HIERARCHICAL MOMENT CLOSURE APPROXIMATION OF THE BOLTZMANN EQUATION

M. Abdel Malik^{*}, E.H. van Brummelen^{*}

*Multiscale Engineering Fluid Dynamics Department of Mechanical Engineering Eindhoven University of Technology Den Dolech 2, 5612 AZ Eindhoven, Netherlands e-mail: M.Abdel.Malik@tue.nl

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Abstract. This work discusses the application of the moment method to a generic form of kinetic equations, given by the Boltzmann equation, to simplify kinetic models of particle systems. Implicit to the method of moments is an approximation of moment closure relations to close the system of equations. The main aim is to explore the opportunities, pertaining to goal-oriented adaptive modeling, presented by the hierarchical structure of moment-closure systems.

1 INTRODUCTION

The Boltzmann equation is the classical model in the kinetic theory of (mono-atomic) fluids, describing rarefied flow by modeling deviations of the velocity distribution from a local equilibrium, thus, accounting for the transitional molecular/continuum regime. Boltzmann's equation provides an evolution equation for the one-particle marginal, viz., the probability density of particles in phase (position/velocity) space. The Boltzmann equation has several fundamental structural properties, notably, conservation of mass, momentum and energy, Galilean invariance and decay of an entropy functional (the celebrated H-theorem). These structural properties underly the connection between the Boltzmann equation and conventional continuum models: all conventional continuum models, such as the Navier-Stokes-Fourier system [1], can be derived as limits of the Boltzmann equation.

Boltzmann's equation poses a formidable challenge for numerical approximation methods, on account of its high dimensional phase-space setting: for a problem in N spatial dimensions, the single molecule phase-space is 2N dimensional. Away from the fluid dynamical regime numerical approximations of kinetic systems are predominantly based on particle methods, such as the Direct Simulation Monte Carlo (DSMC) method. However, the phase-space description of the system results in the prohibitive computational cost of DSMC in the fluid dynamical limit. Moreover, from an approximation perspective, DSMC can be inefficient since it is inherent to Monte-Carlo processes that the approximation error decays only as $n^{-\frac{1}{2}}$ for the number of simulation molecules n [2]. Hence, efficiently modeling gases in the transition regime between the free molecular flow and fluid dynamics remains difficult.

An alternative strategy to describe deviations from fluid dynamics is by means of moment-closure approximations [3,4]. In moment-closure approximations, the Boltzmann equation is projected onto a polynomial space, in the velocity dependence, and the system is closed by providing an approximation to the one-particle marginal based on the same polynomial space. This procedure can in fact be conceived of as a Galerkin approximation. The closure is chosen such that the structural properties of the Boltzmann equation are retained. Results by Schmeiser and Zwirchmayr [5] show that moment equations converge to linear kinetic equations as the order of moment approximation tends to infinity and to a drift-diffusion model in the macroscopic limit, i.e. as the Knudsen number tends to zero. Furthermore, from an adaptive approximation standpoint, the resulting hierarchical structure of the the moment closure system presents promising potential for rigorous model adaptivity. However, fundamental challenges remain to be addressed.

This work discusses the application of the moment method to the Boltzmann equation to derive a closed hierarchy of moment systems that retain structural features of the system in question. In addition opportunities pertaining to goal-oriented adaptive modeling provided by the hierarchical structure exhibited by the resulting closed system of moment equations will be explored. The remainder of this paper is arranged as follows, section 2 enlists the structural properties of the Boltzmann equation that are to be retained by the moment closure approximation; section 3 introduces concepts relevant to moment systems pertaining to subspace approximations as well as the consequential moment closure approximation; section 4 discusses the hierarchical structure of the resulting closed system of moment equations within a multiscale modeling framework and the oppertunities this presents for (goal-oriented) model adaptivity; finally, section 5 gives a concluding summary.

