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2000 J. Phys.: Condens. Matter 12 L665

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LETTER TO THE EDITOR

Lattice Boltzmann nemato-dynamics

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Received 28 September 2000

Abstract. Lattice Boltzmann (LB) methods have been extensively studied for the mesoscopic modelling of isotropic fluids but little attention has been given to the problem of modelling anisotropic fluids. In this paper an LB scheme is presented which recovers the equations of the Ericksen–Leslie–Parodi theory of nemato-dynamics. The scheme introduces a second distribution which advects with the LB momentum densities and which represents the orientation of an ordered fluid element. The momentum evolution scheme requires the use of a linearized LB scheme with an anisotropic scattering matrix and the director evolution is achieved with an LBGK scheme. Results are presented which are in good agreement with the predictions of a Chapman–Enskog analysis of the algorithm. The method provides an initial step in the development of mesoscopic algorithms for modelling the flow of anisotropic fluids.

Over the past decade lattice Boltzmann (LB) methods have been successfully developed as mesoscopic models of isotropic fluids (e.g. [1–3]). The methods show particular promise in multi-component systems (e.g. [4, 5]) and flows in complex geometries (e.g. [6]). However, there are many materials of technological interest which have anisotropic flow properties and it would clearly be of interest to extend LB methods to represent such fluids. However very little work has been reported on this problem.

In this paper we consider nematic liquid crystals [7] which are of interest because of their applications in display devices. Materials which exhibit liquid crystal phases have anisometric molecules which are often modelled as either oblate or prolate ellipsoids [8]. The nematic ordering is characterized by an order tensor whose principal eigenvector defines the director, $n_{\alpha}(x, t)$, a unit vector which essentially defines the 'average orientation' of the molecules.

The continuum theory of the fluid dynamics of incompressible nematics was established by Ericksen, Leslie and Parodi (ELP) (see [7]) and the equations of the ELP theory may be summarized as follows

$$\nabla_{\alpha} v_{\alpha} = 0 \tag{1}$$

$$\frac{Dv_{\beta}}{Dt} = \partial_{\alpha}\sigma_{\alpha\beta} \tag{2}$$

where

$$N_{\alpha} = \frac{Dn_{\alpha}}{Dt} - \varepsilon_{\alpha\beta\gamma}\omega_{\beta}n_{\gamma}.$$
(4)

The first two equations are the equations of continuity (1) and momentum evolution (2). Equation (3) may be considered to be an equation controlling the evolution of the director. In these equations, we have used the repeated index summation convention, D/Dt is the convective derivative, $\sigma_{\alpha\beta}$ is the stress tensor, $A_{\alpha\beta} = \frac{1}{2} \left(\partial_{\alpha} v_{\beta} + \partial_{\beta} v_{\alpha} \right)$ is the symmetric part of the velocity gradient tensor and $\omega_{\alpha} = \frac{1}{2} \varepsilon_{\alpha\beta\gamma} \partial_{\beta} v_{\gamma}$ is the fluid vorticity. The field $h_{\alpha}(x, t)$ is a

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'molecular field' which mediates the effects of (i) the Frank elastic energy and (ii) the effect of any external applied magnetic or electric fields. In this work we adopt the *one constant approximation* in which the three Frank elastic constants are assumed to be equal to a single constant, K, and the molecular field becomes

$$n_{\alpha} = K \partial_{\beta} \partial_{\beta} n_{\alpha} + \gamma_a (\boldsymbol{H} \cdot \boldsymbol{n}) H_{\alpha}$$
⁽⁵⁾

where H_{α} is the external magnetic field. The viscous part of the stress tensor for a nematic may be written in the form

