Mesoscopic kinetic approach for studying nonequilibrium hydrodynamic and thermodynamic effects of shock wave, contact discontinuity, and rarefaction wave in the unsteady shock tube

Ruofan Qiu,† Tao Zhou, Yue Bao, Kang Zhou, Huanhuan Che, and Yancheng You†

School of Aerospace Engineering, Xiamen University, Xiamen 361005, People’s Republic of China

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This paper presents a detailed description of a molecular velocity distribution-based mesoscopic kinetic approach that enables a better understanding of various nonequilibrium hydrodynamic and thermodynamic effects in shock waves, contact discontinuities, and rarefaction waves. This builds on the mesoscopic kinetic approach in a previous investigation into regular reflection shocks by further addressing the mesoscopic physical meaning of kinetic moments from the view of kinetics and the implications of the magnitude and sign of nonequilibrium kinetic moments. To deepen understanding of nonequilibrium effects, this work focuses on the one-dimensional unsteady shock tube problem, which contains the typical and essential features of the discontinuous flows, and has no interference of two-dimensional flow direction. The approach uses a lattice Boltzmann method to solve the flow field, and describes nonequilibrium effects through the nonequilibrium kinetic moments of molecular velocity distribution functions. The mechanism of nonequilibrium effect in discontinuous flows is further probed. This work develops the mesoscopic kinetic approach and clarifies the mesoscopic physics of shock waves, contact discontinuities, and rarefaction waves.

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I. INTRODUCTION

Compressible flows with shock waves, contact discontinuities, and rarefaction waves are widespread in high-speed vehicles and rockets. Macroscopic computational fluid dynamics (CFD), which employs the Euler equations or Navier-Stokes equations, is one of the most widely used computational tools for studying the flow mechanisms and engineering applications of compressible flows. In fact, the macroscopic transport of fluid and heat is essentially the result of the collective motion of matter with random molecular motion at the microscopic level. Pham-Van-Diep et al. [1] experimentally observed the nonequilibrium molecular motion that occurs in a shock wave. Such nonequilibrium molecular motion will lead to nonequilibrium hydrodynamic and thermodynamic effects on a variety of physical properties. The nonequilibrium effects can be manifested in the physical characteristics of the shock wave, contact discontinuity, or rarefaction wave. The macroscopic method, which does not contain molecular information, may not adequately describe nonequilibrium effects in the internal region of the shock wave. The lattice Boltzmann (LB) method [2,3] is a mesoscopic CFD approach that describes fluid flow through the evolution of the molecular velocity distribution based on nonequilibrium statistical mechanics, which is suitable for studying the mechanism of shock waves with nonequilibrium molecular motion. In recent years, the LB method has been successfully applied to various incompressible flows, such as turbulence [4–7], heat transfer problems [8–11], fluid-structure interactions [12–14], porous media flows [15–18], and multiphase flows [19–22]. Its simple boundary treatment, highly efficient parallel computing, and ease of programming make it a promising CFD tool. However, the standard LB model is not suitable for simulating compressible flows.

Efforts have been made to develop compressible LB models that are capable of simulating shock waves. There are three approaches to establish compressible models which can recover the compressible Navier-Stokes equations. The multispeed approach achieves this goal by adding discrete velocities [23–25]. The multispeed models usually have a large number of discrete velocities and suffer from numerical instabilities [26]. The fixed Prandtl number is also a problem unless some additional treatment is done [27]. The second approach is the double-distribution-function (DDF) model, which solves the momentum and energy equations using two distribution functions separately [28,29]. The DDF models have less discrete velocities and good numerical stability. They are easy to obtain adjustable Prandtl numbers [30]. Guo et al. [29] proposed a DDF model based on the total energy distribution function, which is a simple DDF framework. The third one is called the hybrid approach, which solves the momentum and energy equations through the LB model and the macroscopic energy equation, respectively [31–33].

The determination of the equilibrium distribution function is another key issue for establishing a compressible LB model. The popular methods rely on the Gauss-Hermite quadrature-based methodology [34,35], the moment matching approach [25,36,37], or the maximum entropy principle [38–41]. The Gauss-Hermite quadrature-based methodology [34,35] can achieve higher-order approximations to the continuum Boltzmann equation. Based on this approach, Nie et al. [32] developed a hybrid method for transonic flows.
in which the energy dynamics are described by an entropy equation. They adopted the fifth-order Hermite polynomial for the equilibrium density distribution function. The supersonic flow past a wedge in a two-dimensional wind tunnel and the transonic flow around an RAE 2822 airfoil were simulated by their LB model. He et al. [42] introduced the Hermite expansion approach into the DDF framework [29], and simulated a spherical shock wave explosion in a three-dimensional enclosed box. Guo et al. [43] developed a compressible LB model with a Hermite expansion approach based on a hybrid recursive regularization collision operator. Compressible cases of the inviscid supersonic flow over a circular bump and shock-vortex interactions were examined. In the moment matching approach, the equilibrium distribution function is determined based on the kinetic moment relations to recover compressible Navier-Stokes equations. There are several ways to implement this approach [25,36,37]. Among them, the circular function-based equilibrium distribution function proposed by Qu et al. [36] is an effective compressible LB model. The simple circular function is effective for high-Mach-number cases. Li et al. [30] introduced the circular function-based discrete velocity model into the DDF framework for the density equilibrium distribution function. The model was validated through Riemann problems and a double Mach reflection case. Following this idea, Wang et al. [44] proposed a DDF-LB model with polynomial kernel function-based density and total energy equilibrium distribution functions. Recently, we applied Li et al.’s DDF-LB model with the circular function-based density equilibrium distribution function to simulate supersonic viscous flows with a boundary layer [45–47], such as supersonic boundary layers and shock wave and boundary layer interactions. The maximum entropy principle-based compressible LB model is presented by Frapolli et al. [38,39]. Latt et al. [41] extended their compressible LB model deriving exponential discrete equilibria designed to recover an arbitrary number of the Maxwellian moments. The number of discrete velocities in three dimensions can decrease from 343 to 39, by putting more effort into the equilibrium instead of the lattice. In addition to the approach mentioned above, the adaptive velocity discretization is also an effective way for compressible LB models [48–51]. The adaptive LB models can improve the accuracy and the stability for simulating large velocity and temperature variations in compressible flows.

The solving scheme is also an important issue needed to be addressed. The collide-and-stream algorithm is a distinguishing feature of LB method, which can not be easily implemented in compressible LB models. For instance, when using the Gauss-Hermite quadrature-based equilibrium distribution function with standard D2Q9 lattice, the diagonal elements of some velocity moments of equilibrium distribution functions deviate from the related relationship due to the low symmetry of the D2Q9 lattice [52]. This deviation can be removed by introducing a correction term [40,43,52–54]. On the other hand, the finite-difference method is another effective solving scheme for compressible LB model. In the finite-difference LB method, the time step is independent of the grid, and the choice of discrete velocity is free. The high performance of implicit-explicit Runge-Kutta (IMEX-RK) scheme [55] makes it popular in the finite-difference LB method community [27,30,42,44,47]. Besides, the Boltzmann-BGK also can be solved through the finite-volume scheme, such as the discrete unified gas kinetic schemes (DUGKS) [56].

With years of efforts by scholars, the compressible LB method has become more and more mature. However, most studies on compressible LB methods have focused on establishing the theoretical model according to the physical level of the macroscopic method. When the LB method is only regarded as another solving approach for the Navier-Stokes equations, its mesoscopic features are barely reflected. It is expected that the flow mechanism of shock waves with nonequilibrium molecular motion can be explored from the mesoscopic view by the LB method. In recent years, Xu and his coworkers proposed an investigative approach to introduce new physical insights into the hydrodynamic and thermodynamic nonequilibrium behaviors of fluid flows by comparing the nonconserved kinetic moments of the distribution function and those of the corresponding equilibrium distribution function [57–59]. They derived the association between some of the moments and certain macroscopic quantities, such as the viscous stress tensor and heat flux. They applied this approach to investigate shock waves [37], multiphase flows [60–63], and combustion [58,64,65]. For the shock wave problem, they only presented a simple and preliminary analysis of nonequilibrium effects [37].

Inspired by this idea, we recently presented a mesoscopic kinetic approach for nonequilibrium hydrodynamic and thermodynamic effects, and used it to study the inner-scale physics of regular reflection shock waves. This has produced novel insights into the behavior of shock waves, particularly in revealing the mechanism of nonequilibrium effects [66]. In this paper, we describe this mesoscopic kinetic approach in more detail than in Ref. [66], thus enhancing the overall understanding of the physical meaning of nonequilibrium effects occurring in shock waves. Two points are addressed, namely, the mesoscopic physical meaning of kinetic moments based on the view of kinetics and the implications of the magnitude and sign of nonequilibrium kinetic moments. These two points are also the main difference from the approach of Xu et al. First, an alternative understanding of the kinetic moments is proposed, enabling a systematic formulation of the physical meaning of nonequilibrium effects at various physical levels from the view of kinetics. Second, the implications of the magnitude and sign of nonequilibrium effects are presented in terms of the relation between the molecular velocity distributions in the current state and those in the local equilibrium state. Moreover, the nonequilibrium hydrodynamic and thermodynamic effects in contact discontinuities and rarefaction waves, which are also widespread in compressible flows, are studied in addition to shock waves. The one-dimensional unsteady shock tube problem has typical flow characteristics, and there is no interference caused by the two-dimensional flow direction, so it is used as the research object of this paper to study the mechanism of nonequilibrium effect in depth.

