Fokker-Planck model of hydrodynamics

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We present a phenomenological description of the hydrodynamics in terms of the Fokker-Planck (FP) equation for one-particle distribution function. Similar to the Boltzmann equation or the Bhatnager-Gross-Krook (BGK) model, this approach is thermodynamically consistent and has the H theorem. In this model, transport coefficients as well as the equation of state can be provided independently. This approach can be used as an alternate to BGK-based methods as well as the direct simulation Monte Carlo method for the gaseous flows.

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I. INTRODUCTION

Recent years have seen the emergence of a set of new algorithms termed as mesoscale fluid simulations tools. A few examples of such methods are the lattice Boltzmann model (LBM), multiparticle collision dynamics, and dissipative particle dynamics [1–4]. All of them share a common theme of simplified kinetic theory with model collision terms such as Boltzmann BGK, FP, stochastic rotation dynamics, etc. [1–4]. These simplified and computationally attractive microscopic dynamics are quite local in nature, and therefore, ensure better parallel efficiency. These methods are rapidly evolving in terms of their capability to handle applied and fundamental problems in engineering and science [5,6].

A recent addition to mesoscale approaches is direct discretization of the phase space description in terms of the Fokker-Planck equation. In this regard, it was pointed out that a computationally attractive option is to solve the Fokker-Planck collision model via the associated Langevin equation [7–9]. The computational motivation behind the FP approach is that unlike the direct simulation Monte Carlo (DSMC) method [10,11], collision dynamics is simpler and the associated Langevin dynamics is highly computationally efficient [12,13]. The basic model in this approach is that of Lebowitz *et al.* [14], where the Boltzmann collision operator was the model as diffusive Fokker-Planck dynamics in velocity space. Although this model has the correct hydrodynamic limit, this approach leads to the Prandtl number $\mathrm{Pr} = 3/2$. Here, we remember that the Boltzmann equation predicts the Prandtl number of gas to be $\mathrm{Pr} = 2/3$, while the BGK model predicts the Prandtl number to be $\mathrm{Pr} = 1$.

In the present work, we propose a Fokker-Planck model of hydrodynamics which can describe fluid flow for an arbitrary Prandtl number. In addition, similar to the phenomenological hydrodynamic description in terms of Navier-Stoke-Fourier dynamics, in the current description equation of state can also be provided independently. This model is based on Ref. [15], where it was shown that adding a correction term to the free flight of the Boltzmann equation provides an alternate route to tune the equation of state as well as transport coefficients. We show that this approach, when coupled with the Fokker-Planck approach, leads to a simple but quite accurate model with a flexible Prandtl number (Pr). The resulting hydrodynamics equation has the correct hydrodynamic limit and is thermodynamically consistent.

The work is organized as follows: In Sec. II, important aspects of Boltzmann and Enskog collision operators are discussed. In Sec. III, Lebowitz 's *et al.* [14] approach to the Fokker-Planck approximation of the Boltzmann equation is reviewed and the H theorem is proved for this model. In Sec. IV, a phenomenological Fokker-Planck model is proposed and the H theorem is proved for it. Furthermore, transport coefficients and the hydrodynamic limit of this model is discussed in the same section. In Sec. V, the present model is contrasted with the literature and a numerical method for rarified gas flow simulation is provided.

II. KINETIC DESCRIPTION AND PROPERTIES OF COLLISION TERMS

In the kinetic description of fluid, the fundamental quantity of interest is the single-particle distribution function f, where $f(\mathbf{x},\mathbf{c},t)d\mathbf{c}$ provides the probability of finding a particle at location $\mathbf{x}$ with velocity in the range $\mathbf{c}$ to $\mathbf{c}+d\mathbf{c}$. The macroscopic quantities such as mass density ρ, momentum density $j = \rho\mathbf{u}$, and energy density $E = \rho\mathbf{u}^2/2 + e$ (e is the internal energy) can be obtained as the lower order moment of f defined by the relation,

$$\rho = \langle 1, f\rangle, \qquad \rho\mathbf{u} = \langle \mathbf{c}, f\rangle, \qquad e = \left\langle \frac{\xi^2}{2}, f\right\rangle, \tag{1}$$

where $\boldsymbol{\xi} = \mathbf{c} - \mathbf{u}$ is the peculiar velocity and $\mathbf{u}$ represents the mean velocity and the angular bracket denotes the inner product defined as

$$\langle \phi_1(\mathbf{c}), \phi_2(\mathbf{c})\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\mathbf{c}\phi_1\,\phi_2. \tag{2}$$

The temperature T of the gas can be defined in terms of the internal energy as $e = 3\,k_B T/(2m)$, where k_B is the Boltzmann constant and m is the mass of a gaseous particle. In the dilute limit, the dynamics of single-particle distribution f is governed by the Boltzmann equation:

$$\partial_t f + c_\alpha \partial_\alpha f = \Omega^B(f,f), \tag{3}$$

where Ω^B is a bi-linear function of f as follows.

