u} \\ \widetilde{\theta} \end{pmatrix} = P_\star \widetilde{U}. \tag{2.13}$$

Thus, the derivative of the second application is defined by the matrix $P_\star^{-1}$. Finally, we have

$$\nabla_{U_\star} M_{U_\star}(v) = M_{U_\star}(v) \begin{pmatrix} \dfrac{1}{\rho_\star} \\ \dfrac{v - u_\star}{\theta_\star} \\ -\dfrac{N}{2\theta_\star} + \dfrac{|v - u_\star|^2}{2\theta_\star^2} \end{pmatrix}.$$

Then, it turns out that the linearized operator reduces to a projection: let $f \in L^2(M_{U_\star} \, \mathrm{d}v)$, then

$$L_{U_\star} f = \Pi f - f$$

with

$$\Pi f := \frac{1}{M_{U_\star}} \nabla_{U_\star} M_{U_\star} \cdot \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u} \\ \widetilde{\theta} \end{pmatrix} = \frac{\widetilde{\rho}}{\rho_\star} + \frac{v - u_\star}{\theta_\star} \widetilde{u} + \frac{\widetilde{\theta}}{2\theta_\star} \Big(\frac{|v - u_\star|^2}{\theta_\star} - N \Big).$$

and

$$\begin{pmatrix} \widetilde{\rho} \\ \widetilde{\rho} u_\star + \rho_\star \widetilde{u} \\ \widetilde{\rho}(u_\star^2 + N\theta_\star) + 2\rho_\star u_\star \cdot \widetilde{u} + N\rho_\star \widetilde{\theta} \end{pmatrix} = P_\star \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u} \\ \widetilde{\theta} \end{pmatrix} = \int_{\mathbb{R}^N} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f M_{U_\star} \, \mathrm{d}v.$$

Clearly, Π is the orthogonal projection of $L^2(M_{U_\star} \, \mathrm{d}v)$ to the finite dimensional set spanned by the collisional invariants $\{1, v, |v|^2\}$. In fact the asymptotic and boundary layer analysis relies on the following properties of the linearized collision operator:

- $L_{U_\star}$ is self-adjoint for the inner product of $L^2(M_{U_\star}\,\mathrm{d}v)$,
- $\mathrm{Ker}(L_{U_\star}) = \mathrm{Span}\{1, v, |v|^2\}$,
- $\mathrm{Ran}(L_{U_\star}) = \big(\mathrm{Ker}(L_{U_\star})\big)^\perp$ for the inner product of $L^2(M_{U_\star}\,\mathrm{d}v)$,
- and the following dissipation property holds

$$\int_{\mathbb{R}^N} L_{U_\star} f\; f\; M_{U_\star}\,\mathrm{d}v \leq 0.$$

These properties are obviously satisfied by the linearized BGK operator which is a mere projection. But they are fulfilled for the Boltzmann operator as well, at least for hard potentials, see [14] (functional framework for the case of soft potentials is discussed in [34]). Here, for the sake of simplicity we restrict the discussion to the BGK operator.

Assuming that the fluctuation remains small, we get rid of the non linear remainder term in (2.12).[¶] We are thus concerned by the linear problem

$$\left\{\begin{array}{l} \partial_t f + v\cdot\nabla_x f = \dfrac{1}{\tau} L_{U_\star} f, \\ f_{|t=0} = f^{\mathrm{Init}}, \\ \gamma^{\mathrm{inc}} f(t,x,v) = \Psi^{\mathrm{data}}(t,v), \quad \text{ on } \Gamma^{\mathrm{inc}}, \end{array}\right. \tag{2.14}$$

where the boundary condition is given, coming back to (2.6), by

$$\Psi^{\mathrm{data}} = \frac{\Phi^{\mathrm{data}}}{M_{U_\star}} - 1.$$

Now, as $\tau \to 0$ we guess that f looks like an infinitesimal Maxwellian

$$f(t,x,v) \simeq m_{\widetilde{U}(t,x)}(v) = \frac{\widetilde{\rho}(t,x)}{\rho_\star} + \frac{v-u_\star}{\theta_\star}\widetilde{u}(t,x) + \frac{\widetilde{\theta}(t,x)}{2\theta_\star}\Big(\frac{|v-u_\star|^2}{\theta_\star} - N\Big) \in \mathrm{Ker}(L_{U_\star}).$$

Inserting this ansatz in the following moment system (analog for the linearized problem of (2.4))

$$\partial_t \int_{\mathbb{R}^N} \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} f M_{U_\star}\,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^N} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} f M_{U_\star}\,\mathrm{d}v = 0,$$

we are led to the linearized Euler system

$$\left\{\begin{array}{l} \partial_t \widetilde{\rho} + \rho_\star \nabla_x\cdot\widetilde{u} + u_\star\cdot\nabla_x\widetilde{\rho} = 0, \\ \partial_t \widetilde{u} + (u_\star\cdot\nabla_x)\widetilde{u} + \nabla_x\widetilde{\theta} + \dfrac{\theta_\star}{\rho_\star}\nabla_x\widetilde{\rho} = 0, \\ \partial_t \widetilde{\theta} + u_\star\cdot\nabla_x\widetilde{\theta} + \dfrac{2}{N}\theta_\star\nabla_x\cdot\widetilde{u} = 0. \end{array}\right. \tag{2.15}$$

Of course, we obtain the linear system (2.15) when we linearize directly the system of conservation laws (2.5), assuming that the perturbations and their derivatives remain small. The question is now to identify the boundary conditions to be satisfied by $\widetilde{\rho}, \widetilde{u}, \widetilde{\theta}$, that will depend on the kinetic incoming condition in (2.6).

[¶] which makes sense when the amplitude of the deviation f is small compared to τ.

2.4 Slab geometry

For the sake of simplicity, we avoid all difficulties associated to complex geometries and from now on we adopt the following simplified framework: the flow does not depend on the transverse variables $x_2, ..., x_N$ and the particles evolve in the domain $x_1 \in (-\omega, +\omega)$. We slightly change the notation by using x to denote the single coordinate x_1 characterizing this slab geometry. When necessary we shall write $u \in \mathbb{R}^N$ as $(u_1, u_\perp) \in \mathbb{R} \times \mathbb{R}^{N-1}$.

Then the kinetic equation now reads

$$\partial_t F + v_1 \partial_x F = \frac{1}{\tau}\Big(M_{U(t,x)} - F\Big) \qquad t \geq 0,\ x \in (-\omega, +\omega),\ v \in \mathbb{R}^N, \tag{2.16}$$

with ρ, u, θ associated to F by (2.3). The boundary condition becomes

$$\gamma^{\rm inc} F(t, -\omega, v) = \Phi^{\rm data,L}(t, v) \quad \text{for } v_1 > 0, \qquad \gamma^{\rm inc} F(t, +\omega, v) = \Phi^{\rm data,R}(t, v) \quad \text{for } v_1 < 0. \tag{2.17}$$

The linearized equation (2.14) can be recast in a similar fashion: we have

$$\begin{cases} \partial_t f + v_1 \partial_x f = \dfrac{1}{\tau} L_{U_\star} f, \\ f_{|_{t=0}} = f^{\rm Init}, \end{cases} \tag{2.18}$$

endowed with

$$\gamma^{\rm inc} f(t, -\omega, v) = \Psi^{\rm data,L}(t, v) \quad \text{for } v_1 > 0, \qquad \gamma^{\rm inc} f(t, +\omega, v) = \Psi^{\rm data,R}(t, v) \quad \text{for } v_1 < 0, \tag{2.19}$$

where $\Psi^{{\rm data},j} = \Phi^{{\rm data},j} / M_{U_\star} - 1$ for $j = {\rm L}$ or $j = {\rm R}$.

Let us go back to the hydrodynamic equations. In conserved variables the Euler system reads

$$\partial_t \mathscr{U} + \partial_x \mathscr{F}(\mathscr{U}) = 0,$$

where now $\mathscr{F} : \mathbb{R}^{N+2} \to \mathbb{R}^{N+2}$. It is given by the components $\mathscr{F}_{i1}$ of the multi-dimensional case. Precisely we have

$$\mathscr{F}(\mathscr{U}) = \begin{pmatrix} j_1 \\ j_1^2/\rho + 2\mathscr{E}/N - j^2/(N\rho) \\ j_1 j_\perp / \rho \\ \big((N+2)\mathscr{E}/N - j^2/(N\rho)\big) j_1/\rho \end{pmatrix}.$$

As far as the solution is smooth, we can rewrite the equation in the following non conservative form

$$\partial_t \mathscr{U} + \mathscr{A}(\mathscr{U}) \partial_x \mathscr{U} = 0,$$

with

$$\mathscr{A}(\mathscr{U}) = \nabla_{\mathscr{U}} \mathscr{F}(\mathscr{U}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -\frac{j_1^2}{\rho^2} + \frac{j^2}{N\rho^2} & \frac{2j_1}{\rho} - \frac{2j_1}{N\rho} & \left(\frac{2j_\perp}{N\rho}\right)^T & \frac{2}{N} \\ -\frac{j_1 j_\perp}{\rho^2} & \frac{j_\perp}{\rho} & \frac{j_1}{\rho}\mathbb{I}_{N-1} & 0 \\ -\left(\frac{N+2}{N}\mathscr{E} - \frac{j^2}{N\rho}\right)\frac{j_1}{\rho^2} + \frac{j_1 j^2}{N\rho^3} & \left(\frac{N+2}{N}\mathscr{E} - \frac{j^2}{N\rho}\right)\frac{1}{\rho} - \frac{2j_1^2}{N\rho^2} & \left(-\frac{2j_\perp j_1}{N\rho^2}\right)^T & \frac{N+2}{N}\frac{j_1}{\rho} \end{pmatrix}.$$

The linearized version of the Euler system is simply

$$\partial_t \widetilde{\mathscr{W}} + \mathscr{A}(\mathscr{U}_\star)\partial_x \widetilde{\mathscr{W}} = 0.$$

Equivalently we can express the system with the variations of density, velocity and temperature $\widetilde{U} = (\widetilde{\rho}, \widetilde{u}, \widetilde{\theta})$. We remind that they are related to the conservative unknowns by $\widetilde{\mathscr{W}} = P_\star \widetilde{U}$, see (2.13). In the slab geometry, (2.15) becomes

$$\partial_t \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u}_1 \\ \widetilde{u}_\perp \\ \widetilde{\theta} \end{pmatrix} + \underbrace{\begin{pmatrix} u_{\star 1} & \rho_\star & 0 & 0 \\ \dfrac{\theta_\star}{\rho_\star} & u_{\star 1} & 0 & 1 \\ 0 & 0 & u_{\star 1}\mathbb{I}_{N-1} & 0 \\ 0 & 2\theta_\star/N & 0 & u_{\star 1} \end{pmatrix}}_{:=A_\star} \partial_x \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u}_1 \\ \widetilde{u}_\perp \\ \widetilde{\theta} \end{pmatrix} = 0. \tag{2.20}$$

We thus have

$$\partial_t \widetilde{\mathscr{W}} + P_\star A_\star P_\star^{-1} \partial_x \widetilde{\mathscr{W}} = 0,$$

and of course

$$P_\star A_\star P_\star^{-1} = \mathscr{A}(\mathscr{U}_\star).$$

The characteristic speeds of the system are the eigenvalues of $A_\star$, that is $u_{\star 1}$ (with multiplicity N), $u_{\star 1} \pm c_\star$, with $c_\star = \sqrt{\frac{N+2}{N}\theta_\star}$ the sound speed. A difficulty is related to the fact that the number of boundary conditions necessary to complete the problem depends on the number of "incoming characteristics", that is the dimension of the eigenspace associated to positive eigenvalues (at $x = -\omega$, while at $x = +\omega$ we care about negative eigenvalues). This intuition[‖] becomes clear by using the natural symetrization of the system provided by the (relative) entropy.

To this end, we need to introduce a couple of notation, the goal being to rewrite the linearized system in an equivalent form $\partial_t \mathscr{S}_\star \widetilde{\mathscr{W}} + \partial_x \mathscr{Q}_\star \widetilde{\mathscr{W}} = 0$, with $\mathscr{S}_\star$ and $\mathscr{Q}_\star$ symmetric matrices. The definition of $\mathscr{S}_\star$ and $\mathscr{Q}_\star$ are deduced from the expression of the entropy. Since the pioneering works of K. O. Friedrichs and P. D. Lax [27] and S. Godunov [29], this is the standard preliminary step for studying hyperbolic problems. In particular it has an essential role for proving the local well-posedness of the non linear Cauchy problem. For the initial boundary value problem, the new formulation of the system gives rise to the boundary terms that need to be imposed.

Tedious computations yield

$$\nabla_{\mathscr{W}} \eta(\mathscr{W}|\mathscr{U}_\star) = \begin{pmatrix} \ln\Big(\dfrac{\rho}{\rho_\star}\Big(\dfrac{\theta_\star}{\theta}\Big)^{N/2}\Big) + \dfrac{|u-u_\star|^2}{2\theta_\star} - \dfrac{u}{\theta_\star}\cdot(u-u_\star) + \Big(-\dfrac{1}{\theta} + \dfrac{1}{\theta_\star}\Big)\dfrac{|u|^2}{2} \\ \dfrac{u}{\theta} - \dfrac{u_\star}{\theta_\star} \\ -\dfrac{1}{\theta} + \dfrac{1}{\theta_\star} \end{pmatrix}.$$

[‖]The basic tools for the analysis of hyperbolic mixed problems are described e. g. in [53, Chapter 14].

