First-order continuous- and discontinuous-Galerkin moment models for a linear kinetic equation: model derivation and realizability theory

Florian Schneider\textsuperscript{a}, Tobias Leibner\textsuperscript{b}

\textsuperscript{a}Fachbereich Mathematik, TU Kaiserslautern, Erwin-Schrödinger-Str., 67663 Kaiserslautern, Germany, schneider@mathematik.uni-kl.de
\textsuperscript{b}Fachbereich Mathematik und Informatik, WWU Münster, Einsteinstrasse 62, 48149 Münster, tobias.leibner@uni-muenster.de

Abstract

We provide two new classes of moment models for linear kinetic equations in slab and three-dimensional geometry. They are based on classical finite elements and low-order discontinuous-Galerkin approximations on the unit sphere. We investigate their realizability conditions and other basic properties. Numerical tests show that these models are more efficient than classical full-moment models in a space-homogeneous test, when the analytical solution is not smooth.

Keywords: moment models, minimum entropy, kinetic transport equation, continuous Galerkin, discontinuous Galerkin, realizability

1. Introduction

Moment closures are a type of (non-linear) Galerkin approximation typically used in the context of kinetic transport equations. An infinite set of moment equations is defined by taking velocity- or phase-space averages with respect to some basis of this space. A reduced description of the kinetic density is then achieved by truncating this hierarchy of equations at some finite order. Unfortunately, in most cases, the remaining equations are not closed and require information from the equations which were removed. The specification of this information, the so-called moment closure problem, distinguishes different types of moment models. In the context of linear radiative transport, the standard spectral method is commonly referred to as the \( P_N \) closure \cite{P5}, where \( N \) is the degree of the highest-order moments in the model. It is basically a straightforward Galerkin approximation on the unit sphere. The \( P_N \) method is powerful and simple to implement, but does not take into account that the original function to be approximated, the kinetic density, must be non-negative. This often leads to physically meaningless solutions, as the \( P_N \) solutions can, e.g., contain negative values for the local particle density.

In the context of radiative transport, entropy-based moment closures, the so-called \( M_N \) models \cite{M1}, have all the properties one would desire in a moment method, namely positivity of the underlying kinetic density,\footnote{Positivity is actually not gained for every entropy-based moment closure but is in fact a property of those models derived from important, physically relevant entropies.} hyperbolicity of the closed system of equations, and entropy dissipation \cite{M4}. Although there have been a lot of theoretical investigations about minimum-entropy models throughout the last fifty years, see, e.g., \cite{M5, M6, M7, M8, M9, M10}, practical implementations were limited to very low orders (e.g. \( N = 1 \)) \cite{M11, M12, M13, M14} as, generally, \( M_N \) models are too expensive and more difficult to implement compared to, e.g.,
direct Monte Carlo simulations. The reason for this is that they require the (numerical) solution of a non-linear optimization problem at every point on the space-time grid, which tends to be very time-consuming. However, there has been renewed interest in the models recently due to their inherent parallelizability [3, 25].

The property of positivity implies that the system of moment equations only evolves on the set of so-called realizable moments. Realizable moments are simply those moments associated with positive densities, and the set of these moments forms a convex cone which is a strict subset of all moment vectors [4, 14].

To increase the accuracy of the $M_N$ models while maintaining the lower cost for small moment order $N$, partial moment and mixed moment models have been developed [20–22, 41, 48, 50]. They are based on a partition of the velocity space while keeping the moment order fixed, similar to some $h$-refinement for, e.g., finite element approximations [5].

While the partial moment models have been extensively studied for special cases (like half- or quarter-moments in one or two dimensions), we are unaware of any general investigation, especially in the fully three-dimensional setup.

In this paper, which is the first of two parts, we provide realizability theory for general first-order (piece-wise discontinuous) partial moments in one- and three-dimensional geometry, as well as their continuous analogue (compare to the finite element method). An extensive numerical study using a second-order realizability-preserving scheme will be done in the second part. Here, the required realizability can cause problems for numerical methods, as standard high-order numerical solutions (in space and time) can destroy this property if not handled very carefully [4, 12, 39, 44, 46, 49, 54].

This paper is organized as follows. First, the transport equation and its moment approximations are given. Then, the available realizability theory is derived in one and three dimensions, followed by some numerical investigations of the approximation properties of our models. Finally, conclusions and an outlook on future work is given.

2. Modeling

We consider the linear transport equation

$$\frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \sigma_a \psi = \sigma_s \mathcal{C}(\psi) + Q,$$

which describes the density of particles with speed $\mathbf{\Omega} \in S^2$ at position $x \in X \subseteq \mathbb{R}^3$ and time $t \in T = [0, t_f]$ under the events of scattering (proportional to $\sigma_s(t, x)$), absorption (proportional to $\sigma_a(t, x)$) and emission (proportional to $Q(t, x, \mathbf{\Omega})$). Collisions are modeled using the BGK-type collision operator

$$\mathcal{C}(\psi) = \int_{S^2} K(\mathbf{\Omega}', \mathbf{\Omega}) \psi(t, x, \mathbf{\Omega}') \, d\mathbf{\Omega}' - \int_{S^2} K(\mathbf{\Omega}, \mathbf{\Omega}') \psi(t, x, \mathbf{\Omega}) \, d\mathbf{\Omega}'. \quad (2.1b)$$

The collision kernel $K$ is assumed to be strictly positive, symmetric (i.e. $K(\mathbf{\Omega}, \mathbf{\Omega}') = K(\mathbf{\Omega}', \mathbf{\Omega})$) and normalized to $\int_{S^2} K(\mathbf{\Omega}', \mathbf{\Omega}) \, d\mathbf{\Omega}' \equiv 1$. A typical example is isotropic scattering, where $K(\mathbf{\Omega}, \mathbf{\Omega}') \equiv \frac{1}{|S^2|} = \frac{1}{4\pi}$.

The equation is supplemented with initial condition and Dirichlet boundary conditions:

$$\psi(0, x, \mathbf{\Omega}) = \psi_{t=0}(x, \mathbf{\Omega}) \quad \text{for } x \in X, \mathbf{\Omega} \in S^2,$$

$$\psi(t, x, \mathbf{\Omega}) = \psi_b(t, x, \mathbf{\Omega}) \quad \text{for } t \in T, x \in \partial X, \mathbf{n} \cdot \mathbf{\Omega} < 0 \quad (2.1c)$$

where $\mathbf{n}$ is the outward unit normal vector in $x \in \partial X$.

Parameterizing $\mathbf{\Omega}$ in spherical coordinates we obtain

$$\mathbf{\Omega} = \left( \sqrt{1-\mu^2} \cos(\varphi), \sqrt{1-\mu^2} \sin(\varphi), \mu \right)^T = (\Omega_x, \Omega_y, \Omega_z)^T, \quad (2.2)$$
where \( \varphi \in [0, 2\pi] \) is the azimuthal and \( \mu \in [-1, 1] \) the cosine of the polar angle.