$$\sigma_{\alpha\beta}' = \left(\alpha_2 n_\alpha h_\beta + \alpha_3 h_\alpha n_\beta\right) / \gamma_1 + \alpha_1 n_\alpha n_\beta n_\gamma n_\delta A_{\gamma\delta} + \alpha_4 A_{\alpha\beta} \left(\alpha_5 - \alpha_2 \gamma_2 / \gamma_1\right) n_\alpha n_\gamma A_{\gamma\beta} + \left(\alpha_6 - \alpha_3 \gamma_2 / \gamma_1\right) n_\beta n_\gamma A_{\gamma\alpha}$$
(6)

where

$$\gamma_1 = \alpha_3 - \alpha_2 \tag{7}$$

$$\gamma_2 = \alpha_6 - \alpha_5 = \alpha_2 + \alpha_3 \tag{8}$$

We now describe an LB algorithm which will recover the macroscopic equations (1)–(3). The core of an LB algorithm is an evolution equation for the momentum density distribution $f_i(x, t)$ associated with lattice link *i* at the lattice site *x* and time step *t*. The distribution function is a mesoscopic quantity from which the macroscopic flow fields may be recovered through

$$\rho(\boldsymbol{x},t) = \sum_{i} f_{i}(\boldsymbol{x},t) \qquad \rho(\boldsymbol{x},t)u_{\alpha} = \sum_{i} c_{i\alpha}f_{i}(\boldsymbol{x},t)$$
(9)

where the $c_{i\alpha}$ are the velocity vectors associated with the underlying lattice [9, 10].

In order to represent a nematic fluid within a LB scheme it is necessary to introduce a variable which carries information about the orientational order of the fluid elements within the system. For simplicity we specialize to a two-dimensional model in which the director is restricted to lie in the $\{x, y\}$ plane and associate a scalar $\theta_i(x, t)$ with each lattice link in addition to the momentum density distributions $f_i(x, t)$. The 'director' associated with the fluid density in link direction *i* is $n_i = \{\cos \theta_i, \sin \theta_i\}$. The quantity $\theta_i(x, t)$ is assumed to advect with the momentum density $f_i(x, t)$. The ELP equations are recovered from two LB schemes, one for the evolution of the momentum densities, $f_i(x, t)$, and a second for the evolution of the orientation, $\theta_i(x, t)$. These two LB algorithms are run in parallel with the same time increment and on the same underlying lattice. At the end of each propagation step, the values of the orientation and velocity fields are exchanged.

In the method presented here we essentially represent the order of the fluid through the introduction of a vector density. This is in contrast to a nemato-dynamics LB scheme recently reported by Denniston *et al* [11] which introduces the order of the nematic fluid through a tensor density. The Denniston scheme is able to model systems with variable order parameter but does not include the full tensorial coupling of the director and velocity fields achieved by the method described here.

The anisotropy is introduced into a momentum evolution scheme through an anisotropic collision process. Thus the momentum densities are assumed to propagate according a linearized lattice Boltzmann scheme (LLB) [12] of the form

$$f_i(x + \delta c_i, t + \delta) = f_i(x, t) + \sum_j (\Omega_{ij} - S_{ij}) f_j^{(neq)} + F_i$$
(10)

where Ω_{ij} is an anisotropic collision matrix, the matrix S_{ij} is defined below, $f_j^{(neq)} = f_j - f_j^{(0)}$ is the non-equilibrium component of the momentum density distribution and the 'forcing' term, F_i , is of the form

$$F_i = t_p c_{i\beta} \partial_\alpha \left(\alpha_2 n_\alpha h_\beta + \alpha_3 h_\alpha n_\beta \right) / (\gamma_1 c_s^2)$$
⁽¹¹⁾

The parameter t_p is defined below after equation (16). The perturbation, F_i , recovers the momentum evolution arising from the first term of the stress tensor given in equation (6). In order to recover the remaining terms in the stress tensor (6), the matrix Ω_{ij} is taken to be of the form

$$\Omega_{ij} = \frac{\Omega_{ij}^{(0)}}{1 + \lambda_j^{(0)} + \lambda_j^{(2)} + \lambda_j^{(4)}}$$
(12)

where $\Omega_{ij}^{(0)}$ is an *isotropic* collision matrix and

$$\lambda_j^{(0)} = \delta_0(c_{j\alpha}c_{j\alpha}) \qquad \lambda_j^{(2)} = \delta_2(c_{j\alpha}n_\alpha)^2 \qquad \lambda_j^{(4)} = \delta_4(c_{j\alpha}n_\alpha)^4 \tag{13}$$

