A Hybrid Moment Method for Multi-scale Kinetic Equations Based on Maximum Entropy Principle

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Abstract
We propose a hybrid method for the multi-scale kinetic equations in the framework of the hyperbolic moment method (Cai and Li in SIAM J Sci Comput 32(5):2875–2907, 2010). In this method, the fourth order moment system is chosen as the governing equations in the fluid region, while the hyperbolic moment system with arbitrary order is chosen as the governing equations in the kinetic region. When transiting from the fluid regime to the kinetic regime, the maximum entropy principle is adopted to reconstruct the kinetic distribution function, so that the information in the fluid region can be utilized thoroughly. Moreover, only one uniform set of numerical scheme is needed for both the fluid and kinetic regions. Numerical tests validate this new hybrid method.

Keywords Hybrid method · Hyperbolic moment method · Maximum entropy method · Boltzmann equation

1 Introduction

Traditional fluid models, such as the Euler and the Navier–Stokes equations, give accurate descriptions of gas flows when the system is close to an equilibrium state. However, many problems, such as simulations of hypersonic flows, involve non-equilibrium processes, where traditional fluid models break down. In this case, the kinetic equations, such as the Boltzmann equation, are introduced to describe the evolution of the particles. However, due to its high

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dimensionality, the computational cost to simulate the kinetic equation is quite expensive compared to the fluid models such as the Euler or the Navier–Stokes equations. Several parameters are introduced to describe how far the system is from the equilibrium, one of which is the Knudsen number. The Knudsen number is defined as the ratio of the mean free path of the particles to a typical macroscopic length. When the Knudsen number is large, the flow is in the kinetic regime, and simulations are usually done on the kinetic equations, for example the Boltzmann equation. Several kinds of numerical methods have been proposed to solve the Boltzmann equation. The DSMC (Direct Simulation Monte Carlo) method [4] is a stochastic numerical method, which is quite efficient when the Knudsen number is large, but may be expensive for the fluid regime. There are also several classical deterministic methods, for example the discrete velocity method [21,33], and the spectral method such as the Fourier spectral method [19,31,34]. Moreover, the Hermite spectral method is also introduced to solve the Boltzmann equation [20,42], which can be traced back to Grad’s classical paper [22]. Despite the numerous numerical methods that have been proposed, the numerical cost of Boltzmann equations is still quite expensive due to the high dimensionality.

For the multi-scale problems, where the fluid and kinetic regions are both included, the coupling of the kinetic and fluid dynamic equations has become an important research area [17,18,28]. In [28], a moment realizability matrix is introduced to differentiate the fluid region and the kinetic region. Based on this realizability matrix, hybrid methods are proposed in [17,18,43] to solve multi-scale kinetic problems. There are several other hybrid methods, which are based on the local Knudsen number [26] or based on the viscosity and heat flux of the Navier–Stokes equations [2,39]. Moreover, the hybridization of the Monte Carlo method and the finite volume method is proposed in [5,12,13].

Recently a globally hyperbolic moment method is proposed in [6,8] to solve the Boltzmann equation. This method is based on the Grad expansion method [22], where the distribution function is expanded in Hermite series, and the weight function for the expansion is the Maxwellian distribution determined by the local velocity and temperature. It is expected that this expansion for the distribution function extends the validity of the moment equations beyond the continuum regime. A highly efficient numerical scheme has been designed under the framework of this method, which also has been successfully applied to solve Vlasov and Wigner equations [24]. It is also proved that the moment system derived by the hyperbolic moment method contains the fluid dynamic equations such as the Euler and the Navier–Stokes equations. This method is verified to successfully simulate nonequilibrium flows for a wide range of Knudsen number [7,9]. But the expansion order may increase quickly with the increase of the Knudsen number. Therefore, when there is a coupling of kinetic and fluid regimes, for example in the simulations of the hypersonic flows around a space vehicle during the re-entry phase, where there may exist large variations in the Knudsen number, the expansion order for the above hyperbolic moment method is decided by the largest Knudsen number, and the computational cost may be expensive.

In this paper, we propose a hybrid method in the framework of the hyperbolic moment method [8]. Instead of the Euler and the Navier–Stokes equations, the moment equations with low order expansion are utilized as the governing equations in the fluid region. For problems with 1D microscopic velocity space, the moment equations with expansion order four are utilized as the governing equations in the fluid region, considering that in this case, it is the smallest moment system in the maximum entropy theory where the distribution ansatz could characterize non-equilibrium behavior. The maximum entropy ansatz is utilized to reconstruct the kinetic distribution function when changing from fluid to kinetic description. For problems with 3D microscopic velocity space, we only consider problems where the solutions are axial symmetric with respect to axis $x_1$, and only the BGK or Shakhov collision
operator are considered. Under the above restrictions, the Chu reduction [18] could be adopted here to reduce the distribution function in 3D microscopic velocity space into two reduced distribution functions in 1D microscopic velocity space. Thus, for the resulting distribution function with 1D microscopic velocity, the similar fourth order moment system is used in the fluid region. Another important ingredient of a hybrid method is the domain decomposition indicator. In this hybrid method, the domain decomposition indicator is based on the moment realizability matrices proposed in [28] and later used in [17,18]. It has quite a simple form, where instead of the derivatives of the macroscopic variables, only the expansion coefficients of the distribution function with orders smaller than four are used. The criteria from/to hydrodynamic to/from kinetic are proposed based on this indicator. Numerical tests show that this method could describe the evolution of the distribution function in the fluid region with quite few degrees of freedom and is therefore more efficient than the traditional hyperbolic moment method using a uniform number of moments. Another advantage of our method is that we could use the same numerical scheme for both the kinetic and fluid regions. We do not need to strictly discriminate the numerical flux in different domains, especially those at the kinetic and fluid interfaces, since they all have the same form, which simplifies the coupling of different domains. Numerical simulations are done for several benchmark problems. In the numerical tests, the BGK and Shakhov collision terms are applied, and the dimension reduction method in the microscopic velocity space described in [7] is adopted to reduce computation complexity.

The rest of this paper is organized as follows: Sect. 2 introduces the Boltzmann equation, the maximum entropy method [27] and the hyperbolic moment method [8] briefly. The details of this hybrid method are given in Sect. 3, and the numerical algorithm to deal with the numerical flux in the interface of different regions is proposed in Sect. 4. Several numerical examples are exhibited in Sect. 5. Conclusion and future work are discussed in Sect. 6. Detailed description of the numerical scheme, the dimension reduction method and the computation of moments of the maximum entropy distribution function are given in the “Appendix A, B and C”, respectively.

2 Boltzmann Equation and the Moment Method

The Boltzmann equation is considered as the basics of modern gas kinetic theory. It is especially useful for the description of rarefied gas flow. When the system approaches the fluid regime, the Euler or the Navier–Stokes equations could be derived from the Boltzmann equation by applying the Chapman-Enskog expansion. In this section, we will first introduce the Boltzmann equation [36] and some related properties.

2.1 Boltzmann Equation

In the Boltzmann equation, the distribution function \( f(t, x, v) \) is used to describe the fluid state, where \( t \) is time, \( x \) is the spatial space, and \( v \) stands for the velocity of gas molecules. The dimensionless form of the governing equation is

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\epsilon} Q[f], \quad t \in \mathbb{R}^+, \quad x \in \mathbb{R}^D, \quad v \in \mathbb{R}^D,
\]  

(2.1)
where $D$ is the dimension number of the microscopic velocity space. $\epsilon$ is a formal smallness parameter which plays the role of the Knudsen number. $Q[f]$ denotes particle collision, which may have quite a complex form. The collision operator satisfies the following properties:

1. Conservation of the mass, momentum and kinetic energy

$$\int_{\mathbb{R}^D} \left( \frac{1}{v} \right) Q[f] \, dv = 0. \quad (2.2)$$

2. Boltzmann’s H-theorem

$$\int_{\mathbb{R}^D} Q[f] \log f \, dv \leq 0, \quad (2.3)$$

where the equality holds if and only if $f$ is the Maxwellian

$$\mathcal{M} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|v-u|^2}{2\theta}\right). \quad (2.4)$$

which is the steady state of the Boltzmann equation (2.1). Here $\rho(t, x)$ is the density, $u(t, x)$ is the macroscopic velocity and $\theta(t, x)$ is the temperature, whose relationships with the distribution function $f(t, x, v)$ is as below

$$\begin{pmatrix} \rho(t, x) \\ \rho(t, x)u(t, x) \\ \frac{1}{2}\rho|u(t, x)|^2 + \frac{D}{2}\rho(t, x)\theta(t, x) \end{pmatrix} = \int_{\mathbb{R}^D} \left( \frac{1}{v} \right) f(t, x, v) \, dv. \quad (2.5)$$

