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Shock Structure Simulation Using Hyperbolic Moment Models in Partially-Conservative Form

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Abstract. The Boltzmann equation is often used to model rarefied gas flow in the transition or kinetic regime for moderate to large Knudsen numbers. However, standard moment methods like Grad's approach lack hyperbolicity of the equations. We point out the failure of Grad's method and overcome the deficiencies with the help of the new hyperbolic moment models called QBME and HME, derived by an operator projection framework.

The new model equations are in partially-conservative form meaning that a subset of the equations cannot be written in conservative form due to some changes in these equations. This leads to additional numerical difficulties. The influence of the partially-conservative terms on the solution is analyzed and we present a numerical scheme for the solution of the partially-conservative PDE systems, namely the PRICE-C scheme by Canestrelli. Furthermore, a shock structure test case is used to compare the accuracy of the different hyperbolic moment models to a discrete velocity reference solution.

The results show that the new hyperbolic models achieve higher accuracy than the standard Grad model despite the fact that the model equations cannot be fully written in conservative form.

INTRODUCTION

Many applications in rarefied gas dynamics require a solution beyond standard Navier-Stokes simulations, because rarefaction effects need to be taken into account. There are several approaches to achieve accurate solutions especially in the rarefied regime, i.e. for larger Knudsen numbers. One possibility is to extend the validity of the Navier-Stokes equations to the so-called slip regime by modification of the boundary conditions. However, this is only accurate for moderate Knudsen numbers. Another solution method is the stochastic DSMC method [1], which models paths of individual particles and their collisions to derive macroscopic quantities from the ensemble of particles. This becomes more and more costly with increasing number of particles and is thus still too expensive for most applications. Other approaches like the Lattice Boltzmann Method (LBM) have become more and more popular recently, but there are still some limitations for high Mach number flows, see e.g. [2].

The moment method aims to bridge the gap between the two approaches and derive macroscopic model equations for a larger Knudsen number. This is usually done by extending the number of variables, for example in case of the R13 equations with additional evolution equations for heat flux and stress tensor [3]. Another relatively old moment approach is Grad's method, proposed in [4]. The method is based on an expansion of the particle distribution function in velocity space and generates hierarchical moment systems. The model equations are unfortunately not hyperbolic for all values of the state vector, which can lead to unphysical solutions [5].

The maximum entropy method that was developed by Levermore [6] yields a hyperbolic moment system by construction, but it does not have an explicit flux formulation on the other hand. The computation is very difficult for a large number of moments as the solution of a costly optimization problem is necessary in every time step.

The use of a multi-variate Pearson-IV-Distribution by Torrilhon in [7] gave good results but is again difficult to generalize to the case with more higher order moments, similar to the β-closure derived by Schäerer in [8].

Recently, several new moment models have been proposed that are based on Grad's method but are globally hyperbolic which makes them promising candidates for further investigation. Among them are the Hyperbolic Moment Equation (HME) by Cai et al. [5] and the Quadrature-Based Moment Equations (QBME) by Koellermeier [9]. Both methods are very similar and their analytical properties and similarities have been extensively studied before, see

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e.g. [10]. First numerical shock tube simulations study the applicability of different numerical schemes to solve the partially-conservative PDE systems and the results show good agreement with reference solutions [11].

In this paper we consider these two new models HME and QBME and present new numerical results for a shock structure problem. The aim is to study the difference between the hyperbolic models and the original Grad system in comparison to a reference discrete velocity method solution of the model problem. As the focus of this paper is the model comparison, we will for simplicity use the numerical methods described in [11].

The rest of this paper is structured as follows: Section 2 recalls the Boltzmann equation and Grad's method and gives explicit equations for the five moment case as. In Section 3 the new models HME and QBME are presented. A brief description of the numerical method follows in Section 4 before the results of the shock structure test case are presented in Section 5. The paper ends with concluding remarks.

BOLTZMANN TRANSPORT EQUATION

In this paper we are interested in solutions of the 1D Boltzmann transport equation

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

which describes the change of the particle density distribution $f(t,x,c)$ for position $x \in \mathbb{R}$ and microscopic velocity $c \in \mathbb{R}$.

