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Towards higher order lattice Boltzmann schemes

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Abstract. – In this contribution we extend the Taylor expansion method proposed previously by one of us and establish equivalent partial differential equations of the lattice Boltzmann scheme proposed by d’Humières [11] at an arbitrary order of accuracy. We derive formally the associated dynamical equations for classical thermal and linear fluid models in one to three space dimensions. We use this approach to adjust “quartic” relaxation parameters in order to enforce fourth order accuracy for thermal model and diffusive relaxation modes of the Stokes problem. We apply the resulting scheme for numerical computation of associated eigenmodes, compare our results with analytical references and observe fourth-order accuracy when using “quartic” parameters.

Keywords: Lattice Boltzmann Equation, Taylor expansion method, thermics, linearized Navier–Stokes, quartic parameters, formal calculus.

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1 Introduction

- The lattice Boltzmann scheme is a numerical method for simulation of a wide family of partial differential equations associated with conservation laws of physics. The principle is to mimic at a discrete level the dynamics of the Boltzmann equation. In this paradigm, the number $f(x, t) dx dv$ of particles at position x , time t and velocity v with an uncertainty of $dx dv$ follows the Boltzmann partial differential equation in the phase space (see *e.g.* Chapman and Cowling [7]):

$$(1) \quad \frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f).$$

- Note that the left hand side is a simple advection equation whose solution is trivial through the method of characteristics:

$$(2) \quad f(x, v, t) = f(x - vt, v, 0) \quad \text{if } Q(f) \equiv 0.$$

Remark also that the right hand side is a collision operator, local in space and integral relative to velocities:

$$(3) \quad Q(f)(x, v, t) = \int \mathcal{C}(f(x, w, t), x, v, t) dw,$$

where $\mathcal{C}(\bullet)$ describes collisions at a microscopic level. Due to microscopic conservation of mass, momentum and energy, an equilibrium distribution $f^{\text{eq}}(x, v, t)$ satisfy the nullity of first moments of the distribution of collisions:

$$\int Q(f^{\text{eq}})(x, v, t) \begin{pmatrix} 1 \\ v \\ \frac{1}{2} |v|^2 \end{pmatrix} dv = 0.$$

Such an equilibrium distribution f^{eq} satisfies classically the Maxwell-Boltzmann distribution.

- The lattice Boltzmann method follows all these physical recommendations with specific additional options. First, space x is supposed to live in a lattice \mathcal{L} included in Euclidian space of dimension d . Second, velocity belongs to a finite set \mathcal{V} composed by given velocities v_j ($0 \leq j \leq J$) chosen in such a way that

$$x \in \mathcal{L} \text{ and } v_j \in \mathcal{V} \implies x + \Delta t v_j \in \mathcal{L},$$

where Δt is the time step of the numerical method. Then the distribution of particles, f , is denoted by $f_j(x, t)$ with $0 \leq j \leq J$, x in the lattice \mathcal{L} and t an integer multiple of time step Δt .

- In the pioneering work of cellular automata introduced by Hardy, Pomeau and De Pazzis [24], Frisch, Hasslacher and Pomeau [18] and developed by d’Humières, Lallemand and Frisch [13], the distribution $f_j(x, t)$ was chosen as Boolean. Since the so-called lattice Boltzmann equation of Mac Namara and Zanetti [35], Higuera, Succi and Benzi [27], Chen, Chen and Matthaeus [8], Higuera and Jimenez [26] (see also Chen and Doolen [9]), the distribution $f_j(\bullet, \bullet)$ takes real values in a continuum and the collision process follows a linearized approach of Bhatnagar, Gross and Krook [4]. With Qian, d’Humières and Lallemand [38], the equilibrium distribution f^{eq} is determined with a polynomial in velocity. In the work of Karlin *et al* [29], the equilibrium state is obtained with a general methodology of entropy minimization.

- The numerical scheme is defined through the evolution of a population $f_j(x, t)$, with $x \in \mathcal{L}$ and $0 \leq j \leq J$ towards a distribution $f_j(x, t + \Delta t)$ at a new discrete time. The scheme is composed by two steps that take into account successively the left and right hand sides of the Boltzmann equation (1). The first step describes the relaxation $f \rightarrow f^*$ of particle distribution f towards the equilibrium. It is local in space and nonlinear in general. D. d’Humières first introduced in [11] the fundamental notion of moments in the context of lattice Boltzmann schemes. He defines an invertible matrix M with $(J + 1)$ lines and $(J + 1)$ columns and the moments m through a simple linear relation

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

- The first N moments are supposed to be at equilibrium:

$$(5) \quad m_i^* = m_i \equiv m_i^{\text{eq}} \equiv W_i, \quad 0 \leq i \leq N - 1$$

and we introduce the vector $W \in \mathbb{R}^N$ of conserved variables composed of the W_i for $0 \leq i \leq N - 1$: $W_i \equiv m_i^{\text{eq}}$, $0 \leq i \leq N - 1$. The first moments at equilibrium are respectively the total density

$$(6) \quad \rho \equiv \sum_{j=0}^J f_j,$$

momentum

$$(7) \quad q_\alpha \equiv \sum_{j=0}^J v_j^\alpha f_j, \quad 1 \leq \alpha \leq d$$

and possibly the energy [31] for Navier–Stokes fluid simulations. In consequence, we have

$$(8) \quad M_{0j} \equiv 1, \quad 0 \leq j \leq J$$

$$(9) \quad M_{\alpha j} \equiv v_j^\alpha, \quad 1 \leq \alpha \leq d, \quad 0 \leq j \leq J.$$

For the other moments, we suppose given $(J + 1 - N)$ (nonlinear) functions $G_k(\bullet)$

$$(10) \quad \mathbb{R}^N \ni W \longmapsto G_k(W) \in \mathbb{R}, \quad N \leq k \leq J$$

that define equilibrium moments m_k^{eq} according to the relation

$$(11) \quad m_k^{\text{eq}} = G_k(W), \quad N \leq k \leq J.$$

Note also that more complicated models have been developed in Yeomans's group (see *e.g.* Marenduzzo *at al* [36]) for modelling of liquid crystals.

- The relaxation process is related to the linearized collision operator introduced at relation (3). In particular intermolecular interactions (Maxwell molecules with a $1/r^4$ potential), the collision operator is exactly solvable in terms of so-called Sonine polynomials (see *e.g.* Chapman and Cowling [7]) and the eigenvectors are known. Moreover, the discrete model is highly constrained by symmetry and exchanges of coordinates. In the work of d'Humières [11], relaxation parameters (also named as s -parameters in the following) s_k ($N \leq k \leq J$) are introduced, satisfying for stability constraints (see *e.g.* [30]) the conditions

$$0 < s_k < 2, \quad N \leq k \leq J.$$

Then the nonconserved momenta m_k^* after collision are supposed to satisfy

$$(12) \quad m_k^* = m_k + s_k (m_k^{\text{eq}} - m_k), \quad k \geq N$$

and we will denote by S the diagonal matrix of order $J+1-N$ whose diagonal coefficients are equal to s_k :

$$(13) \quad S_{k\ell} \equiv \delta_{k\ell} s_\ell, \quad k, \ell \geq N$$

with $\delta_{k\ell}$ the Kroneker symbol equal to 1 if $k = \ell$ and null in the other cases. Remark that this framework is general: when the matrix S is proportional to identity, the d'Humières scheme degenerates to the popular “BGK” method characterized by a “Single Relaxation Rate”. In this particular case the relaxation operator is diagonal and there is no particular diagonalization basis to work with. The distribution f^* after collision is reconstructed by inversion of relation (4):

$$(14) \quad f_j^* = \sum_{\ell=0}^J M_{j\ell}^{-1} m_\ell^*, \quad 0 \leq j \leq J.$$

- We suppose also that the set of velocities \mathcal{V} is invariant by space reflection:

$$v_j \in \mathcal{V} \implies \exists \ell \in \{0, \dots, J\}, v_\ell = -v_j, v_\ell \in \mathcal{V}.$$

The second step is the advection that mimic at the discrete level the free evolution through characteristics (2):

$$(15) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad x \in \mathcal{L}, 0 \leq j \leq J, v_j \in \mathcal{V}.$$

Note that all physical relaxation processes are described in space of moments. Nevertheless, evolution equation (15) is the key issue of forthcoming expansions.

- The asymptotic analysis of cellular automata (see *e.g.* Hénon [25]) provides evidence supporting asymptotic partial differential equations and viscosity coefficients related to the induced parameter defined by

$$(16) \quad \sigma_k \equiv \frac{1}{s_k} - \frac{1}{2}.$$

The lattice Boltzmann scheme (4) to (15) has been analyzed by d’Humières [11] with a Chapman-Enskog method coming from statistical physics. Remark that the extension of the discrete Chapman-Enskog expansion to higher order already exists (Qian-Zhou [39], d’Humières [12]). But the calculation in the nonthermal case ($N > 1$) is quite delicate from an algebraic point of view and introduces noncommutative formal operators. Recently, Junk and Rheinländer [28] developed a Hilbert type expansion for the analysis of lattice Boltzmann schemes at high order of accuracy. We have proposed in previous works [14, 15] the Taylor expansion method which is an extension to the lattice Boltzmann scheme of the so-called equivalent partial differential equation method proposed independently by Lerat and Peyret [33] and by Warming and Hyett [48]. In this framework, the parameter Δt is considered as the only infinitesimal variable and we introduce a **constant** velocity ratio λ between space step and time step:

$$(17) \quad \lambda \equiv \frac{\Delta x}{\Delta t}.$$

The lattice Boltzmann scheme is classically considered as second-order accurate (see *e.g.* [30]). In fact, the viscosity coefficients μ relative to second-order terms are recovered according to a relation of the type

$$\mu = \zeta \lambda^2 \Delta t \sigma_k$$

for a particular value of label k . The coefficient ζ is equal to $\frac{1}{3}$ for the simplest models that are considered hereafter.

- A natural question is to extend this accuracy to third or higher orders. In the case of single relaxation times (the BGK variant of d’Humières scheme), progresses in this direction have been proposed by Shan *et al* [44, 45] and Philippi *et al* [37] using Hermite

polynomial methodology for the approximation of the Boltzmann equation. The price to pay is an extension of the stencil of the numerical scheme and the practical associated problems for the numerical treatment of boundary conditions. Note also the work of the Italian team (Sbragaglia *et al* [42], Falcucci *et al* [17]) on application to multiphase flows. In the context of scheme with multiple relaxation times, Ginzburg, Verhaeghe and d’Humières have analyzed with the Chapman-Enskog method the “Two Relaxation Times” version of the scheme [22, 23]. A nonlinear extension of this scheme, the so-called “cascaded lattice Boltzmann method” has been proposed by Geier *et al* [19]. It gives also high order accuracy and the analysis is under development (see *e.g.* Asinari [3]). The general nonlinear extension of the Taylor expansion method to third-order of accuracy of d’Humières scheme is presented in [16]. It provides evidence of the importance of the so-called tensor of momentum-velocity defined by

$$(18) \quad \Lambda_{kp}^\ell \equiv \sum_{j=0}^J M_{kj} M_{pj} M_{j\ell}^{-1}, \quad 0 \leq k, p, \ell \leq J.$$

Moreover, it shows also that for athermal Navier Stokes equations, the mass conservation equation contains a remaining term of third-order accuracy that cannot be set to zero by fitting relaxation parameters [16].

- Our motivation in this contribution is to show that it is possible to extend the order of accuracy of an *existing a priori* second-order accurate lattice Boltzmann scheme to higher orders. We use the Taylor expansion method [15] to determine the equivalent partial differential equation of the numerical scheme to higher orders of accuracy. Nevertheless, it is quite impossible to determine explicitly the entire expansion in all generality in the nonlinear case. In consequence, we restrict here to a first step. We propose in the following a general methodology for deriving the equivalent equation of the d’Humières scheme at an arbitrary order when the collision process defined by the functions G_k of relation (10) are **linear**. This calculation leads to explicit developments that can be expanded with the help of formal calculation. This work is detailed in Section 2. In Section 3 we apply the general methodology to classical linear models of thermics and linearized athermal Navier Stokes equations. We treat fundamental examples from one to three space dimensions. When it is possible, the equivalent partial equivalent equations are explicit. In Section 4, we use the fourth-order equivalent equation of two and three-dimensional models to enforce accuracy through a proper choice of “quartic” parameters. For a scalar heat equation, the effect of the precision of the numerical computation of eigenmodes is presented. For linearized athermal Navier Stokes equations, we propose a method for enforcing the precision of the eigenmodes of the associated partial differential equation. First numerical results show that for appropriate tuning values of the parameters, fourth-order precision is achieved.

2 Formal development of linearized d'Humières scheme

• In what follows, we suppose that the collision process is **linear** *i.e.* that the G_k functions introduced in (10) (11) are linearized around some reference state. With this hypothesis, we can write:

$$G_k(W) \equiv \sum_{j=0}^N G_{kj} W_j = \sum_{j=0}^N G_{kj} m_j, \quad k \geq N.$$

To be precise, putting together relations (11) and (12), there exists a $(J+1) \times (J+1)$ matrix Ψ such that the collided momentum m^* defined in (12) is a linear combination of the moments before collision:

$$(19) \quad m^* = \Psi \bullet m, \quad m_k^* = \sum_{j=0}^J \Psi_{kj} m_j.$$

Of course, the conservation (9) implies that Ψ has a structure of the type

$$(20) \quad \Psi = \begin{pmatrix} \mathbf{I} & 0 \\ \Phi & \mathbf{I} - S \end{pmatrix}.$$

The top left block of the right hand side of (20) is the identity matrix of dimension N and the bottom left block is described through the G_k functions introduced in (10) (11):

$$(21) \quad \Phi_{kj} \equiv \Psi_{kj} = s_k G_{kj}, \quad j < N, \quad k \geq N.$$

The bottom right block of the right hand side of (20) contains the coefficients $1 - s_k$ ($k \geq N$) related to relaxation (13).

• In order to make our result explicit, we need some notations. We introduce multi-indices $\gamma, \delta, \varepsilon$ in $\{1, \dots, d\}^q$ in order to represent multiple differentiation with respect to space. If

$$\gamma = \left(\underbrace{1, \dots, 1}_{\alpha_1 \text{ times}}, \dots, \underbrace{d, \dots, d}_{\alpha_d \text{ times}} \right),$$

then

$$\partial_\gamma \equiv \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}$$

and we denote by $|\gamma|$ the length of multi-index γ :

$$|\gamma| \equiv \alpha_1 + \cdots + \alpha_d.$$

Then thanks to the binomial formula for iterated differentiation, we can introduce coefficients $P_{\ell\gamma}$ in order to satisfy the identity

$$(22) \quad \left(- \sum_{\alpha=1}^d M_{\alpha\ell} \partial_\alpha \right)^q \equiv \sum_{|\gamma|=q} P_{\ell\gamma} \partial_\gamma.$$

for any integer q .