Moreover, it also holds that

$$Q(\mathcal{M}) = 0. \quad (2.6)$$

3. Galilean invariance: $Q[f]$ commutes with translational and rotational operators.

In this paper, we are mainly concerned with the hybrid method to solve the Boltzmann equation, therefore, the simplified collision operator is used here, for example the BGK collision operator

$$Q_{BGK}[f] = \frac{1}{\tau} (\mathcal{M} - f), \quad (2.7)$$

where $\tau$ is the relaxation time, which is usually obtained from the first order approximation of the Chapman-Enskog theory [4]. $\tau$ is a parameter related to the Knudsen number $Kn$ and some macroscopic variables such as the density. When $\tau$ is large, very few molecular collisions occur, and the entire flow is rarefied. The classical BGK operator gives the wrong Prandtl number 1, whereas the correct Prandtl number for a monoatomic gas is 2/3. Another simplified collision operator, the Shakhov collision operator, preserves the correct Prandtl number [36]. The Shakhov collision operator has the form

$$Q_{Shakhov}(f) = \frac{1}{\tau} (f_s - f), \quad f_s = P_3(t, x, v)\mathcal{M}(t, x, v), \quad (2.8)$$

with

$$P_3 = 1 + \frac{(1 - Pr)(v - u(t, x)) \cdot q(t, x)}{(D + 2)\rho(t, x)[\theta(t, x)]^2} \left( \frac{|v - u(t, x)|^2}{\theta(t, x)} - (D + 2) \right), \quad (2.9)$$
where Pr is the Prandtl number. $q(t, x)$ is heat flux, which is defined as

$$q_i = \frac{1}{2} \int_{\mathbb{R}^D} |v - u|^2(v_i - u_i) f \, dv, \quad i = 1, 2, \ldots, D. \quad (2.10)$$

There are other physical variables people are interested in, such as the stress tensor $\sigma_{ij}$, which is defined as

$$\sigma_{ij} = \int_{\mathbb{R}^D} \left( (v_i - u_i)(v_j - u_j) - \frac{1}{D} \delta_{ij} |v - u|^2 \right) f \, dv, \quad i, j = 1, 2, \ldots, D. \quad (2.11)$$

Besides, the pressure tensor $p_{ij}$ is defined as

$$p_{ij} = \int_{\mathbb{R}^D} (v_i - u_i)(v_j - u_j) f \, dv, \quad \sigma_{ij} = p_{ij} - \frac{1}{D} \delta_{ij} \sum_{k=1}^{D} p_{kk}. \quad (2.12)$$

**Remark 1** In our numerical test, we choose the VHS model for $\tau$ as

$$\tau = \sqrt{\frac{\pi}{2}} \frac{15Kn}{\sqrt{(5 - 2\omega)(7 - 2\omega)}} \frac{\theta^{\omega-1}}{\rho}, \quad (2.13)$$

where $\omega$ is the viscous index dependent on the type of the particles, and $Kn$ is the Knudsen number. Moreover, $\tau$ is also the same parameter to indicate the regime of the particles in some literature [17,18].

There has been much active research on algorithms to solve the Boltzmann equation numerically, especially for problems in the transitional regime, such as [8,16,19,38]. In this paper, we will focus on developing a hybrid moment method under the framework of the globally hyperbolic moment method [6,8], with a strategy that utilizes the maximum entropy principle [23,27,30]. In the next section, we will briefly introduce these two methods.

### 2.2 Maximum Entropy Moment Method

For simplicity, this section considers the 1D microscopic velocity space case. Define the $k$-th order moment as

$$\mu_k = \langle f \rangle_k = \int_{\mathbb{R}} f v^k \, dv. \quad (2.14)$$

We could obtain the time evolution equation of $\mu_k$ by multiplying (2.1) with $v^k$ and integrating against $v$ over $\mathbb{R}$:

$$\frac{\partial \mu_k}{\partial t} + \frac{\partial \mu_{k+1}}{\partial x} = \left\{ \frac{1}{\epsilon} Q[f] \right\}_k, \quad k \in \mathbb{N}. \quad (2.15)$$

Since the governing equation of $\mu_k$ depends on $\mu_{k+1}$ in (2.15), the full system contains an infinite number of equations, and we do a truncation in order to obtain a reduced model for (2.1). Specifically, we choose a fixed integer $M$ and discard all equations for $\mu_k, k > M$. Still, as the truncated moment system depends on $\mu_{M+1}$, it is not a closed system, so a moment closure is needed in the system. One way of specifying a closure is to construct an ansatz for the distribution function. Specifically, given moments $\mu_k, k = 0, \ldots, M$, one could reconstruct an ansatz of the distribution function $\hat{f}$, which satisfies

$$\langle \hat{f}(v; \mu_0, \cdots, \mu_M) \rangle_k = \mu_k, \quad k = 0, \cdots, M. \quad (2.16)$$
Then the moment closure could be given by

$$\mu_{M+1} = \langle \hat{f}(v; \mu_0, \cdots, \mu_M) \rangle_{M+1},$$  \hspace{1cm} (2.17)$$

The maximum entropy moment method closes the system (2.15) by specifying an ansatz of \( f \) based on the entropy minimization principle [14,25,27,32]. Specifically, the ansatz \( \hat{f} \) gives the most likely distribution function under constraints of the given moments by solving the following functional minimization problem

$$\hat{f} = \operatorname{argmin} H(f), \  \text{s.t.} \langle \hat{f}(v) \rangle_k = \mu_k, \ k = 0, \cdots, M,$$  \hspace{1cm} (2.18)$$

with \( H(f) = \langle f \log f - f \rangle \). Direct computation shows the unique solution of (2.18) has the form

$$\hat{f} = \exp \left( \sum_{k=0}^{M} \beta_k v^k \right),$$  \hspace{1cm} (2.19)$$

where \( \beta_k, k = 0, \cdots, M \) are called the Lagrange multipliers. Since (2.19) is in the integrable function space, the degree of the polynomial \( \sum_{k=0}^{M} \beta_k v^k \) should be even.

The simplest model in the maximum entropy hierarchy that contains all the conserved variables is the Euler equation. It is sufficient to describe the processes in local thermodynamic equilibrium, but even in moderately rarefied gas flows, stronger deviations from equilibrium may be expected, making the closing relationship of Euler equation unsound. The next model in the maximum entropy hierarchy is the fourth order moment model, which extends the validity of the Euler system by including some higher order moments such as the heat flux. Levermore [27] has proved that the maximum entropy moment model has several excellent properties. For example, it is a globally hyperbolic system which gives a positive ansatz of the distribution function and dissipates the physical entropy. Unfortunately, when the moments beyond the second order are included, we should solve an optimization problem (2.18) to get the final expression (2.19), which is numerically expensive [1,30,35].

Recently, a globally hyperbolic moment method [6] is proposed to obtain the hyperbolic closure for the moment system. A numerical scheme also is designed in this framework, making the simulation much more efficient for high order moment systems [8]. We will briefly review the hyperbolic moment method in the next section.

### 2.3 The Hyperbolic Moment Method

The globally hyperbolic moment method was first proposed in [8] to solve the Boltzmann equation. It is validated to be efficient for solving the Wigner and Vlasov equations [24], and has also been applied to radiative transfer problems [15]. Under the framework of the hyperbolic moment method, the distribution function \( f \) is approximated by a series expansion of the basis functions. A special regularization procedure is then adopted to obtain the globally hyperbolic moment systems. Precisely, the distribution function \( f(t, x, v) \) is expanded as

$$f(t, x, v) = \sum_{\alpha \in \mathbb{N}^D} f_\alpha(t, x) \mathcal{H}_\alpha^{u, q}(v),$$  \hspace{1cm} (2.20)$$
where $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_D)$ is a D-dimensional multi-index, and the basis functions $H_{\alpha}^{u,\theta}(v)$ are defined as
\begin{equation}
H_{\alpha}^{u,\theta}(v) = \prod_{i=1}^{D} \frac{1}{\sqrt{2\pi}} \theta^{-\frac{\alpha_i+1}{2}} He_{\alpha_i}(\xi_i) \exp \left( -\frac{\xi_i^2}{2} \right), \quad \xi_i = \frac{v_i - u_i}{\sqrt{\theta}}, \tag{2.21}
\end{equation}
where $He_{\alpha_i}$ is the Hermite polynomial. Under this expansion, the relationship between the moment coefficients $f_\alpha$ and the macroscopic variables are as below
\begin{equation}
f_0 = \rho(t, x), \quad f_{e_i} = 0, \quad \sum_{j=1}^{D} f_{2e_j} = 0, \tag{2.22}
\end{equation}
\begin{equation}
q_i = 2f_{3e_i} + \sum_{d=1}^{D} f_{2ed+e_i}, \quad \sigma_{ij} = (1 + \delta_{ij}) f_{e_i + e_j}, \quad i, j = 1, 2, \cdots, D. \tag{2.23}
\end{equation}
With this expansion, the Maxwellian (2.4) can be expressed by the zeroth-order expansion as
\begin{equation}
\mathcal{M} = f_0(t, x) H_{0}^{u,\theta}(v), \quad f_0 = \rho. \tag{2.23}
\end{equation}
With a truncation on (2.20), we can get a finite order approximation of the distribution function. Precisely, let $M \geq 3$ be a positive number and only retain the coefficients in the set $S = \{ f_\alpha \}_{|\alpha| \leq M}$. Thus, the expansion is truncated as
\begin{equation}
f(t, x, v) \approx \sum_{|\alpha| \leq M} f_\alpha(t, x) H_{\alpha}^{u,\theta}(v). \tag{2.24}
\end{equation}
Following the procedure in [8], we can get the globally hyperbolic moment systems. Precisely, substituting the expansion (2.21) into the Boltzmann equation (2.1) and adopting the regularization in [8], we can derive the globally hyperbolic moment equations (HME) for the Boltzmann equation,
\begin{equation}
\frac{\partial f_\alpha}{\partial t} + \sum_{j=1}^{D} \left( \theta \frac{\partial f_{\alpha-e_j}}{\partial x_j} + u_j \frac{\partial f_\alpha}{\partial x_j} + (1 - \delta_{M,|\alpha|})(\alpha_j + 1) \frac{\partial f_{\alpha+e_j}}{\partial x_j} \right) \\
+ \sum_{d=1}^{D} \frac{\partial u_d}{\partial t} f_{\alpha-e_d} \\
+ \sum_{j,d=1}^{D} \frac{\partial u_d}{\partial x_j} \left( \theta f_{\alpha-e_d-e_j} + u_j f_{\alpha-e_d} + (1 - \delta_{M,|\alpha|})(\alpha_j + 1) f_{\alpha-e_d+e_j} \right) \\
+ \frac{1}{2} \frac{\partial \theta}{\partial t} \sum_{d=1}^{D} f_{\alpha-2e_d} \\
+ \sum_{j,d=1}^{D} \frac{1}{2} \frac{\partial \theta}{\partial x_j} \left( \theta f_{\alpha-2e_d-e_j} + u_j f_{\alpha-2e_d} + (1 - \delta_{M,|\alpha|})(\alpha_j + 1) f_{\alpha-2e_d+e_j} \right) \\
= Q_\alpha, \quad |\alpha| \leq M, \tag{2.25}
\end{equation}
where $\delta$ is the Kronecker’s delta, and $f_\alpha$ is taken as zero if any component of $\alpha$ is negative. $Q_\alpha$ is the expansion of the collision term. If we take the BGK collision model (2.7), then