The right hand side of Equation (1) models the collisions of particles. We consider a BGK collision operator [12]

$$S_{\mathrm{BGK}}(f) = -\frac{1}{\tau}\left(f - f_M\right), \tag{2}$$

but other collision operators are also possible within the framework of this paper. The BGK collision operator (2) models a relaxation of the distribution function towards an equilibrium Maxwellian $f_M(t,x,c)$ given by

$$f_M(t,x,c) = \frac{\rho(t,x)}{\sqrt{2\pi\theta(t,x)}} \exp\left(-\frac{(c-u(t,x))^2}{2\theta(t,x)}\right) \tag{3}$$

with positive relaxation time τ.

The distribution function $f(t,x,c)$ is related to the macroscopic variables. The density $\rho(t,x)$, velocity $u(t,x)$ and temperature $\theta(t,x)$ can be obtained as moments of $f(t,x,c)$.

$$\rho(t,x) = \int_{\mathbb{R}} f(t,x,c)\, dc, \tag{4}$$

$$\rho(t,x)u(t,x) = \int_{\mathbb{R}} c f(t,x,c)\, dc, \tag{5}$$

$$\rho(t,x)\theta(t,x) = \int_{\mathbb{R}} |c-u|^2 f(t,x,c)\, dc. \tag{6}$$

It is possible to relate the Boltzmann equation (1) to the evolution of the macroscopic variables in the same way. Multiplication of Equation (1) with microscopic velocity powers and integration over velocity space yields the conservation laws of mass, momentum and energy, see e.g. [13].

Grad's Moment Method

Especially in multiple spatial dimensions the Boltzmann equation is high-dimensional and thus difficult to discretize directly. It is possible to apply a non-linear velocity transformation to allow for efficient adaptive discretization in the velocity space. The variable transformation reads

$$c \mapsto \frac{c-u(t,x)}{\sqrt{\theta(t,x)}}, \tag{7}$$

which is a shift by the mean macroscopic velocity $u(t,x)$ and a scaling by the velocity variance which is the square root of the temperature $\theta(t,x)$. The Boltzmann equation transforms accordingly and also includes the (unknown) macroscopic variables $u(t,x)$ and $\theta(t,x)$ now, see [14] for more details.

We furthermore use a Grad ansatz [4] to expand the distribution function in the transformed velocity space in a Hermite series around equilibrium as follows

$$f(t,x,c) = \sum_{\alpha\in\mathbb{N}} f_\alpha(t,x)\mathcal{H}_\alpha(c), \tag{8}$$

where $f_\alpha(t,x)$, $\alpha \in \mathbb{N}$, are the expansion coefficients and $\mathcal{H}_\alpha$ are weighted Hermite polynomials, respectively.

Testing the definition of the macroscopic quantities (6) with Hermite polynomials and using their orthogonality relations, we get the following constraints for the first coefficients

$$f_0 = \rho, f_1 = f_2 = 0, \tag{9}$$

which means that we can just replace the first three coefficients by the macroscopic variables ρ, u and θ, such that the vector of unknowns becomes $\boldsymbol{u}_M = (\rho, u, \theta, f_3, ...f_M)$, for $M \in \mathbb{N}$, $M \geq 3$.

Evolution equations for $\boldsymbol{u}_M$ can be easily derived now by testing the transformed Boltzmann equation with Hermite polynomials up to degree M and integrating over velocity space. This yields a set of $M+1$ equations that can be given in analytical form.

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}_{\text{Grad}} \partial_x \boldsymbol{u}_M = -\frac{1}{\tau}\boldsymbol{P}\boldsymbol{u}_M. \tag{10}$$

In this paper, we want to focus on the case $M = 4$, which is known as the five moment case. For Grad's method, the model system matrix $\boldsymbol{A}_{\text{Grad}}$ is given by

$$\boldsymbol{A}_{\text{Grad}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v \end{pmatrix} \tag{11}$$

and the right hand side collision matrix is

$$\boldsymbol{P} = \operatorname{diag}(0,0,0,1,1) \tag{12}$$

leading to a relaxation of the higher order coefficients while keeping conservation of mass momentum and energy in the first three equations.

