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On rotational invariance of lattice Boltzmann schemes

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Abstract

We propose the derivation of acoustic-type isotropic partial differential equations that are equivalent to linear lattice Boltzmann schemes with a density scalar field and a momentum vector field as conserved moments. The corresponding linear equivalent partial differential equations are generated with a new “Berliner version” of the Taylor expansion method. The details of the implementation are presented. These ideas are applied for the D2Q9, D2Q13, D3Q19 and D3Q27 lattice Boltzmann schemes. Some limitations associated with necessary stability conditions are also presented.

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

PACS numbers : 02.60Cb (numerical simulation, solution of equations), 43.20.+g (General linear acoustics), 47.10.+g (Navier-Stokes equations).

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1) Introduction

- Partial differential equations like Navier-Stokes equations are invariant by rotation and all space directions are equivalent. Due to the use of a given mesh, lattice Boltzmann schemes cannot be completely invariant by rotation. This difficulty was present in the early ages of lattice gas automata. The initial model of Hardy, de Pazzis and Pomeau [12] proposed very impressive qualitative results but the associated fluid tensor was not invariant by rotation. With a triangular mesh, the second model of Frisch, Hasslacher and Pomeau [4] gives the correct physics. The lattice Boltzmann scheme with multiple relaxation times is the fruit of the work of Higuera and Jiménez [14], Higuera, Succi and Benzi [15], Qian, d’Humières and Lallemand [21] and d’Humières [16]. It uses in general square meshes and leads to isotropic physics for second order equivalent model as analyzed in [18]. The question of rotational invariance is still present in the lattice Boltzmann community and a detailed analysis of moment isotropy has been proposed by Chen and Orszag [3].
- The invariance by rotation has to be kept as much as possible in order to respect the correct propagation of waves. In [10], using the Taylor expansion method proposed in [9] for general applications, we have developed a methodology to enforce a lattice Boltzmann scheme to simulate correctly the physical acoustic waves up to fourth order of accuracy. But unfortunately, stability is in general guaranteed only if the viscosities of the waves are much higher than authorized by common physics. In this contribution, we relax this constraint and suppose that the equivalent partial differential equation of the scheme are invariant under rotations. The objective of this contribution is to propose a methodology to fix the parameters of lattice Boltzmann schemes in order to ensure the invariance by rotation at a given order.
- The outline is the following. In Section 2, we consider the question of the algebraic form of linear high order “acoustic-type” partial differential equations that are invariant by two dimensional and three-dimensional rotations. In Section 3, we recall the essential properties concerning multiple relaxation times lattice Boltzmann schemes. The equivalent equation of a lattice Boltzmann scheme introduces naturally the notion of rotational invariance at a given order. In the following sections, we develop a methodology to force acoustic-type lattice Boltzmann models to be invariant under rotations. We consider the four lattice Boltzmann schemes D2Q9, D2Q13, D3Q19 and D3Q27 in the sections 4 to 7. A conclusion ends our contribution. The Appendix 1 presents with details the implementation of the “Berliner version” of our algorithm to derive explicitly the equivalent partial differential equations. Some long formulas associated of specific results for D2Q13 and D3Q27 lattice Boltzmann schemes are presented in Appendix 2.

2) Invariance by rotation of acoustic-type equations

• With the help of group theory, and we refer the reader *e.g.* to Hermann Weyl [23] or Goodman and Wallach [11], it is possible to write *a priori* the general form of systems of linear partial differential equations invariant by rotation. More precisely, if the unknown is composed by one scalar field ρ (invariant function under a rotation of the space) and one vector field J (a vector valued function that is transformed in a similar way to how than cartesian coordinates are transformed when a rotation is applied), a linear partial differential equation invariant by rotation is constrained in a strong manner. Using some fundamental aspects of group theory and in particular the Schur lemma (see *e.g.* Goodman and Wallach [11]), it is possible to prove that general linear partial differential equations of acoustic type that are invariant by rotation admit the form described below.

• In the bidimensional case, we introduce the notation

$$(1) \quad \nabla^\perp \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right)^\perp = \left(\frac{\partial}{\partial y}, -\frac{\partial}{\partial x} \right), \quad J^\perp \equiv (J_x, J_y)^\perp = (J_y, -J_x).$$

Then acoustic type partial differential equations are of the form

$$(2) \quad \begin{cases} \partial_t \rho + \sum_{k \geq 0} \left(\alpha_k \Delta^k \rho + \beta_k \Delta^k \operatorname{div} J + \gamma_k \Delta^k \operatorname{div}(J^\perp) \right) = 0, \\ \partial_t J + \sum_{k \geq 0} \left(\delta_k \nabla \Delta^k \rho + \mu_k \Delta^k J + \zeta_k \nabla \operatorname{div} \Delta^k J \right. \\ \quad \left. + \varepsilon_k \nabla^\perp \Delta^k \rho + \nu_k \Delta^k J^\perp + \eta_k \nabla \operatorname{div} \Delta^k J^\perp \right) = 0, \end{cases}$$

where the real coefficients $\alpha_k, \beta_k, \gamma_k, \delta_k, \mu_k, \zeta_k, \varepsilon_k, \nu_k$ and η_k are in finite number. The tridimensional case is essentially analogous. The “acoustic type” linear partial differential equations invariant by rotation take necessarily the form

$$(3) \quad \begin{cases} \partial_t \rho + \sum_{k \geq 0} \left(\alpha_k \Delta^k \rho + \beta_k \operatorname{div} \Delta^k J \right) = 0 \\ \partial_t J + \sum_{k \geq 0} \left(\delta_k \nabla \Delta^k \rho + \mu_k \Delta^k J + \eta_k \nabla \operatorname{div} \Delta^k J + \varphi_k \operatorname{curl} \Delta^k J \right) = 0, \end{cases}$$

with an analogous convention that the sums in the relations (3) contain only a finite number of such terms.

3) Lattice Boltzmann schemes with multiple relaxation times

• Each iteration of a lattice Boltzmann scheme is composed by two steps: relaxation and propagation. The relaxation is local in space: the particle distribution $f(x) \in \mathbb{R}^q$ for x a node of the lattice $\mathcal{L}$, is transformed into a “relaxed” distribution $f^*(x)$ that is non linear in general. In this contribution, we restrict to linear functions $\mathbb{R}^q \ni f \mapsto f^* \in \mathbb{R}^q$. As usual with the d’Humières scheme [16], we introduce an invertible matrix M with q lines and q columns. The moments m are obtained from the particle distribution thanks to the associated transformation

$$(4) \quad m_k = \sum_{j=0}^{q-1} M_{kj} f_j, \quad 0 \leq k \leq q-1.$$

Then we consider the conserved moments $W \in \mathbb{R}^N$:

$$(5) \quad W_i = m_i, \quad 0 \leq i \leq N-1.$$

For the usual acoustic equations for d space dimensions, we have $N = d + 1$. The first moment is the density and the next ones are composed by the d components of the physical momentum. Then we define a conserved value m_k^{eq} for the non-equilibrium moments m_k for $k \geq N$. With the help of ‘‘Gaussian’’ functions $G_k(\bullet)$, we obtain:

$$(6) \quad m_k^{\text{eq}} = G_k(W), \quad N \leq k \leq q-1.$$

In the present contribution, we suppose that this equilibrium value is a linear function of the conserved variables. In other terms, the Gaussian functions are linear:

$$(7) \quad G_{N+\ell}(W) = \sum_{i=1}^{n-1} E_{\ell i} W_i, \quad \ell \geq 0$$

for some equilibrium coefficients $E_{\ell i}$ for $\ell \geq 0$ and $0 \leq i \leq N-1$.

- The relaxed moments m_k^* are linear functions of m_k and m_k^{eq} :

$$(8) \quad m_k^* = m_k + s_k (m_k^{\text{eq}} - m_k), \quad k \geq N.$$

For a stable scheme, we have

$$(9) \quad 0 < s_k < 2.$$

We remark that if $s_k = 0$, the corresponding moment is conserved. In some particular cases, the value $s_k = 2$ can also be used (see *e.g.* [7, 8]). The conserved moments are not affected by the relaxation:

$$m_i^* = m_i = W_i, \quad 0 \leq i \leq N-1.$$

From the moments m_ℓ^* for $0 \leq \ell \leq q-1$ we deduce the particle distribution f_j^* by resolution of the linear system

$$M f^* = m^*.$$

- The propagation step couples the node $x \in \mathcal{L}$ with his neighbours $x - v_j \Delta t$ for $0 \leq j \leq q-1$. The time iteration of the scheme can be written as

$$(10) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad 0 \leq j \leq q-1, \quad x \in \mathcal{L}.$$

- From the knowledge of the previous algorithm, it is possible to derive a set of equivalent partial differential equations for the conserved variables. If the Gaussian functions G_k are linear, this set of equations takes the form

$$(11) \quad \frac{\partial W}{\partial t} - \alpha_1 W - \Delta t \alpha_2 W - \dots - \Delta t^{j-1} \alpha_j W - \dots = 0,$$

where α_j is for $j \geq 1$ is a space derivation operator of order j . We refer the reader to [5] for the presentation of our approach in the general case. In this contribution, we have developed an explicit algebraic linear version of the algorithm detailed in Appendix 1. Moreover, we consider that the lattice Boltzmann scheme is invariant by rotation at order ℓ if the equivalent partial differential equation

$$(12) \quad \frac{\partial W}{\partial t} - \sum_{j=1}^{\ell} \Delta t^{j-1} \alpha_j W = 0$$

obtained from (11) by truncation at the order ℓ is invariant by rotation. For acoustic-type models, the partial differential equation (12) has to be identical to (2) or (3) for dimension 2 or 3. In the following, we determine the equivalent partial differential equations for classical lattice Boltzmann schemes in the general linear case. Then we fit the equilibrium and relaxation parameters of the scheme in order to enforce rotational invariances at all orders between 1 and 4.