$$Q^{\text{BGK}}_\alpha = \begin{cases} -\frac{1}{\tau} f_\alpha, & |\alpha| \geq 2, \\ 0, & \text{otherwise}. \end{cases}$$

(2.26)

For the Shakhov collision model, the collision coefficients $Q_\alpha$ have the form

$$Q^{\text{shakhov}}_\alpha = \begin{cases} \frac{1}{\tau} \left( 1 - \frac{P_r}{D + 2} q_j - f_\alpha \right), & \alpha = 2e_i + e_j, \quad i, j = 1, 2, \ldots, D, \\ Q^{\text{BGK}}_\alpha, & \text{otherwise}. \end{cases}$$

(2.27)

Collecting all the independent variables of $f_\alpha, u$ and $\theta$ as a vector $w$, then the system (2.25) can be written in a quasi-linear form

$$D(w) \frac{\partial w}{\partial t} + \sum_{j=1}^{D} M_j(w) D(w) \frac{\partial w}{\partial x_j} = g(w),$$

(2.28)

where $D \frac{\partial w}{\partial t}$ corresponds to the time derivative in (2.25) while $M_j \frac{\partial w}{\partial x_j}$ describes the convection term in the $x_j$ direction, and $g$ denotes the right hand side of (2.25). More details can be found in [7]. In [6,40], the moment system (2.28) is proved to be globally hyperbolic and a highly efficient numerical scheme is designed in the framework of the hyperbolic moment method, where the finite volume method is used for spatial discretization. The detailed numerical scheme is introduced in “Appendix A”.

However, when the Knudsen number is large, or in other cases when the distribution function deviates significantly from the equilibrium distribution, the hyperbolic moment method would require a large expansion number $M$ in order to adequately approximate the distribution function. Originally, when using the globally hyperbolic moment equations (HME) to approximate the kinetic equation, the expansion number of the distribution function $M$ in all cells are fixed and decided by the largest Knudsen number. For problems with large variation in the Knudsen number, it may result in a rather large waste for the areas where the Knudsen number is small. Therefore, the hybrid kinetic/fluid scheme in the framework of the hyperbolic moment method, where an indicator is designed to adjust the expansion number according to the local Knudsen number, is proposed in this paper to reduce the computation cost.

### 3 Hybrid Hyperbolic Moment Method

Many engineering problems involve both areas belonging to the fluid regime and the kinetic regime. For the fluid regime, the fluid description such as the Euler or the Navier–Stokes equations could describe the problem there. However, for the kinetic regime, kinetic models are usually needed to accurately describe the system. Even though lots of work has been done to design highly efficient numerical schemes for the kinetic equations, it is still much more expensive to solve compared with the fluid models. Therefore, for the sake of computational efficiency, several so-called hybrid kinetic/fluid schemes are proposed [17,18] with an automatic domain-decomposition criterion. In this paper, we will introduce a hybrid method in the framework of HME, and a uniform numerical scheme for solving both the fluid and kinetic regions is designed.
For the hybrid method, we first design an indicator function and a criterion to distinguish the fluid and kinetic regions, then propose a method to reconstruct the distribution function when switching from the fluid to kinetic regime.

### 3.1 Moment Realizability Matrix

In this section, the indicator matrix for the hybrid moment method and the specific criterion to discriminate the fluid and kinetic regions are proposed. We will start from the analysis of the moment system (2.25) derived in the hyperbolic moment method. Following the method in [8], we set $\alpha_e = 0, e_i$ and $2e_i$ to deduce the equations of density, velocity and temperature respectively as

$$
\begin{align*}
\frac{\partial \rho}{\partial t} + \sum_{j=1}^{D} \left( u_j \frac{\partial \rho}{\partial x_j} + \rho \frac{\partial u_j}{\partial x_j} \right) &= 0, \\
\rho \left( \frac{\partial u_d}{\partial t} + \sum_{j=1}^{D} u_j \frac{\partial u_d}{\partial x_j} \right) + \sum_{j=1}^{D} \frac{\partial p_{jd}}{\partial x_j} &= 0, \quad d = 1, 2, \cdots, D, \\
\rho \left( \frac{\partial \theta}{\partial t} + \sum_{j=1}^{D} u_j \frac{\partial \theta}{\partial x_j} \right) + \frac{2}{D} \sum_{j=1}^{D} \left( \frac{\partial q_j}{\partial x_j} + \sum_{d=1}^{D} p_{jd} \frac{\partial u_d}{\partial x_j} \right) &= 0.
\end{align*}
$$

(3.1)

When the distribution function $f$ is Maxwellian (2.4), the stress tensor and heat flux are reduced into

$$
p_{ij} = \delta_{ij} \rho \theta, \quad q_i = 0, \quad i, j = 1, 2, \cdots, D.
$$

(3.2)

Then with some rearrangement, we can find that the moment system (3.1) is reduced into the Euler equations

$$
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0, \\
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \otimes u + \rho \theta \mathbf{1}) &= 0, \\
\frac{\partial E}{\partial t} + \nabla \cdot (u(E + \rho \theta)) &= 0,
\end{align*}
$$

(3.3)

where $E = \frac{1}{2} \rho |u|^2 + \frac{D}{2} \rho \theta$ is the kinetic energy. Similarly, we can also get the Navier–Stokes equation, which has exactly the same form as (3.1). In the NS equations, the relationship between $\sigma, q$ and $u, \theta$ are given by some kind of Fourier law [36], and will lead to a closed equation system. From the analysis above, we can see that Euler and Navier–Stokes equations are included in the moment equations (2.25). With the same procedure, we can find that the high order equations similar to Burnett and Super-Burnett equations can also be deduced.

With the increasing of the expansion number, the moment equations are also validated to describe the fluid flow in the rarefied gas problems.

Then we will introduce the indicator matrix for the moment equations, which could distinguish the fluid region and the kinetic region. We will first introduce the two variables

$$
\mathbf{A}(v) = \xi \otimes \xi - \frac{|\xi|^2}{D} \mathbf{I}, \quad \mathbf{B}(v) = \frac{1}{2} (|\xi|^2 - (D + 2)) \xi, \quad \xi = \frac{v-u}{\sqrt{\theta}}.
$$

(3.4)
If the distribution function $f$ is reduced to Maxwellian, we can get the Euler equations. In this case, it holds that

$$\int_{\mathbb{R}^D} A f \, dv = \int_{\mathbb{R}^D} B f \, dv = 0. \quad (3.5)$$

If $f \approx \mathcal{M}(1 + \epsilon g^{(1)})$, then we can deduce Navier–Stokes equations, in which case,

$$\int_{\mathbb{R}^D} A f \, dv \neq 0, \quad \int_{\mathbb{R}^D} B f \, dv \neq 0. \quad (3.6)$$

Thus, $A$ and $B$ could be used to derive the regime indicators in order to discriminate the particle regimes. This idea has already been successfully used in several works to detect the fluid regions, such as [17,18], where a moment realizability matrix is proposed based on $A$ and $B$ to describe the domain decomposition criteria as

$$M := m \otimes m = \left(1, \xi, \sqrt{\frac{2}{D}} \left(\frac{||\xi||^2}{2} - \frac{D}{2}\right)\right), \quad \xi = \frac{v - u}{\sqrt{\theta}}. \quad (3.7)$$