- We first establish that at first-order of accuracy, we have a representation of nonconserved moments in terms of conservative variables:

$$(23) \quad m_k = \sum_{j=0}^J B_{kj}^0 W_j + O(\Delta t), \quad k \geq N.$$

with

$$(24) \quad B_{kj}^0 \equiv \frac{1}{s_k} \Psi_{kj}, \quad k \geq N, \quad 0 \leq j \leq N-1.$$

We have also the first-order conservation law

$$(25) \quad \frac{\partial W_i}{\partial t} + \sum_{|\gamma|=1} A_{ij}^\gamma \partial_\gamma W_j = O(\Delta t), \quad 0 \leq i \leq N-1.$$

with coefficients A_{ij}^γ given according to

$$(26) \quad A_{ij}^\gamma \equiv \sum_{p=0}^J \Lambda_{\gamma i}^p \left(\Psi_{pj} + \sum_{\ell \geq N} \Psi_{p\ell} \frac{1}{s_\ell} \Psi_{\ell j} \right), \quad |\gamma|=1, \quad 0 \leq i, j \leq N-1.$$

The proof of this result and those that follow of this Section are detailed in Appendix A.

- The expansion of moments (23) can be extended to second-order accuracy:

$$(27) \quad m_k = \sum_{0 \leq |\gamma| \leq 1} \Delta t^{|\gamma|} B_{kj}^\gamma \partial_\gamma W_j + O(\Delta t^2).$$

with

$$(28) \quad \left\{ \begin{array}{l} B_{kj}^\gamma = \frac{1}{s_k^2} \sum_{i=0}^{N-1} \Psi_{ki} A_{ij}^\gamma - \frac{1}{s_k} \sum_{r=0}^J \frac{1}{s_r} \sum_{p=0}^J \Lambda_{\gamma k}^p \Psi_{pr} \Psi_{rj}, \\ |\gamma|=1, \quad k \geq N, \quad 0 \leq j \leq N-1. \end{array} \right.$$

- Then we extend the previous expansions (25) and (27) to any order σ . By induction, we establish that we have an equivalent partial differential equation of the form

$$(29) \quad \frac{\partial W_i}{\partial t} + \sum_{1 \leq |\gamma| \leq \sigma} \Delta t^{|\gamma|-1} \sum_{j=0}^{N-1} A_{ij}^\gamma \partial_\gamma W_j = O(\Delta t^\sigma), \quad 0 \leq i \leq N-1,$$

and an expansion of nonconserved moments as

$$(30) \quad m_k = \sum_{0 \leq |\gamma| \leq \sigma} \Delta t^{|\gamma|} \sum_{j=0}^{N-1} B_{kj}^\gamma \partial_\gamma W_j + O(\Delta t^{\sigma+1}), \quad k \geq N,$$

with the following recurrence relations for defining the coefficients A_{ij}^γ and B_{kj}^γ :

$$(31) \quad C_{ij}^{1,\gamma} = A_{ij}^\gamma, \quad 0 \leq i, j \leq N-1,$$

$$(32) \quad \left\{ \begin{array}{l} C_{ij}^{q+1,\gamma} = - \sum_{\delta \geq q, \varepsilon \geq 1, \delta + \varepsilon = \gamma} \sum_{\ell=0}^J C_{i\ell}^{q,\delta} A_{\ell j}^\varepsilon, \\ 2 \leq q+1 \leq |\gamma|, \quad 0 \leq i, j \leq N-1, \end{array} \right.$$

$$(33) \quad \left\{ \begin{array}{l} A_{ij}^\gamma = - \sum_{q=2}^{|\gamma|} \frac{1}{q!} C_{ij}^{q,\gamma} \\ - \sum_{1 \leq |\delta| \leq |\gamma|, 0 \leq |\varepsilon| \leq |\gamma| - 1, \delta + \varepsilon = \gamma} \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J \frac{1}{|\delta|!} M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} B_{rj}^\varepsilon, \end{array} \right.$$

$$(34) \quad D_{kj}^{0,\gamma} = B_{kj}^\gamma, \quad k \geq N, \quad 0 \leq j \leq N-1,$$

$$(35) \quad \left\{ \begin{array}{l} D_{kj}^{q+1,\gamma} = - \sum_{|\delta| \geq q, |\varepsilon| \geq 1, \delta + \varepsilon = \gamma} \sum_{\ell=0}^J D_{k\ell}^{q,\delta} A_{\ell j}^\varepsilon, \\ 1 \leq q+1 \leq |\gamma|, \quad k \geq N, \quad 0 \leq j \leq N-1, \end{array} \right.$$

$$(36) \quad \left\{ \begin{array}{l} B_{kj}^\gamma = \frac{1}{s_k} \left(- \sum_{1 \leq q \leq |\gamma|} \frac{1}{q!} D_{kj}^{q,\gamma} \right. \\ \left. + \sum_{1 \leq |\delta| \leq |\gamma|, 0 \leq |\varepsilon| \leq |\gamma| - 1, \delta + \varepsilon = \gamma} \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J \frac{1}{|\delta|!} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} B_{rj}^\varepsilon \right), \\ k \geq N, \quad 0 \leq j \leq N-1. \end{array} \right.$$

- Note that the results (33) and (36) are coupled through the relations (31) (32) (34) and (35). For example, the evaluation of coefficient $D_{kj}^{q+1,\gamma}$ uses explicitly $A_{\ell j}^\varepsilon$, the evaluation of A_{ij}^γ uses B_{rj}^ε and the computation of B_{rj}^γ is impossible if $D_{kj}^{q,\gamma}$ is not known.

The proof is detailed in Appendix A. It is an elementary and relatively lengthy algebraic calculation. In particular, our mathematical framework is classical: all differential operators commute and the technical difficulties of noncommutative time derivative operators associated with the use of formal Chapman-Enskog method [12] vanish. As a result, the general expansion of a linearized d’Humières scheme at an arbitrary order can be obtained by making explicit the coefficients A_{ij}^γ and B_{kj}^γ . Remark that the hypothesis of linearity allows making the above formulae explicit and we have done this work with the help of formal calculation. Nevertheless, it is always possible to suppose that the G_k functions are linearized expansions of a nonlinear equilibrium. In this case, the previous equivalent high order partial differential equations (29) give a very good information concerning the behavior of the scheme.

3 Equivalent Thermics and Fluid equations

- We make explicit in this section the fourth-order equivalent equation (29) of some lattice Boltzmann schemes for two fundamental problems of mathematical physics: thermics and linearized athermal Navier-Stokes equations. We treat first advective thermics in one space dimension with the so-called D1Q3 lattice Boltzmann scheme. In order to obtain results presentable on a sheet of paper, we simplify the model and omit the advective term for two (D2Q5) and three (D3Q7) space dimensions. Secondly we study linearized athermal Navier-Stokes equations in one (D1Q3), two (D2Q9) and three (D3Q19) space dimensions. Note that we have to define precisely our results. First the numbering of degrees of freedom *via* corresponding graphics is specified; see Appendix B. The choice of moments, *id est* the M matrix, is also made precise in Appendix B. Secondly the Ψ matrix of relation (19) is specified, later in this section.

- **D1Q3 for advective thermics at fourth-order**

For a thermics problem, we have only one conserved quantity. Then $N = 1$ in relation (5). The two nonconserved moments (momentum q^{eq} and energy ϵ^{eq} ; see (78)) at equilibrium are supposed to be **linear** functions of the conserved momentum ρ :

$$(37) \quad q^{\text{eq}} = u \lambda \rho, \quad \epsilon^{\text{eq}} = \alpha \frac{\lambda^2}{2} \rho.$$

Due to (21) and (37), the matrix Ψ for dynamics relation (19) is given according to

$$\Psi = \begin{pmatrix} 1 & 0 & 0 \\ s_1 u \lambda & 1 - s_1 & 0 \\ \alpha s_2 \lambda^2 / 2 & 0 & 1 - s_2 \end{pmatrix}.$$

We determine without difficulty the equivalent partial differential equation for this lattice Boltzmann scheme at order four, to fix the ideas. For $i = 1, 2$, we introduce σ_i from

relaxation time s_i according to relation (16). When a drift in velocity u is present, note that the diffusion coefficient is a function of mean value velocity. We have

$$(38) \quad \frac{\partial \rho}{\partial t} + u \lambda \frac{\partial \rho}{\partial x} - \sigma_1 \Delta t \lambda^2 (\alpha - u^2) \frac{\partial^2 \rho}{\partial x^2} + \kappa_3 \frac{\Delta t^2 \lambda^3}{12} \frac{\partial^3 \rho}{\partial x^3} + \kappa_4 \frac{\Delta t^3 \lambda^4}{12} \frac{\partial^4 \rho}{\partial x^4} = O(\Delta t^4)$$

with parameters κ_3 and κ_4 given according to

$$\begin{aligned} \kappa_3 &= -u \left(2(1 - 12\sigma_1^2)u^2 + 1 - 3\alpha - 12\sigma_1\sigma_2(1 - \alpha) + 24\sigma_1^2\alpha \right) \\ \kappa_4 &= \left(-9 + 60\sigma_1^2 \right) \sigma_1 u^4 + \left(-5(1 - 3\alpha)\sigma_1 - 3(1 - \alpha)\sigma_2 + \right. \\ &\quad \left. + 12(1 - \alpha)\sigma_1\sigma_2 + 36(1 - \alpha)\sigma_1^2\sigma_2 - 72\sigma_1^3\alpha \right) u^2 \\ &\quad + \alpha \sigma_1 \left(2 - 3\alpha - 12(1 - \alpha)\sigma_1\sigma_2 + 12\alpha\sigma_1^2 \right). \end{aligned}$$

If $u = 0$, then $\kappa_3 = 0$ and the scheme is equivalent to an advection-diffusion equation up to third-order accuracy. In this particular case, the scheme is fourth-order accurate in the previous sense if we set

$$\sigma_2 = \frac{2 - 3\alpha + 12\alpha\sigma_1^2}{12\sigma_1(1 - \alpha)}.$$

- **D2Q5 for pure thermics at fourth-order**

We have $J = 4$ and $N = 1$. The equilibrium energy (momentum m_3 in (79) with the labelling conventions of Section 1) is the only one to be non equal to zero. The matrix Ψ of relation (19) is now given by the relation

$$(39) \quad \Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 - s_1 & 0 & 0 & 0 \\ 0 & 0 & 1 - s_1 & 0 & 0 \\ \alpha s_3 & 0 & 0 & 1 - s_3 & 0 \\ 0 & 0 & 0 & 0 & 1 - s_4 \end{pmatrix}.$$

We have developed the conservation law up to fourth-order:

$$(40) \quad \left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} - \frac{\lambda^2 \Delta t}{10} \sigma_1 (4 + \alpha) \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) \\ + \frac{\Delta t^3 \lambda^4}{1200} \sigma_1 (4 + \alpha) \left(\kappa_{40} \left(\frac{\partial^4 \rho}{\partial x^4} + \frac{\partial^4 \rho}{\partial y^4} \right) + \kappa_{22} \frac{\partial^4 \rho}{\partial x^2 \partial y^2} \right) \end{array} \right. = O(\Delta t^4)$$

and the κ coefficients are explicitated as follows:

$$(41) \quad \kappa_{40} = 8 - 3\alpha + 12(\alpha + 4)\sigma_1^2 - 12(1 - \alpha)\sigma_1\sigma_3 - 60\sigma_1\sigma_4$$

$$(42) \quad \kappa_{22} = -6(\alpha + 4) + 24(\alpha + 4)\sigma_1^2 - 24(1 - \alpha)\sigma_1\sigma_3 + 120\sigma_1\sigma_4.$$

- **D2Q9 for advective thermics at fourth-order**

The lattice Boltzmann model D2Q9 for a passive scalar (see Chen, Ohashi and Akiyama [10], Shan [43], Ginzburg [20]) is obtained from the D2Q5 model by adding four velocities along the diagonals (Figure 21, right). The evaluation of matrix M is absolutely nontrivial and is precised at (80). The dynamics is given by

$$(43) \quad \Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u \lambda s_1 & 1-s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v \lambda s_1 & 0 & 1-s_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_3 s_3 & 0 & 0 & 1-s_3 & 0 & 0 & 0 & 0 & 0 \\ a_4 s_4 & 0 & 0 & 0 & 1-s_4 & 0 & 0 & 0 & 0 \\ a_5 u s_5 & 0 & 0 & 0 & 0 & 1-s_5 & 0 & 0 & 0 \\ a_6 v s_5 & 0 & 0 & 0 & 0 & 0 & 1-s_5 & 0 & 0 \\ a_7 s_7 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_7 & 0 \\ a_8 s_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_8 \end{pmatrix}.$$

The coefficients a_3 to a_8 in relation (43) are chosen in order to obtain the advection diffusion equation at order 2:

$$(44) \quad \frac{\partial \rho}{\partial t} + \lambda \left(u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} \right) - \lambda^2 \xi \sigma_1 \Delta t \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) = O(\Delta t)^2.$$

We have precisely:

$$a_3 = 3(u^2 + v^2) - 4 + 6\xi, \quad a_7 = u^2 - v^2, \quad a_8 = uv$$

as explained in [16]. When $u = v = 0$, the equation (44) takes the form

$$\frac{\partial \rho}{\partial t} - \lambda^2 \xi \sigma_1 \Delta t \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) + \frac{\lambda^4 \Delta t^3 \xi}{36} \left(\kappa_{40} \left(\frac{\partial^4 \rho}{\partial x^4} + \frac{\partial^4 \rho}{\partial y^4} \right) + \kappa_{22} \frac{\partial^4 \rho}{\partial x^2 \partial y^2} \right) = O(\Delta t^4)$$

with coefficients κ_{40} and κ_{22} evaluated according to

$$\begin{aligned} \kappa_{40} &= \sigma_1 \left(2 \sigma_5 (\sigma_7 - \sigma_3) (a_4 - 4) + 6 \xi (1 - \sigma_1 \sigma_7 - 5 \sigma_1 \sigma_3 + 2 \sigma_5 (\sigma_7 - \sigma_3)) \right) \\ \kappa_{22} &= 2 (\sigma_1 + \sigma_5 - 2 \sigma_1 \sigma_5 (\sigma_3 + \sigma_7 + 4 \sigma_8)) (a_4 - 4) \\ &\quad + 12 \xi (\sigma_5 + 3 \sigma_1 - 2 \sigma_1 \sigma_5 (\sigma_3 + \sigma_7) - 2 \sigma_1 \sigma_3 \sigma_5 - 8 \sigma_1 \sigma_8 (\sigma_1 + \sigma_5) + \sigma_1^2 \sigma_7). \end{aligned}$$

Remark that the equivalent partial differential equation of this general lattice Boltzmann scheme has been exactly derived in a complex case where all the time relaxations are *a priori* distinct. The coefficients κ_{40} and κ_{22} of the fourth-order terms are polynomials of degree 3 in the σ coefficients. When we make the ‘‘BGK hypothesis’’ *id est* that all the σ coefficients are equal, a first possibility for killing the coefficients κ_{40} and κ_{22} is given by:

$$\sigma_1 = \sigma_1 = \sigma_3 = \sigma_4 = \sigma_5 = \sigma_7 = \sigma_8 = \frac{1}{6}, \quad \xi = 0.$$

