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Some results on energy-conserving lattice Boltzmann models

Pierre Lallemand [1] and François Dubois [2,3]

[1] *Centre National de la Recherche Scientifique, Paris, France*

[2] *Conservatoire National des Arts et Métiers, Paris, France*

[3] *Department of Mathematics, University Paris Sud, Orsay, France.*

pierre.lallemand1@free.fr , francois.dubois@math.u-psud.fr .

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Abstract

We consider the problem of "energy conserving" lattice Boltzmann models. A major difficulty observed in previous studies is the coupling between the viscous and thermal waves even at moderate wave numbers. We propose a theoretical framework based on the knowledge of the partial equivalent equations of the lattice Boltzmann scheme at several orders of precision. With the help of linearized models (inviscid and dissipative advective acoustics and classical acoustics), we suggest natural sets of relations for the parameters of lattice Boltzmann schemes. The application is proposed for three two-dimensional schemes. Numerical test cases for simple linear and nonlinear waves establish that the main difficulty in the previous contributions can now be overcome.

Key words : Taylor expansion method, linearized Navier-Stokes, isotropy.

PACS numbers : 02.60Cb (numerical simulation, solution of equations), 43.28.-g (aeroacoustics), 47.10.+g (Navier-Stokes equations), 47.11.Mn (molecular dynamics calculations in fluid dynamics), 51.10+y (kinetic and transport theory of gases).

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1) Introduction

The derivation of lattice gas automata taking into account the conservation of mass, momentum and total energy has been initially proposed by McNamara and Alder [13]. In his contribution that fixed the paradigm of multiple relaxation times of lattice Boltzmann schemes, d'Humières [10] presented simulation of compressible fluids with the presence of strong discontinuities. Nevertheless, in order to fit the equilibrium distribution, it is necessary to consider lattice Boltzmann models with a large number of velocities (see *e.g.* Qian [14] and Alexander, Chen and Sterling [3]). In the study of one of us with L.S. Luo [12], it has been established that the D2Q9 scheme (see the Figure 10 and a detailed description in Annex 1) does not allow correctly a variation of sound velocity with the temperature. The contribution [12] enforces the use of higher order stencils as the D2Q13 scheme (see Figure 11 and Annex 2).

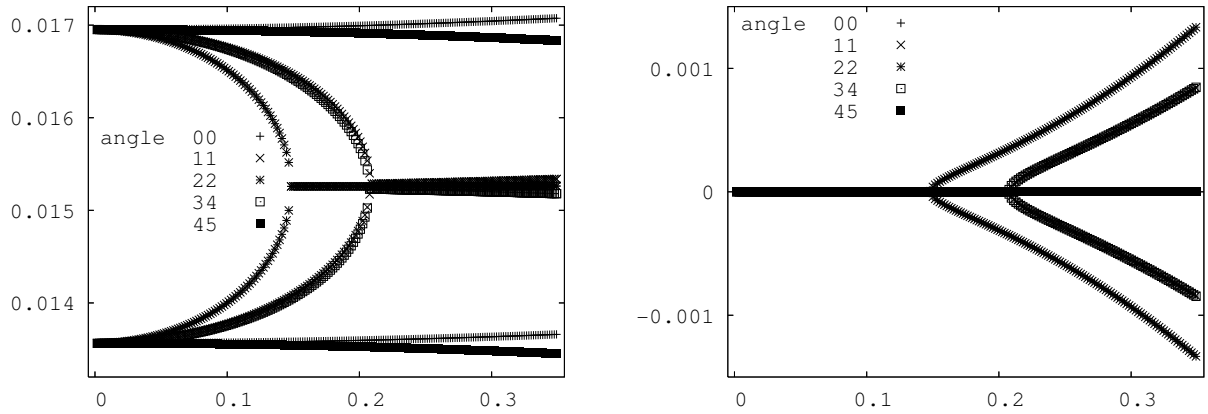

Figure 1. "Zero point" experiment with the D2Q13 lattice Boltzmann scheme. The wave vector is in abscissa and the eigenvalues of the lattice Boltzmann scheme in y-axis. The real part is on the left figure and the imaginary part on the right. Results for two different angles. For a critical wave number, the viscous and thermal modes merge together and the physics is badly approximated. Choice of coefficients defined in the relations (63) and (71) : $c_1 = -1.3$, $\alpha_2 = -25$, $\beta_2 = -1.5$, $\alpha_3 = 5.5$, $\beta_3 = 0$, $s_5 = 1.88$, $s_7 = 1.95$, $s_9 = 1.60$, $s_{11} = 1.75$, $s_{12} = 1.05$, $s_{13} = 1.35$.

• A major difficulty observed in [12] is the coupling between the viscous and thermal waves at moderate wave numbers. Consider a DdQq lattice Boltzmann scheme with discrete velocities ξ_j (see (55), (56), (67) and (74)) and unknowns f_j satisfying a periodicity condition parametrized by a wave number k:

$$f_j(x + \xi_j \, \Delta x, \, t) \, = \, \exp(i \, k \bullet \xi_j \, \Delta x) \, \Phi_j \, , \qquad 0 \leq j \leq q - 1 \, . \tag{1}$$

With a so-called "zero-point experiment", we consider one iteration in time of the d'Humières scheme [10] with an initial condition satisfying (1). Such an iteration is defined according to

$$f_j(x, \, t) \, = \, f_j^*(x - \xi_j \, \Delta x, \, t) \tag{2}$$

with f_j^* detailed in Annex 1 at the relation (66). Then the vector Φ is necessarily an eigenvector of the amplification matrix, as detailed in [11]. The corresponding eigenvalues define the discrete local modes of the linearized scheme. They must be of modulus less than one in order to have a possible stability. A typical numerical experiment as those first used in [12] is described in Figure 1. For a Prandtl number typically of the order one and a wave number greater than a moderate critical wave number, the viscous and thermal modes become coupled. Then the eigenvalues have a non-physical imaginary part, as presented in the picture on the right of Figure 1.

The physical effects of such bad approximation are presented *e.g.* in figure 2. The physical problem is the relaxation of a wave of wave number k. The initial condition is now of the type

$$f_j(x,\,t) \,=\, \exp(i\,k\bullet x)\,\psi_j\,, \qquad 0 \le j \le q-1\,, \tag{3}$$

with a given vector ψ that corresponds to a shear wave and a vertex x in a $N_x \times N_y$ two-dimensional mesh. Periodic boundary conditions are enforced. Physically, this wave relaxes towards a null equilibrium. For a supercritical wave number, the physics is not well approximated by the method: negative values can numerically occur ! A consequence of this major default is that very few compressible experiments are allowed with the lattice Boltzmann schemes.

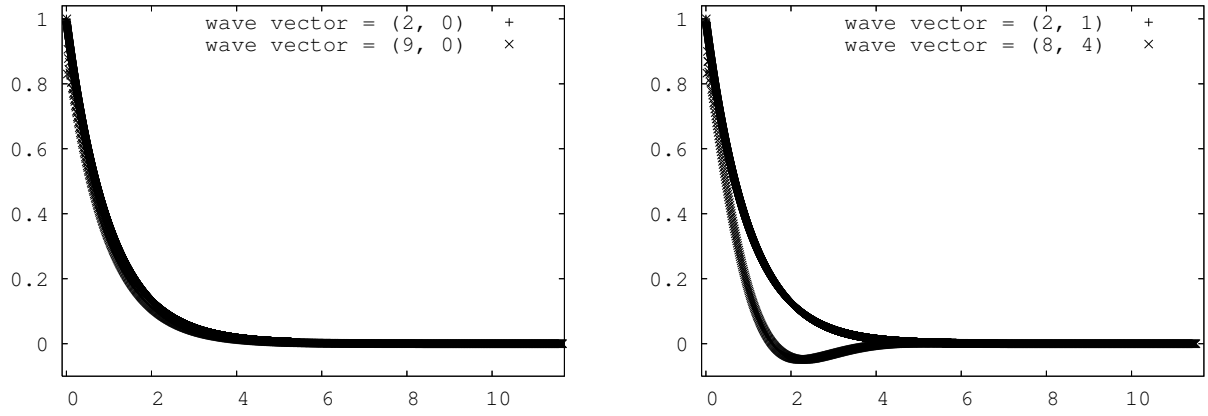

Figure 2. Relaxation of a thermal wave with the D2Q13 lattice Boltzmann scheme. The amplitude of the wave is plotted as a function of the normalized time. Left: wave vector **k** parallel to Ox axis (2 and 9 wavelengths). Right: wave vector **k** at an angle 26.56^0 from Ox. Two values of the wave number are presented, one smaller than the critical value (see Figure 1) and the other larger (respectively 1 and 2 wavelengths along Ox and Oy, and 4 and 8 wavelengths along Ox and Oy). The relaxation is physically correct in the first case but an unphysical undershoot appears in the second case. Domain $N_x \times N_y$ with $N_x = N_y = 61$. Numerical values of the parameters: $s_5 = 1.88, s_7 = 1.9303$, $s_9 = 1.60, s_{11} = 1.05, s_{12} = 1.35, s_{13} = 1.65$, $c_1 = -1.3, \alpha_2 = -25, \beta_2 = -1.5$, $\alpha_3 = 4.5, \beta_3 = 0$.