In the framework of the hyperbolic moment method, we can find that the corresponding coefficient matrix of the moment realizability matrix (3.7) is

$$I = \frac{1}{\rho} \int_{\mathbb{R}^D} M f(t, x, v) \, dv = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{p_{11}}{\rho \theta} & 0 & 0 & \frac{\sqrt{q_{1}}}{\sqrt{D \rho \theta D/2}} \\ 0 & 0 & \ddots & 0 & \vdots \\ 0 & 0 & 0 & \frac{p_{DD}}{\rho \theta^2} & \frac{\sqrt{q_{D}}}{\sqrt{D \rho \theta D/2}} \\ 0 & \frac{\sqrt{q_{1}}}{\sqrt{D \rho \theta D/2}} & \cdots & \frac{\sqrt{q_{D}}}{\sqrt{D \rho \theta D/2}} & C \end{pmatrix}, \quad (3.8)$$

where

$$C = \frac{1}{\rho} \int_{\mathbb{R}^D} \frac{2}{D} \left(\frac{||\xi||^2}{2} - \frac{D}{2}\right)^2 f(t, x, v) \, dv = \frac{12}{D \rho \theta^2} \sum_{j=1}^{D} f_{4e_k} + \frac{2}{D \rho \theta^2} \sum_{i,j=1}^{D} (1 - \delta_{ij}) f_{2e_i + 2e_j} + 1. \quad (3.9)$$

For now, we have introduced the moment realizability matrix composed of the expansion coefficients of the distribution function, the criteria to distinguish the different regions will be proposed next. Instead of Euler or NS equations, we use the moment equations with a small expansion order as the macroscopic model in the fluid model. This is due to our strategy for reconstructing the distribution function when changing from fluid to kinetic regime. We will explain the criteria of the 1D microscopic velocity space case, and the 3D microscopic velocity space case, respectively.
3.2 Regime Indicator and Criterion in 1D Microscopic Velocity Space

We begin from the introduction of the fluid model. For the 1D case, the moment realizability matrix is reduced into

\[
I = \begin{pmatrix}
1 & 0 & 0 & \frac{\sqrt{2} q_1}{\sqrt{\rho}} \\
0 & \frac{\rho_{11}}{\rho d} & \frac{\sqrt{2} q_1}{\sqrt{\rho}} & \frac{12}{\rho d^2} f_4 + 1 \\
0 & \frac{\sqrt{2} q_1}{\sqrt{\rho}} & \frac{12}{\rho d^2} f_4 + 1 \\
\end{pmatrix}
\]  \hspace{1cm} (3.10)

Instead of the Euler and NS equations, the fourth order moment system is utilized in the fluid region. From the deduction in the last section, we can find that the fourth order moment system contains the Euler and Navier–Stokes equation, and the detailed deduction can be found in [8]. Moreover, the fourth-order moment model is the simplest maximum entropy model which could characterized non-equilibrium behavior. Based on this fourth order moment system, we could recover the higher order expansion coefficients based on the maximum entropy principle [14,25] when changing from fluid to kinetic region.

Then, we propose a criterion to discriminate the fluid and kinetic region. We can find that the moment realizability matrix (3.10) is reduced into the Identity matrix for the Euler equations. However, for the four order moment system, at least one of its eigenvalues is different from 1, and remain the same for any higher order model. Therefore, the specific criteria to discriminate the fluid and kinetic region are proposed based on the moment realizability matrix (3.7).

From kinetic to fluid Supposing the eigenvalues of (3.8) other than 1 are $\lambda_i, \ i = 1, 2$. We will first propose the criterion from the kinetic to the fluid region. There are several methods [5,17,18,26,28] to decide how far the gas is from the equilibrium. Here, we adopt the simple comparison between the eigenvalues $\lambda_i$ and 1. The detailed criterion is then as follows: The kinetic description could be reduced into the fluid description if the two conditions below are satisfied.

1. the eigenvalues are all close to the eigenvalues of the Euler equations which all equal 1.

\[
\max_{i=1,2} |\lambda_i - 1| \leq \epsilon_1. 
\]  \hspace{1cm} (3.11)

2. the $l_1$ norm of the expansion coefficients of the distribution function $f_\alpha$ when $|\alpha| > 4$ is small.

\[
\sum_{4<|\alpha| \leq M} |f_\alpha| \leq \epsilon_2. 
\]  \hspace{1cm} (3.12)

If both criteria are satisfied, the expansion number of the distribution function is set as $M = 4$. Then the region is changed from kinetic to fluid regime. In this case, the expansion coefficients $\{f_\alpha, \alpha > 4\}$ are simplify set to zero.

From fluid to kinetic The criterion from fluid region to kinetic region is similar, where the eigenvalues $\lambda_i$ are also utilized. The detailed criterion is then as follows: The fluid description should be recovered to kinetic description if the condition below is satisfied.

1. at least one of the eigenvalues is far from the eigenvalues of the Euler equations.

\[
\max_{i=1,2} |\lambda_i - 1| > \epsilon_1. 
\]  \hspace{1cm} (3.13)
If the criterion is satisfied, the regime should be changed from the fluid region to the kinetic region. In this case, the maximum entropy method, which will give the most likely distribution function given the known information \([27,32]\), is adopted to recover an ansatz of the distribution function and get all the expansion coefficients \(\{f_\alpha, \alpha > 4\}\).

However, the maximum entropy method is known to be expensive to solve numerically. To solve this problem, we speed up a Newton iteration by specifying initial conditions based on interpolation, and using adaptive integration for computing the gradient and the Hessian matrix. It will be discussed in detail in the next section.

### 3.3 Recovering from Fluid to Kinetic Regime

In the fluid region, all the information we have on the distribution function are the expansion coefficients \(\{f_\alpha, \alpha \leq 4\}\). When recovering the distribution function from these coefficients, we construct the “most likely” distribution using the maximum entropy principle. Similar idea has been used in [44] for a different application. This procedure requires solving the optimization problem (2.18) where the constraints are exactly the first four order moments. In this paper, a Newton iteration method is utilized to solve the 1D maximum entropy problem.

Consider the maximum entropy moment problem

\[
\hat{f} = \arg\min_{f\in\mathbb{H}} \int_{\mathbb{R}} f \log f - f \, dv, \quad s.t. (\hat{f}(v))_k = \mu_k, \quad k = 0, \ldots, 4, \tag{3.14}
\]

where

\[
\mathbb{H} := \{ f \geq 0 : (1 + v^{2n}) f \in L^1(\mathbb{R}), f \neq 0 \}, \quad \forall n \in \mathbb{N}.
\]

We follow the approach in [1] to reformulate (3.14) into the unconstrained form

\[
\beta = \arg\min_{\beta\in\mathcal{A}\mathbb{L}} \int_{\mathbb{R}} \exp\left(\sum_{i=0}^{4} \beta_i v^i\right) dv - \sum_{i=0}^{4} \beta_i \mu_i, \quad \tag{3.15}
\]

where

\[
\mathcal{A} \triangleq \left\{ \beta \in \mathbb{R}^5 \mid \beta_4 < 0, \text{ or } \beta_4 = \beta_3 = 0 \text{ with } \beta_2 < 0 \right\}.
\]

The Newton method is utilized to solve this optimization problem as

1. Provide the starting point \(\beta_0\) by a combination of analysis and interpolation from pre-computed data. Compute the corresponding gradient \((\nabla \mathcal{L})_0\) and Hessian matrix \(H_0\).
2. At iteration \(m\), perform the following steps:
   (a) Solve for the direction of descent by
       \[H_m d_m = - (\nabla \mathcal{L})_m;\]
   (b) Find the next iteration point \(\beta_{m+1}\) as
       \[\beta_{m+1} = \beta_m + d_m;\]
   (c) At the new iteration point \(\beta_{m+1}\), compute the gradient \((\nabla \mathcal{L})_{m+1}\) and the Hessian \(H_{m+1}\).
Direct computation shows that

\[(\nabla \mathcal{L})_{m,j} = \int_{\mathbb{R}} v^j \exp\left(\sum_{i=0}^{4} \beta_i v_i\right) dv - \mu_j, \quad H_{m,jk} = \int_{\mathbb{R}} v^{k+j} \exp\left(\sum_{i=0}^{4} \beta_i v_i\right) dv.\]

(3.16)

To ensure fast convergence, we need to specify a good initial condition. In the Newton iteration method, if the given moments are close to the Junk’s line, or are below the Junk’s line and near the Maxwellian point, we use an analytical estimation to determine the initial Lagrangian multiplier \(\beta\). Otherwise, the initial \(\beta\) is determined from interpolation on a database of pre-computed \(\beta\) which is generated by using a fine grid on the realizable region of \((\mu_3, \mu_4)\). The Newton iteration converges with an average three steps, the details of which is shown in [29].

Moreover, providing an efficient algorithm to compute the high order moments of the distribution function will also speed up calculation of the Hessian matrix and gradients of the Lagrange function in (3.16). Computing the high order moments means accurately computing the numerical integration efficiently, which is solved by an adaptive integral formulation in the Newton iteration method. To make the distribution function integrable, it requires that \(\beta_4 = \beta_3 = 0\), or \(\beta_4 < 0\), and therefore the integration can be approximated accurately by integration on a sufficiently large bounded domain. Details for the truncation and applying the numerical quadrature are provided in “Appendix C”.

For now, we have introduced the brief review of the Maximum entropy method to complete the distribution function. The criterion to discriminate the fluid and kinetic regime in the 1D microscopic velocity space case is completed and we will extend it to the 3D microscopic velocity space case.