**Remark 2.1.** Another possibility to model collisions would be the Laplace-Beltrami operator on the unit sphere,

\[
\Delta_{\Omega} \psi = \frac{d}{d\mu} \left( (1 - \mu^2) \frac{d\psi}{d\mu} \right) + \frac{1}{1 - \mu^2} \frac{d^2\psi}{d\varphi^2}.
\]  

It arises, for example, as the result of a non-lectural analysis of the Boltzmann equation under the assumption of small energy loss and deflection, and forward-peaked scattering in the context of electron transport \[23, 26, 40\].

**Definition 2.2.** The vector of functions \( \mathbf{b} : S^2 \to \mathbb{R}^n \) consisting of \( n \) basis functions \( b_i \), \( i = 1, \ldots, n \), of maximal order \( N \) in \( \Omega \) is called a maximal basis. The so-called moments \( \mathbf{u} = (u_0, \ldots, u_n)^T \) of a given distribution function \( \psi \) are then defined by

\[
\mathbf{u} = \int_{S^2} \mathbf{b} \psi \, d\Omega =: \langle \mathbf{b} \rangle \psi,
\]  

where the integration is performed component-wise.

Furthermore, the quantity \( p = \rho(\mathbf{u}) := \langle \psi \rangle \) is called the local particle density. Additionally, \( \mathbf{u}_{iso} = \langle \mathbf{b} \rangle \) is called the isotropic moment.

Equations for \( \mathbf{u} \) can then be obtained by multiplying (2.1) with \( \mathbf{b} \) and integration over \( S^2 \), yielding

\[
\langle \mathbf{b} \partial_t \psi \rangle + \langle \mathbf{b} \nabla_x \cdot \Omega \psi \rangle + \langle \mathbf{b} \sigma_a \psi \rangle = \sigma_s \langle \mathbf{b} \mathcal{C}(\psi) \rangle + \langle \mathbf{b} \mathcal{Q} \rangle.
\]

Collecting known terms, and interchanging integration and differentiation where possible, the moment system has the form

\[
\partial_t \mathbf{u} + \langle \mathbf{b} \nabla_x \cdot \Omega \psi \rangle + \sigma_a \mathbf{u} = \sigma_s \langle \mathbf{b} \mathcal{C}(\psi) \rangle + \langle \mathbf{b} \mathcal{Q} \rangle.
\]  

Depending on the choice of \( \mathbf{b} \) the terms \( \langle \Omega_a \mathbf{b} \psi \rangle \), \( \langle \Omega_b \mathbf{b} \psi \rangle \), \( \langle \Omega_c \mathbf{b} \psi \rangle \), and in some cases even \( \langle \mathbf{b} \mathcal{C}(\psi) \rangle \), cannot be given explicitly in terms of \( \mathbf{u} \). Therefore an ansatz \( \hat{\psi} \) has to be made for \( \psi \) closing the unknown terms. This is called the moment-closure problem.

In this paper the ansatz density \( \hat{\psi} \) is reconstructed from the moments \( \mathbf{u} \) by minimizing the entropy-functional

\[
\mathcal{H}(\psi) = \langle \eta(\psi) \rangle
\]  

under the moment constraints

\[
\langle \mathbf{b} \psi \rangle = \mathbf{u}.
\]  

The kinetic entropy density \( \eta : \mathbb{R} \to \mathbb{R} \) is strictly convex and twice continuously differentiable and the minimum is simply taken over all functions \( \psi = \psi(\Omega) \) such that \( \mathcal{H}(\psi) \) is well defined. The obtained ansatz \( \hat{\psi} = \hat{\psi}_\mathbf{u} \), solving this constrained optimization problem, is given by

\[
\hat{\psi}_\mathbf{u} = \arg\min_{\psi : \eta(\psi) \in L_1} \{ \langle \eta(\psi) \rangle : \langle \mathbf{b} \psi \rangle = \mathbf{u} \}.
\]  

This problem, which must be solved over the space-time mesh, is typically solved through its strictly convex finite-dimensional dual,

\[
\mathbf{a}(\mathbf{u}) := \arg\min_{\mathbf{\alpha} \in \mathbb{R}^n} \langle \eta_s(\mathbf{b}^T \mathbf{\alpha}) \rangle - \mathbf{u}^T \mathbf{\alpha},
\]  

where \( \eta_s \) is the Legendre dual of \( \eta \). The first-order necessary conditions for the multipliers \( \mathbf{a}(\mathbf{u}) \) show that the solution to (2.9) has the form

\[
\hat{\psi}_\mathbf{u} = \eta_s' \left( \mathbf{b}^T \mathbf{a}(\mathbf{u}) \right),
\]
where $\eta_r$ is the derivative of $\eta_r$.

This approach is called the minimum-entropy closure [34]. The resulting model has many desirable properties: symmetric hyperbolicity, bounded eigenvalues of the directional flux Jacobian and the direct existence of an entropy-entropy flux pair (compare [34], [17]).

The kinetic entropy density $\eta$ can be chosen according to the physics being modeled. We follow [25, 34] and use Maxwell-Boltzmann entropy

$$\eta(\psi) = \psi \log(\psi) - \psi,$$

thus $\eta_r(\psi) = \eta_r(\psi) = \exp(\psi)$. This entropy is used for non-interacting particles as in an ideal gas.

Substituting $\psi$ in (2.5) with $\hat{\psi}u$ yields a closed system of equations for $u$:

$$\partial_t u + \partial_x \left\langle \Omega_x b \hat{\psi} u \right\rangle + \partial_y \left\langle \Omega_y b \hat{\psi} u \right\rangle + \partial_z \left\langle \Omega_z b \hat{\psi} u \right\rangle + \sigma_a u = \sigma_s \left\langle b C \left( \hat{\psi} u \right) \right\rangle + \langle b Q \rangle.$$  (2.11)

Remark 2.3. Note that using the entropy $\eta(\psi) = \frac{1}{2} \psi^2$ the linear ansatz

$$\hat{\psi} u = b^T \alpha(u)$$

is obtained, leading to standard continuous/discontinuous-Galerkin approaches. In this case, the optimization problem can be solved analytically yielding

$$\alpha(u) = M^{-1} u$$

where $M_{ij} = \langle b_i b_j \rangle$ [2, 47]. If the angular basis is chosen as spherical harmonics of order $N$, (2.11) turns into the classical $P_N$ model [7, 9, 51].