(1) Collisional invariants. The mass, the momentum, and the energy are not altered by collision term (Ω^B), which implies

$$\langle \Omega^B, \{1, c_\alpha, \mathbf{c}^2\}\rangle = 0. \tag{4}$$

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(2) Zero of collision. The Maxwell-Boltzmann distribution (f^{MB}),

$$f^{\mathrm{MB}} = \rho \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{m}{2k_B T}(c-u)^2\right), \quad (5)$$

is zero of the collision term, i.e.,

$$\Omega^{\mathrm{B}}(f,f) = 0 \Rightarrow f = f^{\mathrm{MB}}. \quad (6)$$

(3) H theorem. The Boltzmann collision term is such that

$$\langle \Omega^{\mathrm{B}}, \ln f \rangle \leqslant 0. \quad (7)$$

Thus, the H function, defined as

$$H^{\mathrm{ID}} = \int d\mathbf{c}(f \ln f - f), \quad (8)$$

is the nonequilibrium generalization of the entropy. This can be seen by writing the evolution equation for the H function,

$$\partial_t H^{\mathrm{ID}} + \partial_\alpha J_\alpha^{\mathrm{H,ID}} = -\sigma^{(\mathrm{B})}, \quad (9)$$

where the entropy flux term and production term are

$$J_\alpha^{\mathrm{H,ID}} = \int d\mathbf{c} c_\alpha (f \ln f - f), \quad \sigma^{(\mathrm{B})} = -\langle \Omega^{\mathrm{B}}, \ln f \rangle, \quad (10)$$

and Eq. (9) is obtained by multiplying Eq. (3) with $\ln f$ and integrating with respect to velocity space ($\mathbf{c}$). Thus, the Boltzmann equation ensures that the entropy production $\sigma^{(\mathrm{B})} \geqslant 0$ and is zero only when $f = f^{\mathrm{MB}}$.

(4) Conservation laws. By taking the appropriate moments of the Boltzmann equation [Eq. (3)], it is evident that macroscopic conservation laws have an expected form:

$$\begin{aligned} \partial_t \rho + \partial_\alpha j_\alpha &= 0, \\ \partial_t j_\alpha + \partial_\beta(\rho u_\alpha u_\beta + p\delta_{\alpha\beta}) + \partial_\beta \sigma_{\alpha\beta} &= 0, \\ \partial_t E + \partial_\alpha((E+p)u_\alpha + \sigma_{\alpha\gamma}u_\gamma) + \partial_\alpha q_\alpha &= 0, \end{aligned} \quad (11)$$

where the pressure term $p = p^{\mathrm{ID}}$ with $p^{\mathrm{ID}} = \rho k_{\mathrm{B}} T/m$, stress tensor $\sigma_{\alpha\beta} = \sigma_{\alpha\beta}^{(\mathrm{K})}$, and heat flux $q_\alpha = q_\alpha^{(\mathrm{K})}$ and the kinetic contribution to stress and heat flux are defined as

$$\sigma_{\alpha\beta}^{(\mathrm{K})} = \langle \overline{\xi_\alpha \xi_\beta} \rangle, \quad q_\alpha^{(\mathrm{K})} = \left\langle \xi_\alpha \frac{\xi^2}{2} \right\rangle, \quad (12)$$

where for any second-order tensor $A_{\alpha\beta}$, its traceless part $\overline{A}_{\alpha\beta}$ is

$$\overline{A}_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} + A_{\beta\alpha}) - \frac{1}{D} A_{\gamma\gamma}\delta_{\alpha\beta}. \quad (13)$$

The reason for this distinction between kinetic contribution and total contribution to stress and heat flux would be apparent in the next section, where a more general framework is used.

Due to the complexity of the Boltzmann collision operator, a simplified description in terms of the BGK collision term [16],

$$\Omega^{\mathrm{BGK}} = \frac{1}{\tau_{\mathrm{BGK}}}\left(f^{\mathrm{MB}} - f\right), \quad (14)$$

is often used and where τ_{BGK} is the mean free time. This model preserves all of the above mentioned properties of the collision operator, and thus provides a qualitatively correct representation of the Boltzmann equation and is widely used in the applications. However, quantitative comparison is often not possible due to the fact that this model predicts the Prandtl number of the monatomic gas to be $\mathrm{Pr} = 1$ instead of $\mathrm{Pr} = 2/3$.

For an arbitrary kinetic model, whenever the collision term conserves mass, momentum, and energy irrespective of the form of the collision term, the conservation laws [Eq. (11)] remain the same. Thus, in the case of dense gases, where dynamics is well described by the Enskog model and its revised form [17], the conservation laws do not change. For the Enskog collision model, too, the collisional invariants remain the same and in the space-independent case, the equilibrium distribution is Maxwell-Boltzmann. However, the H function for the Enskog model ([18]) is

$$H = H^{\mathrm{ID}} - \frac{s^{\mathrm{nID}}(\rho)}{k_{\mathrm{B}}}, \quad (15)$$

where H^{ID} is given by Eq. (8) and the nonideal part of entropy (s^{nID}) is a function of density only in this description. The evolution of the H function is of the form,

$$\partial_t H + \partial_\alpha J_\alpha^{\mathrm{H}} = -\sigma^{(\mathrm{E})}, \quad (16)$$

with entropy production $\sigma^{(\mathrm{E})} \geqslant 0$ and the flux of entropy J_α^{H} is different from the Boltzmann equation due to the nonlocal nature of the collision [18,19]. Thus the model has the H theorem and the minimum of the H function remains Maxwell-Boltzmann only. Thus, a phenomenological model of the hydrodynamics at the kinetic level must satisfy all of the above mentioned restrictions on the collision model and should have a valid H theorem for the H function in the Enskog form [Eq. (15)].