The mesoscopic kinetic approach essentially relies on the Boltzmann–Bhatnagar-Gross-Krook (BGK) equation [67]. As long as the compressible LB model is to solve the Boltzmann-BGK equation, the present mesoscopic kinetic approach can be used. In this work, the finite-difference compressible
DDF-LB model with the density equilibrium distribution function of Qu et al. [36] and the total energy distribution function of Li et al. [30] is adopted for the following considerations. First, the DDF scheme has good numerical stability and is easy to obtain an adjustable Prandtl number. Second, the combination of Qu’s density equilibrium distribution function and Li’s total energy equilibrium distribution function is effective for high-Mach-number flows. Third, the IMEX-RK scheme is suitable for the above LB model.

The remainder of this paper is organized as follows. In Sec. II, the mesoscopic kinetic approach is described and discussed in detail. In Sec. III, the Sod shock tube and reflected shock problems are considered in terms of their nonequilibrium effects, especially at the shock wave, contact discontinuity, and rarefaction wave. Finally, the conclusions to this study are presented in Sec. IV.

II. MESOSCOPIC LB MODEL AND KINETIC NONEQUILIBRIUM METHOD

In this section, the mesoscopic kinetic approach is described in detail. We start with the DDF-LB model in Sec. II A, then discuss the crucial role of nonequilibrium effects in the corresponding macroscopic thermohydrodynamic equation in Sec. II B. On account of these effects, the kinetic-view-based kinetic nonequilibrium method is then presented in terms of equilibrium kinetic moments and nonequilibrium kinetic moments in Sec. II C. For the nonequilibrium kinetic moments, the implications of their magnitude and sign are discussed based on the molecular velocity distribution at the end of Sec. II C 2.

The mesoscopic kinetic method is based on the Boltzmann-BGK equation, which is a simple and effective formulation of the original Boltzmann equation. The basic idea of the Boltzmann-BGK equation is to replace the complex collision term in the original Boltzmann equation by a simplified linear collision term. This linear term describes the molecular collision process through the idea that the particle distribution function tends to the local equilibrium state. Thus, let us start with the compressible LB method based on the Boltzmann-BGK equation.

A. DDF compressible LB method

The LB model derived from the Boltzmann-BGK equation struggles to handle the fixed specific heat ratio and Prandtl number. However, the DDF approach provides good solutions. The compressible DDF-LB model has two distribution functions, describing density and total energy, respectively. Their evolution equations are given as follows [30]:

\begin{equation}
\frac{\partial f_a}{\partial t} + (\mathbf{e}_a \cdot \nabla) f_a = -\frac{1}{\tau_f} (f_a - f_{eq}^a),
\end{equation}

\begin{equation}
\frac{\partial h_a}{\partial t} + (\mathbf{e}_a \cdot \nabla) h_a = -\frac{1}{\tau_h} (h_a - h_{eq}^a)
- \frac{1}{\tau_h} (\mathbf{e}_a \cdot \mathbf{u} - \frac{\mathbf{u}^2}{2}) \left( f_a - f_{eq}^a \right),
\end{equation}

where $f_{eq}^a$ is the density equilibrium distribution function, which represents the molecular velocity distribution in the local equilibrium state and $f_a$ is the molecular distribution function in the current state; $h_{eq}^a$ and $h_a$ represent similar distribution functions for the total energy. The subscript $\alpha$ denotes the discrete velocity direction, $\mathbf{e}_a$ is the lattice velocity, and $\mathbf{u}$ is the macroscopic velocity vector. $\tau_f$ and $\tau_h$ are relaxation times for $f$ and $h$, and $\tau_{hf}$ relates these quantities according to $1/\tau_{hf} = 1/\tau_h - 1/\tau_f$. $\tau_f$ can be determined by the pressure $p = \mu/\tau_f$, where $\mu$ is the dynamic viscosity.

As shown in Eqs. (1) and (2), the key issue for the physical precision of the LB model is the formulation of $f_{eq}^a$ and $h_{eq}^a$. These are determined by the relations of kinetic moments. The seven kinetic moment relations for $f_{eq}^a$ and $h_{eq}^a$ required to recover the compressible Navier-Stokes equations are as follows:

\begin{equation}
M_0(f_{eq}^a) = \sum_\alpha f_{eq}^a = \rho,
\end{equation}

\begin{equation}
M_{1,i}(f_{eq}^a) = \sum_\alpha f_{eq}^a e_{ai} = \rho u_i,
\end{equation}

\begin{equation}
M_{2,ij}(f_{eq}^a) = \sum_\alpha f_{eq}^a e_{ai} e_{aj} = \rho u_i u_j + \rho \delta_{ij},
\end{equation}

\begin{equation}
M_{3,ijk}(f_{eq}^a) = \sum_\alpha f_{eq}^a e_{ai} e_{aj} e_{ak} = \rho u_i u_j u_k + \rho (u_i \delta_{ij} + u_j \delta_{ik} + u_k \delta_{jk}).
\end{equation}

\begin{equation}
M_0(h_{eq}^a) = \sum_\alpha h_{eq}^a = \rho E,
\end{equation}

\begin{equation}
M_{1,i}(h_{eq}^a) = \sum_\alpha h_{eq}^a e_{ai} = (\rho E + p) u_i,
\end{equation}

\begin{equation}
M_{2,ij}(h_{eq}^a) = \sum_\alpha h_{eq}^a e_{ai} e_{aj} = (\rho E + 2p) u_i u_j + p(E + RT) \delta_{ij},
\end{equation}

where the subscripts $i$, $j$, and $k$ indicate the $x$, $y$, and $z$ components. $\delta_{ij}$, $\delta_{ik}$, and $\delta_{jk}$ are Kronecker delta functions. The subscript of $M$ indicates the number of multipliers of lattice velocity. $E = bRT/2 + u^2/2$ is the total energy, in which $T$ is the temperature and $b$ is a constant associated with the specific heat ratio $\gamma$ according to $\gamma = (b + 2)/b$. The Prandtl number is given by $Pr = \tau_f/\tau_h$.

The LB model with the equilibrium distribution functions of the discrete velocity model, which satisfies Eqs. (3) and (4), has the same order of physical precision as the compressible Navier-Stokes equations. Various equilibrium distribution functions based on different approaches have been developed [35–37].

In our previous work, we demonstrated that the DDF-LB model with a circular function-based density equilibrium distribution function has good numerical stability when simulating compressible viscous flows with shock waves [45–47]. Thus, we adopt this approach in this work. The two-dimensional 13-velocity (D2Q13) square discrete velocity model [30,45] is employed. The lattice velocity is defined by $\tilde{c} = \sqrt{RT}$, where $T_c$ is the characteristic temperature. The circular function-based equilibrium density distribution function [36] and the general method for the total energy equilibrium distribution function presented by Li et al. [30] are used.
The formulation details of \( f_{\alpha}^{eq} \) and \( h_{\alpha}^{eq} \) are the same as in Refs. [30,45], and are not repeated here.

### B. Nonequilibrium effects

The relation between the macroscopic thermohydrodynamic equations and the mesoscopic Boltzmann-BGK equation from the view of nonequilibrium effects was described by Gan et al. [27]. Here, we show the relations for the DDF-LB model. Taking the moments of Eq. (1) with the vector \((1, e_\alpha)\), using Eqs. (3a)–(3c) gives the following equations:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{5}
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p - \nabla \cdot \lambda_{f,2}, \tag{6}
\]

where \( \lambda_{f,2,ij} = \sum_{\alpha} (f_\alpha - f_{\alpha}^{eq}) e_{\alpha i} e_{\alpha j} \) represents a kind of nonequilibrium effect. Similarly, taking the moment of Eq. (2) with \( 1 \) using Eqs. (4a) and (4b), the following equation can be obtained:

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = -\nabla \cdot (\rho \mathbf{u}) - \lambda_{h,1}, \tag{7}
\]

where \( \lambda_{h,1,i} = \sum_{\alpha} (h_{\alpha} - h_{\alpha}^{eq}) e_{\alpha i} \). Comparing Eqs. (5)–(7) with the compressible Navier-Stokes equations, it is easy to find the relations between the nonequilibrium effects and the macroscopic physical quantities, namely, \( \lambda_{f,2} = -\Pi \) and \( \lambda_{h,1} = -\mathbf{j}_q - \mathbf{u} \cdot \mathbf{\Pi} \), in which \( \mathbf{\Pi} \) is the viscous stress tensor and \( \mathbf{j}_q \) is the heat flux.

Note that the nonequilibrium terms \( \lambda_{f,2} \) and \( \lambda_{h,1} \) are directly derived from the Boltzmann-BGK equations, and Eqs. (6) and (7) are unclosed. The compressible Navier-Stokes equations can be recovered through the first-order Chapman-Enskog expansion using Eqs. (3d) and (4c). Thus, Eqs. (5)–(7) actually form the general macroscopic thermohydrodynamic equation frame. Equations that require a specific order of physical precision, such as the Navier-Stokes equations, can use the approximate nonequilibrium terms at the corresponding order. For instance, if a higher order of nonequilibrium effects is considered, the equilibrium distribution function should satisfy the moment relations with higher orders beyond Eqs. (3d) and (4c). The corresponding macroscopic thermohydrodynamic equation of the LB model will then have a higher physical precision order than the Navier-Stokes equations. This improvement in the order of physical precision is essentially obtained by introducing higher-order nonequilibrium effects into the model. Thus, the nonequilibrium effects are crucial for complex flows. For example, the Burnett equations [68,69] provide better performance for rarefied gas than the Navier-Stokes equations. In essence, the former has a higher order of nonequilibrium terms \( \lambda_{f,2} \) and \( \lambda_{h,1} \) than the latter, which results in the Burnett equations giving a better description of complex flows with strong nonequilibrium effects. In this paper, we mainly focus on the compressible Navier-Stokes level.