4) D2Q9

The isotropy of the lattice Boltzmann scheme D2Q9 for the acoustic equations has been studied in detail in [1, 2]. We give here only a summary of our results.

- The matrix M for the D2Q9 lattice Boltzmann model is of the form

$$(13) \quad M_{kj} = p_k(v_j), \quad 0 \leq j, k \leq q-1$$

with polynomials p_k detailed in the contribution [17]. With this choice, the moments are named according to the following notations:

$$(14) \quad \left\{ \begin{array}{lll} 0 & 1 & \lambda^0 \\ 1, 2 & X, Y & \lambda^1 \\ 3 & \varepsilon & \lambda^2 \\ 4, 5 & XX, XY & \lambda^2 \\ 6, 7 & q_x, q_y & \lambda^3 \\ 8 & \varepsilon_2 & \lambda^4. \end{array} \right.$$

We have recalled in (14) the degrees of homogeneity of each moment m_k relative to the reference numerical velocity $\lambda \equiv \frac{\Delta x}{\Delta t}$.

- At first order, the invariance by rotation (2) takes the form

$$(15) \quad \left\{ \begin{array}{l} \partial_t \rho + \operatorname{div} J = O(\Delta t) \\ \partial_t J + c_0^2 \nabla \rho = O(\Delta t) \end{array} \right.$$

if the next moments of degree 2 follow the simple equilibrium:

$$(16) \quad \varepsilon^{\text{eq}} = \alpha \lambda^2 \rho, \quad XX^{\text{eq}} = XY^{\text{eq}} = 0.$$

Then the sound velocity c_0 in the equation (15) satisfies

$$(17) \quad c_0^2 = \frac{\lambda^2}{6} (4 + \alpha).$$

- At second order, the invariance by rotation (2) is realized under specific conditions for the third order moments $q \equiv (q_x, q_y)$. This equilibrium condition is defined with the help of Hénnon's [13] parameters σ_k defined from the coefficients s_k according to

$$(18) \quad \sigma_k \equiv \frac{1}{s_k} - \frac{1}{2} \quad \text{when } k \geq 3.$$

The stability condition (9) can be written as

$$(19) \quad \sigma_k > 0, \quad \text{for } k \geq N.$$

We have

$$(20) \quad q^{\text{eq}} = \frac{\sigma_4 - 4\sigma_5}{\sigma_4 + 2\sigma_5} \lambda^2 J.$$

We obtain with these conditions the following equivalent partial differential equations

$$(21) \quad \begin{cases} \partial_t \rho + \text{div} J = O(\Delta t^2) \\ \partial_t J + c_0^2 \nabla \rho - \mu \Delta J - \zeta \nabla \text{div} J = O(\Delta t^2). \end{cases}$$

The physical viscosities μ and ζ can be determined according to

$$(22) \quad \mu = \frac{\sigma_4 \sigma_5}{\sigma_4 + 2\sigma_5} \lambda \Delta x, \quad \zeta = \sigma_3 \frac{(2\sigma_4 - 2\sigma_5 - \alpha \sigma_4 - 2\alpha \sigma_5)}{6(\sigma_4 + 2\sigma_5)} \lambda \Delta x.$$

We observe that the classical isotropy condition $\sigma_4 = \sigma_5$ for the second order moments XX and XY is not necessary for the relaxation at this second order step.

- At third order, the system (2) takes the particular form

$$(23) \quad \begin{cases} \partial_t \rho + \text{div} J + \xi \Delta \text{div} J = O(\Delta t^3) \\ \partial_t J + c_0^2 \nabla \rho - \mu \Delta J - \zeta \nabla \text{div} J + \chi \nabla \Delta \rho = O(\Delta t^3). \end{cases}$$

This is possible if the complementary relations

$$(24) \quad \sigma_4 = \sigma_5, \quad \varepsilon_2^{\text{eq}} = -\frac{\lambda^4 \rho}{2} (3\alpha + 4)$$

hold. Then the heat flux at equilibrium has an expression (20) that can be simply written as

$$(25) \quad q^{\text{eq}} = -\lambda^2 J.$$

The coefficients in the equations (23) are given by the expressions

$$(26) \quad \begin{cases} \mu = \frac{1}{3} \sigma_4 \lambda \Delta x, \quad \zeta = -\frac{1}{6} \sigma_3 \alpha \lambda \Delta x, \quad \xi = \frac{1}{72} (\alpha - 2) \Delta x^2, \\ \chi = \frac{1}{216} (\alpha + 4) (2 + 6\alpha \sigma_3^2 - \alpha - 12\sigma_4^2) \lambda^2 \Delta x^2. \end{cases}$$

We remark that the dissipation of the acoustic waves $\gamma \equiv \frac{\mu + \zeta}{2}$ (see *e.g.* Landau and Lifshitz [19]) is given according to

$$(27) \quad \gamma = \frac{\lambda \Delta x}{12} (2\sigma_4 - \alpha \sigma_3).$$

- The invariance by rotation at fourth order of the D2Q9 lattice Boltzmann scheme does not give completely satisfactory results, as observed previously in [2]. In order to get equivalent equations at order 4 of the type

$$(28) \quad \begin{cases} \partial_t \rho + \text{div} J + \xi \Delta \text{div} J + \eta \Delta^2 \rho = O(\Delta t^4) \\ \partial_t J + c_0^2 \nabla \rho - \mu \Delta J - \zeta \nabla \text{div} J + \chi \nabla \Delta \rho + \mu_4 \Delta^2 J + \zeta_4 \nabla \text{div} \Delta J = O(\Delta t^4), \end{cases}$$

it is necessary to fix some relaxation parameters:

$$(29) \quad \sigma_3 = \sigma_4 = \sigma_8, \quad \sigma_6 = \sigma_7 = \frac{1}{6\sigma_4}.$$

The two viscosities μ and ζ are now dependent and the dissipation of the acoustic waves introduced previously in (27) admits now the expressions

$$(30) \quad \mu = \frac{1}{3} \sigma_4 \lambda \Delta x, \quad \zeta = -\frac{1}{6} \sigma_4 \alpha \lambda \Delta x, \quad \gamma = \frac{\lambda \sigma_4 \Delta x}{12} (2 - \alpha).$$

Observe that the dissipation γ is positive under usual conditions. If the conditions (29) are satisfied, we can specify the coefficients of the fourth order terms in the equations (28):

$$(31) \quad \begin{cases} \eta = \frac{\lambda \Delta x^3}{432} (\alpha + 4) (\alpha - 2), & \mu_4 = \frac{\lambda \Delta x^3}{108} (12 \sigma_4^2 - 1), \\ \zeta_4 = \frac{\lambda \Delta x^3}{216} \sigma_4 (12 - \alpha - 2 \alpha^2 + 12 \sigma_4^2 (\alpha^2 - \alpha - 4)). \end{cases}$$

- In [2], we have conducted a set of numerical experiments that make more explicit the isotropy qualities of four different variants of the D2Q9 lattice Boltzmann scheme for the numerical simulation of acoustic waves. The orders of isotropy precision numerically computed are in coherence with the level of accuracy presented in this section.

5) D2Q13

- Four more velocities are added to the D2Q9 scheme to construct D2Q13. The details can be found *e.g.* in [17]. Nine moments are analogous to those proposed in (14) for D2Q9 and four moments ($r_x, r_y, \varepsilon_3, XX_e$) are new:

$$(32) \quad \begin{cases} 0 & 1 & \lambda^0 \\ 1, 2 & X, Y & \lambda^1 \\ 3 & \varepsilon & \lambda^2 \\ 4, 5 & XX, XY & \lambda^2 \\ 6, 7 & q_x, q_y & \lambda^3 \\ 8, 9 & r_x, r_y & \lambda^5 \\ 10 & \varepsilon_2 & \lambda^4 \\ 11 & \varepsilon_3 & \lambda^6 \\ 12 & XX_e & \lambda^4. \end{cases}$$

- At first order, the invariance by rotation (2) takes again the form (15). The conditions (16) are essentially unchanged, except that the sound velocity is now evaluated according to the relation

$$(33) \quad c_0^2 = \frac{\lambda^2}{26} (28 + \alpha) \equiv c_s^2 \lambda^2.$$

- At second order, the equivalent partial differential equations take the isotropic form (21) when we have :

$$(34) \quad q^{\text{eq}} = \varphi \lambda^2 J, \quad r^{\text{eq}} = \frac{1}{12} \left(\frac{20 \sigma_5 - 85 \sigma_4 - 49 \varphi \sigma_4 - 14 \varphi \sigma_5}{\sigma_4 + \sigma_5} \right) \lambda^4 J.$$