For convenience, we write (2.11) in the standard form of a non-linear hyperbolic system of partial differential equations:

$$\partial_t u + \partial_x F_1(u) + \partial_y F_2(u) + \partial_z F_3(u) = s(u),$$  (2.14)

where

$$F_1(u) = \left\langle \Omega_x b \hat{\psi} u \right\rangle, \quad F_2(u) = \left\langle \Omega_y b \hat{\psi} u \right\rangle, \quad F_3(u) = \left\langle \Omega_z b \hat{\psi} u \right\rangle \in \mathbb{R}^n,$$

$$s(u) = \sigma_s \left\langle b C \left( \hat{\psi} u \right) \right\rangle + \langle b Q \rangle - \sigma_a u.$$  (2.15a)

Due to the notational complexity of the full three-dimensional setting we will first derive the models in slab geometry, which is a projection of the sphere onto the $z$-axis [51]. The transport equation under consideration then has the form

$$\partial_t \psi + \mu \partial_z \psi + \sigma_a \psi = \sigma_s C(\psi) + Q, \quad t \in T, z \in X, \mu \in [-1, 1].$$  (2.16)

The shorthand notation $\langle \cdot \rangle = \int_{-1}^{1} \cdot \, d\mu$ then denotes integration over $[-1, 1]$ instead of $S^2$. Finally, the moment system is given by

$$\partial_t u + \partial_z \left\langle \mu b \hat{\psi} u \right\rangle + \sigma_a u = \sigma_s \left\langle b C \left( \hat{\psi} u \right) \right\rangle + \langle b Q \rangle.$$  (2.17)
3. Angular bases in slab geometry

3.1. Full moments

As in a standard Galerkin approach, a polynomial basis on \([-1, 1]\) is a reasonable choice for an angular basis. It is denoted by the symbol \(b = f_N\). There are two obvious options for \(f_N\), resulting in equivalent models:

- the monomial basis
  \[ f_N = (1, \mu, \ldots, \mu^N)^T; \]  
  \( (3.1) \)
- the Legendre basis
  \[ f_N = (P_0^0, P_1^0, P_2^0, \ldots, P_N^0)^T \]  
  \( (3.2) \)

with the Legendre polynomials \(P_l^l, l = 0, \ldots, N\).

The monomial basis is attractive due to its simplicity, especially for realizability considerations \([15]\). On the other hand, the Legendre polynomials form an orthogonal basis of \(L^2([-1, 1], \mathbb{R})\) and are additionally eigenfunctions of the isotropic-scattering operator \(C\) if \(K \equiv \frac{1}{2}\), diagonalizing the source-term.

3.2. Piecewise-linear angular basis (Hat functions)

As mentioned above, the method of moments is nothing else than a Galerkin approximation of the kinetic equation \((2.16)\). The full-moment \(P_N\) model is equivalent to the finite element method (FEM) with fixed angular mesh-size and increasing order (this method is often referred to as the \(p\)-version, related to the maximal order \(p\) of the polynomial basis \([5]\)). Another natural approach is the standard finite element method, where the polynomial order is fixed but the angular mesh is refined (often referred to as the \(h\)-version, where \(h\) denotes the mesh-size \([5]\)).

Given a set of \(n\) angular “grid” points \(-1 = \mu_1 < \mu_2 < \ldots < \mu_{n-1} < \mu_n = 1\) and corresponding intervals \(I_j = (\mu_j, \mu_{j+1}), j = 1, \ldots, k = n - 1\), the piecewise-linear basis functions \(h_n = (h_1, \ldots, h_n)^T\) (hat functions or B-splines of first order \([17]\)) are defined as

\[
h_i(\mu) = \begin{cases} 
\llbracket_{\mu_i, \mu_{i+1}} \frac{\mu - \mu_{i+1}}{\mu_i - \mu_{i+1}} & \text{if } i = 1, \\
\llbracket_{\mu_{i-1}, \mu_i} \frac{\mu - \mu_{i-1}}{\mu_i - \mu_{i-1}} + \llbracket_{\mu_i, \mu_{i+1}} \frac{\mu - \mu_{i+1}}{\mu_i - \mu_{i+1}} & \text{if } 1 < i < n, \\
\llbracket_{\mu_{i-1}, \mu_i} \frac{\mu - \mu_{i-1}}{\mu_i - \mu_{i-1}} & \text{if } i = n.
\end{cases} \]  
\( (3.3a) \)

Some basis functions of \(h_5\) with equidistant nodes are shown exemplarily in Figure 1.

The isotropic moment vector is given by \(u_{\text{iso}} = \frac{1}{4} \left( \mu_2 - \mu_1, \mu_3 - \mu_1, \ldots, \mu_{i-1} - \mu_{i-2}, \mu_{n-1} - \mu_{n-2} \right)^T\).

One of the most important properties of the hat functions is the following.

Lemma 3.1. The hat functions form a partition of unity, i.e. \( \sum_{i=1}^{n} h_i \equiv 1 \).

Corollary 3.2.

(a) The full moment basis \(f_1\) is equivalent to \(h_2\) (with \(\mu_1 = -1\) and \(\mu_2 = 1\)).

(b) The mixed moment basis \([23, 48]\) \(m_1\) is equivalent to \(h_3\) (with \(\mu_1 = -1, \mu_2 = 0\) and \(\mu_3 = 1\)).
Proof. The claim follows immediately, observing that

(a) \( f_1 = (1, \mu)^T = (h_1 + h_2, -h_1 + h_2)^T \),

(b) \( m_1 = (1, [0,1] \mu, [1,0] \mu)^T = (h_1 + h_2 + h_3, h_3, -h_1)^T \).

\[ \quad \]

Definition 3.3. The resulting linear (compare (2.12)) and nonlinear model (compare (2.10)) will be called HFP\(_n\) and HFM\(_n\), respectively.

Exemplarily, the HFM\(_n\) integrals are given by

\[
\langle \hat{\psi}_u h_i \rangle_{I_j} = \frac{(e^{\alpha_i - 1} - e^{\alpha_i}) (\mu_i - \mu_{i-1})}{(\alpha_{i-1} - \alpha_i)^2} - \frac{e^{\alpha_i} (\mu_i - \mu_{i-1})}{\alpha_{i-1} - \alpha_i} = (\mu_i - \mu_{i-1}) e^{\alpha_i} \sum_{l=2}^{\infty} \frac{(\alpha_{i-1} - \alpha_i)^{l-2}}{l!}
\]

\[
\langle \hat{\psi}_u h_i \rangle_{I_j} = \frac{(e^{\alpha_i} - e^{\alpha_{i+1}}) (\mu_i - \mu_{i+1})}{(\alpha_i - \alpha_{i+1})^2} - \frac{e^{\alpha_i} (\mu_i - \mu_{i+1})}{\alpha_i - \alpha_{i+1}} = (\mu_{i+1} - \mu_i) e^{\alpha_i} \sum_{l=2}^{\infty} \frac{(\alpha_{i+1} - \alpha_i)^{l-2}}{l!}
\]

\[
u_i = \langle \hat{\psi}_u h_i \rangle_{I_j} + \langle \hat{\psi}_u h_i \rangle_{I_{j-1}}
\]

where \( \hat{\psi}_u = \exp \left( \sum_i h_i \alpha_i \right) \) is the minimum-entropy ansatz. Note that for \( \alpha_{i-1} \approx \alpha_i \) or \( \alpha_{i+1} \approx \alpha_i \) (which occurs for example in the isotropic state) the closed formulas become numerically instable. This can be avoided by replacing them in this situation with a Taylor expansion of suitable order.

