A Framework for Hyperbolic Approximation of Kinetic Equations Using Quadrature-Based Projection Methods

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Abstract

We derive hyperbolic PDE systems for the solution of the Boltzmann Equation. First, the velocity is transformed in a non-linear way to obtain a Lagrangian velocity phase space description that allows for physical adaptivity. The unknown distribution function is then approximated by a series of basis functions.

Standard continuous projection methods for this approach yield PDE systems for the basis coefficients that are in general not hyperbolic. To overcome this problem, we apply quadrature-based projection methods which modify the structure of the system in the desired way so that we end up with a hyperbolic system of equations.

With the help of a new abstract framework, we derive conditions such that the emerging system is hyperbolic and give a proof of hyperbolicity for Hermite ansatz functions in one dimension together with Gauss-Hermite quadrature.

AMS subject classification: 35Q20, 35Q35

Key words: Boltzmann equation, kinetic equation, quadrature, hyperbolicity

1 Introduction

Kinetic equations like the Boltzmann Equation are the basis for many different applications and are widely used in industrial and scientific fields (see e.g. [10], [15], [21]). Especially for rarefied flows they provide an efficient setting for the conduction of

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numerical simulations (compare e.g. [23]). As there are regions of the flow in which the application of standard fluid dynamic models like the Euler or Navier-Stokes Equations is not appropriate for a physical solution, one has to apply more suitable kinetic models that are motivated directly by kinetic equations.

Standard methods to solve kinetic equations are DSMC and the discrete velocity method. DSMC actually simulates the movement of particles and the solution converges to the underlying kinetic equation in the limit of infinitely many particles, see [3],[4]. The number of particles is typically very large, which slows down the computation in many cases. In a discrete velocity method, the kinetic equation is evaluated at discrete points in the velocity phase space. The placement of the discrete velocities is not easy, as the microscopic and macroscopic velocities can attain very large values leading to the necessity of a very fine discretization in the velocity space with many unknowns. New methods by Filbet [11] and Mieussens [19] use local grids in the velocity or scale the velocity space to restrict the discrete velocities to a smaller domain. Developments by Kauf [16] show a way to circumvent the problem of the velocity discretization at the expense of a more difficult PDE involving additional terms using a transformation of the velocity space to a Lagrangian velocity phase space to allow for physical adaptivity of a later discretization, even for uniform grids in the transformed velocity variable. We will also use this approach but in multiple dimensions and derive a transformed Boltzmann Equation that enables efficient discretizations.

The standard method to discretize the resulting equation in velocity space according to Grad in [12] is to derive equations for the macroscopic flow variables like density, velocity and temperature of the flow by expanding the unknown distribution function of the Boltzmann Equation in a Hermite series and projecting the equations by multiplication with test functions and integration over the velocity space. This approach is especially useful close to equilibrium. The drawback of this method is that the resulting PDE system can loose hyperbolicity for certain values of higher moments. In these cases, numerical methods can become unstable because the problem is ill-posed. The admissible region of variables for hyperbolicity of the system in fact becomes smaller for higher accuracy of the methods, as shown by Cai in [7], see also [6].

There are some methods for which it can be shown under certain conditions that they are hyperbolic in special cases like one-dimensional flows. One of those is based on multi-variate Pearson-IV-Distributions and was proposed by Torrilhon [24]. Another method to achieve hyperbolic equations has been published by Levermore in [18], but the integrals in his maximum entropy method are unfortunately not given in analytical form in general.

In [7] Cai et al. have successfully performed a regularization of Grad's moment system in one dimension that is globally hyperbolic. They essentially derived the characteristic polynomial of the corresponding matrix analytically and used this information to delete certain entries in the Jacobian matrix so that the new characteristic polynomial has real roots and the system becomes hyperbolic for all values of the variables involved. The approach by Cai et al. is successful but it is not entirely clear how to generalize the procedure to similar problems, e.g. for different ansatz functions.

The main part of this paper is concerned with the setup of a general framework to derive hyperbolic PDEs for the solution of the Boltzmann Equation. With the help of this framework it is feasible to decide about the hyperbolicity of the resulting system a priori, i.e. before inserting a special ansatz and performing projections of the equation, only by the specific choice of the ansatz and the projection method.

We investigate the use of quadrature-based projection methods in particular and analyze the application of those methods to the transformed Boltzmann Equation with respect to the effects on the structure of the equations as well as on the eigenvalues of the system matrix, which is closely related to the hyperbolicity of the system. The framework includes quadrature-based projections and gives concrete conditions under which the system will be hyperbolic. While the framework is applicable for all flow regimes, it is especially useful for the collision dominated and the transition regime, e.g. for Knudsen numbers on the order of one.

The paper is organized as follows: Section 2 is dedicated to the kinetic setting in which we investigate the Boltzmann Equation and the transformed Boltzmann Equation is derived along with a formal closure of the equations by so-called *compatibility conditions*. The deficiencies of standard projection methods like discrete velocities and exact integration are shown in Section 3, as those methods lead to conditionally hyperbolic systems. The framework for developing globally hyperbolic approximations is detailed in Section 4 together with general conditions for hyperbolicity which are afterwards verified for quadrature-based projections using a Hermite ansatz in one dimension in Section 5. The paper ends with concluding remarks.

2 Transformed Boltzmann Transport Equation

2.1 Basics of Kinetic Theory

In kinetic theory the evolution of the mass density function $f(t, \boldsymbol{x}, \boldsymbol{c})$ is described by the Boltzmann Transport Equation

$$\frac{\partial}{\partial t} f(t, \boldsymbol{x}, \boldsymbol{c}) + c_i \frac{\partial}{\partial x_i} f(t, \boldsymbol{x}, \boldsymbol{c}) = S(f), \tag{2.1}$$

where we consider a d-dimensional setting, i.e. we have position $\boldsymbol{x} \in \mathbb{R}^d$ and velocity $\boldsymbol{v} \in \mathbb{R}^d$. Note that we use index notation, whenever the indices are no further specified, e.g. in the transport term of Equation (2.1). The right-hand side collision operator $S(f)$ will be neglected throughout this paper as we focus on the transport part of Equation (2.1). Models for the right-hand side can be found in [2], [8] and [14].

The distribution function $f(t, \boldsymbol{x}, \boldsymbol{c})$ is related to the macroscopic quantities like density ρ, velocity $\boldsymbol{v}$ and energy θ via integration over the velocity space as follows:

$$\rho(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}, \tag{2.2}$$

$$\rho(t, \boldsymbol{x}) \boldsymbol{v}(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} \boldsymbol{c} f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}, \tag{2.3}$$

$$d \cdot \rho(t, \boldsymbol{x}) \theta(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} |\boldsymbol{c} - \boldsymbol{v}|^2 f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}. \tag{2.4}$$

A system of equations for these macroscopic variables can be derived by multiplication of Equation (2.1) with $\left(1, \boldsymbol{c}, c_i^2\right)$ and subsequent integration over the velocity space. The emerging equations are the conservation laws of mass, momentum and energy, see e.g. [23] or (2.13) later.

2.2 Transformation to Lagrangian Velocity Phase Space

A direct discretization of Equation (2.1) leads to the need for many discretization points, as the micro- and macroscopic velocities can attain very large values. An equidistant grid centered around the origin might not be suitable because it misses features of the distribution function for large velocities. In the following, we describe a transformed version of the Boltzmann Equation (2.1) that essentially uses a Lagrangian velocity phase space and thus exhibits physical adaptivity which allows for efficient and yet simple discretizations.

