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On new hyperbolic moment models for the Boltzmann equation

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Abstract. *The Boltzmann equation can be used to model flows in the transition or kinetic regime. However, standard moment methods like Grad's approach lack hyperbolicity. Based on recent developments in this field, we have derived a quadrature-based moment method leading to globally hyperbolic and rotationally invariant moment equations. The method is presented as one example of a newly developed operator projection framework. We discuss a special case of the model equations and compare the new model to standard models by analyzing the structure of the equations.*

Keywords: Boltzmann equation; hyperbolicity; moment method

1 VELOCITY DISCRETIZATION OF THE BOLTZMANN EQUATION

We consider hyperbolic moment models for the solution of the Boltzmann Equation (1)

$$\frac{\partial}{\partial t} f(t,\boldsymbol{x},\boldsymbol{c}) + c_i \frac{\partial}{\partial x_i} f(t,\boldsymbol{x},\boldsymbol{c}) = S(f), \tag{1}$$

where we assume a general d-dimensional setting, i.e. we have position $\boldsymbol{x} \in \mathbb{R}^d$ and velocity $\boldsymbol{c} \in \mathbb{R}^d$. As we focus on the transport part, we set $S(f) = 0$ throughout this paper.
We apply a nonlinear transformation of the velocity variable in order to obtain a Lagrangian velocity phase space and exhibit physical adaptivity, which allows for efficient and yet simple discretizations (see [1] for more details):

$$\boldsymbol{\xi}(t,\boldsymbol{x},\boldsymbol{c}) := \frac{\boldsymbol{c} - \boldsymbol{v}(t,\boldsymbol{x})}{\sqrt{\theta(t,\boldsymbol{x})}}. \tag{2}$$

This yields a shift of the microscopic velocity $\boldsymbol{c}$ by the mean velocity $\boldsymbol{v}$ and a scaling by the temperature θ.
Now, we expand the distribution function in a series of basis functions times coefficients around local equilibrium

$$f(t,\boldsymbol{x},\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} f_{\boldsymbol{\alpha}}(t,\boldsymbol{x}) H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{3}$$

using weighted Hermite polynomial basis functions in the transformed velocity variable $\boldsymbol{\xi}$

$$H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = (-1)^{|\boldsymbol{\alpha}|} \frac{d^{\boldsymbol{\alpha}}}{d\boldsymbol{\xi}^{\boldsymbol{\alpha}}} w(\boldsymbol{\xi}), \quad w(\boldsymbol{\xi}) = \frac{1}{\sqrt{2\pi}^d} \exp\left(-\frac{|\boldsymbol{\xi}|^2}{2}\right). \tag{4}$$

In the following, we will explain different methods to derive moments systems given the ansatz above and discuss a 1D example of the equations.

2 HYPERBOLIC MOMENT MODELS

A straightforward procedure to derive moment equations is to multiply Equation (1), including the inserted transformations (2) and the ansatz (3), with test functions, for example the basis functions themselves, and integrate over the whole velocity space. This is known as projection of the equation on the test functions. However, standard projection methods like Grad [2] do not lead to hyperbolic PDE systems. Hyperbolicity is necessary for physical solutions and stability of the simulation. Recently, different methods have been developed to derive globally hyperbolic systems. The first method leads to the Hyperbolic Moment Equations (HME) by Cai et al. [3]. Another new method yields the Quadrature-Based Moment Equations (QBME) by Koellermeier et al. [4]. The methods can be derived in the same framework. Here we want to give a 1D example of QBME and compare to HME and Grad's approach.

Quadrature-Based Moment Equations can be explained using three different approaches: The first approach is to substitute the exact integration over velocity space by Gaussian quadrature formulas (see [4] for details), which changes some terms as the quadrature is not exact for all occurring terms. On the other hand, it is also possible to cut off higher order terms multiple times during the derivation of the equation system which is equivalent to using a quadrature formula. The same result can be obtained by repeated projection of the equations onto a subspace during the derivation (see [5] for details), which is a more general approach and will be explained in the following section.

3 OPERATOR PROJECTION FRAMEWORK FOR MOMENT MODELS

In 1D the discretization in the transformed velocity space leads to an infinite PDE system of the following form

$$\boldsymbol{M}\boldsymbol{D}\partial_t \boldsymbol{u} + \boldsymbol{C}\boldsymbol{M}\boldsymbol{D}\partial_x \boldsymbol{u} = 0, \tag{5}$$

for an unknown infinite dimensional vector $\boldsymbol{u} = (\rho, v, \theta, f_3, f_4, \dots)$ and matrices corresponding to different steps during the derivation of the equation. The matrices $\boldsymbol{M}, \boldsymbol{D}$ and $\boldsymbol{C}$ correspond to operations like multiplication with ξ or c and derivative with respect to ξ applied to the basis functions, according to the transformed version of the Boltzmann equation (see [1] for the whole equation).