3.3. Partial moments (discontinuous-Galerkin ansatz)

The obvious problem of full-moment models is that averaging over the complete angular domain may remove necessary information. The idea of partial moments is not to average over the full domain at once but to partition the sphere (or its projection) into disjoint parts and define moments separately for every element of the partition \[22, 43\]. One model of this class, which has been successfully applied to radiative transfer in one dimension, is the half-moment approximation \[20\].

Figure 1: Some elements of the hat-function basis \( h_5 \) for five equidistantly-placed nodes (indicated by black, dashed lines).
Although higher-order models are possible, we will stick to first-order approximation, i.e. locally linear polynomials. Let the set of $k + 1$ angular “grid” points $-1 = \mu_1 < \mu_2 < \ldots < \mu_k < \mu_{k+1} = 1$ define the partition given by the intervals $I_j = (\mu_j, \mu_{j+1})$, $j = 1, \ldots, k$.

For every such interval we define moments by

$$u_{I_j} = \langle p_{I_j} \psi \rangle_{I_j} = \int_{I_j} p_{I_j} \psi \, d\mu.$$ 

The basis functions $p_{I_j}$ are monomials on their corresponding intervals and zero elsewhere. Consequently, $p_{I_j} = \mathbb{1}_{I_j}(1, \mu)$, where $\mathbb{1}_{I_j}(\mu)$ is the indicator function on the interval $I_j$. The set of basis functions is then given by the vector $p = (p_{I_1}, \ldots, p_{I_k})^T$. The advantage of considering only first-order moments is that, similar to the piecewise-linear ansatz, the moment integrals in (2.6b) can be calculated exactly.

Assume that the ansatz satisfies $\hat{\psi} u_{I_j} = \exp(\alpha_{j,0} + \alpha_{j,1} \mu)$. Then

$$u_{0,j} := \langle \hat{\psi} u \rangle_{I_j} = -\frac{e^{\alpha_{j,0}} (e^{\alpha_{j,1} \mu_j} - e^{\alpha_{j,1} \mu_{j+1}})}{\alpha_{j,1}} = e^{\alpha_{j,0}} \sum_{l=1}^{\infty} \frac{\alpha_{j,1}^{l-1} (\mu_j - \mu_{j+1})}{l!}$$

$$u_{1,j} := \langle \mu \hat{\psi} u \rangle_{I_j} = e^{\alpha_{j,0}} \sum_{l=2}^{\infty} \frac{\alpha_{j,1}^{l-2} (\mu_{j+1} - \mu_j)(l-1)}{l!}$$

**Definition 3.4.** Let $n = 2k$ be the number of moments associated with $p$. The resulting linear (compare (2.12)) and nonlinear model (compare (2.10)) will be called PMP$_n$ and PMM$_n$, respectively.

**Remark 3.5.** The PMM$_2$ model is equivalent to the full-moment M$_1$ model.

### 4. Angular bases in three dimensions

Although both approaches are not limited to this, we consider moments on spherical triangles.

Let $T_h$ be a spherical triangulation of $S^2$ and $K \in T_h$ be a spherical triangle with vertices $A_K$, $B_K$ and $C_K$ (or A, B, C as short notation). Furthermore, let $K$ be the flat triangle spanned by the vertices $A$, $B$ and $C$, i.e. $K = g(K)$ with $g(x) = x / \|x\|_2$. This is shown exemplarily in Figure 2.

In the following, we will use a dyadic refinement of the quadrants/octants. This is achieved by subdividing every spherical triangle into four new ones, adding vertices at the midpoints of the triangle edges. This is shown in Figure 2b for one quadrant (black) and two refinements (red and green).

**Remark 4.1.** Previous results indicate that the dyadic refinement is better initialized using the vertices of an icosahedron instead of an octahedron [2]. We decided to use this variant regardless to include the quarter-moment model into our sequence of refinements. However, this is only for investigative reasons. Any practical application should start from the icosahedron.

\[2\] Indeed, a generalization of the partial moments to arbitrary convex spherical polygons is straightforward.
4.1. Barycentric-coordinate basis functions

We consider basis functions defined using spherical barycentric coordinates [10, 32, 42]. Basis functions are associated with vertices of the triangulation. Let \( h_{A_K}, h_{B_K}, \) and \( h_{C_K} \) be those basis functions for the vertices of the spherical triangle \( K \). For every point \( \Omega \in \overline{K} \) we have that the values of the basis functions are uniquely defined by requiring that \( \Omega \in \overline{K} \) is the Riemannian center of mass with weights \( h_{A_K}(\Omega), h_{B_K}(\Omega), \) and \( h_{C_K}(\Omega) \), respectively, and \( h_{A_K}(\Omega) + h_{B_K}(\Omega) + h_{C_K}(\Omega) = 1 \).

**Lemma 4.2** ([42]).

(a) At the vertices \( v \in \{ A_K, B_K, C_K \} \) of \( K \):

\[
h_{A_K}(v) = \begin{cases} 1 & \text{if } v = A_K, \\ 0 & \text{else,} \end{cases}
\]

and likewise for \( h_{B_K} \) and \( h_{C_K} \), respectively.

(b) For every interior point \( \Omega \in \text{int}(\overline{K}) \) and every \( v \in \{ A_K, B_K, C_K \} \) it holds that \( h_v(\Omega) > 0 \) and \( h_v(\Omega) \geq 0 \) for every \( \Omega \in S^2 \).

Numbering all vertices as \( v_1, \ldots, v_n \), the full set of basis functions is then given as

\[ h_{n_v} = (h_1, \ldots, h_n). \]

Since the basis functions form a partition of unity, it follows that \( \rho = \sum_{i=1}^n u_i \). We show one example of such a basis function in Figure 3.

As above, the corresponding moment models will be called HFP_{n_v} and HFM_{n_v}, respectively (see Definition 3.3).

4.2. Partial moments on the unit sphere

In this paper we want to focus on (first-order) partial-moment models on the sphere. They have been introduced in reference [21] (although the authors restricted their investigation to quarter moments).

**Definition 4.3.** For \( D \subseteq S^2 \) and \( \psi \in L_2(D, \mathbb{R}) \) we define its \( i^{th} \) tensorial moment, \( i \in \{0, \ldots, N\} \), by

\[
u_i|_D = \langle \mathbb{1}_D \Omega^i \psi \rangle =: \langle \Omega^i \psi \rangle_D, \tag{4.2}
\]

where \( \mathbb{1}_D \) denotes the indicator function on \( D \). The corresponding components of the tensorial moments are given by

\[
u^{(i_x, i_y, i_z)}_D = \langle \Omega_x^{i_x} \Omega_y^{i_y} \Omega_z^{i_z} \psi \rangle_D, \quad i_x, i_y, i_z \geq 0, i_x + i_y + i_z = i. \tag{4.3}
\]
Abusing notation, we define $\mathbf{p}^0_K = \left( \mathbb{1}^0_K, \mathbb{1}^0_K \otimes \Omega^1, \ldots, \mathbb{1}^0_K \otimes \Omega^N \right)$ and $\mathbf{u}^0_K = \langle \mathbf{p}^0_K \psi \rangle$. The angular basis $\mathbf{p}^0_N$ now consists of all element bases $\mathbf{p}^0_K, K \in T_h$. Since we only investigate first-order systems, we have $N = 1$. The local particle density is then given by $\rho = \sum_{K \in T_h} \mathbf{u}^0_K$.