The term $\lambda_j^{(0)}$ only contributes to the isotropic viscosity, a_4 . The term $\lambda_j^{(2)}$ yields the final two terms in the stress tensor (6) and the term $\lambda_j^{(4)}$ gives the term associated with α_1 . In order to recover the terms associated with $\lambda_j^{(2)}$ in the correct form it is necessary for the velocity tensors

$$T^{(n)}_{\alpha_1\alpha_2\dots\alpha_n} = \sum_i t_p c_{i\alpha_1}\dots c_{i\alpha_n}$$
(14)

to be isotropic up to 6th order. Here this is achieved through the use of a two-dimensional lattice with 13 velocity components (D2Q13) based on a three-speed hexagonal lattice with velocity vectors, c_p , given by

$$c_{0} = \{0, 0\}$$

$$c_{1} = c\{\pm 1, 0\}, c\{\pm 1/2, \pm \sqrt{3}/2\}$$

$$c_{2} = c\{0, \pm \sqrt{3}\}, c\{\pm 3/2, \pm \sqrt{3}/2\}$$
(15)

the subscripts 0, 1 and 2 being associated with particles with velocity 0, *c* and $\sqrt{3c}$ respectively. The term associated with $\lambda^{(4)}$ requires isotropy of $T^{(N)}$ to 8th order; this could be achieved by further enhancement of the velocity set but for simplicity this term is omitted in the current analysis.

The isotropic equilibrium distribution function, $f_i^{(0)}(\rho, u)$, for the D2Q13 lattice is determined by the requirements that it satisfies the moments (9), yields 6th order isotropy in the velocity tensors and is Galilean invariant. It is found to $O(u^2)$ to be of the form

$$f_i^{(0)}(\rho, \boldsymbol{u}) = \rho t_p \left(1 + \frac{1}{c_s^2} u_\alpha c_{i\alpha} + \frac{1}{2c_s^2} u_\alpha u_\beta \left(\frac{c_{i\alpha} c_{i\beta}}{c_s^2} - \delta_{\alpha\beta} \right) \right)$$
(16)

where $t_0 = 11/25$, $t_1 = 9/100$ and $t_2 = 1/300$ and the velocity of sound $c_s = (3/10)^{1/2}$. The 13 × 13, isotropic scattering matrix $\Omega_{ij}^{(0)}$ is chosen to be of the form

$$\begin{pmatrix} c & b & d \\ b^T & A & G \\ d^T & G & A \end{pmatrix}$$
(17)

where $b = \{b, b, b, b, b, b\}$, $d = \{d, d, d, d, d\}$, and A and G are 6×6 circulant matrices with first rows

$$\{a_0, a_{60}, a_{120}, a_{180}, a_{120}, a_{60}\} \qquad \{g_{30}, g_{30}, g_{90}, g_{150}, g_{150}, g_{90}\}. \tag{18}$$

The matrix $\Omega_{ij}^{(0)}$ is an extension of that used by Higuera *et al* [12] for the D2Q7 lattice. $\Omega_{ij}^{(0)}$ has the circulant properties required by symmetry and couples the three velocity sets. The requirements of conservation of mass and momentum can be satisfied by a wide choice of matrix elements. We make the following choice in order to recover the required physical behaviour

$$b = \tau/13 \qquad c = -12\tau/13 \qquad d = \tau/13 g_{30} = \tau/13 \qquad g_{90} = \tau/13 \qquad g_{150} = \tau/13$$
(19)

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$$a_0 = -(10\tau + 13\phi)/39 \qquad a_{60} = (6\tau + 13\phi)/78 a_{120} = (-20\tau + 13\phi)/78 \qquad a_{180} = (3\tau - 13\phi)/39.$$
(20)

With this choice of matrix elements, $\Omega_{ij}^{(0)}$ has five eigenvectors with eigenvalues 0, four with eigenvalue $-\phi$ and four with eigenvalue $-\tau$.