III. FOKKER-PLANCK MODEL FOR BOLTZMANN EQUATION

An alternate to the BGK model is the Fokker-Planck model [14], where the Boltzmann collision term is approximated as

$$\Omega^{\mathrm{FP}} = \frac{1}{\tau}\partial_{c_\alpha}\left(A_\alpha f + \mathfrak{D}\frac{\partial f}{\partial c_\alpha}\right), \quad (17)$$

where τ^{-1} is the friction constant, A_α is the drift term, and $\mathfrak{D}$ is the diffusion term. For Lebowitz's model,

$$A_\alpha = \xi_\alpha, \qquad \mathfrak{D} = \frac{k_B T}{m}. \quad (18)$$

It is evident that the collision invariants for this model are the same as the Boltzmann description and zero of the collision is the Maxwell-Boltzmann distribution. Thus, the conservation laws are the same as Eq. (11). The model is thermodynamic consistent, provided the entropy production term $\sigma^{(\mathrm{FP})}$,

$$\sigma^{(\mathrm{FP})} = -\langle \Omega^{\mathrm{FP}}, \ln f \rangle = \frac{1}{\tau}\int d\mathbf{c}\left(\xi_\alpha + \frac{1}{f}\frac{k_{\mathrm{B}}T}{m}\frac{\partial f}{\partial c_\alpha}\right)\frac{\partial f}{\partial c_\alpha}, \quad (19)$$

is positive, i.e., $\sigma^{(\mathrm{FP})} \geqslant 0$. To show that, the entropy production term can be written as

$$\begin{aligned} \sigma^{(\mathrm{FP})} &= -\frac{3\rho}{\tau} + \frac{k_{\mathrm{B}}T}{m\tau}\int d\boldsymbol{\xi}\,\frac{1}{f}\frac{\partial f}{\partial \xi_\alpha}\frac{\partial f}{\partial \xi_\alpha} \\ &= \frac{k_{\mathrm{B}}T}{m\tau}\int d\boldsymbol{\xi}\, f\left(\frac{\partial \ln\left(\frac{f}{f^{\mathrm{MB}}}\right)}{\partial \xi_\alpha}\right)^2 \geqslant 0, \end{aligned} \quad (20)$$

where we have used the identity,

$$\int d\boldsymbol{\xi}\, f\left(\frac{\partial \ln\left(\frac{f}{f^{\mathrm{MB}}}\right)}{\partial \xi_\alpha}\right)^2 = \int d\boldsymbol{\xi}\left[\frac{1}{f}\frac{\partial f}{\partial \xi_\alpha}\frac{\partial f}{\partial \xi_\alpha} + f\frac{\partial \ln f^{\mathrm{MB}}}{\partial \xi_\alpha}\frac{\partial \ln f^{\mathrm{MB}}}{\partial \xi_\alpha} - 2\frac{\partial f}{\partial \xi_\alpha}\frac{\partial \ln f^{\mathrm{MB}}}{\partial \xi_\alpha}\right]$$
$$= \int d\boldsymbol{\xi}\left[\frac{1}{f}\frac{\partial f}{\partial \xi_\alpha}\frac{\partial f}{\partial \xi_\alpha} + f\frac{m^2\xi^2}{k_{\mathrm{B}}^2T^2} + 2\frac{\partial f}{\partial \xi_\alpha}\frac{m\,\xi_\alpha}{k_{\mathrm{B}}T}\right]$$
$$= -\frac{3\,\rho m}{k_{\mathrm{B}}T} + \int d\boldsymbol{\xi}\,\frac{1}{f}\frac{\partial f}{\partial \xi_\alpha}\frac{\partial f}{\partial \xi_\alpha}. \tag{21}$$

Furthermore, in this model every higher order moment has its own relaxation rate (a feature shared with the Boltzmann equation). In particular, the evolution equations for stress and heat flux are

$$\partial_t\sigma_{\alpha\beta} + \partial_\gamma(\sigma_{\alpha\beta}u_\gamma) + 2p\overline{\partial_\alpha u_\beta} + 2\overline{\sigma_{\alpha\gamma}\partial_\gamma u_\beta} + \partial_\gamma Q_{\alpha\beta\gamma} + \frac{4}{D+2}\overline{\partial_\alpha q_\beta} = -\frac{2}{\tau}\sigma_{\alpha\beta}, \tag{22}$$

