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Diffusion Lattice Boltzmann Scheme on a Orthorhombic Lattice

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We present a diffusion lattice Boltzmann (DLB) scheme which is derived from first principles. As opposed to the traditional lattice BGK schemes the DLB is valid for orthorhombic lattices and it has two eigenvalues of the collision operator. It is shown that the diffusion coefficient depends only on one eigenvalue of the collision operator. Hence, the DLB scheme can be optimized with means of the additional eigenvalue of the collision operator and with different lattice spacing along the principal axes. The properties of the DLB scheme concerning consistency, stability, and accuracy are studied with eigenmode analysis. This analysis shows that the DLB scheme is consistent with diffusion for a wide range of diffusion coefficients, it has unconditional stability, and that it has third-order accuracy. Furthermore, it is shown that accuracy is improved by setting the additional eigenvalue to zero and by densifying the lattice spacing along the direction of the density gradient.

KEY WORDS: Lattice Boltzmann; diffusion, eigenmode analysis.

INTRODUCTION

The Lattice Boltzmann scheme is a recently developed technique for modelling physical transport phenomena.(1) The algorithm is quite simple and is derived from basic physical principles. Because of its simple nature it is frequently and successfully used for modelling complex phenomena such as hydrodynamics, multi-phase flow, natural convection and reaction diffusion.(2–6) As the method is relatively new, most studies are done with high symmetry lattices, such as the cubic and square lattice. However engineering problems may demand the use of less symmetric lattices. On this problem little study is performed. We investigate this problem by

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studying the Lattice Boltzmann scheme for isotropic diffusion on a orthorhombic lattice, which has different lattice spacing in the three orthogonal directions.

Diffusion has seldom been the prime focus of studies on LB schemes,[7] though it is a simple phenomenon speaking from both a mathematical and numerical point of view. Isotropic diffusion in a homogeneous medium is mathematically described by the following elliptic partial differential equation:

$$\partial_t \rho_g = D\nabla^2 \rho_g \tag{1}$$

with ρ_g the diffusing physical quantity and D the diffusion coefficient. The solution of elliptical partial differential equations poses little problems for conventional numerical methods.[8] It is conceivable that this is also the case for Lattice Boltzmann schemes. Hence, diffusion is an ideal problem for detailed theoretical analysis of the LB scheme and investigations directed towards generalisation and optimisation of the method. Furthermore we expect that improvements of the Lattice Boltzmann technique found for diffusion can lead to new directions for LB schemes for the more complex phenomena as fluid flow.

In order to find all possible degrees of freedom, which can be used for improving the LB scheme, we construct the DLB scheme from first principles, i.e., the conservation laws and lattice symmetry requirements. The properties of the DLB scheme concerning consistency, stability and accuracy are analysed in terms of eigenmodes.[9, 10] Using the eigenmode analysis we investigate ways of improving the performance of the DLB scheme using its extra degrees of freedom.

LATTICE BOLTZMANN SCHEME

Lattice Boltzmann equation

The general formulation of the Lattice Boltzmann scheme, can be written as cf. ref. 1:

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) + \Omega_{ij}[\, g_j^{eq}(\mathbf{x}, t) - g_j(\mathbf{x}, t)\,] = A_{ij} g_j(\mathbf{x}, t) \tag{2}$$

where the distribution function $g_i(\mathbf{x}, t)$ represents the number of particles on lattice site $\mathbf{x}$ at time t, moving with velocity $\mathbf{c}_i$. The velocities are chosen such that at the next time step $t + \Delta t$ the particles move to neighbouring sites $\mathbf{x} + \Delta \mathbf{x}_i$, i.e., $\mathbf{c}_i = \Delta \mathbf{x}_i / \Delta t$. g_i^{eq} is the equilibrium particle distribution function, and Ω_{ij} is a relaxation matrix. The matrix elements A_{ij} are the transition rates between states associated with a particular velocity $\mathbf{c}_i$. This

formulation of the LB scheme, Eq. (2), is also known as the enhanced collisions LB scheme.[1]