• In this contribution, we propose some solution to try and solve the previous difficulties. We use the Taylor expansion method proposed by one of us [4] and used in previous contributions for the development of "quartic" schemes [6, 7] because the analysis of the full dispersion equation is not practically tractable when the number q of velocities is greater than nine typically. With this method, we analyze the linearized waves of the numerical schemes for different problems and the lattice Boltzmann schemes D2Q9, D2Q13 and D2Q17 presented in Annexes 1, 2 and 3. In Section 2, we show that the inviscid advective acoustics necessarily fixes some moments of degree 2 and 3. Then in Section 3, we consider the second order analysis of the lattice Boltzmann scheme for dissipative advective acoustics. We enforce at first order Galilean invariance for shear and thermal waves. In Section 4, we analyze the waves of the scheme at fourth order accuracy for a possible acoustics simulation. We enforce isotropy of the waves and this condition fixes an important number of parameters of the method. We propose possible values for the three schemes. In the three following sections, we present preliminary numerical experiments for the lattice Boltzmann schemes D2Q9, D2Q13 and D2Q17. Some words of conclusion are proposed in Section 8.

2) Inviscid advective acoustics

We are interested by conservation laws of mass, momentum and energy. The conserved variables

$$W = \left(\rho \, , \; j_x \equiv \rho \, u \, , \; j_y \equiv \rho \, v \, , \; \varepsilon \right)^{\rm t} \tag{4}$$

are related to the particle densities f_j through the relations

$$\rho \equiv \sum_j f_j \, , \;\; j_x \equiv \sum_j v_j^x \, f_j \, , \;\; j_y \equiv \sum_j v_j^y \, f_j \, , \;\; \varepsilon \equiv \frac{1}{2} \sum_j \, | \, v_j \, |^2 \;\, f_j \, + \, {\rm orth.} \tag{5}$$

where "orth" are *ad hoc* terms for enforcing orthogonality, detailed for the various schemes in Annexes 1 to 3. The other second order moments are defined by

$$XX \equiv \sum_j \, \left[\, (v_j^x)^2 - (v_j^y)^2 \, \right] f_j \, , \qquad XY \equiv \sum_j \, v_j^x \; v_j^y \, f_j \, . \tag{6}$$

The first third order moments q_x and q_y are related to heat fluxes:

$$q_x \equiv \sum_j \, \frac{1}{2} \, | \, v_j \, |^2 \; v_j^x \, f_j \, , \quad q_y \equiv \sum_j \, \frac{1}{2} \, | \, v_j \, |^2 \; v_j^y \, f_j \, . \tag{7}$$

In this section these moments at equilibrium are supposed to be **linearized** functions of the conserved moments W defined in (4). We propose a method for determining the 16 corresponding coefficients when we wish to approximate advective acoustics.

• We start from the Euler equations of gas dynamics

$$\frac{\partial W}{\partial t} + \frac{\partial f(W)}{\partial x} + \frac{\partial g(W)}{\partial y} \, = \, 0 \tag{8}$$

with

$$\left\{ \begin{array}{l} f(W) \equiv \big(\, \rho\, u\,,\ \rho\, u^2 + p\,,\ \rho\, u\, v\,,\ u\, \varepsilon + p\, u \big)^{\mathrm{t}} \\ g(W) \equiv \big(\, \rho\, v\,,\ \rho\, u\, v\,,\ \rho\, v^2 + p\,,\ v\, \varepsilon + p\, v \big)^{\mathrm{t}}\,. \end{array} \right. \tag{9}$$

We linearize this system around a given state

$$W_0 \ = \ \big(\ \rho_0\,,\ \rho_0\, u_0\,,\ \rho_0\, v_0\,,\ \rho_0\, E_0\ \big)^{\mathrm{t}}. \tag{10}$$

We introduce the internal specific energy e according to

$$\varepsilon \ \equiv \ \rho\, e + \frac{\rho}{2}\big(u^2 + v^2\big) \tag{11}$$

and we suppose that the pressure is a function of the only internal volumic energy $\rho\, e$:

$$p = \text{function}\big(\rho\, e\big)\,. \tag{12}$$

We linearize the pressure p given at relation (12) around the given state W_0 and after some lines of elementary calculus, with the notation $\beta \equiv \mathrm{d}p/\mathrm{d}(\rho\, e)$ we have

$$\mathrm{d}p = \beta_0 \Big[\, \frac{1}{2}\big(u^2 + v^2\big)\, \mathrm{d}\rho \ - \ u\, \mathrm{d}j_x \ - \ v\, \mathrm{d}j_y + \mathrm{d}\varepsilon \,\Big]\,. \tag{13}$$

The three first linearized equations of system (8)(9) concerning mass and momentum conservation take the form

$$\left\{ \begin{array}{l} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \Big[\Big(\frac{1}{2}\beta_0(u_0^2 + v_0^2) - u_0^2\Big)\, \partial_x - u_0\, v_0\, \partial_y\Big]\rho \ + \ \Big[\partial_t + (2 - \beta_0)\, u_0\, \partial_x + v_0\, \partial_y\Big] j_x \\ \qquad\qquad + \Big[- \beta_0\, v_0\, \partial_x + u_0\, \partial_y\Big] j_y \ + \ \beta_0\, \partial_x \varepsilon \ = \ 0 \\ \Big[- u_0\, v_0\, \partial_x + \Big(\frac{1}{2}\beta_0(u_0^2 + v_0^2) - v_0^2\Big)\, \partial_y\Big]\rho \ + \ \Big[v_0\, \partial_x - \beta_0\, u_0\, \partial_y\Big] j_x \\ \qquad\qquad + \Big[\partial_t + u_0\, \partial_x + (2 - \beta_0)\, v_0\, \partial_y\Big] j_y \ + \ \beta_0\, \partial_y \varepsilon \ = \ 0\,. \end{array} \right. \tag{14}$$

We identify these equations with those obtained by a first order Taylor expansion (see *e.g.* [4]) of the lattice Boltzmann scheme. Then we obtain for the D2Q9, D2Q13 and D2Q17 schemes the following expressions for second order moments at equilibrium

$$XX^{\mathrm{eq}} = -\big(u_0^2 - v_0^2\big)\, \rho + 2\, u_0\, j_x - 2\, v_0\, j_y\,, \ \ XY^{\mathrm{eq}} = -u_0\, v_0\, \rho + v_0\, j_x + u_0\, j_x\,. \tag{15}$$

• The expressions (15) are linear functions of the conserved variables (4) around the reference state W_0 given at relation (10). If we consider the conserved variables (4) as "small variations" of the reference state (10), *id est*

$$\rho = \delta\rho_0\,, \ j_x = \delta(\rho_0\, u_0)\,, \ j_y = \delta(\rho_0\, v_0)\,, \ \epsilon = \delta(\rho_0\, E_0)\,, \tag{16}$$

and skipping the index "zero" for convenience, the expressions (15) can be considered as differential forms:

$$\left\{ \begin{array}{l} \delta XX^{\mathrm{eq}} = -\big(u^2 - v^2\big)\, \delta\rho + 2\, u\, \delta(\rho\, u) - 2\, v\, \delta(\rho\, v) \\ \delta XY^{\mathrm{eq}} = -u\, v\, \delta\rho + v\, \delta(\rho\, u) + u\, \delta(\rho\, v)\,. \end{array} \right. \tag{17}$$

A natural question when considering differential forms is to know whether they are or not the differential of some functions. In other terms, the question is to find functions $\xi(\rho,\, u,\, v)$ and $\eta(\rho,\, u,\, v)$ such that the expressions given in (17) admit also the form

$$\left\{ \begin{array}{l} \delta X X^{\rm eq} \equiv \left(u^2 - v^2 \right) \delta\rho + 2\,\rho\,u\,\delta u - 2\,\rho\,v\,\delta v \; = \; \delta\xi(\rho,\, u,\, v) \\ \delta X Y^{\rm eq} \equiv u\,v\,\delta\rho + \rho\,v\,\delta u + \rho\,u\,\delta v \; = \; \delta\eta(\rho,\, u,\, v)\,. \end{array} \right. \tag{18}$$