### 3.4 Regime Indicator and Criterion in 3D Microscopic Velocity Space

In this section, we will discuss the problem in 3D microscopic velocity space. Since it is the initial paper in the hybrid moment method using the maximum entropy method to recover the distribution function, we will focus on some special cases.

In some benchmark problems, for example the shock wave problem, we only focus on the problems with 1D spatial space and 3D microscopic velocity space. In this case, the distribution function has some symmetric properties in the direction \(v_2\) and \(v_3\). Therefore, the dimension reduction method is always adopted to reduce the computational complexity [18]. In this paper, the dimension reduction method in [7] is utilized for the hyperbolic moment method, where the BGK and Shakhov collision terms are discussed. The total freedom of the distribution function in the 3D microscopic velocity space is described by two distribution functions in 1D microscopic velocity space. The reduced distribution functions are defined as

\[g(t, x, v_1) = \int_{\mathbb{R}^2} f(t, x, \mathbf{v}) dv_2 dv_3,\]

\[h(t, x, v_1) = \int_{\mathbb{R}^2} \frac{v_2^2 + v_3^2}{2} f(t, x, \mathbf{v}) dv_2 dv_3.\]

(3.17)

Assuming the expansion number of the initial distribution function \(f(t, x, \mathbf{v})\) is \(M\), then \(g(t, x, v_1)\) and \(h(t, x, v_1)\) can be approximated as
\[
g(t, x, v_1) \approx \sum_{\alpha_1 \leq M_g} g_{\alpha_1}(t, x) \mathcal{H}_{\alpha_1}^\theta(\xi_1),
\]
\[
h(t, x, v_1) \approx \sum_{\alpha_1 \leq M_h} h_{\alpha_1}(t, x) \mathcal{H}_{\alpha_1}^\theta(\xi_1),
\]
\[
\xi_1 = \frac{v_1 - u_1}{\sqrt{\theta}},
\]
(3.18)

where \(M_g = M\) and \(M_h = M - 2\) and \(\theta\) is the temperature of the distribution function \(f(t, x, v)\). Substituting the expansion (3.18) into the Boltzmann equation, we can derive similar moment equations for \(g(t, x, v_1)\) and \(h(t, x, v_1)\). The details of the moment equations are proposed in “Appendix B”.

For the 3D microscopic velocity problem, the similar fourth-order moment system is also adopted in the fluid regime. In this case, the expansion order is set as \(M_g = 4\) and \(M_h = 2\) in the fluid regime. For the reduced model, the criterion is applied to both distribution functions. Precisely, for the distribution function \(g(t, x, v_1)\), the same criterion as in the 1D microscopic velocity problem is adopted. When the initial distribution function \(f(t, x, v)\) is Maxwellian, the distribution function \(g(t, x, v_1)\), \(h(t, x, v_1)\) also has the form of Maxwellian.

Then the criterion is changed as below: supposing the eigenvalues of the indicator matrix produced by \(g(t, x, v_1)\) is \(\lambda_i, i = 1, 2\), the criterion in both regions is changed into

**From kinetic to fluid**

1. the eigenvalues are all close to the eigenvalues of the Euler equations.
\[
\max_{i=1,2} |\lambda_i - 1| \leq \epsilon_1.
\]
(3.19)

2. the \(l_1\) norm of the expansion coefficients of the distribution function \(g_\alpha\) and \(h_\alpha\) are small.
\[
\sum_{4 < |\alpha| \leq M} |g_\alpha| \leq \epsilon_2, \quad \sum_{2 < |\alpha| \leq M - 2} |h_\alpha| \leq \epsilon_2.
\]
(3.20)

Similarly, when both criteria are satisfied, the region is changed from kinetic to fluid regime. In this case, the expansion numbers of the distribution functions are set as \(M_g = 4\) and \(M_h = 2\).

**From fluid to kinetic**

1. at least one of the eigenvalues is far from the eigenvalues of the Euler equations.
\[
\max_{i=1,2} |\lambda_i - 1| > \epsilon_1.
\]
(3.21)

If this criterion is satisfied, the regime is changed from fluid to kinetic region. In this case, the expansion number of the distribution functions are set as \(M_g = M\) and \(M_h = M - 2\). Moreover, the maximum entropy method is applied on \(g(t, x, v_1)\) to recover the higher order expansion coefficients. For \(h(t, x, v_1)\), since its expansion order in the fluid regime is only \(M_h = 2\), and we do not have any other information, the higher order expansion coefficients are set as zero.

For now, we have introduced the criterion to distinguish different regimes. The detailed numerical scheme which is applied under the framework of the hyperbolic moment method with some adjustment in the interface between the fluid and kinetic regime, will be proposed in the next section.
Remark 2 The application of this hybrid method is only suitable for the problems with 1D spatial space and 3D microscopic velocity space with the BGK and Shakhov collision term, where the dimension reduction method could be utilized. The only information we have about the distribution function is $g$ and $h$, which is the 1D distribution functions in velocity space. Then, we can utilize our method to complete the moment coefficients of higher order. For the general collision term, where the dimension reduction could not be applied, the method could not be applied. Due to the complexity of the maximum entropy problem in the 3D velocity case, we will work on this problem in the future.

4 Numerical Schemes

In the hyperbolic moment method, the standard finite volume discretization is adopted in the spatial space. Firstly, the standard splitting method is applied, where the moment equations are split into the convection step and the collision step.

In the convection step, the standard finite volume method is utilized, and the only difference is the case that the expansion numbers are different in the adjacent cells. Here, we take the 1D spatial space as an example. Suppose $\Gamma_h$ to be a uniform mesh in $\Omega \subset \mathbb{R}$, and each cell is identified by an index $j$. The numerical solution to approximate the distribution function $f$ at $t = t_n$ is denoted as

$$f_h(x, v) = f_j^n(v) = \sum_{|\alpha| \leq M_j^n} f_{\alpha, j}^n \mathcal{H}_\alpha \mu_{\alpha, j}^n (v), \quad x \in \Gamma_j,$$  \hspace{1cm} (4.1)

where $M_j^n$ is the expansion number at cell $j$ and time $t = t_n$ with $u_{1,j}^n$ the first entry of $u_j^n$. Assuming the expansion number on the cell $j + 1$ are $M_{j+1}^n$. If $M_{j+1}$ equals $M_j^n$, then the same HLL flux in [8] is utilized here. However, if they are different, we just take the algorithm below

1. Let $M_j = \max(M_{j+1}^n, M_j^n)$;
2. Reset the expansion number of $f_j^{n+1}$ and $f_j^n$ to $M_j$, where the increased expansion coefficients are set as 0. The reset distribution functions are labeled as $f_j^{n,*}$ and $f_j^{n,*}$;
3. Calculate the numerical flux $F_{n, j+1/2}^{n, *}$ using HLL scheme with $f_j^{n,*}$ and $f_{j+1}^{n,*}$;
4. For the $j-$th cell, derive the numerical flux $F_{n, j+1/2}$ by setting the expansion number of $F_{j+1/2}^{n,*}$ as $M_j^n$, where the expansion coefficients whose orders are higher than $M_j^n$ are simply cut off.

Remark 3 Though in the whole region, the standard finite volume method with HLL flux is utilized in the convection step, we want to emphasize that the expansion numbers in the fluid regime and the kinetic regime are different. Therefore, the computational cost to get the numerical flux is quite different.

The collision step is the same as that in the hyperbolic moment method and we refer [8] for more details. For the completeness of this paper, the detailed numerical method for the hyperbolic moment method is listed in “Appendix A”.

5 Numerical Experiments

In this section, several numerical examples are tested to validate the efficiency of the hybrid method. The BGK or Shakhov collision operators are adopted with the relaxation time co-

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responding to the Maxwell molecules model with $\omega = 1$. Thus (2.13) is reduced into

$$\tau = \frac{Kn}{\rho}. \quad (5.1)$$

The reference solution is computed by the discrete velocity method with mesh fine enough. In the simulation, the linear reconstruction in the spatial space \cite{10} is adopted in the HME and hybrid method to improve the efficiency of the numerical scheme, while the Euler solution is computed using finite volume method with Lax–Friedrichs numerical flux and the mesh fine enough. The time step is determined by the CFL condition (A.10) for all the examples. Computations for the Euler solutions, HME and hybrid method are performed in sequential code on a computer with Intel i7-7500U CPU and 16 GB memory.

### 5.1 Shock Tube Problem

This section considers the shock tube problem for the BGK collision term. The problems in 1D spatial space and 3D microscopic velocity space are studied. The computation domain is infinite but taken to be $[-1.5, 1.5]$ in the simulations. As in \cite{40}, the initial condition is $f(0, x, v) = f_M(\rho, u_1, \theta)$, with

$$\rho(0, x) = \begin{cases} 7.0, & \text{if } x < 0, \\ 1.0, & \text{if } x > 0, \end{cases} \quad p(0, x) = \rho \theta = \begin{cases} 7.0, & \text{if } x < 0, \\ 1.0, & \text{if } x > 0, \end{cases} \quad u_x(0, x) = 0. \quad (5.2)$$

We consider different Knudsen numbers ranging from the fluid limit to the kinetic regime. The numerical solutions we get from the hybrid method and HME are studied, where the Euler solution, the fluid solution which is get by the fourth-order HME system, and the DVM solution are also computed as reference. In all these computations, we take 1000 evenly
Fig. 2 Comparisons of solutions in Sect. 5.1 for $\rho$, $u_x$, $\theta$, and $q_x$ as functions of $x$ for $Kn = 0.05$.