The standard requirements[11] for any LB collision operator are (1) the transition rates are normalised, which guarantees that the collisions are conserving the number of particles and (2) the collision operator must allow a collision invariant equilibrium distribution g_i^{eq}. These requirements impose:

$$\sum_i A_{ij} = 1 \tag{3}$$

$$\sum_j A_{ij} g_j^{eq} = g_i^{eq} \tag{4}$$

Macroscopic parameters are derived from the moments of the particle distribution. For diffusion the number density is sufficient for describing the physical problem. The number density is the number of particles summed over all states i:

$$\rho_g(\mathbf{x}, t) = \sum_i g_i(\mathbf{x}, t) \tag{5}$$

Symmetries

In order to have the Lattice Boltzmann equation describe the desired physical phenomena the lattice and the collision operator should have certain symmetries, cq. Invariance's. In case of isotropic diffusion the constraints are:

(i) The collision operator is invariant under all isometries of the Bravais lattice.

(ii) Second rank tensors are isotropic.

The constraint (ii) guarantees that the diffusivity tensor $D_{\alpha\beta}$ is isotropic, i.e., reduces to $D\delta_{\alpha\beta}$. The standard definitions, Eqs. (3)–(4), combined with constraint (ii) impose the following conditions on g_i^{eq}:[12]

$$\sum_i g_i^{eq} = \rho_g \tag{6}$$

$$\sum_i c_{i,\alpha} g_i^{eq} = 0 \tag{7}$$

$$\sum_i c_{i,\alpha} c_{i,\beta} g_i^{eq} = \rho_g c_s^2 \delta_{\alpha\beta} \tag{8}$$

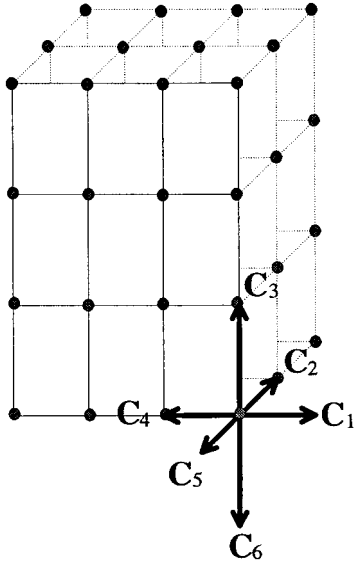

Fig. 1. The six-velocity orthorhombic lattice.

The constant c_s^2 is related to the metric of the Bravais lattice. For fluid flow problems it is identified as the speed of sound of the lattice gas. For diffusion problems it has no direct physical meaning.

Investigation of the conditions Eqs. (6)–(8) shows that they are satisfied when using a lattice with principal axes having two-fold rotation symmetry. Thus in three dimensions the lattice gas can reside on an orthorhombic lattice with lattice spacing, $\Delta x_\alpha = c_\alpha \Delta t$, which are in general unequal. Each lattice site has six states corresponding with the velocity vectors connected to the six nearest neighbour sites, defined as $\mathbf{c}_i = -\mathbf{c}_{i+3} = c_\alpha$. The orthorhombic lattice and its associated particles velocities are drawn in Fig. 1.

The equilibrium distribution satisfying Eqs. (6)–(8), is a weighted function of the number density: $g_i^{eq} = w_i \rho_g$. The weight functions are given by:

$$w_i = \frac{c_s^2}{2c_i^2}, \qquad \text{with} \quad \frac{1}{c_s^2} = \sum_i \frac{1}{2c_i^2} \tag{9}$$

Collision Matrix

The most general collision matrix A_{ij}, taking into account the two-fold rotation symmetry of the orthorhombic lattice, has the form:

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & B_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} & A_{21} & B_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} & A_{31} & A_{32} & B_{33} \\ B_{11} & A_{12} & A_{13} & A_{11} & A_{12} & A_{13} \\ A_{21} & B_{22} & A_{23} & A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & B_{33} & A_{31} & A_{32} & A_{33} \end{pmatrix} \tag{10}$$

Note that the collision matrix is in general not symmetric, i.e. $A_{\alpha\beta} \neq A_{\beta\alpha}$.