2 THE BOLTZMANN EQUATION: PROPERTIES

Consider a gas composed of a single species of identical classical particles, i.e. a monatomic gas, contained within a fixed spatial domain $\Omega \subset \mathbb{R}^D$. Based on kinetic theory the evolution of a non-negative (phase-space) density $f = f(t, \boldsymbol{x}, \boldsymbol{v})$ over a single particle phase $\Omega \times \mathbb{R}^D$ is governed by the (kinetic) Boltzmann equation expressed as

$$\partial_t f + v_j \partial_{x_j} f = \mathcal{C}(f) \tag{1}$$

where the collision operator $f \mapsto \mathcal{C}(f)$ acts only on the \boldsymbol{v} dependence of f locally at each (t, \boldsymbol{x}) . Let $\langle \cdot \rangle$ denote \boldsymbol{v} -integrations of any scalar, vector or matrix valued measurable

function over the D-dimensional Lesbesgue measure dv. All functions considered in this work are understood to be Lebesgue measurable in all variables.

The collision operator C is assumed to be defined over the domain $\mathscr{D}(C)$ that is contained within the set of non-negative functions of v. Furthermore, it is assumed that Chas the following properties [4]:

1. Conservation: Mass, Momentum and Energy Definition A quantity γ is said to be a collision invariant of C if

$$\langle \gamma \mathcal{C}(f) \rangle = 0, \qquad \forall f \in \mathscr{D}(\mathcal{C})$$
 (2)

Denote the collection of collision invariants of C by \mathscr{C} and let the basis for an Ndimensional \mathscr{C} be written as $\{e_i : 1 \leq i \leq N\}$. Relation (2) leads to N independent local conservation laws

$$\partial_t \langle e_i f \rangle + \partial_{x_i} \langle v_j e_i f \rangle = 0 \tag{3}$$

It is assumed that the set of collision invariants is given by

$$\mathscr{C} = \operatorname{span}\{1, \boldsymbol{v}, |\boldsymbol{v}|^2\}$$
(4)

where the notation in (4), adopted throughout this paper, applies to a collection of scalars, vectors and tensors, implying that the span consists of all scalar-valued linear combinations of their components. Assumption (4) implies the Boltzmann equation (1) conserves mass, momentum and energy, and has no other invariants.

2. Entropy Dissipation: H-Theorem **Definition** A convex function $\mathcal{H} = \mathcal{H}(f)$ over \mathbb{R}_+ is called an *entropy* for \mathcal{C} if

$$\langle \mathcal{C}(f)\partial_f \mathcal{H}(f) \rangle \le 0, \qquad \forall f \in \mathscr{D}(\mathcal{C})$$
 (5)

and if for every $f \in \mathscr{D}(\mathcal{C})$ the following statements are equivalent

i.
$$\langle \partial_f \mathcal{H}(f) \mathcal{C}(f) \rangle = 0$$

ii. $\mathcal{C}(f) = 0$ (6)
iii. $\partial_f \mathcal{H}(f) \in \mathscr{C}$

Relations (5) and (6) are abstractions of Boltzmann's H-theorem, where (5) assumes that C dissipates some entropy and (6) characterizes local equilibria of C by vanishing entropy dissipation. Denoting the Legendre transform of the entropy \mathcal{H} by \mathcal{H}^* , i.e.

$$\mathcal{H}(y) + \mathcal{H}^*(z) = yz \tag{7}$$

(5) and (6) suggest that the equilibrium distribution, denoted by f_{eq} , is given by

$$f_{eq} = \partial_z \mathcal{H}^*(z) \qquad \text{for } z \in \mathscr{C}$$
(8)

It is assumed that the entropy of C exists. This assumption implies that solutions of the Boltzmann equation (1) satisfy the local dissipation law corresponding to entropy dissipation

$$\partial_t \langle \mathcal{H}(f) \rangle + \partial_{x_j} \langle v_j \mathcal{H}(f) \rangle = \langle \mathcal{C}(f) \partial_f \mathcal{H}(f) \rangle \le 0 \tag{9}$$

where $\langle \mathcal{H}(f) \rangle$, $\langle v_j \mathcal{H}(f) \rangle$ and $\langle \partial_f \mathcal{H}(f) \mathcal{C}(f) \rangle$ are referred to as entropy density, entropy flux and entropy dissipation rate, respectively.