$$\partial_t q_\alpha + \partial_\beta\left(q_\alpha u_\beta + \frac{R_{\alpha\beta}}{2} + \frac{R'\delta_{\alpha\beta}}{2D}\right) + \frac{(D+2)}{2}p\partial_\alpha\frac{p}{\rho} + \frac{2}{D+2}(q_\gamma\partial_\alpha u_\gamma + q_\alpha\partial_\beta u_\beta)$$
$$-\frac{\sigma_{\alpha\beta}\partial_\beta p}{\rho} + \frac{D+4}{D+2}q_\beta\partial_\beta u_\alpha + Q_{\alpha\beta\gamma}\partial_\beta u_\gamma - \frac{(D+2)p}{2\rho}\partial_\beta\sigma_{\alpha\beta} - \frac{\sigma_{\alpha\kappa}\partial_\beta\sigma_{\kappa\beta}}{\rho} = -\frac{3}{\tau}q_\alpha, \tag{23}$$

where the higher order moments are defined as

$$Q_{\alpha\beta\gamma} = \int d\mathbf{c}\, f\overline{\xi_\alpha\xi_\beta\xi_\gamma}, \quad R' = \int d\mathbf{c}\, f\xi^2\xi^2 - 15\frac{p^2}{\rho}, \quad R_{\alpha\beta} = \int d\mathbf{c}\, f\xi^2\overline{\xi_\alpha\xi_\beta}, \tag{24}$$

with

$$\overline{\xi_\alpha\xi_\beta\xi_\gamma} = \frac{1}{3}(\xi_\alpha\xi_\beta\xi_\gamma + \xi_\beta\xi_\gamma\xi_\alpha + \xi_\gamma\xi_\alpha\xi_\beta) - \frac{1}{D+2}(\xi^2\xi_\alpha\delta_{\beta\gamma} + \xi^2\xi_\beta\delta_{\gamma\alpha} + \xi^2\xi_\gamma\delta_{\alpha\beta}).$$

From Eq. (22) and Eq. (23), it is evident that the Prandtl number (Pr) for this model is 3/2. Furthermore, one can make a correspondence between this model and BGK via setting $\tau = 2\tau_{\mathrm{BGK}}$.

IV. FOKKER-PLANCK MODEL FOR TUNABLE TRANSPORT COEFFICIENT AND EQUATION OF STATE

Recently, an extension to the BGK model was developed [15], where similar to the hydrodynamic description of Navier-Stokes-Fourier, the equation of state and all transport coefficients (viscosity η, and thermal conductivity κ) can be specified independently. The key new idea in this work was that a phenomenological kinetic description can be given in terms of the modified streaming step. In particular, this work suggested that in the streaming step, the shift in trajectory $\Delta x_{i\alpha}$ for the ith molecule with velocity $c_{i\alpha}$ should be of the form,

$$\Delta x_{i\alpha} = c_{i\alpha}\tau + \tau\chi(\rho)(c_{i\alpha} - u_\alpha) - \frac{\tau^2}{2}\lambda^q\left(\xi^2 - \frac{3k_{\mathrm{B}}T}{m}\right)\partial_\alpha \ln T, \tag{25}$$

where τ is mean free time and λ^q is a positive constant related to the Prandtl number and $\chi(\rho)$ is the compressibility factor defined as

$$\chi = \frac{p\,m}{\rho k_{\mathrm{B}}T} - 1 \equiv \frac{m}{\rho k_B}\left(s^{\mathrm{nID}} - \rho\frac{\partial s^{\mathrm{nID}}}{\partial \rho}\right), \tag{26}$$

which is a monotonically increasing function of the density with reference value $\chi(\rho = 0) = 0$ and $s^{\mathrm{nID}}(\rho)$ is the excess entropy. Adopting this description, we propose the following extension of the Fokker-Planck model for the hydrodynamics:

$$\partial_t f + \partial_\alpha\left[\hat{c}_\alpha f\right] = \Omega^{\mathrm{FP}}, \tag{27}$$

where Ω^{FP} is the Fokker-Planck collision operator [Eq. (17)] and the apparent streaming velocity $\hat{c}_\alpha$ is

$$\hat{c}_\alpha = c_\alpha + \underbrace{\chi(\rho)(c_\alpha - u_\alpha) - \frac{\tau}{2}\lambda^q\left(\xi^2 - \frac{3k_{\mathrm{B}}T}{m}\right)\partial_\alpha \ln T}_{B_\alpha}, \tag{28}$$

where the correction to the advection velocity is orthogonal to the mass conservation, thus the added correction term does not change the continuity equation. By taking the appropriate moment of Eq. (27), it is evident that the form of conservation law is still given by Eq. (11) with pressure as $p = p^{\mathrm{ID}}(1+\chi)$. Thus, we see that the conservation laws are consistent with dense gas models such as the Enskog equation. As expected, the term with χ as prefactor contributes the nonideal part of the pressure in the momentum conservation. Furthermore, due to the change in the free flight rule, the expression for the stress tensor and heat flux modifies as

$$\sigma_{\alpha\beta} = (1+\chi)\,\sigma^{\mathrm{K}}_{\alpha\beta} - \tau\lambda^q\, q_\beta\,\partial_\alpha \ln T,$$
$$q_\alpha = q^{\mathrm{K}}_\alpha(1+\chi) - \frac{3}{2}\tau\left(\frac{k_{\mathrm{B}}T}{m}\right)^2\lambda^q\partial_\alpha \ln T - \frac{\tau}{4}\lambda^q R'\partial_\alpha \ln T, \tag{29}$$

which shows that the last term in B_α adds a term to energy conservation which is related to the Prandtl number and does not contribute to momentum conservation.