Then the isotropy coefficients in (15) have the following expressions:

$$(35) \quad \mu = \frac{\lambda \Delta x}{2} \frac{\sigma_4 \sigma_5}{\sigma_4 + \sigma_5} (3 + \varphi), \quad \zeta = \frac{\lambda \Delta x}{26} \sigma_3 (11 + 13 \varphi - \alpha), \quad \sigma_k > 0 \text{ when } k \geq 3.$$

- The invariance by rotation at third order of the mass equation is realized if we impose a unique value for the relaxation coefficients of the second order moments XX and XY introduced in (32):

$$(36) \quad \sigma_4 = \sigma_5.$$

Moreover, the attenuation of sound waves γ does not depend at first order on the advective velocity if (36) is satisfied. For the invariance by rotation of the momentum equation, we must impose also the following equilibrium values for the moments $m_{10} \equiv \varepsilon_2$, $m_{11} \equiv \varepsilon_3$ and $m_{12} \equiv XX_e$:

$$(37) \quad \begin{cases} \varepsilon_2^{\text{eq}} = \left(-5\alpha + \frac{77}{26} \varphi \alpha + \frac{1078}{13} \varphi \right) \lambda^4 \rho \\ \varepsilon_3^{\text{eq}} = \left(\frac{\alpha}{48} - \frac{137}{12} - \frac{135}{208} \alpha \varphi - \frac{945}{52} \varphi \right) \lambda^4 \rho, \quad XX_e^{\text{eq}} = 0. \end{cases}$$

Then the equivalent equations at order 3 of the D2Q13 lattice Boltzmann scheme are still given by the equations (23). The equilibrium condition (34) is now written as

$$(38) \quad r^{\text{eq}} = -\frac{1}{24} (65 + 63 \varphi) \lambda^4 J$$

and the coefficients in the equations (23) can be clarified:

$$(39) \quad \begin{cases} \mu = \frac{1}{4} \sigma_5 (3 + \varphi) \lambda \Delta x, \quad \zeta = \frac{1}{26} \sigma_4 (11 + 13 \varphi - \alpha) \lambda \Delta x, \\ \xi = \frac{1}{624} (2\alpha - 39\varphi - 61) \Delta x^2, \\ \chi = \frac{1}{8112} (28 + \alpha) \left(61 + 39\varphi + 12\alpha\sigma_3^2 - 2\alpha - 78\varphi\sigma_4^2 \right. \\ \left. - 156\varphi\sigma_3^2 - 234\sigma_4^2 - 132\sigma_3^2 \right) \lambda^2 \Delta x^2. \end{cases}$$

- The invariance by rotation at fourth order is satisfied if we add to the previous conditions (36) (37) and (38) the new ones:

$$(40) \quad \begin{cases} q^{\text{eq}} = -\frac{7}{5} \lambda^2 J, \quad \sigma_6 = \sigma_7 = \frac{1}{12 \sigma_4}, \\ \sigma_8 = \sigma_9 = \frac{5}{24} \frac{155 - a}{a - 308} \frac{1}{\sigma_4} + \frac{1}{24} \frac{7a - 1391}{a - 308} \frac{1}{\sigma_3}, \\ \sigma_{10} = \frac{3973}{45} \frac{43a - 16610}{89a - 20680} \frac{5c_s^2 - 4}{1189c_s^2 - 828} \sigma_3 + \\ \quad + \frac{154}{1395} \frac{7a - 1391}{89a - 20680} \frac{725c_s^2 - 418}{1189c_s^2 - 828} a \sigma_4, \\ \sigma_{11} = \frac{a}{155} \sigma_4. \end{cases}$$

If the parameters c_s and α relative to the non-dimensionalized sound velocity are linked together thanks to (33) and if the new parameter a is chosen such that

$$(41) \quad c_s^2 < \frac{418}{25}, \quad -28 < \alpha \leq -\frac{9432}{725} \simeq -13, \quad 155 < a < \frac{1391}{7} \simeq 198,$$

the coefficients σ_8 , σ_{10} and σ_{11} are strictly positive if it is the case for σ_3 and σ_4 . In this case, the stability conditions (19) are satisfied for the coefficients σ_3 , σ_4 , σ_8 , σ_{10} and σ_{11} . With the choice (40) the nontrivial algebraic expressions of the previous conditions (36), (37) and (38) can be written as

$$(42) \quad r^{\text{eq}} = \frac{29}{30} \lambda^4 J, \quad \varepsilon_2^{\text{eq}} = -\left(\frac{1189}{130} \alpha + \frac{7546}{65}\right) \lambda^4 \rho, \quad \varepsilon_3^{\text{eq}} = \left(\frac{547}{39} + \frac{145}{156} \alpha\right) \lambda^4 \rho.$$

With the above conditions (40) and (42) the equivalent equations of the D2Q13 lattice Boltzmann scheme at fourth order are made explicit in (28), with the associated coefficients, except ζ_4 , given according to:

$$(43) \quad \left\{ \begin{array}{l} \xi = \frac{5\alpha - 16}{1560} \Delta x^2, \quad \eta = \frac{\alpha + 28}{40560} (36\sigma_3 + 5\sigma_3 \alpha - 52\sigma_4) \lambda \Delta x^3 \\ \mu = \frac{2}{5} \sigma_4 \lambda \Delta x, \quad \zeta = -\frac{1}{130} \sigma_3 (36 + 5\alpha) \lambda \Delta x \\ \chi = \frac{1}{20280} (28 + \alpha) \left(16 - 5\alpha + 216\sigma_3^2 - 312\sigma_4^2 + 30\alpha\sigma_3^2\right) \lambda^2 \Delta x^2 \\ \mu_4 = \frac{\sigma_4 \lambda \Delta x^3}{300 \sigma_3 (a - 308)} \left(4483\sigma_4 - 5099\sigma_3 - 23a\sigma_4 + 25a\sigma_3 \right. \\ \left. - 14784\sigma_3\sigma_4^2 + 48a\sigma_3\sigma_4^2\right). \end{array} \right.$$

The algebraic expression of the coefficient ζ_4 is quite long. With Hénon's coefficients σ_j defined according to (18), the related moments numbered by the relations (32), the equilibrium of the energy (16) parametrized by α , and the parameter a introduced at (40), the coefficient ζ_4 for the fourth order term in (28) can be evaluated according to:

$$\left\{ \begin{array}{l} \zeta_4 = \frac{\sigma_4 \lambda \Delta x^3}{56581200 \sigma_3 (89a - 20680)} \left(525433428 a \sigma_3 \sigma_4 + 576972000 \alpha^2 \sigma_3^2 \right. \\ + 18001526400 \alpha \sigma_3^3 \sigma_4 + 18001526400 \alpha \sigma_3 \sigma_4^3 + 65975 a^2 \alpha \sigma_3 \sigma_4 \\ + 170558856 a \sigma_4^2 - 334055628 a \sigma_3^2 - 858312 a^2 \sigma_4^2 - 159243217380 \sigma_3 \sigma_4 \\ + 75143778660 \sigma_3^2 + 18001526400 \alpha \sigma_3^2 \sigma_4^2 - 77472720 a \alpha \sigma_3^3 \sigma_4 \\ - 77472720 a \alpha \sigma_3^2 \sigma_4^2 - 77472720 a \alpha \sigma_3 \sigma_4^3 + 504042739200 \sigma_3 \sigma_4^3 \\ + 129610990080 \sigma_3^3 \sigma_4 + 129610990080 \sigma_3^2 \sigma_4^2 + 858312 a^2 \sigma_3 \sigma_4 \\ + 22940190 a \alpha \sigma_3 \sigma_4 + 17841109925 \alpha \sigma_3^2 - 65975 a^2 \alpha \sigma_4^2 \\ + 13110175 a \alpha \sigma_4^2 - 3461832000 \alpha^2 \sigma_3^4 - 85853433600 \alpha \sigma_3^4 \\ - 2483100 a \alpha^2 \sigma_3^2 - 78263065 a \alpha \sigma_3^2 - 438683351040 \sigma_3^4 \\ + 369485280 a \alpha \sigma_3^4 + 14898600 a \alpha^2 \sigma_3^4 + 1887950592 a \sigma_3^4 \\ - 557803584 a \sigma_3^2 \sigma_4^2 - 2169236160 a \sigma_3 \sigma_4^3 - 557803584 a \sigma_3^3 \sigma_4 \\ \left. - 8032585925 \alpha \sigma_3 \sigma_4 \right). \end{array} \right.$$

6) D3Q19

- For the scheme D3Q19, we have 4 conservation laws and a total of 19 moments. We refer *e.g.* to [9] for an algebraic expression of the polynomials p_k in (13):

$$(44) \quad \left\{ \begin{array}{lll} 0 & 1 & \lambda^0 \\ 1, 2, 3 & X, Y, Z & \lambda^1 \\ 4 & \varepsilon & \lambda^2 \\ 5, 6 & XX, WW & \lambda^2 \\ 7, 8, 9 & XY, YZ, ZX & \lambda^2 \\ 10, 11, 12 & q_x, q_y, q_z & \lambda^3 \\ 13 & \varepsilon_2 & \lambda^4 \\ 14, 15 & XX_e, WW_e & \lambda^4 \\ 16, 17, 18 & \text{antisymmetric of order 3} & \lambda^3. \end{array} \right.$$

The results summarized in this Section have been essentially considered (quickly) in the previous contribution [10]. They have been also used by Leriche, Lallemand and Labrosse [20] for the numerical determination of the eigenmodes of the Stokes problem in a cubic cavity.

