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NUMERICAL SOLUTION OF HYPERBOLIC MOMENT MODELS FOR THE BOLTZMANN EQUATION

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KEY WORDS

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ABSTRACT

The Boltzmann equation can be used to model rarefied gas flows in the transition or kinetic regime, i.e. for moderate to large Knudsen numbers. However, standard moment methods like Grad's approach [1] lack hyperbolicity of the equations. This can lead to instabilities and nonphysical solutions. Based on recent developments in this field (see [2], [3] and [4]), we have derived a quadrature-based moment method leading to globally hyperbolic and rotationally invariant moment equations in [5]. We present a 1D case of the equations and use numerical simulations on unstructured spatial grids to compare the new model with standard approaches. The tests are done with dedicated numerical methods to solve the new non-conservative moment equations. These first results using the new method show the accuracy of the new method and its benefits compared with Grad's method or other existing models.

1. INTRODUCTION

Kinetic equations are used in many areas of application (see e.g. [6], [7], [8]). They are especially useful to model rarefied gases and to observe non-equilibrium effects of gas flows at very high velocities and temperatures. A kinetic equation like the Boltzmann equation is usually the basis of a more advanced PDE model that goes beyond the standard fluid dynamics of for example Euler or Navier-Stokes equations. The better approximation quality of the new model equations, which are called moment equations, unfortunately goes together with a higher computational effort when it comes to solving the equations. The reason is that there are additional variables in the model that account for the non-equilibrium behavior of the flow.
The very first approach to the derivation of moment equations has been done by Grad in 1949 (see [1]). The problem with his equations is that they are not globally hyperbolic. Hyperbolicity is related to the existence of finite and real propagation speeds in the system of equations (see [2] for more information about hyperbolic moment systems). This property can be lost in certain regions of the flow, usually already at moderate non-equilibrium. In numerical simulations this can lead to instabilities and most certainly nonphysical solutions. The loss of hyperbolicity is considered to be a major deficiency for Grad's method and has led to relatively few research on Grad's system.

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During the last several years this problem has been investigated in great detail and several new models have been developed that are based on a similar derivation but lead to globally hyperbolic systems of equations. The first system called Hyperbolic Moment Equations (HME) was developed by Cai et al. (see e.g. [3]) and is based on a careful investigation of the characteristic polynomial of the system matrix. Shortly after that, the Quadrature-Based Projection Method was developed (see e.g. [4]) and led to the proposition of another very similar moment system called the Quadrature-Based Moment Equations (QBME). Both systems are very similar even though the idea seems to be very different and the authors have since then worked on a unifying theory and just recently proposed an operator projection framework (see e.g. [5]) that brings together both methods and even includes more general methods.
Apart from the benefits of a globally hyperbolic PDE system, the new equations pose several challenges regarding the numerical solution. The most important difficulty is the lack of a conservation form. Even though the first conservation laws of mass, momentum and energy can be fully recovered, it is no longer possible to write the higher order equations in conservation form. This makes the numerical solution much more difficult as a standard Finite Volume method is no longer applicable and more dedicated numerical methods have to be applied.
It is the purpose of this paper to describe the first successful numerical solution of the QBME system. After a short introduction, we briefly describe the derivation of the method and compare a special case with the existing HME and Grad's approach. We will then present a shock-tube test case where we compute a numerical solution using the PRICE-C algorithm of Canestrelli (see [9]) and again compare with the other models. The results show the good approximation qualities of the new QBME model and are the basis for more advanced test cases.

2. A TRANSFORMED BOLTZMANN EQUATION

In kinetic theory the evolution of the mass density function $f(t, \boldsymbol{x}, \boldsymbol{c})$ is described by the Boltzmann Transport Equation

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

where we consider a d-dimensional setting, i.e. we have position $\boldsymbol{x} \in \mathbb{R}^d$, microscopic velocity $\boldsymbol{c} \in \mathbb{R}^d$ and velocity $\boldsymbol{v} \in \mathbb{R}^d$. Note that we use index notation, whenever the indices are no further specified, e.g. in the transport term of Equation (1). As we focus on the transport part of Equation (1), we first neglect the right-hand side collision operator $S(f)$. However, models for the right-hand exist and in the test Section 6., we will later use a BGK-type model (compare e.g. [10]) to approximate the collision term.
The distribution function $f(t, \boldsymbol{x}, \boldsymbol{c})$ is related to the macroscopic quantities density ρ, velocity $\boldsymbol{v}$ and energy θ via integration over the velocity space as follows:

$$\rho(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}, \tag{2}$$

$$\rho(t, \boldsymbol{x}) \boldsymbol{v}(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} \boldsymbol{c} f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}, \tag{3}$$