The physical precision of these nonequilibrium effects is related to the equilibrium distribution function in the LB model because the nonequilibrium effects are represented by the relations that the equilibrium distribution functions should satisfy. That is, the formulation of the equilibrium distribution function directly influences the physical precision of the LB model. When one establishes an LB model at the level of the Navier-Stokes equations, the equilibrium distribution function may have a higher order in terms of the symmetry of the discrete velocity model and the equations used to construct the approach. Thus, some compressible LB models may have a higher order of physical precision than the Navier-Stokes equations because they consider higher-order nonequilibrium effects.

### C. Kinetic nonequilibrium method

As mentioned above, the nonequilibrium effects are very important in the mechanism of fluid flows. The kinetic nonequilibrium method can extract various nonequilibrium effects. This idea was proposed by Xu and his collaborators [27,37,58]. Inspired by their work, we proposed an intuitive way to understand the kinetic moments and nonequilibrium effects from the view of kinetics, providing a mesoscopic perspective for investigating complex flow phenomena. Furthermore, the implications of the magnitude and sign of nonequilibrium effects can be understood in terms of the relation between the molecular velocity distributions in the current state and those in the local equilibrium state. The kinetic nonequilibrium moments of most interest here are given as

\[
\lambda_{f,n} = M_n (f_\alpha - f_{\alpha}^{eq}), \tag{8}
\]

\[
\lambda_{h,n} = M_n (h_{\alpha} - h_{\alpha}^{eq}), \tag{9}
\]

where \( \lambda_{f,n} \) replaces \( f_{\alpha}^{eq} \) in the corresponding relations of Eq. (3) with \( f_\alpha - f_{\alpha}^{eq} \), \( \lambda_{h,n} \) has a similar definition. Note that the definitions of Eqs. (8) and (9) were given by Xu et al. The difference here is to present a kind of physical explanation for the kinetic moment system from the view of kinetics.

Before we start, some basic concepts should be clarified. The Boltzmann-BGK equation describes the fluid flow based on the nonequilibrium effects, which is the difference between the current distribution function \( f_\alpha \) and the equilibrium distribution function \( f_{\alpha}^{eq} \). Figure 1 shows an example of the particle distribution of a molecular cluster when only the molecular positions are considered. \( f_{\alpha}^{eq} \) represents the distribution in the local equilibrium state, which is symmetric. \( f_\alpha \) is the actual
distribution, which may be asymmetric. In the LB method, the distribution function describes the molecular velocity distribution. It has a similar meaning to the molecular position issue for the current state and the local equilibrium state. Thus, the kinetic moments in Eqs. (3) and (4) are in the local equilibrium state. If $f_{eq\alpha}$ is replaced by $f_{\alpha}$, the kinetic moments will become those in the current state. Moreover, a schematic of the mesoscopic kinetic moment system and its relation with the macroscopic thermohydrodynamic equations is presented in Fig. 2. Equations (3) and (4) give the equilibrium kinetic moments, while Eqs. (8) and (9) give the nonequilibrium kinetic moments. It is easy to find that $M_2(f_{eq\alpha})$ and $M_2(h_{eq\alpha})$ are at the same physical level. Hence, we place the vertical positions of the kinetic moments according to their physical levels in the figure. There are three main relations: (1) the general macroscopic thermohydrodynamic equation frame derived from the Boltzmann equations and the kinetic moments (blue text and arrows), (2) the Navier-Stokes equations obtained by the Chapman-Enskog analysis (red text and arrows), and (3) the equilibrium kinetic moments satisfied by the equilibrium distribution functions (green text and arrows). The kinetic nonequilibrium effects are described by the nonequilibrium kinetic moments, which are obtained through the equilibrium kinetic moments. Therefore, this paper systematically probes the physical meanings of the equilibrium and nonequilibrium kinetic moments from the view of kinetics.

1. Equilibrium kinetic moments

Let us begin with the kinetic moments in the equilibrium state. As given in Eq. (3a), $f_{eq\alpha}$ is the component of mass density. Similarly, $h_{eq\alpha}$ is the component of total energy density. Thus, the overall kinetic moments can be divided into two parts, which are the mass-related moments in Eq. (3) and the total energy-related moments in Eq. (4). In Eq. (3b), the kinetic moment is composed of $f_{eq\alpha}^i$ and $e_{ai}$. It is well known that the mass multiplied by the velocity gives the momentum. Therefore, the moment $\sum_{\alpha} f_{eq\alpha}^i e_{ai}$ can be regarded as the macroscopic quantity of the momentum density. Moreover, $\sum_{\alpha} f_{eq\alpha}^i e_{ai} e_{aj}$ can be seen as some quantity related to the translational kinetic energy density when $i = j$. In the history of physics, people first used momentum $m v$ to describe the motion state of an object. Then, the kinetic energy $\frac{1}{2} m v^2$ was proposed to describe the motion state of the object including the thermodynamic property. The essential difference between the momentum and the kinetic energy from the view of mathematics is that the latter is multiplied by one more velocity term than the former. We can imagine that $m v^3$ is a macroscopic physical quantity for describing the motion state of the object including some dynamical property beyond the kinetic energy. Following this idea, the moment $\sum_{\alpha} f_{eq\alpha}^i e_{ai} e_{aj} e_{ak}$ can be viewed as this kinetic quantity density when $i = j = k$.

We can build a kinetic moment system formed by the product of a physical quantity of some kind of property and a motion multiplier based on the law observed above to better understand the physical meaning of equilibrium moment system as given in Eqs. (3a) and (4). In Eq. (3a), the property is the mass density $f_{eq\alpha}^i$, and the motion multiplier is $e_{ai}$. The moment with $n$ motion multipliers is defined as an $n$th-order kinetic moment. In Eq. (4), the property is the total energy density $h_{eq\alpha}$, and the motion multiplier is still $e_{ai}$. The meaning of the kinetic moment can be understood as a comprehensive characteristic of the physical property and the kinetic effect. The kinetic moment, with more motion multipliers, represents a physical characteristic with a stronger kinetic effect. The definitions of the kinetic moments are given in Table I. To better understand the kinetic moments, we discuss their physical meaning at both the mesoscopic and macroscopic levels.
The basic ideas used to describe fluid flows at the mesoscopic and macroscopic levels are different (Fig. 3). At the mesoscopic level, the fluid flow is made up of molecular clusters. At the macroscopic level, the fluid flow consists of fluid elements. Thus, we need to consider the physical meaning of the kinetic moments from these two different views. The formulations of the mesoscopic kinetic moments and their corresponding macroscopic quantities [the right-hand side of Eqs. (3) and (4)] are the main basis. We give the physical meanings of the kinetic moments at the mesoscopic level and the macroscopic level in Tables II and III. The following explanations are required.

(i) Here, we mainly discuss the physical meaning rather than exact definitions. For instance, the definition of the kinetic energy at the macroscopic level is $\rho u^2$. In this work, $m v^2$ is also recognized as a kind of kinetic energy.

(ii) The physical meaning of some higher-order physical quantities is not easy to understand. We overcome this problem through two approaches. (1) The kinetic moment. The kinetic moment is a generalized definition of the product of a physical quantity of some property and a motion multiplier. For example, the kinetic energy can be viewed as a second-order kinetic moment, in which the property is the mass and the motion multiplier is the velocity. Based on this idea, physical quantities with higher physical levels than the energy can be better understood. (2) The physical units. The derivations of the units are as follows: if

$$\sum_{\alpha} f_{\alpha}^c = 1 \text{ kg/m}^3, \quad \sum_{\alpha} h_{\alpha} = 1 \text{ J/m}^3, \quad e_{ai} = 1 \text{ m/s},$$

and $1 \text{ N} = 1 \text{ kg m/s}^2$, $1 \text{ J} = 1 \text{ N m} = 1 \text{ W s}$, then

$$\sum_{\alpha} f_{\alpha}^c e_{ai} = 1 \text{ (kg/m}^3\text{)(m/s)} = 1 \text{ kg m/s}^2 = 1 \text{ N s/m}^3, \quad \sum_{\alpha} f_{\alpha}^c e_{ai} e_{aj} = 1 \text{ (kg/m}^3\text{)(m/s)(m/s)} = 1 \text{ kg/(m}^2\text{)} = 1 \text{ N/m}^2 = 1 \text{ J/m}, \quad \sum_{\alpha} f_{\alpha}^c e_{ai} e_{aj} e_{ak} = 1 \text{ (N/m}^2\text{)(m/s)} = 1 \text{ N/(m s)} = 1 \text{ J/(m}^2\text{ s)} = 1 \text{ W/m}, \quad \sum_{\alpha} h_{\alpha}^c e_{ai} = 1 \text{ (J/m}^3\text{)(m/s)} = 1 \text{ J/(m}^2\text{ s)} = 1 \text{ W/m}^2 = 1 \text{ N/(s m)}, \quad \sum_{\alpha} h_{\alpha}^c e_{ai} e_{aj} = 1 \text{ J/(m}^3\text{)(m/s)} = 1 \text{ J/(m}^2\text{ s)} = 1 \text{ W/(m s)} = 1 \text{ N/s},$$

where many of the kinetic moments have physical units related to both force and energy. This benefits our understanding of the physical meaning of the right-hand side of Eqs. (3) and (4). For example, in Eq. (3c), $\rho u_i u_j$ is a kind of kinetic energy density, while $p \delta_{ij}$ is the surface compressive stress. Nevertheless, they are at the same physical unit level. It should be noted that the discussion of physical unit here is only for a fluid flow system. When LB methods are used to simulate different types of physics, the approach of units can also be applied to those types of physics for a better understanding of the moments under different unit systems.