Note that the variables f_0, f_1, f_2 have been eliminated using the definitions of the macroscopic variables ρ, v, θ (see [4] for these so-called *compatibility conditions*).

In order to get a finite set of equations we apply projection operators (see [5] for details). For $M+1$ equations the simplest subspace projection operator $\boldsymbol{P}_M$ is given as

$$\boldsymbol{P}_M = (\boldsymbol{I_{M+1}}, \boldsymbol{0}) \in \mathbb{R}^{M+1\times\infty}, M \in \mathbb{N} \tag{6}$$

and can be interpreted as a cut-off of higher order terms which mimics the effect of a Gaussian quadrature rule of respective order. A projection applied to matrices is then defined as $(\cdot)_M := \boldsymbol{P}_M (\cdot) \boldsymbol{P}_M^T$ and for vectors as $(\cdot)_M := \boldsymbol{P}_M (\cdot)$ respectively.

Depending on the subspace projection procedure, different models can be derived:

- **Grad's Equations**
$$(\boldsymbol{M}\boldsymbol{D})_M \partial_t \boldsymbol{u}_M + (\boldsymbol{C}\boldsymbol{M}\boldsymbol{D})_M \partial_x \boldsymbol{u}_M = 0, \tag{7}$$

- **Hyperbolic Moment Equations** (HME)
$$(\boldsymbol{M}\boldsymbol{D})_M \partial_t \boldsymbol{u}_M + \boldsymbol{C}_M (\boldsymbol{M}\boldsymbol{D})_M \partial_x \boldsymbol{u}_M = 0, \tag{8}$$

- **Quadrature-Based Moment Equations** (QBME)
$$\boldsymbol{M}_M\boldsymbol{D}_M\partial_t \boldsymbol{u}_M + \boldsymbol{C}_M\boldsymbol{M}_M\boldsymbol{D}_M\partial_x \boldsymbol{u}_M = 0. \tag{9}$$

We see, that the different models only differ in the way the projections are applied. This leads to different terms in front of the derivatives as we will see in the next section.

4 MODEL COMPARISON

4.1 General Properties

The most important property of the model equations is hyperbolicity as explained in Section 2. The concise procedure of the operator projection leads to globally hyperbolic equations in the case of HME and QBME (see [5] for details) in contrast to the conditionally hyperbolic Grad system. This is valid for arbitrary orders of the expansion and as well as in the multi-dimensional case (see [6] for a straightforward multi-dimensional QBME example).

Furthermore, all systems exhibit rotational invariance. This is particularly interesting for the QBME system, as a standard quadrature approach would spoil this property. But the operator projection framework also works in cases, where there is no rotationally invariant Gaussian quadrature rule and therefore the resulting system is always rotationally invariant.
Due to the projections, the HME and QBME equation systems have some different terms. However, in case of HME only the equations corresponding to the largest degree of the basis functions are changed. The QBME also changes the equations corresponding to the second largest degree due to the additional projection in Equation (9). It is important to say that an arbitrary number of equations can be recovered exactly by choosing a large number of equations in total as in the following example.

4.2 A Five Moment Case

We write the different models in the following form to allow for comparison:

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}\partial_x \boldsymbol{u}_M = 0, \tag{10}$$

where the system matrix $\boldsymbol{A}$ depends on the model. We can analytically derive this matrix for arbitrary M, but here we exemplify a 1D 5-moment case, so it is $M = 4$. The different models result in the following system matrices:

$$\boldsymbol{A}_{\text{Grad}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v \end{pmatrix} \quad \boldsymbol{A}_{\text{HME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v \end{pmatrix} \quad \boldsymbol{A}_{\text{QBME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} - \frac{10f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15f_4}{\rho\theta} & v \end{pmatrix}$$

where terms written in red represent changes with respect to the standard Grad model that originate from the operator projection procedure.
It is widely known that Grad's method is only locally hyperbolic around equilibrium, compare Figure 1. For large deviations from equilibrium (equilibrium is represented by $f_3 = f_4 = 0$), the system of equations is thus not hyperbolic anymore and nonphysical solutions arise or strong numerical oscillations lead to instabilities of the simulations. On the other hand, it can be shown that with the small changes in the system matrix for HME and

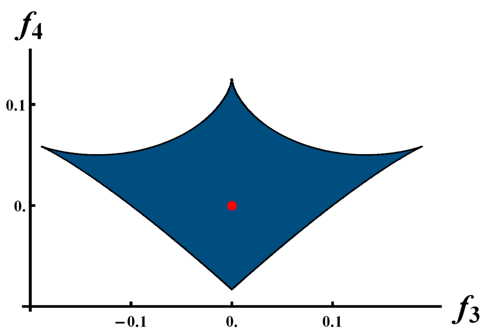

Figure 1: Hyperbolicity region around equilibrium for Grad's method.