We observe that this choice of parameters is without any practical interest because the diffusion term in (44) is null. We observe that a second possibility

$$\xi = \frac{2}{3} \frac{1 - 6\sigma_1^2}{1 - 8\sigma_1^2}, \quad a_4 = -2 \frac{1 - 2\sigma_1^2}{1 - 8\sigma_1^2}$$

induces also a fourth-order accurate lattice Boltzmann scheme. If we replace the strong “BGK hypothesis” by the weaker one associated to “Two Relaxation Times” as suggested by Ginzburg, Verhaeghe and d’Humières in [22, 23], *id est*

$$\sigma_1 = \sigma_5, \quad \sigma_3 = \sigma_4 = \sigma_7 = \sigma_8,$$

we can achieve formal fourth-order accuracy for

$$\sigma_1 = \frac{1}{\sqrt{12}} \quad \text{and} \quad \sigma_3 = \frac{1}{\sqrt{3}}.$$

- **D3Q7 for pure thermics**

For three-dimensional thermics, one only needs a seven point scheme and use the so-called D3Q7 lattice Boltzmann scheme whose stencil is described in Figure 22. The matrix M is given at relation (81). The dynamics of this Boltzmann scheme uses the following matrix for computation of out of equilibrium moments, according to relation (19):

$$\Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 - s_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 - s_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - s_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 - s_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 - s_4 & 0 \\ \alpha s_6 & 0 & 0 & 0 & 0 & 0 & 1 - s_6 \end{pmatrix}.$$

The equivalent thermal scalar conservation law now takes the following form at fourth-order of accuracy:

$$\frac{\partial \rho}{\partial t} - \frac{\lambda^2 \Delta t}{21} \sigma_1 (\alpha + 6) \Delta \rho + \frac{\Delta t^3 \lambda^4}{1764} \sigma_1 (\alpha + 6) \left(\kappa_{400} \left(\frac{\partial^4 \rho}{\partial x^4} + \frac{\partial^4 \rho}{\partial y^4} + \frac{\partial^4 \rho}{\partial z^4} \right) + \kappa_{220} \left(\frac{\partial^4 \rho}{\partial x^2 \partial y^2} + \frac{\partial^4 \rho}{\partial y^2 \partial z^2} + \frac{\partial^4 \rho}{\partial z^2 \partial x^2} \right) \right) = O(\Delta t^4)$$

where the κ coefficients are given by

$$(45) \quad \kappa_{400} = 8 - \alpha + 4\sigma_1^2 (\alpha + 6) - 56\sigma_1 \sigma_4 - 4(1 - \alpha) \sigma_1 \sigma_6$$

$$(46) \quad \kappa_{220} = -2(\alpha + 6) + 8\sigma_1^2 (\alpha + 6) + 56\sigma_1 \sigma_4 - 8(1 - \alpha) \sigma_1 \sigma_6.$$

• After these examples where only one partial differential equation is present, we consider the case of two (D1Q3), three (D2Q9) or four (D3Q19) partial differential equations “emerging” from the lattice Boltzmann algorithm. These equations model macroscopic conservation of mass and momentum of a linearized fluid in our approach in this contribution.

• **D1Q3 for athermal linearized Navier–Stokes at fifth-order**

We have in this case two conservation laws ($N = 2$ in relation (5)) and the equilibrium energy is supposed to be given simply by

$$(47) \quad \epsilon^{\text{eq}} = \alpha \frac{\lambda^2}{2} \rho.$$

Due to (21) and (47), the matrix Ψ for dynamics relation (19) is now given according to

$$\Psi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \alpha s \lambda^2/2 & 0 & 1 - s \end{pmatrix},$$

and σ is related to parameter s according to (16): $\sigma \equiv \frac{1}{s} - \frac{1}{2}$. Then equivalent mass conservation at the order 5 looks like equation (38). We have precisely:

$$(48) \quad \left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} - \frac{\lambda^2 \Delta t^2}{12} (1 - \alpha) \frac{\partial^3 q}{\partial x^3} - \frac{\lambda^4 \Delta t^3}{12} \alpha (1 - \alpha) \sigma \frac{\partial^4 \rho}{\partial x^4} \\ \quad \quad \quad + \frac{\lambda^4 \Delta t^4}{120} (1 - \alpha) (1 + \alpha + 10(1 - 2\alpha)\sigma^2) \frac{\partial^5 q}{\partial x^5} = O(\Delta t^5). \end{array} \right.$$

Conservation of momentum takes the form:

$$(49) \quad \left\{ \begin{array}{l} \frac{\partial q}{\partial t} + \alpha \lambda^2 \frac{\partial \rho}{\partial x} - \lambda^2 \Delta t (1 - \alpha) \sigma \frac{\partial^2 q}{\partial x^2} + \zeta_3 \frac{\lambda^4 \Delta t^2}{6} \frac{\partial^3 \rho}{\partial x^3} \\ \quad \quad \quad + \zeta_4 \frac{\lambda^4 \Delta t^3}{12} \frac{\partial^4 q}{\partial x^4} + \zeta_5 \frac{\lambda^6 \Delta t^4}{120} \frac{\partial^5 \rho}{\partial x^5} = O(\Delta t^5) \end{array} \right.$$

with parameters ζ_3 to ζ_5 given by

$$\begin{aligned} \zeta_3 &= \alpha (1 - \alpha) (1 - 6\sigma^2) \\ \zeta_4 &= -(1 - \alpha) \sigma (1 - 4\alpha - 12(1 - 2\alpha)\sigma^2) \\ \zeta_5 &= \alpha (1 - \alpha) (1 - 4\alpha - 10(5 - 9\alpha)\sigma^2 + 120(2 - 3\alpha)\sigma^4). \end{aligned}$$

When $\sigma = \frac{1}{\sqrt{6}}$, the coefficient ζ_3 of relation (49) is null. In this case, the lattice Boltzmann scheme is formally third-order accurate for the momentum equation. But, as remarked in [16], the mass conservation (48) remains formally second-order accurate, except for the (without any practical interest as it leads to a null viscosity) case $\alpha = 1$.

- **D2Q9 for linearized athermal Navier–Stokes at order four**

The D2Q9 lattice Boltzmann scheme can be used also for simulation of fluid dynamics. For the particular case of conservation of mass and momentum, we just replace matrix Ψ of (43) by the following one, assuming the aim is to simulate an athermal fluid with speed of sound $\sqrt{1/3}$:

$$\Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2s_3 & 0 & 0 & 1-s_3 & 0 & 0 & 0 & 0 & 0 \\ s_4 & 0 & 0 & 0 & 1-s_4 & 0 & 0 & 0 & 0 \\ 0 & -s_5/\lambda & 0 & 0 & 0 & 1-s_5 & 0 & 0 & 0 \\ 0 & 0 & -s_5/\lambda & 0 & 0 & 0 & 1-s_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_7 \end{pmatrix}.$$

We have conservation of mass at fourth-order of accuracy:

$$(50) \quad \frac{\partial \rho}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - \frac{1}{18} \lambda^2 \Delta t^2 \Delta \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) + \frac{\lambda^4 \Delta t^3}{108} (\sigma_3 + \sigma_7) \Delta^2 \rho = O(\Delta t^4)$$

and conservation of two components of momentum:

$$(51) \quad \left\{ \begin{array}{l} \frac{\partial q_x}{\partial t} + \frac{\lambda^2}{3} \frac{\partial \rho}{\partial x} - \frac{\lambda^2}{3} \Delta t \left[\sigma_3 \frac{\partial}{\partial x} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) + \sigma_7 \Delta q_x \right] \\ - \frac{\lambda^4 \Delta t^2}{27} \left(3(\sigma_3^2 + \sigma_7^2) - 1 \right) \frac{\partial}{\partial x} \Delta \rho - \frac{\lambda^4 \Delta t^3}{108} \left(\zeta_{40} \frac{\partial^4 q_x}{\partial x^4} + \zeta_{31} \frac{\partial^4 q_y}{\partial x^3 \partial y} \right. \\ \left. + \zeta_{22} \frac{\partial^4 q_x}{\partial x^2 \partial y^2} + \zeta_{13} \frac{\partial^4 q_y}{\partial x \partial y^3} + \zeta_{04} \frac{\partial^4 q_x}{\partial y^4} \right) = O(\Delta t^4) \end{array} \right.$$

$$(52) \quad \left\{ \begin{array}{l} \frac{\partial q_y}{\partial t} + \frac{\lambda^2}{3} \frac{\partial \rho}{\partial y} - \frac{\lambda^2}{3} \Delta t \left[\sigma_3 \frac{\partial}{\partial y} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) + \sigma_7 \Delta q_y \right] \\ - \frac{\lambda^4 \Delta t^2}{27} \left(3(\sigma_3^2 + \sigma_7^2) - 1 \right) \frac{\partial}{\partial y} \Delta \rho - \frac{\lambda^4 \Delta t^3}{108} \left(\eta_{40} \frac{\partial^4 q_y}{\partial x^4} + \eta_{31} \frac{\partial^4 q_x}{\partial x^3 \partial y} \right. \\ \left. + \eta_{22} \frac{\partial^4 q_y}{\partial x^2 \partial y^2} + \eta_{13} \frac{\partial^4 q_x}{\partial x \partial y^3} + \eta_{04} \frac{\partial^4 q_y}{\partial y^4} \right) = O(\Delta t^4) \end{array} \right.$$

where the coefficients ζ are given by

$$(53) \quad \left\{ \begin{array}{l} \zeta_{40} = \eta_{04} = -\sigma_3 - \sigma_7 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 + 18\sigma_3^2\sigma_5 \\ \quad + 6\sigma_5\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 - 24\sigma_3\sigma_5\sigma_7 + 12\sigma_4\sigma_5\sigma_7 \\ \zeta_{31} = \eta_{13} = -4\sigma_3 - 7\sigma_7 + 18\sigma_3^2\sigma_5 + 18\sigma_5\sigma_7^2 - 12\sigma_3^2\sigma_7 \\ \quad - 12\sigma_3\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 + 12\sigma_3\sigma_5\sigma_7 + 12\sigma_4\sigma_5\sigma_7 + 12\sigma_7^3 \\ \zeta_{22} = \eta_{22} = -13\sigma_3 + 6\sigma_4 - 10\sigma_7 + 18\sigma_3^2\sigma_5 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 \\ \quad + 30\sigma_5\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 + 120\sigma_3\sigma_5\sigma_7 - 60\sigma_4\sigma_5\sigma_7 - 12\sigma_7^3 \\ \zeta_{13} = \eta_{31} = -10\sigma_3 + 6\sigma_4 - 7\sigma_7 + 18\sigma_3^2\sigma_5 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 \\ \quad + 18\sigma_5\sigma_7^2 + 12\sigma_3\sigma_4\sigma_5 + 84\sigma_3\sigma_5\sigma_7 - 60\sigma_4\sigma_5\sigma_7 + 12\sigma_7^3 \\ \zeta_{04} = \eta_{40} = -3\sigma_7 + 24\sigma_5\sigma_7^2 - 12\sigma_7^3. \end{array} \right.$$

- **D3Q19 for linearized Navier–Stokes**

The D3Q19 Lattice Boltzmann scheme is described with details *e.g.* in J. Tölke *et al* [46]. The construction of matrix M that parameterizes the transformation (4) is presented in full detail in relations (82) to (87) in Appendix B. The associated matrix Ψ is also of order 19 and therefore quite difficult to write on a A4 paper sheet. Due to constitutive relations (19) and (20), it is easily obtained from the expression of equilibrium moments. We have taken for this D3Q19 scheme

$$(54) \quad \left\{ \begin{array}{l} m_4^{\text{eq}} = \theta \lambda^2 \\ m_5^{\text{eq}} = m_6^{\text{eq}} = m_7^{\text{eq}} = m_8^{\text{eq}} = m_9^{\text{eq}} = 0 \\ m_{10}^{\text{eq}} = m_{11}^{\text{eq}} = m_{12}^{\text{eq}} = 0 \\ m_{13}^{\text{eq}} = \beta \lambda^4 \\ m_{14}^{\text{eq}} = m_{15}^{\text{eq}} = 0 \\ m_{16}^{\text{eq}} = m_{17}^{\text{eq}} = m_{18}^{\text{eq}} = 0. \end{array} \right.$$

In order to obtain physical equations at first-order of accuracy with a sound velocity c_0 given by $c_0 = \alpha \lambda$ the relation $\theta = 57\alpha^2 - 30$ must be imposed to obtain correct fluid second-order partial differential equations and the parameter β remains free.

- When the number of velocities of the Boltzmann scheme is reduced (up to D2Q9 scheme typically), it is possible to expand the dispersion equation formally and to derive equivalent partial differential equations up to an arbitrary order. We have done the comparison for one-dimensional and bi-dimensional schemes. The process has been extended to models with more velocities and various conserved quantities; however the equations become very complicated and thus will not be reproduced here. Let us just mention that the expressions found are quite similar to those obtained for the previous test cases.

4 The fourth-order accurate lattice Boltzmann scheme

- In this section, we precise how to choose particular “quartic” values of relaxation parameters in order to increase the accuracy of the scheme. We verify with the help of precise numerical experiments for analytical test cases that the numerical precision follows our prediction. We focus first on classical thermics at two and three space dimensions. Then we propose two numerical experiments for athermal linearized Navier-Stokes equations at two and three space dimensions for a nontrivial geometry.

- **The D2Q5 lattice Boltzmann scheme for a thermal problem**

We obtain the order 4 by setting $\kappa_{40} = 0$ and $\kappa_{22} = 0$ in relations (41) and (42) respectively. We obtain :

$$(55) \quad \sigma_3 = \sigma_1 \frac{\alpha + 4}{1 - \alpha} - \frac{1}{12\sigma_1} \frac{2 + 3\alpha}{1 - \alpha}, \quad \sigma_4 = \frac{1}{6\sigma_1}.$$

The BGK condition $\sigma_1 = \sigma_3 = \sigma_4$ leads to $\sigma_1 = \frac{1}{\sqrt{12}}$ and $\alpha = -4$ and thus to a thermal diffusivity equal to 0. Note that the intermediate TRT presented in Ginzburg *et al* [22, 23] supposes simply $\sigma_3 = \sigma_4$. If we insert this constraint inside relations (55), we get

$$\sigma_1 = \frac{1}{\sqrt{12}}, \quad \sigma_3 = \frac{1}{\sqrt{3}}$$

to enforce fourth-order accuracy. Then the d’Humières version of lattice Boltzmann scheme is mandatory for this improvement of the method with a wide family of admissible parameters. In order to study the fourth-order accuracy of the D2Q5 lattice Boltzmann scheme for thermal problem, we use three different approaches. The first two consider the interior scheme and the third one incorporates boundary conditions.