(iii) The physical meaning of the macroscopic terms in Eq. (4c) is difficult to explain due to their high-order physical level. $\rho E u_i u_j$ can be described through the kinetic moment, and $2 \rho u_i u_i$ can be understood with the help of the physical unit. However, the physical meaning of $p(E + RT) \delta_{ij}$ is still unclear. Based on its units, it can be regarded as a kind of acceleration of energy per unit length or acceleration of force.

(iv) The “momentum force” in Table II is a convenient designation. $\rho u_i u_j$ can be recognized as the product of $\rho u_i$ and $u_j$. The former is the momentum density, which can also be regarded as the instantaneous impulse. When multiplied by $e_{ai}$ with units of $m/s$, which can be decomposed into the units of $(1/s)m$, the units $\rho u_i u_j$ become $(N s/m^3)(1/s)m = N m/m^3$. Thus, $\rho u_i u_j$ can be viewed as the work done by the equivalent
TABLE II. Physical meaning of the kinetic moments of the mass.

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Mesoscopic meaning</th>
<th>Macroscopic meaning</th>
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<tbody>
<tr>
<td>$\sum f_a^{\alpha}$</td>
<td>Molecular mass density</td>
<td>Density</td>
</tr>
<tr>
<td>$\sum f_a^{\alpha} e_{ai}$</td>
<td>Molecular momentum density in i direction</td>
<td>Momentum density in i direction</td>
</tr>
<tr>
<td>$\sum f_a^{\alpha} e_{ai} e_{aj} (i = j)$</td>
<td>Molecular translational kinetic energy density in i direction</td>
<td>Sum of kinetic energy density and surface compressive stress in i direction</td>
</tr>
<tr>
<td>$\sum f_a^{\alpha} e_{ai} e_{aj} (i \neq j)$</td>
<td>Work in j direction done by molecular “momentum force” density in i direction</td>
<td>Work in j direction done by “momentum force” density in i direction</td>
</tr>
<tr>
<td>$\sum f_a^{\alpha} e_{ai} e_{aj} e_{ak} (i = j = k)$</td>
<td>First-order kinetic moment of molecular translational kinetic energy density in i direction</td>
<td>Sum of first-order kinetic moment of kinetic energy density in i direction and three times value of power produced by surface compressive stress in i direction</td>
</tr>
<tr>
<td>$\sum f_a^{\alpha} e_{ai} e_{aj} e_{ak} (i \neq j \neq k)$</td>
<td>First-order kinetic moment in k direction of molecular translational kinetic energy density in i direction</td>
<td>Sum of first-order kinetic moment in k of kinetic energy density in i direction and two value of power produced by surface compressive stress in i direction</td>
</tr>
</tbody>
</table>

2. Nonequilibrium kinetic moments

For the LB model at the compressible Navier-Stokes level, Eqs. (3) and (4) give the seven equilibrium kinetic moments that the equilibrium distribution functions must satisfy. Their nonequilibrium kinetic moments can be obtained by Eqs. (8) and (9). Based on the above discussion of the equilibrium kinetic moments, the physical meanings of the nonequilibrium kinetic moments can be better understood: they represent the local nonequilibrium state of the kinetic moments in Tables II and III. Note that the terms with $f_a^{\alpha}$ represent the local equilibrium state, while the terms with $f_a$ represent the current state. Physically, the local nonequilibrium state is the difference between the current state and the local equilibrium state.

As the mass, momentum, and total energy are locally conservative, the kinetic moments in the current state are equal to the local equilibrium kinetic moments, so $\lambda_{f,0} = 0$, $\lambda_{f,1} = 0$, and $\lambda_{h,0} = 0$. As the number of motion multipliers increases, the kinetic feature of the kinetic moments becomes more significant. As a result, the difference between the current state and the local equilibrium state appears. The rest of the nonequilibrium kinetic moments may be nonzero in the fluid flow process. Equations (6) and (7) give the relations $\lambda_{f,2} = -\Pi$ and $\lambda_{h,1} = -\dot{j}_y - a \cdot \Pi$. Combined with the discussions in Sec. II C 1, it is apparent that (1) the nonequilibrium effect of the molecular translational kinetic energy density is equivalent to the negative viscous normal stress, (2) the nonequilibrium effect of the work in the j direction done by the molecular “momentum force” density in the i direction (which is perpendicular to the j direction) is equivalent to the negative viscous shear stress, and (3) the nonequilibrium effect of the first-order kinetic moment of the molecular total energy density is equivalent to the sum of the negative heat flux and the negative power produced by the viscous stress. At the macroscopic level, it is demonstrated that (1) the nonequilibrium effect of the sum of the kinetic energy density and the surface compressive stress is equivalent to the negative viscous normal stress, (2) the nonequilibrium effect of the work in the j direction done by the “momentum force” density in the i direction is equivalent to the negative viscous shear stress, and (3) the nonequilibrium effect

TABLE III. Physical meaning of the kinetic moments of the total energy.

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Mesoscopic meaning</th>
<th>Macroscopic meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sum h_a^{\alpha}$</td>
<td>Molecular total energy density</td>
<td>Total energy density</td>
</tr>
<tr>
<td>$\sum h_a^{\alpha} e_{ai}$</td>
<td>First-order kinetic moment of molecular total energy density</td>
<td>Sum of first-order kinetic moment of total energy density and power produced by surface compressive stress in i direction</td>
</tr>
<tr>
<td>$\sum h_a^{\alpha} e_{ai} e_{aj} (i = j)$</td>
<td>Second-order kinetic moment of molecular total energy density</td>
<td>Sum of second-order kinetic moment of total energy density, twice value of acceleration of surface pressure, and a same-order term in i direction</td>
</tr>
<tr>
<td>$\sum h_a^{\alpha} e_{ai} e_{aj} (i \neq j)$</td>
<td>First-order kinetic moment in j direction of first-order kinetic moment in i of molecular total energy density</td>
<td>Sum of first-order kinetic moment in j direction of first-order kinetic moment in i of total energy density, and first-order kinetic moment in j direction of power produced by surface compressive stress in i direction</td>
</tr>
</tbody>
</table>
of the sum of the first-order kinetic moment of the total energy density and the power produced by the surface compressive stress is equivalent to the sum of the negative heat flux and the negative power produced by the viscous stress. These nonequilibrium effect-based relations also establish the connections among the collision-invariant physical quantities (mass, momentum, total energy), viscous stress, and heat flux. Besides, the Grad’s 13 moment approach [70–72] provides valuable information regarding the space and time evolution of viscous stress and heat flux that have a clear physical meaning. The nonequilibrium kinetic moments $\lambda_{f,2}$ and $\lambda_{h,1}$ can be well understood based on the relations of $\lambda_{f,2} = -\Pi$ and $\lambda_{h,1} = -\hat{j}_q - u \cdot \Pi$ according to the Grad’s 13 moment approach.

As mentioned in Sec. II B, the general macroscopic thermohydrodynamic equation frame can be derived from $M_0(f_{eq}^q), M_1(f_{eq}^q), M_2(f_{eq}^q), M_3(h_{eq}^{q2}), M_4(h_{eq}^{q3}), M_{f,2}$, and $\lambda_{h,1}$. To close Eqs. (5)–(7) at the Navier-Stokes level, $M_2(f_{eq}^q)$ and $M_4(h_{eq}^{q2})$ are needed in the Chapman-Enskog analysis. Therefore, unlike $\lambda_{f,2}$ and $\lambda_{h,1}$, we cannot find the corresponding macroscopic terms of $\lambda_{f,3}$ and $\lambda_{h,2}$ in the macroscopic thermohydrodynamic equations. It is certain that they are quantities with higher physical levels than the viscous stress and the heat flux, and their physical meanings can be explained through the corresponding equilibrium kinetic moments. Indeed, the Navier-Stokes equations are unable to obtain the nonequilibrium effects of $\lambda_{f,3}$ and $\lambda_{h,2}$, but they can easily be calculated using the LB method through $M_3(f_a - f_{eq}^q)$ and $M_4(h_a - h_{eq}^{q2})$.

To evaluate the accuracy of $\lambda_{f,n}$ and $\lambda_{h,n}$ and discuss their implications of the magnitude and sign, we derive the expression of nonequilibrium kinetic moments based on the Chapman-Enskog analysis [73]. The nonequilibrium effect $f_{eq}^{\alpha q}$ can be represented by $f_{eq}^q$ as [35]

$$f_{eq}^{\alpha q} = f_a - f_{eq}^q = -\tau_f \left[ \frac{\partial f_{eq}^q}{\partial t} + \mathbf{u} \cdot \nabla f_{eq}^q \right].$$  (10)

Taking the moments of Eq. (10) with the vector $(1, \ e_{i\alpha}, e_{i\alpha}e_{i\beta}, e_{i\alpha}e_{i\beta}e_{i\gamma}, \ldots)$, the relation between nonequilibrium kinetic moments of $f$ and the corresponding equilibrium kinetic moments can be obtained:

$$\lambda_{f,n,i} = -\tau_f \left[ \frac{\partial M_{n,i}(f_{eq}^q)}{\partial t} + \nabla \cdot \mathbf{M}_{n+1,ij}(f_{eq}^q) \right].$$  (11)

where the subscript $\hat{i}$ represents a certain $i$, $ij$, or $ijk$ in Eqs. (3) and (4), and the subscript $\hat{j}$ of $\mathbf{M}_{n+1,ij}$ represents the vector component obtained by multiplying $e_{ij}$ and $f_{eq}^q$. It should be noted that the subscript $\hat{j}$ corresponds to the direction of the spatial derivative.