QBME, the system becomes globally hyperbolic, see [5]. It is also important to note, that only the last or the last two equations change. The mass, momentum and energy equations thus remain the same as for the Grad case. Only the higher order moments are obtained by different equations.
Rewriting System (10) in terms of the *convective moments* $m_j := \int_{-\infty}^{\infty} f(\xi)\, \xi^j \, d\xi$ and choosing $\boldsymbol{m} = (m_0, \ldots, m_M)$, we obtain a so-called companion matrix for Grad's system. It has the following structure:

$$\partial_t \boldsymbol{m} + \boldsymbol{M}_{\text{Grad}}\, \partial_x \boldsymbol{m} = 0, \quad \boldsymbol{M}_{\text{Grad}} = \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \\ * & \cdots & \cdots & * \end{pmatrix}, \tag{11}$$

where only the last row of $\boldsymbol{M}_{\text{Grad}}$ contains many none zero entries. As the system matrix depends on the moments, we write $\boldsymbol{M}_{\text{Grad}} = \boldsymbol{M}_{\text{Grad}}(\boldsymbol{m})$.
It can be shown that in case of HME, the companion matrix is simply the Grad matrix evaluated at equilibrium, especially for our case $M = 4$.

$$\boldsymbol{M}_{\text{HME}}(\boldsymbol{m}) = \boldsymbol{M}_{\text{Grad}}(\boldsymbol{m}^{eq}), \tag{12}$$

so that the system matrix evaluates to

$$\boldsymbol{M}_{\text{HME}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ v^5 - 10v^3\theta + 15v\theta^2 & -5v^4 + 30v^2\theta - 15\theta^2 & 10v^3 - 30v\theta & -10v^2 + 10\theta & 5v \end{pmatrix}, \tag{13}$$

where $\boldsymbol{m}^{eq}$ with $f_3 = \ldots = f_M = 0$ denotes equilibrium. The hyperbolicity of HME thus originates from the fact, that the convective system matrix is just an evaluation of the standard Grad matrix in equilibrium, where the Grad system is always hyperbolic and the system matrix does not depend on the higher order coefficients any more.

Interestingly, QBME represent a linear deviation from Grad's equilibrium and is still hyperbolic:

$$\boldsymbol{M}_{\text{QBME}}(\boldsymbol{m}) = \boldsymbol{M}_{\text{Grad}}(\boldsymbol{m}^{eq}) + \widetilde{\boldsymbol{M}} \cdot f_M, \tag{14}$$

for some matrix $\widetilde{\boldsymbol{M}}$ depending only on equilibrium values and with only the last two rows containing non-zero entries and defined as follows

$$\widetilde{\boldsymbol{M}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{60}{\rho} - \frac{60v^2}{\theta\rho} & \frac{120v}{\theta\rho} & -\frac{60}{\theta\rho} & 0 & 0 \\ \frac{300v}{\rho} - \frac{300v^3}{\theta\rho} & -\frac{60}{\rho} + \frac{660v^2}{\theta\rho} & -\frac{420v}{\theta\rho} & \frac{60}{\theta\rho} & 0 \end{pmatrix}. \tag{15}$$

We can therefore expect to describe much more complex flow situations with the QBME system, as we do not evaluate the Grad system matrix exactly in equilibrium but use a linear deviation from equilibrium. QBME can thus be seen as an extension of the HME and Grad system respectively. Note that this is also true for $M > 4$, but the case $M = 4$ is especially relevant as it is the smallest system that includes mass, momentum and energy conservation.

5 CONCLUSION

We have presented the operator projection framework that can be used to derive hyperbolic moment models for the Boltzmann equation. The application of a dedicated projection procedure is necessary as standard projection techniques only yield conditionally hyperbolic PDE systems possibly lacking physical solutions. The comparison of three different hyperbolic moment systems led to the interpretation of the QBME as a linear deviation from Grad's equilibrium. This is a new result and justifies a more detailed investigation of the new method. Next steps will be the implementation of special numerical algorithms to solve the (non-conservative) PDE systems and the comparison of the results in different flow regimes and for different test cases.

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