The H function for this model is the same as the Enskog equation and it is given by Eq. (15). The evolution equation for H^{ID} is

$$\partial_t H^{\mathrm{ID}} + \partial_\alpha \int d\mathbf{c}[\hat{c}_\alpha f(\ln f - 1)] - \Bigg(\underbrace{-\partial_\alpha j_\alpha + \int d\mathbf{c}\hat{c}_\alpha \partial_\alpha f}_{\mathscr{I}} \Bigg)$$
$$= -\frac{k_{\mathrm{B}}T}{m\,\tau} \int d\boldsymbol{\xi}\, f \left(\frac{\partial \ln\left(\frac{f}{f^{\mathrm{MB}}}\right)}{\partial \xi_\alpha} \right)^2, \tag{30}$$

where the entropy production due to collision is the same as Eq. (20) and the term $\mathscr{I}$ can be further simplified as

$$\mathscr{I} = \partial_\alpha \left(\frac{m s^{\mathrm{nID}}}{k_{\mathrm{B}}} u_\alpha \right) - \frac{m}{k_{\mathrm{B}}} \left(u_\alpha \partial_\alpha s^{\mathrm{nID}} + \rho \frac{\partial s^{\mathrm{nID}}}{\partial \rho} \partial_\alpha u_\alpha \right)$$
$$- \frac{\tau}{2} \lambda^q \left(\frac{3\rho k_{\mathrm{B}} T}{m} \right) (\partial_\alpha \ln T)^2 . \tag{31}$$

However, using the continuity equation, we have

$$\partial_t \left(\frac{m s^{\mathrm{nID}}}{k_{\mathrm{B}}} \right) + \frac{m}{k_{\mathrm{B}}} \frac{\partial s^{\mathrm{nID}}}{\partial \rho} \partial_\alpha j_\alpha = 0. \tag{32}$$

Substituting for $\mathscr{I}$ from Eq. (31) into Eq. (30), and using Eq. (32), the evolution equation for H can be written as

$$\partial_t H + \partial_\alpha J^H_\alpha = -\Bigg(\frac{k_{\mathrm{B}}T}{m\,\tau} \int d\boldsymbol{\xi}\, f \left(\frac{\partial \ln\left(\frac{f}{f^{\mathrm{MB}}}\right)}{\partial \xi_\alpha} \right)^2$$
$$+ \frac{\tau}{2} \lambda^q \left(\frac{3\rho k_{\mathrm{B}} T}{m} \right) (\partial_\alpha \ln T)^2 \Bigg), \tag{33}$$

where it is evident that the right-hand side of Eq. (33) is negative definite and

$$J^H_\alpha = -\left(\frac{m s^{\mathrm{nID}} u_\alpha}{k_{\mathrm{B}}} \right) + \int d\mathbf{c}\hat{c}_\alpha f(\ln f - 1). \tag{34}$$

Thus, similar to the Enskog equation, we have the evolution equation for H as

$$\partial_t H + \partial_\alpha J^H_\alpha \leqslant 0, \tag{35}$$

which confirms that H theorem for the new model, too. From Eq. (34), it is evident that only the flux term gets affected due to the nonideal equation of state and there is no extra source term for nonideal entropy due to modified streaming velocity. Thus, as expected from a model of repulsive core, the current model does not change entropy production but only changes the entropy flux [18,19]. Similarly, Eq. (33) shows that as expected the change in the Prandtl number manifests itself only in the change of entropy production. Finally, in the space homogenous case the equilibrium distribution remains as the Maxwell-Boltzmann distribution because the collision term is the same as that of Boltzmann.

The physical rationale behind this model can be understood by considering the motion of a tagged particle. According to Eq. (25), when a tagged particle is moving faster than the local average velocity, it gets more displacement. Thus, the tagged particle can avoid joining the locally dense region. Conversely, if a particle is moving slower than the local velocity its speed reduces and thus cluster formation is avoided once again. Thus, on an average, this modification captures the effects of the strong repulsive core of a molecule which does not allow molecules to come very close to each other or to form a cluster. Similarly, if the tagged particle finds itself in a nonhomogenous temperature field, it will get a correction in velocity depending on the local temperature gradient and whether it will move faster or slower than the original velocity will be decided by the sign of the local temperature gradient.