As above, the corresponding moment models will be called PMP$_n$ and PMM$_n$, respectively (see Definition 3.4), where $n = 4 \cdot |T_h|$ is again the number of moments.

5. Realizability

Since the underlying kinetic density to be approximated is non-negative, a moment vector only makes sense physically if it can be associated with a non-negative distribution function. In this case the moment vector is called realizable.

**Definition 5.1.** The realizable set $\mathcal{R}_b$ is

$$\mathcal{R}_b = \{ \mathbf{u} : \exists \psi(\Omega) \geq 0, \rho = \langle \psi \rangle > 0, \text{ such that } \mathbf{u} = \langle \mathbf{b} \psi \rangle \}. \tag{5.1}$$

If $\mathbf{u} \in \mathcal{R}_b$, then $\mathbf{u}$ is called realizable. Any $\psi$ such that $\mathbf{u} = \langle \mathbf{b} \psi \rangle$ is called a representing density. If $\psi$ is additionally a linear combination of Dirac deltas $\{24, 30, 53\}$, it is called atomic $\{12\}$.

**Remark 5.2.**

(a) The realizable set is a convex cone, and

(b) Representing densities are not necessarily unique.

Obviously, $\mathcal{R}_b$ is unbounded (since $\langle \psi \rangle$ is unbounded). Therefore, the following subset of $\mathcal{R}_b$ is important as well.

**Definition 5.3.** The normalized realizable set is defined as

$$\mathcal{R}_b |_{\rho = 1} = \{ \mathbf{u} : \exists \psi(\Omega) \geq 0, \rho = \langle \psi \rangle = 1, \text{ such that } \mathbf{u} = \langle \mathbf{b} \psi \rangle \}. \tag{5.2}$$
Additionally, since the entropy ansatz has the form (2.9), in the Maxwell-Boltzmann case, the optimization problem (2.7) only has a solution if the moment vector lies in the ansatz space $A := \left\{ \langle b \hat{\psi} \rangle : \alpha \in \mathbb{R}^n \right\}$.

In the case of a bounded angular domain, the ansatz space $A$ is equal to the set of realizable moment vectors [28]. Therefore, it is sufficient to focus on realizable moments only.

Unfortunately, the definition of the realizable set is not constructive, making it hard to check if a moment vector is realizable or not. Therefore, other characterizations of $\mathcal{R}_b$ are necessary.

5.1. Slab geometry

**Remark 5.4.** The full-, partial- and mixed-moment, minimum-entropy models of more than first order suffer from the severe drawback that the resulting integrals in the moment equations cannot be expressed in terms of elementary functions. This means that numerical quadrature is strictly necessary to solve these equations. Unfortunately, this has a strong impact on the realizable set and therefore also on the solution of (2.17) [3, 4].

Fortunately, this does not hold for HFM$_n$ and first-order partial-moment models where the integrals can always be evaluated.

5.1.1. Piecewise-linear angular basis

**Theorem 5.5.** A moment-vector $u_{h_n} = (u_1, \ldots, u_n)^T$ is realizable, i.e. $u_{h_n} \in \mathcal{R}_{h_n}$, if and only if

$$u_i \geq 0, \quad \text{for all } i = 1, \ldots, n. \quad (5.2)$$

**Proof.**

Since by construction $h_i \geq 0$, for any $\psi \geq 0$ it holds that $\langle h_i \psi \rangle \geq 0$. Therefore, (5.2) is necessary.

A representing distribution for $u_{h_n}$ is

$$\psi = \sum_{i=1}^{n} u_i \delta(\mu - \mu_i), \quad (5.3)$$

which shows that (5.2) is also sufficient. \qed

**Remark 5.6.** The representing distribution given in (5.3) is obviously not the minimal representing distribution (with respect to the number of nodes). As has been shown in Corollary 5.4, the bases $f_1$ and $m_1$ are special cases of the hat-function basis $h_n$. It can be shown that the minimal representing distribution with respect to $f_1$ has one node (whereas (5.3) requires two). Similarly, it is possible to provide a two-atomic representing distribution with respect to $m_1$ (whereas (5.3) requires three), namely

$$\psi_{m_1} = \frac{u_0}{\phi_{1+} - \phi_{1-}} (\phi_{1+} \delta (\mu - (\phi_{1+} - \phi_{1-})) - \phi_{1-} \delta (\mu + (\phi_{1+} - \phi_{1-}))),$$

where $\phi_{1\pm} = \frac{u_{1\pm}}{u_0}$ are the normalized half moments. In general, we have the following result.

**Corollary 5.7.** The minimal representing distribution for $u_{h_n} = (u_1, \ldots, u_n)^T \in \mathcal{R}_{h_n}$ has $\lceil \frac{n}{2} \rceil$ nodes.
Proof. If \( n = 2k \), the unique representing distribution with \( k \) nodes is given by

\[
\psi = \sum_{i=1}^{k} (u_{2i-1} + u_{2i}) \delta(\mu - \frac{u_{2i-1}\mu_{2i-1} + u_{2i}\mu_{2i}}{u_{2i-1} + u_{2i}}).
\]

It is easy to check, that, provided \( u_i > 0, \frac{u_{2i-1}\mu_{2i-1} + u_{2i}\mu_{2i}}{u_{2i-1} + u_{2i}} \in [\mu_{2i-1}, \mu_{2i}] \) such that (5.2) is again sufficient.

The odd case \( n = 2k - 1 \) is a degenerated version of the even case (just by adding an interior node twice).

This shows that generally the minimal distribution function has at most \( \lceil \frac{n}{2} \rceil \) nodes. In addition, the basis functions \( h_i \) are supported only in \( I_{i-1} \) and \( I_{i} \), and \( h_1 \) and \( h_n \) are supported only in \( I_1 \) and \( I_n \), respectively. Thus, the minimal representing density has to have nodes in \( I_{i-1} \) and \( I_{i} \) and at least in every second interval, which gives at least \( \lceil \frac{n}{2} \rceil \) nodes. \( \square \)

5.1.2. First-order partial moments

**Corollary 5.8.** A moment vector \( \mathbf{u} = (u_{0,1}, u_{1,1}, \ldots, u_{0,k}, u_{1,k})^T \in \mathbb{R}^n \) is realizable with respect to \( \mathbf{p} \), i.e. \( \mathbf{u} \in \mathcal{R}_p \), if and only if the local moments \( (u_{0,j}, u_{1,j}) \) for \( j = 1, \ldots, k \) satisfy

\[
u_{0,j} > 0 \quad \text{and} \quad \frac{u_{1,j}}{u_{0,j}} \in I_j,
\]

(5.4)

**Proof.** Follows immediately from the results in [15, 48]. \( \square \)

5.2. Three dimensions

We will now derive realizability conditions for our models in the fully three-dimensional setting.