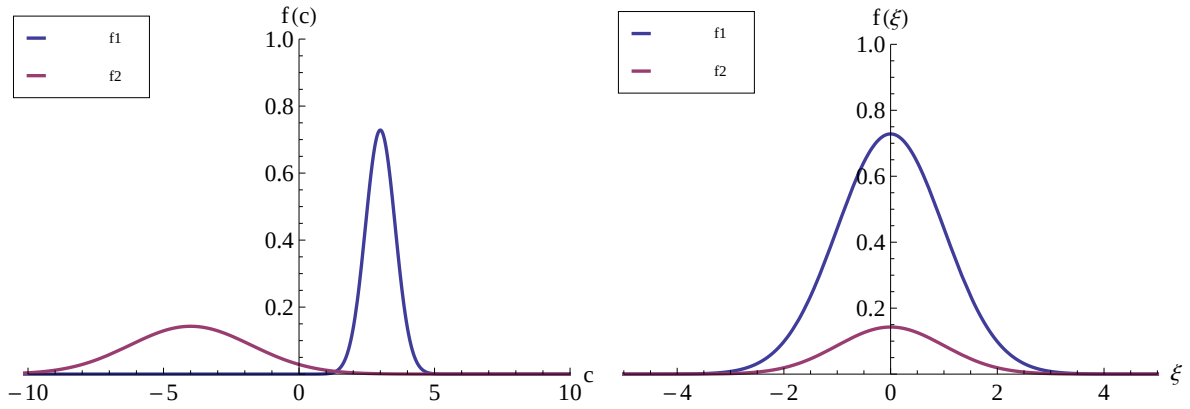
$$d \cdot \rho(t, \boldsymbol{x}) \theta(t, \boldsymbol{x}) = \int_{\mathbb{R}^d} |\boldsymbol{c} - \boldsymbol{v}|^2 \, f(t, \boldsymbol{x}, \boldsymbol{c}) \, d\boldsymbol{c}. \tag{4}$$

The mathematical task is now to derive model equations for the macroscopic quantities that go beyond the standard fluid dynamics equations. One is usually not interested in the actual function f as the macroscopic quantities are of more physical relevance.
A very simple system of equations for these macroscopic variables can be derived by multiplication of Equation (1) with monomials $\left(1, \boldsymbol{c}, c_i^2\right)$ and subsequent integration over the velocity space. The emerging equations are the conservation laws of mass, momentum and energy (see e.g. [11]).
To derive more advanced models, we need to propose an ansatz for the distribution function. In order to be more accurate, we include the macroscopic variables in the ansatz, which can also be interpreted as a

transformation of the equation. We apply a nonlinear transformation of the velocity variable in order to obtain a Lagrangian velocity phase space and exhibit physical adaptivity, which allows for efficient and yet simple discretizations (see [2] for more details):

$$\boldsymbol{\xi}(t,\boldsymbol{x},\boldsymbol{c}) := \frac{\boldsymbol{c}-\boldsymbol{v}(t,\boldsymbol{x})}{\sqrt{\theta(t,\boldsymbol{x})}}. \tag{5}$$

This yields a shift of the microscopic velocity $\boldsymbol{c}$ by the mean velocity $\boldsymbol{v}$ and a scaling by the temperature θ, see also Fig. 1 for the effect of this transformation on two Gaussians. We can later simply use the transformed velocity variable ξ for the discretization in velocity space.



(a) untransformed Gaussians, depending on c

(b) transformed Gaussians, depending on ξ

Figure 1: Gaussians f_1 with $\rho_1 = 1$, $v_1 = 3$, $\theta_1 = 0.3$ and f_2 with $\rho_2 = 0.8$, $v_2 = -4$, $\theta_2 = 5$.