The matrix S_{ij} in equation (10) is defined by

$$S_{ij} = \sum_{\nu=4}^{7} \xi_i^{(\nu)} \xi_j^{(\nu)}$$
(21)

where the summation is over the four eigenvectors, $\xi^{(\nu)}$, with zero eigenvalue which are formed from the velocity vectors c_p . The effect of S_{ij} is to remove the contributions of these eigenvectors from f_i^n for all $n \ge 1$. For the anisotropic scheme described here it is necessary to remove these terms in order to recover the required form for the macroscopic stress tensor. It can be shown from a standard Chapman–Enskog analysis (e.g. [2]) of the momentum evolution equation (10) that the first-order correction to the equilibrium distribution function is given by

$$f_i^{(1)} = (1 + \lambda_i^{(0)} + \lambda_i^{(2)} + \lambda_i^{(4)})g_i^{(1)}$$
(22)

where the $g_i^{(1)}$ are solutions of

$$\frac{t_{\rho}}{c_s^2} \left(c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta} \right) \partial_{\alpha} (\rho u_{\beta}) = \sum_j \Omega_{ij}^{(0)} g_i^{(1)}.$$
⁽²³⁾

The $g_i^{(1)}$ represent first-order corrections to the equilibrium distribution function in the presence of the isotropic scattering matrix $\Omega_{ii}^{(0)}$ and are given by

$$g_{i}^{(1)} = \frac{1}{c_{s}^{2}} \partial_{\alpha} (\rho u_{\beta}) \left(-\frac{t_{p}}{\phi} \left(c_{i\alpha} c_{i\beta} - c_{s}^{2} \delta_{\alpha\beta} \right) + \left(g_{2} \boldsymbol{\xi}_{i}^{(2)} + g_{3} \boldsymbol{\xi}_{i}^{(3)} \right) \delta_{\alpha\beta} \right) + \sum_{\nu=4}^{7} g_{\nu} \boldsymbol{\xi}_{i}^{(\nu)}$$
(24)

where the coefficients g_4 to g_7 in $g_i^{(1)}$ are set to zero by the use of the matrix S_{ij} . Provided the velocity set has the correct isotropy, the form of $f_i^{(1)}$ given by equation (22) leads to the required tensor coupling between the director field and the velocity gradients. Hence, noting that we have set $\lambda_i^{(4)} = 0$, a Chapman–Enskog analysis leads to the following identifications

$$\alpha_4 = -c_s^2 \rho \left(1 - \frac{2}{\phi} - \frac{3\delta_0}{\phi} - \frac{\delta_2}{2\phi} \right) \qquad \alpha_5 = \frac{c_s^2 \rho \delta_2}{\phi} - \alpha_2 \lambda \qquad \alpha_6 = \frac{c_s^2 \rho \delta_2}{\phi} - \alpha_3 \lambda \tag{25}$$

where $\lambda = -\gamma_2/\gamma_1$. Recalling that α_2 and α_3 are introduced through the F_i given by equation (11), we have therefore obtained a momentum evolution scheme which gives direct control over $\alpha_2, \alpha_3, \alpha_4$ and α_5 in the anisotropic stress tensor through the input parameters $\alpha_2, \alpha_3, \delta_0, \delta_2$ and ϕ . In order for the algorithm to be dynamically stable, the parameters associated with the anisotropic scattering matrix, $\{\delta_0, \delta_2, \phi, \tau\}$ must be chosen to ensure that $-2 < \sum_{ij} \xi_i^{\nu} \Omega_{ij} \xi_j^{\nu} < 0$ for each eigenvector, ξ^{ν} , and $|\sum_{ij} \xi_i^{\nu} \Omega_{ij} \xi_j^{\mu}| < 1$ for $\nu \neq \mu$.