According to Kauf (see [16]) who considered the one-dimensional case, the velocity is transformed in a highly non-linear way to allow for intrinsic physical adaptivity of the scheme. We shift the microscopic velocity $\boldsymbol{c}$ by its macroscopic counterpart $\boldsymbol{v}$ and scale by the variance $\sqrt{\theta}$. The corresponding Galilei-invariant variable transformation reads

$$\boldsymbol{c} \mapsto \frac{\boldsymbol{c} - \boldsymbol{v}(t, \boldsymbol{x})}{\sqrt{\theta(t, \boldsymbol{x})}} =: \boldsymbol{\xi}(t, \boldsymbol{x}, \boldsymbol{c}). \tag{2.5}$$

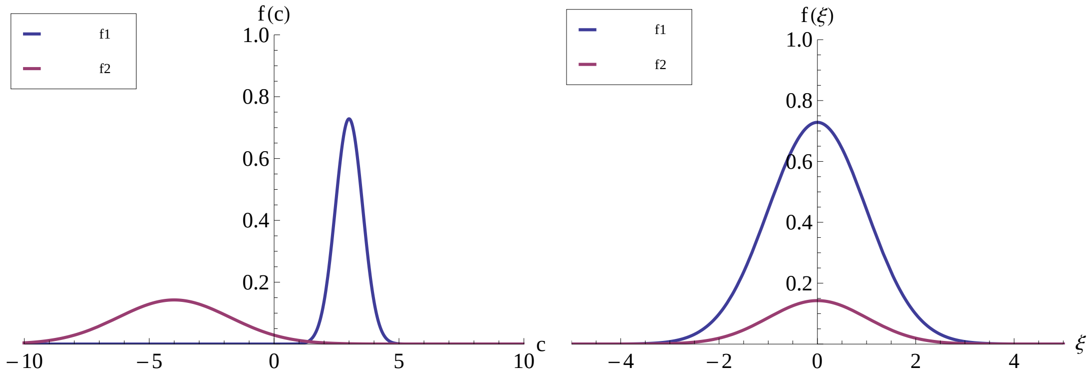
The effect of the transformation for different Gaussian distribution functions with different $\boldsymbol{v}$ and θ is depicted in Figure 1. As shown in [17], Equation (2.1) transforms to

$$D_t f + \sqrt{\theta}\xi_j \partial_{x_j} f + \partial_{\xi_j} f \left(-\frac{1}{\sqrt{\theta}} \left(D_t v_j + \sqrt{\theta}\xi_i \partial_{x_i} v_j \right) - \frac{1}{2\theta} \xi_j \left(D_t \theta + \sqrt{\theta} \xi_i \partial_{x_i} \theta \right) \right) = 0, \tag{2.6}$$

where we used the convective time derivative

$$D_t := \partial_t + v_i \partial_{x_i}. \tag{2.7}$$

Inserting a scaled distribution function according to Equation (2.8) into Equation



(a) untransformed Gaussians, depending on c (b) transformed Gaussians, depending on ξ

Figure 1: Gaussians f_1 with $\rho_1 = 1$, $v_1 = 3$, $\theta_1 = 0.3$ and f_2 with $\rho_2 = 0.8$, $v_2 = -4$, $\theta_2 = 5$.

(2.6), we obtain Equation (2.9).

$$f(t, \boldsymbol{x}, \boldsymbol{\xi}) = \frac{\rho}{\sqrt{\theta}^d} \widetilde{f}(t, \boldsymbol{x}, \boldsymbol{\xi}). \tag{2.8}$$

$$\begin{aligned} &\left(\frac{1}{\rho} D_t \rho - \frac{d}{2\theta} D_t \theta\right) \widetilde{f} + D_t \widetilde{f} + \\ &\sqrt{\theta}\xi_j \left(\left(\frac{1}{\rho}\partial_{x_j}\rho - \frac{d}{2\theta}\partial_{x_j}\theta\right)\widetilde{f} + \partial_{x_j}\widetilde{f}\right) + \\ &\partial_{\xi_j}\widetilde{f}\left(-\frac{1}{\sqrt{\theta}}\left(D_t v_j + \sqrt{\theta}\xi_i \partial_{x_i} v_j\right) - \frac{1}{2\theta}\xi_j\left(D_t\theta + \sqrt{\theta}\xi_i\partial_{x_i}\theta\right)\right) \;=\; 0. \end{aligned} \tag{2.9}$$

Likewise, the computation of the macroscopic quantities (2.2)-(2.4) transforms to compatibility conditions for the scaled distribution function $\widetilde{f}$ as follows:

$$1 = \int_{\mathbb{R}^d} \widetilde{f}(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{2.10}$$

$$0 = \int_{\mathbb{R}^d} \xi_i \widetilde{f}(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \quad i = 1, \ldots, d \tag{2.11}$$

$$d = \int_{\mathbb{R}^d} \xi_i^2 \widetilde{f}(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{2.12}$$

Equation (2.9) is underdetermined, because $\rho, \boldsymbol{v}$ and θ are not known. Analogously to the procedure described in Section 2.1, we can multiply Equation (2.9) with $\left(1, \boldsymbol{\xi}, \xi_i^2\right)$ and integrate over the transformed velocity space to derive the following well-known macroscopic conservation laws that close the equation above.

$$\begin{aligned} D_t\rho + \rho\frac{\partial}{\partial x_i}v_i &= 0, \\ D_t v_k + \frac{1}{\rho}\frac{\partial}{\partial x_j}p_{kj} &= 0, \text{ for } k = 0, \dots, d, \\ D_t\theta + \frac{1}{\rho}\frac{\partial}{\partial x_j}q_j + \frac{2p_{ij}}{\rho}\frac{\partial}{\partial x_i}v_j &= 0. \end{aligned} \tag{2.13}$$

for pressure tensor p_{ij} and heat flux q_i defined as

$$p_{ij} = \rho\theta\int_{\mathbb{R}^d}\xi_i\xi_j\widetilde{f}(t,\boldsymbol{x},\boldsymbol{\xi})\ d\boldsymbol{\xi}, \tag{2.14}$$

$$q_i = \rho\theta^{3/2}\int_{\mathbb{R}^d}\xi_i^2\xi_j\widetilde{f}(t,\boldsymbol{x},\boldsymbol{\xi})\ d\boldsymbol{\xi}, \tag{2.15}$$

which leads to a coupling of the conservation laws to the equation for the unknown distribution function $\widetilde{f}$.

A natural approach to solve the coupled system of equations would be to use point evaluations of Equation (2.9) together with a reasonable finite difference approximation of the derivatives $\partial_{\xi_j}\widetilde{f}$. However, this approach does not lead to a globally hyperbolic system as eigenvalues of the system matrix depend on the unknowns, similar to the examples in Chapter 3. To overcome this problem, we need to apply other methods to derive a system of equations that solves (2.9) as explained in the following sections.

2.3 Expansion of the Distribution Function and Projection

We expand the unknown distribution function $f(t,\boldsymbol{x},\boldsymbol{\xi})$ around its equilibrium Maxwellian with respect to basis functions $\phi_\alpha(\boldsymbol{\xi})$ and corresponding coefficients $\kappa_\alpha(t,\boldsymbol{x})$, obtaining

$$\widetilde{f}(t,\boldsymbol{x},\boldsymbol{\xi}) = \sum_{\alpha=0}^{n}\kappa_\alpha(t,\boldsymbol{x})\phi_\alpha(\boldsymbol{\xi}). \tag{2.16}$$

with ansatz functions $\phi_\alpha(\boldsymbol{\xi}) = w(\boldsymbol{\xi})\varphi_\alpha(\boldsymbol{\xi})$ and weighting function $w(\boldsymbol{\xi}) = \frac{1}{\sqrt{2\pi}^d}\exp\left(-\frac{\xi_i^2}{2}\right)$, because this ansatz is very flexible with respect to the basis functions and allows for a continuous representation of $\widetilde{f}$.

After insertion of Ansatz (2.16) into Equation (2.9), we apply a projection operator $P_\beta(g)$, $\beta = 0, \ldots, n$, which forms a scalar product (in the transformed velocity space $\boldsymbol{\xi}$) of g with test functions $\psi_\beta(\boldsymbol{\xi})$ as follows:

$$P_\beta(g) = \langle \psi_\beta, g \rangle. \tag{2.17}$$

Note that this formulation also includes a discrete velocity model as explained in Section 3.1.