The collision matrix is fully characterised by its eigenvalues μ_α and eigenvectors $v_{\alpha,i}$, where the right and left eigenvectors are respectively defined as:

$$\sum_j A_{ij} w_j v_{a,j} = \mu_a w_i v_{a,i} \tag{11}$$

$$\sum_i v_{a,i} A_{ij} = \mu_a v_{a,i} \tag{12}$$

Using this definition we can construct the eigenvectors following ref. 13.

The first eigenvector follows directly from the standard requirements, Eqs. (3)–(4), which are satisfied if there exists an eigenvector with

$$\mu_0 = 1; \qquad v_{0,i} = 1 \tag{13}$$

This is the so called density mode eigenvector, the left eigenvector is commonly denoted as $\langle 1|$. The density follows from projecting the state vector g_i onto the eigenvector, meaning $\rho = \langle 1 \,|\, g \rangle$.

Next there exist three eigenvectors $\langle v_\alpha|$ of odd parity under inversion of all velocities ($c_i \to -c_i$). These so-called flux modes can be related to Cartesian components of the gradient in the number density $\partial_\alpha \rho \sim \langle v_\alpha \,|\, g \rangle$. In order to have an isotropic diffusion the corresponding eigenvalues must be equal (3-fold degenerate):

$$\mu_\alpha = \lambda; \qquad v_{\alpha,i} = e_{i,\alpha} \tag{14}$$

where $e_{i,\alpha} = c_{i,\alpha}/|c_{i,\alpha}|$.

The remaining two eigenvectors have even parity under velocity inversion, and can be related to second order derivatives of the number density. The corresponding eigenvalues must be equal (2-fold degeneracy) to guarantee isotropic diffusion, requiring:

$$\mu_{\alpha+\beta} = \kappa; \qquad v_{\alpha+\beta,i} = e_{i,\alpha}^2 - e_{i,\beta}^2, \qquad \text{with} \quad \beta \neq \alpha \tag{15}$$

All eigenvectors and corresponding eigenvalues are listed in Table I.

Table I. Eigenvectors $\mathbf{v}_a$ and Eigenvalues of the DLB Scheme μ_a^{DLB} and Lattice BGK Scheme μ_a^{BGK}

a	$\mathbf{v}_a$	μ_a^{DLB}	μ_a^{BGK}
0	$\langle 1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1 \vert$	1	1
1	$\langle 1 \quad 0 \quad 0 \quad -1 \quad 0 \quad 0 \vert$	λ	$1-\omega$
2	$\langle 0 \quad 1 \quad 0 \quad 0 \quad -1 \quad 0 \vert$	λ	$1-\omega$
3	$\langle 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad -1 \vert$	λ	$1-\omega$
4	$\langle 1 \quad -1 \quad 0 \quad 1 \quad -1 \quad 0 \vert$	κ	$1-\omega$
5	$\langle 0 \quad 1 \quad -1 \quad 0 \quad 1 \quad -1 \vert$	κ	$1-\omega$

The collision matrix can now be formulated when imposing the above stated symmetry requirements for the eigenvalues. It is readily seen that the two-fold symmetry of the lattice and the standard requirements Eqs. (3)–(4) are satisfied when the collision matrix meets the detailed balance condition:

$$A_{ij} w_j = A_{ji} w_i \tag{16}$$

Note that this condition implies that the transformed matrix $M_{ij} = 1/\sqrt{w_i}\, A_{ij} \sqrt{w_j}$ is symmetric, which is similar to the collision matrix for a cubic lattice.

After some lengthy, but straightforward algebra using the eigenvalue equations, one finds the expressions for the components of the collision operator:

$$A_{\alpha\alpha} = w_\alpha (1-\kappa) + (1/2)(\kappa+\lambda) \tag{17}$$

$$A_{\beta\alpha} = w_\alpha (1-\kappa), \qquad \text{with} \quad \alpha \neq \beta \tag{18}$$

$$B_{\alpha\alpha} = w_\alpha (1-\kappa) + (1/2)(\kappa-\lambda) \tag{19}$$

We have now formulated the diffusion Lattice Boltzmann (DLB) scheme starting from first principles. The DLB scheme has two degrees of freedom and is valid on lattices with only two-fold symmetry, which holds for the orthorhombic lattice in three dimensions. The DLB scheme has an extra degree of freedom over the Lattice BGK scheme, traditionally used.[14] The DLB scheme becomes equal to the BGK scheme when setting $\lambda = \kappa = 1-\omega$. For comparison we have also listed the set of eigenvectors and eigenvalues for the BGK scheme in Table I.