If the relations (18) are true, we have necessarily $u^2 - v^2 = \frac{\partial \xi}{\partial \rho}$ and there exists some function $\xi_1(u,\, v)$ such that $\xi(\rho,\, u,\, v) \equiv \rho\,(u^2 - v^2) + \xi_1(u,\, v)$. Then we have necessarily $2\,\rho\,u = \frac{\partial \xi}{\partial u} = 2\,\rho\,u + \frac{\partial \xi_1}{\partial u}$ and the function ξ_1 is only function of one single variable: $\xi_1 = \xi_1(v)$. We deduce from (18) the new relation $-2\,\rho\,v = \frac{\partial \xi}{\partial v} = -2\,\rho\,v + \frac{{\rm d}\xi_1}{{\rm d}v}$ and ξ_1 is reduced to some constant. We can proceed in a similar way for the function $\eta(\rho,\, u,\, v)$. First taking the differential of the second relation of (18) relatively to density, we have $u\,v = \frac{\partial \eta}{\partial \rho}$ and there exists some function $\eta_1(u,\, v)$ such that $\eta(\rho,\, u,\, v) \equiv \rho\,u\,v + \eta_1(u,\, v)$. Applying now a derivation relative to u: $\rho\,v = \frac{\partial \eta}{\partial u} = \rho\,v + \frac{\partial \eta_1}{\partial u}$ and $\eta_1 = \eta_1(v)$ only. After a derivation relative to v, we get $\rho\,u = \frac{\partial \eta}{\partial v} = \rho\,u + \frac{{\rm d}\eta_1}{{\rm d}v}$ and η_1 is constant. We have proven the relations

$$\delta X X^{\rm eq} \, = \, \delta\big(\rho\,(u^2 - v^2)\big)\,, \; \delta X Y^{\rm eq} \, = \, \delta\big(\rho\,u\,v\big)\,. \tag{19}$$

The expressions (19) can be integrated up to a constant for nonlinear dynamics (8)(9) and after a simple change of variables, we obtain nonlinear functions of the initial conserved variables (4):

$$X X^{\rm eq} = \frac{j_x^2 - j_y^2}{\rho}\,, \qquad X Y^{\rm eq} = \frac{j_x\,j_y}{\rho}\,. \tag{20}$$

• The conservation of energy is more delicate to fit exactly. It can be achieved if we assume that the equation of state (12) is precisely $p = \rho\,e$ which means that the fluid is a perfect gas with a ratio γ of specific heats equal to 2. In other words, the lattice Boltzmann schemes are well adapted for shallow water equations. For general fluids, we introduce the sound velocity c_0 and the Laplace operator $\Delta \equiv \partial_x^2 + \partial_y^2$. We know that the linearized equations

$$A_0 \bullet W \, = \, {\rm O}(\Delta t) \tag{21}$$

around a given state W_0 admit in this case of two space dimensions the following four eigenvalues

$$\partial_t + u_0\,\partial_x + v_0\,\partial_y \;\; \text{(double)}, \qquad \partial_t + u_0\,\partial_x + v_0\,\partial_y \pm c_0 \sqrt{\Delta} \;\; \text{(acoustics)} \tag{22}$$

with notations used in [7] that are exactly the one used when implementing the approach with a symbolic manipulation software. It is also possible to introduce a Fourier decomposition on harmonic waves of the type $\exp\big(i\,(\omega\,t - \mathbf{k}\bullet\mathbf{x})\big)$. Then we have the usual change of notation: $\partial_t \equiv i\,\omega$, $\nabla \equiv -i\,\mathbf{k}$, $\Delta \equiv -\,|\mathbf{k}|^2$, $\sqrt{\Delta} \equiv i\,|\mathbf{k}|$, *etc.*

• We impose these eigenvalues to the equivalent equations of the lattice Boltzmann schemes D2Q9, D2Q13 and D2Q17. In this way, we obtain 7 independent relationships

that constrain the equilibrium heat flux q given at relation (7) for these three schemes. Independently, we know from (9) that when we linearize the conservation of energy, the coefficients of $\partial_y j_x$ and $\partial_x j_y$ are both equal to zero. In the equivalent equations, we just impose that these two coefficients are equal. In this way, we obtain an eighth equation. We solve these equations and we find for the D2Q9 scheme the following expressions for the linearized heat fluxes q_x and q_y around a given state W_0 :

$$(23)\qquad \left\{ \begin{array}{l} q_x^{\rm eq} = 2\,u_0\,(4\lambda^2-3c_0^2)\,\rho \,+\, (6c_0^2+3v_0^2-3u_0^2-5\lambda^2)\,j_x \,-\, 6u_0v_0\,j_y \,+\, 2u_0\,E \\ q_y^{\rm eq} = 2\,v_0\,(4\lambda^2-3c_0^2)\,\rho \,-\, 6u_0v_0\,j_x \,+\, (6c_0^2+3u_0^2-3v_0^2-5\lambda^2)\,j_y \,+\, 2v_0\,E\,. \end{array} \right.$$

For the D2Q13 lattice Boltzmann scheme, we obtain with the same arguments

$$(24)\qquad \left\{ \begin{array}{l} q_x^{\rm eq} = \dfrac{2}{13}u_0\,(28\lambda^2-13c_0^2)\,\rho \,+\, (2c_0^2+v_0^2-u_0^2-3\lambda^2)\,j_x \,-\, 2u_0v_0\,j_y \,+\, \dfrac{2}{13}u_0\,E \\ q_y^{\rm eq} = \dfrac{2}{13}v_0\,(28\lambda^2-13c_0^2)\,\rho \,-\, 2u_0v_0\,j_x \,+\, (2c_0^2+u_0^2-v_0^2-3\lambda^2)\,j_y \,+\, \dfrac{2}{13}v_0\,E \end{array} \right.$$

and the D2Q17 scheme leads to

$$(25)\qquad \left\{ \begin{array}{l} q_x^{\rm eq} = \dfrac{6u_0}{17}\,(60\lambda^2-17c_0^2)\,\rho - (6c_0^2+3u_0^2-3v_0^2+17\lambda^2)\,j_x \,-\, 6u_0v_0\,j_y \,+\, \dfrac{6\,u_0\,E}{17} \\ q_y^{\rm eq} = \dfrac{6v_0}{17}\,(60\lambda^2-17c_0^2)\,\rho \,-\, 6u_0v_0\,j_x + (6c_0^2+3v_0^2-3u_0^2+17\lambda^2)\,j_y \,+\, \dfrac{6\,v_0\,E}{17}\,. \end{array} \right.$$

We take into account the relations between the physical total energy ε and the orthogonalized total energy E presented at relations (61), (70) and (77). Using an analysis identical to the one presented in details at the relations (17) to (20), and after some lines of elementary calculus, we observe that the relations (23), (24) and (25) are linearizations of the following general relations between the heat flux and the conserved variables. We have precisely

$$(26)\qquad \left\{ \begin{array}{ll} \text{D2Q9}: & \mathbf{q}^{\rm eq} = \Big(\,3\lambda^2 \,-\, 3\,|\,u\,|^2 \,+2\,\dfrac{E}{\rho}\Big)\,\mathbf{j} \\ \text{D2Q13}: & \mathbf{q}^{\rm eq} = \Big(\dfrac{17}{13}\lambda^2 - \,|\,u\,|^2 \,+\dfrac{2}{13}\dfrac{E}{\rho}\Big)\,\mathbf{j} \\ \text{D2Q17}: & \mathbf{q}^{\rm eq} = \Big(\dfrac{71}{17}\lambda^2 \,-\, 3\,|\,u\,|^2 \,+\dfrac{6}{17}\dfrac{E}{\rho}\Big)\,\mathbf{j}\,. \end{array} \right.$$

We observe at this level of analysis that there is no constraint on the higher order vectors $\mathbf{r}$ and τ whenever they exist (see the relations (69) and (76) of Annexes 2 and 3).

3) Dissipative advective acoustics

In the previous section, we have considered the first order eigenvalues given by the expressions (22). We denote by k_0 the kinetic energy of the reference state:

$$(27)\qquad k_0 \equiv \frac{u_0^2+v_0^2}{2}\,.$$

Let us set $\mathrm{u}_0\bullet\nabla \equiv u_0\,\partial_x + v_0\,\partial_y$ and introduce the matrix Λ_0 as the diagonal matrix composed by the eigenvalues:

$$\Lambda_0 \,=\, \mathrm{diag}\big(\partial_t + \mathrm{u}_0\bullet\nabla\,,\ \partial_t + \mathrm{u}_0\bullet\nabla\,,\ \partial_t + \mathrm{u}_0\bullet\nabla + c_0\,\sqrt{\Delta}\,,\ \partial_t + \mathrm{u}_0\bullet\nabla - c_0\,\sqrt{\Delta}\,\big)\,.$$

We observe that the corresponding matrix of eigenvectors, given according to

$$R_0 = \begin{pmatrix} 0 & 1 & \sqrt{\Delta} & \sqrt{\Delta} \\ \partial_y & u_0 & c_0\,\partial_x + u_0\,\sqrt{\Delta} & -c_0\,\partial_x + u_0\,\sqrt{\Delta} \\ -\partial_x & v_0 & c_0\,\partial_y + v_0\,\sqrt{\Delta} & -c_0\,\partial_y + v_0\,\sqrt{\Delta} \\ u_0\,\partial_y - v_0\,\partial_x & k_0 & (c_0^2+k_0)\,\sqrt{\Delta} + c_0\,\mathrm{u}_0 \bullet \nabla & (c_0^2+k_0)\,\sqrt{\Delta} - c_0\,\mathrm{u}_0 \bullet \nabla \end{pmatrix} \tag{28}$$

does **not** depend on the numerical scheme. We consider now the equivalent equations of the lattice Boltzmann scheme at second order accuracy. With the new variables

$$V = R_0 \bullet W \tag{29}$$

obtained by action of the matrix R_0, the equivalent partial differential equations at order 2 take the simple form

$$\big(\Lambda_0 + \Delta t\, P_0\big) \bullet V = \mathrm{O}(\Delta t^2)\,. \tag{30}$$