Differentiating once more and evaluating the Hessian matrix at $\mathscr{U} = \mathscr{U}_\star$ defines the matrix

$$\mathscr{S}_\star = D^2_{\mathscr{U}}\eta(\mathscr{U}|\mathscr{U}_\star)\Big|_{\mathscr{U}=\mathscr{U}_\star} = \begin{pmatrix} \frac{1}{\rho_\star}\Big(1+\frac{N}{2}+\frac{|u_\star|^4}{2N\theta_\star^2}\Big) & -\frac{|u_\star|^2}{N\rho_\star\theta_\star^2}u_\star^T & -\frac{1}{\rho_\star\theta_\star}+\frac{|u_\star|^2}{N\rho_\star\theta_\star^2} \\ -\frac{|u_\star|^2}{N\rho_\star\theta_\star^2}u_\star & \Big(\frac{1}{\rho_\star\theta_\star}+\frac{2|u_\star|^2}{N\rho_\star\theta_\star^2}\Big)\mathbb{I}_N & -\frac{2u_\star}{N\rho_\star\theta_\star^2} \\ -\frac{1}{\rho_\star\theta_\star}+\frac{|u_\star|^2}{N\rho_\star\theta_\star^2} & -\frac{2u_\star^T}{N\rho_\star\theta_\star^2} & \frac{2}{N\rho_\star\theta_\star^2} \end{pmatrix}.$$

Since η is strictly convex (see Lemma 2.1), $\mathscr{S}_\star$ is symmetric positive definite. Now, we evaluate the entropy flux. Since $\eta(\mathscr{U}|\mathscr{U}_\star)$ and $q(\mathscr{U}|\mathscr{U}_\star)$ as well as the gradient of $\eta(\mathscr{U}|\mathscr{U}_\star)$ vanish at $\mathscr{U} = \mathscr{U}_\star$, by differentiating (2.9) we obtain

$$\mathscr{A}(\mathscr{U})^T D^2_{\mathscr{U}}\eta(\mathscr{U}|\mathscr{U}_\star)\Big|_{\mathscr{U}=\mathscr{U}_\star} = D^2_{\mathscr{U}}q(\mathscr{U}|\mathscr{U}_\star)\Big|_{\mathscr{U}=\mathscr{U}_\star}. \tag{2.21}$$

We denote by $\mathscr{Q}_\star$ this matrix. Since it is defined as an Hessian matrix, it is symmetric and we have

$$\mathscr{Q}_\star = \mathscr{A}(\mathscr{U}_\star)^T\mathscr{S}_\star = \mathscr{Q}_\star^T = \mathscr{S}_\star^T\mathscr{A}(\mathscr{U}_\star) = \mathscr{S}_\star\mathscr{A}(\mathscr{U}_\star). \tag{2.22}$$

Considering small fluctuations around $\mathscr{U}_\star$, we can expand the entropy relation (2.10) rewritten as

$$\partial_t\eta(\mathscr{U}_\star+\widetilde{\mathscr{U}}|\mathscr{U}_\star)+\partial_x q(\mathscr{U}_\star+\widetilde{\mathscr{U}}|\mathscr{U}_\star) = 0.$$

At leading order it yields

$$\partial_t(\mathscr{S}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}})+\partial_x(\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}) = 0. \tag{2.23}$$

Of course we can obtain the same relation by remarking that the multiplication of (2.20) by $\mathscr{S}_\star$ leads to

$$\partial_t\mathscr{S}_\star\widetilde{\mathscr{U}}+\partial_x\mathscr{Q}_\star\widetilde{\mathscr{U}} = 0,$$

owing to (2.22). Then we use the symmetry of the matrices $\mathscr{S}_\star$ and $\mathscr{Q}_\star$ to deduce (2.23). The interest of the identity (2.23) relies on the derivation of an energy estimate as follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\omega}^{+\omega}\mathscr{S}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}\,\mathrm{d}x+\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}\Big|_{x=-\omega}^{x=+\omega} = 0.$$

Separating contributions according to their sign yields

$$\begin{aligned} 0 \le \int_{-\omega}^{+\omega}\mathscr{S}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,x)\,\mathrm{d}x+\int_0^t\Big[\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,+\omega)\Big]_+\mathrm{d}t-\int_0^t\Big[\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,-\omega)\Big]_-\mathrm{d}t \\ = \int_{-\omega}^{+\omega}\mathscr{S}_\star\widetilde{\mathscr{U}}^{\mathrm{Init}}\cdot\widetilde{\mathscr{U}}^{\mathrm{Init}}(x)\,\mathrm{d}x+\int_0^t\Big[\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,-\omega)\Big]_+\mathrm{d}t-\int_0^t\Big[\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,+\omega)\Big]_-\mathrm{d}t. \end{aligned} \tag{2.24}$$

Hence we realize that uniqueness is guaranteed when the non negative part of $\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,x=-\omega)$ and the non positive part of $\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}(t,x=+\omega)$ are given.

These considerations are the key ingredients to study the well-posedness of the initial boundary value problem for the linearized system (2.20). We refer to [32] for a crystal-clean overview. The following claim makes the connection between the signature $\sigma_{U_\star}$ of the quadratic form $\widetilde{\mathscr{U}}\longmapsto\mathscr{Q}_\star\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}} = \mathscr{S}_\star\mathscr{A}(\mathscr{U}_\star)\widetilde{\mathscr{U}}\cdot\widetilde{\mathscr{U}}$, see (2.22), and the eigenvalues of the flux matrix $\mathscr{A}(\mathscr{U}_\star)$: the dimension of the eigenspaces associated to positive (resp. negative) eigenvalues of $\mathscr{Q}_\star$ corresponds to the number of positive (resp. negative) eigenvalues of the flux matrix $\mathscr{A}(\mathscr{U}_\star)$, that is, for the left hand boundary $x=-\omega$, the number of "incoming" (resp. "outgoing") characteristics and for the right hand boundary $x=+\omega$, the number of "outgoing" (resp. "incoming") characteristics.

Proposition 2.1. *The signature $\sigma_{U_\star}$ is (n_+, n_-), with $n_+ + n_- + n_0 = N + 2$, n_0 being the dimension of* $\mathrm{Ker}(\mathscr{Q}_\star)$*, and n_+, resp. n_-, is the cardinal of the set of the positive, resp. negative, eigenvalues of $\mathscr{A}(\mathscr{U}_\star)$.*

Combining this statement, which comes from basic linear algebra, to the energy estimate (2.24) we are led to the following well-posedness statement which makes precise the nature of required boundary conditions for solving (2.20).

Proposition 2.2. *Let $E^\pm$ be a subspace of $\mathbb{R}^{N+2}$ such that*

i) For any $\widetilde{\mathscr{U}} \in E^\pm \setminus \{0\}$, we have $\pm \mathscr{Q}_\star \widetilde{\mathscr{U}} \cdot \widetilde{\mathscr{U}} > 0$,

ii) $E^\pm$ is maximal in the sense that any subspace $E \subset \mathbb{R}^{N+2}$ verifying the property stated in i), is included in $E^\pm$.

We set

$$E^{\pm\perp} = \big\{ \widetilde{\mathscr{U}} \in \mathbb{R}^{N+2},\ \text{such that for any } \widetilde{\mathscr{V}} \in E^\pm \text{ we have } \mathscr{Q}_\star \widetilde{\mathscr{U}} \cdot \widetilde{\mathscr{V}} = 0 \big\}.$$

Let $t \longmapsto \widetilde{\mathscr{U}}^{\mathrm{data,L}}(t)$ and $t \longmapsto \widetilde{\mathscr{U}}^{\mathrm{data,R}}(t)$ be integrable functions on $(0,T)$ for any $0 < T < \infty$ such that $\widetilde{\mathscr{U}}^{\mathrm{data,L}}(t) \in E^{-\perp}$ and $\widetilde{\mathscr{U}}^{\mathrm{data,R}}(t) \in E^{+\perp}$. We consider the mixed problem

$$\begin{cases} \partial_t \widetilde{\mathscr{U}} + \mathscr{A}(\mathscr{U}_\star)\partial_x \widetilde{\mathscr{U}} = 0, \\ \widetilde{\mathscr{U}}_{|t=0} = \widetilde{\mathscr{U}}^{\mathrm{Init}} \in H^1([-\omega,\omega]), \\ \widetilde{\mathscr{U}}(t,-\omega) - \widetilde{\mathscr{U}}^{\mathrm{data,L}} \in E^-, \qquad \widetilde{\mathscr{U}}(t,+\omega) - \widetilde{\mathscr{U}}^{\mathrm{data,R}} \in E^+. \end{cases}$$

Suppose that $\widetilde{\mathscr{U}}^{\mathrm{Init}}(x=-\omega) - \widetilde{\mathscr{U}}^{\mathrm{data,L}}(t=0) \in E^-$ and $\widetilde{\mathscr{U}}^{\mathrm{Init}}(x=+\omega) - \widetilde{\mathscr{U}}^{\mathrm{data,R}}(t=0) \in E^+$. Then the mixed problem has a unique solution in $C^1(0,\infty; L^2(-\omega,+\omega))$.

We refer to [20, 32] and [53, Chapter 14] for more details and proofs of these two propositions.

2.5 Boundary layer

As already remarked

$$\mathcal{H}(F|M_{U_\star}) = \int_{\mathbb{R}^N} \Big(F \ln(F/M_{U_\star}) - F + M_{U_\star} \Big)\, \mathrm{d}v \geq 0$$

is the relative entropy associated to the BGK equation (1.1)–(2.2). Then we remark that, for any perturbation f and $0 < \delta \ll 1$,

$$\mathcal{H}(M_{U_\star}(1+\delta f)|M_{U_\star}) = \frac{\delta^2}{2} \int_{\mathbb{R}^N} |f|^2 M_{U_\star}\, \mathrm{d}v + \mathscr{O}(\delta^3).$$

Accordingly,

$$f \longmapsto \int_{\mathbb{R}^N} |f|^2 M_{U_\star}\, \mathrm{d}v$$

defines an entropy for the linearized equation and indeed solutions of (2.18) satisfy

$$\partial_t \int_{\mathbb{R}^N} |f|^2 M_{U_\star}\, \mathrm{d}v + \partial_x \int_{\mathbb{R}^N} v_1 |f|^2 M_{U_\star}\, \mathrm{d}v = \frac{2}{\tau} \int_{\mathbb{R}^N} L_{U_\star} f\ f\ M_{U_\star}\, \mathrm{d}v \leq 0.$$

Evaluating the entropy flux on an infinitesimal Maxwellian defines a quadratic form of the macroscopic quantities:

$$\mathbf{Q} : g = m_{\widetilde{U}} \in \mathrm{Ker}(L_{U_\star}) \mapsto \int_{\mathbb{R}^N} v_1 |g|^2 M_{U_\star} \, \mathrm{d}v$$

satisfies

$$\begin{aligned}
\mathbf{Q}(m_{\widetilde{U}}) &= \int_{\mathbb{R}^N} v_1 \Big| \frac{\widetilde{\rho}}{\rho_\star} + \frac{v-u_\star}{\theta_\star}\widetilde{u} + \frac{\widetilde{\theta}}{2\theta_\star}\Big(\frac{|v-u_\star|^2}{\theta_\star} - N\Big)\Big|^2 M_{U_\star} \, \mathrm{d}v \\
&= \frac{u_{\star 1}}{\rho_\star}\widetilde{\rho}^2 + \frac{\rho_\star u_{\star 1}}{\theta_\star}\widetilde{u}_1^2 + \frac{\rho_\star u_{\star 1}}{\theta_\star}\widetilde{u}_\perp \cdot \widetilde{u}_\perp + N\frac{\rho_\star u_{\star 1}}{2\theta_\star}\widetilde{\theta}^2 + 2\widetilde{\rho}\widetilde{u}_1 + 2\frac{\rho_\star}{\theta_\star}\widetilde{u}_1\widetilde{\theta} \\
&= \begin{pmatrix} \frac{u_{\star 1}}{\rho_\star} & 1 & 0 & 0 \\ 1 & \frac{\rho_\star u_{\star 1}}{\theta_\star} & 0 & \frac{\rho_\star}{\theta_\star} \\ 0 & 0 & \frac{\rho_\star u_{\star 1}}{\theta_\star} & 0 \\ 0 & \frac{\rho_\star}{\theta_\star} & 0 & N\frac{\rho_\star u_{\star 1}}{2\theta_\star^2} \end{pmatrix} \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u}_1 \\ \widetilde{u}_\perp \\ \widetilde{\theta} \end{pmatrix} \cdot \begin{pmatrix} \widetilde{\rho} \\ \widetilde{u}_1 \\ \widetilde{u}_\perp \\ \widetilde{\theta} \end{pmatrix} = \Sigma_\star \widetilde{U} \cdot \widetilde{U}.
\end{aligned}$$

In fact this quantity gives the entropy flux in the variables $(\widetilde{\rho}, \widetilde{u}, \widetilde{\theta})$ instead of the conservative variables, owing to the following claim.

Lemma 2.2. *We have* $\Sigma_\star = P_\star^T \mathscr{Q}_\star P_\star$.

Proof. The identity can be checked by direct inspection. Instead, let us give some hints explaining where the formula comes from. According to the definition of the entropy flux $q(\mathscr{U}|\mathscr{U}_\star)$ in Lemma 2.1, $\mathbf{Q}(m_{\widetilde{U}})$ corresponds to the leading term in the expansion of

$$\int_{\mathbb{R}^N} v \left[M_{U_\star + \widetilde{U}} \ln\Big(\frac{M_{U_\star+\widetilde{U}}}{M_{U_\star}}\Big) - M_{U_\star+\widetilde{U}} + M_{U_\star} \right] \mathrm{d}v.$$

Therefore, by identification with (2.23) and using (2.13), we obtain

$$\mathbf{Q}(m_{\widetilde{U}}) = \Sigma_\star \widetilde{U} \cdot \widetilde{U} = \mathscr{Q}_\star \widetilde{\mathscr{U}} \cdot \widetilde{\mathscr{U}} = \mathscr{Q}_\star P_\star \widetilde{U} \cdot P_\star \widetilde{U} = P_\star^T \mathscr{Q}_\star P_\star \widetilde{U} \cdot \widetilde{U}.$$

□

Let us split the set of infinitesimal Maxwellians according to the sign of the quadratic form $\mathbf{Q}$:

$$\mathrm{Ker}(L_{U_\star}) = \Lambda^+ \oplus \Lambda^- \oplus \Lambda^0,$$

with

$$\mathbf{Q}_{|\Lambda^+} \text{ is positive definite, } \mathbf{Q}_{|\Lambda^-} \text{ is negative definite and } \Lambda^0 = \big\{ g = m_{\widetilde{U}},\ \mathbf{Q}(g) = 0 \big\}.$$

By Lemma 2.2, we note that $g = m_{\widetilde{U}} \in \Lambda^\pm$ means that $\widetilde{\mathscr{U}} = P_\star \widetilde{U}$ verifies $\pm \mathscr{Q}_\star \widetilde{\mathscr{U}} \cdot \widetilde{\mathscr{U}} > 0$ and thus $\widetilde{\mathscr{U}}$ belongs to $E^\pm$ as arising in Proposition 2.2. Owing to Proposition 2.1 and Lemma 2.2, we have

$$\dim(\Lambda^+) = n_+, \qquad \dim(\Lambda^-) = n_-, \qquad \dim(\Lambda^0) = n_0$$

and a correspondence is established between the quadratic form $\mathbf{Q}$ on $\mathrm{Ker}(L_{U_\star})$ and the quadratic form on $\mathbb{R}^{N+2}$ associated to the symmetric matrix $\mathscr{Q}_\star$. According to [20], and as developed in [9,32], it is convenient to introduce the following basis of $\mathrm{Ker}(L_{U_\star})$:

$$\begin{aligned}
\chi_1(v) &= \frac{1}{\sqrt{2N(N+2)}}\Big(\sqrt{N(N+2)}\frac{v_1-u_{\star 1}}{\sqrt{\theta_\star}} + \frac{|v-u_\star|^2}{\theta_\star}\Big),\\
\chi_0(v) &= \frac{1}{\sqrt{2(N+2)}}\Big(\frac{|v-u_\star|^2}{\theta_\star} - N - 2\Big),\\
\chi_k(v) &= \frac{v_k-u_{\star k}}{\sqrt{\theta_\star}} \qquad \text{for } k\in\{2,...,N\},\\
\chi_{N+1}(v) &= \frac{1}{\sqrt{2N(N+2)}}\Big(\sqrt{N(N+2)}\frac{v_1-u_{\star 1}}{\sqrt{\theta_\star}} - \frac{|v-u_\star|^2}{\theta_\star}\Big).
\end{aligned}$$

In what follows, we denote

$$I^{\pm} = \big\{k\in\{0,...,N+1\}, \chi_k\in\Lambda^{\pm}\big\}, \qquad I^0 = \big\{k\in\{0,...,N+1\}, \chi_k\in\Lambda^0\big\}.$$

Note that $\#I^+ = n_+, \#I^- = n_-, \#I^0 = n_0$. The interest of this specific basis relies on the orthogonality properties and useful formula summarized in the following Lemma.

