On the Numerical Solution of the Boltzmann Equation Using Quadrature-Based Projection Methods

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Velocity Discretization of the Boltzmann Equation

We consider hyperbolic moment models for the solution of the Boltzmann Equation

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

where we assume a d-dimensional setting, i.e. we have position $\boldsymbol{x} \in \mathbb{R}^d$ and velocity $\boldsymbol{c} \in \mathbb{R}^d$. 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:

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

We expand the distribution function in a series around local equilibrium

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

using weighted Hermite polynomial basis functions

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

In the following, we will explain different methods and give a 1D example of the equations.

Hyperbolic Moment Models

Standard projection methods like Grad [3] do not lead to hyperbolic PDE systems. Recently, different methods have been developed to derive globally hyperbolic systems:

- Hyperbolic Moment Equations (HME) by Cai et al. [4],
- Quadrature-Based Moment Equations (QBME) by Koellermeier et al. [1].

Quadrature-Based Moment Equations

Quadrature-Based Moment Equations can be explained using three different approaches:

- Gaussian quadrature formulas instead of exact integration (see [1] for details),
- multiple cut-offs of higher order terms during derivation,
- repeated projection of the equations onto a subspace during derivation (see [2] for details).

Operator Projection Framework

The discretization in the transformed velocity space leads to an infinite PDE system of the following form

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

for an unknown infinite vector $\boldsymbol{u} = (\rho, v, \theta, f_3, f_4, \ldots)$ and different matrices corresponding to different steps during the derivation of the equation.
In order to get a finite set of equations we apply projection operators (see [2] for details). The subspace projection operator $\boldsymbol{P}_M$ is given as

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

and can be interpreted as a cut-off of higher order terms.
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**

$$(\boldsymbol{M}\boldsymbol{D})_M \partial_t \boldsymbol{u}_M + (\boldsymbol{C}\boldsymbol{M}\boldsymbol{D})_M \partial_x \boldsymbol{u}_M = 0,$$

- **Hyperbolic Moment Equations** (HME)

$$(\boldsymbol{M}\boldsymbol{D})_M \partial_t \boldsymbol{u}_M + \boldsymbol{C}_M (\boldsymbol{M}\boldsymbol{D})_M \partial_x \boldsymbol{u}_M = 0,$$

- **Quadrature-Based Moment Equations** (QBME)

$$\boldsymbol{M}_M \boldsymbol{D}_M \partial_t \boldsymbol{u}_M + \boldsymbol{C}_M \boldsymbol{M}_M \boldsymbol{D}_M \partial_x \boldsymbol{u}_M = 0.$$

Properties of the Model Equations

The resulting system of equations for QBME exhibits various desirable properties:

- global hyperbolicity,
- exactness of the first $M-1$ equations,
- rotational invariance even for the d-dimensional case.

Comparison of the Equation Systems

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

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

where the system matrix $\boldsymbol{A}$ depends on the model. For the 1D 5-moment case $M = 4$ the different models result in the following system matrices:

Grad

$$\begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 2 & 0 & 0 \\ 0 & \theta & v & \frac{3}{\rho} & 0 \\ 0 & 4f_3 & \rho\theta & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & 3f_3 & \theta & v \end{pmatrix}$$