A. Moment chain and hydrodynamics

The transport coefficient expressions for this model can be derived by writing the evolution equations for the stress tensor $\sigma^{(\mathrm{K})}_{\alpha\beta}$, and the heat flux $q^{(\mathrm{K})}_\alpha$, which, using Eq. (27), are

$$\partial_t \sigma^{\mathrm{K}}_{\alpha\beta} + \partial_\gamma \left(\sigma^{\mathrm{K}}_{\alpha\beta} u_\gamma \right) + 2p\overline{\partial_\alpha u_\beta} + 2\overline{\sigma_{\alpha\gamma}\partial_\gamma u_\beta} + \partial_\gamma (1+\chi) Q_{\alpha\beta\gamma} + \frac{4}{D+2} \overline{\partial_\alpha (1+\chi) q^{\mathrm{K}}_\beta}$$
$$- \frac{1}{2} \partial_k \left(\lambda^q \tau (\partial_k \ln T) \left(R_{\alpha\beta} - \frac{3k_B T}{m} \sigma^{\mathrm{K}}_{\alpha\beta} \right) \right) - (\tau \lambda^q \partial_k \ln T) \overline{q^{\mathrm{K}}_\beta \partial_k u_\alpha} = -\frac{2\sigma^{\mathrm{K}}_{\alpha\beta}}{\tau}, \tag{36}$$

$$\partial_t q^{\mathrm{K}}_\alpha + \partial_\beta \left(q^{\mathrm{K}}_\alpha u_\beta + \frac{(1+\chi) R_{\alpha\beta}}{2} + \frac{(1+\chi) R' \delta_{\alpha\beta}}{2D} \right) + \frac{(D+2)}{2} p \partial_\alpha \frac{p^{\mathrm{ID}}}{\rho} + \frac{2(1+\chi)}{D+2} \left(q^{\mathrm{K}}_\gamma \partial_\alpha u_\gamma + q^{\mathrm{K}}_\alpha \partial_\beta u_\beta \right)$$
$$- \frac{\sigma^{\mathrm{K}}_{\alpha\beta} \partial_\beta p}{\rho} + \frac{(D+4)(1+\chi)}{D+2} q^{\mathrm{K}}_\beta \partial_\beta u_\alpha + (1+\chi) Q_{\alpha\beta\gamma} \partial_\beta u_\gamma - \frac{(D+2) p^{\mathrm{ID}}}{2\rho} \partial_\beta \sigma_{\alpha\beta} - \frac{\sigma^{\mathrm{K}}_{\alpha\kappa} \partial_\beta \sigma_{\kappa\beta}}{\rho}$$
$$- \frac{1}{4} \partial_k \left(\lambda^q \tau (\partial_k \ln T) \left(\Lambda_\alpha - 6 \frac{p^{\mathrm{ID}}}{\rho} q^{\mathrm{K}}_\alpha \right) \right) - \frac{1}{4} (\tau \lambda^q \partial_\beta \ln T) \left(R' + \frac{6 (p^{\mathrm{ID}})^2}{\rho} \right) \partial_\beta u_\alpha$$
$$- \frac{1}{4} (\tau \lambda^q \partial_\beta \ln T) \left(R_{\alpha k} + \frac{R' \delta_{\alpha k}}{D} + \frac{2 (p^{\mathrm{ID}})^2 \delta_{\alpha k}}{\rho} - \frac{3 p^{\mathrm{ID}} \sigma^{\mathrm{K}}_{\alpha k}}{\rho} \right) \partial_\beta u_k = -\frac{3 q^{\mathrm{K}}_\alpha}{\tau}, \tag{37}$$

where $\Lambda_\alpha = \int d\mathbf{c} f \xi^2 \xi^2 \xi_\alpha$. To understand the hydrodynamic limit, we use the Chapman-Enskog expansion procedure, in which the distribution function is expanded in terms of relaxation time τ as

$$f = f^{\mathrm{MB}}(\rho, \mathbf{u}, T) + \tau f^{(1)} + \tau^2 f^{(2)} + \cdots, \tag{38}$$

where conserved moments are left unexpanded. Furthermore, the time derivative of any quantity ϕ is also expanded as

$$\partial_t \phi = \partial_t^{(0)}\phi + \tau\partial_t^{(1)}\phi + \tau^2\partial_t^{(2)}\phi + \cdots, \tag{39}$$

and the time derivatives at every order are defined via conservation laws [Eq. (11)] [20].

Thus, the kinetic parts of the stress tensor and the heat flux (which correspond to moments of the distribution function) can be written as

$$\begin{aligned} \sigma_{\alpha\beta}^{\mathrm{K}} &= \tau\sigma_{\alpha\beta}^{(\mathrm{K},1)} + \tau^2\sigma_{\alpha\beta}^{(\mathrm{K},2)}\ldots\ldots, \\ q_{\alpha}^{\mathrm{K}} &= \tau q_{\beta}^{(\mathrm{K},1)} + \tau^2 q_{\beta}^{(\mathrm{K},2)}\ldots\ldots \end{aligned} \tag{40}$$

Using Eqs. (39) and (40) in Eqs. (36) and (37) and considering terms up to first order in relaxation time τ, we have

$$\begin{aligned} \sigma_{\alpha\beta}^{\mathrm{K}} &= -\tau p^{\mathrm{ID}}(1+\chi)\overline{\partial_\alpha u_\beta}, \\ q_{\alpha}^{\mathrm{K}} &= -\tau\frac{D+2}{6}p^{\mathrm{ID}}(1+\chi)\partial_\alpha\frac{p^{\mathrm{ID}}}{\rho}. \end{aligned} \tag{41}$$