- First of all, we study homogeneous plane waves with a “one point computation”. In that case, we can derive numerically a dispersion equation for scheme (15) associated with (4), (19), (79) and (39), as proposed in [30]. We introduce a wave in the Boltzmann scheme, *id est* $f(x, t) \equiv \widehat{f}(k_x, k_y) \exp(ik_x x + ik_y y)$. Then we have $f(x, t + \Delta t) = G f(x, t)$ with the so-called amplification matrix G (see *e.g.* Richtmyer and Morton [40]) obtained without difficulty from matrices M , Ψ and B defined respectively in (79) (39) and

$$B = \text{diag} \left(1, e^{ik_x \Delta x}, e^{ik_y \Delta x}, e^{-ik_x \Delta x}, e^{-ik_y \Delta x} \right)$$

for the D2Q5 scheme displayed in Figure 21 (left). Then $G = B M^{-1} \Psi M$. Then if $\frac{\partial}{\partial t}$ is formally given by relation (40) and operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ replaced by ik_x and ik_y respectively, the number $z = \exp(\Delta t \frac{\partial}{\partial t})$ is an eigenvalue of matrix G at fourth-order of accuracy. The numerical experiment (see Figure 1) confirms the theoretical

development of the dispersion equation. Note that for situations relaxing to uniform state, the eigenvalues that we determine below are negative; however we shall express results in terms of *positive* relaxation rates with adequate sign changes.

- For inhomogeneous situations, with $N_{\mathcal{L}}$ lattice points (and $N_{\mathcal{L}}(J+1)$ degrees of freedom), one can study the time evolution starting from some initial state. Another approach for linear situations considers that the state $X(t)$ that belongs to $\mathbb{R}^{N_{\mathcal{L}}(J+1)}$ can be decomposed as a sum of eigenmodes of the operator A defined using the discrete evolution scheme:

$$(56) \quad X(t + \Delta t) \equiv A \bullet X(t).$$

The matrix A being of very large size, one can look for some of its eigenmodes using for instance the method proposed by Arnoldi [2]. To accelerate the Arnoldi computations, following a suggestion by L. Tuckerman [47], we replace the determination of the eigenvalues of equation (56) by the determination of the eigenvalues of

$$(57) \quad X(t + (2\ell + 1)\Delta t) \equiv A^{2\ell+1} \bullet X(t),$$

for some $\ell \in \mathbb{N}$, using the fact that the lattice Boltzmann scheme is very fast compared to the inner “working” of the Arnoldi procedure. Replacing problem (56) by problem (57) not only increases the splitting between various eigenmodes, but also helps to discriminate against the acoustic modes by multiplying the logarithm of the imaginary part of the eigenvalues by $2\ell + 1$. Note that choosing an even number of time steps would bring in the “checker-board” type modes. We denote by Γ_{num} any eigenvalue computed with this methodology.

- We first test this method for “internal” lattice, *id est* with a periodic $N_{\mathcal{L}} \equiv N_x \times N_y$ situation and find the same results as those derived from the “one-point” analysis (see Figure 1) with very good accuracy. For this periodic situation, the eigenmodes are plane waves for the wave vector $k_x = 2\pi \frac{I_x}{N_x}$, $k_y = 2\pi \frac{I_y}{N_y}$, where I_x and I_y are integers. We compare the numerical relaxation rates $\Gamma_{\text{num}}(I_x, I_y, N_x, N_y)$ to $\Gamma_{\text{th}} \equiv \kappa(k_x^2 + k_y^2)$ and show in Figure 2 the relative difference between those two quantities (called the “error”) for the particular values $I_x = 5$ and $I_y = 0$ and N_x from 11 to 91. With arbitrarily chosen values of the “non-hydrodynamic” s -parameters, we observe second-order convergence. However for the quartic s -parameters the convergence is of order four with a large decrease in the absolute value of the error. Analogous results are displayed in Figure 2 for D3Q7.

- We now consider a second case with boundary conditions: exact solution for the modes of the Laplace equation in a circle of radius R with homogeneous Dirichlet boundary conditions. Density is defined with (6) applied with $J = 4$ in this particular case.

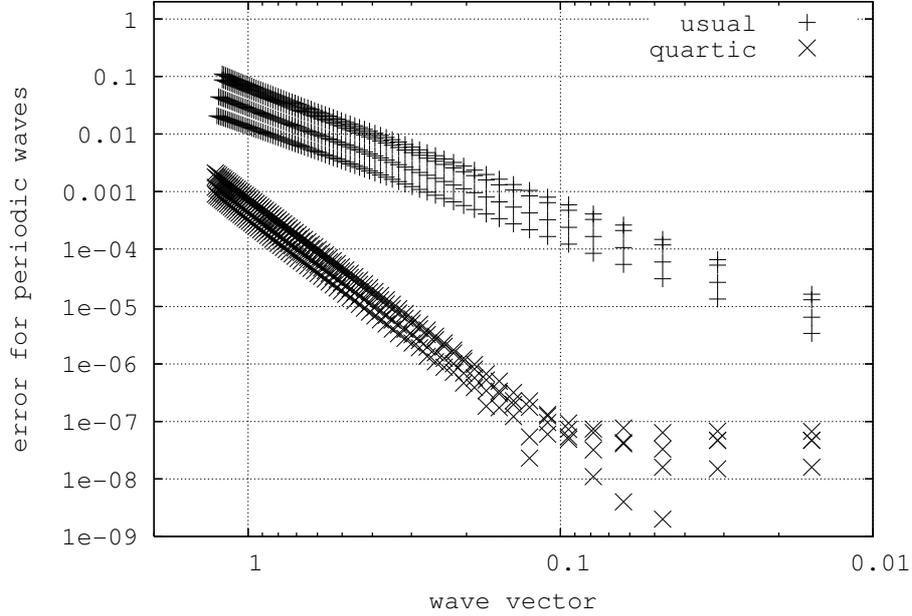


Figure 1: Error $|\frac{\Gamma_{num}}{\Gamma_{th}} - 1|$ of D2Q5 scheme for thermic test case, “one point” simulation. Different curves correspond to different orientation of the wave-vector with respect to the axis, showing the angular dependence of the next order.

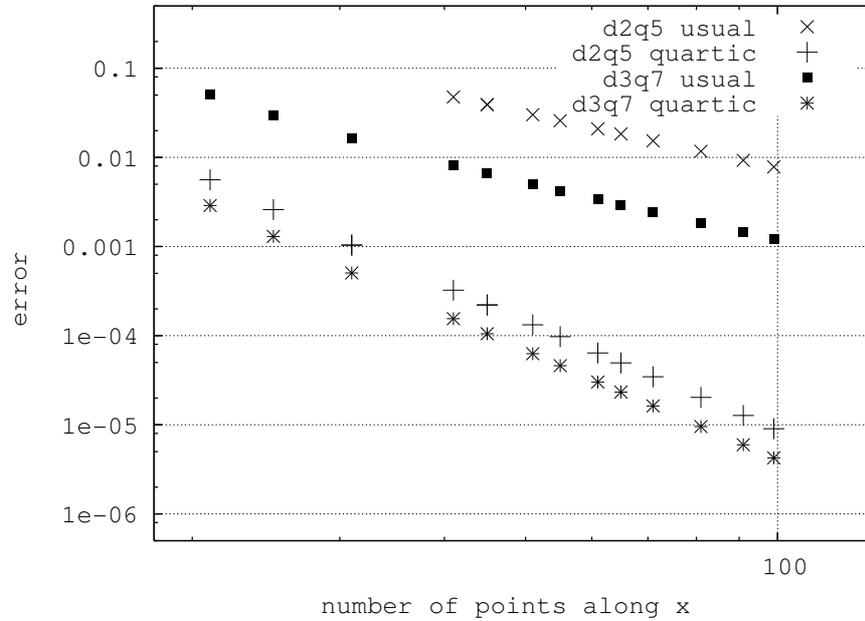


Figure 2: Arnoldi test case for periodic thermics, $I_x = 5$, $I_y = 0$. Various parameters for lattice Boltzmann schemes D2Q5 and D3Q7.

Recall that density follows heat equation $\frac{\partial \rho}{\partial t} - \kappa \Delta \rho = 0$ with $\kappa = \frac{\lambda^2 \Delta t}{10} \sigma_1 (4 + \alpha)$ and homogeneous boundary conditions at $r = R$. The solution of this problem is standard (see *e.g.* Landau and Lifchitz [32], Abramowitz and Stegun [1] or Carslaw and Jaeger [6]) and is parameterized by a pair (ℓ, n) of integers. We introduce ζ_ℓ^n , the n^{th} zero of the Bessel function J_ℓ . Then a solution with time dependence as $\exp(-\Gamma t)$ defines a corresponding eigenvalue Γ (also denoted as Γ_{th} in the following) that satisfies

$$(58) \quad \Gamma = \kappa \left(\frac{\zeta_\ell^n}{R} \right)^2.$$

- The effect of fourth-order accuracy Boltzmann scheme in computing the eigenfunction is spectacular: just compare Figures 3 and 4. Nevertheless, the effect of boundary conditions (we use anti-bounce-back with interpolation *à la* Bouzidi *et al* [5]) cannot be neglected. In Figure 5, we have compared the error defined by $|\frac{\Gamma_{\text{num}}}{\Gamma_{\text{th}}} - 1|$ for two internal schemes (with usual and quartic parameters) and two versions (first and second-order) of simple numerical boundary conditions introduced by Bouzidi *et al* [5]. We still observe a better numerical precision of the schemes (by two orders of magnitude typically) whereas the convergence still remains second-order accurate. We conclude that the effect of boundary conditions is crucial for the determination of the order of convergence. Nevertheless, the choice of quartic parameters gives a higher precision for the lattice Boltzmann scheme.

- **The D3Q7 lattice Boltzmann scheme for a thermal problem**

We obtain the order 4 by setting $\kappa_{400} = 0$ and $\kappa_{220} = 0$ in relations (45) and (46). We obtain :

$$\sigma_4 = \frac{1}{6 \sigma_1}, \quad \sigma_6 = \frac{\alpha + 6}{1 - \alpha} \sigma_1 - \frac{4 + 3\alpha}{12(1 - \alpha)} \frac{1}{\sigma_1}.$$

As for D2Q5, the ‘‘BGK condition’’ $\sigma_1 = \sigma_4 = \sigma_6$ leads to $\sigma_6 = \frac{1}{\sqrt{6}}$ and $\alpha = -6$ and thus to thermal diffusivity equal to 0. Theoretical modes of the Laplace equation in a sphere of radius R with homogeneous Dirichlet boundary conditions are parameterized through the n^{th} zero $\eta_{\ell+1/2}^n$ of semi-integer Bessel function $J_{\ell+1/2}$ and the eigenvalue Γ is given by:

$$(59) \quad \Gamma = \kappa \left(\frac{\eta_{\ell+1/2}^n}{R} \right)^2, \quad \ell \in \mathbb{N}, \quad n \geq 1.$$

- The results of Figures 6 and 7 have been obtained with $R = 17.2$ and $n = 5$. The theoretical value of the eigenvalue is $\Gamma = 5^2 \pi^2 \kappa / R^2$ (as for $m = 0$, the zeros of the semi-integer Bessel function are simply πn). We have used parameters $s_1 = 1.26795$, $s_4 = 1.2$, $s_6 = 1.3$ for the usual computations. The quartic parameters have been chosen as

$$s_1 = 1.26795, \quad s_4 = s_6 = 0.92820.$$

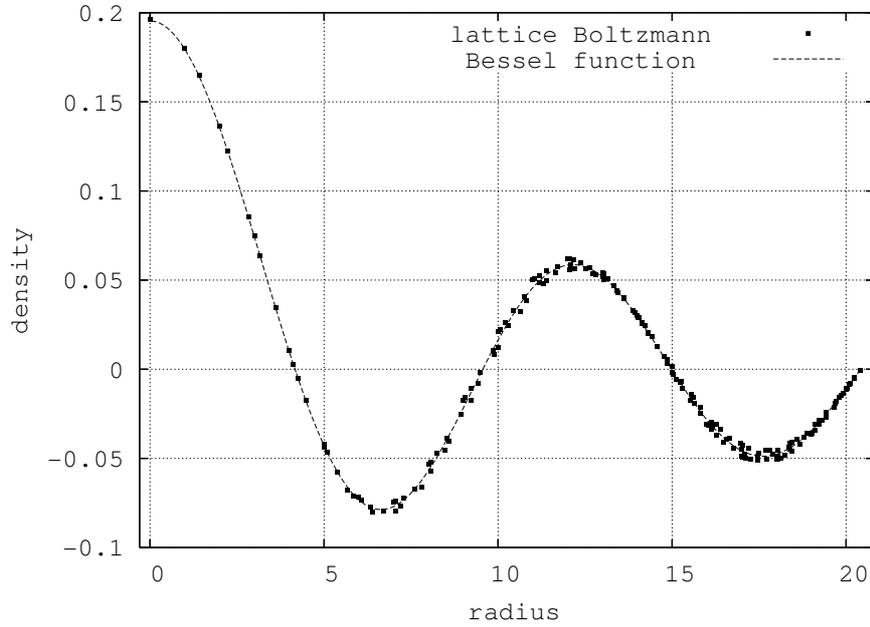


Figure 3: D2Q5 scheme for thermics inside a circle. Eigenmode $n = 4$, $\ell = 0$ for heat equation with Dirichlet boundary conditions. Second-order accuracy with usual parameters for lattice Boltzmann scheme.

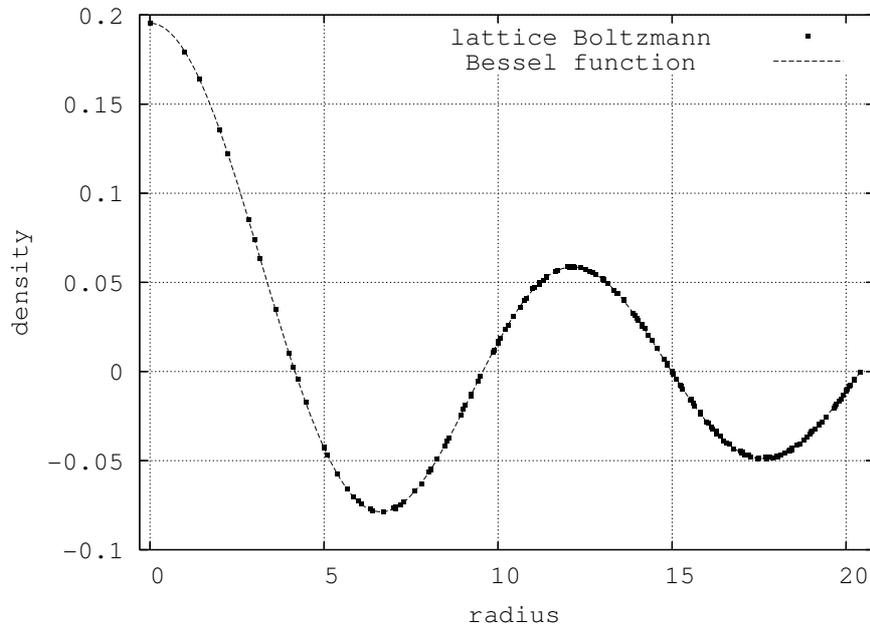


Figure 4: D2Q5 scheme for thermics inside a circle. Eigenmode $n = 4$, $\ell = 0$. Quartic parameters for lattice Boltzmann scheme.