For the BGK scheme the Lattice Boltzmann equation, Eq. (2), is written as:

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) + \omega[\, g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\,] \tag{20}$$

In order to be consistent with existing literature we use below $1 - \omega$ instead of λ for the eigenvalues of the flux modes.

EIGENMODE ANALYSIS

Eigenmodes

Having constructed the diffusion Lattice Boltzmann diffusion scheme with a collision operator A_{ij} satisfying all required symmetry properties, we now determine the properties concerning consistency, stability and accuracy by analyzing the LB equation Eq. (2) in terms of eigenmodes.[9] This approach is very similar to the traditional von Neumann stability analysis of numerical schemes.

Assuming an unbounded or periodic lattice, the eigenmodes of the Lattice Boltzmann equation are given by:

$$g_i(\mathbf{x}, t) = \tilde{g}_i(\mathbf{k}, s) \exp(st + i\mathbf{k} \cdot \mathbf{x}) \tag{21}$$

Here $s = s(k)$ is the relaxation rate of the eigenmode. Substitution of the ansatz Eq. (21) into the LB equation Eq. (2) leads to the eigenvalue equation:

$$\exp(-i\mathbf{k} \cdot \Delta \mathbf{x}_i)\, A_{ij}\, \tilde{g}_j(\mathbf{k}, s) = \exp(s(k)\, \Delta t)\, \tilde{g}_i(\mathbf{k}, s) \tag{22}$$

From the spectrum of the eigenvalues $\mu(k) = \exp(s(k)\, \Delta t)$, information about the consistency, stability and accuracy can be deduced. The number of eigenmodes of the LB equation is equal to the number of states at a lattice site. As LB schemes satisfy conservation laws, the eigenmodes can be divided in slow modes, related to conservation laws, and kinetic modes, which usually decay rapidly.[9, 10] As diffusion is only concerned with conservation of mass, the DLB scheme has only one slow diffusive mode. The scheme will show diffusive behaviour if the relaxation rate of the diffusive eigenmode holds is significantly slower than those of the kinetic modes.

The LB scheme is consistent with diffusion if for the dominant (diffusive) eigenmode holds that $Re(s(\mathbf{k})) \sim -k^2$ and $Im(s(\mathbf{k})) = 0$. Then the time evolution of the number density will be:

$$\rho_g(\mathbf{x}, t) = \sum_i g_i(\mathbf{x}, t) = \rho_0 \exp(-Dk^2 t) \exp(i\mathbf{k} \cdot \mathbf{x}) \tag{23}$$

as follows from the Laplace transformation of Eq. (1). The diffusion coefficient D depends on the eigenvalues of the collision operator A_{ij} and will be derived below with means of the perturbation analysis of the eigenvalue equation.

General Properties

The properties of the LB scheme are discussed using a simple case, for which there exists an analytical solutions of the eigenvalue problem Eq. (22). The case we studied is that of a Lattice BGK scheme applied to a cubic lattice for eigenmodes having wavevectors equal to $\mathbf{k} = k(1, 1, 1)$. The corresponding eigenvalue equation is solved using the algebraic manipulation software package Maple^{TM}:

$$\mu_{0,1}(k) = (1 - \tfrac{1}{2}\omega)\cos(k) \pm [(1 - \tfrac{1}{2}\omega)^2 \cos^2(k) + (\omega - 1)]^{1/2} \quad (24)$$

$$\mu_{2,3}(k) = (1 - \omega)\exp(+ik) \quad (25)$$

$$\mu_{4,5}(k) = (1 - \omega)\exp(-ik) \quad (26)$$

The properties of the LB scheme following from the spectra of the eigenmodes, are shown in Fig. 2, and also hold for more general cases and even for hydrodynamic LB schemes.[10] These properties are:

- The LB scheme has one single diffusive mode which for small k behaves as $\ln(\mu_0(k)) = -Dk^2$. It is dominant over the kinetic modes for a wide range of wavelengths k in the range of $1 \leqslant \omega \leqslant 2$.
- The LB scheme is unconditionally stable, i.e., $|Re(\mu_a(k))| \leqslant 1$ holds for all eigenmodes.
- In the range of $0 \leqslant \omega \leqslant 1$ the diffusive behaviour of the scheme is limited. At relatively large wavelength the diffusive mode becomes mixed with a kinetic mode.
- In the range of $\omega \to 2$, the diffusive mode is not dominant over all kinetic modes. Consequently the LB will show spurious oscillations, due to slowly damped (oscillating) kinetic modes, i.e., $Re(\mu_a(k)) \to -1$ and $Im(\mu_a(k) \neq 0)$.

Take note that these properties hold only for unbounded or periodic lattices. For finite lattices the found results will be valid for the inner part of the lattice, near and at the boundaries the effects of the boundary conditions become significant. Sharp gradients at the boundaries induce instabilities or spurious modes, which cannot be captured with this eigenmodes analysis.

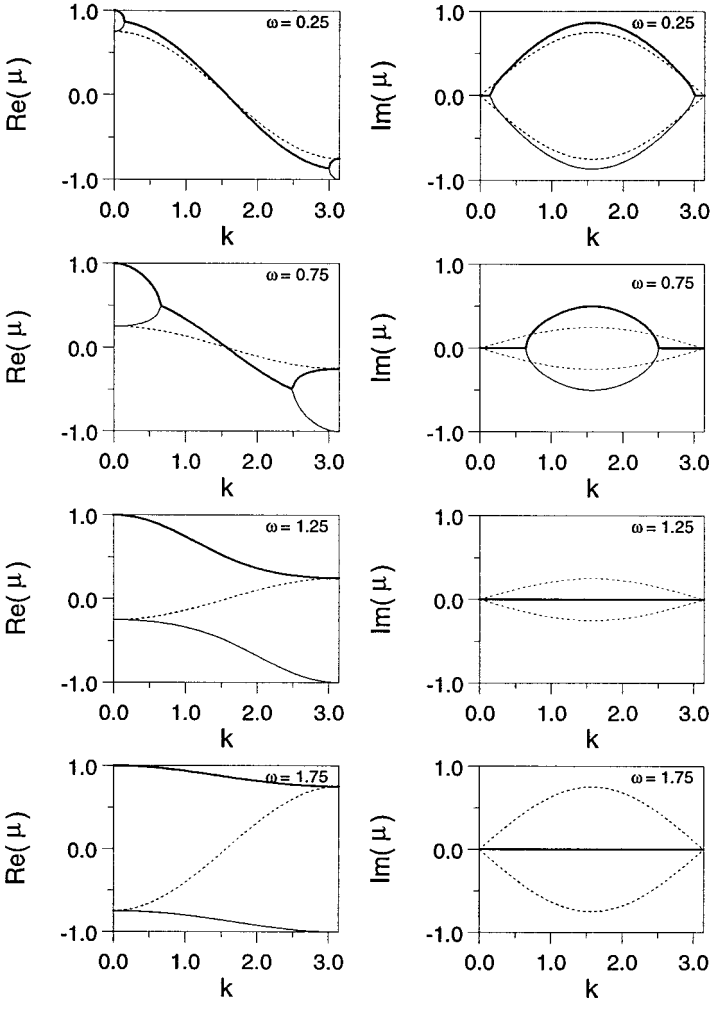

Fig. 2. The spectra of eigenmodes of a Lattice BGK scheme for $\omega = 0.25$, 0.75, 1.25 and 1.75 applied on a cubic lattice, with $\Delta x_i = 1$. The wave vector of the eigenmode is $\mathbf{k} = (k, k, k)$. The thick solid line is the spectrum of the eigenvalue μ_0 of the diffusive mode. The dashed line is the spectrum of eigenvalue μ_1. The other spectra are shown as thin solid lines. Observe that the diffusive mode in the top half of the figure becomes a propagating kinetic mode at finite k.