Lemma 2.3. *We have*

$$\begin{aligned}
&\int_{\mathbb{R}^N} \chi_k\chi_l(v)\, M_{U_\star}\,\mathrm{d}v = \rho_\star\delta_{kl},\\
&\int_{\mathbb{R}^N} v_1\chi_k\chi_l(v)\, M_{U_\star}\,\mathrm{d}v = 0 \qquad \textit{if } k\neq l.
\end{aligned}$$

Furthermore, we observe that

$$\begin{aligned}
&\int_{\mathbb{R}^N} v_1|\chi_1|^2(v)\, M_{U_\star}\,\mathrm{d}v = \rho_\star\Big(u_{\star 1} + \sqrt{\frac{N+2}{N}}\theta_\star\Big) = \rho_\star(u_{\star 1}+c_\star),\\
&\int_{\mathbb{R}^N} v_1|\chi_k|^2(v)\, M_{U_\star}\,\mathrm{d}v = \rho_\star u_{\star 1} \qquad \textit{for } k\in\{0,2,...,N\},\\
&\int_{\mathbb{R}^N} v_1|\chi_{N+1}|^2(v)\, M_{U_\star}\,\mathrm{d}v = \rho_\star\Big(u_{\star 1} - \sqrt{\frac{N+2}{N}}\theta_\star\Big) = \rho_\star(u_{\star 1}-c_\star).
\end{aligned}$$

The final touch consists in introducing an ansatz which takes into account the boundary layer correctors. We expand the solution of (2.18) as follows

$$f(t,x,v) = m_{\widetilde{U}(t,x)}(v) + G^{\mathrm{L}}(t,(x+\omega)/\tau,v) + G^{\mathrm{R}}(t,(\omega-x)/\tau,v) + r_\tau(t,x,v)$$

with r_τ a remainder which is expected to be small as τ goes to 0. The correctors $G^{\mathrm{L}}(t,z=(\omega+x)/\tau,v)$ and $G^{\mathrm{R}}(t,z=(\omega-x)/\tau,v)$ are defined from the following half space problem

$$\left\{\begin{array}{ll} v_1\partial_z G = L_{U_\star}G, & \text{for } z>0 \text{ and } v\in\mathbb{R}^N,\\ \gamma^{\mathrm{inc}}G(0,v) = \mathrm{Y}^{\mathrm{data}}, & \text{for } v_1>0, \end{array}\right. \tag{2.25}$$

where $\mathrm{Y}^{\mathrm{data}}$ has to be suitability defined (the variables of the half-space problem are z and v; in fact we are concerned with data parametrized by the time variable but we omit the time dependence to simplify the notations). We seek a solution which vanishes at infinity: imposing

$$G(z,v) \xrightarrow[z\to+\infty]{} 0 \tag{2.26}$$

means that the influence of the corrector becomes negligible far away from the boundary $x = -\omega$ or $x = +\omega$. The complete analysis of the half-space problem is due to [20] (after the preliminary breakthrough of [6] and formulation of the problem in [13]; for the specific case of the linearized BGK operator the analysis appeared in a different form in [3, 38]). Precisely, we have the following statement [20, Theorem 1.7.1]

Theorem 2.1. *Let V^+ be a subspace of $\mathrm{Ker}(L_{U_\star})$ satisfying*

i) For any $\widetilde{U} \in \mathbb{R}^{N+2} \setminus \{0\}$ such that $m_{\widetilde{U}} \in V^+$ we have $\mathbf{Q}(m_{\widetilde{U}}) \geq 0$,

ii) V^+ is maximal in the sense that any subspace $V \subset \mathrm{Ker}(L_{U_\star})$ verifying the property stated in i) is included in V^+.

Let $\Upsilon^{\mathrm{data}} \in L^2(\mathbb{R}^N, (1+|v|)M_{U_\star}(v)\,\mathrm{d}v)$. Then, for any $m \in \mathrm{Ker}(L_{U_\star})$, there exists a unique $m_\infty \in V^+$ and a unique solution $G \in L^\infty\big(0,\infty; L^2(\mathbb{R}^N, M_{U_\star}\,\mathrm{d}v)\big)$ of (2.25) such that for any $\gamma > 0$ small enough we have

$$e^{\gamma z}\Big(G(z,v) - m - m_\infty(v)\Big) \in L^\infty\big(0,\infty; L^2(\mathbb{R}^N, (1+|v|)M_{U_\star}(v)\,\mathrm{d}v)\big).$$

The statement can be rephrased as follows (using Theorem 2.1 with $m = 0$)

Corollary 2.1. *There exists a linear mapping (that can be called the generalized Chandrasekhar functional)*

$$\begin{array}{rccc} \mathscr{C}_\star : & L^2(\mathbb{R}^N, (1+|v|)M_{U_\star}(v)\,\mathrm{d}v) & \longrightarrow & V^+ \\ & \Upsilon^{\mathrm{data}} & \longmapsto & m_\infty \end{array}$$

with m_∞ the limit as $z \to \infty$ of the unique solution $G \in L^\infty\big(0,\infty; L^2(\mathbb{R}^N, M_{U_\star}\,\mathrm{d}v)\big)$ of (2.25).

This statement defines the necessary boundary condition for the macroscopic field $\widetilde{U}$ at the boundary $x = -\omega$ and $x = +\omega$. Indeed, coming back to (2.18), the boundary layer correctors are defined as follows:

- $G^{\mathrm{L}}(t,z,v) = G(t,z,v)$ with G the solution of (2.25) with incoming data
$$\Upsilon^{\mathrm{data}}(v) = \Psi^{\mathrm{data,L}}(t,v) - m_{\widetilde{U}(t,-\omega)}(v),$$
- $G^{\mathrm{R}}(t,z,v) = G(t,z,\hat{v})$ with G the solution of (2.25) with incoming data
$$\Upsilon^{\mathrm{data}}(v) = \Psi^{\mathrm{data,R}}(t,\hat{v}) - m_{\widetilde{U}(t,+\omega)}(\hat{v}),$$
where if $v = (v_1, v_2, v_3)$, $\hat{v} = (-v_1, v_2, v_3)$.

The n_+ necessary boundary conditions at $x = -\omega$ (resp. the n_- necessary boundary conditions at $x = +\omega$) are provided by the determination of the asymptotic state m_∞ associated to the incoming data. Imposing (2.26) means that

$$\mathscr{C}_\star(\Psi^{\mathrm{data,L}}(t,\cdot)) = \mathscr{C}_\star(m_{\widetilde{U}(t,-\omega)}), \qquad \mathscr{C}_\star(\Psi^{\mathrm{data,R}}(t,\cdot)) = \mathscr{C}_\star(m_{\widetilde{U}(t,+\omega)}). \tag{2.27}$$

In fact it is maybe more intuitive to split $m_{\widetilde{U}(t,-\omega)}$ into its "outgoing part" $m_- = \sum_{k\in I^-} \alpha_k\chi_k$ and its "incoming part" $m_+ = \sum_{k\in I^+\cup I^0} \alpha_k\chi_k$: the former is determined by the flow while the latter has to be imposed as a boundary condition to complete the Euler system. Precisely, let us define $\tilde{G}$ as to be the solution of (2.25) with incoming data $\Upsilon^{\mathrm{data}} = \Psi^{\mathrm{data,L}} - m_-$. Then, the boundary condition for the macroscopic field is obtained by requiring m_+ to be the asymptotic state of $\tilde{G}(z,v)$ as $z \to \infty$ which means

$$\mathscr{C}_\star(m_+(t,.)) = \mathscr{C}_\star(\Psi^{\mathrm{data,L}}(t,.) - m_-(t,.)).$$

A similar reasoning applies for the boundary condition at $x = \omega$. We are going to use this formalism in order to define numerical fluxes.

3 Finite Volume scheme and treatment of the boundary conditions

From now on, we only consider the case $N = 1$ and we assume for the velocity variable $v \in \mathbb{R}$. The space domain reduces to the interval $(-\omega, +\omega)$, where for the simulation we will set $\omega = 0.5$. We wish to compare the simulation of the 1D BGK equation (2.16) endowed with the initial condition $F_{|t=0} = F^{\text{Init}}$ and the given incoming boundary condition (2.17) with the simulation of the Euler system

$$\left\{ \begin{array}{l} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + \rho\theta) = 0, \\ \partial_t\Big(\dfrac{\rho u^2 + \rho\theta}{2}\Big) + \partial_x\Big(\Big(\dfrac{\rho u^2}{2} + \dfrac{3}{2}\rho\theta\Big)u\Big) = 0, \end{array} \right. \tag{3.1}$$

completed with boundary conditions defined through the boundary layer analysis.

We introduce a regular subdivision

$$-\omega = x_0 < x_1 = -\omega + \Delta x < ... < x_i = -\omega + i\Delta x < ... < x_{I+1} = -\omega + (I+1)\Delta x = +\omega.$$

In order to solve the kinetic equation (2.16) we use a simple splitting scheme: given $F^n_{i,p}$, an approximation of F at time $n\Delta t$, position $x_i = -\omega + i\Delta x$ and velocity $p\Delta v$, with $n \in \mathbb{N}$, $i \in \{0, ..., I+1\}$, where $(I+1)\Delta x = +2\omega$, and $p \in \{-P, ..., P\}$

- Firstly, we solve the free transport equation $(\partial_t + v\partial_x)F = 0$ starting from $F_{|n\Delta t} = F^n$. Of course, we treat a discrete version of the equation which casts as

  $$F^{n+1/2}_{i,p} = F^n_{i,p} - \Delta t \mathbb{D}_{i,p} F^n$$

  where $\mathbb{D}$ is a discrete version of the advection operator $v\partial_x$. For instance, we can work with the upwind scheme which leads to

  $$\mathbb{D}_{ip}F = \frac{p\Delta v}{\Delta x}(F_{i,p} - F_{i-1,p}) \quad \text{if } p > 0, \qquad \mathbb{D}_{ip}F = \frac{p\Delta v}{\Delta x}(F_{i+1,p} - F_{i,p}) \quad \text{if } p < 0,$$

  and $\mathbb{D}_{i0}F = 0$. The scheme is completed by using the incoming boundary condition for the fictitious points. The solution at time $(n+1)\Delta t$ defines the state $F^{n+1/2}$.

- Secondly, we solve the collision part $\partial_t F = \frac{1}{\tau}(M[F] - F)$ with initial data $F_{|n\Delta t} = F^{n+1/2}$. Actually, it reduces to a mere ODE since the macroscopic quantities do not change during this time step: since $\int_{\mathbb{R}}(1, v, |v|^2)F\,\mathrm{d}v = \int_{\mathbb{R}}(1, v, |v|^2)F^{n+1/2}\,\mathrm{d}v$, we have $M[F] = M[F^{n+1/2}]$ and therefore we end up with

  $$F^{n+1} = (1 - e^{-\Delta t/\tau})M[F^{n+1/2}] + e^{-\Delta t/\tau}F^{n+1/2}.$$

Actually, we make use of the Strang version of this algorithm which is a straightforward extension intended to reach second order accuracy with respect to time.

Of course as the parameter τ becomes small the resolution of the kinetic equation becomes highly demanding in computational time since the simulation can produce relevant results capturing the microscopic effects only under the constraints $\Delta t, \Delta x \ll \tau$. Thus, when τ goes to 0 there is a clear advantage in using the hydrodynamic equations which furthermore work on a reduced set of variables (since we do not need to consider the velocity variable v). In what follows, the simulation of

(2.16)–(2.17) by using the splitting scheme will serve to obtain a reference solution, at the price of a very long computational time, and validate our numerical treatment of the boundary conditions for the Euler system.

Now, let us explain the scheme for the Euler system (3.1). To this end, let us denote, for any $i \in \{1, ..., I\}$, $C_i = \big(-\omega + (i-1/2)\Delta x, -\omega + (i+1/2)\Delta x\big)$ to be the cell centered on x_i. Similarly, the boundary cells are defined by $C_0 = (-\omega, -\omega + \Delta x/2)$ and $C_{I+1} = (\omega - \Delta x/2, \omega)$. Then $\mathscr{U}_i^n$ is intended to be an approximation of $\frac{1}{\Delta x}\int_{C_i} \mathscr{U}(n\Delta t, x)\,\mathrm{d}x$, the mean value of $\mathscr{U}(n\Delta t, x)$ over the cell C_i. The definition of the scheme is deduced from the integration of (3.1) over the cell $(n\Delta t, (n+1)\Delta t) \times C_i$:

$$\int_{C_i} \mathscr{U}((n+1)\Delta t, x)\,\mathrm{d}x - \int_{C_i} \mathscr{U}(n\Delta t, x)\,\mathrm{d}x + \int_{n\Delta t}^{(n+1)\Delta t} \Big(\mathscr{F}(\mathscr{U})(s, -\omega + (i+1/2)\Delta x) - \mathscr{F}(\mathscr{U})(s, -\omega + (i-1/2)\Delta x)\Big)\,\mathrm{d}s = 0$$

suggests

$$\mathscr{U}_i^{n+1} - \mathscr{U}_i^n = -\frac{\Delta t}{\Delta x}\Big(\mathscr{F}_{i+1/2}^n - \mathscr{F}_{i-1/2}^n\Big)$$

where $\mathscr{F}_{i+1/2}^n$ is an approximation of the flux on the interface $x = -\omega + (i+1/2)\Delta x$ on the time step. This approximation is obtained as a suitable function of the $\mathscr{U}_k^n$'s: in the simplest case, the numerical flux on the interface $x = -\omega + (i+1/2)\Delta x$ is determined by the unknowns in the two neighboring cells

$$\mathscr{F}_{i+1/2}^n = \mathbf{F}(\mathscr{U}_i^n, \mathscr{U}_{i+1}^n)$$

see [28, 43]. In what follows we work with Godunov fluxes (see e. g. [43, Chapter 15]) for the interior cells which correspond to the cells with $i \in \{1, ..., I\}$ since the scheme uses only 3 points, but of course more sophisticated schemes can be used. The question is now to define the boundary fluxes, namely for indices $i = 0$ and $i = I + 1$, in a way that accounts for the boundary layer analysis.