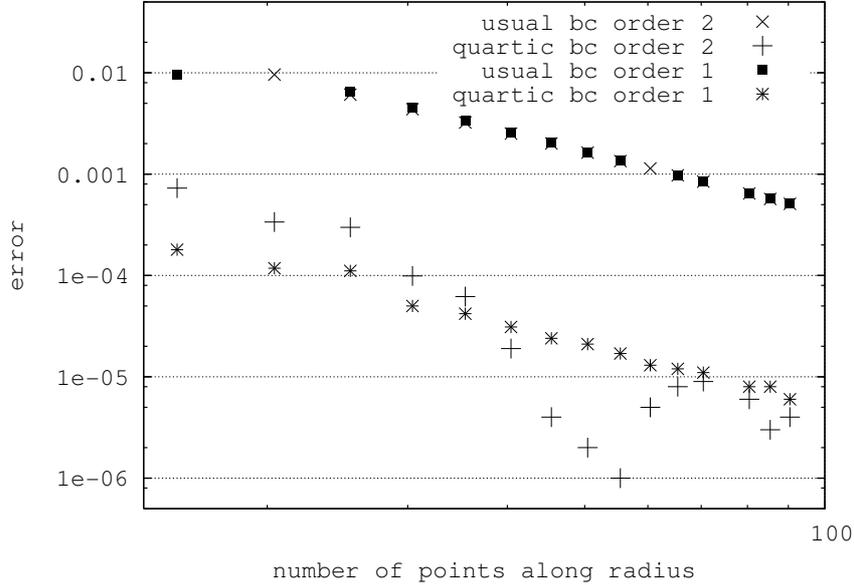


Figure 5: D2Q5 scheme for thermics in a circle. Eigenmode $n = 1$, $\ell = 5$. Errors for various parameters for lattice Boltzmann and boundary schemes.

From results presented in Figure 8, the conclusion is essentially the same as that observed for two-dimensional thermics: the results are improved by two orders of magnitude typically, but the rate of convergence cannot be rigorously measured or still remains of second-order.

- We also made a parameter study of the location of the boundary condition. We plot in Figure 9 the ratio $\Gamma R^2/(\kappa \pi^2)$ with Γ given by relation (59). We use Bouzidi *et al* [5] boundary procedure with linear interpolation. The fluctuation due to the boundary algorithm is around 0.2 %. The gap between second-order usual computation and new fourth-order computation is of the order of 2%. We observe that this gap is **one order of magnitude larger** than the error due to the choice of the boundary condition estimated from the fluctuations with the imposed radius.

- **The D2Q9 for linearized athermal Navier–Stokes at fourth-order**

We consider now the linear fluid model obtained by a D2Q9 lattice Boltzmann scheme. The equivalent partial differential equations are given at the order 4 by relations (51) to (53). The dream would be to enforce high order accuracy. However, this is definitively impossible in the framework considered here due to the never null third-order term for mass conservation (50). Recall notation (5) for conservative variables: $W \equiv (\rho, q_x, q_y)^t$

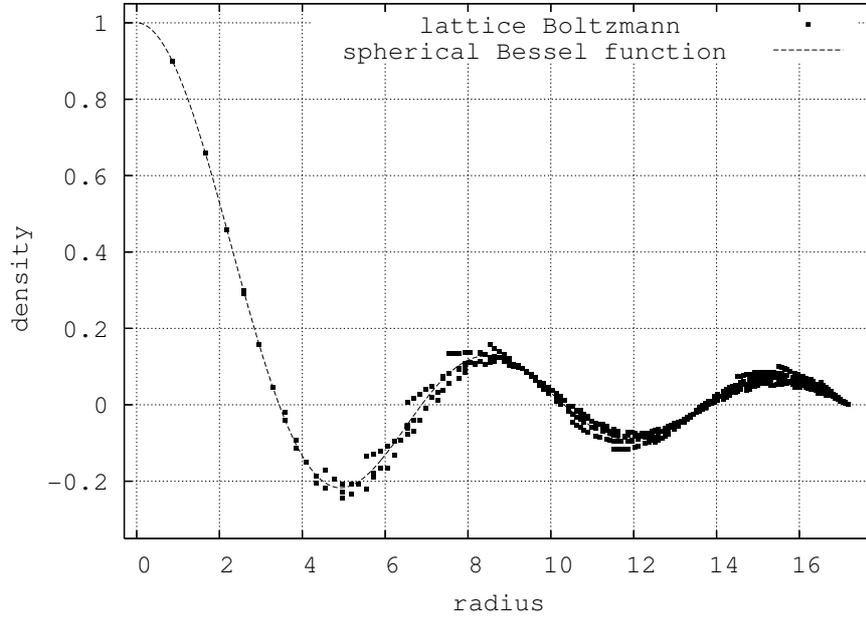


Figure 6: D3Q7 lattice Boltzmann scheme for thermics in a sphere. Eigenmode $n = 5$, $\ell = 1$, $m = 0$ with usual parameters.

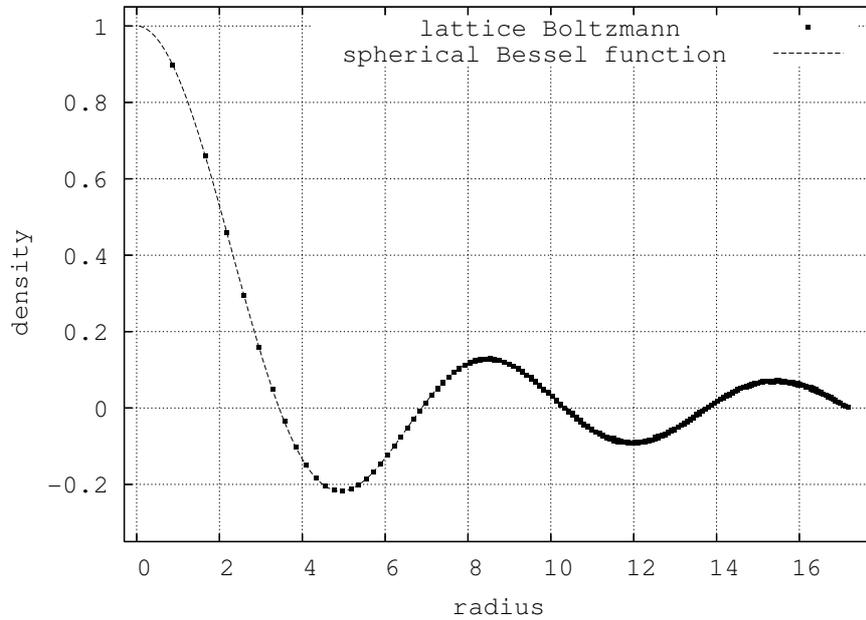


Figure 7: D3Q7 lattice Boltzmann scheme for thermics in a sphere. Eigenmode $n = 5$, $\ell = 1$, $m = 0$ with quartic parameters.

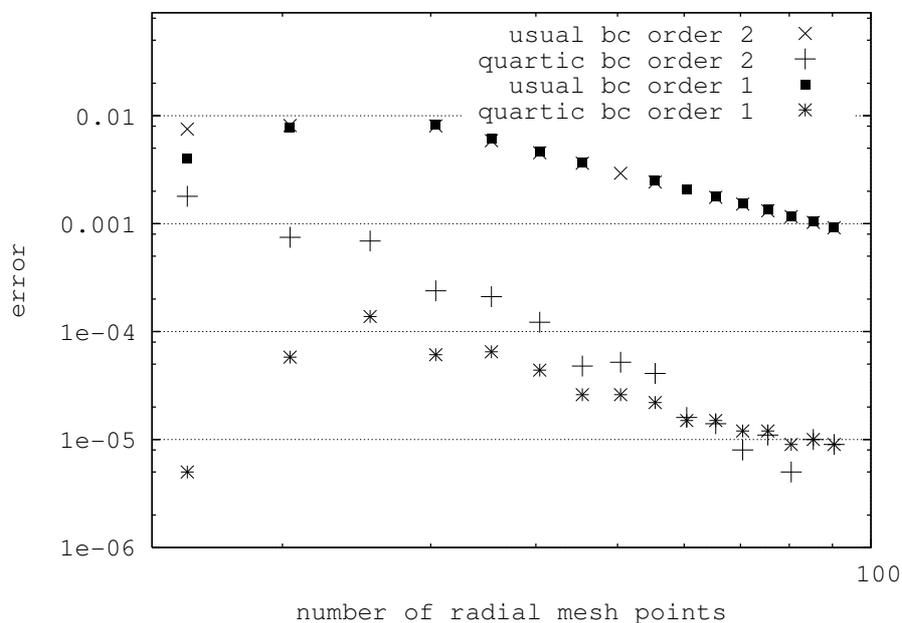


Figure 8: D3Q7 scheme for thermics in a sphere with Dirichlet boundary conditions. Eigenmode $n = 1$, $\ell = 0$. Errors for various parameters for lattice Boltzmann and boundary schemes.

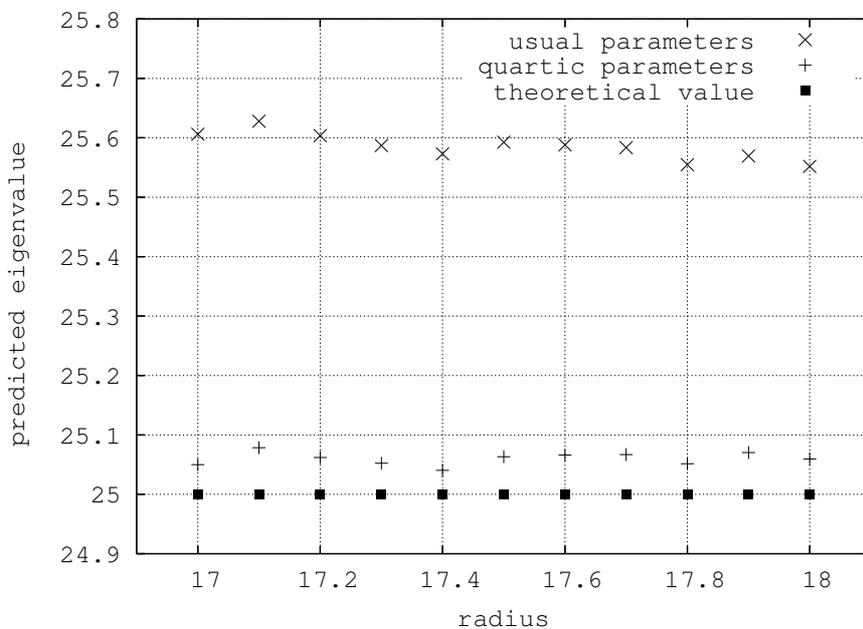


Figure 9: D3Q7 for thermics in a sphere. Eigenmode (in units $\kappa\pi^2/R^2$) for $n = 5$ and $\ell = 0$. Variation of the location of the boundary between $R = 17$ and $R = 18$.

and write the equivalent equations (51)-(53) in the synthetic form:

$$(60) \quad \partial_t W_k + \sum_{j,p,q} A_{kpq}^j \partial_x^p \partial_y^q W_j = O(\Delta t^4).$$

We search for a dissipative mode, *id est* a mode for linear incompressible Stokes problem under the form $W(t) = e^{-\Gamma t + i(k_x x + k_y y)} \widehat{W}$. Then Γ is an eigenvalue of the matrix A defined by

$$A_k^j = \sum_{j,p,q} A_{kpq}^j (i k_x)^p (i k_y)^q.$$

We know (see *e.g.* Landau and Lifchitz [32]) that for Stokes problem (incompressible shear modes), the relation

$$(61) \quad \Gamma = \nu (k_x^2 + k_y^2)$$

is classical. Moreover, as a consequence of (51) and (52)

$$(62) \quad \nu = \frac{\lambda^2}{3} \Delta t \sigma_7$$

for a lattice Boltzmann scheme with multiple relaxation times.

- We propose here to tune the parameters s_ℓ in such a way that the relation (61) is enforced for the modes of (60). Precisely, we search s_ℓ such that

$$(63) \quad \Delta_m \equiv \det \left[A - \left(\frac{\lambda^2}{3} \Delta t \sigma_7 \right) (k_x^2 + k_y^2) \text{Id} \right] = O(\Delta t^7).$$

With an elementary formal computation, the third-order term Δ_m^3 of Δ_m relative to Δt is equal to

$$(64) \quad \left\{ \begin{array}{l} \Delta_m^3 = -\frac{\Delta t^3 \lambda^6}{108} \sigma_7 (k_x^2 + k_y^2) \left((-1 - 4\sigma_7^2 - 8\sigma_5 \sigma_7) (k_x^4 + k_y^4) \right. \\ \left. + 2(1 - 4\sigma_7^2 - 4\sigma_5 \sigma_7) k_x^2 k_y^2 \right). \end{array} \right.$$

It is then clear that the expression (64) is identically null for parameters σ_5 and σ_7 chosen according to

$$(65) \quad \sigma_5 = \frac{\sqrt{3}}{3}, \quad \sigma_7 = \frac{\sqrt{3}}{6}.$$

With this particular choice of parameters, so-called quartic in what follows, the viscosity ν in relation (62) has the following particular value:

$$(66) \quad \nu = \frac{\lambda^2 \Delta t}{\sqrt{108}} \approx 0.096225 \lambda^2 \Delta t.$$

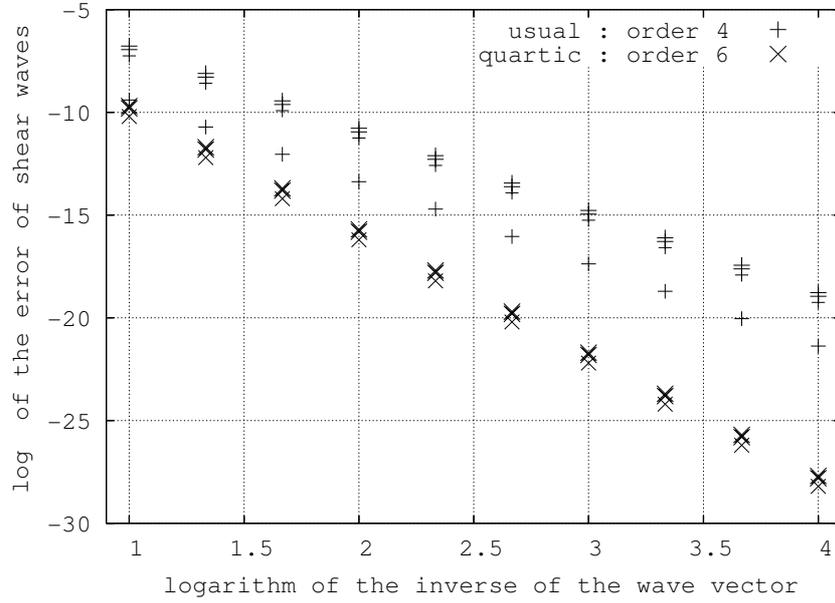


Figure 10: D2Q9 “one point” test case of shear waves for different angles of the wave vector.