The partial differential equations (30) extend naturally the first order expression proposed in (21). The perturbation matrix P_0 has the generic form

$$P_0 = \begin{pmatrix} P_{00} & \begin{pmatrix} * & * \\ * & * \end{pmatrix} \\ \begin{pmatrix} * & * \\ * & * \end{pmatrix} & \begin{pmatrix} * & * \\ * & * \end{pmatrix} \end{pmatrix}. \tag{31}$$

The two by two matrix P_{00} is **not** diagonal. Then the method of perturbations (see *e.g.* [8, 9]) that we used in [7] is not straightforward to deal with. We have *a priori* to diagonalize the perturbation P_{00} which is a difficult task in all generality ! In this contribution, following an idea first proposed by Qian [14], we want to express that the corresponding two first eigenvalues

$$\lambda_1 = \partial_t + u_0\,\partial_x + v_0\,\partial_y + \Delta t\, p_1\,, \quad \lambda_2 = \partial_t + u_0\,\partial_x + v_0\,\partial_y + \Delta t\, p_2 \tag{32}$$

do not depend on the underlying velocity u_0, in a way first suggested by Qian and Zhou [15]. In this contribution, we simply enforce the property that the trace and the determinant of the matrix P_{00} do not depend on u_0, at least up to second order. In other terms, we have

$$\frac{\partial}{\partial u_0}\big(p_j\big) = \frac{\partial}{\partial v_0}\big(p_j\big) = 0\,, \qquad j = 1\,,\, 2\,. \tag{33}$$

We did not study the analogous property for acoustic waves, *id est* the condition (33) for $j = 3$ and 4. Such a study will be considered in future contributions. In the end of this section, we explicit the various constraints that are obtained for the three lattice Boltzmann schemes due to the conditions (33).

- **D2Q9**

We know first from (23) that there exists some relation between the sound velocity c_0 and the coefficient c_1 defined *e.g.* thanks to the relation (62). The previous relation is enforced and the sound velocity is completely imposed:

$$c_0 \,=\, \sqrt{\frac{2}{3}}\,\lambda\,. \tag{34}$$

Moreover, the fifth nonconserved moment is the square of energy E_2. It is a scalar field. The conditions (33) enforce this property and we have

$$E_2^{\rm eq} \,=\, \alpha_2\,\lambda^4\,\rho + \beta_2\,\lambda^2\,E\,. \tag{35}$$

Then the perturbations p_1 and p_2 define the viscosity and the diffusivity at constant volume. They are given by

$$p_1 = -\frac{\lambda^2}{3}\,\sigma_5\,\Delta\,,\quad p_2 = -\frac{\lambda^2}{12}\,\big(4\,+4\,\beta_2-\alpha_2\big)\,\sigma_7\,\Delta\,. \tag{36}$$

- **D2Q13**

There is *a priori* no constraint for the sound velocity. The square of the energy at equilibrium is again given by a relation of the type (35). The vectorial moment $\mathbf{r}$ (with labels 8 and 9 in the family (68)) is proportional to the momentum $\mathbf{j}$:

$$\mathbf{r}^{\rm eq} \,=\, \frac{\lambda^2}{12}\,\big(\,62\,\lambda^2 - 63\,c_0^2\,\big)\;\mathbf{j} \;\equiv\; c_2\,\mathbf{j}\,. \tag{37}$$

There is no condition for the cube E_3 of the energy. The 13th moment named "XX_e" is essential for visco-elastic simulations when the moment XX is quasi-conserved. It admits an equilibrium of the type

$$XX_e^{\rm eq} \,=\, \xi_x(u_0,\,v_0)\,\Big(\,\lambda^4\,\rho + \frac{\lambda^2}{28}\,E\,\Big)\,. \tag{38}$$

Remark that we are not completely satisfied by the relation (38). The left and right hand sides are not of the same tensorial type. If we exchange x and y, the signs of XX_e is changed but it is not the case for scalar moments ρ and E. Nevertheless, this kind of lack of tensorial coherence exists at any order if we consider sufficiently high order moments, as observed with very different methods by Augier *et al.* [1, 2]. Then the viscosity and the diffusivity at constant volume p_1 and p_2 take the form

$$p_1 = -\frac{1}{2}\,c_0^2\,\sigma_5\,\Delta\,,\quad p_2 = -\frac{1}{154}\,\frac{\lambda^4}{c_0^2}\,\big(28\,\beta_2 + 140\,-\alpha_2\big)\,\sigma_7\,\Delta\,. \tag{39}$$

- **D2Q17**

As for the D2Q13 scheme, there is no constraint for the sound velocity. The square of the energy at equilibrium is still obtained by the condition (35). There is no condition for the "powers" three E_3 and four E_4 of the energy. Note that "XX_e" and "XY_e" (labels 12 and 13 in (75)) satisfy conditions close to (38):

$$XX_e^{\rm eq} \,=\, \xi_x(u_0,\,v_0)\,\Big(\,\lambda^4\,\rho + \frac{\lambda^2}{60}\,E\,\Big)\,,\quad XY_e^{\rm eq} \,=\, \xi_y(u_0,\,v_0)\,\Big(\,\lambda^4\,\rho + \frac{\lambda^2}{60}\,E\,\Big)\,. \tag{40}$$

There is no condition on the equilibrium of vector $\mathbf{r}$. But if we introduce the notations

$$\left\{ \begin{array}{l} r_x^{\rm eq} \, = \, \lambda^3 \left(c_x^\rho \, \lambda^2 \, \rho + c_x^x \, \lambda \, j_x + c_x^y \, \lambda \, j_y + c_x^\varepsilon \, E \right) \\ r_y^{\rm eq} \, = \, \lambda^3 \left(c_y^\rho \, \lambda^2 \, \rho + c_y^x \, \lambda \, j_x + c_y^y \, \lambda \, j_y + c_y^\varepsilon \, E \right) , \end{array} \right. \tag{41}$$

where the $c's$ coefficients of relations (41) are *a priori* functions of the advection field $\mathbf{u_0}$, we have the following expressions for the vector $\tau = (\tau_x \, , \, \tau_y) \equiv (X \, E_3 \, + {\rm orth.} \, , \, Y \, E_3 \, + {\rm orth.})$ with labels 10 and 11 at relations (75):

$$\left\{ \begin{array}{l} \tau_x^{\rm eq} \, = \, - \dfrac{31}{2} \, \lambda^5 \left[c_x^\rho \, \lambda^2 \, \rho + \dfrac{\lambda}{124} \Big(124 \, c_x^x + 249 \, \dfrac{c_0^2}{\lambda^2} - 442 \Big) \, j_x + c_x^y \, \lambda \, j_y + c_x^\varepsilon \, E \right] \\ \tau_y^{\rm eq} \, = \, - \dfrac{31}{2} \, \lambda^5 \left[c_y^\rho \, \lambda^2 \, \rho + c_y^x \, \lambda \, j_x + \dfrac{\lambda}{124} \Big(124 \, c_y^y + 249 \, \dfrac{c_0^2}{\lambda^2} - 442 \Big) \, j_y + c_y^\varepsilon \, E \right] . \end{array} \right. \tag{42}$$

Finally the perturbations p_1 and p_2 are given by

$$p_1 = - \frac{1}{2} \, c_0^2 \, \sigma_5 \, \Delta \, , \quad p_2 = - \frac{1}{218} \, \frac{\lambda^4}{c_0^2} \left(60 \, \beta_2 + 620 \, - \alpha_2 \right) \sigma_7 \, \Delta \, . \tag{43}$$

A variant of the relations (39) !

4) Fourth order isotropic acoustics

We suppose in this section that the reference advective state W_0 has a zero velocity : $u_0 = v_0 = 0$. We evaluate the eigenvalues λ_j (for $j = 1$ to 4) at fourth order accuracy by using the general method presented in details in [7]. Then the eigenvalues admit a general expansion of the type

$$\left\{ \begin{array}{l} \lambda_1 \, = \, \partial_t + \Delta t \, p_1 + \Delta t^2 \, \widetilde{p_1} + \Delta t^3 \, \overline{p_1} + {\rm O}(\Delta t^4) \\ \lambda_2 \, = \, \partial_t + \Delta t \, p_2 + \Delta t^2 \, \widetilde{p_2} + \Delta t^3 \, \overline{p_2} + {\rm O}(\Delta t^4) \\ \lambda_3 \, = \, \partial_t + c_0 \, \sqrt{\Delta} + \Delta t \, p_3 + \Delta t^2 \, \widetilde{p_3} + \Delta t^3 \, \overline{p_3} + {\rm O}(\Delta t^4) \\ \lambda_4 \, = \, \partial_t - c_0 \, \sqrt{\Delta} + \Delta t \, p_3 - \Delta t^2 \, \widetilde{p_3} + \Delta t^3 \, \overline{p_3} + {\rm O}(\Delta t^4) \end{array} \right. \tag{44}$$

and we refer to (22) and (32) for advective acoustics at first and second order accuracy. In the following, we enforce isotropy by saying that the eigenvalues λ_j proposed in (44) are isotropic. In other words, the operators p_j , $\widetilde{p_j}$ and $\overline{p_j}$ that appear in (44) are only functions of the Laplacian. This induces a family of equations for the parameters.