Similarly, the nonequilibrium effect $h_{eq}^{\alpha q}$ is given by

$$h_{eq}^{\alpha q} = h_a - h_{eq}^{q2} = -\tau_h \left[ \frac{\partial h_{eq}^{q2}}{\partial t} + \mathbf{u} \cdot \nabla h_{eq}^{q2} \right] - \left( \mathbf{u} \cdot \mathbf{u} - \frac{u^2}{2} \right) \frac{f_{eq}^{\alpha q}}{\tau_{bf}},$$  (12)

and nonequilibrium kinetic moments of $h$ can be written as

$$\lambda_{h,n,i} = -\tau_h \left[ \frac{\partial M_{n,i}(h_{eq}^{q2})}{\partial t} + \nabla \cdot \mathbf{M}_{n+1,ij}(h_{eq}^{q2}) \right] - \frac{1}{\tau_{bf}} \left( \mathbf{u} \cdot \mathbf{f}_{n+1,ij} - \frac{u^2}{2} \lambda_{f,n,i} \right).$$  (13)

Based on Eqs. (11) and (13), we can discuss the accuracy, magnitude, and sign of nonequilibrium kinetic moments. (1) **Accuracy.** The $n$th-order nonequilibrium kinetic moment $\lambda_{f,n,i}$ is composed of the corresponding temporal derivative of $n$th-order equilibrium kinetic moment $\frac{\partial M_{n,i}(f_{eq}^q)}{\partial t}$ and spatial derivative of $(n + 1)$th-order equilibrium kinetic moment $\nabla \cdot \mathbf{M}_{n+1,ij}(f_{eq}^q)$. The $n$th-order nonequilibrium kinetic moment $\lambda_{h,n,i}$ is related to $M_{n,i}(h_{eq}^{q2})$, $M_{n+1,i}(h_{eq}^{q2})$, $M_{n,i}(f_{eq}^q)$, $M_{n+1,i}(f_{eq}^q)$, $M_{n+2,i}(f_{eq}^q)$. In the present LB model, the accuracy of the nonzero nonequilibrium kinetic moments $\lambda_{f,2}$ and $\lambda_{h,1}$ is guaranteed since their related equilibrium kinetic moments satisfy relations in Eqs. (3) and (4). Besides, the accuracy of higher-order equilibrium kinetic moments $M_{4,i}(f_{eq}^q)$ and $M_{3,i}(h_{eq}^{q2})$ is not restricted. Then, for $\lambda_{f,3}$ and $\lambda_{h,2}$, the accuracy can be guaranteed for terms other than $M_{4,i}(f_{eq}^q)$ and $M_{3,i}(h_{eq}^{q2})$ related terms. Therefore, the present LB model can accurately obtain $\lambda_{f,2}$ and $\lambda_{h,1}$, while for $\lambda_{f,3}$ and $\lambda_{h,2}$, there may exist errors in terms related to $M_{4,i}(f_{eq}^q)$ and $M_{3,i}(h_{eq}^{q2})$. Thus, this work mainly focuses on $\lambda_{f,2}$ and $\lambda_{h,1}$, and $\lambda_{f,3}$ and $\lambda_{h,2}$ are regarded as references. (2) **Magnitude and sign.** The magnitude and sign of nonequilibrium kinetic moments are basically determined by the magnitude and sign of temporal and spatial derivative of equilibrium kinetic moments. For instance, the sum of temporal derivative of $n$th-order equilibrium kinetic moment $\frac{\partial M_{n,i}(f_{eq}^q)}{\partial t}$ and spatial derivative of $(n + 1)$th-order equilibrium kinetic moment $\nabla \cdot \mathbf{M}_{n+1,ij}(f_{eq}^q)$ can determine the magnitude and sign of $\lambda_{f,n,i}$ [see Eq. (11)]. The positive $\frac{\partial M_{n,i}(f_{eq}^q)}{\partial t}$ means $M_{n,i}$ increases over time. The positive $\nabla \cdot \mathbf{M}_{n+1,ij}(f_{eq}^q)$ indicates that $\mathbf{M}_{n+1,ij}$ increases along the gradient direction, such as $x$. Although the expression of $\lambda_{h,n,i}$ is more complicated than the expression of $\lambda_{f,n,i}$, the factors that determine the magnitude and sign are still directly related to the temporal and spatial derivatives of equilibrium kinetic moments.

It is still not easy to understand the implications of the magnitude and sign of the nonequilibrium kinetic moments on account of the above discussions. Hence, we further discuss the implications of the magnitude and sign of the nonequilibrium kinetic moments using the basic idea of the Boltzmann-BGK equation, which describes fluid flows based on the local nonequilibrium state of the particle distribution function. The equilibrium distribution function $f_{eq}^q$ is symmetrically distributed according to the discrete velocity model, while the distribution function in the current state $f_a$ may have an asymmetrical distribution (Fig. 4). Their low-order kinetic moments are identical. However, the asymmetrical distribution of $f_a$ amplifies the asymmetry of the high-order current kinetic moments, as they have more motion multipliers. Thus, differences may appear between the current and equilibrium kinetic moments, which are the nonequilibrium effects described by the nonequilibrium kinetic moments.
Physically, the distribution function describes the molecular distribution in the cluster. \( f_a \) represents the actual molecular distribution, whereas \( f_{eq} \) is the molecular distribution in the local equilibrium state. For instance, \( M_{2,xx}(f_a) \) is the molecular translational kinetic energy density in the current state, and \( M_{2,xx}(f_{eq}) \) is that in the local equilibrium state. Their difference is the nonequilibrium effect at this physical level, which is equivalent to the negative viscous normal stress.

The sign of the nonequilibrium kinetic moment reflects the deviation in the direction of the current kinetic moment from the local equilibrium state. For instance, for a fluid flow with the macroscopic velocity \( u_0 \), the positive nonequilibrium kinetic moment in the \( x \) direction indicates that the kinetic moment in the current state deviates from the local equilibrium state along the positive \( x \) direction, which means the former has a stronger kinetic effect than the latter.

In fact, this deviation reflects the activity of the molecular motion mapped to the corresponding physical level of the mass and the total energy. The deviation direction can be regarded as the direction of the molecular motion relative to its corresponding equilibrium state. The magnitudes of the nonequilibrium effects represent the degree of the local “instability” of the molecular motions at the corresponding physical levels.

In addition, the mesoscopic kinetic approach is mainly based on nonequilibrium kinetic moments \( M_1(f_a - f_{eq}) \) and \( M_h(h_a - h_{eq}) \). As long as the compressible LB model is to solve the Boltzmann-BGK equation, present mesoscopic kinetic approach can be used. Regardless of whether it is DDF or single distribution function LB model, there is no difference in the application of the mesoscopic kinetic approach. It should be noted that the accuracy of nonequilibrium kinetic moments are related to the equilibrium kinetic moments as presented in Eqs. (11) and (13). LB models with equilibrium distribution function satisfying Eqs. (3) and (4) can obtain the same \( \lambda_{f,2} \) and \( \lambda_{h,1} \), while results of \( \lambda_{f,3} \) and \( \lambda_{h,2} \) may not be the same since the relations of \( M_{4,ij}(f_{eq}) \) and \( M_{3,ij}(h_{eq}) \) are not restricted. Therefore, at this level, \( \lambda_{f,2} \) and \( \lambda_{h,1} \) of LB models are accurate, and \( \lambda_{f,3} \) and \( \lambda_{h,2} \) can be used as reference physical quantities for flow mechanism analysis due to possible high-order errors of \( M_{4,ij}(f_{eq}) \) and \( M_{3,ij}(h_{eq}) \).

III. RESULTS AND DISCUSSION

This section presents the results from several shock tube problems that are investigated to study the mesoscopic kinetic nonequilibrium effects. These shock tube problems are selected because they contain the typical compressible flow features of shock waves, contact discontinuities, and rarefaction waves. The numerical implementations of the discretization for Eqs. (1) and (2) are similar to methods used with the conventional macroscopic equations. The spatial discretization is realized by the finite-difference method using the third-order weighted nonscoillatory and non-free-parameter dissipation (WNND) scheme [74,75] with the nonlinear weight of Hu et al. [76]. The implementation details can be found in Ref. [47]. The third-order IMEX-RK scheme [30,55] is adopted for the time discretization. The reference length \( L_0 \), reference velocity \( u_0 = \sqrt{RT_0} \), and reference time \( t_0 = L_0/u_0 \) are used in the simulations. The parameters are as follows: \( Pr = 0.73, b = 5.0 \) for a specific heat ratio of 1.4, \( R = 1.0, T_0 = 1.0, \mu_0 = 1.86 \times 10^{-5} \). The Courant-Friedrichs-Lewy (CFL) number is defined as CFL = \( \Delta t \max \{ |u_a| \} / \min \{ |\Delta x| \} \) [77], giving CFL = 1.0 in the simulations.

