NAS Technical Report
NAS-06-006
July 2006

On Discontinuous Galerkin Approximations of Boltzmann Moment Systems With Levermore Closure

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Abstract

This work considers the discontinuous Galerkin (DG) finite element discretization of first-order systems of conservation laws derivable as moments of the kinetic Boltzmann equation with Levermore (1996) closure. Using standard energy analysis techniques, a new class of energy stable numerical flux functions are devised for the DG discretization of Boltzmann moment systems. Simplified energy stable numerical fluxes are then constructed which replace exact state space integration in the numerical flux with Gauss-Lobatto quadrature. Numerical results for supersonic flow over a cylinder geometry in the continuum and transistional regimes using 5 and 10 moment approximations are presented using the newly devised DG discretizations.

Key words: Nonlinear Conservation Laws, Kinetic Boltzmann Equation, Levermore Boltzmann Moment Closure, Entropy Symmetrization, Discontinuous Galerkin Finite Element Method

1 Introduction

Gases are frequently modeled as either a collection of particles described in terms of position and velocity or as a continuum media modeled in terms macroscopic quanties such as density, temperature, and velocity. The Boltzmann equation describes the evolution of particle distributions. This equation is efficiently solved using direct simulation Monte Carlo (DSMC) methods when particles in the gas have a mean free path that is large relative to some characteristic macroscopic length scale, see Bird (1994). Dense gases with short

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Preprint accepted to appear in Computer Methods in Applied Mechanics and Engineering

mean free path are well described and efficiently solved using macroscopic continuum descriptions such as the Navier-Stokes equations. An important parameter in characterizing the applicability and efficiency of each model is the Knudsen number defined as the ratio of the particle mean free path distance to the characteristic macroscopic length scale. As the Knudsen number increases the validity of continuum models such as the Navier-Stokes equations deteriorates. As the Knudsen number decreases, the arithmetic complexity of the DSMC method increases rapidly. Difficulties arise in the "transitional" regime when the Knudsen number is of the order 10^{-3} to 10^{-1}. In this regime, DSMC methods are too expensive and the Navier-Stokes equations too inaccurate. To overcome this computational difficulty, various extended macroscopic models have been proposed that are constructed by taking a finite sequence of moments of the Boltzmann equation together with a closure assumption. This extends the range of applicability of continuum approximations into the transitional regime. An early example of such a closed system is the 13 moment model due to Grad (1949). Unfortunately, this model exhibits a loss of hyperbolicity in certain flow regimes and is generally not used in numerical simulations. More recently, Levermore (1996) has suggested a closure assumption based on a *minimum entropy principle*. An important property of Boltzmann moment systems with Levermore closure is the guarantee of hyperbolicity using a canonical exponential conjugate entropy. This structure is exploited in the remainder of this paper in both the analysis and the construction of energy stable DG discretizations for Boltzmann moment systems. Although special consideration is given here to moment systems that are extensions of the Euler and Navier-Stokes equations, the Levermore closure technique has been applied to a wide variety of particle-continuum problems ranging from relativistic gas dynamics with gravitation as discussed in Banach (2003) to semiconductor device simulation, see Anile and Hern (2002).

Discretization techniques for Boltzmann moment systems have been developed previously in LeTallec and Perlat (1997); Junk (1997); Struchtrup (2000). Stable discretizations have been constructed using "half fluxes" obtained by splitting the Boltzmann equation and then taking moments. If exact integration is used for particle phase space integrations, the half fluxes used in these methods then reduce to the kinetic flux vectors previously developed by Deshpande (1986b) in the special case of polytropic gases. Using half fluxes together with first order upwind differencing, LeTallec and Perlat prove that numerical solutions satisfy a discrete entropy inequality and are guaranteed to have positive fluid density. This paper considers numerical discretization of Boltzmann moment systems using the discontinuous Galerkin finite method. As will be shown, the DG formulation permits discretization on arbitrary unstructured meshes using arbitrary order polynomial approximation while retaining a discrete entropy inequality property. The present work differs significantly from the previous work in several respects. Unlike the previous methods, symmetrization variables are used as the basic unknowns. These

variables play a central role in the Levermore closure theory. For the steady-state calculations shown later, the entire discontinuous Galerkin method has been implemented in these symmetric variables so that the transformation to and from the macroscopic conservation variables in never needed except for the specification of initial data and in some instances specification of boundary data. This is a major practical consideration since the calculation of the conservation variables from the symmetrization variables can be problematic as well as expensive. Although the computation of conservation law variables from symmetrization variables is a direct integration in particle phase space, the transformation from conserved variables to symmetrization variables is not. LeTallec and Perlat suggest a numerical minimization procedure for this purpose. Unfortunately, even though the function to be minimized in this procedure is convex, Junk (1998) shows that this minimization can fail because the domain of definition in the minimization is not convex. Using generalizations of Maxwellian and Gaussian distributions, this realizability problem becomes most important when moments involving polynomials of degree greater than two are used. The present work also develops an alternative to the half fluxes described above. The new flux formula utilizes mean value linearization via path integation in state space and flux difference splitting. Using this numerical flux, we prove a rigorous discrete entropy inequality and prove that the path integration can be replaced by Gauss-Lobatto quadrature without sacrificing the discrete entropy inequality property.

2 Background

Consider the Cauchy initial value problem for a system of m coupled first-order differential equations in d space coordinates and time which represents a conservation law process. Let $\mathbf{u}(x,t) : \mathbb{R}^d \times \mathbb{R}^+ \mapsto \mathbb{R}^m$ denote the dependent solution variables and $\mathbf{f}(\mathbf{u}) : \mathbb{R}^m \mapsto \mathbb{R}^{m\times d}$ the flux vector. The model Cauchy problem is then given by

$$\begin{cases} \mathbf{u}_{,t} + \mathbf{f}_{i,x_i} = 0 \\ \mathbf{u}(x,0) = \mathbf{u}_0(x) \end{cases} \tag{1}$$

with implied summation on the index $i = 1, \ldots, d$. Additionally, the system is assumed to possess a convex scalar entropy extension. Let $U(\mathbf{u}) : \mathbb{R}^m \mapsto \mathbb{R}$ and $F(\mathbf{u}) : \mathbb{R}^m \mapsto \mathbb{R}^d$ denote an entropy-entropy flux pair for the system such that in addition to (1) the following inequality holds

$$U_{,t} + F_{i,x_i} \leq 0 \tag{2}$$

with equality for classical (smooth) solutions. In the symmetrization theory for first-order conservation laws Godunov (1961); Mock (1980); Harten (1983), one seeks a mapping $\mathbf{u}(\mathbf{v}) : \mathbb{R}^m \mapsto \mathbb{R}^m$ applied to (1) so that when transformed

$$\mathbf{u}_{,\mathbf{v}}\mathbf{v}_{,t} + \mathbf{f}_{i,\mathbf{v}}\,\mathbf{v}_{,x_i} = 0 \tag{3}$$

the matrix $\mathbf{u}_{,\mathbf{v}}$ is symmetric positive definite (SPD) and the matrices $\mathbf{f}_{i,\mathbf{v}}$ are symmetric. Clearly, if twice differentiable functions $\mathcal{U}(\mathbf{v}) : \mathbb{R}^m \mapsto \mathbb{R}$ and $\mathcal{F}_i(\mathbf{v}) : \mathbb{R}^m \mapsto \mathbb{R}$ can be found so that

$$\mathbf{u} = \mathcal{U}^T_{,\mathbf{v}}, \quad \mathbf{f}_i = \mathcal{F}^T_{i,\mathbf{v}} \tag{4}$$

then the matrices

$$\mathbf{u}_{,\mathbf{v}} = \mathcal{U}_{,\mathbf{vv}}, \quad \mathbf{f}_{i,\mathbf{v}} = \mathcal{F}_{i,\mathbf{vv}}$$

are symmetric. Further, we shall require that $\mathcal{U}(\mathbf{v})$ be a convex function such that

$$\lim_{\mathbf{v}\to\infty} \frac{\mathcal{U}(\mathbf{v})}{|\mathbf{v}|} = +\infty \tag{5}$$

so that $U(\mathbf{u})$ can be interpreted as a Legendre transform of $\mathcal{U}(\mathbf{v})$

$$U(\mathbf{u}) = \sup_{\mathbf{v}} \{\mathbf{v}\cdot\mathbf{u} - \mathcal{U}(\mathbf{v})\} \quad .$$

From (5), it follows that $\exists\, \mathbf{v}^* \in \mathbb{R}^m$ such that $\mathbf{v}\cdot\mathbf{u} - \mathcal{U}(\mathbf{v})$ achieves a maximum at $\mathbf{v}^*$

$$U(\mathbf{u}) = \mathbf{v}^*\cdot\mathbf{u} - \mathcal{U}(\mathbf{v}^*) \quad . \tag{6}$$

At this maximum $\mathbf{u} = \mathcal{U}_{,\mathbf{v}}(\mathbf{v}^*)$ which can be locally inverted to the form $\mathbf{v}^* = \mathbf{v}(\mathbf{u})$. Elimination of $\mathbf{v}^*$ in (6) yields the simplified duality relationship

$$U(\mathbf{u}) = \mathbf{v}(\mathbf{u})\cdot\mathbf{u} - \mathcal{U}(\mathbf{v}(\mathbf{u})) \quad .$$