Using Eq. (41) in Eq. (29) and taking terms up to first order in τ, we obtain

$$\begin{aligned} \sigma_{\alpha\beta} &= -2\left(\frac{\tau p^{\mathrm{ID}}(1+\chi)^2}{2}\right)\overline{\partial_\alpha u_\beta}, \\ q_\alpha &= -\tau\left(\frac{D+2}{6}p^{\mathrm{ID}}(1+\chi)^2\partial_\alpha\frac{p^{\mathrm{ID}}}{\rho}\right. \\ &\quad \left. + \frac{3}{2}\rho\left(\frac{k_{\mathrm{B}}}{m}\right)^2 T\lambda^q\partial_\alpha T\right). \end{aligned} \tag{42}$$

Thus, we have the viscosity coefficient (μ) and heat conductivity (κ) as

$$\begin{aligned} \mu &= \frac{\tau p^{\mathrm{ID}}(1+\chi)^2}{2}, \\ \kappa &= \tau\left(\frac{D+2}{6}p^{\mathrm{ID}}(1+\chi)^2 + \frac{3}{2}\rho\left(\frac{k_{\mathrm{B}}}{m}\right)^2 T\lambda^q\right), \end{aligned} \tag{43}$$

which implies that the Prandtl number is

$$\mathrm{Pr} = \frac{3(1+\chi)^2 C_p}{2(1+\chi)^2 C_p + 9\lambda^q(k_{\mathrm{B}}/m)}, \tag{44}$$

where C_p is specific heat at constant pressure. Equation (44) allows us to set the Prandtl number independently in interval $(0, \frac{3}{2}]$.

V. OUTLOOK

To conclude, the Fokker-Planck approach of [14] was extended so that the Prandtl number and equation of state can be provided as an input to the kinetic description. Such a framework is quite useful for numerical implementation and may provide an alternate to methods such as DSMC or the recent set of works where a nonlinear extension to Ref. [14] was proposed for dilute gases [7–9]. In particular, our model needs to be contrasted with Ref. [8] where the Fokker-Planck model was extended to have the Prandtl number $\mathrm{Pr} = 2/3$ by using a nonlinear cubic drift term,

$$A_\alpha = c_{\alpha\beta}\xi_\beta + y_\alpha\left(\xi^2 - \frac{3k_BT}{m}\right) + \Lambda\left(\xi^2\xi_\alpha - \frac{2q_\alpha}{\rho}\right), \tag{45}$$

where $c_{\alpha\beta}$, y_α, and Λ are the macroscopic coefficients. Although the nonlinear extension of the drift term in the Fokker-Planck model is a good computational tool, one cannot show the H theorem and the existence of Maxwell-Boltzmann as the equilibrium solution in the space-independent case. Thus, the current model is preferable over Ref. [8] (at least for theoretical consistency reasons) as an approximation for the Boltzmann equation with the correct Prandtl number 2/3.

Furthermore, similar to Ref. [8], we do expect the current approach to be numerically efficient. This can be seen by writing equivalent Langevin stochastic differential equations for the Fokker-Planck equation [Eq. (27)],

$$\frac{dx_\alpha}{dt} = c_\alpha + \chi(c_\alpha - u_\alpha) - \frac{\tau}{2}\lambda^q(\partial_\alpha \ln T)\left(\xi^2 - D\frac{k_BT}{m}\right), \tag{46}$$

$$\frac{dc_\alpha}{dt} = -\frac{A_\alpha}{\tau} + \sqrt{2\,\mathfrak{D}}\frac{dW_\alpha}{dt}, \tag{47}$$

where A_α and $\mathfrak{D}$ are the same as the Lebowitz's Fokker-Planck model and $dW(t)$ is the standard Weiner process, which is a rapidly varying random force with $\langle dW_\alpha\rangle = 0$ and $\langle dW_\alpha dW_\beta\rangle = dt\delta_{\alpha\beta}$. Here, we want to point out that unlike Ref. [8], we have the linear Langevin equation for the velocity update. It is essential to note that the change in the internal energy due to the drift term is statistically matched with change in the internal energy due to the diffusion term for all time. To solve the Langevin equations [Eqs. (46) and (47)], the stochastic version of the Verlet algorithm ([21]) can be used. As an illustration, we consider the case of dilute gas where $\chi = 0$. In this case, the stochastic Verlet

TABLE I. Algorithm for implementation of current scheme.

1. Computational domain is divided into the finite number of cells with cell size similar to mean free path.
2. In each cell based on local density a finite number of particles is introduced with random location and velocity distributed according to the Maxwell-Boltzmann distribution.
3. In every cell, compute cell average velocity, temperature, and number density.
4. Update position and velocity of each particle using Eq. (48) and diffusive boundary condition.
5. Sort the particles in different cells based on their new location.
6. Repeat steps 3–5 until desired final time is achieved.