A. Magnitude and sign of nonequilibrium kinetic moments

In this section, the LB model adopted in this paper is validated through the Sod shock tube problem. A preliminary analysis of the equilibrium and nonequilibrium kinetic moments is then carried out. The initial conditions are specified as follows:

\[
(\rho, u_x, p) = \begin{cases} 
(1.0, 0, 1.0), & 0 \leq x/L_0 \leq 0.5, \\
(0.125, 0, 0.1), & 0.5 < x/L_0 \leq 1.0.
\end{cases}
\]

A uniform \( N_x \times N_y = 400 \times 5 \) grid is used, where \( N_x \) and \( N_y \) are lattice numbers along the \( x \) and \( y \) directions, respectively. \( f_a = f_{eq} \) and \( h_a = h_{eq} \) are set along the boundaries in the \( x \) direction, and a periodic boundary condition is applied in the \( y \) direction. The reference length \( L_0 = 2.0 \) and the characteristic temperature \( T_c = 2.5T_0 \). The viscosity is \( \mu_0 \). The simulation results for the Sod shock tube at \( t = 0.1644t_0 \) using the present LB model for the density, velocity, pressure, and temperature are given in Fig. 5. The numerical results are in good agreement with the exact solutions.

The equilibrium and nonequilibrium kinetic moments of the Sod shock tube at \( t = 0.1644t_0 \) are presented in Figs. 6 and 7. As \( \lambda_{f,0} = \lambda_{f,1} = \lambda_{h,0} = \lambda_{h,1} = 0 \), and the shock problems are one dimensional in this case, we focus on the nonzero nonequilibrium kinetic moments and their corresponding equilibrium kinetic moments in the \( x \) direction. Note that although we placed the kinetic moments in one coordinate system, the magnitudes do not represent their relations quantitatively as they belong to different physical levels. Thus, we only discuss them qualitatively. The fluid flow field can be divided into five regions with a contact discontinuity near \( x = 1.3 \) and a shock wave near \( x = 1.57 \). Region A covers \( 0 \leq x \leq 0.6 \), region B (rarefaction wave) covers \( 0.6 < x \leq 1.0 \), region C covers \( 1.0 < x < 1.3 \), region D covers \( 1.3 < x \leq 1.57 \), and region E covers \( 1.57 < x \leq 2.0 \). According to the discussion in Sec. II C, \( M_{1,xx}(h_{eq}) \), \( M_{3,xx}(f_{eq}) \), \( \lambda_{f,2,xx} \), and \( \lambda_{h,2,xx} \) are the kinetic moments based on the mass density, whereas the others are kinetic moments based on the total energy. The values of \( M_{1,xx}(h_{eq}) \) and \( M_{3,xx}(f_{eq}) \) are very similar, indicating that they are at the same physical level. The former is the first-order kinetic moment of the total energy density,
FIG. 5. Simulation results for the Sod shock tube at $t = 0.1644t_0$ using the present LB model for (a) density, (b) velocity, (c) pressure, and (d) temperature.

and the latter is the first-order kinetic moment of the molecular translational kinetic energy density. In regions A, C, D, and E, the equilibrium kinetic moments are constants similar to the macroscopic variables, such as density, velocity, and pressure. The values of the nonequilibrium kinetic moments are zero in regions A, C, D, and E, which means the fluid flow system remains in the equilibrium state. In the region of the rarefaction wave (region B), the values of the equilibrium kinetic moments change along the $x$ direction, while the values of the nonequilibrium kinetic moments become nonzero. Moreover, the equilibrium kinetic moments change dramatically near the contact discontinuity (at the interface of regions C and D) and the shock wave (at the interface of regions D and E), while the nonequilibrium kinetic moments reach a sharp peak (valley).

Here, we focus on the regions with nonzero nonequilibrium effects. The schematic of nonequilibrium effect is given in Fig. 8. In this Sod shock tube problem, the fluid velocity direction is consistent with the direction of kinetic moments. Therefore, the positive nonequilibrium kinetic moment indicates that the actual kinetic moment is stronger than the kinetic moment in the local equilibrium state, while the opposite is true for the negative nonequilibrium kinetic moments.

FIG. 6. Equilibrium kinetic moments of the Sod shock tube at $t = 0.1644t_0$.

FIG. 7. Nonequilibrium kinetic moments of the Sod shock tube at $t = 0.1644t_0$.

FIG. 8. Schematic representation of nonequilibrium effect: (a) positive instability, (b) negative instability.
moment. For convenience, we define the positive nonequilibrium kinetic moment with the same fluid velocity direction as “positive instability” and the negative nonequilibrium kinetic moment as “negative instability.” Moreover, the magnitude of nonequilibrium kinetic moment represents the gap between the actual kinetic moment and the local equilibrium kinetic moment. Then, we can obtain and understand the nonequilibrium effects at various physical levels based on the nonequilibrium kinetic moments.

(i) In the region of the rarefaction wave (region B), $M_{2,xx}(f_{eq}^2)$ and $M_{2,xx}(h_0^2)$ are decreasing along the $x$ direction, while the other nonequilibrium effects are increasing. This is strongly influenced by the velocity distribution, which is zero in region A. $M_{2,xx}(f_{eq}^2)$ and $M_{2,xx}(h_0^2)$ have terms that are independent of the velocity, such as the surface compressive stress. In terms of the nonequilibrium kinetic moments, $\lambda_{h,1,x}$ is negative, while the other moments are positive. This indicates that the first-order kinetic moment of the molecular total energy density in the current state is weaker than that in the local equilibrium state, while the opposite is true for the other moments.

(ii) At the contact discontinuity near $x = 1.3$, $M_{2,xx}(h_0^2)$ increases rapidly, but the other equilibrium kinetic moments decrease. The nonequilibrium kinetic moment $\lambda_{f,2,xx}$ remains close to zero, while the others reach their peak values. This indicates that the activity of the molecular motion mapped to the molecular translational kinetic energy density is close to its equilibrium state, while those mapped to the other physical levels exhibit an obvious “positive instability.” Specifically, compared with the nonequilibrium effects at rarefaction wave, $\lambda_{h,1,x}$ is positive and stronger, $\lambda_{f,3,xx}$ has the same direction and similar magnitude, $\lambda_{h,2,xx}$ has same direction but larger peak value.

(iii) At the shock wave near $x = 1.57$, all the equilibrium kinetic moments decrease drastically with strong negative nonequilibrium effects reaching the valley. It can be seen that the nonequilibrium effects at the shock wave are much stronger than those at the contact discontinuity, and their current kinetic moments exhibit opposite deviation directions. Thus, distinguishing inner-scale physical feature can be found in shock wave, contact discontinuity, and rarefaction wave. The dramatic activity of the molecular motion is responsible for the strong “negative instability” of the local physical properties. This can be explained by a mesoscopic perception of the conventional understanding of strong physical features near the shock wave. Moreover, the degree of instability in the local physical properties can be easily described through the nonequilibrium kinetic moments.

Combined with the physical meaning of the nonequilibrium kinetic moments discussed in Sec. II C, the nonequilibrium effects at various physical levels can be identified. For instance, the distribution of $\lambda_{f,2,xx}$ shows that the nonequilibrium effects of the molecular translational kinetic energy density at the contact discontinuity are quite small, whereas those at the shock wave are significant. In other words, the molecular translational kinetic energy density at the contact discontinuity is close to the equilibrium state, while it deviates dramatically from the equilibrium state at the shock wave. This provides the mesoscopic nonequilibrium (or instability) features of molecular translational kinetic energy density at the contact discontinuity and shock wave, which deepens our understanding of the fluid flow mechanism. One can further study the nonequilibrium effects at a specific physical level according to the characteristics of interest in various complex fluid flows.

Compared with the macroscopic quantities in the equilibrium state, the nonequilibrium effects reflect certain characteristics of the fluid flows more clearly near regions with rapidly changing physical properties. Moreover, the nonequilibrium kinetic moments can act as indicators for the shock wave, contact discontinuity, and rarefaction wave, as they contain different features.

B. Viscous influence on nonequilibrium effects

In the one-dimensional study, there is no shear, hence, the dynamic viscosity boils down to the bulk viscosity, where the latter directly controls the dissipation rates of compression and rarefaction waves. The viscosity $\mu$ is proportional to the Knudsen number $Kn$ when the other quantities remain unchanged. The influence of the viscosity $\mu$ is actually the influence of Knudsen number $Kn$. The influence of $Kn$ on the nonequilibrium effects in the shock wave was preliminarily clarified in our previous work [66]. Here, we further study the influence of $Kn$ on the contact discontinuity and rarefaction wave, and probe the mechanism of $Kn$’s influence.

The equilibrium and nonequilibrium kinetic moments of the Sod shock tube with different $Kn$ are plotted in Figs. 9 and 10. The Knudsen number $Kn$ here is defined based on the left fluid. The values of the equilibrium kinetic moments are very close for all $Kn$. The obvious changes are near the turning points, which become smoother as $Kn$ increases due to the viscous effects. Nevertheless, the nonequilibrium effects change significantly as $Kn$ increases. The change between the nonequilibrium effects with $Kn = 1.1 \times 10^{-7}$ and with $Kn = 1.1 \times 10^{-5}$ is not obvious, which indicates that the viscous effect is very weak. At $Kn = 1.1 \times 10^{-4}$, the nonequilibrium effects decrease compared with those at $Kn = 1.1 \times 10^{-5}$. The deviations of the current kinetic moments of $\lambda_{h,1,x}$ and $\lambda_{h,2,xx}$ reverse direction in the rarefaction wave (region B) and near the contact discontinuity, suggesting that they are more sensitive to viscous effects than the other moments. As $Kn$ increases, all the deviation directions of the current kinetic moments take the opposite directions ($Kn = 3.3 \times 10^{-4}$). At $Kn = 1.1 \times 10^{-3}$, the absolute values of the nonequilibrium effects increase significantly. The peak value of $\lambda_{h,2,xx}$ at $Kn = 3.3 \times 10^{-3}$ is 0.038; this grows to 0.12 at $Kn = 1.1 \times 10^{-1}$. Thus, the viscosity has a strong influence on the nonequilibrium effects in the contact discontinuity and rarefaction wave, as well as in the shock wave, in terms of both the magnitude and direction.