Differentiation of this expression

$$U^T_{,\mathbf{u}} = \mathbf{v} + \mathbf{v}_{,\mathbf{u}}\mathbf{u} - \mathbf{v}_{,\mathbf{u}}\,\mathcal{U}^T_{,\mathbf{v}} = \mathbf{v} \tag{7}$$

gives an explicit formula for the entropy variables $\mathbf{v}$ in terms of derivatives of the entropy function $U(\mathbf{u})$. Using the mapping relation $\mathbf{v}(\mathbf{u})$, a duality pairing for entropy flux components is defined

$$F_i(\mathbf{u}) = \mathbf{v}(\mathbf{u}) \cdot \mathbf{f}_i(\mathbf{u}) - \mathcal{F}_i(\mathbf{v}(\mathbf{u})) \ .$$

Differentiation then yields the flux relation

$$F_{i,\mathbf{u}} = \mathbf{v} \cdot \mathbf{f}_{i,\mathbf{u}} + \mathbf{v}_{,\mathbf{u}} \mathbf{f}_i - \mathbf{v}_{,\mathbf{u}} \mathcal{F}_{i,\mathbf{v}}^T = \mathbf{v} \cdot \mathbf{f}_{i,\mathbf{u}}$$

and the fundamental relationship for classical solutions

$$\mathbf{v} \cdot (\mathbf{u}_{,t} + \mathbf{f}_{i,x_i}) = U_{,t} + F_{i,x_i} = 0 \ .$$

Discrete versions of this relationship are often exploited in the energy analysis of numerical methods for scalar and system conservation laws, e.g. Galerkin least-squares finite element analysis as in Hughes et al. (1986); Hughes and Mallet (1986); Shakib (1988); Szepessy (1989); Johnson and Szepessy (1990), finite volume analysis such as given in Osher (1984a); Schonbek (1985); Merriam (1988); Tadmor (1987); Perthame (1990); Sonar (1992); LeFloch et al. (2002), and discontinuous Galerkin analysis as presented in Jiang and Shu (1994); Cockburn and Shu (1997); Barth (1998). This latter analysis for the DG method is discussed in detail for systems of conservation laws in Sect. 3.

2.1 Boltzmann Moment Closure

Consider the particular case of moment systems derived from the kinetic Boltzmann equation with Levermore (1996) closure. Boltzmann's equation is given by

$$f(x, v, t)_{,t} + v \cdot \nabla_x f(x, v, t) = C(f)(x, v, t) \ ,$$

with $f(x, v, t)$ a nonnegative density function, $v \in \mathbb{R}^d$ the particle velocity, and $C(f) : \mathbb{R} \mapsto \mathbb{R}$ the collision operator. Moment systems are obtained by integrating the Boltzmann equation in velocity space over a vector $\mathbf{m}(v)$ of linearly independant polynomials in velocity,

$$\langle\!\langle \mathbf{m}\, f \rangle\!\rangle_{,t} + \langle\!\langle v_i\, \mathbf{m}\, f \rangle\!\rangle_{,x_i} = \langle\!\langle \mathbf{m}\, C(f) \rangle\!\rangle \tag{8}$$

where $\langle\!\langle \psi \rangle\!\rangle$ denotes the integral of a measurable function ψ over velocity space. Without further assumption, the fluxes $\langle\!\langle v_i\, \mathbf{m}\, f \rangle\!\rangle$ cannot be expressed as functions of $\mathbf{u} = \langle\!\langle \mathbf{m}\, f \rangle\!\rangle$. The closure of the system is performed by assuming that

the distribution function f has a prescribed form, $f = f_{\mathrm{B}}(\mathbf{u})$, given by the *minimum entropy principle*

$$H[f_{\mathrm{B}}] = \min\{H[g] \mid \langle\!\langle g\,\mathbf{m}\rangle\!\rangle = \mathbf{u}\} \tag{9}$$

where $H[g] = \langle\!\langle g \ln g\rangle\!\rangle$ is Boltzmann's celebrated H-function. Since H is a convex function, the minimization problem (9) is formally equivalent to

$$f_{\mathrm{B}} = \exp(\mathbf{v}\cdot\mathbf{m})$$

where $\mathbf{v} = \mathbf{v}(\mathbf{u})$ serves as the Lagrange multiplier associated with the constraint $\langle\!\langle g\,\mathbf{m}\rangle\!\rangle = \mathbf{u}$ or equivalently under the closure assumption

$$\mathbf{u} = \langle\!\langle \mathbf{m}\,\exp(\mathbf{v}\cdot\mathbf{m})\rangle\!\rangle \ .$$

The moment system (8) can then be rewritten as

$$\mathbf{u}_{,t} + \mathbf{f}_{i,x_i} = \mathbf{r}(\mathbf{u}) \tag{10}$$

with

$$\mathbf{f}_i = \langle\!\langle v_i\,\mathbf{m}\,\exp(\mathbf{v}\cdot\mathbf{m})\rangle\!\rangle \ . \tag{11}$$

Observe that using the kinetic Boltzmann structure, we have that

$$\mathcal{U}(\mathbf{v}) = \langle\!\langle f_{\mathrm{B}}\rangle\!\rangle = \langle\!\langle \exp(\mathbf{v}\cdot\mathbf{m})\rangle\!\rangle \tag{12}$$

is a suitable conjugate entropy function and that

$$U(\mathbf{u}) = \langle\!\langle (\mathbf{v}(\mathbf{u})\cdot\mathbf{m} - 1)\,\exp(\mathbf{v}(\mathbf{u})\cdot\mathbf{m})\rangle\!\rangle \tag{13}$$

is the corresponding entropy function so that the duality relationship (2) holds.

A well-known moment system is obtained by selecting $\mathbf{m}(v) = (1, v, |v|^2/2)^T$ corresponding to mass, momentum, and kinetic energy. In this instance, the collision integral vanishes identically ($\mathbf{r}(\mathbf{u}) = 0$) and (10) reduces to the system of Euler equations (5 moments) for a monotonic gas. More complex systems with 10, 14 or 35 moments have been considered in the literature, c.f. Groth et al. (1995); Levermore (1996); LeTallec and Perlat (1997). In Appendix A, the compressible Euler equations for a γ-law (polytropic) gas are readily obtained by increasing the dimension of the particle velocity integration space to include internal energy I and utilizing the moments $\mathbf{m}(v, I) = (1, v, |v|^2/2 + I^\delta)^T$ for $\delta = (1/(\gamma-1) - d/2)^{-1}$.

3 The DG Finite Element Method

Let Ω denote a spatial domain composed of stationary nonoverlapping elements K_i, $\Omega = \cup K_i$, $K_i \cap K_j = \emptyset$, $i \neq j$ and time slab intervals $I^n \equiv [t_+^n, t_-^{n+1}], n = 0, \ldots, N-1$. Both continuous in time approximation and full space-time approximation on tensor space-time elements $K_i \times I^n$ will be considered in the analysis. It is useful to also define the element set $\mathcal{T} = \{K_1, K_2, \ldots\}$ and the interface set $\mathcal{E} = \{e_1, e_2, \ldots\}$ with interface members $\overline{K}_i \cap \overline{K}_j, i \neq j$ of measure $d-1$ corresponding to edges in 2-D and faces in 3-D. For brevity, we avoid the introduction of trace operators and instead use a shorthand notation for trace quantities associated with an interface with normal $\mathbf{n}$, i.e. $f_\pm \equiv \lim_{\epsilon \to 0} f(\mathbf{v}(\mathbf{x} \pm \epsilon \mathbf{n}))$, $\langle f \rangle_-^+ \equiv (f_- + f_+)/2$ and $[f]_-^+ = f_+ - f_-$. Let $\mathcal{P}_k(Q)$ denote the set of polynomials of degree at most k in a domain $Q \subset \mathbb{R}^d$. In the discontinuous Galerkin method, the approximating functions are discontinuous polynomials in both space and time

$$\mathcal{V}^h = \left\{ \mathbf{w} \,|\, \mathbf{w}_{|_{K \times I^n}} \in \left(\mathcal{P}_k(K \times I^n) \right)^m \;\; , \forall K \in \mathcal{T}, n = 0, \ldots, N-1 \right\} \;\; .$$

Alternatively, Cockburn et al. (1989, 1990); Shu (1999) utilize a semi-discrete formulation of the DG method together with Runge-Kutta time integration. In this case, the set of approximating functions are discontinuous polynomials in space and continuous functions in time denoted by $\mathcal{V}_c^h$.