Actually, the question is two–fold. The first difficulty consists in performing the non linear boundary layer analysis and deriving the hydrodynamic boundary condition coming from (2.17) in the fluid regime. To our knowledge the theory is not developed as for the linearized problem, except certainly for scalar equations as discussed in [56]. Next, the underlying half-space problems are usually not affordable for the numerical simulation since their resolution is at least as difficult as the original kinetic problem. Hence, we need an additional approximation procedure. The approach we propose is based on the linearized theory described above. It has the advantage of offering a neat framework and a natural way to determine the number and the nature of the needed boundary conditions for the hyperbolic system (3.1). The first attempt would be to use directly (2.27) as a boundary condition: as we shall see it could be valid as far as the solution of the kinetic equation remains close to the reference state $M_{U_\star}$. But of course, using this boundary condition, which comes from a purely linear theory, is certainly questionable since it relies on the permutation of the linearization limit where the amplitude of the fluctuation vanishes and the small mean free path limit (hydrodynamic limit) $\tau \to 0$ in (2.12). Clearly inverting these limits is not valid and the linearized theory cannot be applied in general cases. Nevertheless, we can go beyond this naive idea and we shall use the neat picture offered by the linearized theory to design numerical fluxes based on a local linearization, considering the values in the closest cells to the boundaries as the reference state. Let us describe how the numerical approximation works. In what follows we explain the construction of the numerical fluxes and

details on the underlying formulae are given in the Appendix.

Linearized equations. Let us start by considering the linearized situation which assumes that the solution reads $\mathscr{U} = \mathscr{U}_\star + \widetilde{\mathscr{U}}$, where $\widetilde{\mathscr{U}}$ is a "small" perturbation of the constant state $\mathscr{U}_\star$. Therefore (2.20) can be considered as an approximation of the non linear equations (3.1). In particular, the number of necessary boundary conditions is entirely determined by the reference state $\mathscr{U}_\star$ and we shall distinguish the cases:

- $u_\star - \sqrt{3\theta_\star} > 0$: the signature $\sigma_{U_\star}$ is $(3,0)$ and we do need 3 incoming data at $x = -\omega$, and all fields are outgoing at $x = +\omega$,
- $u_\star > 0 > u_\star - \sqrt{3\theta_\star}$: the signature $\sigma_{U_\star}$ is $(2,1)$ and we need to prescribe 2 incoming data at $x = -\omega$, only 1 at $x = +\omega$,
- $u_\star + \sqrt{3\theta_\star} > 0 > u_\star$: the signature $\sigma_{U_\star}$ is $(1,2)$ and we need to prescribe 1 incoming data at $x = -\omega$, and 2 at $x = +\omega$,
- $u_\star = \sqrt{3\theta_\star}$, $u_\star = 0$ and $u_\star = -\sqrt{3\theta_\star}$ correspond to degenerate cases where there exists a field which is characteristic at the boundary; the signature $\sigma_{U_\star}$ is $(2,0)$, $(1,1)$ or $(0,2)$ respectively which means that 2 or 1 or 0 data are needed at $x = -\omega$ (respectively 0, or 1 or 2 at $x = +\omega$).

Let us focus on the non-degenerate cases. At the boundary, for the left–hand boundary the flux that we seek has the following expression

$$\mathcal{F}_{\rm bd} = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} \Phi^{\rm data}\, {\rm d}v + \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} \big(1 + m_{\rm bd} + \gamma^{\rm out} G(0,v)\big)\, M_{U_\star}\, {\rm d}v, \quad (3.2)$$

with

$$M_{U_\star}(v) = \frac{\rho_\star}{\sqrt{2\pi\theta_\star}}\, \exp\left(-\frac{(v-u_\star)^2}{2\theta_\star}\right),$$

the reference Maxwellian,

$$m_{\rm bd}(v) = \frac{\rho_{\rm bd}}{\rho_\star} + u_{\rm bd}\frac{v-u_\star}{\theta_\star} + \frac{\theta_{\rm bd}}{2\theta_\star}\Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big)$$

an infinitesimal Maxwellian and G solution of the half-space problem (2.25) with incoming data $\Upsilon^{\rm data} = M_{U_\star}^{-1}\big(\Phi^{\rm data} - M_{U_\star}(1+m_{\rm bd})\big)$. These quantities are well defined by Theorem 2.1, however their exact computation is out of reach. Therefore, we seek a suitable definition of the triple $(\rho_{\rm bd}, u_{\rm bd}, \theta_{\rm bd})$, together with the outgoing distribution $\gamma^{\rm out}G(0,v)$, for $v < 0$, intended to approximate the actual quantities.

Let us introduce a few notation, restricting our discussion to the boundary $x = -\omega$ (the boundary $x = +\omega$ is treated in a similar way, changing the sign of the velocity variable and adapting the definition of the outgoing/incoming characteristics). Let $\bar U = (\bar\rho, \bar u, \bar\theta)$ stand for the value of the hydrodynamic unknowns in the boundary cell (that is in C_0 for the left–hand case where $\bar U = U_0^n$ and in C_{I+1} for the right–hand case where $\bar U = U_{I+1}^n$). We set

$$U_{\rm fluc} = \bar U - U_\star = (\rho_{\rm fluc}, u_{\rm fluc}, \theta_{\rm fluc})$$

to which we associate the infinitesimal Maxwellian

$$m_{U_{\rm fluc}}(v) = \frac{\rho_{\rm fluc}}{\rho_\star} + u_{\rm fluc}\frac{v-u_\star}{\theta_\star} + \frac{\theta_{\rm fluc}}{2\theta_\star}\Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big).$$

Remind that we can work with a suitable basis

$$\begin{aligned}
\chi_1(v) &= \frac{1}{\sqrt{6}}\Big(\sqrt{3}\frac{v-u_\star}{\sqrt{\theta_\star}} + \frac{|v-u_\star|^2}{\theta_\star}\Big),\\
\chi_0(v) &= \frac{1}{\sqrt{6}}\Big(\frac{|v-u_\star|^2}{\theta_\star} - 3\Big),\\
\chi_2(v) &= \frac{1}{\sqrt{6}}\Big(\sqrt{3}\frac{v-u_\star}{\sqrt{\theta_\star}} - \frac{|v-u_\star|^2}{\theta_\star}\Big),
\end{aligned} \tag{3.3}$$

of $\mathrm{Ker}(L_{M_{U_\star}})$, which is orthogonal for the quadratic form

$$\mathbf{Q} : f \mapsto \int_{\mathbb{R}} v|f|^2 M_{U_\star}\,\mathrm{d}v,$$

and we split this subspace according to the signature of the quadratic form $\mathbf{Q}$: it defines the subspaces $\Lambda^\pm$ (Λ^0 being reduced to $\{0\}$ in the non-degenerate cases). Now, to define $m_{\rm bd}$, we proceed as follows.

- Firstly, we associate to $m_{U_{\rm fluc}}$ its projection on Λ^-:

$$m_-(v) = \sum_{k\in I^-}\alpha_k\chi_k, \qquad \alpha_k = \frac{\displaystyle\int_{\mathbb{R}} v\, m_{U_{\rm fluc}}\chi_k\, M_{U_\star}\,\mathrm{d}v}{\displaystyle\int_{\mathbb{R}} v\,|\chi_k|^2\, M_{U_\star}\,\mathrm{d}v}.$$

- Secondly, we define m_+ as to be an infinitesimal Maxwellian with fluxes imposed by the half-space problem (2.25)-(2.26), with $\Upsilon^{\rm data} = \Psi^{\rm data,L} - m_-$, where we remind that the boundary data is given by $\Psi^{\rm data,L} = \Phi^{\rm data,L}/M_{U_\star} - 1$. Of course, the resolution of the half-space problem is usually not affordable and we shall use an approximation device. Integrating the half space problem (2.25) over the velocity variable, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}z}\int_{\mathbb{R}} v\begin{pmatrix}1\\ v\\ |v|^2\end{pmatrix} G(z,v)M_{U_\star}(v)\,\mathrm{d}v = 0. \tag{3.4}$$

  By using the incoming boundary condition and (2.26) it follows that

$$\begin{aligned}
&\int_{\mathbb{R}} v\begin{pmatrix}1\\ v\\ |v|^2\end{pmatrix} G(0,v)M_{U_\star}\,\mathrm{d}v = \int_{\mathbb{R}} v\begin{pmatrix}1\\ v\\ |v|^2\end{pmatrix} G(\infty,v)M_{U_\star}\,\mathrm{d}v = 0\\
&= \int_{v>0} v\begin{pmatrix}1\\ v\\ |v|^2\end{pmatrix}\Upsilon^{\rm data}(v)M_{U_\star}\,\mathrm{d}v + \int_{v<0} v\begin{pmatrix}1\\ v\\ |v|^2\end{pmatrix}\gamma^{\rm out}G(0,v)M_{U_\star}\,\mathrm{d}v.
\end{aligned}$$

  Then, we make an approximation which has been already proposed by Maxwell [45]. It is related to the Marshak approximation [44] introduced in radiative transfer and it is precisely discussed for gas dynamics in [2], see also [30, 33]. We suppose that the outgoing distribution

coincides with the distribution at infinity: $\gamma^{\rm out} G(0,v) = G(\infty,v)$, which, coming back to (2.26), leads to $\gamma^{\rm out} G(0,v) = 0$. Hence we determine the coefficients of m_+ in the basis $\{\chi_k,\ k \in I^+\}$ by equating the incoming fluxes

$$\int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} (\Psi^{\rm data} - m_-)(v) M_{U_\star}\, {\rm d}v - \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} m_+(v) M_{U_\star}\, {\rm d}v = 0.$$

Except in the case $\#I^+ = \dim(\Lambda^+) = 3$ this system is overdetermined. Therefore instead we solve the optimization problem

$$\inf_{m_+ = \sum_{k\in I^+} \alpha_k \chi_k \in \Lambda^+} \left| \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} (\Psi^{\rm data} - m_-)(v) M_{U_\star}\, {\rm d}v - \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} m_+(v) M_{U_\star}\, {\rm d}v \right|^2 . \tag{3.5}$$

It can be recast in matrix formulation

$$\min_{B^+\alpha = 0} |A\alpha - b^{\rm data}|^2,$$

where the coefficients of the 3×3 matrix A only depend on the reference state $U_\star$ and the coefficients of $b^{\rm data} \in \mathbb{R}^3$ depend on $U_\star$, $\Psi^{\rm data}$ and m_-, while B^+, having $n_+ \in \{0,...,3\}$ raws and 3 columns, is associated to the constraint $m^+ \in \Lambda^+$ and only depends on $U_\star$ (see formulae in the Appendix). The solution is obtained by solving the linear system

$$\begin{pmatrix} A^T A & B^{+T} \\ B^+ & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \lambda \end{pmatrix} = \begin{pmatrix} A^T b^{\rm data} \\ 0 \end{pmatrix} \tag{3.6}$$

with $\lambda \in \mathbb{R}^{I^+}$ the Lagrange multiplier associated to the constraint $\alpha \in {\rm Ker}(B^+)$.

- Eventually, we define the needed Maxwellian by

$$m_{\rm bd} = m_+ + m_-.$$

Clearly if the signature of $\mathbf{Q}$ is $(3,0)$ (resp. $(0,3)$), then $m_- = 0$ since $I^- = \emptyset$ (resp. $m_- = m_{U_{\rm fluc}}$ since $I^+ = \emptyset$).

Having disposed of this construction of $m_{\rm bd}$ and using the Maxwell approximation, we go back to (3.2) and we are led to the following definition of the (left–)boundary flux to be used in the numerical scheme:

$$\mathcal{F}_{\rm bd} = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} \Phi^{\rm data}\, {\rm d}v + \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} \left(1 + m_- + m_+\right) M_{U_\star}\, {\rm d}v.$$

In this formula, m_- is determined by the "outgoing" part of the hydrodynamic flow, while the coefficients of m_+ are determined by the resolution of a certain linear system.

Remark 3.1. *Instead of solving the minimization problem, another possibility is simply to pick as many relations as needed among the three fluxes identities. This is the definition proposed in [2, 33].*

This linearized approach produces satisfying results, but its applicability remains very limited. Indeed, starting from a given state, due to the incoming boundary condition, the solution of the BGK equation might be conducted far away from the reference state. In particular it might happen that, next to the boundary, the flow changes type, with modification of the number of incoming/outgoing characteristics. The fully linearized approach, that will be referred to as the global linearization, is not able to capture such phenomena and therefore produces wrong results as time becomes large (see Figures 1 and 2).

Local linearization. Nevertheless, we can adapt the ideas by reasoning locally. Knowing the numerical approximation $U^\ell = (\rho^\ell, u^\ell, \theta^\ell)$ for $\ell \in \{0, ..., n\}$, the first step consists in defining a convenient reference state. Let $0 \leq \nu < 1$. We find an approximation of $\frac{2}{\Delta x}\int_{C_0} U((n+\nu)\Delta t, y)\,\mathrm{d}y$ by linear interpolation and we set $U_\star = U^n + \nu(U^n - U^{n-1})$. (In practice, we work with $\nu = 1/2$.) Then we consider the unknown in the boundary cell as a perturbation of the reference state: we write $U_0^n = U_\star + U_{\mathrm{fluc}}$. Now, we construct the boundary fluxes by repeating the strategy detailed above. The noticeable point is that now all the coefficients of A, b^{data}, B^+ arising from (3.5) need to be updated at each time step. It thus requires the evaluation of several integrals, which has a non negligible computational cost (but of course, it still remains far less costly than the computation of the kinetic equation!). By the way, we notice that the evaluation of these integrals should be performed with enough accuracy, a basic requirement being to preserve the constant solutions when the initial data and boundary condition coincide with the reference state $F^{\mathrm{Init}} = \Psi^{\mathrm{data}} = M_\star$ (the simulations presented here are obtained using the fourth order Simpson rule). Figures 1 compare the results of a kinetic simulation to the simulation of the hydrodynamic system with both the linearized and the localized approaches.

In the simulation $(\rho^{\mathrm{Init}}, u^{\mathrm{Init}}, \theta^{\mathrm{Init}}) = (\rho_\star, u_\star, \theta_\star) = (1, 0.1, 1)$ such that $\sigma_{U_\star}$ is (2,1). At the boundary we choose $\Phi^{\mathrm{data}} = 0$ and $t = 0.1$ as final time. As for section 4, we take $\Delta x_{\mathrm{hydro}} = \Delta x_{\mathrm{kin}} = 1/1500$ and Δt is determined by the CFL condition. Moreover the computation of the integrals respect to v are performed with regularly spaced nodes on the domain $[-16, 16]$. Finally we work with $\tau = 10^{-3}$.

It shows that the localized approach noticeably improves the hydrodynamic approximation. Figure 2 gives the evolution in time of the eigenvalues for the same test case of figure 1. Clearly at the beginning we have as signature $\sigma_{U_\star} = (2, 1)$ and after a short time, this signature becomes (0,3) for the right boundary and (3,0) for the left one. This explain why the local linearization is better: the globally linearized scheme works well for short times but it is not able to adapt to the change of type (sub/supersonic) induced by the boundary conditions.