The changes to the nonequilibrium effects in the shock wave, contact discontinuity, and rarefaction wave with respect to $Kn$ can be clearly seen in Fig. 11, which shows the peak or valley values along with $Kn$. Because $\lambda_{f,2,xx}$ is close to zero for all $Kn$, it is not plotted in Fig. 11(b). At small values of $Kn$ ($Kn < 1.0 \times 10^{-5}$), the nonequilibrium effects remain broadly unchanged. As $Kn$ increases, the peak value in the contact discontinuity decreases, while the valley value at the shock wave increases. The nonequilibrium
kinetic moments reach zero at around $\text{Kn} = 1.0 \times 10^{-4}$. Thus, the nonequilibrium effects near $\text{Kn} = 1.0 \times 10^{-4}$ for both the shock wave and the contact discontinuity are weak, which means the current distribution functions are close to the equilibrium state. The directions of the nonequilibrium effects change after reaching zero. Their absolute values increase dramatically with increases in $\text{Kn}$. In the rarefaction wave, $\lambda_{h,1,x}$ increases as $\text{Kn}$ increases when $\text{Kn} > 1.1 \times 10^{-5}$, while the other moments decrease. As presented in Ref. [66], the magnitudes of nonequilibrium effects are close to zero in the shock wave when the flow system is at the equilibrium Knudsen number $\text{Kn}_{eq}$. Similarly, it can be found that the magnitudes of nonequilibrium effects are close to zero at a certain $\text{Kn}$ in the contact discontinuity and rarefaction wave [see Figs. 11(b) and 11(c), respectively]. In this flow system, $\text{Kn}_{eq}$ is similar in the shock wave, contact discontinuity, and rarefaction wave, i.e., $\text{Kn}_{eq} \simeq 1.0 \times 10^{-4}$.

Figure 12 shows the schematic representation of Kn’s influence on nonequilibrium effect. When Kn is small enough, nonequilibrium effect is positive or negative instabilities. As Kn increases, the magnitude of nonequilibrium kinetic moment decreases. When $\text{Kn} = \text{Kn}_{eq}$, the nonequilibrium effect reaches a nearly stable state. As Kn continues to increase, the direction of instability becomes opposite and the magnitude increases. The nearly stable point also can be regarded as a transition point between negative and positive instabilities of nonequilibrium effect. Besides, the strength of nonequilibrium effect is a rough but effective index to investigate the overall feature of a flow system [60,62,65]. The strength of nonequilibrium effect is related to the magnitude of nonequilibrium kinetic moment. It is interesting that the strength of nonequilibrium effect first decreases and then increases as Kn increases. This can be explained that when Kn is small enough, the nonequilibrium effect is caused by the pure molecular motion. As Kn increases, molecular motion is affected by the viscosity effect, leading to decrease in strength of nonequilibrium effect. Therefore, the nonequilibrium effect gets a transition point at some specific Kn. As Kn continues to increase, the enhanced viscosity effect results in an opposite direction of “instability” with increasing strength.

C. Dynamic and interactional features of nonequilibrium effects

The above study is for the nonequilibrium effect at a certain moment in the Sod shock tube case. Here we further focus on the nonequilibrium effect feature during a dynamic evolution process and in the interaction between different waves. The dynamic and interactional features of the nonequilibrium effects can be studied through an unsteady simulation of reflected shock problem in a shock tube [78], in which the initial conditions are defined as follows:

$$
(\rho, u_x, p) = \begin{cases} 
(120, 0, 120/\gamma), & 0 \leq x/L_0 \leq 0.5, \\
(1.2, 0, 1.2/\gamma), & 0.5 < x/L_0 \leq 1.0.
\end{cases}
$$
A uniform grid of $N_x \times N_y = 1000 \times 5$ is adopted. The reflecting wall is imposed on boundaries in the $x$ direction, and the periodic boundary condition is applied in the $y$ direction. The reference length is $L_0 = 1.0$, and the viscosity is determined through the Reynolds number $Re = 200$ by $\mu = 1.0/Re$. The value of $Re = 200$ is a typical case presented by Daru and Tenaud [78], and the corresponding viscosity is greater than $100\mu_0$, and so the equilibrium and nonequilibrium kinetic moments will exhibit significant viscous effects. The other conditions are the same as those in the Sod shock tube simulation described above.

Daru and Tenaud [78] presented the evolution of the density in the $x$-$t$ plane of the reflected shock problem, as shown in Fig. 13. Initially, a shock wave, followed by a contact discontinuity, moves towards the right wall. The shock wave reaches the right wall at approximately $t = 0.2$. The reflected shock wave then moves to the left, and interacts with the contact discontinuity at around $t = 0.3$. The shock wave continues to move left, while the contact discontinuity remains stationary close to the right wall. Later, the shock wave interacts with the rarefaction wave at around $t = 0.4$. According to this evolution, the equilibrium and nonequilibrium kinetic moments at several time points are studied; these are noted in Fig. 13 by the blue dashed lines.

Figures 14 and 15 present the evolution of the equilibrium and nonequilibrium kinetic moments, respectively, during the reflected shock process. As the viscosity is greater than $100\mu_0$, the curves of the equilibrium kinetic moments are smoother than those in Fig. 9(d), and the nonequilibrium kinetic moments have larger values in nonzero regions. The equilibrium and nonequilibrium kinetic moments have similar distributions, but not positions, at $t = 0.1$ and 0.2. The nonequilibrium kinetic moments have large positive values at the shock wave and negative values at the contact discontinuity. $\lambda_{f,2,xx}$ is still close to zero at the contact discontinuity. The nonequilibrium kinetic moments at the rarefaction wave have much smaller absolute values. When the shock wave interacts with the contact discontinuity ($t = 0.3$), $M_{2,xx}(h_0^{\alpha})$ increases rapidly near the right wall, while the other kinetic moments retain small values. As the reflected shock wave continues to move left, the values of $M_{2,xx}(f_{heq}^{\alpha})$, $M_{1,xx}(h_0^{\alpha})$, and $M_{3,xxx}(f_{heq}^{\alpha})$ behind the shock wave are almost constant; $M_{2,xx}(f_0^{\alpha})$ is greater than the value before the shock wave, whereas $M_{1,xx}(h_0^{\alpha})$ and $M_{3,xxx}(f_0^{\alpha})$ are smaller (close to zero). In contrast, $M_{2,xx}(h_0^{\alpha})$ displays different characteristics. It exhibits a sharp rise near the contact discontinuity, and remains near to the maximum value of $M_{2,xx}(h_0^{\alpha}) = 690$ when $t > 0.45$. Its value behind the shock wave is greater than before the shock. Behind the shock wave, $M_{2,xx}(h_0^{\alpha})$ rises relatively smoothly to the vicinity of the contact discontinuity, then drops to a small valley. These characteristics can be explained from the definitions of the kinetic moments. Both
FIG. 11. Peak or valley value of nonequilibrium kinetic moments at (a) shock wave, (b) contact discontinuity, and (c) rarefaction wave.

$M_{1,xx}(h^{eq}_a)$ and $M_{3,xxx}(f^{eq}_a)$ have a velocity multiplier, and the velocity is close to zero behind the shock wave after the interaction between the shock wave and the contact discontinuity. Hence, they have values close to zero. Conversely, $M_{2,xx}(h^{eq}_a)$ has a surface compression term, which is nonzero behind the shock wave, giving this moment a higher value. In addition, $M_{2,xx}(h^{eq}_a)$ has a term without a velocity multiplier at a high physical level, which leads to large values.

The nonequilibrium kinetic moments, after the shock wave reaches the right wall, contain more information on the shock wave, contact discontinuity, and rarefaction wave. At $t = 0.3$, the shock wave interacts with the contact discontinuity, resulting in the characteristic changes in the nonequilibrium effects. The nonequilibrium kinetic moments of the shock wave drop rapidly, and the influence of the interaction on the contact discontinuity is relatively small, with the absolute value of $\lambda_{h,1,xx}$ decreasing and those of $\lambda_{h,2,xx}$ and $\lambda_{f,3,xxx}$ increasing slightly. After this interaction, $\lambda_{f,2,xx}$ and $\lambda_{h,2,xx}$ are close to the equilibrium state, while the other moments remain negative at the stationary contact discontinuity. The nonequilibrium effect of $\lambda_{h,1,xx}$ is stronger than that of $\lambda_{f,3,xxx}$.

Figure 16 shows the evolution of peak or valley value of the nonequilibrium kinetic moments at the shock wave. In the period $0.3 < t < 0.45$, the shock wave continues to move left and then interacts with the rarefaction wave. During this period, the nonequilibrium kinetic moments of the shock wave decrease to negative values. The decreasing trend in the

FIG. 12. Schematic representation of Kn’s influence on nonequilibrium effect.

$M_{2,xx}(h^{eq}_a)$ has a term without a velocity multiplier at a high physical level, which leads to large values.