Projecting Equation (2.9), the PDE system for the coefficients κ_α then reads for $\beta = 0, \ldots, n$

$$\begin{aligned}
&\left(\frac{1}{\rho}D_t\rho - \frac{d}{2\theta}D_t\theta\right)\kappa_\alpha\langle\psi_\beta,\phi_\alpha\rangle + D_t\kappa_\alpha\langle\psi_\beta,\phi_\alpha\rangle \\
&+\sqrt{\theta}\left(\left(\frac{1}{\rho}\partial_{x_j}\rho - \frac{d}{2\theta}\partial_{x_j}\theta\right)\kappa_\alpha\langle\psi_\beta,\xi_j\phi_\alpha\rangle + \partial_{x_j}\kappa_\alpha\langle\psi_\beta,\xi_j\phi_\alpha\rangle\right) \\
&-\frac{1}{\sqrt{\theta}}\left(D_t v_j\kappa_\alpha\langle\psi_\beta,\partial_{\xi_j}\phi_\alpha\rangle + \sqrt{\theta}\partial_{x_i}v_j\kappa_\alpha\langle\psi_\beta,\xi_i\partial_{\xi_j}\phi_\alpha\rangle\right) \\
&-\frac{1}{2\theta}\left(D_t\theta\kappa_\alpha\langle\psi_\beta,\xi_j\partial_{\xi_j}\phi_\alpha\rangle + \sqrt{\theta}\partial_{x_i}\theta\kappa_\alpha\langle\psi_\beta,\xi_i\xi_j\partial_{\xi_j}\phi_\alpha\rangle\right) \quad = 0.
\end{aligned} \tag{2.18}$$

2.4 Compatibility Conditions

Apart from the $n+1$ coefficients κ_α, System (2.18) also contains the macroscopic quantities $\rho, \boldsymbol{v}, \theta$, so that we need additional relations to close the system. We could in principle use the conservation laws (2.13) to do so (which would be equivalent to choosing the first $d+2$ test functions as $(\psi_0, \ldots, \psi_{d+1}) = \big(1, \xi_1, \ldots, \xi_d, \xi_i^2\big)$), but in order to keep the flexibility of our model we want to proceed in a different way as follows: Using (2.16), we get $d+2$ *compatibility conditions* from Equations (2.10)-(2.12)

$$1 = \kappa_\alpha\langle\phi_\alpha(\boldsymbol{\xi}), 1\rangle, \tag{2.19}$$

$$0 = \kappa_\alpha\langle\phi_\alpha(\boldsymbol{\xi}), \xi_i\rangle, \quad i = 1, \ldots, d \tag{2.20}$$

$$d = \kappa_\alpha\langle\phi_\alpha(\boldsymbol{\xi}), \xi_i^2\rangle. \tag{2.21}$$

Equations (2.19)-(2.21) can be used to reduce the number of unknowns in (2.18) to obtain a closed PDE system similar to the general procedure described in [13]. We thus use $\boldsymbol{Q} \in \mathbb{R}^{l\times(n+1)}, \boldsymbol{c} = (1, 0, \ldots, 0, 1)^T \in \mathbb{R}^l$ and write the $l = d + 2$ Equations (2.19)-(2.21) in matrix-vector form to define $\boldsymbol{Q}$ by

$$\boldsymbol{Q}\boldsymbol{\kappa} = \boldsymbol{c}. \tag{2.22}$$

Every real matrix $\boldsymbol{Q} \in \mathbb{R}^{l\times(n+1)}$ can be decomposed as follows:

$$\boldsymbol{Q} = \boldsymbol{S}\boldsymbol{M}\boldsymbol{T}^{-1}, \text{ with } \boldsymbol{S} \in \mathbb{R}^{l\times l},\ \boldsymbol{M} \in \mathbb{R}^{l\times(n+1)},\ \boldsymbol{T} \in \mathbb{R}^{(n+1)\times(n+1)}, \tag{2.23}$$

for invertible square matrices $\boldsymbol{S}$ and $\boldsymbol{T}$. The matrix $\boldsymbol{M}$ has the form

$$\boldsymbol{M} = \begin{pmatrix} \sigma_1 & & & 0 & \ldots & 0 \\ & \ddots & & \vdots & \ddots & \vdots \\ & & \sigma_l & 0 & \ldots & 0 \end{pmatrix} =: \left(\widehat{\boldsymbol{Q}}, \boldsymbol{0}\right), \tag{2.24}$$

for example with the singular values of $\boldsymbol{Q}$ on the diagonal in case of a singular value decomposition.

We introduce a set of transformed variables $\widehat{\boldsymbol{\beta}} \in \mathbb{R}^{n+1}$ by the definition

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} \boldsymbol{\beta_0} \\ \boldsymbol{\beta} \end{pmatrix} := \boldsymbol{T}^{-1}\boldsymbol{\kappa}, \tag{2.25}$$

for $\boldsymbol{\beta_0} \in \mathbb{R}^l$ and $\boldsymbol{\beta} \in \mathbb{R}^{n+1-l}$, so that we can directly solve for l entries of $\widehat{\boldsymbol{\beta}}$, namely the first l variables $\boldsymbol{\beta_0}$, using the compatibility conditions from Equation (2.22), (see [17] for details)

$$\boldsymbol{\beta_0} = \widehat{\boldsymbol{Q}}^{-1}\boldsymbol{S}^{-1}\boldsymbol{c}. \tag{2.26}$$

We can thereby close the system of PDEs by inserting

$$\boldsymbol{\kappa} = \boldsymbol{T}\begin{pmatrix} \boldsymbol{\beta_0} \\ \boldsymbol{\beta} \end{pmatrix} = (\boldsymbol{T}_1, \boldsymbol{T}_2)\begin{pmatrix} \boldsymbol{\beta_0} \\ \boldsymbol{\beta} \end{pmatrix} = \boldsymbol{T}_1\widehat{\boldsymbol{Q}}^{-1}\boldsymbol{S}^{-1}\boldsymbol{c} + \boldsymbol{T}_2\boldsymbol{\beta}, \tag{2.27}$$

with a proper splitting of the columns of $\boldsymbol{T} = (\boldsymbol{T}_1, \boldsymbol{T}_2)$.

With the help of the compatibility conditions, the set of $n+1$ basis coefficients $\boldsymbol{\kappa}$ is thus reduced to a set of $n+1-l$ variables $\boldsymbol{\beta}$ that leads to a closed PDE system with the same number of equations and unknowns.

By insertion of Equation (2.27) into the PDE System (2.18), we obtain a closed system of equations for the variables $\boldsymbol{u} := (\rho, \boldsymbol{v}, \theta, \boldsymbol{\beta})$ of the form

$$\boldsymbol{B}(\boldsymbol{u}) \frac{D}{Dt} \boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{A}_i(\boldsymbol{u}) \frac{\partial}{\partial x_i} \boldsymbol{u} = 0, \tag{2.28}$$

where $\boldsymbol{B}(\boldsymbol{u}), \boldsymbol{A}_i(\boldsymbol{u}) \in \mathbb{R}^{(n+1)\times(n+1)}$ for $i = 1, \ldots, d$.

The important question is, if System (2.28) can be shown to be globally hyperbolic according to the following definition:

A coupled system of PDEs in d dimensions for $\boldsymbol{u} \in \mathbb{R}^{n+1}$ and $\boldsymbol{A}_i(\boldsymbol{u}) \in \mathbb{R}^{(n+1)\times(n+1)}$ for $i = 1, \ldots, d$, e.g.

$$\boldsymbol{B}(\boldsymbol{u}) \frac{\partial}{\partial t} \boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{A}_i(\boldsymbol{u}) \frac{\partial}{\partial x_i} \boldsymbol{u} = 0, \tag{2.29}$$

is *globally hyperbolic* if $\boldsymbol{B}(\boldsymbol{u})$ is invertible and the eigenvalues of the matrix

$$\boldsymbol{A}_{sys}(\boldsymbol{u}) = \sum_{i=1}^{d} n_i \left(\boldsymbol{B}(\boldsymbol{u})\right)^{-1} \boldsymbol{A}_i(\boldsymbol{u}) \tag{2.30}$$

are real for every $u \in \mathbb{R}^{n+1}$ and every unit vector $\boldsymbol{n} \in \mathbb{R}^d$ with $\|\boldsymbol{n}\|_2 = 1$, see [9] or [13] for more details.

The question of hyperbolicity for System (2.28) will be addressed in the subsequent chapters.

3 Failure of Classical Methods

For the concrete discretization of the transformed Boltzmann Equation, one has to choose a specific ansatz for $\widetilde{f}(t, \boldsymbol{x}, \boldsymbol{\xi})$ or ansatz functions $\phi_\alpha(\boldsymbol{\xi})$ as well as a projection operator $P_\beta(\cdot)$ using test functions ψ_β. Unfortunately, the resulting PDE system is not globally hyperbolic for standard ansatz functions and projection methods as we will show in the following section for simple 1D examples.