For ease of exposition, the spatial domain Ω is assumed either periodic in all space dimensions or nonperiodic with compactly supported initial data. This purposely avoids analysis of boundary conditions for Boltzmann moment systems which is somewhat delicate and beyond the scope of this paper. Furthermore, the inclusion of boundary conditions into the analysis is not anticipated to effect the design of interior numerical fluxes. Next, consider the first-order Cauchy initial value problem

$$\begin{cases} \mathbf{u}_{,t} + \mathbf{f}_{i,x_i} = 0 \\ \mathbf{u}(x, t_-^0) = \mathbf{u}_0(x) \end{cases} \tag{14}$$

with convex entropy extension

$$U_{,t} + F_{i,x_i} \leq 0 \;\; . \tag{15}$$

The DG method for the time interval $[t_+^0, t_-^N]$ with weakly imposed initial data $\mathbf{v}_h(x, t_-^0)$ obtained from a suitable projection of the initial data $\mathbf{v}(\mathbf{u}_0(x))$ is given by the following statement:

DG FEM: Find $\mathbf{v}_h \in \mathcal{V}^h$ such that

$$B_{\mathrm{DG}}(\mathbf{v}_h, \mathbf{w}) = 0 \ , \ \forall\, \mathbf{w} \in \mathcal{V}^h \tag{16}$$

with

$$\begin{aligned} B_{\mathrm{DG}}(\mathbf{v}, \mathbf{w}) = \sum_{n=0}^{N-1} \Bigg(& \sum_{K \in \mathcal{T}} \int\!\!\int_{I^n K} -(\mathbf{u}(\mathbf{v}) \cdot \mathbf{w}_{,t} + \mathbf{f}_i(\mathbf{v}) \cdot \mathbf{w}_{,x_i})\, dx\, dt \\ & + \sum_{K \in \mathcal{T}} \int_{I^n} \int_{\partial K} \mathbf{w}(x_-) \cdot \mathbf{h}(\mathbf{v}(x_-), \mathbf{v}(x_+); \mathbf{n})\, ds\, dt \\ & + \sum_{K \in \mathcal{T}} \int_K \left(\mathbf{w}(t_-^{n+1}) \cdot \mathbf{u}(\mathbf{v}(t_-^{n+1})) - \mathbf{w}(t_+^n) \cdot \mathbf{u}(\mathbf{v}(t_-^n)) \right) dx \Bigg) \end{aligned} \tag{17}$$

with suitable modifications (not shown here) when source terms are present. In this statement $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) : \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}^d \mapsto \mathbb{R}^m$ denotes a numerical flux function, a vector-valued function of two interface states $\mathbf{v}_\pm$ and an oriented interface normal $\mathbf{n}$ with the following consistency and conservation properties:

- Consistency with the true flux, $\mathbf{h}(\mathbf{v}, \mathbf{v}; \mathbf{n}) = \mathbf{f}(\mathbf{v}) \cdot \mathbf{n}$
- Discrete cell conservation, $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = -\mathbf{h}(\mathbf{v}_+, \mathbf{v}_-; -\mathbf{n})$.

For a given symmetrizable system with entropy function $U(\mathbf{u})$, the DG method is uniquely specified once $\mathcal{V}^h$, the entropy function $U(\mathbf{u})$, and the numerical flux function $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ are chosen. In this formulation, the finite-dimensional space of symmetrization variables $\mathbf{v}_h$ are the basic unknowns in the trial space $\mathcal{V}^h$ and the dependent variables are then derived via $\mathbf{u}(\mathbf{v}_h)$. When not needed for clarity, this mapping is sometimes explicitly omitted, e.g. $U(\mathbf{v}_h)$ is written rather than $U(\mathbf{u}(\mathbf{v}_h))$. An important product of the DG energy analysis given below are sufficient conditions to be imposed on the numerical flux so that discrete entropy inequalities and total entropy bounds of the following form are obtained for the discretization of the Cauchy initial value problem:

- A local cell entropy inequality assuming continuous in time approximation, $\mathbf{v}_h \in \mathcal{V}_c^h$

  $$\frac{d}{dt} \int_K U(\mathbf{v}_h)\ dx + \int_{\partial K} \overline{F}(\mathbf{v}_{-,h}, \mathbf{v}_{+,h}; \mathbf{n})\, ds \leq 0 \ , \quad \text{for each } K \in \mathcal{T} \tag{18}$$

  where $\overline{F}(\mathbf{v}_{-,h}, \mathbf{v}_{+,h}; \mathbf{n})$ denotes a conservative numerical entropy flux. Summing over all elements then yields the global inequality

  $$\frac{d}{dt} \int_\Omega U(\mathbf{v}_h)\, dx \leq 0 \ . \tag{19}$$

- A total entropy bound assuming full space-time approximation, $\mathbf{v}_h \in \mathcal{V}^h$

$$\int_\Omega U(\mathbf{u}^*(t_-^0))\; dx \leq \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^N)))\, dx \leq \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^0))\, dx \qquad (20)$$

where $\mathbf{u}^*(t_-^0)$ denotes the minimum total entropy state of the projected initial data

$$\mathbf{u}^*(t_-^0) \equiv \frac{1}{\text{meas}(\Omega)} \int_\Omega \mathbf{u}(\mathbf{v}_h(x,t_-^0))\, dx \;\; .$$

Under the assumption that the symmetrizer $\mathbf{u}_{,\mathbf{v}}$ remains positive definite and spectrally bounded in space-time, i.e. there exist positive constants c_0 and C_0 independent of $\mathbf{v}_h$ such that

$$0 < c_0 \left\|\mathbf{z}\right\|^2 \leq \mathbf{z} \cdot \mathbf{u}_{,\mathbf{v}}(\mathbf{v}_h(x,t))\, \mathbf{z} \leq C_0 \left\|\mathbf{z}\right\|^2$$

for all $\mathbf{z} \neq 0$, the following L_2 stability result is then readily obtained for the Cauchy problem

$$\left\|\mathbf{u}(\mathbf{v}_h(\cdot,t_-^N)) - \mathbf{u}^*(t_-^0)\right\|_{L_2(\Omega)} \leq (c_0^{-1}C_0)^{1/2} \left\|\mathbf{u}(\mathbf{v}_h(\cdot,t_-^0)) - \mathbf{u}^*(t_-^0)\right\|_{L_2(\Omega)} \;\; .$$

3.1 DG Energy Analysis for Conservation Law Systems

Consider the DG method applied to the nonlinear system (14). An energy analysis assuming continuous in time functions, $\mathbf{v}_h \in \mathcal{V}_c^h$, yields the semi-discrete cell-wise entropy inequality (18) whenever the numerical flux satisfies certain properties dictated by the energy analysis. Specifically, the following semi-discrete cell entropy theorem extends the previous DG scalar conservation law energy analysis in Jiang and Shu (1994); Jaffre et al. (1995) to symmetrizable systems using the symmetrization theory given in Sect. 2. This result is also given in Cockburn and Shu (1997) using a different proof technique. The semi-discrete results are then generalized to full space-time in Theorem 2 using the concept of a minimum entropy state.

Theorem 1 (DG Semi-Discrete Cell Entropy Inequality) *Let* $\mathbf{v}_h \in \mathcal{V}_c^h$ *denote a numerical solution obtained using the discontinuous Galerkin method (17) assuming a continuous in time approximation for the Cauchy initial value problem (14) with convex entropy extension (15). Assume the numerical flux* $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ *satisfies the system E-flux condition*

$$[\mathbf{v}]_-^+ \cdot (\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n}) \leq 0 \;\; , \quad \forall \theta \in [0,1] \qquad (21)$$

where $\mathbf{v}(\theta) = \mathbf{v}_- + \theta\; [\mathbf{v}]_-^+$. *The numerical solution* $\mathbf{v}_h$ *then satisfies the local*

semi-discrete cell entropy inequality

$$\frac{d}{dt}\int_K U(\mathbf{v}_h)\ dx + \int_{\partial K} \overline{F}(\mathbf{v}_{-,h}, \mathbf{v}_{+,h}; \mathbf{n})\, ds \leq 0\ , \quad \textit{for each } K \in \mathcal{T} \tag{22}$$

with

$$\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \equiv \langle \mathbf{v} \rangle_-^+ \cdot \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \langle \mathcal{F} \cdot \mathbf{n} \rangle_-^+ \tag{23}$$

as well as the global semi-discrete entropy inequality

$$\frac{d}{dt}\int_\Omega U(\mathbf{v}_h)\ dx \leq 0\ . \tag{24}$$

Proof: Evaluate the energy, $B_{\mathrm{DG}}(\mathbf{v}_h, \mathbf{v}_h)$, for a single stationary element K assuming continuous in time functions

$$\begin{aligned}
\int_K \mathbf{v} \cdot \mathbf{u}_{,t}\ dx &= \frac{d}{dt}\int_K U\, dx \\
&= -\left(\int_K -\mathbf{v}_{,x_i} \cdot \mathbf{f}_i\ dx + \int_{\partial K} \mathbf{v}_- \cdot \mathbf{h}\, ds \right) \\
&= -\left(\int_K -\mathcal{F}_{i,x_i}\, dx + \int_{\partial K} \mathbf{v}_- \cdot \mathbf{h}\ ds \right) \\
&= -\int_{\partial K} (-\mathcal{F}_- \cdot \mathbf{n} + \mathbf{v}_- \cdot \mathbf{h})\ ds \\
&= -\int_{\partial K} (\ \underbrace{\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})}_{\text{Conservative Flux}} + \underbrace{D(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})}_{\text{Entropy Dissipation}}\ )\ ds
\end{aligned}$$

for carefully chosen conservative entropy flux and entropy dissipation functions

$$\begin{aligned}
\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) &\equiv \langle \mathbf{v} \rangle_-^+ \cdot \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \langle \mathcal{F} \cdot \mathbf{n} \rangle_-^+ \\
D(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) &\equiv -\frac{1}{2}([\mathbf{v}]_-^+ \cdot \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - [\mathcal{F} \cdot \mathbf{n}]_-^+)\ .
\end{aligned}$$

Observe that the chosen form of $\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ is a consistent and conservative approximation to the true entropy flux $F(\mathbf{v})$

- $\overline{F}(\mathbf{v}, \mathbf{v}; \mathbf{n}) = (\mathbf{v} \cdot \mathbf{f} - \mathcal{F}) \cdot \mathbf{n} = F \cdot \mathbf{n}$ (consistency)
- $\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = -\overline{F}(\mathbf{v}_+, \mathbf{v}_-; -\mathbf{n})$ (conservation) .