5.2.1. Spherical barycentric

**Theorem 5.9.** Let \( \mathbf{u} = (u_1, \ldots, u_n)^T \in \mathbb{R}^n \) be a vector of moments. Then it is necessary and sufficient for the existence of a non-negative measure \( \psi \) which realizes \( \mathbf{u} \) with respect to \( h_n \) that

\[
u_i \geq 0 \quad \text{for all} \quad i = 1, \ldots, n_v.
\]

(5.5)

**Proof.** The proof works similar to the one-dimensional setting (compare (5.2)). We first show that equation (5.5) is necessary. Let \( \psi \geq 0 \) be arbitrary. By Lemma [4.2(2)] it holds that \( h_i \geq 0 \) which implies that \( u_i = (h_i \psi) \geq 0 \) and thus (5.5).

Assume that \( \mathbf{u} \) satisfies (5.5). A representing distribution is given by

\[
\psi = \sum_{i=1}^{n_v} u_i \delta(\Omega - v_i).
\]

(5.6)

Due to (4.1) it follows that

\[
\langle h_j \psi \rangle = \sum_{i=1}^{n_v} u_i h_j (v_i) = \sum_{i=1}^{n_v} u_i \delta_{ij} = u_j.
\]

**Remark 5.10.** We want to note that the above proof is not limited to barycentric coordinates but also works for other bases with values in \([0,1]\) and the Lagrange interpolation property (4.1).
5.2.2. Partial moments

**Theorem 5.11.** Let \( \mathbf{u} = \left( u_{[0]}^K, u_{[1]}^K \right)^T \in \mathbb{R}^4 \) be a vector of moments. Then it is necessary and sufficient for the existence of a non-negative measure \( \psi \) which realizes \( \mathbf{u} \) with respect to \( p_\rho^K \) that

\[
\frac{u_{[0]}^K}{u_{[0]}^K} > 0
\]

(5.7a)

and the normalized first moment

\[
\phi_{[1]}^K := \frac{u_{[1]}^K}{u_{[0]}^K}
\]

(5.7b)

satisfies \( \phi_{[1]}^K \in \text{conv}(\hat{K}) \), where \( \text{conv}(\cdot) \) denotes the convex hull.

**Proof.** The necessity of (5.7) follows immediately, since by assumption \( \psi \geq 0 \) is supported in \( \hat{K} \) and integration is a linear operation.

To show the sufficiency of (5.7) we give a realizing distribution function under this assumption. The boundary of the convex hull \( \text{conv}(\hat{K}) \) is given by \( \hat{K} \) and \( K \). First, we give realizing distributions on these boundary parts. Due to the convexity of the convex hull and the linearity of the integral, every interior point can then be reproduced by a suitable convex combination of these two candidates.

Assume that \( \| \phi_{[1]}^K \|_2 = 1 \), i.e. \( \phi_{[1]}^K \in \hat{K} \). A realizing distribution is given by

\[
\psi_{\hat{K}} = u_{[0]}^K \delta (\Omega - \phi_{[1]}^K),
\]

(5.8)

where \( \delta \) denotes the multi-dimensional Dirac-delta distribution\(^3\). By assumption, \( \psi_{\hat{K}} \) is supported in \( \hat{K} \).

Thus

\[
\langle \psi_{\hat{K}} \rangle = u_{[0]}^K \quad \text{and} \quad \langle \Omega \psi_{\hat{K}} \rangle = u_{[0]}^K \phi_{[1]}^K = u_{[1]}^K.
\]

If \( \phi_{[1]}^K \in K \) (the opposite boundary of the convex hull), a realizing distribution is

\[
\psi_K = u_{[0]}^K (\lambda_A \delta (\Omega - A) + \lambda_B \delta (\Omega - B) + \lambda_C \delta (\Omega - C)),
\]

(5.9)

where \( \lambda_A, \lambda_B, \lambda_C \) are the barycentric coordinates of \( \phi_{[1]}^K \) with respect to the vertices \( A, B \) and \( C \) on \( K \), i.e. \( \lambda_A + \lambda_B + \lambda_C = 1 \) and \( \lambda_A A + \lambda_B B + \lambda_C C = \phi_{[1]}^K \). It immediately follows that \( \psi_K \) is supported in \( \hat{K} \) and realizes \( \mathbf{u} \).

If \( \phi_{[1]}^K \) is in the interior of the convex hull, we find that \( \| \phi_{[1]}^K \|_2 \) can be realized by (5.8) and the intersection point of the line from the origin \((0,0,0)\) and \( \phi_{[1]}^K \) with \( K \) can be realized by (5.9). Certainly, \( \phi_{[1]}^K \) lies on the same line and can thus be realized by a convex combination of these two distribution functions.

---

\(^3\)We assume for notational simplicity that \( \delta \) has mass 1 even on the boundary of integration.

\(^4\)This is no longer true if \( \| \phi_{[1]}^K \|_2 < 1 \).
5.3. Numerically realizable set

In general, we cannot solve the integrals in (5.1) analytically and have to approximate them by a numerical quadrature $Q$. We thus define the numerically realizable set

$$\mathcal{R}_b^Q = \{ u : \exists \psi(\Omega) \geq 0, \rho = \langle \psi \rangle_Q > 0, \text{ such that } u = \langle b(\psi) \rangle_Q \subset \mathcal{R}_b, \}$$

(5.10)

where for an integrable function $f$, $\langle f \rangle_Q = \sum_{i=1}^{n_Q} w_i f(\Omega_i) \approx \langle f \rangle$ is the approximation of the corresponding integral $\langle \cdot \rangle$ with the quadrature rule $Q$.

The numerically realizable set can also be described as the convex hull of the basis function values at the quadrature nodes (see [3] for the Legendre basis, the proof can be easily adapted for the other bases)

$$\mathcal{R}_b^Q|_{\rho=1} = \text{int} (\text{conv} \{ b(\Omega_i) \}_{i=1}^{n_Q})).$$

(5.11)

If $\rho$ depends linearly on $u$ it follows

$$\mathcal{R}_b^Q|_{\rho<1} = \text{int} (\text{conv} \{ 0, b(\Omega_i) \}_{i=1}^{n_Q})).$$

(5.12)

In general, $\mathcal{R}_b^Q$ is a strict subset of $\mathcal{R}_b$, i.e., there are some moments that are realizable analytically but cannot be realized with $Q$. For the hat functions and one-dimensional partial moments, however, the numerically-realizable set and the realizable set agree for suitable quadratures.