We now consider the evolution of the director whose governing equation, (3), which may be written in the form

$$\partial_t \theta + v_\beta \partial_\beta \theta = \frac{K}{\gamma_1} \nabla^2 \theta + \omega_z + \frac{\gamma_2}{2\gamma_1} \left[\sin(2\theta) (\partial_x u_x - \partial_y u_y) - \cos(2\theta) (\partial_x u_y + \partial_y u_x) \right]$$
(26)

where $\omega_z = [\nabla \times u]_z$. The corresponding macroscopic observable, $\theta(x, t)$, is defined through the following choice of an average orientation

$$\theta(\boldsymbol{x},t) = \frac{1}{N_i} \sum_{i}^{N_i} \theta_i(\boldsymbol{x},t)$$
(27)

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where N_i is the number of lattice links. The inversion symmetry of the director is introduced by calculating the order tensor (cf [7]) of the orientation vectors at each site and adjusting all the angles θ_i to lie within $\pm \pi/2$ of the local director before the average in (27) is calculated. This definition, together with the subsequent definition of the equilibrium distribution function leads to the correct macroscopic behaviour.

In the spirit of LBGK simulation we evolve $\theta_i(x, t)$ according to:

$$\theta_i(\boldsymbol{x} + \delta \boldsymbol{c}_i, t + \delta) = \theta_i(\boldsymbol{x}, t) + \omega \left(\overline{\theta}_i - \theta_i(\boldsymbol{x}, t) \right) + A(\theta, \nabla \boldsymbol{u}) - \frac{1}{c_s^2} \boldsymbol{c}_i \times \boldsymbol{u}$$
(28)

where

$$\overline{\theta}_i = \frac{\theta(\boldsymbol{x}, t) f_i}{\rho(\boldsymbol{x}, t)} \qquad K = \frac{c_s^2 \gamma_1}{2} \left(\frac{2}{\omega} - 1\right).$$
(29)

The time step for angular evolution is chosen to be identical with that used for the momentum evolution. The equilibrium distribution, $\overline{\theta}_i$, has been defined in equation (29) to have the property $\sum_i \overline{\theta}_i = \theta(x, t)$. This ensures that $\sum_i \theta_i^{(n)} = 0$ for $n \ge 1$, a common requirement in LBE formalism [2]. The forcing term, $A(\theta, \nabla u)$, is set to be [13]

$$A(\theta, \nabla u) = t_p \frac{\gamma_2}{2\gamma_1} \left[\sin(2\theta)(\partial_x v_x - \partial_y v_y) - \cos(2\theta)(\partial_x v_y \partial_y v_x) \right]$$
(30)

and this generates all the outstanding terms in the macro-dynamics with an error term $(2\tau - 1)\varepsilon_{z\alpha\beta}\partial_{\alpha}\partial_{\gamma}v_{\gamma}v_{\beta}$ which is small in the target creeping flow applications. The effect of an external magnetic field may be included in the LB director evolution scheme by the addition of a term of the form

$$\frac{\gamma_a}{\gamma_1} \left(H_x H_y \cos(2\theta) + \frac{H_y^2 - H_x^2}{2} \sin(2\theta) \right)$$
(31)

to the forcing term equation (30).