HYPERBOLIC MOMENT MODELS

A system of PDEs as given by (10) is *hyperbolic* if the system matrix is diagonalizable with real eigenvalues. In case of Grad's equations, the system is only locally hyperbolic around equilibrium $\boldsymbol{u}_M^0 = (\rho, u, \theta, 0, 0)$ [5]. The characteristic polynomial contains the two last coefficients f_3 and f_4, such that the hyperbolicity depends on these two values. For moderate to large deviation from equilibrium, the equations loose hyperbolicity. This can cause breakdowns of numerical simulations and most certainly unphysical results. This has already been observed in shock tube tests for small Knudsen numbers [11].

Operator Projection Method

A general framework called Operator Projection framework for the derivation of hyperbolic systems of moment equations has been proposed in [10]. The framework relies on a special projection technique during the derivation. This leads to differences in the final form of the equations. These differences with respect to Grad's system render the new system globally hyperbolic, i.e. the hyperbolicity does not depend on the values of higher order coefficients any more. For more details we refer to [10].

Using the Operator Projection framework proposed in the previously mentioned paper, it is possible to derive different hyperbolic moment systems. We will now present two of those and later compare them in a shock structure test case.

Hyperbolic Moment Equations

The so-called Hyperbolic Moment Equations (HME) have been previously derived in [15] using a specific modification of the original Grad system to change the characteristic polynomial. However, it has been shown that the system can also be derived in the Operator Projection framework using a certain projection [10]. In the case of M=4, the system matrix $\boldsymbol{A}_{\text{HME}}$ differs from [11]

$$\boldsymbol{A}_{\text{HME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v \end{pmatrix} \tag{13}$$

with changes with respect to Grad's system only in the last equation, here marked in red. This especially means that the first three equations modeling conservation of mass, momentum and energy have not been changed. Note that the system matrix does no longer contain f_4.

The system is globally hyperbolic and the eigenvalues are real and do not depend on the higher order coefficients anymore in contrast to Grad's system.

Quadrature-Based Moment Equations

The so-called Quadrature-Based Moment Equations (QBME) have been derived in [9] and have been extended to the multi-dimensional case in [14]. The idea is a replacement of the integration over velocity space by Gaussian quadrature during the derivation. This leads to a modification of some terms in the last equations such that the system becomes globally hyperbolic. Similar to the HME system above the QBME equations can also be derived using the Operator Projection framework. The projection is slightly more complicated than for HME, but the QBME equations are recovered in the same way, see [10] for details. The system matrix $\boldsymbol{A}_{\text{QBME}}$ for the five moment case ($M = 4$) is given by

$$\boldsymbol{A}_{\text{QBME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} - \frac{10 f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15 f_4}{\rho\theta} & v \end{pmatrix} \tag{14}$$

with changes with respect to Grad's system matrix in the last and the second but last equation, again marked in red. The conservation laws are again not changed. In contrast to the HME system, the QBME system matrix still contains all non-equilibrium variables f_3, f_4.

Due to the changes in the system matrix, the eigenvalues are all real and in fact the same as for the HME system.

PARTIALLY-CONSERVATIVE NUMERICAL METHODS

The changes in the system matrices of HME and QBME lead to global hyperbolicity of the systems. It can be shown that the systems can unfortunately no longer be written in conservation form. This means there exists no flux function $\boldsymbol{F}(\boldsymbol{u}_M)$ such that the convective term of the system can be written as

$$\boldsymbol{A}\frac{\partial \boldsymbol{u}_M}{\partial x} = \frac{\partial \boldsymbol{F}(\boldsymbol{u}_M)}{\partial x}. \tag{15}$$

We can therefore not apply a standard finite volume scheme for the numerical solution of the PDE system as we do not have an analytical flux function. Note that a simple finite difference solution is also no useful, because we still want to recover conservation of mass, momentum and energy.