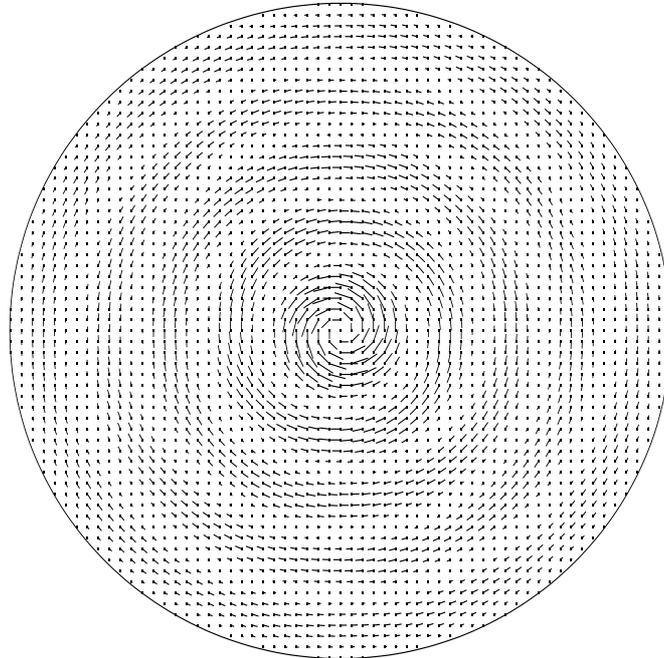


Figure 11: D2Q9 scheme for linear Navier–Stokes. Eigenmode $n = 5$ $\ell = 1$ for the Stokes problem in a circle.

Then it is very simple to verify that the determinant Δ_m is null up to terms of order seven and relation (63) is satisfied.

- As in the particular case of D2Q5 scheme, we have verified with periodic boundary conditions that the relaxation rate of a transverse wave is determined with error of order six and relative fourth-order precision, as shown in Figure 10. The detailed numerical convergence plot is very similar to Figure 2.

- We have also validated our results for eigenmodes of the Stokes problem inside a circle. With the notations introduced previously, the eigenvalues Γ are given [32] by

$$(67) \quad \Gamma = \nu \left(\frac{\zeta_\ell^n}{R} \right)^2.$$

The result for $R = 30.07$, $\ell = 1$ and $n = 5$ is presented in Figure 11 for the velocity field with a mesh included in a square of size 61×61 . The alternance of directions for the vector field is clearly visible on Figure 11 and we use around seven meshpoints between two zeros of the Bessel function. We have compared with the same mesh the results obtained with the lattice Boltzmann scheme with the usual parameters that does not satisfy relation (65) but such that $\nu = \frac{\lambda^2 \Delta t}{10}$ which is very close to (66) and quartic parameters. The radial profile of the tangential velocity is shown in Figures 12 to 14. The difference is visually spectacular. As for the thermics case, we observe that simple boundary conditions (here we use those of Bouzidi *et al.* [5]) prevent fourth-order convergence for the Stokes problem. Use of more sophisticated boundary conditions (see Ginzburg and d’Humières [21]) may help to improve the convergence; however for models with limited number of velocities, it is not clear whether the choice of s -parameters will be the same for “fourth-order volume” and “accurate Poiseuille type boundary conditions”.

- **The D3Q19 for linearized athermal Navier–Stokes at fourth-order**

The D3Q19 model is analyzed as was done above for the D2Q9 model. We detail in Appendix C the way to enforce the precision of eigenmodes for the Stokes problem. We obtain a set of eight equations for the coefficients σ ’s. These equations have only one nontrivial family of solutions given according to

$$(68) \quad \left\{ \begin{array}{llll} \text{energy} & \sigma_4 = \frac{1}{s_4} - \frac{1}{2} & s_4 = & ad\ libitum \\ \text{stress tensor} & \sigma_5 = 1/\sqrt{12} & s_5 = & 3 - \sqrt{3} \\ \text{energy flux} & \sigma_{10} = 1/\sqrt{3} & s_{10} = & 4\sqrt{3} - 6 \\ \text{square of energy} & \sigma_{13} = \frac{1}{s_{13}} - \frac{1}{2} & s_{13} = & ad\ libitum \\ \text{other moments of kinetic energy} & \sigma_{14} = 1/\sqrt{12} & s_{14} = & 3 - \sqrt{3} \\ \text{third-order antisymmetric} & \sigma_{16} = 1/\sqrt{3} & s_{16} = & 4\sqrt{3} - 6. \end{array} \right.$$

Note these results are incompatible with BGK hypothesis (all σ equal) but are compatible with the “two relaxation times” hypothesis which enforces equality of even moments

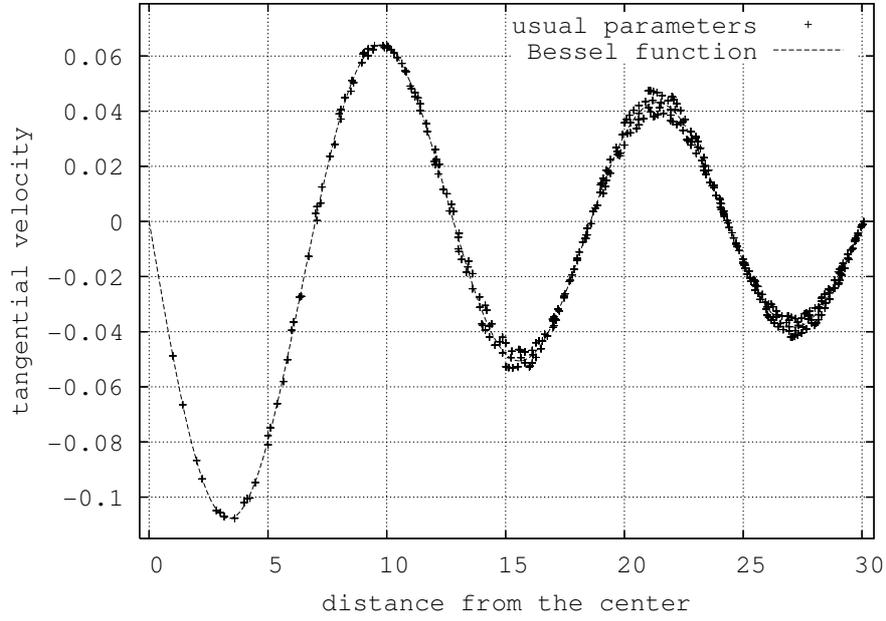


Figure 12: D2Q9 scheme for linear Navier–Stokes in a circle. Eigenmode $n = 5$, $\ell = 1$ for the Stokes problem. Usual parameters.

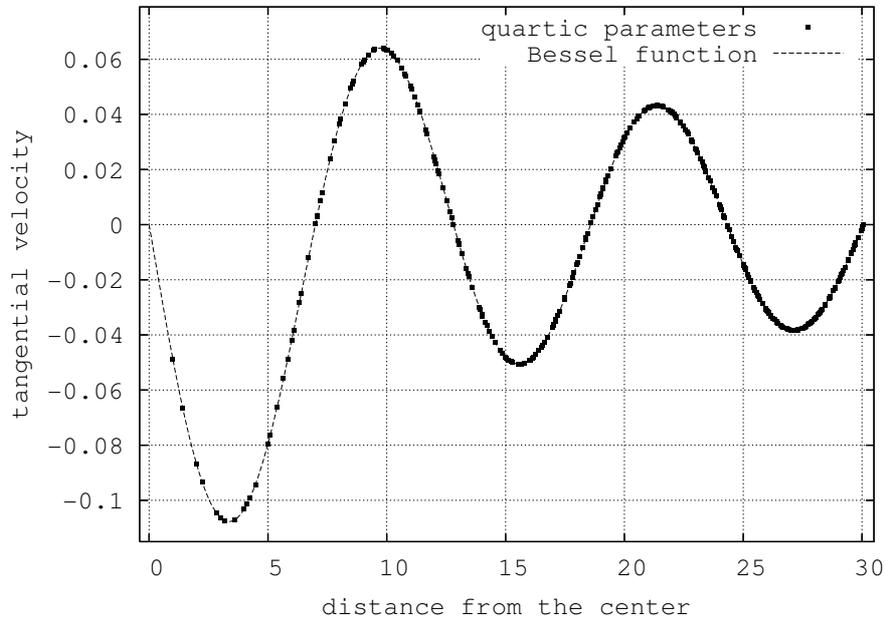


Figure 13: D2Q9 scheme for linear Navier–Stokes in a circle. Eigenmode $n = 5$, $\ell = 1$ for the Stokes problem. Quartic parameters.

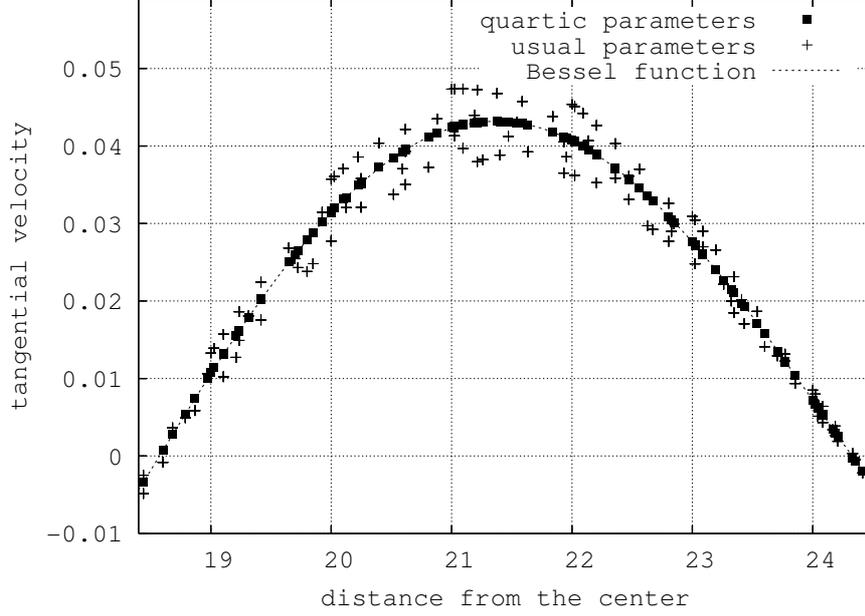


Figure 14: D2Q9 scheme for linear Navier–Stokes in a circle. Eigenmode $n = 5$, $\ell = 1$ for the Stokes problem. Zoom of the figures 12 and 13.

$\sigma_4 = \sigma_5 = \sigma_{13} = \sigma_{14}$, and of odd moments: $\sigma_{10} = \sigma_{16}$. We remark that the relaxation rate for energy (linked to the bulk viscosity) is not constrained. Note that the shear viscosity ν takes the value $1/\sqrt{108}$ as in (66). As for D2Q9 there is no decoupling at order 3 of shear and acoustic modes, and thus, at least at the present stage, we make no claim concerning possible improvements for the acoustic modes. We will study this question in a forthcoming contribution.

- We have performed the same kind of numerical analysis as for the two-dimensional D2Q9 case and find quite similar results. We illustrate our results first with a “one point experiment”. We introduce numerical wave vectors k close to zero and compute the eigenmodes numerically. The shear mode is close to $\frac{\lambda^2}{3} \sigma_5 |k|^2$ and we plot in Figure 15 the experimental error. With ordinary coefficients, the error is of order 4, whereas with the so-called “quartic coefficients”, the error is of order 6 and the relative error of order 4.

- We also illustrate our results for the problem of Stokes modes in a sphere which has an analytical solution in terms of Bessel functions. The Stokes problem searches for a velocity field $\mathbf{u}(r, t)$ with $\mathbf{u} = 0$ on the surface of a sphere of radius R . An analysis similar to that for the Stokes problem in a circle, leads to an eigenvalue problem, with solutions

$$\Gamma = \nu \left(\frac{\zeta_{\ell+1/2}^n}{R} \right)^2, \quad \ell \geq 1,$$

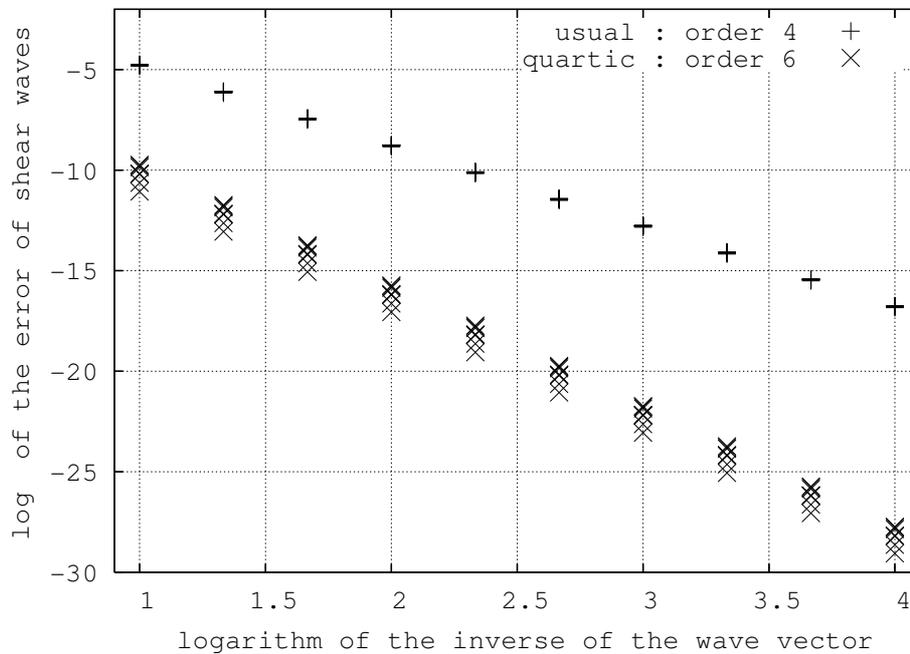


Figure 15: D3Q19 for “one point” experiment and various directions of the wave vector.

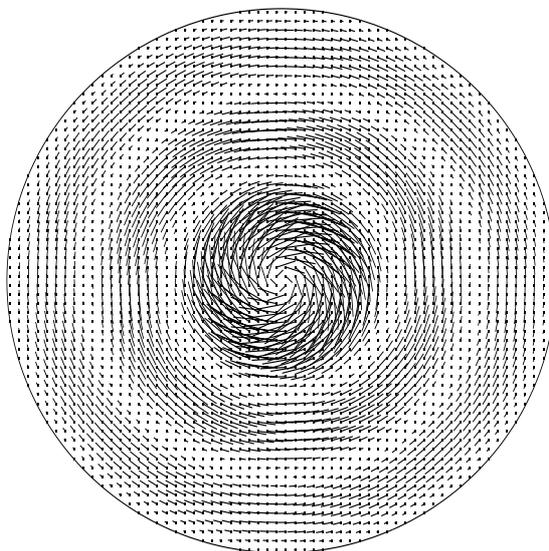


Figure 16: D3Q19 for linear Navier–Stokes in a sphere. Eigenmode $n = 3$, $\ell = 1$ for Stokes problem with Dirichlet boundary conditions. Tangential velocity vector field for a plane through the center of the sphere.