The only remaining task is to determine sufficient conditions in the design of the numerical flux $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ so that $D(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \geq 0$. Rewriting the jump term appearing in the entropy dissipation term as a path integration in state space

$$\begin{aligned} D(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) &= -\frac{1}{2}([\mathbf{v}]_-^+ \cdot \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - [\mathcal{F} \cdot \mathbf{n}]_-^+) \\ &= -\frac{1}{2}[\mathbf{v}]_-^+ \cdot \left(\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \int_0^1 \mathcal{F}_{,\mathbf{v}}^T(\mathbf{v}(\theta)) \cdot \mathbf{n} \; d\theta \right) \\ &= -\frac{1}{2}[\mathbf{v}]_-^+ \cdot \left(\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \int_0^1 \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n} \; d\theta \right) \\ &= -\frac{1}{2} \int_0^1 [\mathbf{v}]_-^+ \cdot (\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n}) \; d\theta \; . \end{aligned}$$

A sufficient condition for nonnegativity of $D(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ and the local cell entropy inequality (22) when finite-dimensional subspaces are employed is that the integrand be nonpositive. This yields a system generalization of Osher's famous E-flux condition for scalar conservation laws given in Osher (1984b)

$$[\mathbf{v}]_-^+ \cdot (\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n}) \leq 0 \; , \quad \forall \theta \in [0,1] \; . \tag{25}$$

Summation of (22) over all elements in the mesh together with the conservative telescoping property of $\overline{F}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ yields the global entropy inequality (24). ■

In Sects. 3.2 and 3.3, specific examples of kinetic Boltzmann moment system E-fluxes are given. Use of the system E-flux condition in the fully-discrete space-time DG discretization is also sufficient to construct the following two-sided bound on the total entropy not previously elucidated for the DG method.

Theorem 2 (DG Fully-discrete Total Entropy Bounds) *Let $\mathbf{v}_h \in \mathcal{V}^h$ denote the space-time numerical solution obtained using the discontinuous Galerkin method (17) for the Cauchy initial value problem (14) with convex entropy extension (15). Assume the numerical flux $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ satisfies the system E-flux condition*

$$[\mathbf{v}]_-^+ \cdot (\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n}) \leq 0 \; , \quad \forall \theta \in [0,1]$$

where $\mathbf{v}(\theta) = \mathbf{v}_- + \theta \; [\mathbf{v}]_-^+$. The numerical solution $\mathbf{v}_h$ then satisfies the total

entropy bound

$$\int_\Omega U(\mathbf{u}^*(t_-^0))\; dx \le \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^N)))\, dx \le \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^0))\, dx \qquad (26)$$

where $\mathbf{u}^*(t_-^0)$ *denotes the minimum total entropy state of the initial projected data*

$$\mathbf{u}^*(t_-^0) \equiv \frac{1}{\mathrm{meas}(\Omega)} \int_\Omega \mathbf{u}(\mathbf{v}_h(x,t_-^0))\, dx \;\; .$$

Proof: Analysis of the spatial terms follows the same path taken in Theorem 1 (omitted here) with an additional integration performed in the time coordinate. Consider the energy of the remaining time evolution terms in (17) after integration-by-parts for a single time slab interval I^n

$$\begin{aligned}\int_{I^n}\int_\Omega \mathbf{v}\cdot\mathbf{u}_{,t}\, dx\, dt + \int_\Omega \mathbf{v}(t_+^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n}\; dx &= \int_\Omega \int_{I^n} U_{,t}\, dt\, dx + \int_\Omega \mathbf{v}(t_+^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n}\; dx \\ &= \int_\Omega \left([U]_{t_-^n}^{t_-^{n+1}} - [U]_{t_-^n}^{t_+^n} + \mathbf{v}(t_+^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n} \right) dx \;\; .\end{aligned}$$

Taylor series with integral remainder together with the duality relationship (2) yields

$$[U]_{t_-^n}^{t_+^n} - \mathbf{v}(t_-^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n} + R^n = 0 \;\; , \;\; R^n \equiv \int_0^1 (1-\theta)\; [\mathbf{v}]_{t_-^n}^{t_+^n} \cdot \mathbf{u}_{,\mathbf{v}}(\mathbf{v}(\theta))\, [\mathbf{v}]_{t_-^n}^{t_+^n}\, d\theta \ge 0$$

where $\mathbf{v}(\theta) = \mathbf{v}(t_-^n) + \theta\; [\mathbf{v}]_{t_-^n}^{t_+^n}$. Inserting into the time evolution terms

$$\int_{I^n}\int_\Omega \mathbf{v}\cdot\mathbf{u}_{,t}\, dx\, dt + \int_\Omega \mathbf{v}(t_+^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n}\, dx = \int_\Omega \left([U]_{t_-^n}^{t_-^{n+1}} + R^n \right) dx \;\; .$$

Summing over all time slabs, the first term on the right-hand side of this equation vanishes except for initial and final time slab contributions. Utilizing nonnegativity of the remainder terms R^n then yields the following inequality for the time evolution terms

$$\sum_{n=0}^{N-1} \left(\int_{I^n}\int_\Omega \mathbf{v}\cdot\mathbf{u}_{,t}\, dx\, dt + \int_\Omega \mathbf{v}(t_+^n)\cdot[\mathbf{u}]_{t_-^n}^{t_+^n}\, dx \right) \ge \int_\Omega \left(U(t_-^N) - U(t_-^0) \right) dx \;\; .$$

Assume satisfaction of the system E-flux condition, the spatial term analysis used in the proof of Theorem 1 reduces to the inequality

$$\sum_{n=0}^{N-1} \sum_{K\in\mathcal{T}} \sum_{K} \int_{I^n} \left(\int_K -\mathbf{v}_{,x_i} \cdot \mathbf{f}_i \; dx + \int_{\partial K} \mathbf{v}_- \cdot \mathbf{h} \, ds \right) \; dt \geq 0 \;\; .$$

Combining temporal and spatial results yields

$$0 = B_{\mathrm{DG}}(\mathbf{v},\mathbf{v}) \geq \int_\Omega \left(U(t_-^N) - U(t_-^0) \right) \; dx \;\; .$$

Hence, the desired upper bound in (26) is established when finite-dimensional subspaces are employed

$$\int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^N))) \, dx \leq \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x,t_-^0)) \, dx \;\; . \tag{27}$$

To obtain the lower bound in (26), we exploit the well-known thermodynamic concept of a *minimum total entropy state* (see for example Merriam (1988)). Define the integral average state $\mathbf{u}^*$ at time slab boundaries

$$\mathbf{u}^*(t_-^n) \equiv \frac{1}{\mathrm{meas}(\Omega)} \int_\Omega \mathbf{u}(\mathbf{v}_h(x,t_-^n)) \, dx \;\; , \quad n = 0, \ldots, N \;\; .$$

For the DG space-time discretization of the Cauchy initial value problem, $\mathbf{u}^*$ is invariant when evaluated at time slab boundaries, i.e.

$$\mathbf{u}^*(t_-^n) = \mathbf{u}^*(t_-^{n-1}) = \ldots = \mathbf{u}^*(t_-^0) \tag{28}$$

owing to discrete conservation in both space and time. A Taylor series with integral remainder expansion of the entropy function given two states $\mathbf{u}^*(t_-^n)$ and $\mathbf{u}(\mathbf{v}_h(x,t_-^n))$ for a fixed n yields

$$U(\mathbf{u}) = U(\mathbf{u}^*) + \mathbf{v}(\mathbf{u}^*) \cdot (\mathbf{u} - \mathbf{u}^*) + \int_0^1 (1-\theta))(\mathbf{u} - \mathbf{u}^*) \cdot U_{,\mathbf{uu}}(\theta)(\mathbf{u} - \mathbf{u}^*) \, d\theta \;\; .$$

When integrated over Ω, the second right-hand side term vanishes identically by the definition of $\mathbf{u}^*$

$$\int_\Omega U(\mathbf{u}) \, dx = \int_\Omega U(\mathbf{u}^*) \, dx + \int_\Omega \int_0^1 (1-\theta))(\mathbf{u} - \mathbf{u}^*) \cdot U_{,\mathbf{uu}}(\theta)(\mathbf{u} - \mathbf{u}^*) \, d\theta \, dx \;\; .$$

From strict convexity of the entropy function, it follows that $\mathbf{u}^*$ is a minimum total entropy state since $\int_\Omega U\,dx$ is minimized when $\mathbf{u} = \mathbf{u}^*$. Finally, since $\mathbf{u}^*(t_-^n)$ is constant for $n = 0, \ldots, N$, then

$$\int_\Omega U(\mathbf{u}^*(t_-^0))\;dx = \int_\Omega U(\mathbf{u}^*(t_-^N))\;dx \leq \int_\Omega U(\mathbf{u}(\mathbf{v}_h(x, t_-^N)))\,dx \;\;.$$

This establishes the lower bound in (26). ■

3.2 Kinetic Boltzmann Moment System E-Fluxes

Both Theorems 1 and 2 assume satisfaction of the system E-flux condition. A new class of system E-fluxes for the discontinuous Galerkin method is suggested by the kinetic Boltzmann moment closure flux formula (11). Following a strategy similar to that taken by Deshpande (1986b) in the different context of flux vector splitting, a kinetic mean-value (KMV) numerical flux was proposed in Barth and Charrier (2001). The following lemma shows that this flux is a valid system E-flux.