Following the theory of path-conservative schemes, we apply the PRICE-C scheme developed by Canestrelli [16] to discretize the non-conservative products of the equation. The update formula of the scheme for the next flow variable $\boldsymbol{u}_i^{n+1}$ is given as

$$\boldsymbol{u}_i^{n+1} = \boldsymbol{u}_i^n - \frac{\Delta t}{\Delta x}\left(\boldsymbol{A}^-_{i+\frac{1}{2}}\left(\boldsymbol{u}_{i+1}^n - \boldsymbol{u}_i^n\right) + \boldsymbol{A}^+_{i-\frac{1}{2}}\left(\boldsymbol{u}_i^n - \boldsymbol{u}_{i-1}^n\right)\right), \tag{16}$$

where the matrices $\boldsymbol{A}^{\pm}_{i+\frac{1}{2}}$ are computed using a special quadrature procedure along a chosen path connecting the two adjacent states, see [16] for details. This enables the method to recover exact conservation for the subset of equations that can be written in conservative form. In our tests we can therefore guarantee conservation of mass, momentum and energy in case a proper choice of variables is used.

The PRICE-C scheme is a centered scheme and thus adds numerical diffusion to the solution. However, it has been shown in previous tests that there is almost no difference between the solution for different numerical schemes applied to the systems given in Section a), see for example [11]. The reason for this is that the non-conservative terms are only in the last or the last two equations, as shown in (13) and (14). The first three conservation laws are never changed. This makes the solution of the system very insensitive to the non-conservative scheme, as long as a proper path discretization is used for the computation of the matrix evaluation in (16).

In general, the choice of the set of variables is also important for a non-conservative system, as it can be shown that different variables may lead to different solutions. Previous test have also proven that this does not influence our equations for problems with usual conditions, such as shock tube test cases. Small deviations only appeared for very large Knudsen numbers or collisionless cases, see [11]. We therefore use the PRICE-C scheme with primitive variables for all our numerical simulations.

NUMERICAL SIMULATION OF THE SHOCK STRUCTURE PROBLEM

As previous tests analyzed the shock tube, see e.g. [5], we will present first results for the numerical simulation of the shock structure problem using hyperbolic moment models. The test case is chosen according to [8].

Shock Structure Test Case

We want to find a traveling shock wave solution to the moment systems where the shock travels with constant shock speed. The boundary conditions $\boldsymbol{u}_L$ upstream and $\boldsymbol{u}_R$ downstream are chosen in local thermodynamic equilibrium and can be computed using the Rankine-Hugoniot conditions [17].

Here we choose a Mach number of $\mathrm{Ma} = 1.8$ to match the results from [8]. This leads to the following values for the boundary conditions upstream

$$\rho_L = 1, \tag{17}$$
$$u_L = \mathrm{Ma} \cdot \sqrt{3} \approx 3.118, \tag{18}$$
$$\theta_L = 1 \tag{19}$$

and downstream

$$\rho_R = \rho_L \cdot \frac{2\mathrm{Ma}^2}{\mathrm{Ma}^2 + 1} \approx 1.528, \tag{20}$$
$$u_R = u_L \cdot \frac{\mathrm{Ma}^2 + 1}{2\mathrm{Ma}^2} \approx 2.040, \tag{21}$$
$$\theta_R = \theta_L \cdot \frac{\left(1 + \mathrm{Ma}^2\right)\left(3\mathrm{Ma}^2 - 1\right)}{4\mathrm{Ma}^2} \approx 2.853. \tag{22}$$

For the relaxation time on the right-hand side, we use a constant $\tau = 0.01$.

We compute the steady-state solution using a time marching from discontinuous initial conditions according to the boundary conditions. After the solution has converged, we scale the density using

$$\widetilde{\rho} = \frac{\rho - \rho_L}{\rho_R - \rho_L} \Rightarrow \widetilde{\rho} \in [0, 1]. \tag{23}$$

As the shock position changes, the numerical solutions needs to be shifted to be comparable. Here we match the values $\widetilde{\rho} = 1/2$.