- **D2Q9** at third order accuracy.

For the D2Q9 lattice Boltzmann scheme, we have a total of 5 equations (respectively one equation) to achieve isotropy at the fourth (respectively third) order. We have no solution at the fourth order. Third order isotropy can be enforced, *i.e.* the dispersion of ultrasonic waves is isotropic in this case, by adding to the relations (34) and (35) the constraint

$$\sigma_7 = \frac{1}{12 \, \sigma_5} \, . \tag{45}$$

- **D2Q13**

For this scheme, a total of 6 equations is necessary to obtain fourth order isotropy. They can be solved by adding to the previous conditions (37) and (38) the constraint (45) and the following specific relations

$$c_0 \;=\; \frac{2}{\sqrt{5}}\,\lambda\,, \tag{46}$$

and

$$E_3^{\rm eq} \;=\; \alpha_3\,\lambda^6\,\rho + \beta_3\,\lambda^4\,E\,. \tag{47}$$

The coefficients α_3 and β_3 of the relation (47) are associated to the coefficients α_2 and β_2 introduced at relation (35) according to

$$\left\{\begin{array}{l} \alpha_3 = \dfrac{1}{1716}\;\dfrac{N_\alpha}{384\,\sigma_5^2+7}\;, \qquad \beta_3 = \dfrac{1}{216216}\;\dfrac{N_\beta}{384\,\sigma_5^2+7}\;, \\ N_\alpha = 41922 - 2505\,\alpha_2 + 54800\,\beta_2 + \big(14098944 + 97440\,\alpha_2 + 1315200\,\beta_2\big)\,\sigma_5^2 \\ N_\beta = -2756851 + 34250\,\alpha_2 - 889970\,\beta_2 \\ \qquad\qquad -\big(204329472 - 822000\,\alpha_2 + 41211840\,\beta_2\big)\,\sigma_5^2\,. \end{array}\right. \tag{48}$$

The coefficient ξ_x in the relation (38) is null and we have also the following relations between the dissipation coefficients defined in (65) from the $s's$:

$$\sigma_9 = \sigma_7\,, \qquad \sigma_{13} = \sigma_5 \tag{49}$$

- **D2Q17**

In this case, fourth order isotropy induces a total of 9 equations. They can be solved analytically (with the help of a formal software for the algebra) first by considering the relations (35) and (40). Secondly, the sound velocity c_0 has not to be imposed. We have to enforce (49) and we add the condition

$$\sigma_{15} = \sigma_7\,. \tag{50}$$

Relation (47) is supplemented by an analogous one for the fourth power of the energy:

$$E_4^{\rm eq} \;=\; \alpha_4\,\lambda^8\,\rho + \beta_4\,\lambda^6\,E\,. \tag{51}$$

The coefficients α's and β's satisfy now

$$\left\{\begin{array}{l} \alpha_3 = -\dfrac{5}{436}\,(2696442 + 7519\,\alpha_2)\,, \quad \beta_3 = -\dfrac{1}{2616}\,(2949247 + 225570\,\beta_2)\,, \\ \alpha_4 = -\dfrac{1}{177888}\,(69687842 + 139145\,\alpha_2)\,,\; \beta_4 = -\dfrac{5}{355776}\,(940101 + 55658\,\beta_2)\,. \end{array}\right. \tag{52}$$

Moreover, the vectors $\mathbf{q}$, $\mathbf{r}$ and τ considered previously satisfy at equilibrium the relations

$$\left\{\begin{array}{c} \mathbf{q}^{\rm eq} \;=\; c_1\,\mathbf{j}\,, \qquad \mathbf{r}^{\rm eq} \;=\; c_2\,\mathbf{j}\,, \qquad \tau^{\rm eq} \;=\; c_3\,\mathbf{j} \\ c_1 = 6\,c_0^2 - 17\,\lambda^2\,, \quad c_2 = \dfrac{\lambda^2}{6}\,(31\,\lambda^2 - 21\,c_0^2)\,, \quad c_3 = \dfrac{\lambda^4}{24}\,(555\,c_0^2 - 596\,\lambda^2)\,. \end{array}\right. \tag{53}$$

We have also the simple equilibria

$$XX_e^{\rm eq} \;=\; 0\,, \qquad XY_e^{\rm eq} \;=\; 0\,. \tag{54}$$

5) Numerical experiments with the D2Q9 scheme

We first consider a "zero point" analysis as described in the introduction. We observe in Figure 3 (left) that the unphysical coupling of waves is present with an arbitrary value of the parameter σ_7 which is proportional to the diffusivity κ at constant volume as indicated at the relation (36). When fourth order isotropy is enforced according to the relation (45), this coupling disappears, as observed in Figure 3 (right).

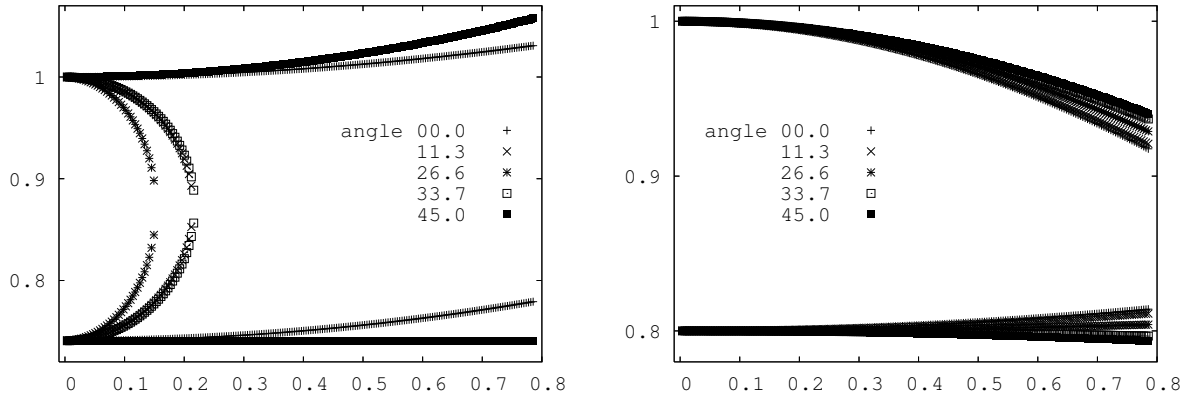

Figure 3. D2Q9 "zero point". Value of the eigenmode divided by k^2 and normalized by the diffusivity κ *vs* the wave number. Left figure : shear and thermal waves with σ_7 chosen arbitrarily. We see clearly a strong coupling between the viscous and diffusive waves for an angle $\theta = 26.565$ degrees. Right figure : the relation (45) is satisfied. The coupling has disappeared but there is still an angular dependency that characterizes this third order isotropy.

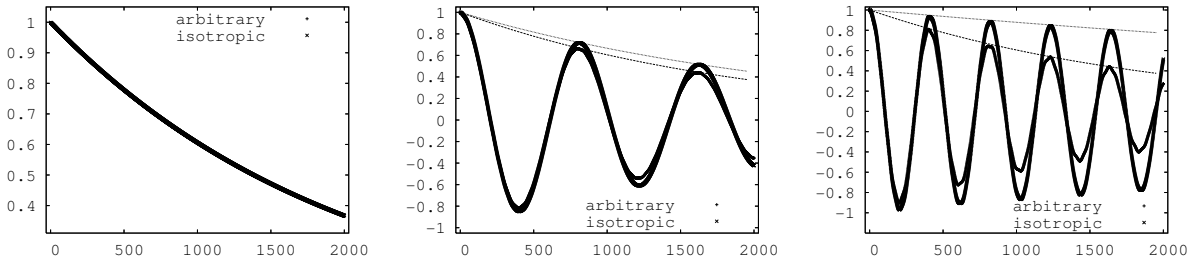

Figure 4. Relaxation of a nonlinear diffusion wave with D2Q9 "energy conserving" lattice Boltzmann scheme. The parameters of the scheme are the following: $s_5 = 1.8181$, $s_9 = 1.1765$, $\alpha_2 = -1$, $\beta_2 = 0.1$ (see the relation (35)), $s_7 = 0.4615$ when the condition (45) is not satisfied, $\alpha_2 = -0.15$, $\beta_2 = -1$ (see the relation (35)), $s_7 = 1.8305$ when the condition (45) is satisfied. Left: $v_{advec} = 0$, Middle: $v_{advec} = 0.05$, Right: $v_{advec} = 0.10$. The light exponential lines correspond to the velocity corrected damping (following complicated expressions not given here).