- We write the four equivalent partial differential equations at first order with the method explained in Appendix 1. Then we impose that the associated modes are isotropic, *i.e.* contain only partial differential operators that are invariant by rotation. In Fourier space, the coefficients of the associated determinant must contain only powers of the wave vector. The associated equations are highly nonlinear relative to the coefficients of the equilibrium matrix introduced in (7). We have obtained a family of parameters by enforcing the linearity of the solution of the isotropic equations. With this constraint, we have to impose a relation for the “energy” moment $m_4 \equiv \varepsilon$ at equilibrium:

$$(45) \quad \varepsilon^{\text{eq}} = \alpha \lambda^2 \rho.$$

Moreover, the equilibrium values for the moments m_5 to m_9 of degree two introduced in (44) are equal to zero:

$$(46) \quad XX^{\text{eq}} = WW^{\text{eq}} = XY^{\text{eq}} = YZ^{\text{eq}} = ZX^{\text{eq}} = 0.$$

When the conditions (45) and (46) are realized, the isotropic equivalent system is given by the system of first order acoustic equations (15). Moreover, the sound velocity c_0 satisfies

$$(47) \quad c_0^2 = \frac{\alpha + 30}{57} \lambda^2 \equiv c_s \lambda^2.$$

- Invariance by rotation at second order is realized if we impose on one hand

$$(48) \quad q^{\text{eq}} = 2 \frac{3\sigma_5 - 4\sigma_7}{\sigma_5 + 2\sigma_7} \lambda^2 J$$

and on the other hand

$$(49) \quad \sigma_5 = \sigma_6, \quad \sigma_7 = \sigma_8 = \sigma_9.$$

Then the equivalent partial differential equations of the D3Q19 lattice Boltzmann scheme take the form (21). The associated coefficients are given according to

$$(50) \quad \begin{cases} \mu = \frac{\sigma_5 \sigma_7}{\sigma_5 + 2 \sigma_7} \lambda \Delta x \\ \zeta = \frac{\lambda \Delta x}{57 (\sigma_5 + 2 \sigma_7)} (27 \sigma_4 \sigma_5 + 19 \sigma_5 \sigma_7 - 22 \sigma_4 \sigma_7 - \alpha \sigma_4 \sigma_5 - 2 \alpha \sigma_7 \sigma_4 \alpha) . \end{cases}$$

• At third order, if we impose the previous relations (45) (46) (48) and (49), *id est* an equilibrium for the “energy square” ε_2 given below, a null value for m_{14}^{eq} and m_{15}^{eq} and a supplementary condition for the relaxation coefficients, *id est*

$$(51) \quad \varepsilon_2^{\text{eq}} = \frac{42 + 9 \alpha}{9} \lambda^2 \rho, \quad XX_e^{\text{eq}} = WW_e^{\text{eq}} = 0, \quad \sigma_5 = \sigma_7,$$

the equivalent equations of the D3Q19 lattice Boltzmann scheme are exactly given by (23). We observe that the relation (48) takes now the form

$$(52) \quad q^{\text{eq}} = -\frac{2}{3} \lambda^2 J$$

and the coefficients associated to the equations (23) can be deduced through an elementary process:

$$(53) \quad \begin{cases} \mu = \frac{1}{3} \sigma_5 \lambda \Delta x, \quad \zeta = \frac{\lambda \Delta x}{171} (5 \sigma_4 + 19 \sigma_5 - 3 \alpha \sigma_4), \quad \xi = \frac{\Delta x^2}{684} (\alpha - 27), \\ \chi = \frac{\lambda^2 \Delta x^2}{19494} (\alpha + 30) (27 + 6 \alpha \sigma_4^2 - 10 \sigma_4^2 - 152 \sigma_5^2 - \alpha). \end{cases}$$

The bulk viscosity $\zeta_b \equiv 3 \zeta - \mu$ (see *e.g.* Landau and Lifshitz [19]) is essentially function of the relaxation parameter associated to the energy ε :

$$(54) \quad \zeta_b = \frac{\lambda \sigma_4 \Delta x}{57} (5 - 3 \alpha).$$

• We have found also a variant of the previous relations to enforce third order isotropy. We can replace the relations (51) by the following ones, with an undefined parameter β :

$$(55) \quad \begin{cases} \varepsilon_2^{\text{eq}} = \beta \lambda^2 \rho, \quad XX_e^{\text{eq}} = WW_e^{\text{eq}} = 0, \quad \sigma_5 = \sigma_7, \\ \sigma_{10} = \sigma_{11} = \sigma_{12} = \frac{1}{12 \sigma_5}, \quad \sigma_{16} = \frac{1}{8 \sigma_5}, \quad \sigma_{17} = \frac{1}{4 \sigma_5}, \quad \sigma_{18} = \frac{1}{12 \sigma_5}. \end{cases}$$

The relations (52), (53) and (54) are not changed, except that the coefficient χ in the second line of (23) is now given by

$$(56) \quad \begin{cases} \chi = \frac{\lambda^2 \Delta x^2}{409374 \sigma_5} \left(16212 \sigma_5 + 126 \alpha^2 \sigma_4^2 \sigma_5 + 3570 \alpha \sigma_4^2 \sigma_5 - 6300 \sigma_4^2 \sigma_5 \right. \\ \quad \left. - \sigma_5 \alpha^2 - 234 \alpha \sigma_5 + 361 \beta \sigma_4 + 171 \alpha \sigma_4 \right. \\ \quad \left. + 798 \sigma_4 - 3192 \alpha \sigma_5^3 - 95760 \sigma_5^3 - 361 \beta \sigma_5 \right). \end{cases}$$

• The invariance by rotation at fourth order has also been considered. But due to the low number of remaining parameters, the family of Boltzmann schemes that we have obtained impose constraints between physical parameters. We must have in particular

$$(57) \quad \sigma_4 = \sigma_5$$

and this relation induces some *a priori* relationship between the shear viscosity μ of relation (50) and the bulk viscosity ζ_b presented in (54). Moreover, the relations (51) (52) must be satisfied and H  non's parameters of the multiple relaxation times have to follow, with an ordering proposed in (44), the complementary conditions

$$(58) \quad \sigma_{10} = \sigma_{11} = \sigma_{12} = \frac{1}{6\sigma_5}, \quad \sigma_{13} = \sigma_{14} = \sigma_{15} = \sigma_5, \quad \sigma_{16} = \sigma_{17} = \sigma_{18} = \frac{1}{6\sigma_5}.$$

Then the fourth order isotropic equivalent equations (28) are satisfied and the associated coefficients can be clarified:

$$(59) \quad \begin{cases} \xi = \frac{\alpha - 27}{684} \Delta x^2, \quad \eta = \frac{(\alpha + 30)(\alpha - 27)}{38988} \sigma_5 \lambda \Delta x^3, \quad \mu_4 = \frac{12\sigma_5^2 - 1}{108} \sigma_5 \lambda \Delta x^3 \\ \zeta_4 = \frac{\sigma_5 \lambda \Delta x^3}{38988} \left(2062 + 45\alpha - 4\alpha^2 - 5304\sigma_5^2 - 612\alpha\sigma_5^2 + 24\alpha^2\sigma_5^2 \right). \end{cases}$$

7) D3Q27

- For the schemes D3Q27, we refer *e.g.* to [10] for an algebraic expression of the polynomials p_k of the relation (13). The moments follow now the nomenclature

$$(60) \quad \left\{ \begin{array}{lll} 0 & 1 & \lambda^0 \\ 1, 2, 3 & X, Y, Z & \lambda^1 \\ 4 & \varepsilon & \lambda^2 \\ 5, 6 & XX, WW & \lambda^2 \\ 7, 8, 9 & XY, YZ, ZX & \lambda^2 \\ 10, 11, 12 & q_x, q_y, q_z & \lambda^3 \\ 13, 14, 15 & r_x, r_y, r_z & \lambda^5 \\ 16 & \varepsilon_2 & \lambda^4 \\ 17 & \varepsilon_3 & \lambda^6 \\ 18, 19 & XX_e, WW_e & \lambda^4 \\ 20, 21, 22 & XY_e, YZ_e, ZX_e & \lambda^4 \\ 23, 24, 25 & \text{antisymmetric of order 3} & \lambda^3 \\ 26 & XYZ & \lambda^3. \end{array} \right.$$