3. VELOCITY DISCRETIZATION

We expand the distribution function in a series of basis functions times coefficients around local equilibrium

$$f(t,\boldsymbol{x},\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} f_{\boldsymbol{\alpha}}(t,\boldsymbol{x}) H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{6}$$

using weighted Hermite polynomial basis functions in the transformed velocity variable $\boldsymbol{\xi}$ defined as

$$H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = (-1)^{|\boldsymbol{\alpha}|} \frac{d^{\boldsymbol{\alpha}}}{d\boldsymbol{\xi}^{\boldsymbol{\alpha}}} w(\boldsymbol{\xi}), \quad w(\boldsymbol{\xi}) = \frac{1}{\sqrt{2\pi}^d} \exp\left(-\frac{|\boldsymbol{\xi}|^2}{2}\right). \tag{7}$$

Using the ansatz (6), it is now possible to multiply the transformed Boltzmann equation with test functions and integrate over velocity space to end up with a PDE in space and time with reduced dimension. This system of PDEs is called a moment system, because one is taking the moments of the Boltzmann equation.
There exist different moment models and we will explain some of them which are using the ansatz from above.

4. HYPERBOLIC MODELS USING OPERATOR PROJECTIONS

A straightforward procedure to derive moment equations is to multiply Equation (1) including the inserted transformations (5) and the ansatz (6) with test functions, for example the basis functions themselves,

and integrate over the whole velocity space. This is known as projection of the equation on the test functions. However, standard projection methods like Grad (see [1]) do not lead to hyperbolic PDE systems. As explained before, hyperbolicity is necessary for physical solutions and stability of the simulation. The loss of hyperbolicity already occurs for moderate values of the higher order non-equilibrium basis coefficients in the expansion (6) as can be seen in Figure 2 where the hyperbolicity region is colored in blue depending on f_3 and f_4 in a 1D case with $M = 4$.

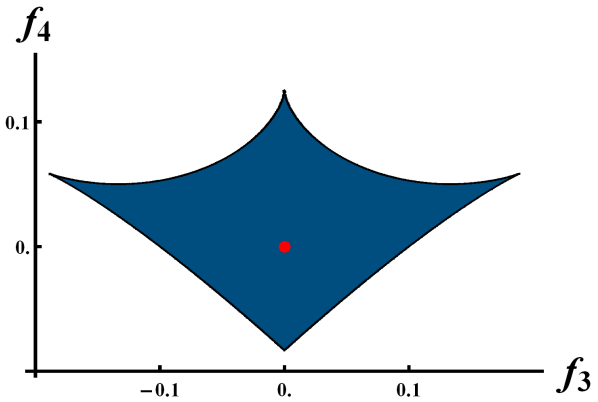


Figure 2: Hyperbolicity region of Grad's method for $M = 4$.

Recently, different methods have been developed to derive globally hyperbolic systems. The first method leads to the Hyperbolic Moment Equations (HME) by Cai et al. [3]. Another new method yields the Quadrature-Based Moment Equations (QBME) by Koellermeier et al. [4]. The methods can be derived in the same framework. Here we want to give a 1D example of QBME and compare to HME and Grad's approach.
The Quadrature-Based Moment Equations can be explained using three different approaches: The first approach is to substitute the exact integration over velocity space by Gaussian quadrature formulas (see [4] for details), which changes some terms as the quadrature is not exact for all occurring terms. On the other hand, it is also possible to cut off higher order terms multiple times during the derivation of the equation system which is equivalent to using a quadrature formula. The same result can be obtained by repeated projection of the equations onto a subspace during the derivation (see [5] for details), which is a more general approach. For details on the projection approach, we would like to refer the reader to [5]. Due to the similar derivation, the different models Grad, HME and QBME are actually very similar and only differ in some terms of the higher order equations. The rest of the equations is the same, especially the first equations including the conservation laws.

5. A 1D FIVE MOMENT EXAMPLE

As an example of the moment equations, we want to exemplify the 1D five moment case. This case is especially important as it corresponds to the 13 moment case in 3D and is the smallest test case including heat flux and stress tensor.
We write the different models in the following form to allow for comparison:

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}\partial_x \boldsymbol{u}_M = 0, \tag{8}$$

where the system matrix $\boldsymbol{A}$ depends on the model. We can analytically derive this matrix for arbitrary M, but here we consider a 1D five moment case, so it is $M = 4$. For the variable vector $\boldsymbol{u}_4 = (\rho, u, \theta, f_3, f_4)$

the different models result in the following system matrices:

$$\boldsymbol{A}_{\text{Grad}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & \frac{3f_3}{2} & \theta & v \end{pmatrix}, \tag{9}$$

$$\boldsymbol{A}_{\text{HME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} & v & 4 \\ -\frac{f_3\theta}{\rho} & 0 & -f_3 & \theta & v \end{pmatrix}, \tag{10}$$

$$\boldsymbol{A}_{\text{QBME}} = \begin{pmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & 0 & 0 \\ 0 & 2\theta & v & \frac{6}{\rho} & 0 \\ 0 & 4f_3 & \frac{\rho\theta}{2} - \frac{10f_4}{\theta} & v & 4 \\ -\frac{f_3\theta}{\rho} & 5f_4 & -f_3 & \theta + \frac{15f_4}{\rho\theta} & v \end{pmatrix}, \tag{11}$$

where terms written in red represent changes with respect to the standard Grad model that originate from the operator projection procedure (see also [5]). Other models with $M > 4$ have the same structure and also only differ from the Grad model in some entries of the last equations, the same is valid for the multi-dimensional case.
It is important to note that these small changes in the last equations suffice to make the equation system globally hyperbolic. The eigenvalues of the HME and the QBME system are in fact the same and are all finite and real.

6. NUMERICAL SIMULATION OF A SHOCK TUBE

In order to test our equation systems, we consider the following shock tube problem:

$$\partial_t \boldsymbol{u}_M + \boldsymbol{A}\partial_x \boldsymbol{u}_M = -\frac{1}{\tau}\boldsymbol{P}\boldsymbol{u}_M, \tag{12}$$

$$\boldsymbol{u}_M = \begin{cases} \boldsymbol{u}_M^L & \text{if } x < 0 \\ \boldsymbol{u}_M^R & \text{if } x > 0, \end{cases} \tag{13}$$

where the collisions have been modelled using a BGK operator with relaxation time $\tau = \frac{\text{Kn}}{\rho}$, which leads to the following form of the matrix $\boldsymbol{P}$ after the projections

$$\boldsymbol{P} = \text{diag}\,(0, 0, 0, 1, \ldots, 1) \tag{14}$$

for the variable vector $\boldsymbol{u}_M = (\rho, u, \theta, f_3, \ldots, f_M)$, $M \geq 4$. In the special case $M = 4$ the matrix $\boldsymbol{A}$ can be directly substituted by one of the model matrices $\boldsymbol{A}_{\text{Grad}}$, $\boldsymbol{A}_{\text{HME}}$ or $\boldsymbol{A}_{\text{QBME}}$ from Section 5.
According to the tests by Cai et al. (see [12]) the left and right states are chosen as

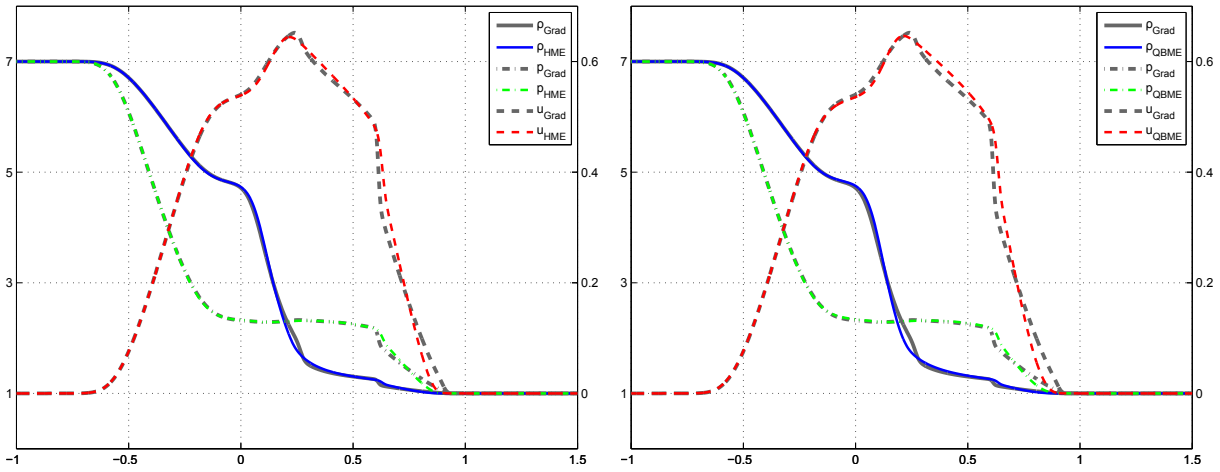
$$\boldsymbol{u}_M^L = (7, 0, 1, 0, \ldots, 0)^T, \qquad \boldsymbol{u}_M^R = (1, 0, 1, 0, \ldots, 0)^T, \tag{15}$$

corresponding to a jump in density at the discontinuity at $x = 0$. We therefore expect a rarefaction wave travelling to the left, a contact discontinuity travelling right and a faster shock wave also travelling right in front of the contact discontinuity.

