A Lattice BGK Model for Viscoelastic Media

Yue-Hong Qian[1] and Yue-Fan Deng[2]
[1]Department of Applied Physics, Columbia University, New York, New York 10027
[2]Department of Applied Mathematics and Statistics, SUNY-Stony Brook, Stony Brook, New York 11794
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A two- and three-dimensional lattice Bhatnager-Gross-Krook model is proposed to simulate viscoelastic media. Large-scale equations are derived using the Chapman-Enskog expansion. A simple linear relationship between the parameter E which is introduced to characterize the elastic behavior and the transverse velocity is obtained. Numerical simulations further confirm the analytical predictions. [S0031-9007(97)04196-3]

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We investigate a new lattice-based model for simulating viscoelastic media with the Bhatnager-Gross-Krook (BGK) approximation [1]. A decade ago, lattice gas models for hydrodynamics were introduced by Frisch *et al.* [2–5] and much research effort has led to encouraging progress [6–9]. These models have several appealing advantages over conventional methods for complex flows such as multiphase flows [10,11], flows in porous media [12], and reaction-diffusion systems [13]. The inconveniences such as statistical noise [14,15] and non-Galilean invariance [4,5,16] in the original lattice gas models have been overcome by the use of lattice Boltzmann equations [17–20]. Another difficulty in lattice gas models, the existence of extra conserved quantities [21–24] which are not physically meaningful, was recently solved by using a fractional propagation procedure [25]. The introduction of the BGK approximation to lattice-based models [20,26–28] simplified the complicated collision processes, increased computing efficiency, and offered new flexibility. These models have been quite effective for solving fluid problems. However, they have not been paid enough attention to in tackling solid or fluid-solid problems [29–31]. The study of viscoelastic behavior of materials done by d'Humières and Lallemand [32] based on a lattice gas model successfully produced transverse waves and the propagation speed. Their prediction was also confirmed nicely by numerical simulations. However, their model requires an internal variable to describe "legal" collisions responsible for propagation of transverse waves and is clumsy in extension of their model to three dimensions.

The equation used in lattice BGK models has the following form [20,26–28]:

$$f_i(\vec{x} + \vec{c}_i, t + 1) = f_i(\vec{x}, t) + \omega[f_i^e(\vec{x}, t) - f_i(\vec{x}, t)], \tag{1}$$

where f_i is the particle distribution density with *predefined* discrete velocity $\vec{c}_i$ and ω the relaxation parameter ($0 \le \omega \le 2$) and i runs over the discrete velocity set. A suitable equilibrium f_i^e leading to the Navier-Stokes equations is [20,26]

$$f_i^e = t_p \rho \left[1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} u_\alpha u_\beta \right], \tag{2}$$

where t_p is a lattice weight factor (the index p is equal to c_i^2) and c_s a constant. Greek subscripts α and β denote the space directions in Cartesian coordinates. The hydrodynamic quantities p and $\vec{u}$ are defined as

$$\rho \equiv \sum_i f_i = \sum_i f_i^e, \qquad \rho \vec{u} \equiv \sum_i f_i \vec{c}_i = \sum_i f_i^e \vec{c}_i . \tag{3}$$

We propose a simple lattice BGK model for viscoelastic materials. Unlike the internal variable needed in [32], a parameter E is introduced to characterize the elasticity. Choosing an equilibrium distribution is much more flexible in lattice BGK models than in the lattice gas models. In fact, adding a term to the equilibrium (2) to model the transverse waves is convenient,

$$f_i^e = t_p \rho \left[1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} u_\alpha u_\beta + E \frac{(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2c_s^4} \frac{(u_\alpha I_\beta + u_\beta I_\alpha)}{2} \right]. \tag{4}$$