Perturbation Analysis

As diffusive behaviour is obtained in the long wave length regime ($k < 1$), we can determine the accuracy of the LB scheme by expanding the eigenvalue equation Eq. (22) in powers of the wave vector k cf. ref. 9. Furthermore this perturbation analysis gives us the relation between the diffusion coefficient and the eigenvalues of the collision operator.

In this analysis we apply the wave-vector expansion for the particle distribution $\tilde{g}_i$ and the relaxation rate s:

$$\tilde{g}_i(\mathbf{k}) = \tilde{g}_i^{(0)} + ik\tilde{g}_i^{(1)} + (ik)^2\, \tilde{g}_i^{(2)} + O(k^3) \tag{27}$$

$$s(k) = (ik)\, s_1 + (ik)^2\, s_2 + (ik)^3\, s_3 + O(k^4) \tag{28}$$

The particle distribution function is expanded as a series of perturbations $\tilde{g}_i^{(n)}$ of the equilibrium distribution $\tilde{g}_i^{(0)} = g_i^{eq}$. As there are no propagation modes for the diffusion problem, the eigenvalue $s(k)$ is an even function of the wave number, i.e., $s_1 = 0$ and $s_3 = 0$.

After substitution of the expansions, Eq. (27)–(28), in the eigenvalue equation Eq. (22) and performing a Taylor expansion, we obtain

$$ik\tilde{g}_i^{(1)}(\mathbf{k}) = -\frac{i\mathbf{k}\cdot \Delta\mathbf{x}_i}{\omega}\, w_i \rho(\mathbf{k}) \tag{29}$$

$$(ik)^2\, \tilde{g}_i^{(2)}(\mathbf{k}) = -\frac{1}{\kappa}\left(\frac{1}{\omega} - \frac{1}{2}\right)\left[(i\mathbf{k}\cdot \Delta\mathbf{x}_i)^2 - (ik)^2\, \Delta x_s^2\right] w_i \rho(\mathbf{k}) \tag{30}$$

where $\Delta x_s^2 = c_s^2\, \Delta t^2$. For s_2 we find

$$s_2 = c_s^2 \left(\frac{1}{\omega} - \frac{1}{2}\right) \tag{31}$$

so the relaxation rate of the diffusive mode is $s \sim -k^2 D + O(k^4)$. The diffusion LB scheme is accurate up to the third order of the wave number k. The expression for the diffusion coefficient in Eq. (31), i.e., $D = c_s^2(1/\omega - 1/2)\, \Delta t$, is identical to the one for the Lattice BGK scheme on a cubic lattice.[7] It depends only on the eigenvalue of the flux modes. The effects of the different lattice spacing are totally absorbed in the constant c_s^2.

OPTIMIZATION OF THE DLB SCHEME

Free Parameter κ

As is shown above the diffusion coefficient is only dependent on the eigenvalue of the flux modes $1 - \omega$. This means that the eigenvalue κ of the

collision operator can be used for optimization of the consistency and accuracy of the LB scheme.

An obvious choice for the free parameter κ is to set it to zero, such that the associated kinetic modes will die out immediately.[1, 10] It is expected that this choice of $\kappa = 0$ will lead to improved diffusive behaviour. We have checked this hypothesis numerically by comparing the spectra of the eigenmodes for the DLB scheme with those for the Lattice BGK scheme. We have computed the spectra for $\mathbf{k} = (k, 0, 0)$ and for four values of the relaxation parameter ω with results shown in figure.

In the right part of the figure the ratio between the computed value of the relaxation rate and the theoretical value ($s(k) = -Dk^2$) is shown. Deviation of this ratio from 1 means deviation from diffusive behaviour. As such from Fig. 3 one can observe that the DLB scheme has improved diffusive behaviour over the BGK scheme, as for $\omega \geqslant 3/4$ the relaxation rate $s(k) = -Dk^2$ for a larger range of wavelengths. From the left part of Fig. 3 one can see that spurious oscillations occur with the BGK scheme, but have vanished with the DLB scheme, as for all eigenmodes $Im(s(k)) = 0$ in the range of $\omega \geqslant 3/4$. It must be noted that the elimination of spurious oscillations occurs only for certain directions of the wave-vector. If $\mathbf{k} = (k, k, k)$ the flux modes will show oscillating behaviour, which is not eliminated by setting $\kappa = 0$.