Lemma 3 (Kinetic Boltzmann Moment System E-Flux) *The kinetic mean-value (KMV) numerical flux*

$$\mathbf{h}_{\mathrm{KMV}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = \langle \mathbf{f}\cdot\mathbf{n}\rangle_-^+ - \frac{1}{2}\int_0^1 \left\langle\!\!\left| v\cdot\mathbf{n}\right|\mathbf{m}\otimes\mathbf{m}\,\exp(\mathbf{v}(\theta)\cdot\mathbf{m})\right\rangle\!\!\right\rangle\,[\mathbf{v}]_{x_-}^{x_+}\,d\theta \tag{29}$$

with $\mathbf{v}(\theta) = \mathbf{v}_- + \theta\;[\mathbf{v}]_-^+$ *satisfies the system E-flux condition*

$$[\mathbf{v}]_-^+ \cdot (\mathbf{h}_{\mathrm{KMV}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) - \mathbf{f}(\mathbf{v}(\xi))\cdot\mathbf{n}) \leq 0 \;\;, \quad \forall\,\xi\in[0,1] \;\;.$$

Proof: Consider the following identities $\forall\,\xi\in[0,1]$

$$\begin{aligned}
\frac{1}{2}\left(\mathbf{f}_+ - \mathbf{f}(\mathbf{v}(\xi))\right)\cdot\mathbf{n} &= \frac{1}{2}\int_\xi^1 \left\langle\!\!\left|(v\cdot\mathbf{n})\,\mathbf{m}\,\exp(\mathbf{v}(\theta)\cdot\mathbf{m})\right\rangle\!\!\right\rangle\cdot[\mathbf{v}]_\xi^+\,d\theta \\
&= \frac{1}{2}\int_\xi^1 \left\langle\!\!\left|(1-\xi)\,(v\cdot\mathbf{n})\,\mathbf{m}\,\exp(\mathbf{v}(\theta)\cdot\mathbf{m})\right\rangle\!\!\right\rangle\cdot[\mathbf{v}]_-^+\,d\theta \\
\frac{1}{2}\left(\mathbf{f}_- - \mathbf{f}(\mathbf{v}(\xi))\right)\cdot\mathbf{n} &= -\frac{1}{2}\int_0^\xi \left\langle\!\!\left|(v\cdot\mathbf{n})\,\mathbf{m}\,\exp(\mathbf{v}(\theta)\cdot\mathbf{m})\right\rangle\!\!\right\rangle\cdot[\mathbf{v}]_-^\xi\,d\theta
\end{aligned}$$

$$= -\frac{1}{2} \int_0^{\xi} \langle\!\langle \xi \, (v \cdot \mathbf{n}) \, \mathbf{m} \, \exp(\mathbf{v}(\theta) \cdot \mathbf{m}) \rangle\!\rangle \cdot [\mathbf{v}]_-^+ \, d\theta \ .$$

The stated lemma follows immediately from

$$\begin{aligned}
[\mathbf{v}]_-^+ \cdot (\mathbf{h}_{\mathrm{KMV}} - \mathbf{f}(\mathbf{v}(\xi)) \cdot \mathbf{n}) &= \frac{1}{2} \int_{\xi}^{1} \langle\!\langle ((1-\xi)(v \cdot \mathbf{n}) - |v \cdot \mathbf{n}|)(\mathbf{m} \cdot [\mathbf{v}]_-^+)^2 \exp(\mathbf{v}(\theta) \cdot \mathbf{m}) \rangle\!\rangle \, d\theta \\
&\quad - \frac{1}{2} \int_0^{\xi} \langle\!\langle \xi \, (v \cdot \mathbf{n}) + |v \cdot \mathbf{n}|)(\mathbf{m} \cdot [\mathbf{v}]_-^+)^2 \exp(\mathbf{v}(\theta) \cdot \mathbf{m}) \rangle\!\rangle \, d\theta \\
&\leq \frac{1}{2} \int_{\xi}^{1} (1-\xi) \, \langle\!\langle (v \cdot \mathbf{n})^- (\mathbf{m} \cdot [\mathbf{v}]_-^+)^2 \exp(\mathbf{v}(\theta) \cdot \mathbf{m}) \rangle\!\rangle \, d\theta \\
&\quad - \frac{1}{2} \int_{\xi}^{1} \xi \, \langle\!\langle (v \cdot \mathbf{n})^+ (\mathbf{m} \cdot [\mathbf{v}]_-^+)^2 \exp(\mathbf{v}(\theta) \cdot \mathbf{m}) \rangle\!\rangle \, d\theta \\
&\leq 0 \ . \ \blacksquare
\end{aligned}$$

3.3 Simplified Kinetic Boltzmann Moment System E-Fluxes

The kinetic Boltzmann moment system E-flux (29) of Sect. 3.2 requires the evaluation of the state space path integration connecting $\mathbf{v}_{\pm}$ as well as the particle integrations appearing in $\langle\!\langle \cdot \rangle\!\rangle$. Except for the simplest systems, these integrations cannot be carried out in closed form. Fortunately, the results of Theorems 1 and 2 are retained using other simpler numerical fluxes $\mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ for which the following comparison principle is satisfied, see also Barth (1998, 1999)

$$[\mathbf{v}]_-^+ \cdot \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \leq [\mathbf{v}]_-^+ \cdot \mathbf{h}_{\mathrm{KMV}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \leq [\mathbf{v}]_-^+ \cdot \mathbf{h}_{\mathrm{EFlux}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \ .$$

The following lemma presents a discrete kinetic Boltzmann moment E-flux which replaces exact path integration in state space with q-point Gauss-Lobatto quadrature.

Lemma 4 (Discrete Kinetic Boltzmann Moment E-Flux) *Let $\omega_{i,q} \in \mathbb{R}^+$ and $\xi_{i,q} \in [0,1]$ denote q-point Gauss-Lobatto quadrature weights and locations. The discrete kinetic Boltzmann moment numerical flux*

$$\mathbf{h}_{\mathrm{DKMV(q)}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = \langle \mathbf{f} \cdot \mathbf{n} \rangle_-^+ - \frac{1}{2} \, \mathbf{h}^d_{\mathrm{DKMV(q)}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) \tag{30}$$

with

$$\mathbf{h}^d_{\mathrm{DKMV(q)}}(\mathbf{v}_-,\mathbf{v}_+;\mathbf{n}) = \sum_{i=1}^{q} \omega_{i,q} \langle\!\langle |v\cdot n|\, \mathbf{m}\otimes\mathbf{m}\, \exp(\mathbf{v}(\xi_{i,q})\cdot\mathbf{m}(v))\rangle\!\rangle\, [\mathbf{v}]^+_-$$

and $\mathbf{v}(\xi_{i,q}) = \mathbf{v}_- + \xi_{i,q}\ [\mathbf{v}]^+_-$ *satisfies the system E-flux comparison principle*

$$[\mathbf{v}]^+_-\cdot\mathbf{h}_{\mathrm{DKMV(q)}}(\mathbf{v}_-,\mathbf{v}_+;\mathbf{n}) \le [\mathbf{v}]^+_-\cdot\mathbf{h}_{\mathrm{KMV}}(\mathbf{v}_-,\mathbf{v}_+;\mathbf{n})$$

for $q \ge 2$.

Proof: Begin with the definition of $\mathbf{h}^d_{\mathrm{KMV}}$ appearing in the KMV flux (29)

$$\begin{aligned}
[\mathbf{v}]^+_-\cdot\mathbf{h}^d_{\mathrm{KMV}} &= [\mathbf{v}]^+_-\cdot\int_0^1 \langle\!\langle |v\cdot\mathbf{n}|\,\mathbf{m}(v)\otimes\mathbf{m}(v)\,\exp\left(\mathbf{v}(\theta)\cdot\mathbf{m}(v)\right)\rangle\!\rangle\,[\mathbf{v}]^+_-\,d\theta \\
&= [\mathbf{v}]^+_-\cdot\langle\!\langle |v\cdot\mathbf{n}|\,\mathbf{m}(v)\otimes\mathbf{m}(v)\int_0^1 \exp\left(\mathbf{v}(\theta)\cdot\mathbf{m}(v)\right)d\theta\rangle\!\rangle\,[\mathbf{v}]^+_- \\
&= \langle\!\langle |v\cdot\mathbf{n}|\,([\mathbf{v}]^+_-\cdot\mathbf{m}(v))^2\int_0^1 \exp\left(\mathbf{v}(\theta)\cdot\mathbf{m}(v)\right)d\theta\rangle\!\rangle\ .
\end{aligned}$$

Consider the following scalar function representing the integrand of the path integration

$$g(\theta) = \exp\left(\mathbf{v}(\theta)\cdot\mathbf{m}\right)$$

followed by $2k$-times differentiation

$$g^{(2k)}(\theta) = ([\mathbf{v}]^+_-\cdot\mathbf{m})^{2k}\,\exp\left(\mathbf{v}(\theta)\cdot\mathbf{m}\right) \ge 0\ .$$