3.1 Discrete Velocity Method

In a discrete velocity setting, we consider evaluations of Equation (2.9) at discrete ξ_β, for $\beta = 0, \dots, n$. In other words, the corresponding projection operator and functions read

$$\begin{aligned} \phi_\alpha(\xi) &= \delta(\xi - \xi_\alpha), &(3.1)\\ \psi_\beta(\xi) &= \delta(\xi - \xi_\beta), &(3.2)\\ P_\beta(g) &= \int_{\mathbb{R}} g(t,x,\xi)\ \delta(\xi - \xi_\beta) d\xi = g(t,x,\xi_\beta). &(3.3)\end{aligned}$$

The distribution function is only given at discrete points and thus expanded using delta functions from Equation (3.1) as follows:

$$\widetilde{f}(t,x,\xi) = \sum_{\alpha=0}^{n} f_\alpha(t,x)\delta(\xi - \xi_\alpha). \tag{3.4}$$

The compatibility conditions from Equations (2.10)-(2.12) give three equations from which we can eliminate the first three unknowns, so that we end up with $n+1$ equivalent variables $\boldsymbol{u} = (\rho, v, \theta, f_3, \dots, f_n)$.

Using the procedure of the previous chapter, we want to write down the PDE system for $\boldsymbol{u}$. As there is no continuous representation of $\widetilde{f}$ according to Equation (3.4), we cannot directly evaluate the derivative terms $\partial_\xi \widetilde{f}$ in Equation (2.9) and consider finite difference approximations of the following kind:

$$\begin{aligned} \partial_\xi \widetilde{f}\Big|_{\xi_0} &\approx \frac{f_1 - f_0}{\xi_1 - \xi_0}, &(3.5)\\ \partial_\xi \widetilde{f}\Big|_{\xi_\beta} &\approx \frac{f_{\beta+1} - f_{\beta-1}}{\xi_{\beta+1} - \xi_{\beta-1}}, \text{ for } \beta = 1, \dots, n-1, &(3.6)\\ \partial_\xi \widetilde{f}\Big|_{\xi_n} &\approx \frac{f_n - f_{n-1}}{\xi_n - \xi_{n-1}}, &(3.7)\end{aligned}$$

i.e. central differences in the interior and single-sided differences for the outer point evaluations.

Evaluating the terms in Equation (2.9), we can write down the emerging PDE system for the unknown vector $\boldsymbol{u}$ similar to System (2.28):

$$\boldsymbol{B}\frac{D}{Dt}\boldsymbol{u} + \boldsymbol{A}\frac{\partial}{\partial x}\boldsymbol{u} = 0. \tag{3.8}$$

Hyperbolicity of the system requires the generalized eigenvalues of $\boldsymbol{A}$ with respect to the matrix $\boldsymbol{B}$ to be real. Observing, that we have $\boldsymbol{A} = \widehat{\boldsymbol{A}}\boldsymbol{B}$ with some regular diagonal matrix $\widehat{\boldsymbol{A}} \in \mathbb{R}^{(n+1)\times(n+1)}$ (for details, see Section 4) due to the structure of the projected System (2.9), we write down the corresponding characteristic polynomial as

$$\chi_{\mathrm{DVM}}(\lambda) = \det\left(\boldsymbol{A} - \lambda\boldsymbol{B}\right) = \det\left(\widehat{\boldsymbol{A}} - \lambda\boldsymbol{I}_{n+1}\right)\det\left(\boldsymbol{B}\right), \tag{3.9}$$

so that we have arbitrary (and possibly imaginary) eigenvalues if $\det\left(\boldsymbol{B}\right) = 0$, i.e. $\boldsymbol{B}$ is singular. The expression $\det\left(\boldsymbol{B}\right) \neq 0$ thus gives a condition for hyperbolicity. Another explanation is that a singular matrix $\boldsymbol{B}$ leads to an ill-posed system, as we can reduce the set of equations by the dimension of the kernel of $\boldsymbol{B}$ resulting in an underdetermined system of equations.

For the five moment case $n = 4$, equidistant discrete velocities $\boldsymbol{\xi} = (-2, -1, 0, 1, 2)^T$ and derivatives as defined in Equations (3.5)-(3.7), we obtain

$$\det\left(\boldsymbol{B}\right) = 2.625 - 8.25 f_3 - 34.5 f_4 + 36 f_3 f_4 + 108 f_4^2. \tag{3.10}$$

The condition $\det\left(\boldsymbol{B}\right) = 0$ is fulfilled for infinitely many positive point values f_β for $\beta = 0, \ldots, 4$, leading to a possible loss of hyperbolicity for reachable values during simulations.

We performed computations using different discrete velocities ξ_β, including equally spaced points centered around zero and Hermite roots, as well as different derivative approximations, but $\det\left(\boldsymbol{B}\right) \neq 0$ always yielded a constraint for the hyperbolicity that can be violated by realizable states. The system is thus not globally hyperbolic in all investigated cases.

3.2 Hermite Ansatz Using Exact Projections

Choosing Hermite functions for the ansatz and test space (compare Definition (A.1)), we have

$$\phi_\alpha(\xi) = w(\xi)H_\alpha(\xi) \tag{3.11}$$

$$\psi_\beta(\xi) = H_\beta(\xi), \tag{3.12}$$

$$P_\beta(\phi_\alpha) = \int_{\mathbb{R}} \psi_\beta(\xi)\phi_\alpha(\xi)d\xi = \delta_{\alpha,\beta}, \tag{3.13}$$

because of orthogonality of the Hermite polynomials with respect to the weighting function $w(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right)$, see also Equation (2.16).

The compatibility conditions from Equations (2.19)-(2.21) translate to

$$\kappa_0 = 1,\ \kappa_1 = 0,\ \kappa_2 = 0, \tag{3.14}$$

so that we can directly set the corresponding values and have a closed system for $n+1$ variables $\boldsymbol{u} = (\rho, v, \theta, \kappa_3, \dots, \kappa_n)$.

It is possible to apply the recursion formulas given in the appendix (Equations (A.3)-(A.6)) to obtain a PDE system for the unknowns. We will not do so here, see e.g. [7] for the full system or [17] for a detailed description of simple cases.

Writing the resulting system after some simplifications as

$$\frac{D}{Dt}\boldsymbol{u} + \boldsymbol{A}\frac{\partial}{\partial x}\boldsymbol{u} = 0, \tag{3.15}$$

we can check the system for hyperbolicity by investigation of the characteristic polynomial $\chi_{\boldsymbol{A}}(\lambda)$ of the system matrix $\boldsymbol{A} \in \mathbb{R}^{(n+1)\times(n+1)}$ from Equation (3.15).

The calculation of $\chi_{\boldsymbol{A}}(\lambda)$ can be done analytically according to [7] or via computer algebra systems for given $n \in \mathbb{N}$ and leads to the following simple result (after scaling with $\sqrt{\theta}$):

$$\chi_{\boldsymbol{A}}(\lambda) = \sqrt{(n+1)!}H_{n+1}(\xi) + \gamma_1 \left(1 - \lambda^2 \kappa_{n-1}\right) + \gamma_2 \kappa_n, \tag{3.16}$$

where $\gamma_1, \gamma_2 \in \mathbb{R}$ are independent of the unkowns. Equation (3.16) shows that the roots of $\chi_{\boldsymbol{A}}(\lambda)$ and thus the eigenvalues of $\boldsymbol{A}$ are imaginary for certain realizable values of κ_{n-1} and κ_n, leading to a loss of hyperbolicity in these situations.

4 Framework for Hyperbolic System of Equations

As shown in Section 3, standard methods fail to derive globally hyperbolic PDE systems for the transformed Boltzmann Equation (2.9). With the help of a newly developed framework, we will show that quadrature-based projection methods are capable of modifying the equations such that the emerging system becomes globally hyperbolic.

4.1 Projection and Derivation of Constrained PDE System

Consider the following quadrature-based projection operator that can be seen as an approximation to the continuous operator defined in Equation (3.13)

$$P_\beta(g) = \sum_{k=0}^{n} w_k g(\boldsymbol{\xi}_k) \psi_\beta(\boldsymbol{\xi}_k) \tag{4.1}$$

with positive quadrature weights w_k and pairwise distinct quadrature points $\boldsymbol{\xi}_k \in \mathbb{R}^d$, for $k = 0, \ldots, n$. Apart from the standard quadrature rules, it is possible to construct non-classical rules with computational tools like the package described in [20].