Remark 3.2. *It might be tempting to use as a reference state the value U_1^n in the first internal cell. Then, the fluctuation would be $U_1^n - U_0^n$, which resembles $\Delta x \partial_x U$; when discontinuities are produced this quantity becomes large and thus it is not a good candidate for being seen as a fluctuation. This strategy indeed leads to unstabilities.*

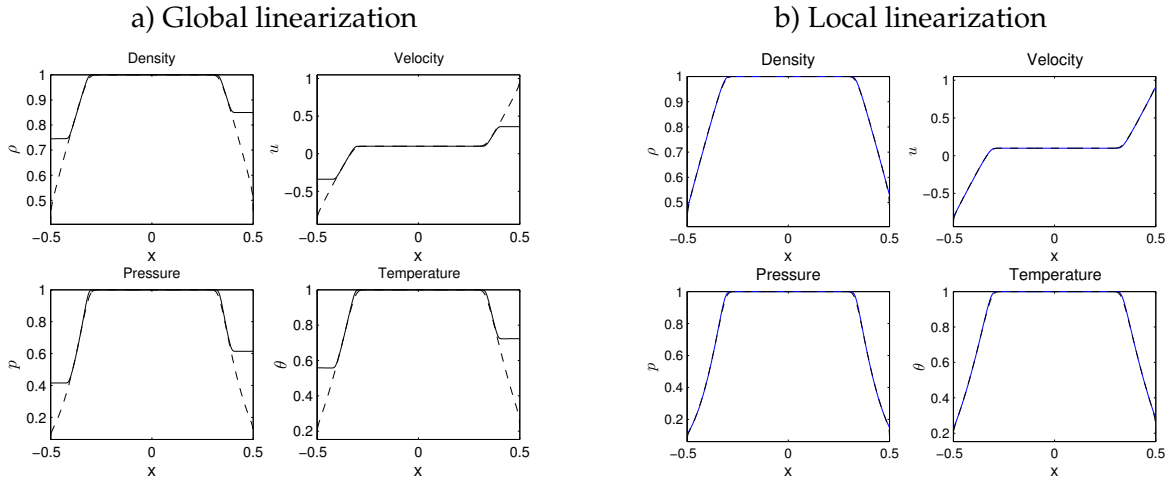

Figure 1: Local linearization vs. global linearization in the case $(\rho_\star, u_\star, \theta_\star) = (1, 0.1, 1)$, $\Phi^{\rm data} = 0$ in (2.6), final time $t = 0.1$. Dashed line: kinetic simulation, solid line: hydrodynamic simulation.

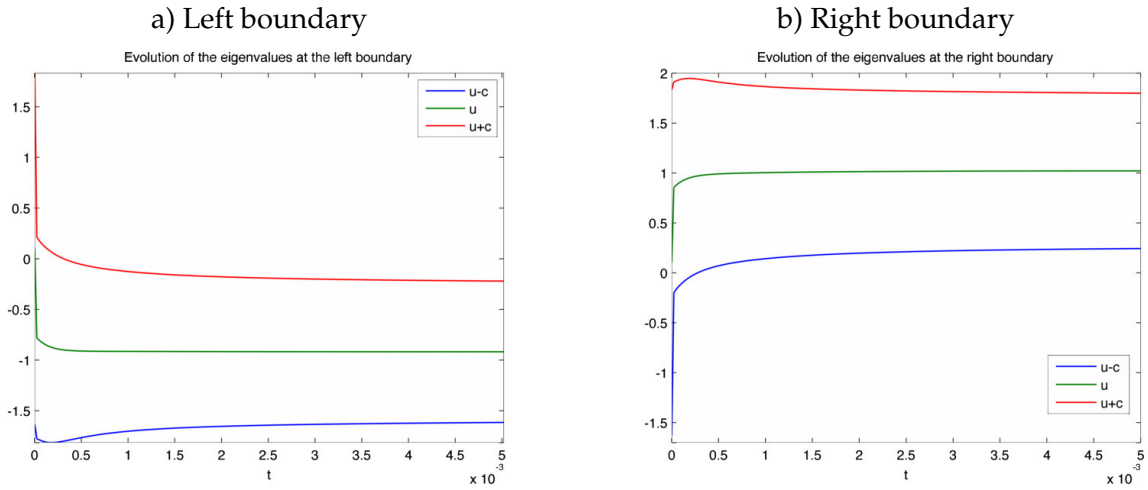

Figure 2: Evolution of the eigenvalues on right and left boundaries for the simulation of figure. 1

The degenerate case $u_\star = 0$. Let us explain how the previous machinery is modified in the specific degenerate case $u_\star = 0$ which yields $\sigma_{U_\star} = (1, 1)$. The starting point consists in remarking that $v\chi_0(v) = \frac{1}{\sqrt{6}} v\big(\frac{|v|^2}{\theta_\star} - 3\big)$ is orthogonal to $\mathrm{Ker}(L_{U_\star})$ since

$$\int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} v\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\, M_{(\rho_\star, 0, \theta_\star)}\, \mathrm{d}v = 0.$$

Therefore, since $\big(\mathrm{Ker}(L_{U_\star})\big)^\perp = \mathrm{Ran}(L_{U_\star})$, we can (uniquely) define the auxiliary function λ verify-

ing

$$L_{U_\star}\lambda = v\chi_0, \text{ with } \int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \lambda \, M_{(\rho_\star,0,\theta_\star)} \, \mathrm{d}v = 0.$$

For the BGK operator, we simply have

$$\lambda(v) = -\frac{1}{\sqrt{6}} v\Big(\frac{|v|^2}{\theta_\star} - 3\Big) = -v\chi_0(v).$$

Then, we observe that the solution of the half-space problem satisfies

$$\frac{\mathrm{d}}{\mathrm{d}z}\int_{\mathbb{R}} v\lambda(v)\, G(z,v)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = \frac{1}{\sqrt{6}}\int_{\mathbb{R}} v\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\, G(z,v)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = K_0$$

which does not depend on z since we bear in mind that (3.4) holds. Hence, if G is a bounded solution of the half-space problem, it imposes an additional conservation law: $K_0 = 0$ that is

$$\int_{\mathbb{R}} v\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\, G(z,v)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = 0, \tag{3.7}$$

and

$$\int_{\mathbb{R}} v\lambda(v)\, G(z,v)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = K \quad \text{(constant independent on } z\text{)}.$$

But we do not have any knowledge of the value of the constant K; this is the reason why we use a two steps method: the first step provides an evaluation of K, which in turn can be used to define the asymptotic state. Having defined m_- as before, we construct $m_+ = \sum_{k\in I^0\cup I^+} \alpha_k\chi_k$ by taking into account this information. We follow the method presented in [30, 33]: it relies on a simple iteration argument, but it can be interpreted as the result of a variational problem. It is convenient to set $\tilde{G}(z,v) = G(z,v) + m_+$ which thus verifies the half space problem

$$\begin{cases} v\partial_z\tilde{G} = L_{U_\star}\tilde{G}, \\ \gamma^{\mathrm{inc}}\tilde{G}(0,v) = \Psi^{\mathrm{data,L}}(v) - m_-(v) \qquad \text{for } v > 0, \end{cases}$$

and, as detailed in Theorem 2.1, $m_+ \in \Lambda^+ \oplus \Lambda^0$ is the equilibrium state at infinity

$$\lim_{z\to\infty} \tilde{G}(z,v) = m_+(v) = \alpha_0\chi_0(v) + \alpha_1\chi_1(v)$$

that we seek.

The first step consists in using the Maxwell approximation to find a preliminary guess for m_+. We have

$$\int_{\mathbb{R}} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \tilde{G}(z,v) M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = \int_{\mathbb{R}} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} m_+(v) M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v.$$

We assume that the outgoing trace coincides with the distribution at infinity. The obtained system is overdetermined since it contains 3 equations while we search for the two components of m_+ in the basis (χ_0,χ_1). Hence, we pick two relations among the system and we define $\tilde{m}_+ = \tilde{\alpha}_0\chi_0(v) + \tilde{\alpha}_1\chi_1(v)$ as to be the solution of

$$\int_{v>0} v \begin{pmatrix} 1 \\ |v|^2 \end{pmatrix} (\Psi^{\mathrm{data,L}} - m_-) M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = \int_{v>0} v \begin{pmatrix} 1 \\ |v|^2 \end{pmatrix} \tilde{m}_+ \, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v.$$

Note that it is useless to use (3.7) as a constraint for defining m_+ since (3.7) is satisfied by any infinitesimal Maxwellian (see below). For the second step, we use $\tilde{m}_+$ as the outgoing distribution to evaluate the two following conserved quantities

$$\int_{v>0} v \begin{pmatrix} \lambda(v) \\ v \end{pmatrix} \big(\Psi^{\mathrm{data,L}} - m_-\big) M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v + \int_{v<0} v \begin{pmatrix} \lambda(v) \\ v \end{pmatrix} \tilde{m}_+ M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = \begin{pmatrix} \tilde{K} \\ \tilde{K}' \end{pmatrix}.$$

Having these quantities at hand, we define $m_+(v) = \alpha_0\chi_0(v) + \alpha_1\chi_1(v)$ as the solution of

$$\int_{\mathbb{R}} v \begin{pmatrix} \lambda(v) \\ v \end{pmatrix} m_+(v) M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = \begin{pmatrix} \tilde{K} \\ \tilde{K}' \end{pmatrix}.$$

As a matter of fact, we remark that this construction is consistent with (3.7). Indeed, on the one hand, the asymptotic state m_+ fulfills the constraint

$$\begin{aligned}\int_{\mathbb{R}} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\, m_+\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v &= \int_{\mathbb{R}} v\chi_0\big(\alpha_0\chi_0 + \alpha_1\chi_1\big)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v \\ &= \alpha_0 \int_{\mathbb{R}} v|\chi_0|^2\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v + \alpha_1 \int_{\mathbb{R}} v\chi_0\chi_1\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = 0\end{aligned}$$

by definition of χ_0 and χ_1. On the other hand at the boundary we have

$$\begin{aligned}&\int_{v>0} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\big(\Psi^{\mathrm{data,L}} - m_-\big)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v + \int_{v<0} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\tilde{m}_+\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v \\ &\quad= \int_{v>0} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\big(\Psi^{\mathrm{data,L}} - m_-\big)\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v \\ &\qquad- \int_{v>0} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\tilde{m}_+\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v + \int_{\mathbb{R}} \frac{v}{\sqrt{6}}\Big(\frac{|v|^2}{\theta_\star} - 3\Big)\tilde{m}_+\, M_{(\rho_\star,0,\theta_\star)}(v)\,\mathrm{d}v = 0\end{aligned}$$

by using the definition of $\tilde{m}_+$.

Here we have detailed the computations for the left hand boundary $x = -\omega$. The right hand boundary $x = +\omega$ is of course treated analogously, except that integration over $v \in (0, +\infty)$ (resp. $v \in (-\infty, 0)$) is replaced by integration over $v \in (-\infty, 0)$ (resp. $v \in (0, +\infty)$).

Remark 3.3. *The treatment of the boundary condition differs from those presented by S. Dellacherie [22, 23]. There, the idea can be summarized as follows:*

- *Firstly we define hydrodynamic quantities $(\rho_{\mathrm{gh}}, u_{\mathrm{gh}}, \theta_{\mathrm{gh}})$ in a ghost cell by solving*

$$\int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} M_{(\rho_{\mathrm{gh}},u_{\mathrm{gh}},\theta_{\mathrm{gh}})}\,\mathrm{d}v = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \Phi^{\mathrm{data,L}}\,\mathrm{d}v.$$

  Namely, we consider the Maxwellian having the same outgoing fluxes as the data. A first attempt would be to use these values as Dirichlet conditions, but a better approach is proposed.

- *Secondly, the flux at the interface between the ghost cell and the computational domain is determined by using a kinetic scheme, as introduced in [49, 50], see also [12]: we set*

$$\mathcal{F}^n_{\mathrm{bd}} = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} M_{(\rho_{\mathrm{gh}},u_{\mathrm{gh}},\theta_{\mathrm{gh}})}\,\mathrm{d}v + \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} M_{(\rho^n_0,u^n_0,\theta^n_0)}\,\mathrm{d}v.$$

Consequently, owing to the specific definition of the numerical fluxes, we do not have to solve the nonlinear system in step 1, we simply use the relation

$$\mathcal{F}_{\rm bd}^n = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} \Phi^{\rm data,L}\,{\rm d}v + \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2/2 \end{pmatrix} M_{(\rho_0^n,u_0^n,\theta_0^n)}\,{\rm d}v.$$

This definition is very natural in the framework adopted in [22] where the resolution of the Euler system is precisely based on the use of a kinetic scheme. The definition of the numerical fluxes can be interpreted as a relevant version of the Enquist–Osher scheme [25] and [50, Chap. 6 & 8]. As crude as it might appear this definition of boundary fluxes is quite performing. We will go back in a future work to further comparison in the context of fluid/kinetic interfaces.

Remark 3.4. *The discussion of Knudsen layers and their numerical treatment is strongly related to the question of finding relevant matching condition between the kinetic equation and the hydrodynamic system in a domain decomposition approach. This issue is discussed in details, with various numerical approaches, in [2, 12, 22, 23, 30–33, 41]. The mathematical analysis of such matching condition is highly delicate, and we refer to the breakthrough of A. Vasseur concerning nonlinear scalar conservation laws [56]. We shall go back to this problem elsewhere and we will also consider the effect of a coupling with an electric potential [19]. We also point out that our approach can be improved by using a more involved approximation of the half-space problem, while here the computations are simply based on the Maxwell approximation: the iterative procedure described in [33] looks quite appealing for this purpose. This refinement will be explored elsewhere.*

Reflection boundary conditions. It is relevant to consider generalized boundary conditions where the incoming distribution of particles depends on the outgoing distribution: such boundary condition is intended to describe the complex interaction between the impinging particles and the boundary. The simplest case corresponds to the specular reflection law

$$\gamma^{\rm inc}F(t,x=-\omega,v) = \alpha\gamma^{\rm out}F(t,x=-\omega,-v) \qquad \text{for } v>0,$$

where $0 \le \alpha \le 1$, but it is certainly too crude to model realistic boundary phenomena. More generally, the boundary condition is defined through a non–local relation

$$\gamma^{\rm inc}F(t,-\omega,v) = \alpha\int_{v'<0} k(v,v')\,\gamma^{\rm out}F(t,-\omega,v')\,|v'|\,{\rm d}v' = \mathcal{R}\big(\gamma^{\rm out}F(t,-\omega,\cdot)\big)(v) \qquad \text{for } v>0$$

where all the physics is embodied in the kernel k and the coefficient $0 \le \alpha \le 1$. We refer for the derivation of boundary kernels and comments to [14, 15, 21, 36, 37, 42]. It is natural to require:

Non-negativity:	$k(v,v') \ge 0$,
Mass conservation:	$\displaystyle\int_{v>0} k(v,v')\,v\,{\rm d}v = 1$,
Reciprocity principle:	There exists a Maxwellian $M_{\rm w}$ verifying $\displaystyle M_{\rm w}(v) = \int_{v'<0} k(v,v')M_{\rm w}(v')\,|v'|\,{\rm d}v'$.