**Lemma 5.12.** Let $b$ be an angular basis in one dimension with piece-wise linear (possibly discontinuous) basis functions, i.e., there exist $-1 \leq \mu_0 < \mu_1 < \ldots < \mu_n \leq 1$ such that the restriction on the interval $(\mu_{j-1}, \mu_j)$ satisfies $b_i(\mu_{j-1}, \mu_j) \in P^1(\mu_{j-1}, \mu_j)$ for all $j = 1, \ldots, n$. Additionally, let $\mu_j$ be part of the node set of the numerical quadrature

$$\langle f \rangle_Q := \sum_{i=1}^{n_Q} w_i f(\mu_i) \approx \langle f \rangle, \quad w_i > 0, \mu_i \in [-1, 1],$$

i.e., $\mu_j \in \{ \hat{\mu}_i | i = 1, \ldots, n_Q \}$. Then we have

$$\mathcal{R}_b^Q := \left\{ u \in \mathbb{R}^n : \exists \psi_i \in \mathbb{R}_{>0} \text{ s.t. } u = \sum_{i=1}^{n_Q} w_i b(\hat{\mu}_i) \psi_i =: \langle b \psi \rangle_Q \right\} = \mathcal{R}_b.$$

(5.13)

**Proof.** It is straight-forward to show that (generally) $\mathcal{R}_b^Q \subset \mathcal{R}_b$. Thus let $u \in \mathcal{R}_b$. Since the basis is piecewise linear, we can find a representing density $\hat{\psi}(\mu) = \sum_{j=1}^{n} \alpha_j \delta(\mu - \mu_j)$ with suitably chosen $\alpha_j \in \mathbb{R}_+$ (compare Theorem 5.5 and Corollary 5.8). Setting

$$\psi_i = \begin{cases} \frac{\alpha_j}{w_i} & \text{if } \mu_j = \hat{\mu}_i, \\ 0 & \text{else,} \end{cases}$$

shows that $u \in \mathcal{R}_b^Q$. □

With a very similar proof, it can be shown that $\mathcal{R}_h^Q = \mathcal{R}_h$ also in three dimensions if the quadrature contains the vertices of the triangulation $\alpha_i$. For the partial moment basis in three dimensions, however, the analytical and numerical realizable set differ as the quadrature would have to contain all points on $K$ to reproduce the whole realizable set.

Note that this gives a numerical equivalent to the analytical realizability conditions Theorem 5.11.
Lemma 5.13. Let \( \mathbf{u} = \begin{pmatrix} \mathbf{u}[0]_K \\ \mathbf{u}[1]_K \end{pmatrix} \in \mathbb{R}^4 \) be a vector of moments, and let \( Q \) be a quadrature on \( \overline{K} \). Then \( \mathbf{u} \in R_{\mathbf{p}_K}^Q \) iff 
\[ \phi[1]_K = \frac{\mathbf{u}[1]_0}{\mathbf{u}[0]_K} \in \text{conv} \left\{ \Omega_i : \Omega_i \in Q \right\}. \] 
(5.14)

Proof. Follows directly from (the proof of) (5.11) and the definition of \( \mathbf{p}_K \).

6. Results

To test the approximation properties of the regarded models, we investigate convergence against some prescribed distribution \( \psi \). For each basis \( \mathbf{b} \), the moment vector \( \mathbf{u} \) is calculated as \( \mathbf{u} = \langle \mathbf{b} \psi \rangle \). Then the ansatz distributions are computed by (2.9).

6.1. Slab geometry

In one dimension, we prescribe the following distributions.

\[ \psi_{\text{gauss}}(\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( \frac{(\mu - \bar{\mu})^2}{-2\sigma^2} \right) \text{ where } \sigma = 0.5, \bar{\mu} = 0, \] 
(6.1)

\[ \psi_{\text{heaviside}}(\mu) = \begin{cases} \frac{10^{-n}}{2} & \text{if } \mu < 0 \\ 1 & \text{else} \end{cases} \] 
(6.2)

Exemplary ansatz functions are shown in Figures 4 and 5. The convergence results can be found in Figure 6 and Tables 1 and 2, where we only used those models/moment numbers which did not exactly reproduce the ansatz. For the Gaussian distribution, as expected [27], the \( P_N \) models show exponential convergence whereas the \( M_N \) models are exact (up to numeric errors) starting from order 2. This is to be expected as the Gaussian can be written as (2.9) if \( N \geq 2 \). For the piecewise linear models, second-order convergence is expected [16, 17], which is confirmed by the results both in \( L_1 \) norm and \( L_\infty \) norm.

| \( n \) | \( E^1_h \) | \( \nu \) | \( E^\infty_h \) | \( \nu \) | \( E^1_h \) | \( \nu \) | \( E^\infty_h \) | \( \nu \) | \( E^1_h \) | \( \nu \) | \( E^\infty_h \) | \( \nu \) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 4.111e-01 | --- | 3.693e-01 | --- | 4.110e-01 | --- | 3.693e-01 | --- |
| 4 | 5.398e-02 | 2.9 | 9.541e-02 | 2.0 | 1.074e-01 | 1.9 | 2.115e-01 | 1.8 | 9.429e-02 | 2.1 | 1.315e-01 | 1.5 |
| 6 | 1.950e-02 | 2.5 | 3.976e-02 | 2.2 | 5.151e-02 | 1.8 | 1.036e-01 | 1.8 | 1.506e-02 | 4.5 | 2.683e-02 | 3.9 |
| 8 | 9.999e-03 | 2.3 | 2.094e-02 | 2.2 | 2.967e-02 | 1.9 | 6.310e-02 | 1.7 | 1.834e-03 | 7.3 | 3.368e-03 | 6.7 |
| 10 | 6.048e-03 | 2.3 | 1.286e-02 | 2.2 | 1.920e-02 | 1.9 | 4.057e-02 | 2.0 | 1.802e-04 | 10.4 | 4.320e-04 | 9.8 |
| 12 | 4.048e-03 | 2.2 | 8.666e-03 | 2.2 | 1.342e-02 | 2.0 | 2.889e-02 | 1.9 | 1.488e-05 | 13.4 | 3.940e-05 | 13.1 |
| 14 | 2.898e-03 | 2.2 | 6.231e-03 | 2.1 | 9.894e-03 | 2.0 | 2.199e-02 | 2.0 | 1.049e-06 | 17.2 | 3.068e-06 | 16.6 |
| 16 | 2.177e-03 | 2.1 | 4.692e-03 | 2.1 | 7.594e-03 | 2.0 | 1.641e-02 | 1.9 | 6.507e-08 | 20.8 | 2.929e-08 | 20.3 |
| 18 | 1.695e-03 | 2.1 | 3.659e-03 | 2.1 | 6.010e-03 | 2.0 | 1.294e-02 | 2.0 | 3.596e-09 | 24.6 | 1.198e-09 | 24.0 |
| 20 | 1.357e-03 | 2.1 | 2.935e-03 | 2.1 | 4.874e-03 | 2.0 | 1.055e-02 | 1.9 | 1.729e-10 | 28.5 | 6.294e-10 | 27.9 |
| 22 | 1.100e-03 | 2.1 | 2.403e-03 | 2.1 | 4.031e-03 | 2.0 | 8.705e-03 | 2.0 | 8.097e-12 | 32.5 | 2.999e-12 | 31.9 |
| 24 | 9.257e-04 | 2.1 | 2.004e-03 | 2.1 | 3.390e-03 | 2.0 | 7.347e-03 | 2.0 | 3.363e-13 | 36.6 | 1.305e-12 | 36.0 |
| 26 | 7.835e-04 | 2.1 | 1.697e-03 | 2.1 | 2.890e-03 | 2.0 | 6.250e-03 | 2.0 | 1.290e-14 | 40.7 | 5.285e-14 | 40.1 |
| 28 | 6.717e-04 | 2.1 | 1.456e-03 | 2.1 | 2.493e-03 | 2.0 | 5.406e-03 | 2.0 | 7.057e-16 | 39.2 | 2.082e-15 | 43.6 |
| 30 | 5.822e-04 | 2.1 | 1.262e-03 | 2.1 | 2.172e-03 | 2.0 | 4.703e-03 | 2.0 | 5.947e-16 | 24.4 | 7.772e-16 | 14.3 |