Fig. 3 Comparisons of solutions in Sect. 5.1 for $\rho$, $u_x$, $\theta$, and $q_x$ as functions of $x$ for $Kn = 0.5$. 
Fig. 4 Comparisons of solutions in Sect. 5.1 for \( \rho \), \( u_x \), \( \theta \) and \( q_x \) as functions of \( x \) for \( Kn = 5 \)

spaced grids in spatial space for the hybrid method, both fourth order and full HME, while the Euler solution is computed on a sufficiently fine mesh to ensure convergence. For the full HME system and the hybrid model, the maximum expansion order is set as \( M = 40 \). The ending time is \( t = 0.3 \). In our test, the Knudsen number is set as \( Kn = 0.0001, 0.05, 0.5 \) and \( 5 \), indicating the problem changes from the fluid regime to the kinetic regime.

In Figs. 1, 2, 3 and 4, the numerical solutions of density \( \rho \), macroscopic velocity in the \( x \) direction \( u_x \), temperature \( \theta \) and heat flux in the \( x \) direction \( q_x \) for the hybrid method and HME with different Knudsen numbers are plotted. From these figures, we can see that for all these Knudsen numbers, the numerical solutions by the hybrid method and HME are all on top of each other. Though there is some difference between the HME solution and DVM solution for \( q_x \) when \( Kn = 10^{-4} \), the error is quite small. In other cases, they all matches well with the reference solutions by DVM. This means that the hybrid method could capture the evolution of the fluid flow for all the regimes.

When \( Kn = 0.0001 \) where it belongs to the fluid regime, it is expected that Euler equations could accurately describe the properties of the fluid flow. From Fig. 1, we can see that the numerical solutions of the hybrid method and HME are all consistent with that of the Euler equation and the fluid solver. With the increase of the Knudsen number, the numerical solutions moves further and further away from that of the Euler equations and the fluid solver. When \( Kn = 0.05 \), the solutions of the hybrid method and HME deviates from the Euler solution, but still agrees well with the solutions of the fluid solver. This is consistent with the fact that the fluid solver, which is a fourth-order HME, remains valid for a wider range of Knudsen number than the Euler equation. When \( Kn = 0.5 \) and \( Kn = 5 \), the fluid flow is in the transitional area, and can only be described by the kinetic theory. From Fig. 4, we can find that numerical solutions of the hybrid method and HME are still almost the same,
but all these solutions are quite different from the Euler solution. The solutions of the fluid solver are somewhere between the solutions of HME and the Euler solutions. This shows that for $Kn = 0.5$ and $Kn = 5$, the fluid solver is no longer adequate for describing the evolution of the system, and a hybrid method where a kinetic solver is also imposed is indeed necessary.

In order to show the efficiency of the hybrid method, the time variation of the expansion order for each grid used by the hybrid method is tested. Figure 5 shows the change of the expansion order, where the blue region is those with order 4 and the yellow region is those with the maximum order. From it, we can find that when $Kn = 0.0001$, most of the region is blue, which means that the flow is in the fluid regime. With the increase of $Kn$, the yellow region becomes larger. Based on the numerical results shown from Figs. 1, 2, 3 and 4, we can find that for all the Knudsen numbers tested, the middle part of the spatial area belongs to the kinetic regime, which is also consistent with the expansion order showed in Fig. 5. This indicates that the new hybrid method could accurately detect different regimes. The computation time of the hybrid method and HME for the different Knudsen numbers is compared in Table 1. We could see that the hybrid method could save the computational time for all the Knudsen numbers, which means that it works effectively in all the regimes. For the fluid regime, the hybrid method saves up to almost half of the computation cost. Even for $Kn = 5$ when it is in the kinetic regime, the hybrid solver reduces the computation cost by around 30%.

Fig. 5 The maximum order used in each region at each time step for different Knudsen numbers in Sect. 5.1
Fig. 6 Comparisons of solutions for $\rho$, $u_x$, $\theta$ and $q_x$ as functions of $x$ for $Kn = 0.01$ in Sect. 5.2.

Fig. 7 Comparisons of solutions for $\rho$, $u_x$, $\theta$ and $q_x$ as functions of $x$ for $Kn = 1$ in Sect. 5.2.
Table 1 Comparison of computational time of the hybrid method and HME with different Knudsen numbers in Sect. 5.1

| Kn       | Full HME (s) | Hybrid (s) |
|----------|--------------|------------|
| 0.0001   | 223          | 112        |
| 0.05     | 220          | 143        |
| 0.5      | 221          | 152        |
| 5        | 222          | 153        |

Fig. 8 The maximum order used in each spatial grid at each time step for different Knudsen numbers in Sect. 5.2

Table 2 Comparison of computational time of the hybrid method and HME with different Knudsen numbers in Sect. 5.2

| Kn       | HME (s) | Hybrid (s) |
|----------|---------|------------|
| 0.01     | 74      | 43         |
| 1        | 75      | 44         |

5.2 Shock Tube Problem with Two Rarefaction Waves

The shock tube problem with two rarefaction waves is tested in this section, a similar set-up of which could be found in [2]. The problems in 1D spatial space and 3D microscopic velocity space are studied. The computation domain is infinite but taken to be $[-1.5, 1.5]$ in the simulation. The initial condition is $f(0, x, v) = f_M(\rho, u_x, \theta)$, with

$$
\rho(0, x) = 1.0, \quad u_x(0, x) = \begin{cases} 
-1.0, & \text{if } x < 0, \\
1.0, & \text{if } x > 0,
\end{cases} \quad \theta = 1.0.
$$

(5.3)

The numerical solution with $Kn = 0.01$ and $Kn = 1$ for the Shakhov collision operator is studied. In the test, the grid size is set as $N = 1000$ and the maximum expansion order is $M = 40$.

Figures 6 and 7 show the macroscopic variables $\rho, u_x, \theta$ and $q_x$ at $t = 0.12$ with different Knudsen numbers. When $Kn = 0.01$, we can find that the numerical solutions by the hybrid method are almost the same as HME. Though some small deviations from DVM solutions can be observed in $\theta$ and $q_x$, the relative error is small. When $Kn = 1$, we can find that the numerical solutions by the hybrid method and HME are also on top of each other, which all agree with the reference by DVM. This means that for problems with two rarefaction waves, the hybrid method can capture the fluid flow. For this test case, when $Kn = 0.01$, the Euler...
solution already deviates somewhat from the kinetic solution, while the solutions of the fluid solver is still in rough agreement with the solutions of the hybrid method and HME. When $Kn = 1$, the solutions of both the Euler and the fluid solver fail to accurately capture the nonequilibrium behaviour, with the fluid solver solutions showing better performance than the Euler solutions. This, therefore, validates the need for the hybrid method. The efficiency of the hybrid method is also tested. Figure 8 shows the time evolution of the maximum order actually used by the hybrid method for each grid in this example. As in the previous example, the blue region indicates a maximum expansion order of 4, while the yellow region means a maximum expansion order of 40. From it, we can find that in the middle of the spatial area, where it is the kinetic regime, the expansion order reaches the maximum, while in the left and right sides of the spatial area, the expansion order four is retained. This means that the hybrid scheme could detect the rarefied zones correctly for the rarefaction wave problems. In Table 2, we compare the computation time for the hybrid method and HME for the two Knudsen numbers. For both cases, we see almost 40 percent of reduction of the computation cost, which shows the efficiency of the hybrid method.

### 5.3 Blast Wave

In this section, a similar blast wave problem as in [17] is tested. The problems in 1D spatial space and 3D in microscopic velocity space with Shakhov collision model are studied. The computation domain is taken to be $[-1, 1]$ in the simulations. The initial condition is $f(0, x, v) = f_M(\rho, u_x, \theta)$, with

$$
\rho(0, x) = 1.0, \quad u_x(0, x) = \begin{cases} 
1.0, & \text{if } x \leq -0.3, \\
0, & \text{if } -0.3 < x < 0.3, \\
-1.0, & \text{if } x \geq 0.3,
\end{cases}
$$

$$
\theta = \begin{cases} 
1.5, & \text{if } x \leq -0.3, \\
1.0, & \text{if } -0.3 < x < 0.3, \\
1.5, & \text{if } x \geq 0.3.
\end{cases}
$$

We take $Kn = 0.001$ and $Kn = 0.01$. In the test, the grid size is set as $N = 1000$ and the maximum expansion order is $M = 40$.