The last term involving E stems from the fact that one simple elastic behavior is wavelike propagation, like a vibrating string. The vector symbol I_α appearing in the above equilibrium is defined as

$$I_\alpha \equiv 1, \qquad \forall\ \alpha = x, y, z .$$

The Chapman-Enskog expansion [16,20,33] is used to derive the large-scale dynamical equations up to second order of the Knudsen number,

$$\partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0, \tag{5}$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha P + \nu[\partial_{\beta\beta}(\rho u_\alpha) + \partial_{\alpha\beta}(\rho u_\beta)] - \frac{E}{2}[\partial_s(\rho u_\alpha) + \partial_\beta(\rho u_\beta) I_\alpha] - \frac{E\nu}{2}[\partial_{s\alpha}\rho + \partial_{\beta\beta}(\rho) I_\alpha] - \frac{3E^2\nu}{4c_s^2}\partial_{s\beta}(\rho u_\beta) I_\alpha - \frac{E^2\nu}{4c_s^2}\partial_{ss}(\rho u_\alpha), \quad (6)$$

where ∂_s is defined through I_α,

$$\partial_s \equiv I_\alpha \partial_\alpha \equiv \partial_x + \partial_y + \partial_z .$$

As expected, the usual Navier-Stokes equations are recovered when $E = 0$. The shear viscosity ν and the pressure P are

$$\nu = \frac{c_s^2}{2}\left(\frac{2}{\omega} - 1\right), \qquad P = c_s^2 \rho . \quad (7)$$

The models considered here are thus isothermal models.

These results are in lattice units. In order to compare with real world systems, we need to keep the same similarity laws, i.e., the same values of *Mach* number M_a ($= u_0/c_s$ in lattice units) and *Reynolds* number R_e ($= u_0 L/\nu$ in lattice units) for both lattice-based models and real systems. For elastic media discussed here, a dimensionless material parameter $e \equiv E/(2c_s)$ also appears in the following dimensionless momentum equation after rescaling in time, space, and velocity (density ρ is linear in every term and thus is rescalable by any constant),

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\frac{1}{M_a^2}\partial_\alpha\rho + \frac{1}{R_e}[\partial_{\beta\beta}(\rho u_\alpha) + \partial_{\alpha\beta}(\rho u_\beta)] - \frac{e}{M_a}[\partial_s(\rho u_\alpha) + \partial_\beta(\rho u_\beta) I_\alpha] - \frac{e}{M_a R_e}[\partial_{s\alpha}\rho + \partial_{\beta\beta}(\rho) I_\alpha] - \frac{3e^2}{R_e}\partial_{s\beta}(\rho u_\beta) I_\alpha - \frac{e^2}{R_e}\partial_{ss}(\rho u_\alpha). \quad (8)$$

In what follows, the small-amplitude wave propagations in transverse and longitudinal directions are considered. If there is only the shear mode $v_y(x) = U_0 \cos(2\pi x)$ initially with density $\rho = 1.0$ and vanishing longitudinal component $v_x(x) = 0.0$, the shear wave propagates at a speed V_{sh} with decay rate γ,

$$V_{\text{sh}} = \frac{E}{2}, \qquad \gamma = \left(1 - \frac{E^2}{4c_s^2}\right)\nu = (1 - e^2)\nu . \quad (9)$$

For the longitudinal waves, there exist two modes which are the solution of the following dispersion relation (with perturbation of the form $e^{i(\Omega t - kx)}$):

$$\Omega^2 - \left[Ek + i\left(2 - \frac{E^2}{c_s^2}\right)\nu k^2\right]\Omega - c_s^2 k^2 + i\nu E k^3 = 0 ;$$

the solution is

$$\Omega = \frac{Ek}{2} + i\left(1 - \frac{E^2}{2c_s^2}\right)\nu k^2 \pm k\sqrt{c_s^2 + \frac{E^2}{4} - \left(1 - \frac{E^2}{2c_s^2}\right)^2 \nu^2 k^2 - i\frac{E^3}{2c_s^2}\nu k} . \quad (10)$$

The physics behind the choice of equilibrium Eq. (4) leading to the viscoelastic behavior is easy to understand. The viscous media act as a spring in both transverse and longitudinal directions, and the parameter E acts as Young's modulus. Since the viscous stress and elastic stress discussed here compound for the total stress, our present model is good only for the Kelvin-Voigt-like materials.