The systems (8) as well as (12) are clearly not in conservation form. It turns out that in fact both the HME and QBME model cannot be written in conservation form. For the solution of the equations special numerical methods have to be used as a standard Finite Volume scheme is not applicable. We developed a software that enables the solution of the model equations on unstructured grids and uses the PRICE-C scheme of Canestrelli (see also [9]) to discretize the non-conservative products of the equations.
For the numerical tests, we consider two cases Kn $= 0.05$ and Kn $= 0.5$ and run the simulation starting at $t = 0$ until $t = 0.3$ with a time step size of $\Delta t = 0.0001$ according to a CFL number of approximately 0.45. For this numerical benchmark problem, the Knudsen number has no direct physical meaning and only changes the influence of the collision operator on the right hand side. For larger Knudsen number, the collision operator has less influence.
In general, we can say that our simulation results agree very well with the simulations carried out by Cai et al. in [12] where they also compared with a kinetic solver.
The test case with Kn $= 0.05$ is done with all three models, i.e. Grad, HME and QBME. The results are shown in Figure 3. Comparing Grad's method with the other two methods, we see only very small differences in the values of ρ, p and u. However, some deviations from Grad's results can be seen in the right half of the domain for $x > 0$, as the initial difference in density leads to a much larger relaxation time, which makes the differences between all methods more visible. Also the non-equilibrium variables f_3 and f_4 are very similar, despite their smaller scale. Again the deviation from Grad's results are more obvious in the region with lower density due to the larger relaxation time. Comparing HME and QBME for this Knudsen number yields almost no difference, which is also because of the large effect of the collision operator on the right hand side for Kn $= 0.05$.
The test case Kn $= 0.5$ is more interesting and also more difficult for standard methods, as the influence of the collision term on the right hand side is much smaller which makes differences in the transport part of the equations appear much earlier. The solution for a larger Knudsen number is in fact equivalent to the solution of the same system with smaller Knudsen number and proper scaling in the x-direction at an earlier time. A very important consequence is the effect on the stability of the methods. Even in the case Kn $= 0.05$ Grad's equations were at the edge of the hyperbolicity region, but now for Kn $= 0.5$ the state vector leaves the region of hyperbolicity and the small effects of the collision operator do not suffice to keep the stability of the computation. In our simulations the computation broke down after a relatively small number of time steps for Grad's method due to this instability. This is why we do not show a comparison with Grad's method. HME and QBME, however, are globally hyperbolic and thus always yield stable results. As can be seen in Figure 4, the differences are again more visible in the region where we have $x > 0$. Deviations can be seen in front of the first density shock wave at approximately $x = 0.6$ as well as in the maximum value of the velocity right at the contact discontinuity around $x = 0.2$. The differences are due to the changes in the equation as shown in Section 5. According to the smaller scale, the comparison of the higher order coefficients f_3 and f_4 shows larger differences which are most obvious at the different minima and maxima of the variables. As before, the differences are amplified in the region of smaller density due to the larger relaxation time. Note that the position of the maxima as well as the position of the shocks is almost the same as the eigenvalues of both the HME and the QBME system are equal.