• In order to confirm this good performance of the D2Q9 lattice Boltzmann scheme with conservation of energy, we have simulated the relaxation of a thermic wave on a 81×81 lattice. We have incorporated the nonlinear terms given by relations (20) for the moments

XX and XY at equilibrium. For the "heat flux" $\mathbf{q}$ at equilibrium, we have considered the expressions (26), but the quadratic term relative to velocity has been neglected. The results are presented in Figure 4. For a small wave vector k and an advection velocity V parallel to the wave vector, the waves are correctly advected, whatever the direction of the wave vector. In other terms, we have isotropy of the Galilean factor.

6) Numerical experiments with the D2Q13 scheme

With the methodology presented in sections 2 to 4, it is possible to remove the spurious coupling of shear and thermal modes depicted in the introduction. Precisely, if the parameters of the scheme satisfy the relations (37), (45), (46), (47), (49), (73), there exists a situation where the scheme is linearly stable for fluid and thermal applications and also for pure acoustics. Moreover we obtain a correct Prandtl number and appropriate attenuations :

$$Pr = 0.728\,, \quad \nu = 0.006\,\lambda\,\Delta x\,, \quad \kappa = 0.008236\,\lambda\,\Delta x\,, \quad \gamma = 0.003487\,\lambda\,\Delta x$$

The results are proposed in Figure 5.

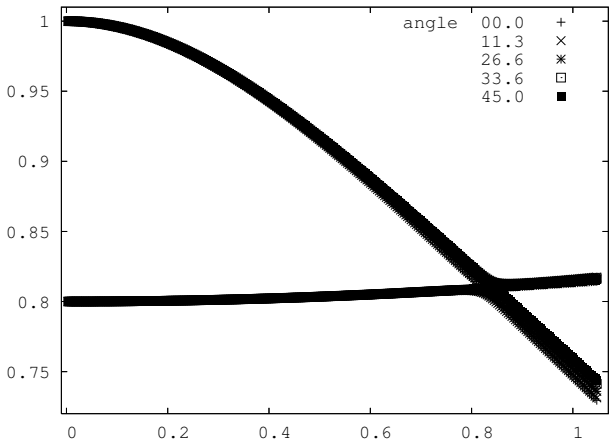

Figure 5. "Zero point" experiment with the D2Q13 lattice Boltzmann scheme. Viscous and diffusive modes for a moderate wave number k and several angles. There is clearly isotropy and the two waves are decoupled. The diffusive wave at $k = 0$ is on the order of 1.025. Note that the small oscillations at this point reflect the numerical difficulties due to the approximation of the eigenvalue 1 at fourth order accuracy. The viscous wave at $k = 0$ is on the order of 0.72. At $k \simeq 0.78$ the two modes cross perfectly without merging. Note that this perfectly isotropic test case is also very dispersive.

- The relaxation of a diffusive wave is presented Figure 6.

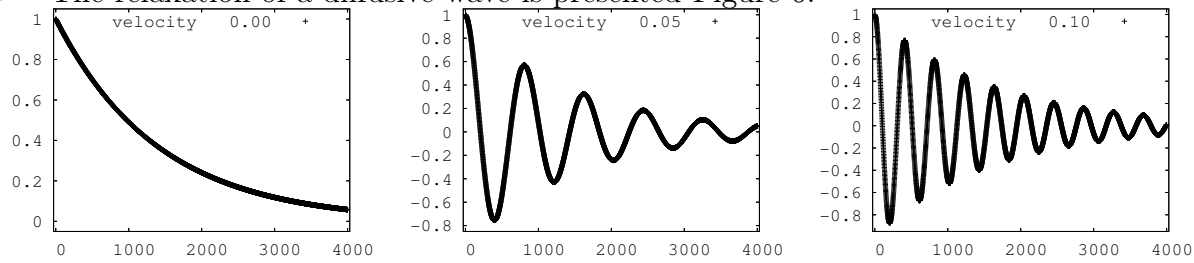

Figure 6. Relaxation of a nonlinear diffusive wave as function of time with the D2Q13 "energy conserving" lattice Boltzmann scheme in a 91×91 domain (2 wave lengths along Ox and 1 wave length along Oy). Parameters are set to have a Prandtl number of .80. Mean velocity parallel to the wavevector of amplitude 0.0, 0.05 and 0.10.

- As an illustration of the potential of this "conserving energy lattice Boltzmann scheme", we present in Figure 7 the propagation of a sound wave in a disc.

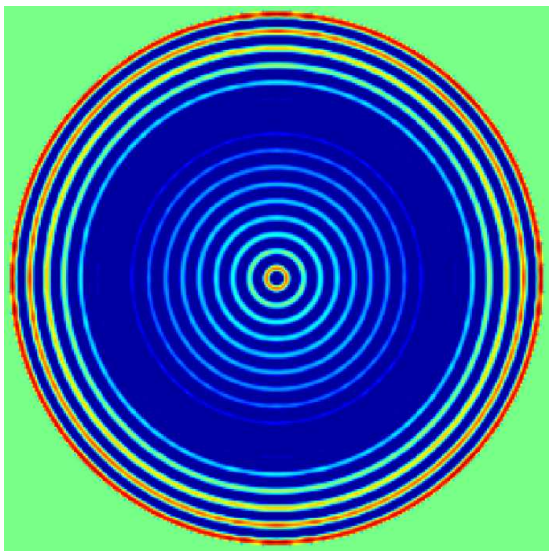

Figure 7. Sound wave propagation in a circle with an "anti bounce - back" numerical boundary condition with the D2Q13 lattice Boltzmann scheme conserving the energy.

7) Numerical experiments with the D2Q17 scheme

With the methodology presented in Sections 2 to 4, the D2Q17 scheme depicted in Figure 10 and in Annex 3 admits parameters satisfying the numerical constraints made explicit in relations (15), (20), (26), (40), (41), (42), (50), (51), (52), (53), (54) and (78).

- Some results are shown for the "zero-point" analysis. In a first case, we have taken the parameters in a simple way. The results are presented in Figure 8. The shear and

eigenmodes are decoupled and show very little angular dependence The decoupling of viscous and thermal modes is correct.

$$Pr = 0.74182\,,\ c_0 = \sqrt{\frac{7}{6}}\,,\ \frac{\nu}{\lambda\,\Delta x} = 0.029167\,,\ \frac{\kappa}{\lambda\,\Delta x} = 0.039318\,,\ \frac{\gamma}{\lambda\,\Delta x} = 0.055959\,.$$

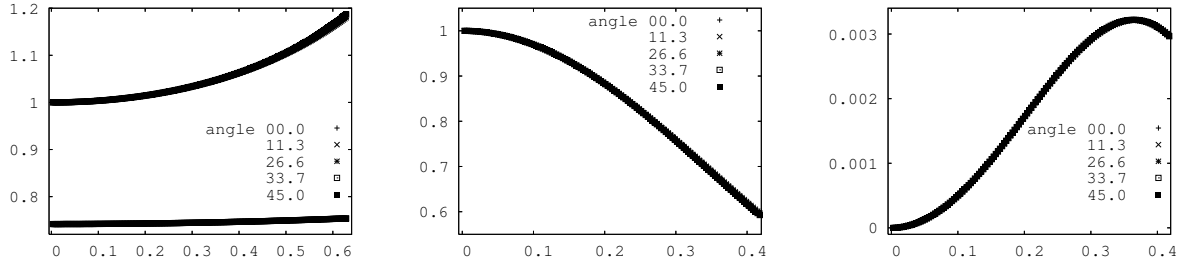

Figure 8. "Zero point" experiment for the D2Q17 scheme. Left : effective viscosity and diffusivity κ *vs* the wave vector k for several directions. Middle : attenuation of the sound waves. Right : $(v_{son}/c_0) - 1$ *vs* k. Choice of parameters: $\alpha_2 = -619$, $\beta_2 = -20.55$, $s_5 = 1.81812$, $s_{11} = 1.9230$, $s_{12} = 1.818$, $s_{17} = 1.111$.

• In a second case, we show that one can reduce significantly the physical dissipations by a better tuning of the parameters. The associated physical parameters are given by

$$Pr = 0.69817\,,\ c_0 = \sqrt{\frac{7}{6}}\,,\ \frac{\nu}{\lambda\,\Delta x} = 0.001167\,,\ \frac{\kappa}{\lambda\,\Delta x} = 0.001671\,,\ \frac{\gamma}{\lambda\,\Delta x} = 0.000651\,.$$

The dissipation is reduced by one order of magnitude if we refer to the previous example. The results are presented in Figure 9. We observe that the isotropy of the waves is not rigorously satisfied. A systematic search in the space of free parameters of the model would certainly lead to better behavior, especially in order to increase the numerical stability of the model which, as presented here, is not very good. We refer for this approach to Xu and Sagaut [16].