The specular law corresponds to the case where k is the Dirac mass $\delta(v'=-v)$. A more relevant example of such a boundary condition is the Maxwell law where

$$k(v,v') = \frac{M_{\rm w}(v)}{Z_{\rm w}}, \qquad M_{\rm w}(v) = \frac{\rho_{\rm w}}{\sqrt{2\pi\theta_{\rm w}}}\,e^{-|v|^2/(2\theta_{\rm w})}, \qquad Z_{\rm w} = \int_{v>0} v\,M_{\rm w}(v)\,{\rm d}v.$$

In other words, the particles are reflected according to the Maxwellian distribution $M_{\rm w}(v)$, proportionally to the outgoing mass flux:

$$\gamma^{\rm inc}F(t,-\omega,v) = \alpha\,\frac{M_{\rm w}(v)}{Z_{\rm w}}\,\int_{v'<0}\gamma^{\rm out}F(t,-\omega,v')\,|v'|\,{\rm d}v' \qquad \text{for } v>0. \tag{3.8}$$

Remark that such a boundary condition can be derived from the simple specular reflection law through an homogenization analysis [4]. The parameter α is the so–called accomodation coefficient and it defines the fraction of reflected particles. Indeed, we have

$$\begin{aligned}\int_{\mathbb{R}} vF(t,-\omega,v)\,{\rm d}v &= \int_0^\infty v\gamma^{\rm inc}F(t,-\omega,v)\,{\rm d}v + \int_{-\infty}^0 v\gamma^{\rm out}F(t,-\omega,v)\,{\rm d}v\\ &= (1-\alpha)\int_{-\infty}^0 v\gamma^{\rm out}F(t,-\omega,v)\,{\rm d}v \le 0.\end{aligned}$$

In particular, when $\alpha = 1$ the mass flux vanishes.

The method described above can be adapted to treat these boundary conditions. Again, we restrict our purpose to the boundary $x=-\omega$. We obtain the following boundary condition for the half-space problem

$$\begin{aligned}M_{U_\star}\,\gamma^{\rm inc}G(0,v) \;&=\; \mathcal{R}\big(M_{U_\star}(1+m)\big) - M_{U_\star}(1+m)\\ &\quad +\mathcal{R}\big(M_{U_\star}\gamma^{\rm out}G(0,v)\big) \quad \text{for } v>0,\end{aligned} \tag{3.9}$$

where we use the shorthand notation $\mathcal{R} : L^1(v<0,|v|\,{\rm d}v) \to L^1(v>0,|v|\,{\rm d}v)$ to denote the reflection operator, which in the simulation corresponds either to the diffuse Maxwell law or to the specular law. We detail in the Appendix the precise form of the linear systems to be solved for defining the boundary flux in this case. Note however that the specular reflection law (partial or total) is excluded from the boundary layer analysis in [20], while the diffuse condition can be considered (see Section 2 and Theorem 2.1.1 in [20]).

In the specific case of a totally reflexive boundary condition, $\alpha = 1$ in (3.8), it is worth pointing out that the mass flux vanishes. Indeed, by combining (2.26) and (3.4) we observe that

$$\int_{\mathbb{R}} v\,G(0,v)M_{U_\star}(v)\,{\rm d}v = 0.$$

Therefore, integrating (3.9) yields

$$\begin{aligned}&\int_{v>0} v\Big(\mathcal{R}\big(M_{U_\star}(1+m)\big) - M_{U_\star}(1+m)\Big)\,{\rm d}v = 0\\ &\quad = \int_{v<0}|v|M_{U_\star}(1+m)(v)\,{\rm d}v - \int_{v>0} vM_{U_\star}(1+m)(v)\,{\rm d}v.\end{aligned}$$

We remind that m splits as $m_- + m_+$ and we arrive at the constraint

$$\int_{\mathbb{R}} vm_+M_{U_\star}\,{\rm d}v = -\int_{\mathbb{R}} v(1+m_-)M_{U_\star}\,{\rm d}v$$

to be satisfied by the asymptotic state m_+. It simply means that the numerical mass flux is set to 0 and this is exactly what our definition does.

Remark 3.5. *For the specular reflection and $\alpha = 1$, both the mass and energy fluxes vanish; in this very specific case the boundary condition for the hydrodynamic system are simply the wall condition that corresponds to use a ghost cell and to reverse the velocity in the ghost cell while keeping the same density and temperature.*

4 Numerical results

As a preliminary remark, we point out that direct comparisons between hydrodynamic and kinetic simulations should be considered with caution since they could be slightly unfair. Indeed, using the Euler system makes sense when the scaling parameter τ is very small. Positive values of τ naturally induce diffusion effects, and Navier-Stokes correction should be taken into account. In particular diffusion will certainly become sensible for large time simulation. Next, performing kinetic simulations with $\tau \ll 1$ is numerically demanding since capturing layer effects requires to make use of resolved meshes, with $\Delta x \ll \tau$. Additionally to the large size of the unknown in such conditions, the stability constraint associated to the advection term makes rapidly the simulation not affordable, especially with the quite naive scheme we are using (performances can be improved by using AP scheme, as introduced in [26,40]). Nevertheless, we shall see below that the comparison is qualitatively satisfactory, and of course, the hydrodynamic simulations run much faster than the microscopic simulations. Furthermore, we observe that the mesh size can be safely increased in the hydrodynamic simulation without altering that much the solution.

A relevant test case corresponds to the simulation of evaporation-condensation phenomena. The problem is presented in great details in works of Y. Sone and K. Aoki [1, 54, 55], we also refer to the survey [9]. The incoming data are given by two Maxwellians with different macroscopic quantities

$$\Phi^{\text{data,L}} = \frac{\rho_{\text{w}}^{\text{L}}}{\sqrt{2\pi\theta_{\text{w}}^{\text{L}}}} \exp\Big(-\frac{|v|^2}{2\theta_{\text{w}}^{\text{L}}}\Big), \qquad \Phi^{\text{data,R}} = \frac{\rho_{\text{w}}^{\text{R}}}{\sqrt{2\pi\theta_{\text{w}}^{\text{R}}}} \exp\Big(-\frac{|v|^2}{2\theta_{\text{w}}^{\text{R}}}\Big). \tag{4.1}$$

where $\rho_{\text{w}}^{\text{L}}$, $\theta_{\text{w}}^{\text{L}}$ can differ from $\rho_{\text{w}}^{\text{R}}$, $\theta_{\text{w}}^{\text{R}}$. We start either from a constant state $(\rho^{\text{Init}}, u^{\text{Init}}, \theta^{\text{Init}})$ which can be not in equilibrium with the incoming data or from a discontinuous profile. For the kinetic equation the initial data is the Maxwellian defined by these macroscopic quantities.

Of course, the basic requirement is that the code preserves the equilibrium: for $(\rho^{\text{Init}}, u^{\text{Init}}, \theta^{\text{Init}}) = (\rho_{\text{w}}^{\text{L}}, 0, \theta_{\text{w}}^{\text{L}}) = (\rho_{\text{w}}^{\text{R}}, 0, \theta_{\text{w}}^{\text{R}})$ the solution remains constant. We check that it is indeed the case, the error being governed by the accuracy of the computation of the integrals arising in (3.5). The same conclusion applies if the reference velocity does not vanish. We do not present a specific figure but an evidence of the ability of the scheme in preserving equilibrium can be seen in the far right hand side of Figures 3, 4 and 5: the data at $x = +\omega$ coincides with the initial Maxwellian and we stop the simulation at a short time so that the perturbation arising from the boundary $x = -\omega$ has not crossed the domain.

In Figures 3, 4 and 5, we compare the results of the kinetic simulation to the hydrodynamic simulation for $(\rho_{\text{w}}^{\text{R}}, u_{\text{w}}^{\text{R}}, \theta_{\text{w}}^{\text{R}}) = (\rho^{\text{Init}}, u^{\text{Init}}, \theta^{\text{Init}}) = (1, 0, 0.5)$ and for several values of $(\rho_{\text{w}}^{\text{L}}, \theta_{\text{w}}^{\text{L}}) \neq (\rho^{\text{Init}}, \theta^{\text{Init}})$. The computational parameters are

$$\Delta x_{\text{hydro}} = 1/1500$$

and Δt is determined by the CFL condition. The computation of the integrals with respect to the v variable are performed using the Simpson approximation rule with regularly spaced nodes in the domain $[-16, +16]$. For the kinetic simulations we work with the scaled mean free path $\tau = 1/1000$ and

$$\Delta x_{\text{kin}} = 1/1500$$

in order to resolve the fine scales. We observe a remarkable agreement between the microscopic and the macroscopic simulations; the definition of the numerical fluxes is able to capture the boundary phenomena issued from the kinetic model. We point out that the kinetic model produces inherently

diffusion terms, typically of size $\mathscr{O}(\tau)$: for long time simulation this effect would become sensible and it would become more realistic for such a value of τ to compare with the Navier-Stokes equations, having $\mathscr{O}(\tau)$ viscous terms. Performing simulations with smaller τ's requires a considerable numerical effort as it has been done in [1,54,55]. These effects are also visible as the density ratio increases: in Figure 5 the discrepancies between kinetic and hydrodynamic models appear essentially in smoother profiles for the temperature and the velocity produced by the microscopic simulation. In Figure 6 we show the results of the simulation of the hydrodynamic system for long times. The solution reaches a stationary state, which is entirely determined by the boundary data, in agreement with the observation and analysis in [1,54,55]. (Note that these references deal with the case $v \in \mathbb{R}^3$ so that it does not make sense to compare directly the asymptotic states, the values of which depend on the velocity dimension.)

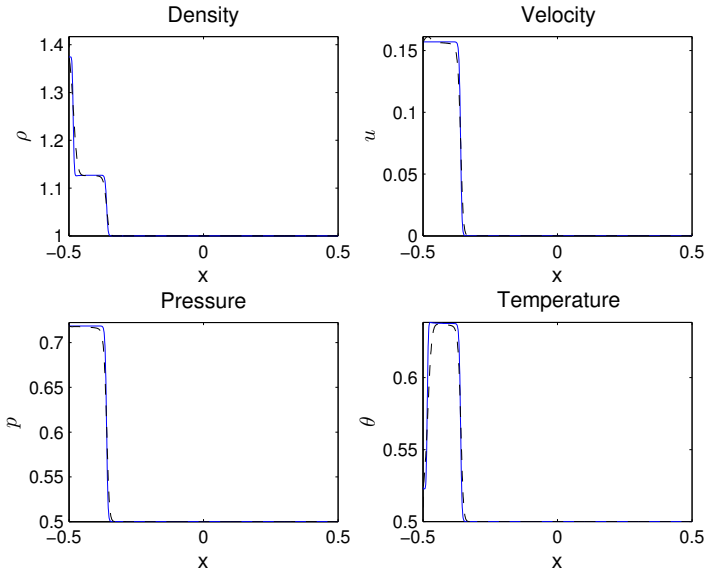

Figure 3: Evaporation-condensation problem: kinetic simulation (dashed line) vs. the hydrodynamic simulation (solid line) for $\rho_{\mathrm{w}}^{\mathrm{L}} = 2/1.2$, $\theta_{\mathrm{w}}^{\mathrm{L}} = 1.2/2$, and a final time $t = 0.1$.

Figures 7, 8, 9 are concerned with examples of a diffusive reflection law. Simulations are done with $(\rho^{\mathrm{Init}}, u^{\mathrm{Init}}, \theta^{\mathrm{Init}}) = (1, 0.1, 1)$, $\alpha = 0.5$, $\rho_{\mathrm{w}}^{\mathrm{L}} = \rho_{\mathrm{w}}^{\mathrm{R}} = 1$, $\theta_{\mathrm{w}}^{\mathrm{L}} = \theta_{\mathrm{w}}^{\mathrm{R}} = 1$ and a final time $t = 0.1$ for figure 7. In figure 8 the differences are uniquely that $u^{\mathrm{Init}} = -0.1$ and $\theta_{\mathrm{w}}^{\mathrm{R}} = 0.5$. Finally figure 9 corresponds to the same case as figure 8 but with $\theta_{\mathrm{w}}^{\mathrm{L}} = 0.5$, $\theta_{\mathrm{w}}^{\mathrm{R}} = 1$ and $\alpha = 1$. It turns out that this simulation is highly sensible to the value of the mean free path τ; a fair comparison with the hydrodynamic simulation is obtained with $\tau = 10^{-5}$ (and thus accordingly $\Delta x = 10^{-5}$ at least for the kinetic run). Again, we point out that the scheme preserves the equilibrium solution. Note also that the velocity vanishes at the boundary for the reflection coefficient equal to one, and, the construction of the numerical fluxes does its job. We point out also that the values of the hydrodynamic quantities in the extreme cells fit with the kinetic simulation, hence capturing the boundary layer (even if this is not visible on the graphs).

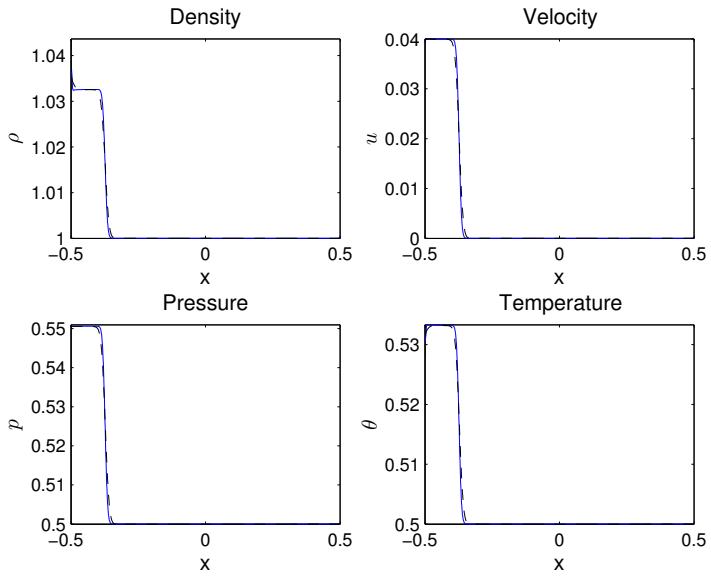

Figure 4: Evaporation-condensation problem: kinetic simulation (dashed line) vs. the hydrodynamic simulation (solid line) for $\rho_{\rm w}^{\rm L} = 1.2/1.1$, $\theta_{\rm w}^{\rm L} = 1.1/2$ and a final time $t = 0.1$.

A Details on the construction of the boundary fluxes

Let us consider a general boundary condition at $x = -\omega$ which combines a given source to the reflection of particles as follows

$$\gamma^{\rm inc} F(t,-\omega,v) = \Phi^{\rm data,L}(t,v) + \mathcal{R}\big(\gamma^{\rm out} F(t,-\omega,\cdot)\big)(v), \qquad \text{for } v > 0.$$

Let us describe the construction of the numerical boundary fluxes that we propose for the hydrodynamic equations, restricting the discussion to the boundary $x = -\omega$.