Using these projections for $\beta = 0, \ldots, n$ System (2.18) can be written in matrix-vector form as follows:

$$\boldsymbol{\Psi}^T \boldsymbol{W} \boldsymbol{A} \boldsymbol{\Lambda} \frac{D}{Dt} \widetilde{\boldsymbol{u}} + \sum_{i=1}^{d} \boldsymbol{\Psi}^T \boldsymbol{W} \boldsymbol{\Xi}_i \boldsymbol{A} \boldsymbol{\Lambda} \sqrt{\theta} \frac{\partial}{\partial x_i} \widetilde{\boldsymbol{u}} = 0, \tag{4.2}$$

with unknowns

$$\widetilde{\boldsymbol{u}} = (\rho, v_1, \ldots, v_d, \theta, \kappa_0, \ldots, \kappa_n)^T \in \mathbb{R}^{n+d+3}, \tag{4.3}$$

a columnwise defined system matrix

$$\boldsymbol{A} = \left(\boldsymbol{\Phi}\boldsymbol{\kappa}, -\frac{\partial \boldsymbol{\Phi}}{\partial \xi_1}\boldsymbol{\kappa}, \ldots, -\frac{\partial \boldsymbol{\Phi}}{\partial \xi_d}\boldsymbol{\kappa}, -d\boldsymbol{\Phi}\boldsymbol{\kappa} - \boldsymbol{\Xi}_j \frac{\partial \boldsymbol{\Phi}}{\partial \xi_j}\boldsymbol{\kappa}, \boldsymbol{\Phi} \right) \in \mathbb{R}^{(n+1)\times(n+d+3)}, \tag{4.4}$$

consisting of matrices (for $i, j = 0, \ldots, n$ and $k = 1, \ldots, d$)

$$\boldsymbol{\Psi}_{i,j} = \psi_j(\boldsymbol{\xi}_i), \tag{4.5}$$

$$\boldsymbol{\Phi}_{i,j} = \phi_j(\boldsymbol{\xi}_i), \tag{4.6}$$

$$\left(\frac{\partial \boldsymbol{\Phi}}{\partial \xi_k}\right)_{i,j} = \partial_{\xi_k}\phi_j\big|_{\boldsymbol{\xi}_i}, \tag{4.7}$$

$$(\boldsymbol{\Xi}_k)_{i,j} = (\boldsymbol{\xi}_i)_k\, \delta_{ij}, \tag{4.8}$$

$$\boldsymbol{W}_{i,j} = \omega_i \delta_{ij} \tag{4.9}$$

and a matrix storing the macroscopic variables

$$\boldsymbol{\Lambda} = \begin{pmatrix} \frac{1}{\sqrt{\theta}} & & & \\ & \frac{\rho}{\theta}\boldsymbol{I}_d & & \\ & & \frac{\rho}{2\theta^{3/2}} & \\ & & & \frac{\rho}{\sqrt{\theta}}\boldsymbol{I}_{n+1} \end{pmatrix} \in \mathbb{R}^{(n+d+3)\times(n+d+3)}. \tag{4.10}$$

The very compact form of Equation (4.2) allows for a straightforward analysis of the properties of the system, but we first have to reduce the number of unknowns using the compatibility conditions (see Equations (2.19)-(2.21)).

4.2 Incorporation of Compatibility Conditions

Using the notation from Section 2.4, we can solve the compatibility conditions for $d+2$ constant transformed variables $\boldsymbol{\beta_0}$. Inserting the solution for $\boldsymbol{\kappa}$ (compare Equation (2.27)), namely

$$\boldsymbol{\kappa} = \boldsymbol{T}_1 \widehat{\boldsymbol{Q}}^{-1} \boldsymbol{S}^{-1}\boldsymbol{c} + \boldsymbol{T}_2\boldsymbol{\beta}, \tag{4.11}$$

into System (4.2), we obtain a closed PDE system for the $n+1$ variables $\boldsymbol{u} = (\rho, \boldsymbol{v}, \theta, \boldsymbol{\beta})^T$.

Rewriting System (4.2) with the help of the reduced variables, we get

$$\boldsymbol{\Psi}^T \boldsymbol{W} \boldsymbol{A}_{\boldsymbol{\beta}} \boldsymbol{\Lambda}_{\beta} \frac{D}{Dt}\boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{\Psi}^T \boldsymbol{W} \boldsymbol{\Xi}_i \boldsymbol{A}_{\boldsymbol{\beta}} \boldsymbol{\Lambda}_{\beta} \sqrt{\theta} \frac{\partial}{\partial x_i}\boldsymbol{u} = 0 \tag{4.12}$$

with a new columnwise defined system matrix $\boldsymbol{A}_{\boldsymbol{\beta}}$ of which the first $d+2$ columns include the transformed coefficients $\boldsymbol{\beta}$:

$$\boldsymbol{A}_{\boldsymbol{\beta}} = \left(\boldsymbol{\Phi}_{\boldsymbol{\beta}}, -\frac{\partial \boldsymbol{\Phi}}{\partial \xi_1}_{\boldsymbol{\beta}}, \ldots, -\frac{\partial \boldsymbol{\Phi}}{\partial \xi_d}_{\boldsymbol{\beta}}, -d\boldsymbol{\Phi}_{\boldsymbol{\beta}} - \boldsymbol{\Xi}_j \frac{\partial \boldsymbol{\Phi}}{\partial \xi_j}_{\boldsymbol{\beta}}, \boldsymbol{\Phi}\boldsymbol{T}_2 \right) \in \mathbb{R}^{(n+1)\times(n+1)}. \tag{4.13}$$

Additionally, we use the definition of the matrices (for $i, j = 0, \ldots, n$ and $k = 1, \ldots, d$)

$$\begin{aligned} \boldsymbol{\Phi}_{\boldsymbol{\beta}} &= \boldsymbol{\Phi} \left(\boldsymbol{T}_1 \widehat{\boldsymbol{Q}}^{-1} \boldsymbol{S}^{-1} \boldsymbol{c} + \boldsymbol{T}_2 \boldsymbol{\beta} \right), & (4.14) \\ \frac{\partial \boldsymbol{\Phi}}{\partial \xi_k}_{\boldsymbol{\beta}} &= \frac{\partial \boldsymbol{\Phi}}{\partial \xi_k} \left(\boldsymbol{T}_1 \widehat{\boldsymbol{Q}}^{-1} \boldsymbol{S}^{-1} \boldsymbol{c} + \boldsymbol{T}_2 \boldsymbol{\beta} \right), & (4.15) \end{aligned}$$

$$\boldsymbol{\Lambda}_{\beta} = \begin{pmatrix} \frac{1}{\sqrt{\theta}} & & & \\ & \frac{\rho}{\theta} \boldsymbol{I}_d & & \\ & & \frac{\rho}{2\theta^{3/2}} & \\ & & & \frac{\rho}{\sqrt{\theta}} \boldsymbol{I}_{n-d-1} \end{pmatrix}. \tag{4.16}$$

The subscript bold $\boldsymbol{\beta}$ thus denotes a dependence of the corresponding matrix on the unknowns $\boldsymbol{\beta}$.

4.3 Conditions for Hyperbolicity

From the compact version of the PDE system as written in System (4.12), it is easy to derive general conditions for the hyperbolicity of the system. As the diagonal matrix $\boldsymbol{\Xi}_i$ contains only real entries, the system is hyperbolic if the matrix $\boldsymbol{\Psi}^T \boldsymbol{W} \boldsymbol{A}_{\boldsymbol{\beta}} \boldsymbol{\Lambda}_{\beta}$ in front of $\frac{D}{Dt}\boldsymbol{u}$ is invertible. The conditions for hyperbolicity are given by Theorem 1.

Theorem 1 *The semidiscrete System* (4.12) *derived from the transformed Boltzmann Equation* (2.6) *using quadrature-based projections is globally hyperbolic if the following* *conditions hold for the matrices defined above:*

$$\begin{aligned}
&(1)\ \textit{Regularity of matrix } \boldsymbol{\Psi}, \\
&(2)\ \textit{Regularity of matrix } \boldsymbol{W} \textit{ or equivalently } \omega_i \neq 0,\ \forall i = 0, \ldots, n, \\
&(3)\ \textit{Regularity of matrix } \boldsymbol{\Lambda}_\beta, \\
&(4)\ \textit{Regularity of matrix } \boldsymbol{A_\beta} \textit{ or equivalently rank} \boldsymbol{A_\beta} = n+1.
\end{aligned} \tag{4.17}$$

The real-valued generalized eigenvalues λ_k for $k = 0, \ldots, n$ of the system can be derived analytically and read

$$\lambda_k = \sum_{i=1}^{d} n_i \left((\boldsymbol{\xi}_k)_i \sqrt{\theta} + v_i \right), \ \textit{for } k = 0, \ldots, n. \tag{4.18}$$

for unit vector $\boldsymbol{n} \in \mathbb{R}^d$ with $\|\boldsymbol{n}\|_2 = 1$.