Figures 9 and 10 show the behavior of $\rho, u_x, \theta$ and $q_x$ at time $t = 0.05, 0.15$ and 0.35 for the Knudsen number $Kn = 0.001$ and 0.01. For all these cases, we see good agreement between the hybrid solver and HME, as well as the reference solution. When $Kn$ is small, we can find that the numerical solutions of HME and the hybrid method agree well with that of Euler equations. In Fig. 11, the time evolution of the maximum order actually used by the hybrid method is again plotted. We can find that for the kinetic region in the middle of the spatial space, the expansion order is 40, which is the yellow region. For the fluid regime, the expansion order is 4, which is the blue region. Note that when $Kn = 0.001$, the spatial position of the yellow region changes as time evolves. This is probably because the relaxation...
Fig. 9 Comparisons of solutions for $\rho$, $u_x$, $\theta$ and $q_x$ as functions of $x$ for $Kn = 0.001$ at time $t = 0.05, 0.15$ and 0.35 in Sect. 5.3

time depends on $Kn/\rho$, and as shown in Fig. 9, the position of the peak values of $\rho$ changes in space with time evolution. This shows that this hybrid method could detect the fluid and kinetic regimes. Moreover, when $Kn = 0.001$, the blue region with expansion order 4 is much larger than that of $Kn = 0.01$, which means that more area belongs to the fluid regime when Knudsen number is smaller. Table 3 compares the computation cost of the hybrid method and HME, we can find that when $Kn = 0.001$, almost 40% of the total computational cost will be saved, while one fourth will be saved when $Kn = 0.01$. Moreover, when $Kn = 0.001$, the hybrid method is more efficient than the case $Kn = 0.01$, which is also consistent with our intuition that usually for smaller Knudsen number, larger area of the flow is in the fluid regime.
5.4 Fourier Flow

In order to show the ability of the hybrid method to capture boundary layer, the Fourier flow is studied. In the Fourier flow, the motion of gas between two infinite stationary parallel plates with different temperatures is studied. Similar problems can be found in [3,9,41]. Since we only want to study the ability of the hybrid method to capture the boundary layer, the simple 1D spatial space and 1D microscopic velocity space with BGK collision term is tested. Same as in [9,37], the Maxwell boundary condition is utilized here, where the boundary conditions are fixed wall temperature, and the initial conditions are linear functions connecting the wall temperature. We choose the wall temperature as

$$T_{wl} = 1, \quad T_{wr} = 1.1. \quad (5.5)$$

Fig. 10 Comparisons of solutions for $\rho, u_x, \theta$ and $q_x$ as functions of $x$ for $Kn = 0.01$ at time $t = 0.05, 0.15$ and $0.35$ in Sect. 5.3
Fig. 11 The maximum order used in all spatial grids at each time step for different Knudsen numbers in Sect. 5.3

Fig. 12 Comparisons of solutions for $\rho$, $\theta$ and $q$ as functions of $x$ for $Kn = 0.001$, 0.01 and 0.1

In the test, the uniform mesh with $N = 200$ is utilized and the maximum expansion order is $M = 30$. The Knudsen number is chosen as $Kn = 0.001$, 0.01 and 0.1. The HME solution is the numerical solution produced by the HME method with the expansion number $M = 30$, while the fluid solution is the numerical solution computed by the HME method with the expansion number $M = 4$. Figure 12 shows the density, temperature and heat flux at the steady state. For all the Knudsen number, the kinetic region is near the boundary. Also, the area of the kinetic region increases with the increase of the Knudsen number. Near the plate,
the gas may be in the non-equilibrium state, and the kinetic model should be adopted. We can find that the hybrid solution is almost the same as that of the HME solution when $Kn$ is small, such as $Kn = 0.01$ and $0.001$. Moreover, we can find obvious difference between the fluid solution and the HME solution. This means that the fluid model could not capture the evolution of the system well compared to the hybrid model. When $Kn$ is large, the heat flux of the hybrid solution does not match well with the HME solution, which may be due to the reason that there is model error between the hybrid model and the HME model.

6 Conclusion

This work aims at a uniform hybrid moment method for the multi-scale kinetic problems. The method is proposed in the framework of the hyperbolic moment method. Instead of Euler or Navier–Stokes equations, the fourth order moment system is utilized as the governing equations in the fluid region, in which case only one set of the numerical scheme is needed for both fluid and kinetic regions. Moreover, with the fourth order moment systems, the maximum entropy method is applied here to derive the high order expansion coefficients of the distribution function in the interface area from the fluid regime to the kinetic regime. Several numerical experiments show that this hybrid numerical algorithm can capture the evolution of the systems in different regions accurately and efficiently.

The method will be further validated in the numerical tests for more complex kinetic models, which is one of the ongoing work. The extension of the method to high dimensional problems will also be studied in future work.

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Data Availability Data available on request from the authors. The data that support the findings of this study are not openly available due to the reason that the code to simulate the examples is not open source, and are available from the corresponding author upon reasonable request for scientific usage.

Declarations

Conflict of interest The authors declare that no conflicts of interest.

Code Availability Code available on request from the authors.

Appendix A: Numerical Scheme for the Regularized Moment Method

In this section, we will introduce the numerical scheme of the dimensional reduced regularized moment method. We refer readers [7] for more details. Let $\omega = (\omega^{(f)}, \omega^{(h)})$ be the variables of the reduced system, where $\omega^{(f)}$, $f = g, h$ is the corresponding variable of the distribution...
function $f$ in (2.28). The reduced moment system is written as

$$\frac{\partial \omega}{\partial t} + \sum_{j=1}^{2} B_j \frac{\partial \omega}{\partial x} = Q \omega. \quad \text{(A.1)}$$

Splitting method is adopted here, where (A.1) is split into the convection part and the collision part:

- **convection part**:
  $$\frac{\partial \omega}{\partial t} + \sum_{j=1}^{2} B_j \frac{\partial \omega}{\partial x} = 0. \quad \text{(A.2)}$$

- **collision part**:
  $$\frac{\partial \omega}{\partial t} = Q \omega. \quad \text{(A.3)}$$

The detailed algorithm is as below,

1. Let $n = 0$, and give the initial value of $\omega^n_i$.
2. Calculate the time step length $\Delta t_n$ by CFL condition.
3. Solve the convection part using the finite volume method with the HLL flux, and denote the result as $\omega^{n,*}_i$.
4. Update the collision step using $\omega^{n,*}_i$ as the initial condition.
5. Let $t \leftarrow t + \Delta t_n$ and $n \leftarrow n + 1$; then go to Step 2.

The numerical scheme for the convection step and the collision is listed below in detail.

**Convection step** For the convection part, the moment equation (A.2) is reformulated as

$$\frac{\partial \omega}{\partial t} + \frac{\partial F(\omega)}{\partial x} + R(\omega) \frac{\partial \omega}{\partial x} = 0. \quad \text{(A.4)}$$

Then, the finite volume method is utilized here, and the detailed scheme is

$$\omega^{n,*}_i = \omega^n_i - \frac{\Delta t_n}{\Delta x} \left( \hat{F}^{n+}_{i+1/2} - \hat{F}^{n-}_{i-1/2} \right) - \frac{\Delta t_n}{\Delta x} \left( \hat{R}^{n+}_{i+1/2} - \hat{R}^{n-}_{i-1/2} \right), \quad \text{(A.5)}$$

where $\hat{F}^{n+}_{i+1/2}$ is the HLL numerical flux defined as

$$\hat{F}^{n+}_{i+1/2} = \begin{cases} F(\omega^n_i), & \lambda_{i+1/2}^{L,n} \geq 0, \\ \frac{\lambda_{i+1/2}^{R,n} F(\omega^n_{i+1}) - \lambda_{i+1/2}^{L,n} F(\omega^n_{i})}{\lambda_{i+1/2}^{R,n} - \lambda_{i+1/2}^{L,n}}, & \lambda_{i+1/2}^{L,n} < 0 < \lambda_{i+1/2}^{R,n}, \\ \lambda_{i+1/2}^{L,n} \leq 0. & \\ F(\omega^n_{i+1}), & \lambda_{i+1/2}^{R,n} \leq 0. \end{cases} \quad \text{(A.6)}$$
The numerical flux for the non-conservation part \( \hat{R}_{i+1/2}^n \) is

\[
\hat{R}_{i+1/2}^n = \begin{cases} 
0, & \lambda_{i+1/2}^{L,n} \geq 0, \\
-\frac{\lambda_{i+1/2}^{L,n}}{\lambda_{i+1/2}^{L,n} - \lambda_{i+1/2}^{R,n}} g_{i+1/2}^n, & 0 < \lambda_{i+1/2}^{R,n}, \\
g_{i+1/2}^n, & \lambda_{i+1/2}^{R,n} \leq 0,
\end{cases}
\]

(A.7)

with

\[
g_{i+1/2}^n = \int_0^1 R(\Phi(s; q_i^n, q_{i+1}^n)) \frac{\partial \Phi}{\partial s}(s; q_i^n, q_{i+1}^n) \, ds,
\]

(A.8)

where \( \Phi(s; \cdot, \cdot) \) is a path that connects the two states. We refer [11] for more details. The characteristic speeds \( \lambda_{i+1/2}^{R,n} \) and \( \lambda_{i+1/2}^{L,n} \) are

\[
\lambda_{i+1/2}^{R,n} = \max \left( u_{1,i}^n + C_{M+1} \sqrt{\theta_i^n}, u_{1,j}^n + C_{M+1} \sqrt{\theta_{i+1}^n} \right), \\
\lambda_{i+1/2}^{L,n} = \max \left( u_{1,i}^n - C_{M+1} \sqrt{\theta_i^n}, u_{1,j}^n - C_{M+1} \sqrt{\theta_{i+1}^n} \right),
\]