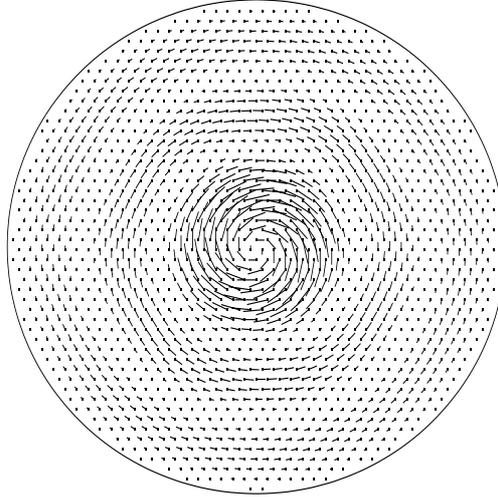


Figure 17: D3Q19 for linear Navier–Stokes in a sphere. Eigenmode $n = 3$, $\ell = 1$ for Stokes problem with Dirichlet boundary conditions. Tangent vector field for a plane orthogonal to vector $(1, 1, 1)$.

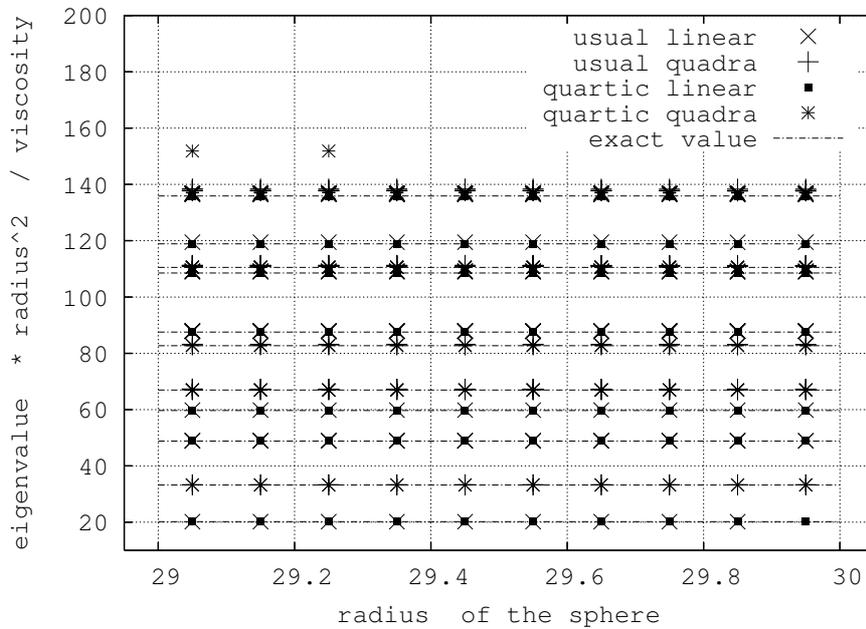


Figure 18: D3Q19 for linear Navier–Stokes in a sphere. First eigenmodes for stationary Stokes problem with Dirichlet boundary conditions.

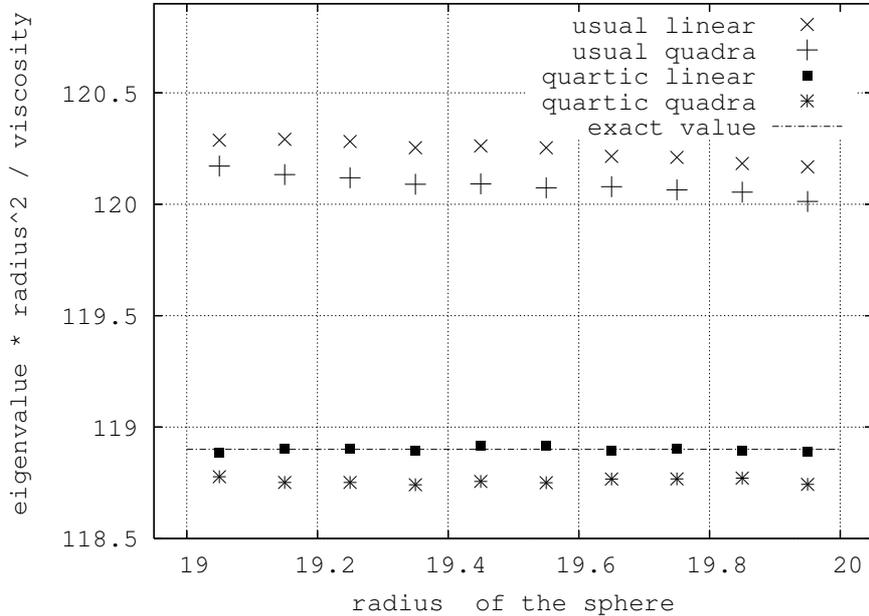


Figure 19: D3Q19 for linear Navier–Stokes in a sphere. Eigenmode for stationary Stokes problem. Zoom of various schemes for Dirichlet eigenmode close to 118.8998692.

analogous to (59), with $\zeta_{\ell+1/2}^n$ equal to the n^{th} zero of the “semi-integer” Bessel function $J_{\ell+1/2}$ as defined in Abramowitz and Stegun [1]. Using the Arnoldi technique, we can determine a few eigenvalues and verify that they are close to the theoretical formula. We present Figures 16 and 17 an example of a typical result obtained with this framework. We find that these eigenvalues have the expected degeneracy $2\ell + 1$. Note however that, the computations being made for a rather small radius R , there are small splittings of the degenerate eigenvalues due to the fact that lattice Boltzmann computations have cubic symmetry.

- For a more detailed analysis, we take advantage of the symmetry of the Stokes problem and therefore perform computations on an eighth of the sphere, taking proper account of the symmetry with respect to the planes perpendicular to the coordinates x , y , z , through the center of the cube (symmetry or anti-symmetry). Using four different combinations of symmetries on the planes, we can determine all the eigenvalues, the other combinations leading to the same eigenvalues with only a permutation in the coordinates for the eigenmodes. Note that due to the rather high complexity of the Arnoldi procedure, this allows a reduction in computer time of two orders of magnitude.
- We present in Figure 18 the effect of boundary conditions for a number of values of the radius from 29 to 30. We give in Figure 19 some details for R between 19 and 20 for

the $m = 1, n = 6$ mode. There are two sets of data, one for usual s -parameters

$$s_4 = 1.3, \quad s_5 = 1.25, \quad s_{10} = 1.2, \quad s_{13} = 1.4, \quad s_{14} = 1.25, \quad s_{16} = 1.3$$

and one for the quartic s -parameters given precedingly in (68) with

$$s_4 = 1.3, \quad s_{13} = 1.4.$$

Similar work has been done for a cube. The results are published in Leriche *et al* in [34].

5 Conclusion

- The expansion of equivalent equations that are satisfied by the mean quantities determined by the lattice Boltzmann method has been described in this contribution and explicit formulae given for a few models up to order four in space derivatives. Extending either to more complicated models or to higher order derivatives is very simple and does not imply new conceptual developments, in particular careful treatment of non commuting terms that appear in the Chapman-Enskog procedure. The developments imply only simple algebraic manipulations that can be performed by a “formal language” program, as used here. Note that these developments have a rather high complexity as seen by the fact that each order takes roughly ten times as much computer time as the preceding one.
- With the Taylor expansion method, we can obtain explicit formulae which, then, enable us to tune some parameters of the lattice Boltzmann scheme initially proposed by d’Humières in order to capture, up to fourth-order accuracy, shear waves. Of course, this extra-precision obtained with a classical scheme is possible only if the viscosity is essentially fixed and the expansion done around zero velocity. Even though very few situations were studied here, it can be said that tuning the accuracy of the “internal code” independently from the method to take care of boundary conditions allows us to get useful information concerning these two sources of errors in lattice Boltzmann simulations. Future extension of this work will be to try and discriminate between some of the numerous proposed ways to deal with boundaries to be able to estimate their contributions to errors in comparison to those due to the “internal code”.

Appendix A. Taylor expansion method

- We start from relation (15) for iteration of the lattice Boltzmann scheme and take the momentum of order k . Then

$$\begin{aligned}
m_k(x, t + \Delta t) &= \sum_{\ell=0}^J M_{k\ell} f_\ell^*(x - v_\ell \Delta t, t) \\
&= \sum_{\ell=0}^J \sum_{p=0}^J M_{k\ell} M_{\ell p}^{-1} m_p^*(x - v_\ell \Delta t, t) \quad \text{due to (14)} \\
&= \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} m_r(x - v_\ell \Delta t, t)
\end{aligned}$$

due to (19). We have

$$(69) \quad m_k(x, t + \Delta t) = \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} m_r(x - v_\ell \Delta t, t), \quad 0 \leq k \leq J.$$

We expand now momentum $m_r(x - v_\ell \Delta t, t)$ with a Taylor formula of infinite length:

$$(70) \quad m_r(x - v_\ell \Delta t, t) = \sum_{q=0}^{+\infty} \frac{(\Delta t)^q}{q!} \left(- \sum_{\alpha=1}^d M_{\alpha\ell} \partial_\alpha \right)^q m_r(x, t).$$

Then due to (69), (70) and (22), we have

$$(71) \quad m_k(x, t + \Delta t) = \sum_{\gamma} \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} \frac{\Delta t^{|\gamma|}}{|\gamma|!} P_{\ell\gamma} \partial_\gamma m_r, \quad 0 \leq k \leq J.$$

We can also expand the left hand side of (71) and we have finally

$$(72) \quad \sum_{q=0}^{\infty} \frac{\Delta t^q}{q!} \partial_t^q m_k = \sum_{\gamma} \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} \frac{\Delta t^{|\gamma|}}{|\gamma|!} P_{\ell\gamma} \partial_\gamma m_r, \quad 0 \leq k \leq J.$$

- We consider relation (72) at order zero relative to time step for a conserved component of momentum (*id est* $0 \leq k \equiv i \leq N-1$). The left hand side of (72) is equal to $m_i + O(\Delta t)$

and we have

$$\begin{aligned}
W_i + \text{O}(\Delta t) &= \sum_{\ell=0}^J \sum_{p=0}^J \sum_{r=0}^J M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} m_r + \text{O}(\Delta t) \\
&= \sum_{p=0}^J \sum_{r=0}^J \delta_{ip} \Psi_{pr} m_r + \text{O}(\Delta t) \\
&= \sum_{r=0}^J \Psi_{ir} m_r + \text{O}(\Delta t) \quad \text{with } 0 \leq i \leq N \\
&= \sum_{r=0}^J \delta_{ir} m_r + \text{O}(\Delta t) \quad \text{due to (20)} \\
&= m_i + \text{O}(\Delta t)
\end{aligned}$$

and no information is contained at this first step. Consider now the same development for $k \geq N$. We pass over some repeated summations:

$$\begin{aligned}
m_k + \text{O}(\Delta t) &= M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} m_r + \text{O}(\Delta t) \\
&= \sum_{j=0}^{N-1} M_{k\ell} M_{\ell p}^{-1} \Psi_{pj} m_j + \sum_{r \geq N} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} m_r + \text{O}(\Delta t) \\
&= \sum_{j=0}^{N-1} \delta_{kp} \Psi_{pj} W_j + \sum_{r \geq N} M_{k\ell} M_{\ell p}^{-1} \delta_{pr} (1 - s_r) m_r + \text{O}(\Delta t) \\
&\hspace{15em} \text{due to (19) and (20)} \\
&= \sum_{j=0}^{N-1} \Psi_{kj} W_j + M_{k\ell} M_{\ell p}^{-1} (1 - s_p) m_p + \text{O}(\Delta t) \\
&= \delta_{kp} (1 - s_p) m_p + \sum_{j=0}^{N-1} \Psi_{kj} W_j + \text{O}(\Delta t) \\
&= (1 - s_k) m_k + \sum_{j=0}^{N-1} \Psi_{kj} W_j + \text{O}(\Delta t).
\end{aligned}$$

We deduce from the previous calculation the relation (23) with the expression (24) of the coefficients B_{kj}^0 . Then we can go now one step further.

- At first order, relation (72) becomes

$$(73) \quad m_k + \Delta t \frac{\partial m_k}{\partial t} + \text{O}(\Delta t^2) = m_k^* - \Delta t \sum_{\alpha=1}^d M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} M_{\alpha\ell} \partial_\alpha m_r + \text{O}(\Delta t^2).$$

For conserved variables (5) (*id est* $0 \leq k \equiv i \leq N - 1$), we have after dividing by Δt ,

$$\begin{aligned}
\frac{\partial W_i}{\partial t} + O(\Delta t) &= - \sum_{\alpha=1}^d M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} M_{\alpha\ell} \partial_\alpha m_r + O(\Delta t) \\
&= - \sum_{\alpha=1}^d \Lambda_{\alpha i}^p \Psi_{pr} \partial_\alpha m_r + O(\Delta t) \quad \text{due to (18)} \\
&= \sum_{\alpha=1}^d \Lambda_{\alpha i}^p \left(\sum_{j < N} \Psi_{pj} \partial_\alpha W_j + \sum_{\ell \geq N} \Psi_{p\ell} \partial_\alpha m_\ell \right) + O(\Delta t) \\
&= \sum_{\alpha=1}^d \Lambda_{\alpha i}^p \sum_{j < N} \left(\Psi_{pj} \partial_\alpha W_j + \sum_{\ell \geq N} \Psi_{p\ell} \partial_\alpha \left(\frac{1}{s_\ell} \Psi_{\ell j} W_j \right) \right) + O(\Delta t) \\
&= \sum_{j=0}^{N-1} \sum_{\alpha=1}^d \sum_{p=0}^J \Lambda_{\alpha i}^p \left(\Psi_{pj} + \sum_{\ell \geq N} \Psi_{p\ell} \frac{1}{s_\ell} \Psi_{\ell j} \right) \partial_\alpha W_j + O(\Delta t).
\end{aligned}$$

For an index γ between 1 and d , we define A_{ij}^γ according to the relation (26) and the previous calculation can be written as a conservation law at first-order

$$(74) \quad \frac{\partial W_i}{\partial t} + \sum_{|\gamma|=1} A_{ij}^\gamma \partial_\gamma W_j = O(\Delta t), \quad 0 \leq i \leq N - 1.$$

- We start again from relation (73) with nonconservative indices k ($k \geq N$):

$$m_k = -\Delta t \frac{\partial m_k}{\partial t} + (1-s_k) m_k + \sum_{j=0}^{N-1} \Psi_{kj} W_j - \Delta t \sum_{\alpha=1}^d M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} M_{\alpha\ell} \partial_\alpha m_r + O(\Delta t^2).$$

Then due to (23),

$$\begin{aligned}
m_k &= \frac{1}{s_k} \left(\Psi_{kj} W_j - \Delta t \frac{1}{s_k} \Psi_{ki} \frac{\partial W_i}{\partial t} - \Delta t \Lambda_{\alpha k}^p \Psi_{pr} \partial_\alpha \left(\frac{1}{s_r} \Psi_{rj} W_j \right) \right) + O(\Delta t^2) \\
&= \frac{1}{s_k} \left(\Psi_{kj} W_j + \frac{\Delta t}{s_k} \Psi_{ki} \sum_{|\gamma|=1} A_{ij}^\gamma \partial_\gamma W_j - \frac{\Delta t}{s_r} \Lambda_{\gamma k}^p \Psi_{pr} \Psi_{rj} \partial_\gamma W_j \right) + O(\Delta t^2).
\end{aligned}$$