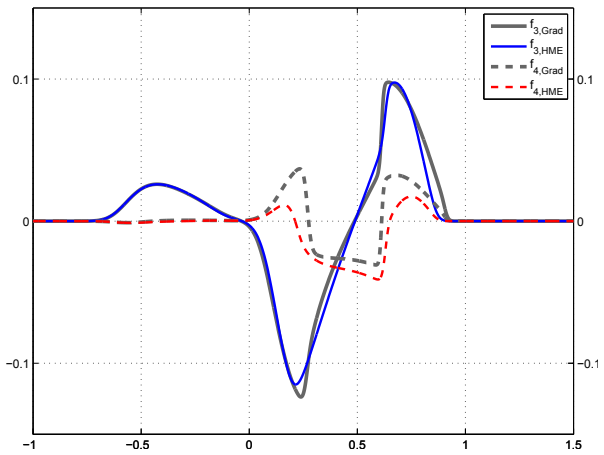
7. CONCLUSIONS

We have presented the Quadrature-Based Moment Equations (QBME) as a new set of globally hyperbolic equations to model rarefied gas flows. In the 1D case, the derivation is particularly easy as it only requires the application of a quadrature formula instead of exact integration. The derivation of the method can be generalized to a projection procedure, that is also applicable to many other models. In an example with the five moment case in 1D, we show that the equations are actually very similar to Grad's model and the existing HME system.
The five moment case is used to simulate a shock tube for the first time with QBME and a comparison with HME and Grad's model yields very similar results. An important advantage of the method with respect to Grad's system is the global hyperbolicity which allows also simulations where a computation

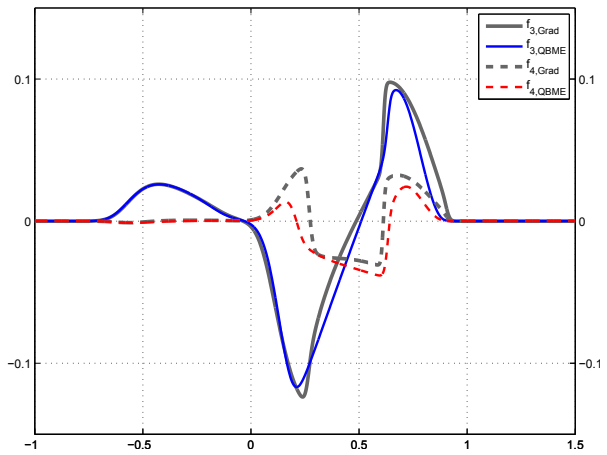


(a) Grad and HME comparison of ρ, p and u

(b) Grad and QBME comparison of ρ, p and u



(c) Grad and HME comparison of f_3 and f_4



(d) Grad and QBME comparison of f_3 and f_4

Figure 3: Numerical results of the shock tube problem for Kn $= 0.05$. In Figure 3a and Figure 3b the left y-axis is for ρ and p and the right axis is for u.

with other methods becomes unstable.
We can see this first results as a starting point for more detailed simulation results with the new model equations and plan to perform fully two-dimensional tests as well as to apply different numerical methods for comparison in the near future.

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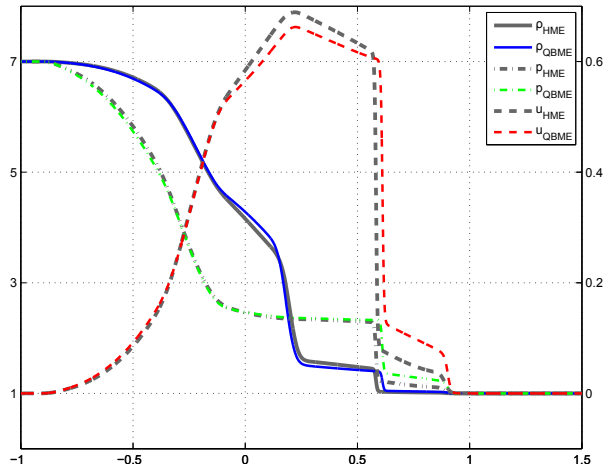
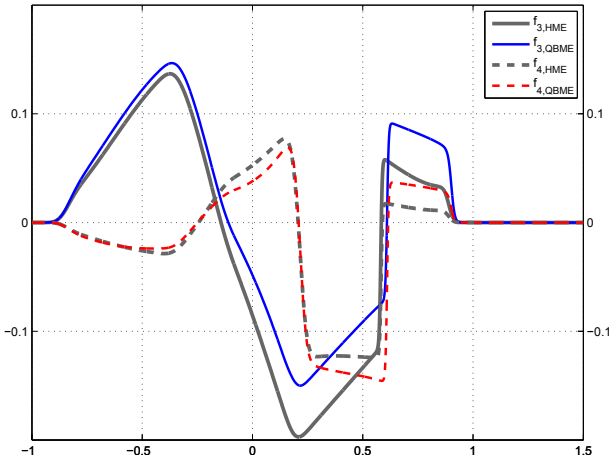


(a) HME and QBME comparison of ρ, p and u



(b) HME and QBME comparison of f_3 and f_4

Figure 4: Numerical results of the shock tube problem for Kn $= 0.5$. In Figure 4a the left y-axis is for ρ and p and the right axis is for u.

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