3. Symmetry: Galilean Invariance

The operator C is assumed to commute with translational and orthogonal transformations. Specifically, given any $g = g(t, \boldsymbol{x}, \boldsymbol{v})$ for every vector $\boldsymbol{u} \in \mathbb{R}^D$ and for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$ define transformed functions $\mathcal{T}_u f$ and $\mathcal{T}_O f$ by

$$\mathcal{T}_{u}g = \mathcal{T}_{u}g(t, \boldsymbol{x}, \boldsymbol{v}) \equiv g(t, \boldsymbol{x} - \boldsymbol{u}t, \boldsymbol{u} - \boldsymbol{v}), \quad \mathcal{T}_{O}g = \mathcal{T}_{O}g(t, \boldsymbol{x}, \boldsymbol{v}) \equiv g(t, O^{\top}\boldsymbol{x}, O^{\top}\boldsymbol{v})$$
(10)

It is assumed that if $f \in \mathscr{D}(\mathcal{C})$ then so are $\mathcal{T}_u f$ and $\mathcal{T}_O f$:

$$\mathcal{T}_u \mathcal{C}(f) = \mathcal{C}(\mathcal{T}_u f), \qquad \mathcal{T}_O \mathcal{C}(f) = \mathcal{C}(\mathcal{T}_O f)$$
 (11)

Assumption (11) implies that if f satisfies (1) so does the image of f under a Galilean group.

3 MOMENT CLOSURE

Physically, one may be more interested in functions of f (observables), from which macroscopic properties can be extracted, than in f itself. Such reasoning motivates the derivation of equations for such observables instead. That is, rather than resolving equation (1) for f, one could resolve moment systems (or weighted averages) of f, which would govern the evolution of a finite set of velocity moments of f. In resolving the moment equations instead of (1), the velocity dependence of f is replaced by a finite number of parameters, thus reducing the complexity of the problem [6].

To derive the moment equations, consider a finite linear subspace Θ of functions of \boldsymbol{v} (taken to be polynomials) with dimension θ and basis $\{\vartheta_i = \vartheta_i(\boldsymbol{v})\}_{i=1}^{\theta}$. Denote the column θ -vector of these basis elements by $\boldsymbol{\vartheta} = \boldsymbol{\vartheta}(\boldsymbol{v})$, so that every $\boldsymbol{\vartheta} \in \Theta$ has a unique representation in the form $\boldsymbol{\vartheta}(\boldsymbol{v}) = \boldsymbol{\alpha}^{\top} \boldsymbol{\vartheta}(\boldsymbol{v})$ for some $\boldsymbol{\alpha} \in \mathbb{R}^{\theta}$. Taking the moments, i.e. weighted average, of equation (1) over the vector $\boldsymbol{\vartheta}(\boldsymbol{v})$ yields

$$\partial_t \langle \boldsymbol{\vartheta} f \rangle + \partial_{x_j} \langle v_j \boldsymbol{\vartheta} f \rangle = \langle \boldsymbol{\vartheta} \mathcal{C}(f) \rangle \tag{12}$$

thus, a weaker form of equation (1) is formally expressed as a hierarchy of moment systems of partial differential equations in (12) in the sense that a solution of (1) would also satisfy (12). In general, it is not known whether the quantities appearing in this equation are well defined for every solution f of a given kinetic equation. Since, it has been shown that this is the case for the spatially homogenous equation [7], following Levermore [4] it shall be assumed here that these quantities are well defined.

Furthermore, it is observed that in equations (12) the flux in one equation appears as the density in the subsequent one, i.e. the expansion at some order n contains the moments at orders $n \pm 1$. Moreover, the equations contain the production terms which are related to the distribution function f through the collision term C(f). Therefore, in order to have a complete set of equations for the moments, constitutive relations are needed to express the densities $\langle \vartheta f \rangle$, fluxes $\langle \vartheta \vartheta f \rangle$ and collisional terms $\langle \vartheta C(f) \rangle$ as a function of θ variables, thus forming a closed system. Generally, this is achieved by finding a relation between the moments and the distribution function. Deriving such a relation is called the moment closure problem.