Proof If Conditions (4.17) are fulfilled, inversion of the corresponding matrices in System (4.12) leads to

$$\frac{D}{Dt}\boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{\Lambda}_\beta^{-1} \boldsymbol{A_\beta}^{-1} \boldsymbol{\Xi}_i \boldsymbol{A_\beta} \boldsymbol{\Lambda}_\beta \sqrt{\theta} \frac{\partial}{\partial x_i} \boldsymbol{u} = 0, \tag{4.19}$$

so that we have similar to Equation (2.30)

$$\boldsymbol{A}_{sys} = \boldsymbol{\Lambda}_\beta^{-1} \boldsymbol{A_\beta}^{-1} \left(\sqrt{\theta} \sum_{i=1}^{d} n_i \boldsymbol{\Xi}_i \right) \boldsymbol{A_\beta} \boldsymbol{\Lambda}_\beta \tag{4.20}$$

denoting a similarity transformation of the middle part, which leads to real eigenvalues of the system (note the definition of the convective time derivative $\frac{D}{Dt}$ in Equation (2.7))

$$\lambda_k = \sum_{i=1}^{d} n_i \left((\boldsymbol{\xi}_k)_i \sqrt{\theta} + v_i \right), \ \text{for } k = 0, \ldots, n. \tag{4.21}$$

As all eigenvalues λ_k are real (independent of the values $\boldsymbol{\beta}$), System (4.12) is globally hyperbolic.

■

The Conditions (4.17) in Theorem 1 are thus an easy way to prove global hyperbolicity of the resulting system. The following section shows an example for the application of Theorem 1 with Hermite ansatz and test functions and projections using the corresponding Gauss-Hermite quadrature.

5 Globally Hyperbolic System Using Hermite Ansatz and Quadrature

In order to show that the framework developed in Section 4 can be successfully applied, we will give a one-dimensional example with normalized Hermite functions as basis and test functions and Gauss-Hermite quadrature for the projections. We verify the conditions from Theorem 1 and prove global hyperbolicity of the emerging PDE system.

Consider the following expansion of the unknown distribution function for $x, \xi \in \mathbb{R}$

$$
\begin{aligned}
f(t,x,\xi) &= \frac{\rho}{\sqrt{\theta}} \widetilde{f}(t,x,\xi), && (5.1)\\
\widetilde{f}(t,x,\xi) &= \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2} \sum_{i=0}^{n} \kappa_i(t,x) H_i(\xi), && (5.2)
\end{aligned}
$$

for normalized Hermite functions H_n as defined in (A.1). This fits in the framework of Section 4 by setting (compare Equations (3.11),(3.12))

$$
\begin{aligned}
\phi_\alpha(\xi) &= w(\xi) H_\alpha(\xi), && (5.3)\\
w(\xi) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right), && (5.4)\\
\psi_\beta(\xi) &= H_\beta(\xi). && (5.5)
\end{aligned}
$$

For the projections we use Gauss-Hermite quadrature according to Equation (4.1). Quadrature points are the roots of $H_{n+1}(\xi)$ and the weights are chosen as

$$
\omega_i = \frac{\widetilde{\omega}_i}{w(\xi_i)} \quad \text{for } i = 0, \dots, n \tag{5.6}
$$

to account for the weighting function $w(\xi)$ that is included in the ansatz. For $\widetilde{\omega}_i$, see Equation (A.8).

Using the method above it is important to note that the first 3 equations of System (4.12) are linear combinations of the conservation laws, as we use polynomials $\psi_\beta(\xi)$ up to degree 3 for the projections, compare Section 2.1. The conservation laws for mass, momentum and energy are coupled to the other coefficients $\boldsymbol{\beta}$, so that the remaining equations can be seen as a closure for the conservation laws.

Deriving the matrices used in Theorem 1, we can check the conditions for hyperbolicity. The result is given by Theorem 2.

Theorem 2 *Using Hermite basis and test functions as specified in Equations* (5.3)-(5.5) *together with Gauss-Hermite quadrature, the conditions of Theorem 1 are fulfilled and the resulting PDE system is globally hyperbolic.*

Proof We construct the corresponding matrices one after another and show regularity. As matrix $\boldsymbol{\Psi} \in \mathbb{R}^{(n+1)\times(n+1)}$, we have due to Equations (4.5) and (5.5)

$$\boldsymbol{\Psi} = \begin{pmatrix} H_0(\xi_0) & \cdots & H_n(\xi_0) \\ \vdots & \ddots & \vdots \\ H_0(\xi_n) & \cdots & H_n(\xi_n) \end{pmatrix} =: (\boldsymbol{H}_0, \dots, \boldsymbol{H}_n) \tag{5.7}$$

for evaluations of the j-th normalized Hermite polynomial at the discrete quadrature points $\boldsymbol{H}_j \in \mathbb{R}^{n+1}$ and $j = 0, \dots, n$.

This matrix is invertible due to the construction of the quadrature rule, see also [22] and the comments in [17]. The columns $\boldsymbol{H}_j$ are thus all linearly independent.

Evaluating the ansatz functions to construct $\boldsymbol{\Phi}$, we observe according to Equation (5.3)

$$\boldsymbol{\Phi} = diag\left(w(\xi_0), \dots, w(\xi_n)\right) \boldsymbol{\Psi} \tag{5.8}$$

and because of the derivative recursion (see Equation (A.5)) a similar result holds for the matrix $\frac{\partial \boldsymbol{\Phi}}{\partial \xi}$, so that the diagonal matrix with the evaluations of the weighting functions can be factored out of the whole matrix $\boldsymbol{A_\beta}$, see [17] for details.

The matrix $diag\,(w(\xi_0),\dots,w(\xi_n))$ in fact cancels out with the multiplication of $\boldsymbol{W}$, because the diagonal entries of $\boldsymbol{W}$ include the corresponding values in the denominator, see Equation (5.6). We will therefore only consider the basis functions $H_i(\xi)$ in the following and not the multiplication with the weighting function $w(\xi)$.

The weighting matrix

$$\boldsymbol{W} = diag\,(\omega_0,\dots,\omega_n) \in \mathbb{R}^{(n+1)\times(n+1)} \tag{5.9}$$

is also invertible, because the diagonal entries are the quadrature weights as defined in (5.6) and they are guaranteed to be positive for Gauss-Hermite quadrature.

The matrix $\boldsymbol{\Lambda}_\beta$ is regular, if and only if $\rho \neq 0$ and $\theta \neq 0$. We assume this to be true, because Ansatz (2.16) would not make sense otherwise.

The last thing to check is the regularity of the matrix $\boldsymbol{A_\beta}$, which we will do in the following deliberations:

In one spatial dimension, we have three constraints to fulfill (see also Equations (2.10)-(2.12)) from which we get three explicit values for κ_0, κ_1 and κ_2:

$$\kappa_0 = 1, \quad \kappa_1 = 0, \quad \kappa_2 = 0, \tag{5.10}$$

if we evaluate the integrals in the compatibility conditions using Gauss-Hermite quadrature exactly. In terms of Section 2.4, we can identify

$$\boldsymbol{Q} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 \\ 1 & 0 & \sqrt{2} & 0 & \dots & 0 \end{pmatrix} \in \mathbb{R}^{3\times(n+1)} \text{ and } \boldsymbol{c} = (1,0,1)^T. \tag{5.11}$$

This allows for the following decomposition of $\boldsymbol{Q}$:

$$\boldsymbol{Q} = \boldsymbol{S}\boldsymbol{M}\boldsymbol{T}^{-1} \tag{5.12}$$

with

$$\boldsymbol{S} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \tag{5.13}$$

$$\boldsymbol{M} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & \sqrt{2} & 0 & \dots & 0 \end{pmatrix}, \text{ so that } \widehat{\boldsymbol{Q}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}, \tag{5.14}$$

and

$$\boldsymbol{T} = \boldsymbol{I}_{n+1}, \tag{5.15}$$

which leads to a very simple new transformed variable $\widehat{\boldsymbol{\beta}}$ (compare Definition (2.25))

$$\boldsymbol{\kappa} = \boldsymbol{T}\widehat{\boldsymbol{\beta}} = \widehat{\boldsymbol{\beta}}. \tag{5.16}$$

It is then possible to explicitly compute

$$\boldsymbol{\beta_0} = \widehat{\boldsymbol{Q}}^{-1}\boldsymbol{S}^{-1}\boldsymbol{c} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{5.17}$$

On the other hand, this is equivalent to setting $(\boldsymbol{\kappa}_0, \boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2) = (1, 0, 0)$ as shown above.