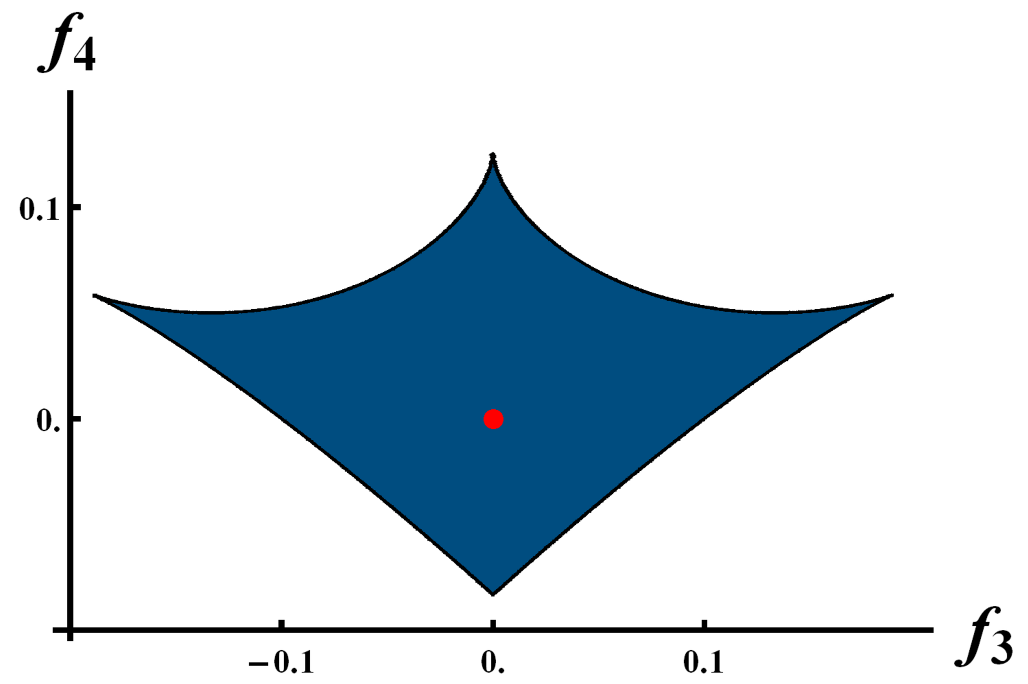
HME

$$\begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 2 & 0 & 0 \\ 0 & \theta & v & \frac{3}{\rho} & 0 \\ 0 & 4f_3 & \rho\theta & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -2f_3 & \theta & v \end{pmatrix}$$

QBME

$$\begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 2 & 0 & 0 \\ 0 & \theta & v & \frac{3}{\rho} & 0 \\ 0 & 4f_3 & \rho\theta - \frac{20 f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -2f_3 & \theta + \frac{15 f_4}{\rho\theta} & v \end{pmatrix}$$

It is widely known that Grad's method is only locally hyperbolic around equilibrium:



Hyperbolicity region around equilibrium for Grad's method.

It can be shown that with the small changes in the system matrix for HME and QBME, the system becomes **globally hyperbolic**.

Rewriting the system in terms of the convective moments $m_j = \int_{-\infty}^{\infty} f(t, x, \xi)\, \xi^j d\xi$ 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:

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

As $\boldsymbol{M}_{\text{Grad}}$ 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:

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

where $\boldsymbol{m}^{eq}$ with $f_3 = \ldots = f_M = 0$ denotes equilibrium.
Additionally, QBME represent a linear deviation from Grad's equilibrium:

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

for some matrix $\widetilde{\boldsymbol{M}}$ with only the last two rows containing non-zero entries.

Next Steps

- Working with new projection operators to obtain more advanced model equations.
- Extension of a numerical solver for the non-conservative QBME and investigation of approximation properties compared to Grad and HME.

References

[1] J. Koellermeier, R. P. Schaerer and M. Torrilhon. A Framework for Hyperbolic Approximation of Kinetic Equations Using Quadrature-Based Projection Methods, *Kinet. Relat. Mod.* **7(3)** (2014), 531–549

[2] Y. Fan, J. Koellermeier, J. Li, R. Li and M. Torrilhon. Model Reduction of Kinetic Equations by Operator Projection, *submitted*

[3] H. Grad. On the kinetic theory of rarefied gases, *Comm. Pure Appl. Math.*, **2** (1949), 331–407.

[4] Z. Cai, Y. Fan and R. Li. Globally hyperbolic regularization of Grad's moment system, *Comm. Pure Appl. Math.*, **67** (2014), 464–518.