Compared with the models of Navier-Stokes-like equations for viscoelastic media, this model has five features: (i) New for studying viscoelastic properties of materials, (ii) complementary to existing approaches particularly for systems of small scales that the hydrodynamical description breaks down, (iii) bridging the microscopic and macroscopic descriptions of physics, (iv) flexible for analyzing different media [different choices of the equilibrium (4)], and (v) easy for numerical simulations.

The above results are valid for any spatial dimension. We performed tests by the following two-dimensional model which was found recently to have six order isotropy of velocity tensors [34] and no extra spurious invariants [25]. This model has 13 discrete particles' velocities (in lattice units): $(0,0)$, $(\pm 1, 0)$, $(0, \pm 1)$, $(\pm 1, \pm 1)$, $(\pm 2, 0)$, and $(0, \pm 2)$; the four weight factors are $t_0 = 2/5$, $t_1 = 8/75$, $t_2 = 1/25$, and $t_4 = 1/300$. The constant c_s is equal to $\sqrt{10}/5$ in lattice units.

As in all lattice BGK simulations, we solve Eqs. (1), (3), and (4) by time splitting. A time step consists of two substeps: collision and propagation. The collision substep is purely local and it involves only the relaxation term in Eq. (1). While during the propagation substep, particles hop from one site $\vec{x}$ at time t to another $\vec{x} + \vec{c}_i$ at time $t + 1$ according to the *given* discrete velocity $\vec{c}_i$.

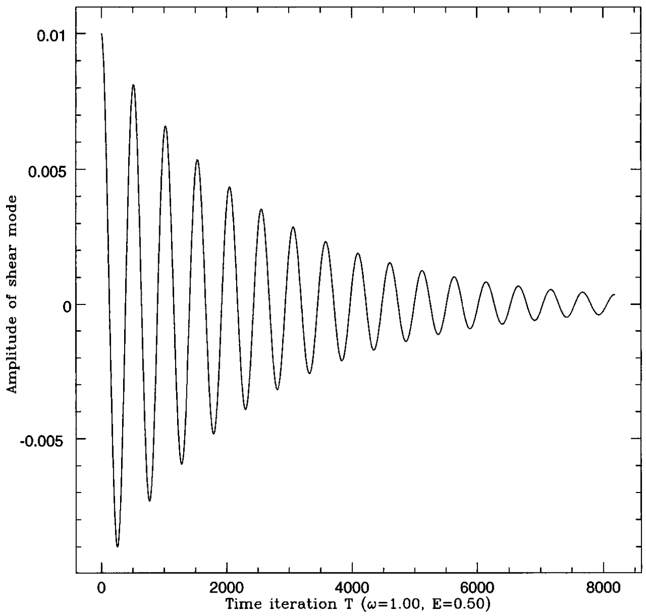

FIG. 1. Oscillation decay of transverse shear mode with time ($\omega = 1.00$, $E = 0.50$).

In Fig. 1 we show the oscillation of a shear mode with time. The initial condition is uniform density and zero longitudinal velocity; the transverse velocity is $v_y(x) = U_0 \cos(2\pi x)$. Instead of a pure decay, the transverse wave propagates along the longitudinal direction. From Fig. 1, the propagating speed and the decay rate are measured and compared with $E/2$ and $\gamma = (1 - E^2/4c_s^2)\nu$. The square and triangular points in Fig. 2 are the numerical measurements while the curves are the predictions. A good agreement is achieved. Figure 3 plots the longitudinal wave speed and decay rate; the curves are the solution of Eq. (10). We again see a satisfactory confirmation between theory and simulations.