Appealing to the well known theory of q-point Gauss-Lobatto numerical quadrature with weights $\omega_{i,q}\in\mathbb{R}^+$ and locations $\xi_{i,q}\in[0,1]$ for $g(\theta)\in C^{2q-2}[0,1]$ (see for example Abramowitz and Stegun (1970))

$$\sum_{i=1}^{q}\omega_{i,q}\,g(\xi_{i,q}) - \int_0^1 g(\theta)\,d\theta = \frac{q(q-1)^3((q-2)!)^4}{(2q-1)((2q-2)!)^3}g^{(2q-2)}(\eta) \ge 0 \tag{31}$$

for some $\eta\in[0,1]$. Consequently, using Gauss-Lobatto quadrature with $q\ge 2$

$$
\begin{aligned}
[\mathbf{v}]_{x_-}^{x_+} \cdot \mathbf{h}^d_{\mathrm{KMV}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) &= [\mathbf{v}]_{x_-}^{x_+} \cdot \int_0^1 \langle\!\langle |v \cdot \mathbf{n}|\, \mathbf{m} \otimes \mathbf{m}\, \exp(\mathbf{v}(\theta) \cdot \mathbf{m}(v)) \rangle\!\rangle\, [\mathbf{v}]_-^+ d\theta \\
&\leq [\mathbf{v}]_{x_-}^{x_+} \cdot \sum_{i=1}^{q} \omega_{i,q} \langle\!\langle |v \cdot \mathbf{n}|\, \mathbf{m} \otimes \mathbf{m}\, \exp(\mathbf{v}(\xi_{i,q}) \cdot \mathbf{m}(v)) \rangle\!\rangle\, [\mathbf{v}]_-^+ \\
&= [\mathbf{v}]_{x_-}^{x_+} \cdot \mathbf{h}^d_{\mathrm{DKMV(q)}} \ .
\end{aligned}
$$

Using this result, the stated lemma is readily obtained. ■

4 Numerical Results

In this section, moment approximations are considered for a monatomic gas with density ρ, velocity $u \in \mathbb{R}^3$, and temperature θ. Two specific moment approximations considered below are

- 5 moments, $\mathbf{m}(v) = (1, v, |v|^2)^T$ with Maxwellian f

$$
f = \exp(\mathbf{v} \cdot \mathbf{m}(v)) = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(-\frac{1}{2\theta}|v-u|^2\right) \ . \tag{32}
$$

  The corresponding symmetrization variables are given by

$$
\mathbf{v} = \left(\log\left(\frac{\rho}{(2\pi\theta)^{3/2}}\right) - \frac{1}{2\theta}|u|^2, \frac{u}{\theta}, -\frac{1}{2\theta}\right)^T \ . \tag{33}
$$

  Upon performing moment integrations, all collision terms vanish yielding the Euler equations for a monatomic gas

$$
\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho u \\ \rho|u|^2 + 3\rho\theta \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho u \\ \rho u \otimes u + \rho\theta \\ \rho u(|u|^2 + 5\theta) \end{pmatrix} = 0 \ . \tag{34}
$$

- 10 moments, $\mathbf{m} = [1, v, v \otimes v]$ with Gaussian f

$$
f = \exp(\mathbf{v} \cdot \mathbf{m}(v)) = \frac{\rho}{((2\pi)^3 \det(\Theta))^{1/2}} \exp\left(-\frac{1}{2}(v-u)^T \Theta^{-1}(v-u)\right) \tag{35}
$$

where $\Theta \in \mathbb{R}^{3\times 3}$ is a symmetric positive definite generalized temperature matrix and $\theta \equiv \frac{1}{3}\mathrm{trace}(\Theta)$. In this case, the symmetrization variables are given by

$$
\mathbf{v} = \left(\log\left(\frac{\rho}{((2\pi)^3 \det(\Theta))^{1/2}}\right) - \frac{1}{2}u^T\Theta^{-1}u, \Theta^{-1}u, -\frac{1}{2}\Theta^{-1}\right)^T \ . \tag{36}
$$

The moment equations are given by

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho u\otimes u+\rho\Theta\end{pmatrix}+\nabla\cdot\begin{pmatrix}\rho u\\ \rho u\otimes u+\rho\Theta\\ \rho u\otimes u\otimes u+\rho\Theta\otimes u\end{pmatrix}=\begin{pmatrix}0\\ 0\\ Q(\rho,\Theta)\end{pmatrix} \quad (37)$$

where the right-hand side collision term has been modeled assuming Maxwell molecules as suggested in Levermore and Morokoff (1998)

$$Q(\rho,\Theta)=\frac{\rho\theta}{\mu(\theta)}(\theta\,\mathrm{I}-\Theta)$$

with the viscosity law for Argonne gas used in calculations

$$\frac{\mu}{\mu_{\mathrm{ref}}}=\left(\frac{\theta}{\theta_{\mathrm{ref}}}\right)^{.72} \quad .$$

Further details concerning these two systems can be found in Levermore and Morokoff (1998).

4.1 Velocity Space Integration

For most moment closure models involving moment polynomials of degree greater than four, it is impossible to evaluate the needed integrals $\langle\!\langle\ \cdot\ \rangle\!\rangle$ in closed form. At first glance, the prospect of approximating the velocity space integration using numerical quadrature appears computationally inefficient. Fortunately, extremely efficient quadrature formulas for the 5 and 10 moment approximations exist. For higher order moment approximations that are perturbations of these models, the numerical quadratures developed for the 5 and 10 moment models may still be very accurate approximations near equilibrium. In LeTallec and Perlat (1997), they construct optimal quadrature points and weights for polynomial moments of the Maxwellian distribution written in spherical coordinates. A different but related strategy is given here optimized for polynomial moments of the Gaussian distribution. Consider for illustrative purposes the state calculation

$$\langle\!\langle \mathbf{m}(v)\,\exp(\mathbf{m}(v)\cdot\mathbf{v})\rangle\!\rangle=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathbf{m}(v)\,\frac{\rho}{((2\pi)^3\det(\Theta))^{1/2}}\,e^{-1/2(v-u)^T\Theta^{-1}(v-u)}dv$$

Next, construct a factorization matrix $C\in\mathbb{R}^{3\times3}$ of the SPD Θ matrix

$$C^TC=2\Theta$$

for use in the linear transformation

$$v = u + C^T w$$

so that the Gaussian distribution is canonically transformed

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathbf{m}(v)\, e^{-1/2(v-u)^T\Theta^{-1}(v-u)} dv = \det(C^T) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathbf{m}(v(w))\, e^{-w\cdot w} dw$$

where $\mathbf{m}(v(w))$ remain polynomials moments if $\mathbf{m}(v)$ are polynomial moments. Optimal n-point quadrature locations and weights are obtained from roots of Hermite polynomials $H(n, w)$ and $H(n-1, w)$ with an error term depending on $2n$ derivatives of the transformed moments, see Abramowitz and Stegun (1970). For terms such as $\langle\!\langle |v \cdot \mathbf{n}| \mathbf{m}(v) \exp(\mathbf{v} \cdot \mathbf{m}(v)) \rangle\!\rangle$, a final normal aligned rotation transformation is utilized, $z = R(\mathbf{n})w$. Because $R(\mathbf{n})$ is a rotation, $w \cdot w = z \cdot z$ and

$$v \cdot n = u \cdot n + n^T C^T w = u \cdot n + n^T C^T R^T(\mathbf{n}) z = u \cdot n + \|C\, n\| z_1$$

if the chosen rotation satisfies

$$R(\mathbf{n})\, C\, n = \|C\, n\| (1, 0, 0)^T \quad .$$

This isolates all the nondifferentiability associated with $|v \cdot \mathbf{n}|$ with the transformed z_1 coordinate associated with the normal direction.

4.2 Jacobian Linearization

For implicit methods such as Newton's method, one is also often interested in derivatives of this numerical flux. Recall the discrete kinetic Boltzmann moment numerical flux proposed for the discontinuous Galerkin method after rewriting the first term

$$\begin{aligned}\mathbf{h}_{\mathrm{DKMV(q)}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = &\langle\!\langle (v \cdot \mathbf{n}) \mathbf{m}(v) (\exp(\mathbf{v}_- \cdot \mathbf{m}) + \exp(\mathbf{v}_+ \cdot \mathbf{m}))/2 \rangle\!\rangle \\ &- \frac{1}{2} \sum_{i=1}^{q} \omega_{i,q} \langle\!\langle |v \cdot n|\, \mathbf{m} \otimes \mathbf{m}\, \exp(\mathbf{v}(\xi_{i,q}) \cdot \mathbf{m}(v)) \rangle\!\rangle\, [\mathbf{v}]_-^+\end{aligned}$$

and $\mathbf{v}(\xi_{i,q}) = \mathbf{v}_- + \xi_{i,q}\, [\mathbf{v}]_-^+$. This form makes the computation of derivatives straightforward. For example, derivatives with respect to $\mathbf{v}_-$ are given by

$$\frac{\partial \mathbf{h}_{\mathrm{DKMV(q)}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})}{\partial \mathbf{v}_-} = \langle\!\langle (v \cdot \mathbf{n}) \mathbf{m} \otimes \mathbf{m} \exp(\mathbf{v}_- \cdot \mathbf{m})/2 \rangle\!\rangle$$