As $\boldsymbol{T} = \boldsymbol{I}_{n+1}$, the application of $\boldsymbol{T}_2$ to a matrix is equal to the effect of deleting the first three columns of that matrix and a multiplication with $\boldsymbol{T}_1$ is equal to an extraction of the first three columns, compare Equation (2.27).

The matrices in the definition of $\boldsymbol{A}_{\boldsymbol{\beta}}$ from Equation (4.13) are then obtained by (see also Equation (4.14), (4.15) and the remark corresponding to Equation (5.8))

$$\boldsymbol{\Phi}_{\boldsymbol{\beta}} = \boldsymbol{\Phi}\left(\boldsymbol{T}_1\widehat{\boldsymbol{Q}}^{-1}\boldsymbol{S}^{-1}\boldsymbol{c} + \boldsymbol{T}_2\boldsymbol{\beta}\right) = \boldsymbol{H}_0 \cdot 1 + \sum_{i=3}^{n} \boldsymbol{H}_i \kappa_i, \tag{5.18}$$

$$\boldsymbol{\Phi}\boldsymbol{T}_2 = \left(\boldsymbol{H}_3, \dots, \boldsymbol{H}_n\right), \tag{5.19}$$

and with the help of the recursion formula from Equation (A.5) we can derive

$$\frac{\partial \boldsymbol{\Phi}}{\partial \xi} = -\begin{pmatrix} \sqrt{1}H_1(\xi_0) & \cdots & \sqrt{n+1}H_{n+1}(\xi_0) \\ \vdots & \ddots & \vdots \\ \sqrt{1}H_1(\xi_n) & \cdots & \sqrt{n+1}H_{n+1}(\xi_n) \end{pmatrix}. \tag{5.20}$$

The reduced matrix $\frac{\partial \boldsymbol{\Phi}}{\partial \xi_k}_{\boldsymbol{\beta}}$ is then computed in a straightforward way as

$$\begin{aligned} \frac{\partial \boldsymbol{\Phi}}{\partial \xi}_{\boldsymbol{\beta}} &= \frac{\partial \boldsymbol{\Phi}}{\partial \xi}\left(\boldsymbol{T}_1\widehat{\boldsymbol{Q}}^{-1}\boldsymbol{S}^{-1}\boldsymbol{c} + \boldsymbol{T}_2\boldsymbol{\beta}\right) \\ &= -\boldsymbol{H}_1 - \sum_{i=4}^{n} \sqrt{i+1}\boldsymbol{H}_{i+1}\kappa_i \\ &= -\boldsymbol{H}_1 - \sum_{i=4}^{n-1} \sqrt{i+1}\boldsymbol{H}_{i+1}\kappa_i, \end{aligned} \tag{5.21}$$

where we used $\boldsymbol{H}_{n+1} = 0$, as the quadrature points are the roots of H_{n+1}, in the last step.

The term $\Xi\frac{\partial \boldsymbol{\Phi}}{\partial \xi}_{\boldsymbol{\beta}}$ in the third column of the matrix $\boldsymbol{A}_{\boldsymbol{\beta}}$ is derived using the second recursion formula for the derivative in Equation (A.6) as follows:

$$\begin{aligned} \Xi\frac{\partial \boldsymbol{\Phi}}{\partial \xi}_{\boldsymbol{\beta}} &= \sum_{i=0}^{n} \left(\xi_k\ \partial_\xi \Phi_i(\xi_k)\right)\kappa_i \\ &= -\left(\xi_k\ \sqrt{n+1}\Phi_{n+1}(\xi_k)\right)\kappa_n + \sum_{i=0}^{n-1} \left(\xi_k\ \partial_\xi \Phi_i(\xi_k)\right)\kappa_i \\ &= 0 - \sum_{i=0}^{n-1} \sqrt{i+1}\left(\sqrt{i+2}\Phi_{i+2}(\xi_k) + \sqrt{i+1}\Phi_i(\xi_k)\right)\kappa_i. \end{aligned} \tag{5.22}$$

With the help of

$$\boldsymbol{z}_i := \sqrt{i+1}\left(\sqrt{i+2}\boldsymbol{H}_{i+2}(\xi_k) + \sqrt{i+1}\boldsymbol{H}_i(\xi_k)\right) \tag{5.23}$$

we can write the vector $\Xi\frac{\partial\boldsymbol{\Phi}}{\partial\xi}_{\boldsymbol{\beta}}$ as a sum of $\boldsymbol{z}_i\kappa_i$:

$$\Xi\frac{\partial\boldsymbol{\Phi}}{\partial\xi}_{\boldsymbol{\beta}} = -\sum_{i=0}^{n-1}\boldsymbol{z}_i\kappa_i. \tag{5.24}$$

Since $(\kappa_0,\kappa_1,\kappa_2) = (1,0,0)$, we obtain the following equation for the term:

$$\begin{aligned}\Xi\frac{\partial\boldsymbol{\Phi}}{\partial\xi}_{\boldsymbol{\beta}} &= -\sqrt{1}\left(\boldsymbol{H}_2\sqrt{2} + \boldsymbol{H}_0\sqrt{1}\right) - \sum_{i=3}^{n-1}\boldsymbol{z}_i\kappa_i \\ &= -\boldsymbol{H}_0 - \sqrt{2}\boldsymbol{H}_2 - \sum_{i=3}^{n-1}\boldsymbol{z}_i\kappa_i. \end{aligned}\tag{5.25}$$

Now we check the columns of $\boldsymbol{A_\beta}$ for linear independence which will lead to regularity of the matrix.

As discussed above, every column of $\boldsymbol{A_\beta}$ is a linear combination of some $\boldsymbol{H}_i$. We can therefore prove linear independence by checking where each column $\boldsymbol{H}_i$ appears. In total, we must not have more than n columns $\boldsymbol{H}_i$ involved and all columns of $\boldsymbol{A_\beta}$ have to be linearly independent of each other.

(1) $\boldsymbol{\Phi T}_2$ (see Equation (5.19)) has linear independent columns $\boldsymbol{H}_3,\ldots,\boldsymbol{H}_n$,

(2) $-\frac{\partial\boldsymbol{\Phi}}{\partial\xi}_{\boldsymbol{\beta}}$ (see Equation (5.21)) is a linear combination of the columns of $\boldsymbol{\Phi T}_2$ plus an additional $\boldsymbol{H}_1$ and thus linearly independent of $\boldsymbol{\Phi T}_2$,

(3) $\boldsymbol{\Phi_\beta}$ (see Equation (5.18)) is a linear combination of columns of $\boldsymbol{\Phi T}_2$ plus $\boldsymbol{H}_0$ and thus linearly independent of the others,

(4) $-\boldsymbol{\Phi_\beta} - \Xi\frac{\partial\boldsymbol{\Phi}}{\partial\xi}_{\boldsymbol{\beta}}$ (see Equations (5.18) and (5.25)) is a linear combination of columns of $\boldsymbol{\Phi T}_2$ plus $\sqrt{2}\boldsymbol{H}_2$ and thus linearly independent of the others.

Matrix $\boldsymbol{A_\beta}$ therefore has full rank and is regular. Condition (4) of (4.17) is thus fulfilled. The PDE system is hyperbolic for all values $\boldsymbol{\kappa} \in \mathbb{R}^{n+1}$.

■

According to Theorem 1, the eigenvalues in this one-dimensional example read

$$\lambda_k = \xi_k \sqrt{\theta} + v, \text{ for } k = 0, \dots, n. \tag{5.26}$$

We see that the quadrature-based projection method in fact leads to a globally hyperbolic system for the unknown basis coefficients and macroscopic variables.

5.1 Comparison with Existing Models

Compared with exact projections like the Grad ansatz [12] or the method proposed by Cai [7] certain terms change or become zero due to the approximation by the quadrature rule of exactness up to order $2n+1$. A detailed investigation of the single terms is shown in [17].

For the one-dimensional case described above, we can identify the terms of the system's matrices occurring in Equation (4.12) that differ from the formulation in Section (3.2). We rewrite System (4.12) in 1D as

$$\boldsymbol{T} \frac{D}{Dt} \boldsymbol{u} + \boldsymbol{X} \frac{\partial}{\partial x} \boldsymbol{u} = 0 \tag{5.27}$$

and note that the one-dimensional Hermite ansatz with exact integration leads to a different system

$$\widetilde{\boldsymbol{T}} \frac{D}{Dt} \boldsymbol{u} + \widetilde{\boldsymbol{X}} \frac{\partial}{\partial x} \boldsymbol{u} = 0, \tag{5.28}$$

with different matrices $\boldsymbol{T}, \boldsymbol{X}, \widetilde{\boldsymbol{T}}, \widetilde{\boldsymbol{X}} \in \mathbb{R}^{(n+1)\times(n+1)}$.