(A.9)

where \( C_{M+1} \) is the maximal root of Hermite polynomial of degree \( M + 1 \). The time step length is also decided by the characteristic velocity as

\[
\Delta t^n \max_i \left\{ \left| \lambda_{i+1/2}^{R,n} \right|, \left| \lambda_{i+1/2}^{L,n} \right| \right\} \leq CFL.
\]

(A.10)

**Collision step** For the BGK and Shakhov model, the collision part can be solved exactly in the reduced regularized moment method. For neatness, the superscript \( n, n + 1 \) and the subscripts \( i \) are omitted. The solutions are as below:

- For the BGK model:

\[
g_\alpha = g_\alpha^* \exp \left( -\frac{\Delta t}{\tau} \right), \quad 2 \leq |\alpha| \leq M, \\
h_0 = g_0^* \theta^* \left( 1 - \exp \left( \frac{\Delta t}{\tau} \right) \right) + h_0^* \exp \left( -\frac{\Delta t}{\tau} \right), \\
h_\alpha = h_\alpha^* \exp \left( -\frac{\Delta t}{\tau} \right), \quad 1 \leq |\alpha| \leq M - 2.
\]

(A.11)
For the Shakhov model:

\[ g_{3e_1} = g_{3e_1}^* \exp \left( -\frac{\Delta t}{\tau} \right) + \frac{1}{5} g_i^* \left( \exp \left( -\frac{\Pr \Delta t}{\tau} \right) - \exp \left( -\frac{\Delta t}{\tau} \right) \right), \]
\[ g_\alpha = g_\alpha^* \exp \left( -\frac{\Delta t}{\tau} \right), \quad |\alpha| = 2 \text{ or } 4 \leq |\alpha| \leq M, \]
\[ h_0 = g_0^* \theta^* \left( 1 - \exp \left( -\frac{\Delta t}{\tau} \right) \right) + h_i^* \exp \left( -\frac{\Delta t}{\tau} \right), \]
\[ h_{e_1} = h_{e_1}^* \exp \left( -\frac{\Delta t}{\tau} \right) + \frac{1}{5} g_i^* \left( \exp \left( -\frac{\Pr \Delta t}{\tau} \right) - \exp \left( -\frac{\Delta t}{\tau} \right) \right), \]
\[ h_{3e_1} = h_{3e_1}^* \exp \left( -\frac{\Delta t}{\tau} \right) + \frac{\theta^*}{5} g_i^* \left( \exp \left( -\frac{\Pr \Delta t}{\tau} \right) - \exp \left( -\frac{\Delta t}{\tau} \right) \right), \]
\[ h_\alpha = h_\alpha^* \exp \left( -\frac{\Delta t}{\tau} \right), \quad |\alpha| = 2 \text{ or } 4 \leq |\alpha| \leq M - 2. \]

**Appendix B: Reduced Moment System**

When the distribution function has some symmetric properties in the direction \( v_2 \) and \( v_3 \), the Chu reduction is utilized here and we refer [7] for more details. With this dimension reduction method, we will introduce two distribution functions in 1D microscopic velocity space (3.17), which is approximated as (3.18). The reduced Boltzmann with Shakhov collision model for \( g(t, x, v_1) \) and \( h(t, x, v_1) \) is

\[
\frac{\partial g}{\partial t} + v_1 \frac{\partial g}{\partial x} = \frac{1}{\epsilon} \left( g^N - g \right),
\]
\[
\frac{\partial h}{\partial t} + v_1 \frac{\partial h}{\partial x} = \frac{1}{\epsilon} \left( h^N - h \right),
\]

where

\[
g^N = \left[ 1 + \frac{(1-\Pr)(v_1 - u_1(t,x))q(t,x)}{5\rho(t,x)[\theta(t,x)]^2} \left( \frac{|v_1 - u_1(t,x)|^2}{\theta(t,x)} - 5 \right) \right] g_{eq},
\]
\[
h^N = \left[ 1 + \frac{(1-\Pr)(v_1 - u_1(t,x))q(t,x)}{5\rho(t,x)[\theta(t,x)]^2} \left( \frac{|v_1 - u_1(t,x)|^2}{\theta(t,x)} - 3 \right) \right] h_{eq},
\]

with

\[
g_{eq} = \frac{\rho}{\sqrt{2\pi}\theta} \exp \left( -\frac{(v_1 - u_1(t,x))^2}{2\theta} \right), \quad h_{eq} = \theta g_{eq}.
\]

The relationship of the macroscopic variables and the distribution functions are

\[
\rho = \int_R g(t,x,v_1) \, dv_1, \quad \rho u_1 = \int_R v_1 g(t,x,v_1) \, dv_1,
\]
\[
\frac{3}{2} \rho \theta = \int_R \left( \frac{1}{2} |v_1 - u_1|^2 g + h \right) \, dv_1, \quad q_1 = \int_R (v_1 - u_1) \left( \frac{1}{2} |v_1 - u_1|^2 g + h \right) \, dv_1.
\]
Substituting (3.18) into (B.1), and matching order of the basis functions, we can derive the moment equations for the reduced distribution function as

\[
\frac{\partial \psi}{\partial t} + \left( \theta \frac{\partial \psi}{\partial x} + u_1 \frac{\partial \psi}{\partial x_1} + (1 - \delta_{N,i}) (i + 1) \frac{\partial \psi_{i+1}}{\partial x} \right) + \frac{\partial u_1}{\partial t} \psi_{i-1} \\
+ \frac{\partial u_1}{\partial x} \left[ \theta \psi_{i-2} + u_1 \psi_{i-1} + (1 - \delta_{N,i}) (i + 1) \psi_i \right] + \frac{1}{2} \frac{\partial \theta}{\partial t} \psi_{i-2} \\
+ \frac{1}{2} \left[ \psi_{i-3} + u_1 \psi_{i-2} + (1 - \delta_{N,i}) (i + 1) \psi_{i-1} \right] = \frac{1}{\epsilon} (\Delta_i (\psi) - \psi_i), \quad i \leq N,
\]

where \( \psi = g, h \). When \( \psi = g, N = M \), while \( N = M - 2 \), if \( \psi = h \). Here \( \Delta_i (\psi) \) is the deduced by the collision term as

\[
\Delta_i (g) = \begin{cases} 
  g_0, & i = 0, \\
  (1 - \Pr) q_i / 5, & i = 3, \\
  0, & \text{otherwise,}
\end{cases} \quad \Delta_i (h) = \begin{cases} 
  \theta g_0, & i = 0, \\
  (1 - \Pr) q_i / 5, & i = 1, 3, \\
  0, & \text{otherwise,}
\end{cases}
\]

Appendix C: Integration Algorithm in Computing the Maximum Entropy Distribution Function

For computing the gradient and Hessian matrix when applying the Newton iteration to solve the maximum entropy distribution ansatz, we need to compute the high order moments of the distribution ansatz. We employ an adaptive integration technique based on the location of the peaks of the distribution function. Since the maximum entropy distribution function takes the form of \( \exp(P(v)) \), where \( P(v) \) is a quartic function, its peak values could be computed by taking the roots of \( P'(v) \). In [29], the detailed algorithm has been provided, and we briefly review it here. Since the distribution function decays exponentially, we truncate the integration domain from \( \mathbb{R} \) to one or two bounded intervals, by taking the intercept of \( P(v) \) at a certain value, such that \( P(v) \) is cut somewhere sufficiently low below its peak values. The truncation procedure is done by considering two possible scenarios separately.

Let \( P(v) = \sum_{i=0}^{4} \beta_i v^i \),

1. If \( P(v) \) has only one peak, which we denote as \( v_1 \), the integration interval is decided as \([c_1, c_2]\), where \( c_1, c_2 \) are the two roots of \( P(v) = (P(v_1) - c) = 0, \)

with \( c \) a sufficiently large constant.

2. If \( P(v) \) has two peaks \( v_1 \) and \( v_2 \), we solve

\[
P(v) - (P(v_1) - c) = 0, \quad P(v) - (P(v_2) - c) = 0,
\]

to obtain the two intervals as \([c_1, c_2]\) and \([c_3, c_4]\). If \( c_2 > c_3 \), then the interval \([c_1, c_4]\) is used for computation.

The value of \( c \) is taken according to experience, such that it is sufficiently large. In our computation, it is usually enough to take \( c = 50 \). There are two additional special cases which we treat separately:

1. If \( |\beta_4| < 10^{-16} \) and \( \beta_2 < 0 \), the distribution function is almost Maxwellian. In this case, we could directly specify the integration interval, as the position of the peak is simply
Considering that the smaller the value of $|\beta_2|$, the larger the integration interval needs to be, we take the length of the truncated integration interval to be $4\sqrt{-\frac{50}{\beta_2}}$.

2. If $\beta_4 < -50$, the moments are close to the boundary of the realizable region. In this case, $c$ needs to be larger as the peaks are very sharp. Considering that the larger $|\beta_4|$ is, the sharper the peaks are, for moments near the boundary we modify the value of $c$ to be $c = 50\sqrt{-\frac{\beta_4}{10}}$.

Once the integration interval is determined, we use Gauss–Chebyshev quadrature to calculate the integral. In our numerical examples, 400 quadrature points are used to evaluate each integration. If there are two intervals, the quadrature points are divided between the two intervals proportional to the interval lengths.

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