The nonequilibrium kinetic moments, after the shock wave reaches the right wall, contain more information on the shock wave, contact discontinuity, and rarefaction wave. At $t = 0.3$, the shock wave interacts with the contact discontinuity, resulting in the characteristic changes in the nonequilibrium effects. The nonequilibrium kinetic moments of the shock wave drop rapidly, and the influence of the interaction on the contact discontinuity is relatively small, with the absolute value of $\lambda_{h,1,xx}$ decreasing and those of $\lambda_{h,2,xx}$ and $\lambda_{f,3,xxx}$ increasing slightly. After this interaction, $\lambda_{f,2,xx}$ and $\lambda_{h,2,xx}$ are close to the equilibrium state, while the other moments remain negative at the stationary contact discontinuity. The nonequilibrium effect of $\lambda_{h,1,xx}$ is stronger than that of $\lambda_{f,3,xxx}$.

Figure 16 shows the evolution of peak or valley value of the nonequilibrium kinetic moments at the shock wave. In the period $0.3 < t < 0.45$, the shock wave continues to move left and then interacts with the rarefaction wave. During this period, the nonequilibrium kinetic moments of the shock wave decrease to negative values. The decreasing trend in the

FIG. 13. Schematic of the density $x-t$ diagram of the reflected shock in a shock tube presented by Daru and Tenaud [78]. The blue dashed lines are the time points at which we study the nonequilibrium effects. The markers correspond to those in Figs. 14 and 15.
FIG. 14. Evolution of equilibrium kinetic moments in the process of reflected shock in a shock tube at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, (d) $t = 0.45$, (e) $t = 0.5$, (f) $t = 0.53$, (g) $t = 0.6$, (h) $t = 0.8$, and (i) $t = 1.0$. Nonequilibrium kinetic moments of the interaction between the shock wave and the contact discontinuity extends to $t = 0.4$. At the beginning of the interaction between the shock wave and the rarefaction wave ($0.4 < t < 0.45$), the absolute value of $\lambda_{h,1,x}$ continues to increase, while the other moments decrease slightly. As a result, the absolute value of $\lambda_{h,1,x}$ is greater than $\lambda_{h,2,xx}$. Later, the former value drops close to zero while the others rise dramatically to relatively large positive values at around $t = 0.5$. This sudden rise may be caused by two interactions. The first interaction, near $t = 0.3$, causes the nonequilibrium kinetic moments at the shock wave to drop to negative values. After the shock wave has separated from the contact discontinuity, its nonequilibrium kinetic moments are unstable because they were positive before the interaction. The second interaction with the rarefaction wave exacerbates the instability, leading to a strong rebound in the nonequilibrium effects. At $t = 0.53$, the nonequilibrium effects of the shock wave quickly reduce to a very low level, where $\lambda_{h,1,x}$ is negative and the other moments transition from a peak behind the shock wave to a valley in front of it. The nonequilibrium effects of the rarefaction wave ahead of the shock wave are negligible. In general, $\lambda_{f,2,xx}$ and $\lambda_{h,1,x}$ are close to zero, while the other moments have small negative values compared with those at the shock wave. In the period $0.6 < t < 1.0$, the shock wave continues to interact with the rarefaction wave. The nonequilibrium effects change over a small range during this process. Finally ($t = 1.0$), the nonequilibrium effects at the shock wave become relatively small.

Thus, the nonequilibrium effects in the shock wave, contact discontinuity, and rarefaction wave will be influenced by the interactions among them. The nonequilibrium effects at the shock wave are more unstable than those at the contact discontinuity. The instability of the nonequilibrium effects at the shock wave may cause a sudden rise in the magnitudes of the nonequilibrium kinetic moments during the interaction process.
FIG. 15. Evolution of nonequilibrium kinetic moments in the process of reflected shock in a shock tube at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, (d) $t = 0.45$, (e) $t = 0.5$, (f) $t = 0.53$, (g) $t = 0.6$, (h) $t = 0.8$, and (i) $t = 1.0$.

D. Deviation of high-order nonequilibrium kinetic moments

As discussed in Sec. II C 2, the nonequilibrium kinetic moments can be expressed by the equilibrium kinetic moments and the accuracy of the nonequilibrium kinetic moments $\lambda_{f,2}$ and $\lambda_{h,1}$ are guaranteed since their related equilibrium kinetic moments satisfy relations in Eqs. (3) and (4) in the present LB model. However, the accuracy of $\lambda_{f,3}$ and $\lambda_{h,2}$ can be guaranteed for terms other than $M_{4,ijkl}(f_{eq})$ and $M_{3,ijkl}(h_{eq})$ related terms. Here, we show the deviation of high-order nonequilibrium kinetic moments ($\lambda_{f,3}$ and $\lambda_{h,2}$) calculated by the nonequilibrium distribution function ($f_{\alpha} - f_{eq}$ or $h_{\alpha} - h_{eq}$) compared with nonequilibrium kinetic moments obtained by the macroscopic definition presented in Eqs. (11) and (13). The equilibrium and nonequilibrium kinetic moments in the Sod shock tube problem with $Kn = 1.1 \times 10^{-3}$, which has a strong nonequilibrium effect, are addressed.

According to Eqs. (11) and (13), $\lambda_{f,3}$ and $\lambda_{h,2}$ can be split into two parts. One part is the terms defined in Eqs. (3) and
FIG. 17. Comparison between equilibrium kinetic moments calculated by the equilibrium distribution function and equilibrium kinetic moments obtained by the macroscopic definition: $M_{2,xx}(f_{eq}^\alpha)$, $M_{1,xxx}(h_{eq}^\alpha)$, $M_{3,xx}(f_{eq}^\alpha)$, $M_{2,xxx}(h_{eq}^\alpha)$.

(4), while the other part is $M_{4,ijkl}(f_{eq}^\alpha)$ and $M_{3,ijk}(h_{eq}^\alpha)$ related terms. Figure 17 shows the comparison between equilibrium kinetic moments calculated by the equilibrium distribution function and equilibrium kinetic moments obtained by the macroscopic definition for the ones defined in Eqs. (3) and (4). The equilibrium kinetic moments obtained by the macroscopic definition [right-hand side of Eqs. (3) and (4)] are superscripted with #. They are in good agreement. To analyze $M_{4,ijkl}(f_{eq}^\alpha)$ and $M_{3,ijk}(h_{eq}^\alpha)$, their macroscopic definitions are needed. We can find them in the literature [27] considering the LB method with higher order than the Navier-Stokes equation. Then the comparison between equilibrium kinetic moments calculated by the equilibrium distribution function and equilibrium kinetic moments obtained by the macroscopic definition for $M_{4,xxxx}(f_{eq}^\alpha)$, $M_{3,xxx}(h_{eq}^\alpha)$ is given in Fig. 18. It can be seen that the deviation appears since the LB model used in this work does not require the high-order equilibrium distribution function $M_{4,xxxx}(f_{eq}^\alpha)$, $M_{3,xxx}(h_{eq}^\alpha)$ to satisfy the macroscopic definition as we discussed above.

Based on the comparison of equilibrium kinetic moment, the comparison between nonequilibrium kinetic moments calculated by the nonequilibrium distribution function and nonequilibrium kinetic moments obtained by the macroscopic definition: (a) $\lambda_{f,3,xxx}$, (b) $\lambda_{h,2,xx}$.

FIG. 18. Comparison between equilibrium kinetic moments calculated by the equilibrium distribution function and equilibrium kinetic moments obtained by the macroscopic definition: $M_{4,xxxx}(f_{eq}^\alpha)$, $M_{3,xxx}(h_{eq}^\alpha)$.

FIG. 19. Comparison between nonequilibrium kinetic moments calculated by the nonequilibrium distribution function and nonequilibrium kinetic moments obtained by the macroscopic definition: (a) $\lambda_{f,3,xxx}$, (b) $\lambda_{h,2,xx}$.
IV. CONCLUSIONS

This paper has presented a detailed description of a mesoscopic kinetic approach for understanding the kinetic moments of the LB method. The nonequilibrium effects of shock waves, contact discontinuities, and rarefaction waves have been investigated using this approach. Sod shock tube and reflected shock problems were considered to study the mechanism of nonequilibrium effects. The main contributions and findings of this research can be summarized as follows:

(i) The physical meaning of the equilibrium and nonequilibrium kinetic moments of the molecular velocity distribution functions at various physical levels have been systematically formed in terms of kinetics.

(ii) The implications of the magnitude and sign of nonequilibrium effects were explored in terms of the relation between the molecular velocity distributions in the current state and those in the local equilibrium state. They can be understood as the positive or negative instability of the kinetic moments.

(iii) The nonequilibrium effects in the shock wave are more significant than those in the contact discontinuity and rarefaction wave. They are inconsistent in terms of their deviation directions. Additionally, more flow features were revealed through the nonequilibrium kinetic moments than the equilibrium kinetic moments in flow regions with nonequilibrium molecular motions, such as the shock wave, contact discontinuity, or rarefaction wave.

(iv) The Kn$^{eq}$ phenomenon, that the current kinetic moments are near the local equilibrium state, can be explained by the influence of viscosity on molecular motion. Moreover, the influence of viscosity on the nonequilibrium effects in the contact discontinuity and rarefaction wave was found to be similar to those in the shock wave.

(v) The interactional features of the nonequilibrium effects between the shock wave and contact discontinuity and rarefaction wave were probed by investigating the evolution of a reflected shock problem. Although the nonequilibrium effects in the shock wave are strong, they are not stable. The interaction with the contact discontinuity changes the shock wave’s nonequilibrium effects to the opposite direction, while the interaction with the rarefaction wave leads to a sharp crest in most nonequilibrium kinetic moments.

The mesoscopic kinetic approach and nonequilibrium effect results presented in this paper will be useful in helping to understand the inner-scale physics in shock waves, contact discontinuities, and rarefaction waves. In addition, this mesoscopic information may also be helpful to the development of numerical models for compressible flows.

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