We have at hand the numerical approximation $\mathscr{U}_i^\ell$, $n \in \mathbb{N}$, $i \in \{0,...,I+1\}$, $\ell \in \{0,...,n\}$. As explained above, the evolution of the discrete unknowns is governed by a finite volume scheme, here using Godunov's definition for the internal fluxes. In the boundary cell C_0, the evolution is driven by

$$\mathscr{U}_0^{n+1} = \mathscr{U}_0^n - \frac{\Delta t}{\Delta x}(\mathcal{F}_{1/2}^n - \mathcal{F}_{\rm bd}^n)$$

where $\mathcal{F}_{1/2}^n$ is the standard Godunov flux between the cell C_0 and the cell C_1 and we are going to detail the construction of the boundary flux $\mathcal{F}_{\rm bd}^n$. The reference state $U_\star$ is therefore defined by the density, velocity and temperature associated to the $\mathscr{U}_0^\ell$'s by interpolation, e. g. $U_\star = U_0^n + \nu(U_0^n - U_0^{n-1})$ for some $0 \le \nu \le 1$. We consider the value of the numerical unknown in the cell C_0 as a fluctuation from the reference state, defining $U_{\rm fluc} = (\rho_{\rm fluc}, u_{\rm fluc}, \theta_{\rm fluc}) = U_0^n - U_\star$. The strategy is to define the numerical fluxes $\mathcal{F}_{\rm bd}^n$ by a formula involving integrals of $M_{U_\star}(1 + m_{\rm bd})$, with the decomposition $m_{\rm bd} = m_+ + m_-$. The infinitesimal Maxwellian

$$m_- = \frac{\rho_-}{\rho_\star} + \frac{v - u_\star}{\theta_\star} u_- + \frac{\theta_-}{2\theta_\star}\Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big) = \sum_{k \in I^-} \alpha_{-,k} \chi_k$$

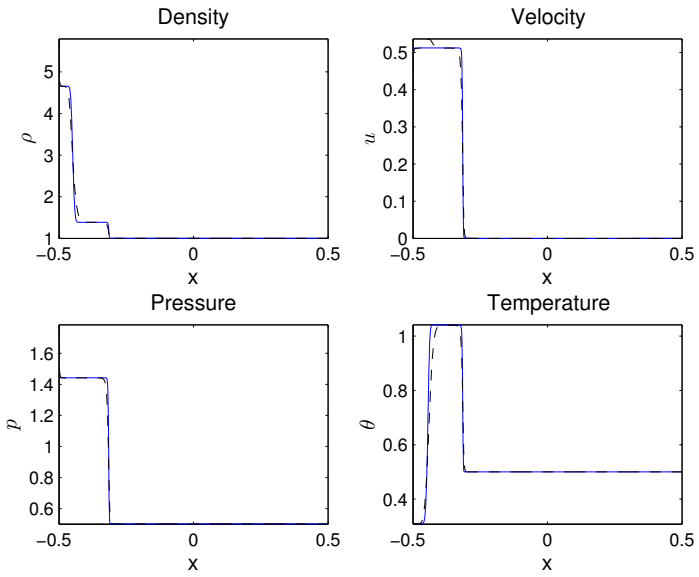

Figure 5: Evaporation-condensation problem: kinetic simulation (dashed line) vs. the hydrodynamic simulation (solid line) for $\rho_{\rm w}^{\rm L} = 10/1.1$, $\theta_{\rm w}^{\rm L} = 1.1/2$ and a final time $t = 0.1$.

is the projection on $\Lambda^- = \mathrm{Span}\{\chi_k,\ k \in I^-\}$ of

$$m_{\rm fluc} = \frac{\rho_{\rm fluc}}{\rho_\star} + \frac{v-u_\star}{\theta_\star}u_{\rm fluc} + \frac{\theta_{\rm fluc}}{2\theta_\star}\Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big).$$

Namely, the coefficients $\alpha_{-,k}$ are given by

$$\alpha_{-,k} = \frac{\displaystyle\int_{\mathbb{R}} v m_{\rm fluc}\,\chi_k M_{U_\star}\,\mathrm{d}v}{\displaystyle\int_{\mathbb{R}} v|\chi_k|^2 M_{U_\star}\,\mathrm{d}v}$$

and the macroscopic quantities are obtained with

$$\begin{pmatrix} \rho_- \\ u_- \\ \theta_- \end{pmatrix} = \int_{\mathbb{R}} \begin{pmatrix} 1 \\ \dfrac{v-u_\star}{\rho_\star} \\ \dfrac{\theta_\star}{\rho_\star}\Big(\dfrac{|v-u_\star|^2}{\theta_\star} - 1\Big) \end{pmatrix} m_- M_{U_\star}\,\mathrm{d}v -$$

We now need to define the infinitesimal Maxwellian

$$m_+(v) = \frac{\rho_+}{\rho_\star} + \frac{v-u_\star}{\theta_\star}u_+ + \frac{\theta_+}{2\theta_\star}\Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big) = \sum_{k\in I^+}\alpha_{+,k}\chi_k \in \Lambda^+.$$

The boundary condition for the half space problem is obtained with the approximation $F(t,x,v) \simeq M_{U_\star}(1 + m_{\rm bd}(v) + G^{\rm L}(t,(x+\omega)/\tau,v))$ next to the boundary $x = -\omega$. We are led to

$$M_{U_\star}\big(1 + m_{\rm bd} + \gamma^{\rm inc}G^{\rm L}\big)(t,0,v) = \Phi^{\rm data,L}(t,v) + \mathcal{R}\big(M_{U_\star}(1 + m_{\rm bd} + \gamma^{\rm out}G^{\rm L})\big)(t,0,v),$$

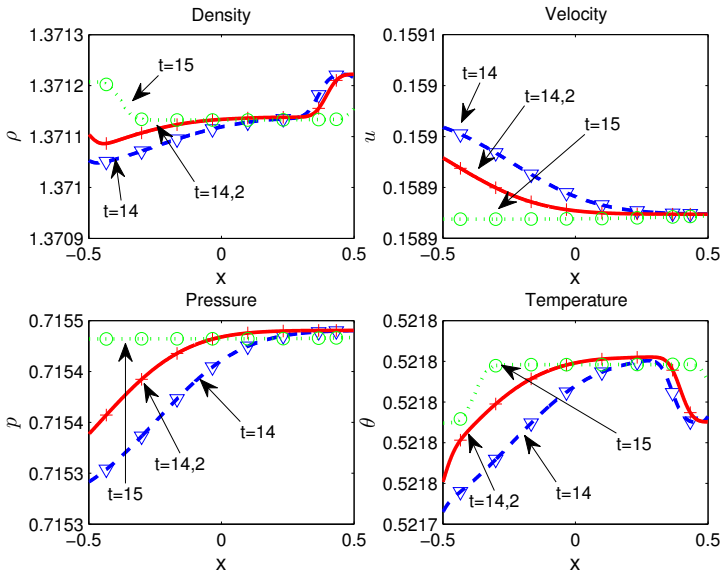

Figure 6: Evaporation-condensation problem and convergence towards a stationary state: long time behaviour for the hydrodynamic simulation for $\rho_{\rm w}^{\rm L} = 2/1.2$, $\theta_{\rm w}^{\rm L} = 1.2/2$ and a final time $t = 15$.

for $v > 0$. The conservation laws impose

$$\int_{\mathbb{R}} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} G^{\rm L}(t,0,v) M_{U_\star} \,{\rm d}v = \lim_{z\to\infty} \int_{\mathbb{R}} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} G^{\rm L}(t,z,v) M_{U_\star} \,{\rm d}v = 0,$$

which therefore recasts as

$$\int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \left[\frac{\Phi^{\rm data,L} + \mathcal{R}\big(M_{U_\star}(1 + m_{\rm bd} + \gamma^{\rm out} G^{\rm L})\big)}{M_{U_\star}} - (1 + m_{\rm bd}) \right] (t,0,v) M_{U_\star} \,{\rm d}v$$
$$+ \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \gamma^{\rm out} G^{\rm L}(t,0,v) M_{U_\star} \,{\rm d}v = 0.$$

We define m_+ by

- using the Maxwell approximation, which consists in approximating the outgoing distribution $\gamma^{\rm out} G^{\rm L}$ by its asymptotic state, that is 0,
- minimizing the obtained system under the constraints associated to the fact that m_+ is searched for in the subspace Λ^+.

Let us define the matrix A such that

$$A \begin{pmatrix} \rho_+ \\ u_+ \\ \theta_+ \end{pmatrix} = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \left[m_+ - \frac{\mathcal{R}\big(M_{U_\star} m_+\big)}{M_{U_\star}} \right] M_{U_\star} \,{\rm d}v.$$

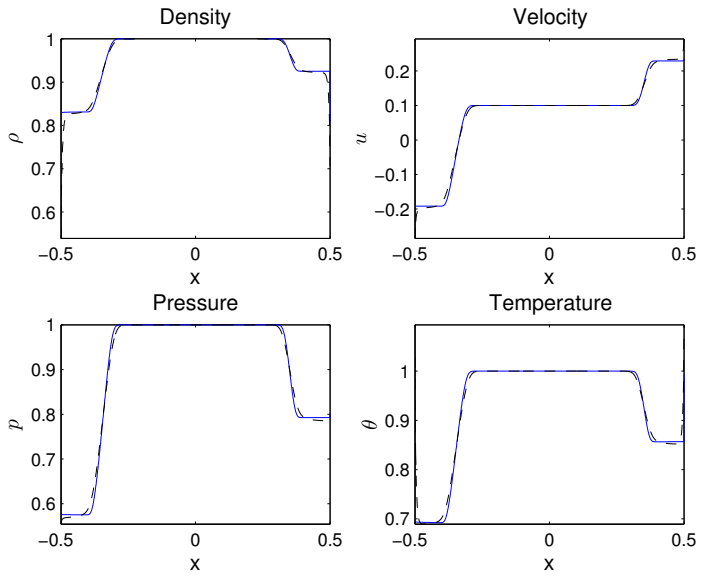

Figure 7: Example of diffusive reflection law with $(\rho_\star, u_\star, \theta_\star) = (1, 0.1, 1)$ and $\alpha = 0.5$, $\rho_{\rm w}^{\rm L} = 1, \rho_{\rm w}^{\rm R} = 1, \theta_{\rm w}^{\rm L} = 1, \theta_{\rm w}^{\rm R} = 1$ for a final time $t = 0.1$. Dashed line: kinetic simulation, solid line: hydrodynamic simulation.

For $\mathcal{R} = 0$, we simply have

$$\begin{aligned} A_{k1} &= \frac{1}{\rho_\star}\int_{v>0} v^k M_{U_\star}\,\mathrm{d}v, \\ A_{k2} &= \frac{1}{\theta_\star}\int_{v>0} v^k (v-u_\star) M_{U_\star}\,\mathrm{d}v, \\ A_{k3} &= \frac{1}{2\theta_\star}\int_{v>0} v^k \Big(\frac{(v-u_\star)^2}{\theta_\star} - 1\Big) M_{U_\star}\,\mathrm{d}v. \end{aligned}$$

We also set

$$b^{\rm data} = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \left[\frac{\mathcal{R}(M_{U_\star}) + \Phi^{\rm data,L}}{M_{U_\star}} - 1 + \frac{\mathcal{R}(M_{U_\star} m_-)}{M_{U_\star}} - m_- \right] M_{U_\star}\,\mathrm{d}v$$

We are thus led to consider the following cases:

- if $\sigma_{U_\star} = (0,3)$ all characteristics are outgoing, Λ^+ is reduced to $\{0\}$ and m_+ simply vanishes;
- if $\sigma_{U_\star} = (3,0)$ all characteristics are incoming, $m_- = 0$ and m_+ is defined by the linear system

$$A \begin{pmatrix} \rho_+ \\ u_+ \\ \theta_+ \end{pmatrix} = b^{\rm data};$$

- if $\sigma_{U_\star} = (2,1)$ or $(1,2)$ we solve the system (3.6)

$$\begin{pmatrix} A^T A & B^{+T} \\ B^+ & 0 \end{pmatrix} \begin{pmatrix} \alpha_+ \\ \lambda \end{pmatrix} = \begin{pmatrix} A^T b^{\rm data} \\ 0 \end{pmatrix}$$

  where B^+ accounts for the constraints:

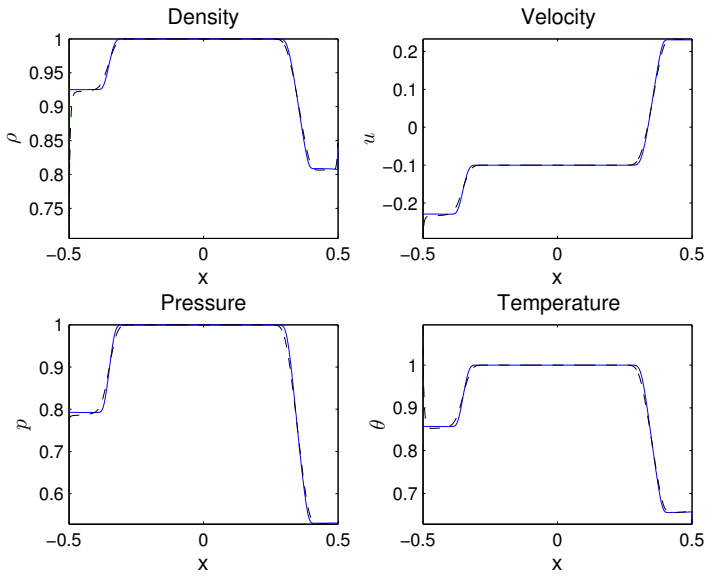

Figure 8: Example of diffusive reflection law with $(\rho_\star, u_\star, \theta_\star) = (1, -0.1, 1)$ and $\alpha = 0.5$, $\rho_{\mathrm{w}}^{\mathrm{L}} = 1, \rho_{\mathrm{w}}^{\mathrm{R}} = 1, \theta_{\mathrm{w}}^{\mathrm{L}} = 1, \theta_{\mathrm{w}}^{\mathrm{R}} = 0.5$ for a final time $t = 0.1$. Dashed line: kinetic simulation, solid line: hydrodynamic simulation.

- when $\sigma_{U_\star} = (2,1)$, Λ^+ is two-dimensional, hence there is one constraint relating the coefficients (ρ_+, u_+, θ_+); it reads:

$$B^+ = \begin{pmatrix} \dfrac{1}{\rho_\star} & -\dfrac{3}{\sqrt{3\theta_\star}} & \dfrac{1}{\theta_\star} \end{pmatrix};$$

- when $\sigma_{U_\star} = (1,2)$, Λ^+ is one-dimensional, hence there are two constraints relating the coefficients (ρ_+, u_+, θ_+); we get

$$B^+ = \begin{pmatrix} \dfrac{1}{\rho_\star} & 0 & -\dfrac{1}{2\theta_\star} \\ 0 & \dfrac{1}{\sqrt{3\theta_\star}} & -\dfrac{1}{2\theta_\star} \end{pmatrix};$$

- in the very specific case where $u_\star = 0$, and thus $\sigma_{U_\star} = (1,1)$, m_+ is evaluated by the two steps iteration procedure described in Section 3.