Lattice Spacing

Another way of improving the diffusive behaviour of the LB scheme is to increase the number of lattice sites along the direction of the density gradient $\nabla \rho_g$. We show this by computing the spectra of the DLB scheme (with $\kappa = 0$) for different lattice spacing along the direction of wave vector $\mathbf{k} = (k, 0, 0)$. We have set $\Delta x = 1/2$, 1, and 2, $\Delta y = \Delta z = 1$. The computed spectra argue shown in Fig. 4. Again we have plotted the ratio of the computed value and the theoretical value of the relaxation rate of the diffusive mode as a function of the wave number, for $\omega = 1.25$ and $\omega = 1.75$. This ratio is about 1 for a larger range of wavenumbers for $\Delta x = 1/2$ especially for high ω. Consequently the deviation from pure diffusive behaviour is smallest for $\Delta x = 1/2$.

Hence, if there is prior knowledge about the gradients in the density field, the metrics of the lattice can be optimised for that particular case. The lattice should be densified along the direction of the gradient. On the other hand the lattice can be stretched along the opposite directions, such that the total number of lattice sites can be kept limited.

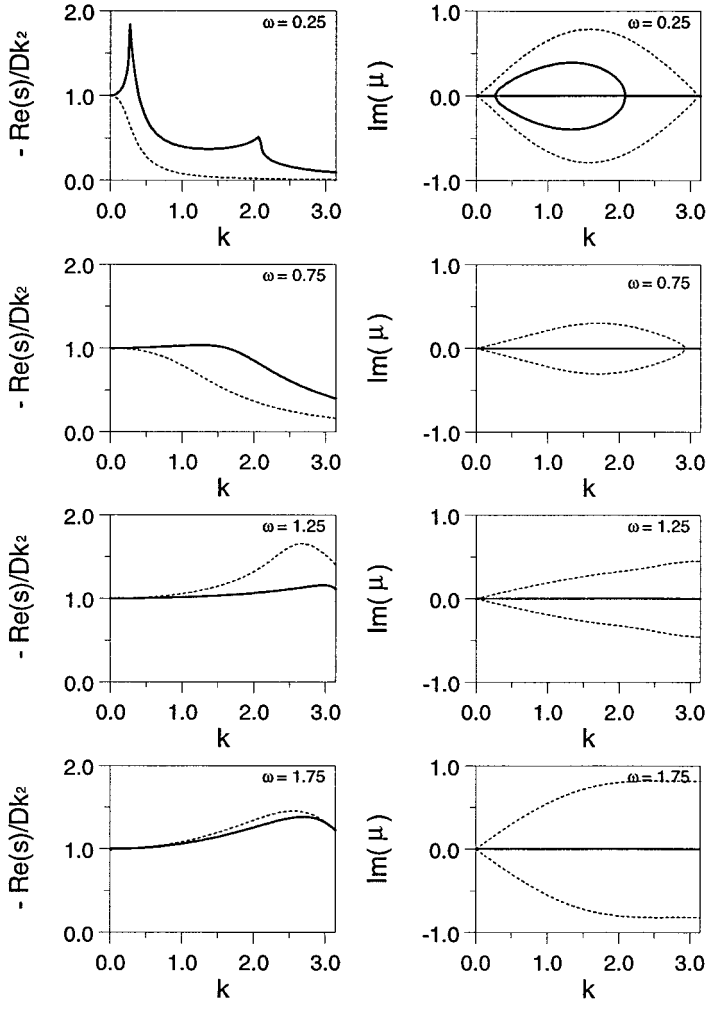

Fig. 3. The eigenmode spectra of the BGK scheme (dashed lines) and the DLB scheme (solid lines) for $\omega = 0.25$, 0.75, 1.25 and 1.75 applied on a cubic lattice with $\Delta x_i = 1$. The wavevector of the eigenmode is $\mathbf{k} = (k, 0, 0)$. In the left part of the figure the ratio of the real part of the relaxation coefficient of the diffusive mode $Re(s)$ and the theoretical dispersion relation $D = -Dk^2$ is shown. In the right part the imaginary part of the eigenvalue $Im(\mu)$ for all eigenmodes are shown.