Subtracting one system from the other, we can define the regularization term $\boldsymbol{R} \in \mathbb{R}^{n+1}$ as follows:

$$\boldsymbol{R} = \left(\boldsymbol{T} - \widetilde{\boldsymbol{T}}\right) \frac{D}{Dt} \boldsymbol{u} + \left(\boldsymbol{X} - \widetilde{\boldsymbol{X}}\right) \frac{\partial}{\partial x} \boldsymbol{u} \tag{5.29}$$

The components of $\boldsymbol{R}$ can be computed analytically and read for our quadrature-based projection method

$$
\begin{aligned}
R_i &= 0, \quad \text{for } i = 0, \ldots, n-2 && (5.30)\\
R_{n-1} &= -\frac{n+1}{2}\sqrt{n}\alpha_n \frac{\rho}{\theta}\partial_x \theta && (5.31)\\
R_n &= -\frac{n+1}{2}\alpha_n \frac{\rho}{\theta^{3/2}} D_t\theta - (n+1)\alpha_n \frac{\rho}{\sqrt{\theta}}\partial_x v - \frac{n+1}{2}\sqrt{n}\frac{\rho}{\theta}\alpha_{n-1} && (5.32)
\end{aligned}
$$

Now we obtain the regularized system (5.27) by adding the vector $\boldsymbol{R}$ to the left-hand side of System (5.28). According to Theorem 2 hyperbolicity is guaranteed with the help of the additional regularization terms that are added to the last two equations according to the definition of R_{n-1} and R_n, see Equations (5.31) and (5.32).

The regularization developed above with the help of quadrature-based projection methods is also different from the regularization proposed by Cai in [7]. In our setting, Cai's additional regularization terms are

$$
\begin{aligned}
R_i^C &= 0, \quad \text{for } i = 0, \ldots, n-1 && (5.33)\\
R_n^C &= -(n+1)\alpha_n \frac{\rho}{\sqrt{\theta}}\partial_x v - \frac{n+1}{2}\sqrt{n}\frac{\rho}{\theta}\alpha_{n-1} && (5.34)
\end{aligned}
$$

In addition to Cai, the quadrature-based projection also changes the second but last equation due to $R_{n-1} \neq 0$, but we have $R_{n-1}^C = 0$. Another term is added to the time derivative part.

Cai's closure apparently uses less terms and only changes the last equation, which was one constraint for the construction of Cai's specific regularization (see [7]). It is important to note that we can recover this version by using the quadrature based projection only for the transport term of the last equation and using exact projections (possibly higher order quadrature rules) for all the other terms. Cai's regularization can thus be seen as a special case of our general approach to use quadrature-based projection methods, especially as our method is not restricted to this type of ansatz functions.

The proof of global hyperbolicity is furthermore very compact compared to the tedious computation of each minor according to Laplace's Formula conducted in [7] and the new framework gives additional insight into the underlying theoretical foundations of the new regularization.

6 Conclusion

6.1 Summary

Starting with the transformation of the velocity variable of the Boltzmann Equation in multiple dimensions, we use a Lagrangian velocity phase space that allows for physical adaptivity of the following discretizations. We have derived the corresponding transformed Boltzmann Equation and developed a constructive method to deal with the compatibility conditions that restrict the basis coefficients to a realizable subset.

The emerging PDE system for the macroscopic variables ρ, v, θ together with the basis expansion coefficients has been shown to be only locally hyperbolic for standard methods like discrete velocity or exact integration as projection operators.

Considering a flexible basis expansion of the distribution function, the general PDE system includes the conservation laws, which result from the projection with the first three monomials using the compatibility conditions. The inclusion of the conservation laws in our model is important for numerical simulations as we can thereby guarantee the conservation of the macroscopic quantities mass, momentum and energy using proper numerical schemes.

With the help of quadrature-based projection methods, we developed a framework in which concrete conditions for global hyperbolicity could be derived for arbitrary ansatz functions. The approach is multi-dimensional and the presented framework also allows for an easy a priori computation of the eigenvalues of the PDE system. Choosing specific basis and test functions together with a projection method, the framework can be used to show global hyperbolicity for different discretization approaches.

In the last Section, we applied the framework to the one-dimensional expansion of the distribution function in Hermite polynomials. For the projections we use Gauss-Hermite quadrature. The proof for global hyperbolicity refers to the hyperbolicity conditions derived with the help of the abstract framework and uses properties of the quadrature rule as well as recursion formulas of the Hermite polynomials. In this example, we showed that quadrature-based projection methods succeed in the hyperbolic approximation of the transformed Boltzmann Equation.

6.2 Further Work

The conceptual work of this paper opens many different areas for further research.

A straightforward next step is the extension of the proof for Hermite ansatz functions to the general d-dimensional setting and to more arbitrary functions and quadrature formulas. It is, however, not yet clear how to construct the appropriate quadrature rules, e.g. for spherical harmonics combined with Laguerre functions in radial direction of a three-dimensional setting.

The techniques of the proof could in principle be used for the generalization to orthogonal basis functions together with their respective Gauss quadrature formulas. The results of this work are planned to be presented in subsequent publications.

A detailed investigation of the resulting PDE system using quadrature-based projections is also in preparation and will be supplemented by numerical examples investigating the approximation quality of the quadrature-based methods with respect to standard methods.

A Appendix

A.1 Hermite Polynomials

We consider orthonormal Hermite polynomials $H_n(\xi)$ derived from the traditional version of the probabilists' Hermite polynomials $\widetilde{H}_n(\xi)$ (see e.g. [1]) as follows:

$$H_n(\xi) := \frac{1}{\sqrt{n!}} \widetilde{H}_n(\xi), \quad \text{for} \quad n \in \mathbb{N}. \tag{A.1}$$

The $H_n(\xi)$ are orthonormal with respect to the scalar product

$$\langle \phi, \psi \rangle_w = \int_{-\infty}^{+\infty} \phi(\xi)\psi(\xi)w(\xi)d\xi, \quad \text{for} \quad w(\xi) := \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2}. \tag{A.2}$$

Using $H_0(\xi) = 0$ the following recursion formulas can be derived from Definition (A.1):

$$\begin{aligned}
\xi H_n(\xi) &= \sqrt{n+1} H_{n+1}(\xi) + \sqrt{n} H_{n-1}(\xi), && \text{(A.3)}\\
H_n'(\xi) &= \sqrt{n} H_{n-1}(\xi), && \text{(A.4)}\\
\frac{d}{d\xi}\Big(H_n(\xi)w(\xi)\Big) &= -w(\xi)\sqrt{n+1} H_{n+1}(\xi), && \text{(A.5)}\\
\xi \frac{d}{d\xi}\Big(H_n(\xi)w(\xi)\Big) &= -w(\xi)\sqrt{n+1}\Big(\sqrt{n+2} H_{n+2}(\xi) + \sqrt{n+1} H_n(\xi)\Big). && \text{(A.6)}
\end{aligned}$$

A.2 Gauss-Hermite Quadrature

Gauss-Hermite quadrature is a special case of Gauss quadrature to approximate integrals of functions by a weighted sum of function evaluations. As integration weight, we again have $w(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2}$. The quadrature formula of order $N \in \mathbb{N}$ reads

$$\int_{-\infty}^{+\infty} f(\xi)w(\xi)d\xi \approx \sum_{i=0}^{N-1} \widetilde{\omega}_i f(\xi_i) \tag{A.7}$$

for *quadrature weights* $\widetilde{\omega}_i$ and *sampling points* ξ_i. In the case of Gauss-Hermite quadrature, the sampling points are the zeros of the N-th Hermite polynomial $H_N(\xi)$ and the corresponding quadrature weights can be calculated by the following formula:

$$\widetilde{\omega}_i = \frac{1}{N H_{N-1}(\xi_i)^2}, \quad \text{for} \quad i = 0, \ldots, N-1. \tag{A.8}$$

It is easy to show that all $\widetilde{\omega}_i$ are finite and positive, the sampling points are furthermore symmetrically placed around zero.

As a special case of Gauss quadrature, Gauss-Hermite quadrature is exact for polynomials up to degree $2N-1$, see [5] or [22] for more details about quadrature formulas.

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