The moment solutions for Grad, HME and QBME are computed on a grid with $[x_L, x_R] = [-78, 78]$ and $N_x = 7500$ cells with a CFL number of approximately 0.5. A discrete velocity method (DVM) reference solution was taken from [8]. This solution included $N_c = 400$ velocity points and $N_x = 4000$ spatial cells. Note that the DVM solution needs much more computational time due to the larger number of variables at every spatial point.

The results of the shock structure problem for the different moment models are shown in Figure 1. In Figure 1(a) the normalized density is plotted and we see a relatively good agreement of all moment models with the DVM solution. Grad's method seems to perform worse than the hyperbolic models with slightly more accurate results for the HME model. The appearance of the subshocks in front of the shock is due to properties of the moment method in general and is not changed by the hyperbolic regularizations. However, we can see that the error for Grad's method just behind the first subshock is much larger than for the other two hyperbolic models. The graphs for u in Figure 1(b) and θ in Figure 1(c) look almost identically to the density plot apart from the scaling of the variables.

Figure 1(d) displays the normalized heat flux as computed from the moment solution and from the DVM, respectively, by the following formula

$$Q = \frac{6 f_3}{\rho \theta^{3/2}}. \tag{24}$$

Because of the subshocks, we see a relatively large error for Q for all methods. Especially the region just in front of the shock is far away from the DVM solution. The positions of the subshocks are in agreement with the results for the density ρ where the positions were similar.