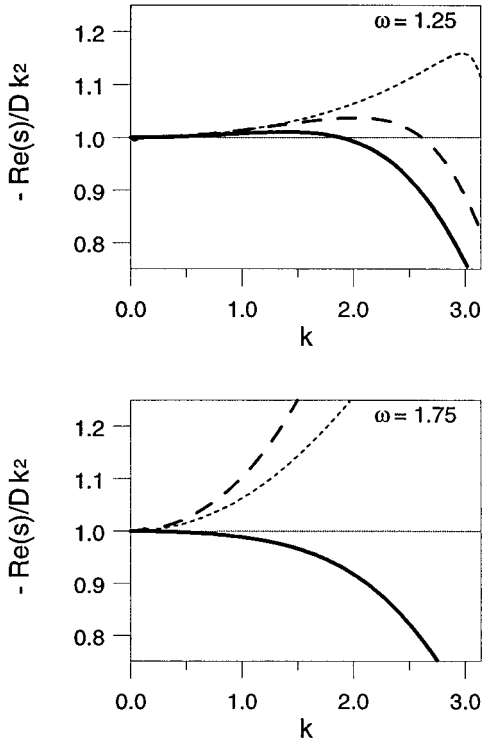

Fig. 4. The ratio of the real part of the relaxation rate of the diffusive mode $Re(s(k))$ with the theoretical value $-Dk^2$, as a function of the normalized wavenumber $k\Delta x$. The wave vectpr of the eigenmode is $\mathbf{k} = (k, 0, 0)$. Lattice spacings in are $\Delta x = 1/2$ (solid lines), 1 (dashed lines), 2 (points) and $\Delta y = \Delta z = 1$.

DISCUSSION

A diffusion Lattice Boltzmann (DLB) scheme is constructed from first principles, i.e., lattice symmetry requirements and the conservation laws. Isotropic diffusive behaviour is obtainable with orthorhombic lattices with six particle velocities. The collision operator of the DLB scheme has two eigenvalues, of which only one is related to the diffusion coefficient. The other eigenvalue can be chosen freely and is used for improving the performance of the DLB scheme.

The procedure of constructing of the DLB scheme from first principles can equally well be applied to other phenomena such as convection-diffusion and hydrodynamics. The Lattice-BGK schemes currently used for convection diffusion and hydrodynamics, can be made more general, as

indicated by the existence of a hydrodynamic LB scheme for 2-D rectangular lattices with nine velocities,[2] and by the two-parameter LB scheme for hydrodynamics.[10]

The eigenmode analysis is a valuable tool for analysing the properties of the DLB schemes concerning consistency, stability and accuracy. The properties of the diffusion DLB scheme are:

- The behaviour of the DLB scheme is consistent with diffusion for a wide range of ω and wave number k.
- The validity of the DLB scheme is poor for $0 < \omega < 1$.
- The validity of the DLB scheme for $\omega \approx 2$ is limited to low wave numbers. Sharp gradients as occur near boundary conditions will lead to spurious oscillations.
- The DLB scheme is unconditionally stable.
- The DLB scheme has at least second order accuracy.
- By setting free eigenvalues (κ) to zero, both the range of consistency with diffusion and the damping of spurious oscillations are improved.
- The diffusive behaviour of the DLB scheme is improved if the lattice spacing is densified along the direction of the gradient.

These properties the DLB scheme hold also for hydrodynamic LB schemes[10] and probably for LB schemes in general.

Recent studies have recognised that LB schemes are a special discretization of the classical Boltzmann equation.[15, 16] They show that other discretization schemes, as employed by the Finite Difference method, and non-regular lattice spacing may equally well be applied with LB schemes. The construction procedure and the method of analysis presented in this paper can be valuable tools for investigation of the properties of such new schemes. It may be worthwhile to perform this investigation first for diffusion, as this is the simplest phenomenon that can be modelled with LB schemes while the findings probably also hold for more complex phenomena as hydrodynamics.

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