The LB scheme described above has been implemented for some simple flow regimes in order to validate the method. A standard experimental approach is to measure the viscosity of the liquid crystal in a simple shear field in the presence of strong director aligning fields in order to determine the Miesowicz viscosities (see e.g. [7, 14]). It is found that the effective viscosities in a shear flow in which the director is parallel and perpendicular to the flow, $\eta_{\parallel} \left[= \frac{1}{2} (\alpha_4 + \alpha_6 + \alpha_3) \right]$ and $\eta_{\perp} = \left[\frac{1}{2} (\alpha_4 + \alpha_5 - \alpha_2) \right]$, are given respectively by

$$\eta_{\parallel} = -\frac{\alpha_3^2}{\alpha_2 - \alpha_3} + c_s^2 \rho \left(-\frac{1}{2} + \frac{1}{\phi} + \frac{3\delta_0}{2\phi} + \frac{3\delta_2}{4\phi} \right)$$

$$\eta_{\perp} = -\frac{\alpha_2^2}{\alpha_2 - \alpha_3} + c_s^2 \rho \left(-\frac{1}{2} + \frac{1}{\phi} + \frac{3\delta_0}{2\phi} + \frac{3\delta_2}{4\phi} \right).$$
(32)

Simulation results for these two Miesowicz viscosities are plotted in figure 1 as a function of $|1/\phi|$ for the parameter set { $\tau = -1, \delta_0 = 0.06, \delta_2 = -0.07761, \gamma_1 = 0.04698, \gamma_2 = -0.04842$ }. The ratio of the slope to the intercept for each of these two sets of data agrees with the predicted value to better than 0.02%. For $\phi = -1.962$ this parameter set gives Leslie coefficients in the same ratio as those of N-(p-methoxybenzylidene)-p-n-butyl-aniline (MBBA) at 25° [15]; $\alpha_2/\alpha_4 = -0.956, \alpha_3/\alpha_4 = -0.0144, \alpha_5/\alpha_4 = 0.556$ and $\alpha_6/\alpha_4 = -0.413$. The ratio of the two Miesowicz viscosities is found to be 4.383 which is in agreement with the predicted value to within 0.2%. The method has also been used to replicate the flow of p-methoxy-p'-butylazoxybenezene and p,p'-dibutylazoxybenzene (DIBAB) over the range of temperatures reported in [16].



Figure 1. Simulation results for the Miesowicz viscosities as a function of $1/\phi$ for director orientations of 0° (Δ) and 90° (\Box). Solid lines from equations (32)



Figure 2. Simulation results for bulk director orientation in shear flow as a function of $-\gamma_2/\gamma_1$. The continuous curve is $\cos(2\theta) = -\gamma_1/\gamma_2$.

In figure 2 we show a comparison between the theoretical and simulation results for the variation in the director orientation in a shear flow. The simulation results have been obtained using the director evolution scheme given in equation (28). In order to test the director evolution algorithm we considered the response of the director field to a shear flow for which it is predicted that far from the walls the director angle is given by

$$\cos(2\theta) = -\gamma_1/\gamma_2 \tag{33}$$

if the director is pinned perpendicular to the walls. This behaviour is correctly recovered as is

shown in figure 2.

In this letter we have proposed an LB scheme for an nematic fluid and demonstrated that the algorithm is able to recover the equations of the ELP theory of nemato-dynamics. The scheme introduces a variable to represent the director field which advects with the LB momentum densities. The momentum evolution scheme requires the use of a linearized LB scheme with an anisotropic scattering matrix and the director evolution is achieved with an LBGK scheme. The momentum evolution equation requires isotropy of the velocity tensors up to 8th order to recover the full ELP equations. Results have been presented for the scheme which recover four of the five Leslie coefficients using a velocity set which has 6th order isotropy and using a particular form of the scattering matrix. The results are in good agreement with the predictions of the Chapman–Enskog analysis.

Whilst the momentum scheme described here could be generalized straightforwardly to three dimensions, the angular evolution scheme is specialized for a two-dimensional director field. The extension of the angular scheme to three dimensions would require a reworking of the methodology and is currently being developed. In future work it is hoped first to address the important problem of materials with a spatially varying order parameter.

We thank D Cleaver, A Masters, P Olmsted, L-S Luo, J Yeomans and C Denniston for useful conversations. The work is part funded by EPSRC grant number GR/L86135.

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