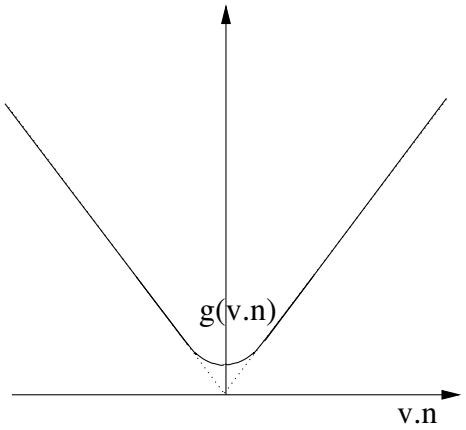


Fig. 1. Smooth upper approximation $g(v \cdot \mathbf{n})$ to the function $|v \cdot \mathbf{n}|$.

$$+\frac{1}{2}\sum_{i=1}^{q}\omega_{i,q}\langle\!\langle |v\cdot n|\,\mathbf{m}\otimes\mathbf{m}\,\exp(\mathbf{v}(\xi_{i,q})\cdot\mathbf{m})\rangle\!\rangle$$
$$-\frac{1}{2}\sum_{i=1}^{q}\omega_{i,q}(1-\xi_{i,q})\langle\!\langle |v\cdot n|\,\mathbf{m}\otimes\mathbf{m}\otimes\mathbf{m}\,\exp(\mathbf{v}(\xi_{i,q})\cdot\mathbf{m})\rangle\!\rangle\,[\mathbf{v}]_{-}^{+}$$

The second term containing $|v \cdot \mathbf{n}|$ should be rotated to a normal aligned coordinate. In addition, it should be mentioned that $|v\cdot\mathbf{n}|$ can be approximated by a smooth upper approximation without compromising the cell entropy inequality, i.e. let $g(v \cdot \mathbf{n})$ be a piecewise smooth function such that $|v \cdot \mathbf{n}| \leq g(v\cdot\mathbf{n})$, see Fig. 1. It is then straightforward to prove that the modified discrete Boltzmann moment numerical flux

$$\mathbf{h}_{\mathrm{DKMV(q)}}(\mathbf{v}_-,\mathbf{v}_+;\mathbf{n}) = \langle\!\langle (v\cdot\mathbf{n})\mathbf{m}(v)(\exp(\mathbf{v}_-\cdot\mathbf{m})+\exp(\mathbf{v}_+\cdot\mathbf{m}))/2\rangle\!\rangle$$
$$-\frac{1}{2}\sum_{i=1}^{q}\omega_{i,q}\langle\!\langle g(v\cdot n)\,\mathbf{m}\otimes\mathbf{m}\,\exp(\mathbf{v}(\xi_{i,q})\cdot\mathbf{m}(v))\rangle\!\rangle\,[\mathbf{v}]_{-}^{+}$$

is also a system E-flux as described earlier.

4.3 Discontinuous Galerkin Stabilization

All the flow fields computed below contain strong discontinuities. Except when piecewise constant polynomials are employed, numerical solutions computed with the discontinuous Galerkin method do not possess a discrete maximum (minimum) principle. Consequently, additional nonlinear stabilization is added to the baseline DG method (17) near discontinuities, see also Jaffre et al. (1995); Barth (1998). In the present calculations, the following stabilization term has been added to the method (suitably modified when source terms are

present)

$$B_{\text{Stab}}(\mathbf{v}_h, \mathbf{w}_h) = \sum_{n=0}^{N-1} \int_{I^n} \sum_{K \in \mathcal{T}^n} \int_K \epsilon_K \ \nabla \mathbf{v}_h \cdot \mathbf{u}_{,\mathbf{v}} \nabla \mathbf{w}_h \, dx \, dt \tag{38}$$

$$\epsilon_K \equiv \frac{h}{\|\nabla \mathbf{v}_h\|_{\mathbf{u},\mathbf{v},T}} \left(C_K \, R_T + h^{-1/2} \, C_{\partial K} \, R_{\partial T} \right)$$

utilizing the element interior and trace space-time residuals

$$R_K \equiv \|\text{div}(\mathbf{f}(\mathbf{v}_h))\|_{\mathbf{u}_{,\mathbf{v}}^{-1},K} \ , \ \ R_{\partial K} \equiv \|\mathbf{h}(\mathbf{v}_{-,h}, \mathbf{v}_{+,h}; \mathbf{n}) - \mathbf{f}(\mathbf{v}_{-,h}) \cdot \mathbf{n}\|_{\mathbf{u}_{,\mathbf{v}}^{-1},\partial K}$$

for chosen constants C_K and $C_{\partial K}$.

4.4 5 Moment Results

The first test problem consists of Mach=5 supersonic 2D flow over a cylinder geometry. Calculations using linear elements have been performed on an adapted simplicial mesh containing 25K 2D elements using the full 5 moment (3D) numerical flux. A 4x4x4 velocity quadrature space has been used for all particle velocity integrations except those integrations involving $|v \cdot \mathbf{n}|$ in which case 12 quadrature points have been used in the normal direction. Comparison calculations have been performed using the a Lax-Friedrichs numerical flux function (see Cockburn et al. (1990)) for a monatomic ($\gamma = 5/3$) gas. Figure 2 shows solution iso-density and Mach number contours comparing the

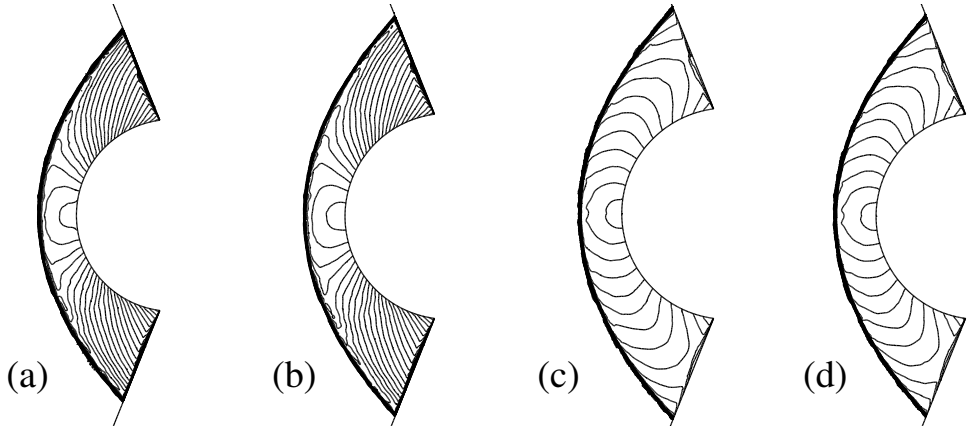


Fig. 2. Supersonic flow (Mach=5) over a cylinder geometry computed using the discontinuous Galerkin method. Solution iso-density contours using the 5 moment numerical flux are shown in (a) and Lax-Friedrichs flux in (b). Solution Mach number contours for the 5 moment numerical flux are shown in (c) and Lax-Friedrichs flux in (d).

5 moment numerical flux and the standard Lax-Friedrichs flux. Very little differences are observed between the solutions obtained using the 5 moment and Lax-Friedrichs numerical fluxes. A small solution defect is seen in the Mach number contours along the top-bottom symmetry line using both fluxes. This is frequently observed in high Mach number bow shock computations. Figure

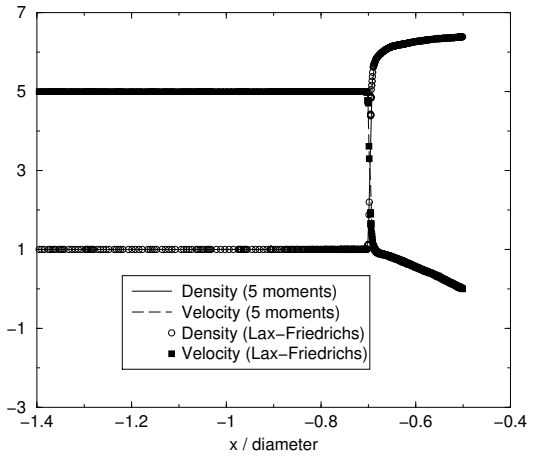


Fig. 3. Supersonic flow (Mach=5) over cylinder geometry computed using the discontinuous Galerkin method. Density and velocity sampled along the top-bottom symmetry line for solutions obtained using the 5 moment and Lax-Friedrichs fluxes.

3 graphs density and velocity profiles along the symmetry line for the solutions obtained with the 5 moment and Lax-Friedrichs numerical fluxes. Once again very little differences are observed between solutions obtained using the two numerical fluxes.

The total computing time for the 5 moment numerical flux is easily one order of magnitude larger than the compute time for the Lax-Friedrichs flux. For this particular problem, the Lax-Friedrichs flux seems the most appropriate choice. As mentioned earlier, a motivation for developing the kinetic numerical flux discussed in this paper is the ability to discretize moment approximations (usually employing moments of large polynomial degree) for which closed formed expressions of the flux function may not be possible. In these cases, the Lax-Friedrichs flux is problematic to implement.

4.5 10 Moment Results for Rarefied Gases

To validate the implementation of the 10 moment model, the 10 moment (3D) numerical flux has been used in the discontinuous Galerkin method with linear elements to compute the 1D stationary shockwave problem posed in Levermore and Morokoff (1998). Figure 4 graphs discontinuous Galerkin solution density profiles obtained for preshock Mach numbers of 1.2, 1.34, 3.0,

and 5.0. Normalized density profiles are graphed in nondimensional mean free path units x/λ. The theory predicts that smooth solutions cease to exist at a critical Mach number of 1.34 or greater. The numerical computations also predict this critical Mach number. At higher preshock Mach numbers, a small shockwave forms followed by a smooth viscous profile. Figure 4 also compares computed $M = 5$ shockwave profiles with the reduced 10 moment equations given in Levermore and Morokoff (1998) as well as DSMC calculations (see Bird (1994)) and a Navier-Stokes solution assuming no heat transfer present as discussed in the Levermore paper. The agreement between the 10 moment solution results and the reduced equation solution is excellent.