- At first order, we follow the same methodology as the one presented for the previous schemes. We keep the relation (45) for the momentum $m_4 \equiv \varepsilon$ at equilibrium. As for the D3Q19 scheme, the equilibrium values for the moments m_5 to m_9 of degree two introduced in (60) are equal to zero and the relation (46) still holds. Then the first order isotropic equivalent system is given by (15). Observe that the sound velocity c_0 now satisfies

$$(61) \quad c_0^2 = \frac{\alpha + 2}{3} \lambda^2 \equiv c_s \lambda^2.$$

- At second order the equilibrium values have to be constrained: the ‘‘heat flux’’ at equilibrium is given by the relation

$$(62) \quad q^{\text{eq}} = 2 \frac{\sigma_5 - 4\sigma_7}{\sigma_5 + 2\sigma_7} \lambda^2 J$$

and a null value for the equilibrium of the third order moments is imposed:

$$(63) \quad m_{23}^{\text{eq}} = m_{24}^{\text{eq}} = m_{25}^{\text{eq}} = m_{26}^{\text{eq}} = 0.$$

Moreover, the relations (49) between Hénon's parameters of second order moments still have to be imposed. Then the second order equivalent equations are isotropic and the coefficients of (21) follow the non-traditional relations

$$(64) \quad \mu = \frac{\sigma_5 \sigma_7}{\sigma_5 + 2 \sigma_7} \lambda \Delta x, \quad \zeta_b \equiv 3 \zeta - \mu = \frac{\lambda \sigma_4 \Delta x}{\sigma_5 + 2 \sigma_7} (\sigma_5 - 2 \sigma_7 - \alpha \sigma_5 - 2 \alpha \sigma_5).$$

- At third order, we have two options as for the D3Q19 scheme. If we suppose that the heat flux at equilibrium and only one time relaxation are fixed, *id est*

$$(65) \quad \begin{cases} q^{\text{eq}} = -2 \lambda^2 J, & \varepsilon_2^{\text{eq}} = -(2 + 3 \alpha) \lambda^2 \rho, \\ XX_e^{\text{eq}} = WW_e^{\text{eq}} = XY_e^{\text{eq}} = YZ_e^{\text{eq}} = ZX_e^{\text{eq}} = 0, & \sigma_5 = \sigma_7, \end{cases}$$

the third order equivalent equations of the D3Q27 lattice Boltzmann scheme are given by the expressions (23). The coefficients in these equations are simple to evaluate with a software of formal calculus:

$$(66) \quad \begin{cases} \mu = \frac{1}{3} \sigma_5 \lambda \Delta x, & \zeta_b = -\frac{1}{3} \sigma_4 (1 + 3 \alpha) \lambda \Delta x, & \xi = \frac{1}{36} (\alpha - 1) \Delta x^2, \\ \chi = \frac{1}{54} (\alpha + 2) (1 + \alpha + 6 \alpha \sigma_4^2 - 2 \sigma_4^2 + 8 \sigma_5^2) \lambda^2 \Delta x^2. \end{cases}$$

- The second solution for third order isotropy does not specify completely the “square of the energy” ε_2 but fixes an important number of relaxation times:

$$(67) \quad \begin{cases} q^{\text{eq}} = -2 \lambda^2 J, & \varepsilon_2^{\text{eq}} = \beta \lambda^2 \rho, & \sigma_5 = \sigma_7, \\ \sigma_{10} = \sigma_{11} = \sigma_{12} = \frac{1}{12 \sigma_5}, & \sigma_{23} = \frac{1}{12 \sigma_5}, & \sigma_{24} = \frac{1}{4 \sigma_5}, & \sigma_{25} = \frac{1}{8 \sigma_5}, \\ XX_e^{\text{eq}} = WW_e^{\text{eq}} = XY_e^{\text{eq}} = YZ_e^{\text{eq}} = ZX_e^{\text{eq}} = 0. \end{cases}$$

The parameters μ , ζ , ζ_b and ξ are still given by the relations (66). But the value of the parameter χ is modified:

$$(68) \quad \begin{cases} \chi = \frac{1}{162 \sigma_5} \left(4 \sigma_5 + 2 \sigma_4 + 3 \alpha \sigma_4 - 6 \alpha \sigma_5 - 3 \alpha^2 \sigma_5 + 18 \alpha^2 \sigma_4^2 \sigma_5 + 42 \alpha \sigma_4^2 \sigma_5 \right. \\ \quad \left. + 12 \sigma_4^2 \sigma_5 - 24 \alpha \sigma_5^3 - 48 \sigma_5^3 + \beta \sigma_4 - \beta \sigma_5 \right) \lambda^2 \Delta x^2. \end{cases}$$

- The search of an isotropic form of the fourth order equivalent partial differential equations like (28) leads to a nonlinear system of 33 equations. We have obtained a first solution with the following particular parameters:

$$(69) \quad r^{\text{eq}} = 2 \lambda^4 J, \quad \sigma_{10} = \sigma_{11} = \sigma_{12}, \quad \sigma_{18} = \sigma_{19}, \quad \sigma_{23} = \sigma_{24} = \sigma_{25}.$$

It is possible to fix the other parameters of the scheme with the ratio ψ of Hénon's parameters associated with the moments XX_e and XX . With the notations proposed in (60), we set

$$(70) \quad \psi \equiv \frac{\sigma_{18}}{\sigma_5}.$$

When we impose the following relations between the coefficients of relaxations (all defined through their associated Hénon's parameter introduced at the relation (20)),

$$(71) \quad \left\{ \begin{array}{l} \sigma_4 = \sigma_5 \frac{3\psi^3 - 4\psi^2 - 13\psi + 32}{3\psi^3 - 22\psi^2 + 23\psi + 14}, \\ \sigma_{10} = \sigma_{11} = \sigma_{12} = \frac{1}{12\sigma_5} \frac{(3\psi - 7)(\psi - 4)}{3\psi^2 - 11\psi + 14}, \\ \sigma_{16} = \sigma_5 \frac{6\psi^5 - 24\psi^4 + 100\psi^3 - 267\psi^2 + 506\psi - 364}{(4\psi - 7)(3\psi^3 - 22\psi^2 + 23\psi + 14)}, \\ \sigma_{18} = \sigma_{19} \equiv \psi \sigma_5, \\ \sigma_{23} = \sigma_{24} = \sigma_{25} = \frac{1}{12\sigma_5} \frac{3\psi^2 - 7\psi + 16}{3\psi^2 - 11\psi + 14}, \\ \sigma_{26} = \frac{1}{18\sigma_5} \frac{21\psi^2 - 73\psi + 100}{3\psi^2 - 11\psi + 14}, \end{array} \right.$$

the equivalent partial differential equations of the D3Q27 lattice Boltzmann scheme are isotropic at fourth order of accuracy. We can make more explicit graphically the previous result. We observe in Figure 1 that the fundamental stability property $\sigma_{16} > 0$ can be maintained only if $0 < \psi < 1.5$. With this restriction, we see in Figure 1 again that Hénon's parameters σ_{10} , σ_{16} and σ_{18} remain positive only if

$$(72) \quad 1 < \frac{\sigma_4}{\sigma_5} < 2.25.$$

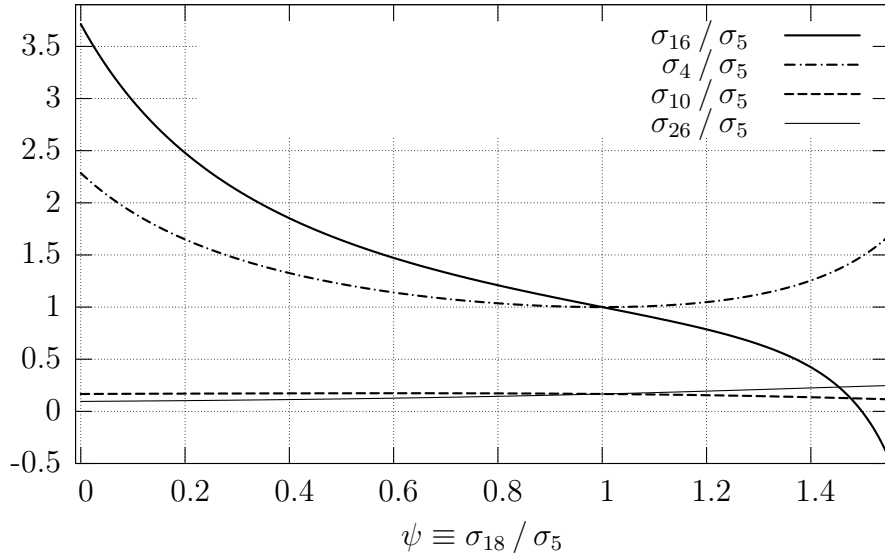


Figure 1. Fourth order isotropy parameters for the D3Q27 lattice Boltzmann scheme.

Due to the expressions (66) of the shear and the bulk viscosities, the inequality (72) imposes significant restrictions for the physical parameters μ and ζ_b . The coefficients η

and μ_4 associated with the fourth order equation (28) can be evaluated easily:

$$(73) \quad \begin{cases} \eta = \frac{\sigma_5 \lambda \Delta x^3}{108} \frac{N_\eta}{14 + 23\psi - 22\psi^2 + 3\psi^3}, \\ N_\eta = (\alpha + 2)(32\alpha - 8 - 13\alpha\psi - 35\psi - 4\alpha\psi^2 + 28\psi^2 + 3\alpha\psi^3 - 3\psi^3) \\ \mu_4 = \frac{\sigma_5 \lambda \Delta x^3}{108} \frac{132\psi\sigma_5^2 - \psi + 36\psi^2\sigma_5^2 + 168\sigma_6^2 + 3\psi^2 - 8}{3\psi^2 - 11\psi + 14}. \end{cases}$$

The expression of ζ_4 is quite long and is reported in the relation (114) of Appendix 2.