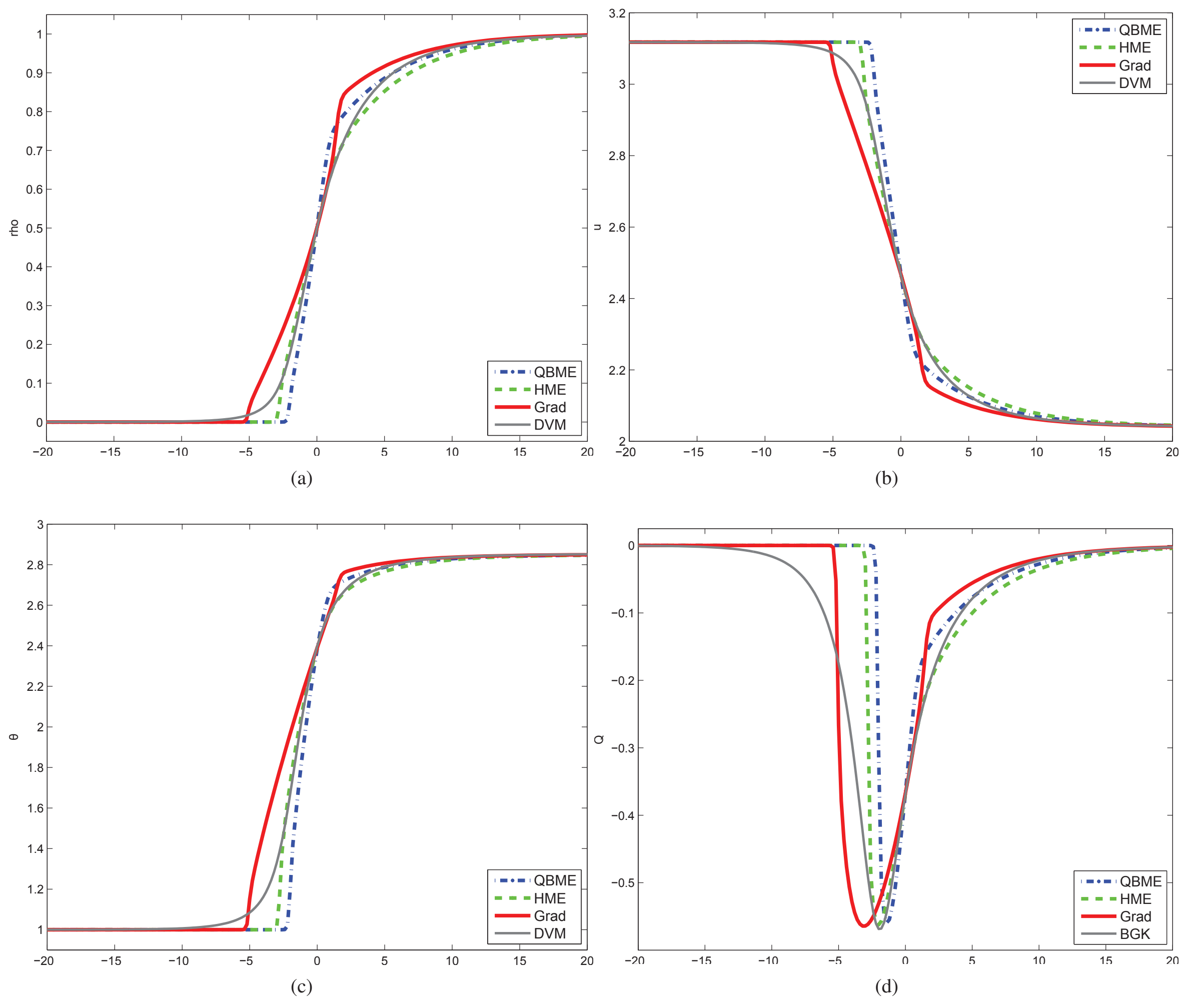

FIGURE 1. Density $\widetilde{\rho}$ (a), velocity u (b), temperatures θ (c) and heat flux Q (d) of moment model comparison for Ma = 1.8 shock structure problem.

TABLE 1. Relative L_1 errors for moment models.

	ρ	u	p	Q
Grad	4.2%	0.8%	2.5%	29%
HME	2.2%	0.4%	1.4%	34%
QBME	3.3%	0.7%	2.3%	47%

To allow for an easier comparison, we computed the L_1 error on the displayed domain $[x_L, x_R] = [-20, 20]$ for the different models and the respective variables. In case of the density, the error is computed using

$$\epsilon_{\rho,\text{model}} = \frac{\|\rho_{\text{model}} - \rho_{\text{DVM}}\|_{L_1}}{\|\rho_{\text{DVM}}\|_{L_1}} \Rightarrow \widetilde{\rho} \in [0, 1], \tag{25}$$

and similarly for the other variables.

The errors are shown in Table 1 for ρ, u, p and Q. The errors thus behave very similarly for ρ, u, p. In all these cases Grad's method shows a slightly larger error, whereas the HME method has the smallest error.

This is different for the normalized heat flux Q where the error is relatively large in the first place and the hyperbolic models end up with even larger errors than Grad's method. One explanation is the different behavior of Q for the true solution. Q is only non-zero close to the shock, this leads to larger values in the relative L_1 errors. The absolute error is in fact comparable or even smaller than for the other variables. Another point is the effect of the position of the subshock. We clearly see that a later subshock (e.g. as in the case of QBME) leads to a larger error in the Q variable. However, the position of the extremum in the heat flux is more accurate for QBME and especially HME when compared to Grad's method, which shows a larger offset in the position of the minimum of Q. The fact that HME has a smaller heat flux error than QBME could be attributed to the fact that the HME matrix has only two different entries with respect to Grad and also only in the last equation. QBME on the other hand changes the last two equations which has a stronger effect on the heat flux as the heat flux is related to the variable f_3 by Equation (24).

CONCLUSION

In this paper, we showed a numerical solution to the shock structure problem using hyperbolic moment models. We gave a short overview of the derivation of the moment models and showed explicit equations for the five moment case. We briefly discussed the importance of non-conservative numerical schemes and the PRICE-C scheme used to solve the non-conservative hyperbolic PDE system. The numerical results showed that the two new models HME and QBME can indeed accurately solve the shock structure problem. We have seen very small relative errors in the first macroscopic variables. The error for the heat flux was larger, but the overall agreement with the DVM solution was still good.

Further work on the new moment models should include other test cases such as two-dimensional problems.

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