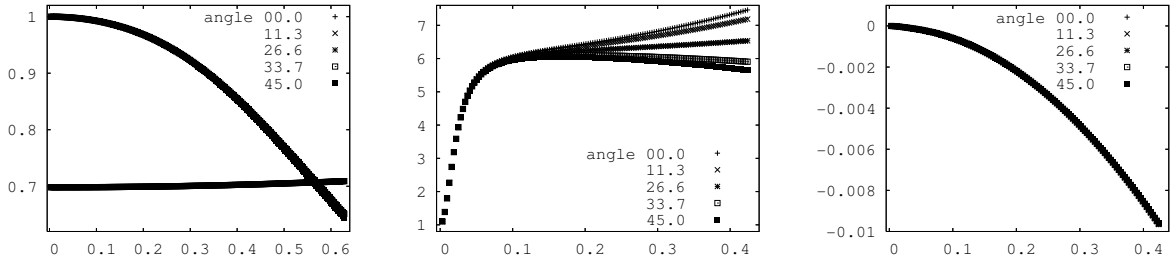

Figure 9. "Zero point" experiment for the D2Q17 scheme. Left : effective viscosity and diffusivity κ *vs* the wave vector k for several directions. Middle : attenuation of the sound waves. Right : $(v_{son}/c_0) - 1$ *vs* k. Choice of parameters: $\alpha_2 = -641.17$ $\beta_2 = -21.01933$, $s_5 = 1.9920$, $s_{11} = 1.9230$, $s_{12} = 1.818$, $s_{17} = 1.25$.

8) Conclusion

We have considered the problem of "energy conserving" lattice Boltzmann models. Not completely satisfying results were proposed in the literature with the classic version of D2Q13 LB scheme [12] even for very elementary situations as a shear wave and diffusive wave. We have added two new ideas : add nonlinear terms and remove the "spurious coupling" with a fourth order analysis of the equivalent partial equivalent equation. More precisely, our theoretical analysis is founded of the knowledge of the partial equivalent equations of the lattice Boltzmann scheme at several orders of precision. At the first order the linear nondissipative advective acoustics suggest which nonlinear terms should be included in the equilibrium values of the second order moments and the third order heat flux. At the second order the linear dissipative advective acoustics establish general relations for the viscosity and diffusivity from the necessary isotropic behavior of the LBE model leads to constraint on the linear dependence of higher order moments. It is possible to enforce Galilean invariance at first order accuracy for shear, thermal and acoustic waves. The analysis of classical acoustics allows the computation of parameters that are compatible with isotropic waves. Satisfactory results are shown for the shear wave for three versions of the lattice Boltzmann model considered here. This breakthrough has to be confirmed for other test cases, lattice Boltzmann models and higher dimensions !

Acknowledgments

The authors thank Nikolaos Prasianakis for his suggestion to incorporate the D2Q9 lattice Boltzmann scheme in the framework of this contribution.

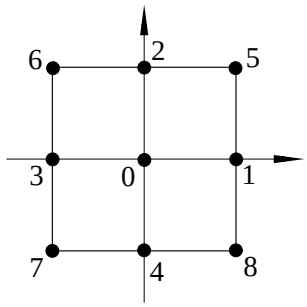

Figure 10. Stencil of 9 velocities for the D2Q9 lattice Boltzmann scheme.

Annex - 1. D2Q9 lattice Boltzmann scheme

The velocity set v_j for $0 \leq j \leq q-1$ of a DdQq lattice Boltzmann scheme is given by the general relation

$$v_j = \xi_j \, \lambda \, , \tag{55}$$

where λ is some scale velocity. For the D2Q9 scheme [11] illustrated in Figure 10, the ξ_j's of relation (55) are given by the expressions

$$\left\{ \begin{array}{l} \xi_0 = (0,\, 0) \, , \ \xi_1 = (1,\, 0) \, , \ \xi_2 = (0,\, 1) \, , \ \xi_3 = (-1,\, 0) \, , \ \xi_4 = (0,\, -1) \, , \\ \xi_5 = (1,\, 1) \, , \ \xi_6 = (-1,\, 1) \, , \ \xi_7 = (-1,\, -1) \, , \ \xi_8 = (1,\, -1) \, . \end{array} \right. \tag{56}$$

The d'Humières moments [10] are defined with the help of a family p_k $(0 \leq k \leq q-1)$ of two variables polynomials. They are ordered by increasing degree. For the D2Q9 scheme, $p_j \in \mathcal{P}_{\mathrm{D2Q9}}$ with

$$(57) \qquad \left\{ \begin{array}{l} p_0 = 1\,, \quad p_1 = X\,, \quad p_2 = Y\,, \quad p_3 = -4\,\lambda^2 \,+\, 3\,(X^2+Y^2) \\ p_4 = X^2 - Y^2\,, \quad p_5 = X\,Y \\ p_6 = X\,\big(-5\,\lambda^2 + 3\,(X^2+Y^2)\big)\,,\; p_7 = Y\,\big(-5\,\lambda^2 + 3\,(X^2+Y^2)\big) \\ p_8 = 4\,\lambda^4 \,-\, \dfrac{21}{2}\,\lambda^2\,(X^2+Y^2) \,+\, \dfrac{9}{2}\,(X^2+Y^2)^2\,. \end{array} \right. .$$

The coefficients of the matrix M are simply given by nodal values in the velocity space:

$$(58) \qquad M_{kj} = p_k(v_j)\,, \qquad 0 \leq\, j\,,\; k\, \leq q-1\,.$$

The moments m_k for $0 \leq k \leq q-1$ are defined with the help of this matrix:

$$(59) \qquad m_k \,=\, \sum_j M_{kj}\, f_j\,, \qquad 0 \leq\, k\, \leq q-1\,.$$

The moments defined by the relations (57) and (58) are, due to (63), the eigenvectors of the relaxation operator of the Boltzmann equation with a finite number of velocities, as noticed in [5]. In particular in this contribution,

$$(60) \qquad \left\{ \begin{array}{l} \rho \equiv \displaystyle\sum_j f_j\,,\;\; j_x \equiv \sum_j v_j^x\, f_j\,,\;\; j_y \equiv \sum_j v_j^y\, f_j\,,\;\; E \equiv \sum_j p_3(v_j)\, f_j\,, \\ XX \equiv \displaystyle\sum_j p_4(v_j)\, f_j\,,\;\; XY \equiv \sum_j p_5(v_j)\, f_j\,, \\ q_x \equiv \displaystyle\sum_j p_6(v_j)\, f_j\,,\;\; q_y \equiv \sum_j p_7(v_j)\, f_j\,. \end{array} \right.$$

We observe that due to the orthogonalization procedure, the "numerical" total energy E proposed at relations (60) and effectively used in the simulations is related to the "physical" total energy ε introduced in (4) as the fourth conserved variable thanks to the relation

$$(61) \qquad E = 6\,\varepsilon - 4\,\lambda^2\,\rho\,.$$

In a first approach, we choose the equilibria for the nonconserved moments as follows :

$$(62) \qquad XX^{\mathrm{eq}} \,=\, 0\,, \quad XY^{\mathrm{eq}} \,=\, 0\,, \quad \mathbf{q}^{\mathrm{eq}} \,= c_1\,\lambda^2\,\mathbf{j}\,, \quad E_2^{\mathrm{eq}} \,=\, \alpha_2\,\lambda^4\,\rho + \beta_2\,\lambda^2\,E\,.$$

The coefficients s_k that determine the relaxation of the d'Humières moments

$$(63) \qquad m_k^* \,=\, m_k \,+\, s_k\,\big(m_k^{\mathrm{eq}} - m_k\big)$$

are defined according to

$$(64) \qquad s_{XX} \equiv s_5\,, \quad s_{XY} \equiv s_5\,, \quad s_{qx} \equiv s_7\,, \quad s_{qy} \equiv s_7\,, \quad s_{E2} \equiv s_9\,.$$

We set also

$$(65) \qquad \sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}\,.$$

Recall that the distribution f_j^* of particles after relaxation is defined from the moments m and the inversible matrix M according to

$$(66) \qquad f_j^* \,=\, \sum_k \big(M^{-1}\big)_{jk}\, m_k^*\,.$$

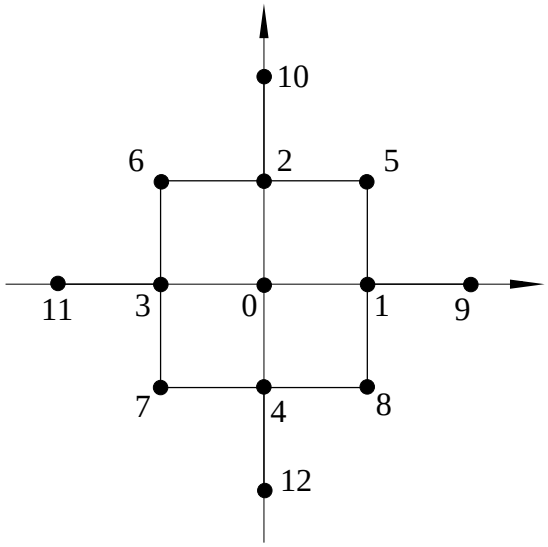

Figure 11. Stencil of 13 velocities for the D2Q13 lattice Boltzmann scheme.