8) Conclusion

- In this contribution, we have presented the “Berliner version” of the Taylor expansion method in the linear case. This is done with explicit algebra and allows a huge reduction of computer time for formal analysis. We have also considered in all generality acoustic type partial differential equations that are rotationally invariant at an arbitrary order.
- The generalization of a methodology of group theory for discrete invariance groups of a lattice Boltzmann scheme remains still under question, in the spirit of the previous study of Rubinstein and Luo [22].
- Concerning the fundamental examples considered in this contribution, the D2Q9 scheme can be invariant by rotation at third order. At fourth order, physical parameters have to be strongly correlated. The D2Q13 scheme is invariant by rotation at fourth order for an *ad hoc* fitting of the parameters. We have not explored all the possible solutions of the strongly nonlinear set of equations that is necessary to solve in order to fit the fourth order isotropy. Numerical experiments have to confirm our theoretical considerations. The D3Q19 lattice Boltzmann scheme admits two sets of coefficients in order to impose rotational invariance at third order. Particular physics has to be imposed to satisfy fourth order isotropy. The D3Q27 scheme is rotationally invariant at fourth order for a parameterized set of parameters. Our analysis imposes restrictions for the physical parameters to guarantee the stability. A complementary numerical experiment will be welcome !

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Appendix 1. Formal expansion in the linear case

• We present in this Appendix the “Berliner version” [6] of the algorithm proposed in all generality in our contribution [9]. We suppose having defined a lattice Boltzmann scheme “DdQq” with d space dimensions and q discrete velocities at each vertex. The invertible matrix M between the particles and the moments is given:

$$(74) \quad m_k = \sum_{j=0}^{q-1} M_{kj} f_j \equiv (M \bullet f)_k, \quad 0 \leq k \leq q-1.$$

The lattice Boltzmann scheme generates N conservation laws: the first moments

$$m_k \equiv W_k, \quad 0 \leq k \leq N-1$$

are conserved during the collision step :

$$(75) \quad m^* = m_k = W_k.$$

The $q - N$ “slave” moments Y with

$$(76) \quad Y_\ell \equiv m_{N+\ell}, \quad 0 \leq \ell \leq q - N - 1$$

relax towards an equilibrium value Y_ℓ^{eq} . This equilibrium value is supposed to be a **linear** function of the state W . We introduce a constant rectangular matrix E with $N - q$ lines and N columns to represent this linear function:

$$(77) \quad Y_\ell^{\text{eq}} = \sum_{k=0}^{N-1} E_{\ell k} W_k, \quad 0 \leq \ell \leq q - N - 1.$$

The relaxation step is obtained through the usual algorithm [16] that decouples the moments:

$$(78) \quad Y_\ell^* = Y_\ell + s_\ell (Y_\ell^{\text{eq}} - Y_\ell), \quad s_\ell > 0, \quad 0 \leq \ell \leq q - N - 1.$$

Observe that the numbering of the “ s ” coefficients used in (78) differ just a little from the one used for the equation (8) and the four examples considered previously. With a matricial notation, the relaxation can be written as:

$$(79) \quad m^* = J_0 \bullet m$$

with a matrix J_0 of order q decomposed by blocks according to

$$(80) \quad J_0 = \begin{pmatrix} I_N & 0 \\ S \bullet E & I_{q-N} - S \end{pmatrix}$$

and a diagonal matrix S of order $q - N$ defined by $S \equiv \text{diag}(s_0, s_1, \dots, s_{q-N-1})$. The discrete advection step follows the method of characteristics:

$$(81) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad 0 \leq j \leq q-1.$$

• With the d’Humières’s lattice Boltzmann scheme [16] previously defined, we can proceed to a formal Taylor expansion:

$$\begin{aligned}
 m_k(t + \Delta t) &= \sum_j M_{kj} f_j^*(x - v_j \Delta t) = \sum_{j\ell} M_{kj} M_{j\ell}^{-1} m_\ell^*(x - v_j \Delta t) \\
 &= \sum_{j\ell} M_{kj} M_{j\ell}^{-1} \sum_{n=0}^{\infty} \frac{\Delta t^n}{n!} \left(- \sum_{\alpha=1}^d v_j^\alpha \partial_\alpha \right)^n m_\ell^* \\
 &= \sum_{n=0}^{\infty} \frac{\Delta t^n}{n!} \sum_{j\ell p} M_{kj} M_{j\ell}^{-1} \left(- \sum_{\alpha=1}^d v_j^\alpha \partial_\alpha \right)^n (J_0)_{\ell p} m_p.
 \end{aligned}$$

We introduce a derivation matrix of order $n \geq 0$, defined by blocks of space differential operators of order n :

$$(82) \quad \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix}_{kp} \equiv \frac{1}{n!} \sum_{j\ell} M_{kj} (M^{-1})_{j\ell} \left(- \sum_{\alpha=1}^d v_j^\alpha \partial_\alpha \right)^n (J_0)_{\ell p}, \quad n \geq 0.$$

We observe that in the relation (82), the blocks A_n and D_n are square matrices of order N and $q-N$ respectively. The matrices B_n and C_n are rectangular of order $N \times (q-N)$ and $(q-N) \times N$ respectively. We remark also that at order zero, the matrices A_0 , B_0 , C_0 and D_0 are known:

$$(83) \quad \begin{pmatrix} A_0 & B_0 \\ C_0 & D_0 \end{pmatrix} = J_0 = \begin{pmatrix} I_N & 0 \\ S \bullet E & I_{q-N} - S \end{pmatrix}.$$

The previous Taylor expansion can now be written under a matricial form:

$$(84) \quad \begin{pmatrix} W \\ Y \end{pmatrix}(x, t + \Delta t) = \sum_{n=0}^{\infty} \Delta t^n \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix} \bullet \begin{pmatrix} W \\ Y \end{pmatrix}(x, t).$$

- At order zero relative to Δt we have:

$$\begin{pmatrix} W \\ Y \end{pmatrix}(x, t) + O(\Delta t) = J_0 \bullet \begin{pmatrix} W \\ Y \end{pmatrix} + O(\Delta t) = \begin{pmatrix} W \\ S \bullet E \bullet W + (I - S) \bullet Y \end{pmatrix} + O(\Delta t)$$

and the non-conserved moments are close to the equilibrium:

$$(85) \quad Y(x, t) = E \bullet W(x, t) + O(\Delta t).$$

- We make now the hypothesis of a general form for the expansion of the nonconserved moments:

$$(86) \quad Y(x, t) = \left(E + \sum_{n \geq 1} \Delta t^n \beta_n \right) \bullet W(x, t)$$

and the hypothesis of a formal linear partial differential system of arbitrary order for the conserved variables W :

$$(87) \quad \frac{\partial W}{\partial t} = \left(\sum_{\ell \geq 0} \Delta t^\ell \alpha_{\ell+1} \right) \bullet W(x, t),$$

where α_ℓ and β_n are space differential operators of order ℓ and n respectively. We develop the first equation of (84) up to first order:

$$\begin{aligned} W + \Delta t \frac{\partial W}{\partial t} + O(\Delta t^2) &= W + \Delta t (A_1 W + B_1 Y) + O(\Delta t^2) \\ &= W + \Delta t (A_1 W + B_1 E W) + O(\Delta t^2) \end{aligned}$$

due to (85). Then

$$(88) \quad \frac{\partial W}{\partial t} = (A_1 + B_1 E) \bullet W + O(\Delta t)$$

and the relation (87) is satisfied at order one, with

$$(89) \quad \alpha_1 = A_1 + B_1 E.$$

The “Euler equations” are emerging ! We have an analogous calculus for the second equation of (84) :

$$Y + \Delta t \frac{\partial Y}{\partial t} + O(\Delta t^2) = S E W + (I - S) Y + \Delta t (C_1 W + D_1 E W) + O(\Delta t^2).$$

We clarify the time derivative $\partial_t Y$ at order zero by differentiating (formally !) the relation (85) relative to time:

$$\frac{\partial Y}{\partial t} = E \frac{\partial W}{\partial t} + O(\Delta t) = E \alpha_1 W + O(\Delta t).$$

We introduce this expression inside the previous calculus. Then:

$$S Y + \Delta t E \alpha_1 W + O(\Delta t^2) = S E W + \Delta t (C_1 W + D_1 E W) + O(\Delta t^2).$$