Finally, still using the Maxwell approximation, we set

$$\mathcal{F}_{\mathrm{bd}}^n = \int_{v>0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \left(\Phi^{\mathrm{data,L}} + \mathcal{R}(M_{U_\star}(1+m_{\mathrm{bd}}))\right) \mathrm{d}v + \int_{v<0} v \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} M_{U_\star}(1+m_{\mathrm{bd}})\, \mathrm{d}v$$

When the reflection operator $\mathcal{R}$ is conservative ($\alpha = 1$ for the diffuse reflection operator), the mass flux at the boundary is given by

$$\int_{\mathbb{R}} vF\, \mathrm{d}v = \int_{v>0} v\Phi^{\mathrm{data}}\, \mathrm{d}v.$$

It can be recast as

$$\int_{\mathbb{R}} vM_{U_\star}\left(1 + m_{\mathrm{bd}} + G^{\mathrm{L}}(t,0,v)\right) \mathrm{d}v = \int_{v>0} v\Phi^{\mathrm{data}}\, \mathrm{d}v.$$

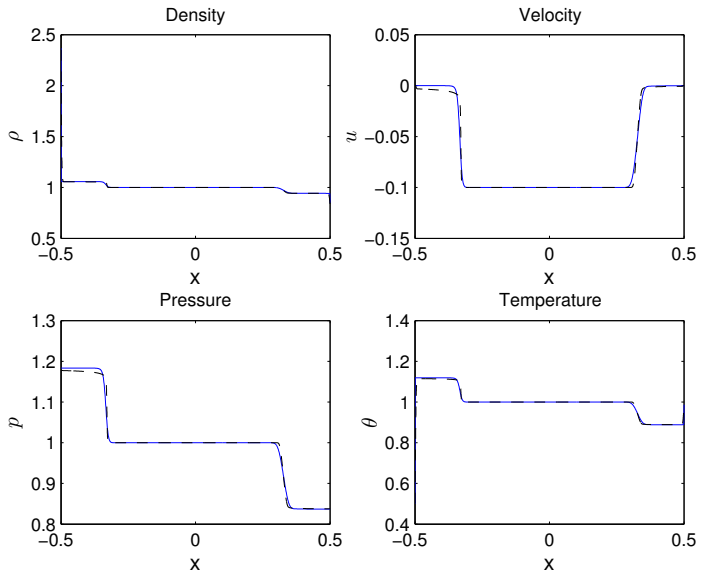

Figure 9: Example of diffusive reflection law with $(\rho_\star, u_\star, \theta_\star) = (1, -0.1, 1)$ and $\alpha = 1$, $\rho_{\rm w}^{\rm L} = 1, \rho_{\rm w}^{\rm R} = 1, \theta_{\rm w}^{\rm L} = 0.5, \theta_{\rm w}^{\rm R} = 1$ for a final time $t = 0.1$. Dashed line: kinetic simulation (with $\tau = 10^{-5}$), solid line: hydrodynamic simulation.

The Maxwell approximation replaces $\gamma^{\rm out} G^{\rm L}$ by 0 so that we are led to

$$\int_{\mathbb{R}} v M_{U_\star} \big(1 + m_- + m_+\big)\, {\rm d}v = \int_{v>0} v \Phi^{\rm data}\, {\rm d}v.$$

Therefore, our construction guarantees that the numerical boundary mass flux is given by

$$\mathcal{F}_{\rm bd}^n = \int_{v>0} v \Phi^{\rm data}\, {\rm d}v.$$

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While preparing the final version of this paper, we learn that similar questions have been addressed by L. Wang, J. Liu and S. Jin for relaxation models with numerical treatment by domain decomposition methods, [58].

References

[1] K. Aoki and N. Masukawa. Gas flows caused by evaporation and condensation on two parallel condensed phases and the negative temperature gradient: Numerical analysis by using a nonlinear kinetic equation. *Phys. Fluids*, 6(3):1379–1395, 1994.

[2] A. Arnold and U. Giering. An analysis of the Marshak conditions for matching Boltzmann and Euler equations. *Math. Models Methods Appl. Sci.*, 7(4):557–577, 1997.

[3] M. Arthur and C. Cercignani. Non-existence of a steady rarefied supersonic flow in a half-space. *ZAMP*, 31:635–645, 1980.

[4] H. Babovsky. Derivation of stochastic reflection laws from specular reflection. *Transport Theory Statist. Phys*, 16(1):113–126, 1987.
[5] C. Bardos. Problèmes aux limites pour les équations aux dérivées partielles du premier ordre à coefficients réels; théorèmes d'approximation; application à l'équation de transport. *Ann. Sci. École Norm. Sup. (4)*, 3:185–233, 1970.
[6] C. Bardos, R. Caflisch, and B. Nicolaenko. The Milne and Kramers problems for the Boltzmann equation of a hard sphere gas. *Comm. Pure Appl. Math.*, 39:323–352, 1986.
[7] C. Bardos, F. Golse, and D. Levermore. Fluid dynamic limits of kinetic equations. I. Formal derivations. *J. Statist. Phys.*, 63(1-2):323–344, 1991.
[8] C. Bardos, F. Golse, and D. Levermore. Fluid dynamic limits of kinetic equations. II. Convergence proofs for the Boltzmann equation. *Comm. Pure Appl. Math.*, 46(5):667–753, 1993.
[9] C. Bardos, F. Golse, and Y. Sone. Half-space problems for the Boltzmann equation: a survey. *J. Stat. Phys.*, 124(2-4):275–300, 2006.
[10] R. Beals and V. Protopopescu. Abstract time-dependent transport equations. *J. Math. Anal. Appl.*, 121:370–405, 1987.
[11] P. L. Bhatnagar, E. P. Gross, and M. Krook. A model for collision processes in gases. i. small amplitude processes in charged and neutral one-component systems. *Phys. Rev.*, 94:511–525, 1954.
[12] J.-F. Bourgat, P. Le Tallec, B. Perthame, and Y. Qiu. Coupling Boltzmann and Euler equations without overlapping. In A. Quarteroni, J. Periaux, Y. Kutznetsov, and O. Widlund, editors, *Domain Decomposition Methods in Science and Engineering, The sixth international conference on domain decomposition, Como, Italy, June 1992*, volume 157 of *Contemp. Math.*, pages 377–398. AMS, 1994.
[13] C. Cercignani. Half-space problems in the kinetic theory of gases. In E. Kröner and K. Kirchgässner, editors, *Trends to Applications of Pure Mathematics to Mechanics*, volume 249 of *Lecture Notes in Physics*, pages 35–51. Springer-Verlag, 1987.
[14] C. Cercignani. *The Boltzmann equation and its applications*, volume 67 of *Applied Mathematical Sciences*. Springer-Verlag, 1988.
[15] C. Cercignani. Scattering kernels for gas-surface interaction. In *Proceedings of the Workshop on Hypersonic Flows for Reentry Problems, INRIA, Antibes*, volume I, pages 9–29, 1990.
[16] C. Cercignani, M. Lampis, and A. Lentati. A new scattering kernel in kinetic theory of gases. *Transport Theory Statist. Phys.*, 24(9):1319–1336, 1995.
[17] M. Cessenat. Théorèmes de trace L^p pour des espaces de fonctions de la neutronique. *C. R. Acad. Sci. Paris Sér. I Math*, 299:831–834, 1984.
[18] M. Cessenat. Théorèmes de trace pour des espaces de fonctions de la neutronique. *C. R. Acad. Sci. Paris Sér. I Math*, 300:89–92., 1985.
[19] F. Charles, N. Vauchelet, C. Besse, T. Goudon, I. Lacroix-Violet, J.-P. Dudon, and L. Navoret. Numerical approximation of Knudsen layesr for Euler–Poisson system. Technical report, Cemracs 2010, 2011.
[20] F. Coron, F. Golse, and C. Sulem. A classification of well-posed kinetic layer problems. *Comm. Pure Appl. Math.*, 41(4):409–435, 1988.
[21] J.-S. Darrozès and J.-P. Guiraud. Généralisation formelle du théorème H en présence de parois. *C. R. Acad. Sci. Paris*, 262:369–371, 1966.
[22] S. Dellacherie. Coupling of the Wang Chang-Uhlenbeck equations with the multispecies Euler system. *J. Comput. Phys.*, 189:239–276, 2003.
[23] S. Dellacherie. *Etude et discrétisation de modèles cinétiques et de modèles fluides à bas nombre de Mach.* Habilitation à diriger des recherches, Univ. Paris 6, 2010.
[24] R. J. DiPerna and P.-L. Lions. On the Cauchy problem for Boltzmann equations: global existence and weak stability. *Ann. of Math.*, 130(2):321–366, 1989.
[25] B. Enquist and S. Osher. Stable and entropy satisfying approximations for transonic flow calculations. *Math. Comp.*, 31:45–75, 1981.
[26] J. Filbet and S. Jin. A class of asymptotic–preserving schemes for kinetic equations and related problems with stiff sources. *J. Comp. Phys.*, 229(20):7625–7648, 2010.
[27] K. O. Friedrichs and P. D. Lax. Systems of conservation equations with a convex extension. *Proc. Nat. Acad. Sci. U.S.A.*, 68:1686–1688, 1971.

[28] E. Godlewski and P.-A. Raviart. *Numerical approximation of hyperbolic systems of conservation laws*, volume 118 of *Applied Mathematical Sciences*. Springer, New-York, 1996.
[29] S. K. Godounov. Lois de conservation et intégrales d'énergie des équations hyperboliques. In C. Carasso, P.-A. Raviart, and D. Serre, editors, *Nonlinear hyperbolic problems (St. Etienne, 1986)*, volume 1270 of *Lecture Notes in Math.*, pages 135–149. Springer, Berlin, 1987.
[30] F. Golse. Applications of the Boltzmann equation within the context of upper atmosphere vehicle aerodynamics. *Comp. Methods Appl. Mech. Engng.*, 75:299–316, 1989.
[31] F. Golse. Knudsen layers from a computational viewpoint. *Transport Theory Statist. Phys.*, 21(3):211–236, 1992.
[32] F. Golse. Boundary and interface layers for kinetic models. Technical report, GdR SPARCH–CNRS, September 1997. Lecture Notes of the 4th Summer School of the GdR SPARCH, St Pierre d'Oléron.
[33] F. Golse and A. Klar. A numerical method for computing asymptotic states and outgoing distributions for kinetic linear half-space problems. *J. Statist. Phys.*, 80(5-6):1033–1061, 1995.
[34] F. Golse and F. Poupaud. Stationary solutions of the linearized Boltzmann equation in a half-space. *Math. Meth. Appl. Sci.*, 11:486–502, 1989.
[35] F. Golse and L. Saint-Raymond. The Navier-Stokes limit of the Boltzmann equation for bounded collision kernels. *Invent. Math.*, 155(1):81–161, 2004.
[36] T. Goudon. Existence of solutions of transport equations with nonlinear boundary conditions. *European J. Mech. B Fluids*, 16(4):557–574, 1997.
[37] T. Goudon. *Sur quelques questions relatives à la théorie cinétique des gaz et à l'équation de Boltzmann*. PhD thesis, Université Bordeaux 1, 1997.
[38] W. Greenberg and C. V. M. van der Mee. An abstract approach to evaporation models in rarefied gas dynamics. *Z. Angew. Math. Phys.*, 35(2):156–165, 1984.
[39] K. Hamdache. Initial-boundary value problems for the Boltzmann equation: global existence of weak solutions. *Arch. Rational Mech. Anal.*, 119(4):309–353, 1992.
[40] S. Jin. Efficient asymptotic–preserving (AP) schemes for some multiscale kinetic equations. *SIAM J. Sci. Comput.*, 21(2):441–454, 1999.
[41] A. Klar. Domain decomposition for kinetic problems with nonequilibrium states. *European J. Mech. B Fluids*, 15(2):203–216, 1996.
[42] I. Kuscer. Phenomenological aspects of gas-surface interaction. In E. Cohen and W. Fiszdon, editors, *Fundamental problems in statistical mechanics*, volume IV, pages 441–467, 1978.
[43] R. J. LeVeque. *Finite volume methods for hyperbolic problems*. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge, 2002.
[44] R. E. Marshak. Note on the spherical harmonic method as applied to the Milne problem for a sphere. *Phys. Rev.*, 71:443–446, 1947.
[45] J. C. Maxwell. On stresses in rarefied gases arising from inequalities of temperature. *Phil. Trans. Royal Soc. London*, 170:231–256, 1879.
[46] S. Mischler. On the trace problem for solutions of the Vlasov equation. *Comm. Partial Differential Equations*, 25(7-8):1415–1443, 2000.
[47] S. Mischler. Kinetic equations with Maxwell boundary condition. Technical report, Univ. Paris Dauphine, 2010. `hal-00346628`.
[48] B. Perthame. Global existence to the BGK model of Boltzmann equation. *J. Differential Equations*, 82(1):191–205, 1989.
[49] B. Perthame. Second order Boltzmann schemes for compressible Euler equations in one and two space dimensions. *SIAM J. Numer. Anal.*, 29(1):1–19, 1992.
[50] B. Perthame. *Kinetic formulation of conservation laws*, volume 21 of *Oxford Lecture Series in Math. and its Appl.* Oxford Univ. Press, 2002.
[51] B. Perthame and M. Pulvirenti. Weighted L^∞ bounds and uniqueness for the Boltzmann BGK model. *Arch. Rational Mech. Anal.*, 125(3):289–295, 1993.
[52] D. Serre. *Systems of conservation laws. Volume 1: Hyperbolicity, entropies, shock waves*. Cambridge University Press, Cambridge, 1999.
[53] D. Serre. *Systems of conservation laws. Volume 2: Geometric structures, oscillation and mixed problems*. Cam-

bridge University Press, Cambridge, 2000.

[54] Y. Sone. *Kinetic theory and fluid dynamics*. Modeling and simulation in science, engineering and technology. Birkhauser, 2002.

[55] Y. Sone, T. Ohwada, and K. Aoki. Evaporation and condensation on a plane condensed phase: Numerical analysis of the linearized Boltzmann equation for hard-sphere molecules. *Phys. Fluids*, 1(8):1398–1405, 1989.

[56] A. Vasseur. Rigorous derivation of the kinetic/fluid coupling involving a kinetic layer on a toy problem. *Archiv. Rat. Mech. Anal.*, 2010. To appear.

[57] C. Villani. Limites hydrodynamiques de l'équation de Boltzmann (d'après C. Bardos, F. Golse, C. D. Levermore, P.-L. Lions, N. Masmoudi, L. Saint-Raymond). *Astérisque*, (282):Exp. No. 893, ix, 365–405, 2002. Séminaire Bourbaki, Vol. 2000/2001.

[58] L. Wang, J. Liu, and S. Jin. Domain decomposition method for a two-scale hyperbolic system. Technical report, UW-Madison, 2011.