Annex - 2. D2Q13 lattice Boltzmann scheme

For the D2Q13 scheme [14, 17] illustrated in Figure 11, the first nine ξ_j's of relation (55) are the one given at the relation (56). The last four are

$$\xi_9 = (2,\,0)\,,\ \xi_{10} = (0,\,2)\,,\ \xi_{11} = (-2,\,0)\,,\ \xi_{12} = (0,\,-2)\,, \tag{67}$$

The family $\mathcal{P}_{\rm D2Q13}$ of two-variable polynomials that define the moments according to relation (58) are detailed as follows:

$$\left\{ \begin{array}{l} p_0 = 1\,, \quad p_1 = X\,, \quad p_2 = Y\,, \quad p_3 = -28 \,+\, 13\,(X^2+Y^2) \\ p_4 = X^2 - Y^2\,, \quad p_5 = X\,Y \\ p_6 = X\,(-3\,\lambda^2 + X^2 + Y^2)\,,\ p_7 = Y\,(-3\,\lambda^2 + X^2 + Y^2) \\ p_8 = X\,\Big(\dfrac{101}{6}\lambda^4 - \dfrac{63}{4}\lambda^2\,(X^2+Y^2) + \dfrac{35}{12}\,(X^2+Y^2)^2\Big) \\ p_9 = Y\,\Big(\dfrac{101}{6}\lambda^4 - \dfrac{63}{4}\lambda^2\,(X^2+Y^2) + \dfrac{35}{12}\,(X^2+Y^2)^2\Big) \\ p_{10} = 140\,\lambda^4 - \dfrac{361}{2}\lambda^2\,(X^2+Y^2) + \dfrac{77}{2}\,(X^2+Y^2)^2 \\ p_{11} = -12\,\lambda^6 + \dfrac{581}{12}\lambda^4\,(X^2+Y^2) - \dfrac{273}{8}\lambda^2\,(X^2+Y^2)^2 + \dfrac{137}{24}\,(X^2+Y^2)^3 \\ p_{12} = (X^2-Y^2)\,\Big(-\dfrac{65}{12}\lambda^2 + \dfrac{17}{12}\,(X^2+Y^2)\Big)\,. \end{array} \right. \tag{68}$$

The moments $m_k \equiv \sum p_k(v_j)\,f_j$ have usual names given in (60) and for the D2Q13 scheme by the complementary relations

$$m_8 \equiv r_x\,, \quad m_9 \equiv r_y\,, \quad m_{10} \equiv E_2\,, \quad m_{11} \equiv E_3\,, \quad m_{12} \equiv X X_e\,. \tag{69}$$

We observe also for this scheme that the "numerical" total energy E is a simple function of the "physical" total energy ε. We have

$$E = 26\,\varepsilon - 28\,\lambda^2\,\rho \tag{70}$$

In the first approach presented in the introduction, we choose the equilibria for the non-conserved moments as follows :

$$\left\{ \begin{array}{l} XX^{\rm eq} = 0\,, \quad XY^{\rm eq} = 0\,, \quad \mathbf{q}^{\rm eq} = c_1\,\lambda^2\,\mathbf{j}\,, \quad \mathbf{r}^{\rm eq} = c_2\,\lambda^4\,\mathbf{j}\,, \\ E_2^{\rm eq} = \alpha_2\,\lambda^4\,\rho + \beta_2\,\lambda^2\,E\,, \quad E_3^{\rm eq} = \alpha_3\,\lambda^6\,\rho + \beta_3\,\lambda^4\,E\,, \quad XX_e^{\rm eq} = 0\,. \end{array} \right. \tag{71}$$

The relaxation rates s_k that determine the relaxation (63) of the moments are associated according to

$$\left\{ \begin{array}{l} s_{XX} \equiv s_5\,, \quad s_{XY} \equiv s_5\,, \quad s_{qx} \equiv s_7\,, \quad s_{qy} \equiv s_7\,, \quad s_{rx} \equiv s_9\,, \quad s_{ry} \equiv s_9\,, \\ s_{E2} \equiv s_{11}\,, \quad s_{E3} \equiv s_{12}\,, \quad s_{XXe} \equiv s_{13}\,. \end{array} \right. \tag{72}$$

The coefficient c_1 is related to the sound velocity c_0 according to

$$c_1 = 2\,c_0^2 - 3\,. \tag{73}$$

Annex - 3. D2Q17 lattice Boltzmann scheme

For the D2Q17 scheme illustrated in Figure 12, the thirteen ξ_j's of relation (55) are those given at the relation (67). The last four are

$$\xi_{13} = (2,\,2)\,,\ \xi_{14} = (-2,\,2)\,,\ \xi_{15} = (-2,\,-2)\,,\ \xi_{16} = (2,\,-2)\,,. \tag{74}$$

In a way analogous to (68), the two-variable polynomials family $\mathcal{P}_{\rm D2Q17}$ are given according to:

$$\left\{ \begin{array}{l} p_0 = 1\,, \quad p_1 = X\,, \quad p_2 = Y\,, \quad p_3 = -60 \,+\, 17\,(X^2+Y^2) \\ p_4 = X^2 - Y^2\,, \quad p_5 = X\,Y \\ p_6 = X\,(-17\,\lambda^2 + 3\,(X^2+Y^2))\,, \quad p_7 = Y\,(-17\,\lambda^2 + 3\,(X^2+Y^2)) \\ \quad {\rm p}_r = \dfrac{47}{6}\lambda^4 - \dfrac{17}{4}\lambda^2\,(X^2+Y^2) + \dfrac{5}{12}\,(X^2+Y^2)^2 \\ p_8 = X\,{\rm p}_r\,, \quad p_9 = Y\,{\rm p}_r \\ \quad {\rm p}_\tau = -\dfrac{7429}{42}\lambda^6 + \dfrac{1565}{8}\lambda^4(X^2+Y^2) - \dfrac{2635}{48}\lambda^2(X^2+Y^2)^2 + \dfrac{465}{112}(X^2+Y^2)^3 \\ p_{10} = X\,{\rm p}_\tau\,, \quad p_{11} = Y\,{\rm p}_\tau \\ p_{12} = (X^2-Y^2)\,\Big(-\dfrac{65}{12}\lambda^2 + \dfrac{17}{12}\,(X^2+Y^2)\Big) \\ p_{13} = \,X\,Y\,\Big(-\dfrac{65}{12}\lambda^2 + \dfrac{17}{24}(X^2+Y^2)\Big) \\ p_{14} = 620\,\lambda^4 - \dfrac{969}{2}\lambda^2\,(X^2+Y^2) + \dfrac{109}{2}\,(X^2+Y^2)^2 \\ p_{15} = -16740\,\lambda^6 + \dfrac{330361}{12}\lambda^4\,(X^2+Y^2) - \dfrac{74485}{8}\lambda^2\,(X^2+Y^2)^2 + \cdots \\ \qquad\qquad + \dfrac{18445}{24}\,(X^2+Y^2)^3 \\ p_{16} = 84\,\lambda^8 - \dfrac{24055}{56}\lambda^6(X^2+Y^2) + \dfrac{35425}{96}\lambda^4\,(X^2+Y^2)^2 + \cdots \\ \qquad\qquad - \dfrac{6035}{64}\lambda^2\,(X^2+Y^2)^3 + \dfrac{9193}{1344}(X^2+Y^2)^4\,. \end{array} \right. \tag{75}$$

The first moments are precise at the relations (60). The new moments introduced with the D2Q17 scheme with the help of relations (58) and (75) are

$$\left\{ \begin{array}{l} m_8 \equiv r_x\,, \quad m_9 \equiv r_y\,, \quad m_{10} \equiv \tau_x\,, \quad m_{11} \equiv \tau_y\,, \quad m_{12} \equiv XX_e\,, \\ m_{13} \equiv XY_e\,, \quad m_{14} \equiv E_2\,, \quad m_{15} \equiv E_3\,, \quad m_{16} \equiv E_4\,. \end{array} \right. \tag{76}$$

We observe between the "numerical" and "physical" total energies a relation very analogous to (61) and (70). We have for the D2Q17 lattice Boltzmann scheme:

$$E = 34\,\varepsilon - 60\,\lambda^2\,\rho \tag{77}$$

Due to natural isotropy conditions, the σ's coefficients defined by (65), satisfy the relations

$$\sigma_4 = \sigma_5\,, \quad \sigma_6 = \sigma_7\,, \quad \sigma_8 = \sigma_9\,, \quad \sigma_{10} = \sigma_{11}\,, \quad \sigma_{12} = \sigma_{13}\,. \tag{78}$$

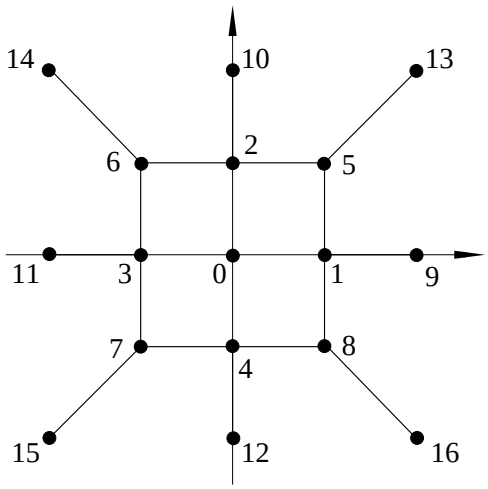

Figure 12. Stencil of 17 velocities for the D2Q17 lattice Boltzmann scheme.

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