Consequently we have established the expansion of the nonconserved moments at order one:

$$(90) \quad Y = E W + \Delta t S^{-1} (C_1 + D_1 E - E \alpha_1) W + O(\Delta t^2)$$

with

$$(91) \quad \beta_1 = S^{-1} (C_1 + D_1 E - E \alpha_1).$$

Now, we have formally

$$\frac{\partial^2 W}{\partial t^2} = \frac{\partial}{\partial t} (\alpha_1 W + O(\Delta t)) = \alpha_1 \frac{\partial W}{\partial t} + O(\Delta t) = \alpha_1 (\alpha_1 W) + O(\Delta t) = \alpha_1^2 W + O(\Delta t)$$

and we recognize the “wave equation”

$$(92) \quad \frac{\partial^2 W}{\partial t^2} - \alpha_1^2 W = O(\Delta t).$$

• We can derive a formal expansion at order two. We go one step further in the Taylor expansion of equation (84) :

$$\begin{aligned} W + \Delta t \frac{\partial W}{\partial t} + \frac{1}{2} \Delta t^2 \alpha_1^2 W + O(\Delta t^3) &= \\ &= W + \Delta t (A_1 W + B_1 Y) + \Delta t^2 (A_2 W + B_2 Y) + O(\Delta t^3) \\ &= W + \Delta t (A_1 W + B_1 (E W + \Delta t \beta_1 W)) + \Delta t^2 (A_2 W + B_2 E W) + O(\Delta t^3) \end{aligned}$$

and dividing by Δt , we obtain a “Navier-Stokes type” second order equivalent equation:

$$\frac{\partial W}{\partial t} = \alpha_1 W + \Delta t \left(B_1 \beta_1 + A_2 + B_2 E - \frac{1}{2} \alpha_1^2 \right) W + O(\Delta t^2).$$

With the notations introduced in (87), we have made explicit the partial differential equations for the conserved variables at the order two:

$$\frac{\partial W}{\partial t} = \alpha_1 W + \Delta t \alpha_2 W + O(\Delta t^2)$$

with

$$(93) \quad \alpha_2 = A_2 + B_2 E + B_1 \beta_1 - \frac{1}{2} \alpha_1^2.$$

We remark that this Taylor expansion method can be viewed as a “numerical Chapman Enskog expansion” relative to a specific numerical parameter Δt instead of a small physical relaxation time step. For the moments Y out of equilibrium, we expand the first order derivative of Y relative to time with a formal derivation of the relation (90):

$$\begin{aligned} \frac{\partial Y}{\partial t} &= \frac{\partial}{\partial t} (E W + \Delta t \beta_1 W) + O(\Delta t^2) \\ &= E (\alpha_1 W + \Delta t \alpha_2 W) + \Delta t \beta_1 \alpha_1 W + O(\Delta t^2) \\ &= (E \alpha_1 + \Delta t (E \alpha_2 + \beta_1 \alpha_1)) W + O(\Delta t^2). \end{aligned}$$

Then

$$(94) \quad \frac{\partial Y}{\partial t} = (E \alpha_1 + \Delta t (E \alpha_2 + \beta_1 \alpha_1)) W + O(\Delta t^2).$$

Analogously for the second order time derivative:

$$(95) \quad \frac{\partial^2 Y}{\partial t^2} = E \alpha_1^2 W + O(\Delta t).$$

We re-write the second line of the expansion of the equation (84) at second order accuracy:

$$\begin{aligned} Y + \Delta t \frac{\partial Y}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 Y}{\partial t^2} + O(\Delta t^3) &= \\ &= S E W + (I - S) Y + \Delta t (C_1 W + D_1 Y) + \Delta t^2 (C_2 W + D_2 Y) + O(\Delta t^3) \end{aligned}$$

and we get

$$\begin{aligned} S Y &= S E W - \Delta t (E \alpha_1 + \Delta t (E \alpha_2 + \beta_1 \alpha_1)) W - \frac{\Delta t^2}{2} E \alpha_1^2 W \\ &\quad + \Delta t (C_1 W + D_1 (E + \Delta t \beta_1) W) + \Delta t^2 (C_2 W + D_2 E W) + O(\Delta t^3) \\ Y &= E W + \Delta t S^{-1} (C_1 + D_1 E - E \alpha_1) W \\ &\quad + \Delta t^2 S^{-1} (C_2 + D_2 E + D_1 \beta_1 - E \alpha_2 - \beta_1 \alpha_1 - \frac{1}{2} E \alpha_1^2) W + O(\Delta t^3). \end{aligned}$$

It is exactly the expansion (87) at second order :

$$Y = E W + \Delta t \beta_1 W + \Delta t^2 \beta_2 W + O(\Delta t^2)$$

with

$$(96) \quad \beta_2 = S^{-1} \left[C_2 + D_2 E + D_1 \beta_1 - E \alpha_2 - \beta_1 \alpha_1 - \frac{1}{2} E \alpha_1^2 \right]$$

• For the general case, we proceed by induction. We suppose that the developments (86) and (87) are correct up to the order k , that is:

$$(97) \quad \begin{cases} \frac{\partial W}{\partial t} = (\alpha_1 + \Delta t \alpha_2 + \dots \Delta t^{k-1} \alpha_k) W + O(\Delta t^k) \\ Y = (E + \Delta t \beta_1 + \Delta t^2 \beta_2 + \dots \Delta t^k \beta_k) W + O(\Delta t^{k+1}). \end{cases}$$

We expand the relation (84) at order $k+2$, we eliminate the zeroth order term and divide by Δt . We obtain

$$(98) \quad \frac{\partial W}{\partial t} + \sum_{j=2}^{k+1} \frac{\Delta t^{j-1}}{j!} (\partial_t^j W) + O(\Delta t^{k+1}) = \sum_{j=1}^{k+1} \Delta t^{j-1} (A_j W + B_j Y) + O(\Delta t^{k+1}).$$

The term $\partial_t^j W = (\sum_{\ell=1}^{\infty} \Delta t^{\ell-1} \alpha_{\ell})^j$ on the left hand side of (98) can be evaluated by taking the formal power of the equation (87) at the order j . We define the coefficients Γ_m^j according to:

$$(99) \quad \left(\sum_{\ell=1}^{\infty} \Delta t^{\ell-1} \alpha_{\ell} \right)^j \equiv \sum_{\ell=0}^{\infty} \Delta t^{\ell} \Gamma_{j+\ell}^j, \quad j \geq 0.$$

They can be evaluated without difficulty from the coefficients α_{ℓ} , taking care of the non-commutativity of the product of two matrices. We report the corresponding terms and we identify the coefficients in factor of Δt^k between the two sides of the equation (98), with the help of the induction hypothesis (97). We deduce:

$$(100) \quad \alpha_{k+1} = A_{k+1} + \sum_{j=1}^{k+1} B_j \beta_{k+1-j} - \sum_{j=2}^{k+1} \frac{1}{j!} \Gamma_{k+1}^j.$$

We do the same operation with the second relation of (84) :

$$(101) \quad \left\{ \begin{array}{l} Y + \sum_{j=1}^{k+1} \frac{\Delta t^j}{j!} (\partial_t^j Y) + O(\Delta t^{k+2}) = \\ = S E W + (I - S) Y + \sum_{j=1}^{k+1} \Delta t^j (C_j W + D_j Y) + O(\Delta t^{k+2}). \end{array} \right.$$

As in the previous case, we suppose that we have evaluated formally the temporal derivative

$$\begin{aligned} \partial_t^j Y &= \partial_t^j \left[(E + \Delta t \beta_1 + \Delta t^2 \beta_2 + \dots + \Delta t^k \beta_k + \dots) W \right] \\ &= (E + \Delta t \beta_1 + \Delta t^2 \beta_2 + \dots + \Delta t^k \beta_k + \dots) (\partial_t^j W) \\ &= (E + \Delta t \beta_1 + \Delta t^2 \beta_2 + \dots + \Delta t^k \beta_k + \dots) (\alpha_1 + \Delta t \alpha_2 + \dots + \Delta t^{\ell} \alpha_{\ell} + \dots)^j W \end{aligned}$$

relatively to the space derivatives. Then with the help of the induction hypothesis

$$(102) \quad \left(E + \sum_{m=1}^{\infty} \Delta t^m \beta_m \right) \left(\sum_{p=1}^{\infty} \Delta t^{p-1} \alpha_p \right)^j \equiv \sum_{\ell=0}^{\infty} \Delta t^{\ell} K_{j+\ell}^j, \quad j \geq 0,$$

we identify the two expressions of the coefficient of Δt^{k+1} issued from the equation (101):

$$(103) \quad S \beta_{k+1} = C_{k+1} + \sum_{j=1}^{k+1} D_j \beta_{k+1-j} - \sum_{j=1}^{k+1} \frac{1}{j!} K_{k+1}^j.$$

• The explicitation of the coefficients $\Gamma_{j+\ell}^j$ and K_{k+1}^j of the matricial formal series is now easy, due to the relations (99) and (102). We specify the coefficients $\Gamma_{j+\ell}^{\ell}$ obtained

in the matricial formal series (99). For $j = 0$, the power in relation (99) is the identity. Then

$$(104) \quad \Gamma_0^0 = I, \quad \Gamma_\ell^0 = 0, \quad \ell \geq 1.$$

When $j = 1$, the initial series is not changed. Then

$$(105) \quad \Gamma_\ell^1 = \alpha_\ell, \quad \ell \geq 1.$$

For $j = 2$, we have to compute the square of the initial series, paying attention that the matrix operators α_ℓ do not commute. Observe that with the formal Chapman-Enskog method used *e.g.* in [16], non-commutation relations have also to be taken into consideration for higher order terms in the case of several conserved moments. We have

$$\left(\sum_{\ell=1}^{\infty} \Delta t^\ell \alpha_{\ell+1} \right) \left(\sum_{j=1}^{\infty} \Delta t^j \alpha_{j+1} \right) = \sum_{p=0}^{\infty} \Delta t^p \sum_{\ell+j=p} \alpha_{\ell+1} \alpha_{j+1}$$

and we have in particular

$$(106) \quad \Gamma_2^2 = \alpha_1^2, \quad \Gamma_3^2 = \alpha_1 \alpha_2 + \alpha_2 \alpha_1, \quad \Gamma_4^2 = \alpha_1 \alpha_3 + \alpha_2^2 + \alpha_3 \alpha_1.$$