In summary, we have studied a simple lattice BGK model for viscoelastic materials. A parameter E characterizing the elasticity is introduced in the equilibrium distribution (4). Large-scale dynamical equations are derived by the Chapman-Enskog expansion. Our model accurately describes transverse wave propagations. All predictions made by the model are confirmed by numerical simulations. Compared with the lattice gas model [32], this new model is flexible and straightforward for a three-dimensional extension.

Various potential applications of this model may include the P waves and S waves in seismology, polymer fluids [35], turbulence modeling [36], and magnetic sensitive transport coefficients of some materials [37]. A concrete three-dimensional model with consideration of thermal effect is in progress.

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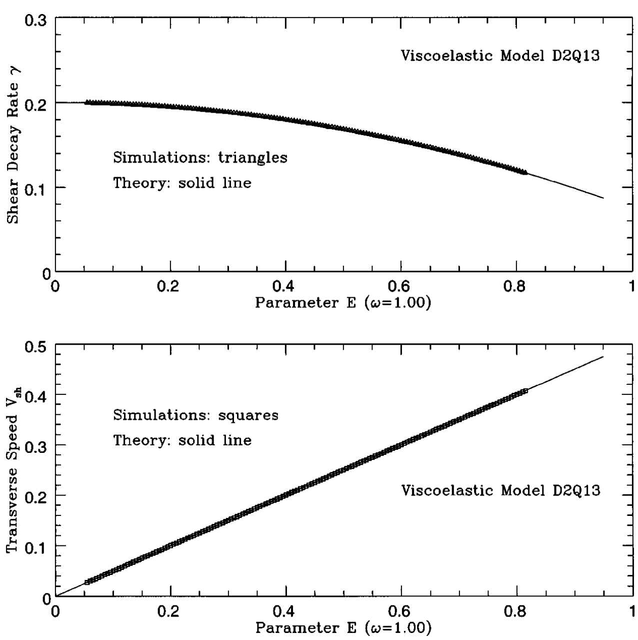

FIG. 2. Transverse shear speed V_{sh} as function of parameter E (bottom). Shear mode decay rate in function of E (top). Squares and triangles are numerical results and solid curves are predictions of the transverse velocity $V_{sh} = E/2$ and the decay rate $\gamma = (1 - e^2)\nu$.

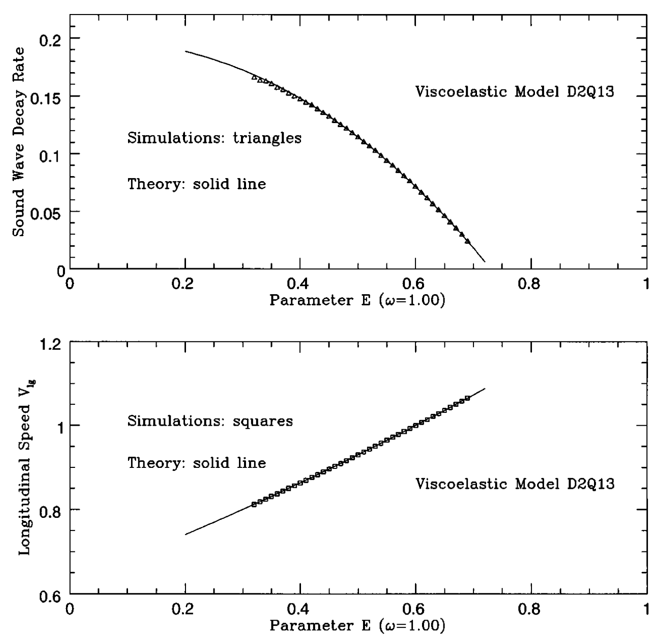

FIG. 3. Longitudinal wave propagation speed V_{lg} in function of parameter E (bottom). Longitudinal sound decay rate in function of E (top). Squares and triangles are numerical results, and solid curves are predictions of Eq. (10).

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