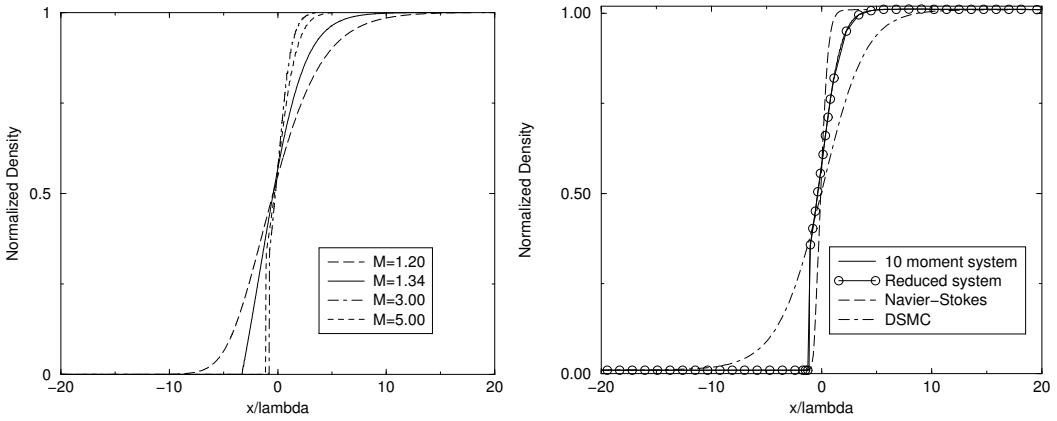


Fig. 4. Normalized density profiles for 1D shockwaves computed using the 10 moment approximation. The left figure graphs profiles obtained for various preshock Mach numbers. The right figure compares the 10 moment solution at M=5 to Navier-Stokes and DSMC calculations as well as the reduced equations given in Levermore and Morokoff (1998).

In the last numerical example, supersonic 2D flow (M=5) is computed over the sample cylinder geometry assuming 273°K Argon gas at a transistional Kudsen number of 1/10. The final adapted 2D mesh contains approximately 20K simplices. As expected at this transistional Knudsen number, the resulting

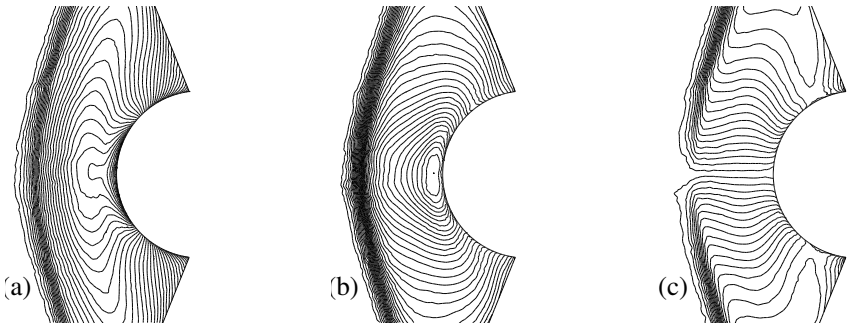


Fig. 5. Supersonic flow (Mach=5) over cylinder geometry computed using the discontinuous Galerkin method with the 10 moment model. Shown are (a) iso-density contours , (b) Θ_{11} contours, and (c) Θ_{12} contours.

contour plots show a significant thickening of the shockwave profile due to the collision model in the the 10 moment system. This effect ultimately changes the bow shock location and shape. In these calculations, we have used a slip wall boundary condition although the 10 moment equations would permit a noslip boundary condition to be imposed as well. The 10 moment numerical flux was also used for farfield imposition of data. The smooth boundary contours suggest the favorable characteristic imposition of data owing to the upwind properties of the 10 moment numerical flux.

5 Conclusions

This paper establishes sufficient conditions to be imposed on the numerical flux function so that energy stability of the discontinuous Galerkin method is obtained for the class of first-order systems obtained as moments of a Boltzmann equation with Levermore closure. The kinetic mean-value numerical flux $\mathbf{h}_{\mathrm{KMV}}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n})$ is then proposed and shown to satisfy the sufficient conditions for energy stability. The structure of Levermore closure is then further exploited so that path integration appearing in this flux can be replaced by Gauss-Lobatto quadrature without compromising energy stability of the DG method.

In ongoing work, these results are further generalized to include perturbed Levermore closures for 35 moment systems and other kinetic systems such as those occuring in radiative transfer and semi-conductor device simulation.

A The Boltzmann Moment Structure for a Polytropic Gas

For a γ-law (polytropic) gas, one has with suitable nondimensionalization

$$p = (\gamma - 1)\rho\epsilon, \quad T = (\gamma - 1)\epsilon$$

where ρ denotes fluid density, p pressure, T temperature, and ϵ the internal energy. Following Perthame (1990), we consider the following Maxwellian in $\mathbb{R}^d$ for a γ-law gas:

$$f(\rho, u, T; v, I) = \frac{\rho}{\alpha(\gamma, d)\, T^{d/2+1/\delta}}\, e^{-(|u-v|^2/2+I^\delta)/T} \tag{A.1}$$

with

$$\delta = \frac{1}{\frac{1}{\gamma-1} - \frac{d}{2}}$$

and

$$\alpha(\gamma, d) = \int_{\mathbb{R}^d} e^{-|v|^2/2} dv \cdot \int_{\mathbb{R}^+} e^{-I^\delta} dI \ .$$

Using this particular form, Perthame shows that the Euler equations for a γ-law gas are obtained as the following moments

$$\mathbf{m}(v, I) = \begin{pmatrix} 1 \\ v \\ |v|^2/2 + I^\delta \end{pmatrix} \tag{A.2}$$

so that

$$\mathbf{u} = \langle\!\langle \mathbf{m}\, f \rangle\!\rangle, \quad \mathbf{f}_i = \langle\!\langle v_i\, \mathbf{m}\, f \rangle\!\rangle, \quad \langle\!\langle \cdot \rangle\!\rangle \equiv \int_{\mathbb{R}^d} \int_{\mathbb{R}^+} (\cdot)\, dI\, dv \ .$$

The nonobvious energy moment $|v|^2/2 + I^\delta$ was devised by Perthame rather than the more standard moment $|v|^2/2+I$ (see for example Deshpande (1986a,b)) in order that a classical Boltzmann entropy $H(f) = f \ln f$ be obtained.

It is straightforward to verify that this choice of moments yields an exponential form for the conjugate entropy function

$$\mathcal{U}(\mathbf{v}) = \langle\!\langle f \rangle\!\rangle = \langle\!\langle \exp(\mathbf{v} \cdot \mathbf{m}(v, I)) \rangle\!\rangle \ .$$

Inserting the expression for δ into the temperature term appearing in the Maxwellian yields

$$f(\rho, u, T; v, I) = \frac{1}{\alpha(\gamma, d)} \frac{\rho}{T^{1/(\gamma-1)}} e^{-(|u-v|^2/2+I^\delta)/T} \ . \tag{A.3}$$

Alternatively, the expression for $\exp(\mathbf{v}\cdot\mathbf{m})$ obtained using the entropy function

$$U(\mathbf{u}) = \text{Constant} - \frac{\rho s}{(\gamma - 1)}$$

with

$$s = \ln \frac{(\gamma - 1)\varepsilon}{\rho^{\gamma-1}} + (\gamma - 1) \left(\ln \alpha + \frac{\gamma}{\gamma - 1} \right)$$

yields

$$\mathbf{v} = U^T_{,\mathbf{u}} = \begin{pmatrix} -\frac{s}{\gamma-1} - \frac{|u|^2}{2T} \\ \frac{u}{T} \\ -\frac{1}{T} \end{pmatrix} = \begin{pmatrix} \ln\left(\frac{\rho}{\alpha T^{1/(\gamma-1)}}\right) - \frac{|u|^2}{2T} \\ \frac{u}{T} \\ -\frac{1}{T} \end{pmatrix}$$

and consequently

$$\exp(\mathbf{v}\cdot\mathbf{m}(v,I)) = \frac{\rho}{\alpha T^{1/(\gamma-1)}}\, e^{-(|u-v|^2/2+I^\delta)/T} \quad .$$

Comparing with (A.3), an exponential form for the conjugate entropy function is verified

$$\mathcal{U}(\mathbf{v}) = \langle\!\langle f \rangle\!\rangle = \langle\!\langle \exp(\mathbf{v}\cdot\mathbf{m}(v,I)) \rangle\!\rangle \quad .$$

Moreover, a straightforward computation shows that

$$U(\mathbf{u}) = \langle\!\langle (\mathbf{v}\cdot\mathbf{m} - 1)\, \exp(\mathbf{v}\cdot\mathbf{m}) \rangle\!\rangle$$

so that the desired duality relationship

$$U(\mathbf{u}) + \mathcal{U}(\mathbf{v}(\mathbf{u})) = \mathbf{v}(\mathbf{u})\cdot\mathbf{u}$$

is obtained.

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