A subspace Θ will be called admissible if it satisfies (see [4])

i. $\mathscr{C} \subseteq \Theta$:

In this condition, the collection of collision invariants \mathscr{C} is contained within Θ . More specifically, the constant functions are included in Θ so that any moment closure will include the conservation law for mass. It also includes multiples of the polynomial \boldsymbol{v} , which gives a balance law for momentum. Multiples of $|\boldsymbol{v}|^2$ give a balance law for the energy. This is needed if any fluid dynamical approximation is to be recovered.

ii. Θ is invariant under actions of \mathcal{T}_u and \mathcal{T}_o : More specifically, this means that Θ is unchanged when $\boldsymbol{v} \mapsto O^{\top} \boldsymbol{v}$ or $\boldsymbol{v} \mapsto \boldsymbol{v} - \boldsymbol{u}$, for every vector $\boldsymbol{u} \in \mathbb{R}^D$ and for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$. This is a prerequisite of classical dynamics, in particular, that Galilean invariance holds.

Closure of (12) is attained if there exists a function \mathcal{F} (and is made known) such that $f(t, \boldsymbol{x}, \boldsymbol{v}) = \mathcal{F}(\langle f, \boldsymbol{\vartheta} \rangle, \boldsymbol{v})$. Then the flux terms $\langle \boldsymbol{v}\boldsymbol{\vartheta}f \rangle$ and the collision terms $\langle \boldsymbol{\vartheta}\mathcal{C}(f) \rangle$ can be related to the densities $\langle \boldsymbol{\vartheta}\mathcal{F} \rangle$ to provide a closed system of the form

$$\partial_t \langle \boldsymbol{\vartheta} \mathcal{F} \rangle + \partial_{x_i} \langle v_j \boldsymbol{\vartheta} \mathcal{F} \rangle = \langle \boldsymbol{\vartheta} \mathcal{C}(\mathcal{F}) \rangle \tag{13}$$

Note that f is an element of an infinite dimensional vector space and typically cannot be expressed by any finite number of components. Therefore, any closure will require the approximation of f. The aim is to devise an approximation that, in addition to providing well-posedness of (13), maintains the aforementioned structural features of (1) listed in section 2. Moreover, the closure relation should result in a tractable system.

Remark Considering the smallest admissible subspace $\Theta \equiv \mathscr{C}$ reduces (13) to the Euler equations for a monatomic gas.

Previous studies of moment closure approximations can be found in [3, 4, 6, 8]. Grad's moment closure [3] is based on an expansion of the one-molecule marginal using Hermite polynomials, modulated by the local equilibrium distribution. A deficiency of Grad's moment closure system is the potential occurrence of locally negative and therefore inadmissible phase-space distributions, and potential loss of hyperbolicity [9, 10]. Later, Levermore [4] developed a moment closure system based on entropy minimization, which leads to an exponential closure. However, it was subsequently shown by Junk [11] that Levermore's moment closure system suffers from a realizability problem, i.e. there exist moments for which the minimum entropy solution is undefined. On the other hand, results by Junk [11, 12], Schneider [13] and Pavan [14], show that a relaxation of the entropy minimization problem is well-posed while retaining exponential closure. However, employing the relaxed minimization problems leads to loss of the one-to-one correspondence between the entropy minimizing distribution and the moments of the single-particle phase-space densities. An additional deficiency of Levermore's entropy-based closure is the potential occurrence of singularities owing to the fact that densities describing local thermodynamic equilibrium may belong to the boundary of the set containing all degenerate densities [11, 12, 15]. Another fundamental complication pertaining to the implementation of the moment-closure systems based on exponential closure, is that the resulting formulation requires the evaluation of moments of exponentials of polynomials of, in principle, arbitrary orders. It is generally accepted that the derivation of closed-form expressions for such moments is intractable, and accurate approximation of the moments is a notoriously difficult problem [16].