In the general case, we have

$$\left(\sum_{\ell=0}^{\infty} \Delta t^\ell \alpha_{\ell+1} \right)^j = \sum_{\ell=0}^{\infty} \Delta t^\ell \sum_{\ell_1+\dots+\ell_j=\ell} \alpha_{\ell_1+1} \dots \alpha_{\ell_j+1}$$

and in consequence

$$(107) \quad \Gamma_{p+j}^j = \sum_{\ell_1+\dots+\ell_j=p} \alpha_{\ell_1+1} \dots \alpha_{\ell_j+1}.$$

We have in particular for $j = 3$ and $j = 4$:

$$(108) \quad \Gamma_3^3 = \alpha_1^3, \quad \Gamma_4^3 = \alpha_1^2 \alpha_2 + \alpha_1 \alpha_2 \alpha_1 + \alpha_2 \alpha_1^2, \quad \Gamma_4^4 = \alpha_1^4.$$

For the explicitation of the coefficients K_{k+1}^j , we can replace the power of the formal series of the relation (99) in the relation (102). We obtain, with the notation $\beta_0 \equiv E$,

$$\left(\sum_{m=0}^{\infty} \Delta t^m \beta_m \right) \left(\sum_{\ell=0}^{\infty} \Delta t^\ell \Gamma_{j+\ell}^j \right) \equiv \sum_{p=0}^{\infty} \Delta t^p K_{j+p}^j$$

then we have by induction

$$(109) \quad K_{j+p}^j = \sum_{m+\ell=p} \beta_m \Gamma_{j+\ell}^j.$$

For $j = 0$, we deduce

$$(110) \quad K_0^0 = E, \quad K_p^0 = 0, \quad p \geq 1$$

and for $j = 1$, we have a simple product of two formal series:

$$(111) \quad K_p^1 = E \alpha_p + \beta_1 \alpha_{p-1} + \dots + \beta_{p-1} \alpha_1, \quad p \geq 1.$$

We specify some particular values of the coefficients K_{j+p}^j when $j = 2$, $j = 3$ and for $j = 4$:

$$(112) \quad \begin{cases} K_2^2 = E \Gamma_2^2, & K_3^2 = E \Gamma_3^2 + \beta_1 \Gamma_2^2, & K_4^2 = E \Gamma_4^2 + \beta_1 \Gamma_3^2 + \beta_2 \Gamma_2^2, \\ K_3^3 = E \Gamma_3^3, & K_4^3 = E \Gamma_4^3 + \beta_1 \Gamma_3^3, & K_4^4 = E \Gamma_4^4. \end{cases}$$

- It is now possible to make explicit up to fourth order to fix the ideas the matricial coefficients of the expansion (86) of the nonconserved moments and of the associated partial differential equation (87). We have, following the natural order of the algorithm:

$$(113) \quad \left\{ \begin{array}{l} \beta_0 = E \\ \alpha_1 = A_1 + B_1 E \\ \beta_1 = S^{-1} (C_1 + D_1 E - K_1^1) \\ \alpha_2 = A_2 + B_2 E + B_1 \beta_1 - \frac{1}{2} \Gamma_2^2 \\ \beta_2 = S^{-1} \left[C_2 + D_2 E + D_1 \beta_1 - K_2^1 - \frac{1}{2} K_2^2 \right] \\ \alpha_3 = A_3 + B_1 \beta_2 + B_2 \beta_1 + B_3 E - \frac{1}{2} \Gamma_3^2 - \frac{1}{6} \Gamma_3^3 \\ \beta_3 = S^{-1} \left[C_3 + D_1 \beta_2 + D_2 \beta_1 + D_3 E - K_3^1 - \frac{1}{2} K_3^2 - \frac{1}{6} K_3^3 \right] \\ \alpha_4 = A_4 + B_1 \beta_3 + B_2 \beta_2 + B_3 \beta_1 + B_4 E - \frac{1}{2} \Gamma_4^2 - \frac{1}{6} \Gamma_4^3 - \frac{1}{24} \Gamma_4^4. \end{array} \right.$$

Observe that with the explicit relations (113), the computer time for deriving formally the equivalent partial equation like (97) at fourth order of accuracy has been reduced by three orders of magnitude (!) in comparison with the algorithm presented in the contribution [9].

Appendix 2. A specific algebraic coefficient

- With Hénon's coefficients σ_j defined according to (18), a numbering of the D3Q27 moments proposed in (60), the equilibrium of the energy (16) parametrized by α , and the parameter ψ introduced in (70), the coefficient ζ_4 for the fourth order term in (28) can be evaluated according to:

$$(114) \quad \left\{ \begin{aligned} \zeta_4 &= \frac{1}{108} \frac{\sigma_5 \lambda \Delta x^3}{(4\psi - 7)(3\psi^2 - 11\psi + 14)(14 + 23\psi - 22\psi^2 + 3\psi^3)^3} N_4 \\ N_4 &= -526848 - 13105344\sigma_5^2 + 56334931\psi^6\alpha - 3413088\psi^2 \\ &\quad + 29925576\psi^3 + 44310000\sigma_5^2\psi^3\alpha^2 + 2458624\alpha^2 - 7776\sigma_5^2\psi^{12} \\ &\quad + 116153808\sigma_5^2\psi^7 + 16213680\sigma_5^2\psi^9 - 56871552\sigma_5^2\psi^8 - 2696976\sigma_5^2\psi^{10} \\ &\quad + 803992\psi\alpha - 16250948\psi^2\alpha + 15057742\psi^3\alpha + 236520\sigma_5^2\psi^{11} \\ &\quad - 47554008\sigma_5^2\psi^5\alpha^2 + 414648\sigma_5^2\psi^9\alpha^2 + 5924856\sigma_5^2\psi^7\alpha^2 \\ &\quad - 3520104\sigma_5^2\psi^8\alpha^2 + 7776\sigma_5^2\psi^{12}\alpha^2 - 73224\sigma_5^2\psi^{11}\alpha^2 - 1805156\psi^8\alpha^2 \\ &\quad - 1316084\psi^7\alpha^2 + 13802956\psi^6\alpha^2 - 29063324\psi^5\alpha^2 + 25708132\psi^4\alpha^2 \\ &\quad - 1230152\psi^3\alpha^2 + 3742816\alpha^2\psi + 27756\psi^{11}\alpha^2 - 3429\psi^{11}\alpha \\ &\quad - 187851264\sigma_5^2\alpha^2\psi^2 + 198524928\sigma_5^2\alpha^2\psi + 195048\sigma_5^2\psi^{10}\alpha^2 \\ &\quad - 12827088\psi^4 + 100016448\sigma_5^2\psi - 10762392\sigma_5^2\psi^3 \\ &\quad - 287184\sigma_5^2\psi^5 - 117365232\sigma_5^2\psi^6 + 102921792\sigma_5^2\psi^4 - 131926368\sigma_5^2\psi^2 \\ &\quad - 6082272\psi + 22678777\psi^4\alpha - 58798343\psi^5\alpha + 316283520\sigma_5^2\psi\alpha \\ &\quad - 421440000\sigma_5^2\psi^2\alpha + 148286280\sigma_5^2\psi^3\alpha + 2458624\alpha - 1296\psi^{12}\alpha^2 \\ &\quad - 324\psi^{12}\alpha - 12657680\psi^2\alpha^2 + 169965\psi^{10}\alpha - 1834629\psi^9\alpha \\ &\quad + 9787591\psi^8\alpha - 30298973\psi^7\alpha - 235980\psi^{10}\alpha^2 + 989292\psi^9\alpha^2 \\ &\quad + 55400808\sigma_5^2\psi^4\alpha^2 - 3888\sigma_5^2\psi^{12}\alpha + 223236\sigma_5^2\psi^{11}\alpha \\ &\quad - 2725812\sigma_5^2\psi^{10}\alpha + 15619428\sigma_5^2\psi^9\alpha - 48491916\sigma_5^2\psi^8\alpha \\ &\quad + 75338436\sigma_5^2\psi^7\alpha + 8771448\sigma_5^2\psi^6\alpha^2 - 78989568\sigma_5^2\alpha \\ &\quad - 6400920\psi^9 - 56568924\psi^7 + 24275088\psi^8 + 3240\psi^{12} - 88452\psi^{11} \\ &\quad - 46884384\psi^5 + 76942908\psi^6 + 151481100\sigma_5^2\psi^4\alpha - 12989436\sigma_5^2\psi^6\alpha \\ &\quad - 141331668\sigma_5^2\psi^5\alpha + 1015308\psi^{10} - 77070336\sigma_5^2\alpha^2. \end{aligned} \right.$$

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