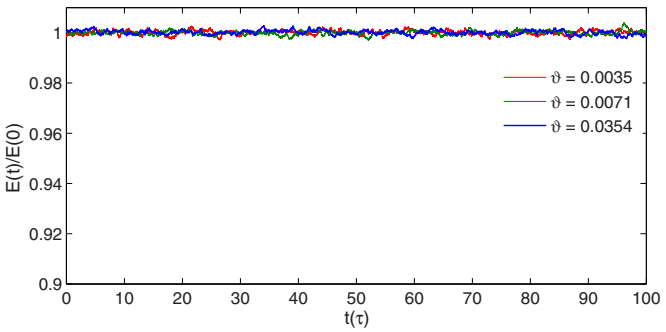

FIG. 1. (Color online) Energy with time.

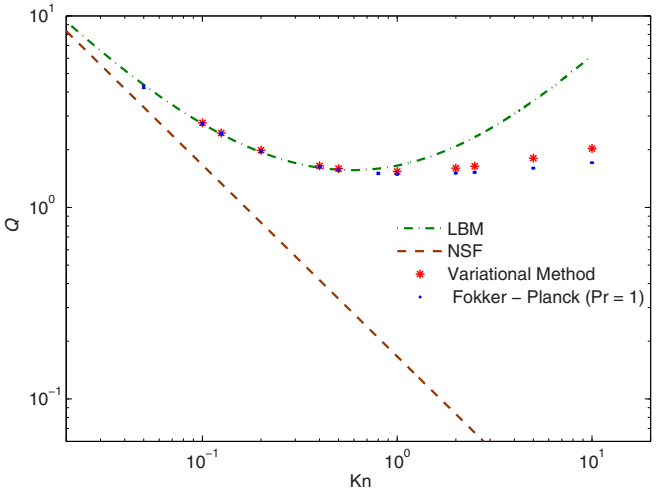

FIG. 2. (Color online) Poiseuille flow.

algorithm is

$$x_\alpha^{(1)} = x_\alpha + \frac{1}{2}\left(c_\alpha(t) - \frac{\tau}{2}\lambda^q(\partial_\alpha \ln T) \times \left(\xi^2 - D\frac{k_B T}{m}\right)\right)\Delta t,$$

$$c_\alpha(t+\Delta t) = c_\alpha(t) - \frac{\vartheta}{1+\vartheta/2}(c_\alpha(t) - U_\alpha) + \frac{\sqrt{2\,\mathfrak{D}\vartheta}}{1+\vartheta/2}\phi_t,$$

$$x_\alpha(t+\Delta t) = x_\alpha^{(1)} + \frac{1}{2}\left(c_\alpha(t+\Delta t) - \frac{\tau}{2}\lambda^q(\partial_\alpha \ln T) \times \left(\xi^2 - D\frac{k_B T}{m}\right)\right)\Delta t, \quad (48)$$

where $\vartheta = \frac{\Delta t}{\tau}$ and random noise ϕ_t is normal distributed with mean 0 and variance 1. This scheme works efficiently for the small time step, i.e., $\vartheta < 0.01$.

An algorithmic overview of this method is provided in Table I. To check the accuracy of the above scheme for the proposed Fokker-Planck approximation to the Boltzmann equation, we have initialized 10^5 gaseous particles with random Maxwellian velocities in a single cubic box with periodic wall conditions and no external force is applied. Figure 1 depicts the ability of the Verlet scheme to conserve the energy for the small time step.

Finally, to present accuracy of the current scheme, poiseuille flow is simulated using the stochastic Verlet scheme. For this setup, Yudistiawan *et al.* [22] had analytically solved a discrete velocity model solved by higher order LBM and obtained an expression for the dimensionless flow rate (Q) as

$$Q = \frac{0.166667}{\mathrm{Kn}} + 1.08152 + 2\mathrm{Kn} - \frac{0.17096 + 2.06084\mathrm{Kn} + 6.21071\mathrm{Kn}^2}{1 + 1.0433\coth\left(\frac{0.248039}{\mathrm{Kn}}\right)}, \quad (49)$$

where Knudsen number for a channel of height L is defined as

$$\mathrm{Kn} = \frac{\tau}{L}\sqrt{\frac{k_\mathrm{B}T_0}{2m}} = \frac{\tau_\mathrm{BGK}}{L}\sqrt{\frac{2k_\mathrm{B}T_0}{m}}. \quad (50)$$

In Fig. 2, we contrast FP results with semianalytical results of BGK, NSF solution, as well as this approximate expression. It is evident that this algorithm provides quite good results even in the transitional regime ($0.1 \leqslant \mathrm{Kn} \leqslant 5$) as compared to LBM and NSF and the Knudsen minimum effect predicted by this model matches quite well with the BGK results ([23]).

To conclude, we have developed a Fokker-Planck-based kinetic model which allows for an independent transport coefficient and a nonideal equation of state. The model has the correct hydrodynamic limit and H theorem. It is expected that the present model can be used as a numerical tool for solving kinetic equations. In subsequent works, we will present a detailed comparison of the present model and DSMC for the finite Knudsen regime.

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