Abdel Malik and Van Brummelen [8] have recently investigated moment-closure systems based on approximations of the exponential of the form given by an even-order Taylor-series approximation about a Maxwellian. The even-order of the Taylor-series approximation ensures non-negativity of the approximation. The results in [8] convey that in this manner, it is possible to construct well-posed moment-closure systems that retain the structural features of the Boltzmann equation listed in section 2, but for which the evaluation of moments of exponentials of arbitrary polynomials is replaced by the evaluation of high-order moments of Gaussians. Such high-order moments of Gaussians can be evaluated in closed form. It has been noted that Grad's moment closure can be perceived as a first order approximation of Levermore's exponential closure [6, 17]. The results of [8] can be conceived as a refinement of Grad's moment system as it overcomes potentially negative densities and potential loss of hyperbolicity by incorporating higher order approximations.

4 MULTISCALE HIERARCHY: MODEL ADAPTIVITY

Moment-closure systems potentially offer efficient hierarchical approximations of the Boltzmann equation, by exploiting the fact that its solutions converge to functions in a particular class, the equilibrium distributions. Adaptivity between the Boltzmann equation (micro model) and the Euler equations (macro model) has been propounded by several authors, e.g., E and Engquist [18]. However, no methodology to this purpose has been developed so far. The scale disparity between the Euler equations and the Boltzmann equations is enormous, which renders direct adaptivity between these two models infeasible. The hierarchy of moment-closure systems can be conceived of as a gradual transition from the Euler equations to the Boltzmann equations. The goal-oriented error estimate provides a systematic refinement criterion.

This section aims to explore the potential opportunities provided by the hierarchical structure of the moment equations in (13) for numerical approximation of the Boltzmann equation, more specifically, for goal-oriented model adaptivity.

4.1 Towards Goal-Oriented Model Adaptivity

The general procedure for performing goal-oriented adaptivity consists of repeated application of the following operations [19]:

$\mathsf{SOLVE} \to \mathsf{ESTIMATE} \to \mathsf{MARK} \to \mathsf{REFINE}$

Given an initial mesh, the first step concerns the solution of the finite-element problem on that mesh. The second step is the construction of a computable a-posteriori estimate of the error in the finite-element approximation, based on the current approximation and exogenous data. In the third step, the error estimate is decomposed into element-wise contributions, and the elements which yield the largest contributions to the error in the goal functional are marked according to some marking strategy. In the final stage, the marked elements are refined.

In the context of the hierarchy of moment-closure systems, it is envisaged that the above procedure can be extended to include both mesh-adaptivity and hierarchical-rank adaptivity. That is, not only estimate the error in the numerical solution, but also the error in the moment-closure system itself. Accordingly, the adaptive procedure locally adapts the element size and the hierarchical rank to arrive at an optimal approximation. The challenges in the development of the a-posteriori error estimate and the adaptive-refinement procedure, are the construction of a computable error estimate for the moment-closure hierarchy, and the (nonstandard) decomposition of the error into contributions from the model error (i.e., the finite rank of the considered moment-closure system) and the finite-element approximation error (i.e., the finite mesh width). For the a posteriori error estimation, one could employ duality-based techniques [20–22]. Moreover, by virtue of the fact that moment-closure systems assume the form of a hierarchy of hyperbolic systems, the discontinuous-Galerkin formulation is well suited to discretize these systems, and element-wise refinement indicators can then be derived in a similar manner as in [23].

5 CONCLUSION

The enormous potential of moment-closure approximations of the Boltzmann equation in the context of numerical-approximation techniques, lies in the fact that such approximations assume the form of a hierarchy of systems of hyperbolic partial-differential equations, which puts the full arsenal of approximation techniques for this class of problems at our disposal, in particular, (goal-)adaptive finite-element methods based on a-posteriori error estimates. The hierarchical structure of the moment-closure systems, engendered by the inclusion relation acting on the polynomials, implies that the solution of each system can be regarded as an approximation to the solution to the next member in the hierarchy. Hence, by virtue of the hierarchical structure, a-posteriori error estimates can be constructed by evaluating the residual of the next member in the hierarchy. Based on this observation, we propounded an adaptive numerical approach, in which not only the mesh width and order of approximation in the finite-element method are locally adapted for one particular moment-closure system, but in which also the hierarchical rank of the moment-system is locally adapted, in accordance with an a-posteriori error estimate.