Table 1: \( L_1/L_\infty \) errors and observed order of convergence \( \nu \) for different models and moment numbers in the Gauss slab geometry case.
In the Heaviside test, the PMP\(_n\) and PMM\(_n\) models are exact if an even number of intervals is used. All other tested models and the PMP\(_n\) and PMM\(_n\) models for an odd number of intervals show the expected first-order convergence in \(L_1\) norm \([31, 52]\). Notably, the HFM\(_n\) models with an even number of intervals give errors that are several orders of magnitude lower than the other models though the rate of convergence is not improved. In \(L_\infty\) norm, no convergence can be observed in this testcase, due to the well-known Gibbs phenomenon (see Figure 5).

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**Figure 4:** Distributions of selected models for the slab geometry Gauss test.

**Figure 5:** Distributions of selected models for the slab geometry Heaviside test.
Figure 6: Approximation errors for prescribed distributions in slab geometry.
Table 2: $L_1/L_\infty$ errors and observed order of convergence $\nu$ for different models and moment numbers in the Heaviside slab geometry case.

| Model | $L_1$ | $L_\infty$ | $\nu$ | $E_h^1$ | $E_h^\infty$ | $\nu$ | $E_h^1$ | $E_h^\infty$ | $\nu$ | $E_h^1$ | $E_h^\infty$ | $\nu$ |
|-------|-------|------|------|-------|------|------|-------|------|------|-------|------|------|
| HFM   | 2     | 5.446e-01 | -     | 5.446e-01 | -     | 5.446e-01 | -     | 5.447e-01 | -     | 5.447e-01 | -     |
| PMM   | 6     | 1.604e-01 | 0.2   | 1.815e-01 | 1.0   | 8.478e-01 | -0.0  | 1.603e-01 | 1.1   | 6.453e-01 | 0.2   |
| MN    | 10    | 9.085e-02 | 0.0   | 1.089e-01 | 1.0   | 8.478e-01 | 0.0   | 1.017e-01 | 0.9   | 6.308e-01 | 0.0   |
|       | 14    | 1.604e-01 | 0.2   | 1.604e-01 | 1.0   | 8.478e-01 | -0.0  | 3.732e-01 | 0.0   | 7.632e-01 | 0.0   |
|       | 18    | 4.817e-02 | 0.0   | 6.051e-02 | 1.0   | 8.478e-01 | 0.0   | 5.208e-02 | 1.2   | 6.236e-01 | 0.1   |
|       | 22    | 3.899e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 26    | 3.276e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 30    | 2.824e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 34    | 2.481e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 38    | 2.213e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 42    | 1.997e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 46    | 1.820e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |
|       | 50    | 1.671e-02 | 0.0   | 1.0     | 0.0   | 8.478e-01 | -0.0  | 0.599e-02 | 0.1   | 6.329e-01 | -0.1  |

Table 3: $L_1/L_\infty$ errors and observed order of convergence $\nu$ for different models and moment numbers in the Gauss 3D case.

For the discontinuous square distribution, as in one dimension, first-order convergence in the grid width (for the piecewise linear models) is expected in the $L_1$-norm [27]. This corresponds to a convergence rate of $1/2$ in $n$. The observed convergence rate for the piecewise-linear models is achieved in average, with slightly varying values (from 0.3 to 0.8) between different refinement iterations. The full moment models (MN and PN) converge (in average) slightly slower, with an observed convergence rate of approximately 0.38. In $L_\infty$ norm, none of the models converges due to the famous Gibbs phenomenon. For completeness, we also show a selection of ansatz functions for the Gauss (Figure 8) and the Square test (Figure 9).
Table 4: $L_1/L_\infty$ errors and observed order of convergence $\nu$ for different models and moment numbers in the Square 3D case.

Figure 7: Approximation errors for prescribed distributions in three dimension.
We observe that, qualitatively, the piece-wise linear models cannot compete with the full moment models in the smooth Gauss test. This is expected due to the exponential convergence of full moment models. Besides that, it is clearly visible that switching from the linear model (e.g. PMP_n) to the non-linear model (e.g. PMM_n) significantly improves the approximation quality. A direct comparison between the two piece-wise linear basis functions is unfortunately impossible due to the difference in the degrees of freedom (comparing e.g. HFM_{18} with PMM_{32} yields a better result while the next refinement HFM_{66} outperforms PMM_{32} (not shown)). In the non-smooth Square test, the hat function basis yields better results than the partial moment ansatz. In particular, the hat function basis can compete with the full moment ansatz which is much more challenging and costly in the implementation. Note that the Gibbs oscillations can be observed along the boundaries of the square for all models.

7. Conclusions and outlook

We have derived minimum-entropy models for continuous and discontinuous piece-wise linear basis functions in one dimension and on the unit sphere. Additionally, we gave the corresponding realizability conditions, which also provide the set of moments for which these minimum-entropy models are hyperbolic and well-defined. Finally, numerical tests show the expected second- and first-order convergence to smooth and discontinuous distributions, respectively.

The sequel of this paper will deal with higher-order realizability-preserving numerical schemes for this type of moment models and an extensive numerical analysis for several classical benchmark problems. Additionally, we investigate the effects of numerical quadrature on the realizability set.

In future work, generalizations of the continuous piece-wise linear basis function to higher-order splines on the unit sphere [1] could be considered, as well as higher-order partial moments. However, realizability theory even for second order is challenging and has yet to be found, except for very few special cases like the full moment basis [29]. Additionally, the development of Kershaw closures as in [35, 46, 50] for these new bases would be particularly interesting, as they provide a realizable moment method while avoiding the costly non-linear optimization problem of the minimum-entropy model.

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Figure 8: Distributions of selected models for the three-dimensional Gauss test. The value of the distribution is represented by the color, restricted to the interval \([0, \tfrac{2}{\pi}]\).
Figure 9: Distributions of selected models for the three-dimensional square test. The value of the distribution is represented by the color, restricted to the interval $[0, \frac{3}{2}]$. 

(a) Reference

(b) $M_8(n = 81)$

(c) PMM$_{128}$

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