REFERENCES

- [1] L. Saint-Raymond. *Hydrodynamic Limits of the Boltzmann Equation*. Number v. 1971 in Lecture Notes in Mathematics. Springer, 2009.
- [2] A. Klenke. Probability Theory: A Comprehensive Course. Universitext (1979). Springer, 2008.
- [3] H. Grad. On the kinetic theory of rarefied gases. Communications on Pure and Applied Mathematics, 2(4):331407, 1949.
- [4] C. Levermore. Moment closure hierarchies for kinetic theories. Journal of Statistical Physics, 83:10211065, 1996.
- [5] C. Schmeiser and A. Zwirchmayr. Convergence of Moment Methods for Linear Kinetic Equations. SIAM Journal on Numerical Analysis, 36(1):pp. 7488, 1998.
- [6] H. Struchtrup. Macroscopic Transport Equations for Rarefied Gas Flows: Approximation Methods in Kinetic Theory. Interaction of Mechanics and Mathematics Series. Springer, 2005.
- [7] T. Elmroth. Global boundedness of moments of solutions of the Boltzmann equation for forces of infinite range. Archive for Rational Mechanics and Analysis, 82:112, 1983.
- [8] M.R.A. Abdel Malik and E.H. van Brummelen. Numerical approximation of the boltzmann equation: Moment closure. Technical Report 12-30, Eindhoven University of Technology, 2012.

- [9] F. Brini. Hyperbolicity region in extended thermodynamics with 14 moments. Continuum Mechanics and Thermodynamics, 13:18, 2001.
- [10] M. Torrilhon. Characteristic waves and dissipation in the 13-moment-case. Continuum Mechanics and Thermodynamics, 12:289301, 2000.
- [11] M. Junk. Domain of Definition of Levermore's Five-Moment System. Journal of Statistical Physics, 93:11431167, 1998.
- [12] M. Junk. Maximum entropy for reduced moment problems. Mathematical Models and Methods in Applied Sciences, 10:10011025, 2000.
- [13] J. Schneider. Entropic approximation in kinetic theory. ESAIM. Mathematical Modelling and Numerical Analysis, 38:541561, 2004.
- [14] V. Pavan. General Entropic Approximations for Canonical Systems Described by Kinetic Equations. *Journal of Statistical Physics*, 142:792827, 2011.
- [15] M. Junk and A. Unterreiter. Maximum entropy moment systems and Galilean invariance. Continuum Mechanics and Thermodynamics, 14:563576, 2002.
- [16] J.B. Lasserre. Moments, Positive Polynomials and Their Applications. Imperial College Press Optimization Series. Imperial College Press, 2010.
- [17] W. Dreyer, M. Junk, and M. Kunik. On the Approximation of Kinetic Equations By Moment Systems. *Nonlinearity*, 14, 2000.
- [18] E W. and B. Engquist. The heterognous multiscale methods. Comm. Math. Sci, 1:87132, 2003.
- [19] W. Dörfler. A convergent adaptive algorithm for poisson's equation. SIAM Journal on Numerical Analysis, 33(3):1106–1124, 1996.
- [20] M. Ainsworth and J.T. Oden. A Posteriori Error Estimation in Finite Element Analysis. Pure and Applied Mathematics: A Wiley Series of Texts, Monographs and Tracts. Wiley, 2011.
- [21] W. Bangerth and R. Rannacher. Adaptive Finite Element Methods for Differential Equations. Lectures in Mathematics. Birkhuser Basel, 2003.
- [22] Endre Süli. A posteriori error analysis and adaptivity for finite element approximations of hyperbolic problems. In Dietmar Krner, Mario Ohlberger, and Christian Rohde, editors, An Introduction to Recent Developments in Theory and Numerics for Conservation Laws, volume 5 of Lecture Notes in Computational Science and Engineering, page 123194. Springer Berlin Heidelberg, 1999.

[23] W. Hoitinga. Goal Adaptive Discretization of a One-dimensional Boltzmann Equation. PhD thesis, 2011.