We introduce B_{kj}^γ for $|\gamma|=1$ according to (28) and due to previous calculation, relation (23) can be extended as

$$(75) \quad m_k = \sum_{0 \leq |\gamma| \leq 1} \Delta t^{|\gamma|} B_{kj}^\gamma \partial_\gamma W_j + O(\Delta t^2).$$

- We generalize the relations (74) and (75) at the order σ through a recurrence hypothesis (29) (30). In order to treat the left-hand side of relation (72), we observe that

we have

$$\begin{aligned}\partial_t^2 W_i &= - \sum_{1 \leq |\gamma| \leq \sigma} \Delta t^{|\gamma|-1} A_{ij}^\gamma \partial_\gamma \left(\partial_t W_j \right) + O(\Delta t^\sigma) \\ &= \sum_{1 \leq |\delta| \leq \sigma} \Delta t^{|\delta|-1} A_{i\ell}^\delta \partial_\delta \left(\sum_{1 \leq |\varepsilon| \leq \sigma} \Delta t^{|\varepsilon|-1} A_{\ell j}^\varepsilon \partial_\varepsilon W_j \right) + O(\Delta t^\sigma)\end{aligned}$$

and if we introduce $C_{ij}^{1,\gamma}$ according to (31) and

$$C_{ij}^{2,\gamma} \equiv - \sum_{|\delta| \geq 1, |\varepsilon| \geq 1, \delta + \varepsilon = \gamma} A_{i\ell}^\delta A_{\ell j}^\varepsilon, \quad 2 \leq |\gamma| \leq \sigma + 1,$$

we have for the second time derivative a relation quite analogous to (29):

$$\partial_t^2 W_i + \sum_{2 \leq |\gamma| \leq \sigma+1} \Delta t^{|\gamma|-2} C_{ij}^{2,\gamma} \partial_\gamma W_j = O(\Delta t^\sigma), \quad 0 \leq i \leq N-1.$$

This relation can be generalized at an arbitrary order according to

$$(76) \quad \partial_t^q W_i + \sum_{q \leq |\gamma| \leq \sigma+q-1} \Delta t^{|\gamma|-q} C_{ij}^{q,\gamma} \partial_\gamma W_j = O(\Delta t^\sigma), \quad 0 \leq i \leq N-1.$$

If relation (76) is true at order q , we have by differentiation with respect to time,

$$\begin{aligned}\partial_t^{q+1} W_i &= - \sum_{q \leq |\gamma| \leq \sigma+q-1} \Delta t^{|\gamma|-q} C_{ij}^{q,\gamma} \partial_\gamma \left(\partial_t W_j \right) + O(\Delta t^\sigma) \\ &= \sum_{q \leq |\delta| \leq \sigma+q-1} \Delta t^{|\delta|-q} C_{i\ell}^{q,\delta} \partial_\delta \left(\sum_{1 \leq |\varepsilon| \leq \sigma} \Delta t^{|\varepsilon|-1} A_{\ell j}^\varepsilon \partial_\varepsilon W_j \right) + O(\Delta t^\sigma) \\ &\equiv \sum_{q+1 \leq |\gamma| \leq \sigma+q} \Delta t^{|\gamma|-q-1} C_{ij}^{q+1,\gamma} \partial_\gamma \left(\partial_t W_j \right) + O(\Delta t^\sigma)\end{aligned}$$

and relation (76) is satisfied at the order $q+1$ with $C_{ij}^{q+1,\gamma}$ given by the recurrence relation (32). In an analogous way, we have

$$(77) \quad \partial_t^q m_k = \sum_{q \leq |\gamma| \leq \sigma+q} \Delta t^{|\gamma|-q} D_{kj}^{q,\gamma} \partial_\gamma W_j + O(\Delta t^{\sigma+1}), \quad k \geq N,$$

with $D_{kj}^{0,\gamma}$ defined according to (34). If the relation (77) is satisfied at order q , we have by differentiation relative to time,

$$\begin{aligned}\partial_t^{q+1} m_k &= \sum_{q \leq |\gamma| \leq \sigma+q} \Delta t^{|\gamma|-q} D_{kj}^{q,\gamma} \partial_\gamma \left(\partial_t W_j \right) + O(\Delta t^{\sigma+1}) \\ &= - \sum_{q \leq |\delta| \leq \sigma+q} \Delta t^{|\delta|-q} D_{k\ell}^{q,\delta} \partial_\delta \left(\sum_{1 \leq |\varepsilon| \leq \sigma} \Delta t^{|\varepsilon|-1} A_{\ell j}^\varepsilon \partial_\varepsilon W_j \right) + O(\Delta t^{\sigma+1}) \\ &\equiv \sum_{q+1 \leq |\gamma| \leq \sigma+q+1} \Delta t^{|\gamma|-(q+1)} D_{kj}^{q+1,\gamma} \partial_\gamma W_j + O(\Delta t^{\sigma+1})\end{aligned}$$

with coefficients $D_{kj}^{q+1,\gamma}$ determined according to the relation (35). We observe that for the particular value $|\gamma| = \sigma + 1$ the coefficient $D_{kj}^{q+1,\gamma}$ is well defined for $0 \leq q \leq \sigma$. In other words, the coefficient $D_{kj}^{q,\gamma}$ is well defined for $1 \leq q \leq |\gamma|$.

• We verify now by induction that the recurrence relations (29) and (30) are satisfied. It is the case at order 1 as we have shown in (74) and (75). We first consider a label i such that $0 \leq i \leq N - 1$. Then according to (72), we have at the order $\sigma + 2$:

$$\left\{ \begin{array}{l} W_i + \Delta t \frac{\partial W_i}{\partial t} + \sum_{q=2}^{\sigma+1} \frac{\Delta t^q}{q!} \partial_t^q W_i + O(\Delta t^{\sigma+2}) = \\ W_i + M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} \sum_{1 \leq |\delta| \leq \sigma+1} \frac{\Delta t^{|\delta|}}{|\delta|!} P_{\ell\delta} \partial_\delta \left(\sum_{0 \leq |\varepsilon| \leq \sigma} \Delta t^{|\varepsilon|} B_{rj}^\varepsilon \partial_\varepsilon W_j \right) + O(\Delta t^{\sigma+2}). \end{array} \right.$$

We use relation (76) for the left hand side of previous relation. We get after dividing by Δt

$$\left\{ \begin{array}{l} \frac{\partial W_i}{\partial t} - \sum_{q=2}^{\sigma+1} \frac{\Delta t^{q-1}}{q!} \sum_{q \leq |\gamma| \leq \sigma+q-1} \Delta t^{|\gamma|-q} C_{ij}^{q,\gamma} \partial_\gamma W_j + O(\Delta t^{\sigma+1}) = \\ \sum_{1 \leq |\delta| \leq \sigma+1, 0 \leq |\varepsilon| \leq \sigma} M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} \frac{\Delta t^{|\delta|+|\varepsilon|-1}}{|\delta|!} B_{rj}^\varepsilon \partial_{\delta+\varepsilon} W_j + O(\Delta t^{\sigma+1}). \end{array} \right.$$

and the relation (29) is extended one step further with a coefficient A_{ij}^γ defined for $|\gamma| = q + 1$ by the recurrence relation (33). For the nonconserved moments ($k \geq N$), the relation (72) can be written at the order $\sigma + 2$ as

$$\left\{ \begin{array}{l} m_k + \sum_{q=1}^{\sigma+1} \frac{\Delta t^q}{q!} \partial_t^q m_k + O(\Delta t^{\sigma+2}) = \\ (1 - s_k) m_k + \sum_{1 \leq |\delta| \leq \sigma+1} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} \frac{\Delta t^{|\delta|}}{|\delta|!} P_{\ell\delta} \partial_\delta \left(\sum_{0 \leq |\varepsilon| \leq \sigma} \Delta t^{|\varepsilon|} B_{rj}^\varepsilon \partial_\varepsilon W_j \right) + O(\Delta t^{\sigma+2}). \end{array} \right.$$

We use the relation (77) and we deduce:

$$\left\{ \begin{array}{l} s_k m_k = - \sum_{q=1}^{\sigma+1} \frac{\Delta t^q}{q!} \sum_{q \leq |\gamma| \leq \sigma+q} \Delta t^{|\gamma|-q} D_{kj}^{q,\gamma} \partial_\gamma W_j \\ + \sum_{1 \leq |\delta| \leq \sigma+1, 0 \leq |\varepsilon| \leq \sigma} \frac{\Delta t^{|\delta|+|\varepsilon|}}{|\delta|!} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} B_{rj}^\varepsilon \partial_{\delta+\varepsilon} W_j + O(\Delta t^{\sigma+2}). \end{array} \right.$$

We set, with $|\gamma| = \sigma + 1$, $k \geq N$, $0 \leq j \leq N - 1$,

$$B_{kj}^\gamma = \frac{1}{s_k} \left(- \sum_{1 \leq q \leq \sigma+1} \frac{1}{q!} D_{kj}^{q,\gamma} + \sum_{1 \leq |\delta| \leq \sigma+1, 0 \leq |\varepsilon| \leq \sigma, \delta+\varepsilon=\gamma} \frac{1}{|\delta|!} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} B_{rj}^\varepsilon \right)$$

and the relation (36) is established by induction. \square

Appendix B.

Notations for classical lattice Boltzmann schemes

In order to define precisely our results, the numbering of degrees of freedom must be defined and we make this point precise in this Appendix with the help of usual graphics. The choice of moments, *id est* the M matrix (relation (4)) is also made explicit.

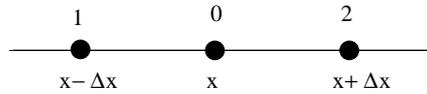


Figure 20: Stencil for the D1Q3 lattice Boltzmann scheme

- **D1Q3 for advective thermics**

Recall first that the D1Q3 lattice Boltzmann scheme ($J = 2$ in relation (4)) uses three neighbours for a given node x : the vertex x itself and the first neighbours located at $\pm\Delta x$ from x (see Figure 20). We introduce λ as in (17) and adopt a labelling for matrix M of relation (4) as in Figure 20:

$$(78) \quad M = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2/2 & 0 & \lambda^2/2 \end{pmatrix}.$$

- **D2Q5 for classical thermics**

We have now four ($J = 4$) nontrivial possible directions for propagation of particles (Figure 21, left). We adopt for the M matrix of relation (4) the following choice:

$$(79) \quad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 \\ 0 & 0 & \lambda & 0 & -\lambda \\ -4 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 1 & -1 \end{pmatrix}.$$

- **D2Q9 for classical thermics**

The lattice Boltzmann model D2Q9 is obtained from the D2Q5 model by adding four velocities along the diagonals (Figure 21, right). The evaluation of matrix M is entirely nontrivial. We refer the reader to [30], and the reader can also consult our introduction

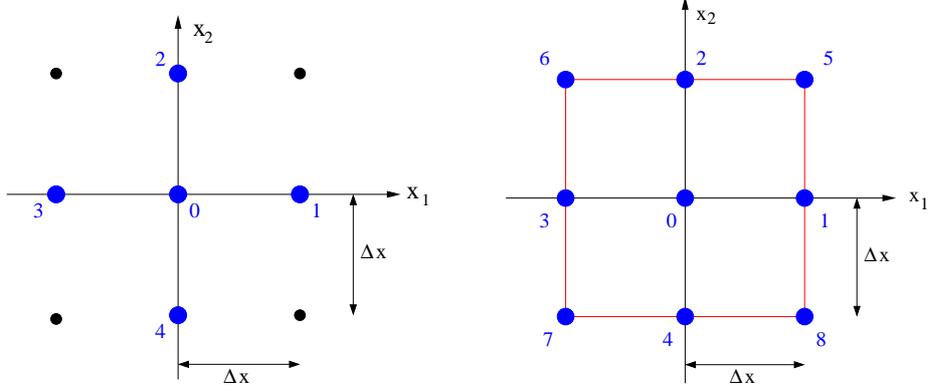


Figure 21: Stencils for D2Q5 and D2Q9 lattice Boltzmann schemes

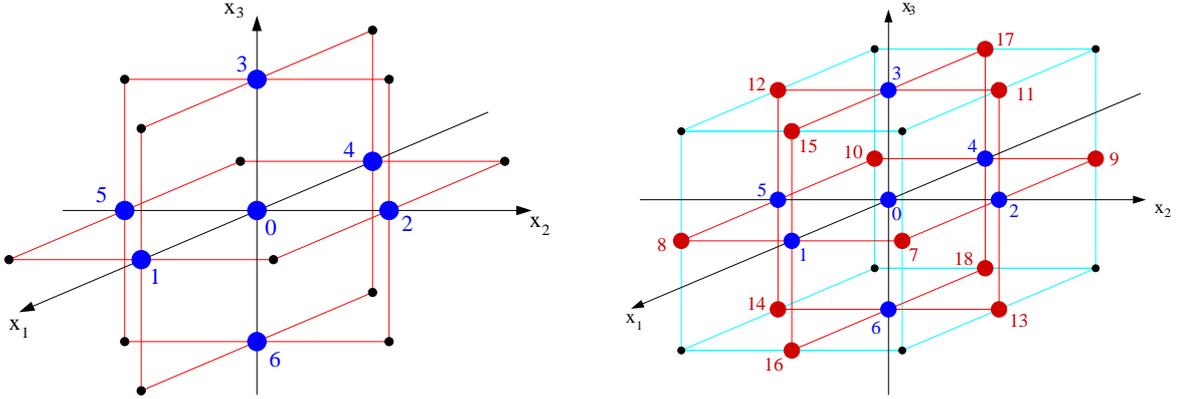


Figure 22: Stencils for D3Q7 and D3Q19 lattice Boltzmann schemes

[14]. We have:

$$(80) \quad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}.$$

- **D3Q7 for pure thermics**

For three-dimensional thermics, one only needs a seven point scheme and can use the so-called D3Q7 lattice Boltzmann scheme whose stencil is described in the left part of

Figure 22. The matrix is not very difficult to construct. We follow [31]:

$$(81) \quad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & \lambda & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & \lambda & 0 & 0 & -\lambda \\ 0 & -1 & -1 & 2 & -1 & -1 & 2 \\ 0 & 1 & -1 & 0 & 1 & -1 & 0 \\ -6 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

- **D3Q19 for linearized Navier–Stokes**

The D3Q19 Lattice Boltzmann scheme is described with details *e.g.* in J. Tölke *et al* [46] and the stencil is presented in Figure 22 (right). The matrix M that parameterizes the transformation (4) looks like this:

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & 0 & -\lambda & 0 & 0 & \lambda & \lambda & -\lambda & -\lambda & 0 & 0 & 0 & 0 & \lambda & \lambda & -\lambda & -\lambda \\ 0 & 0 & \lambda & 0 & 0 & -\lambda & 0 & \lambda & -\lambda & \lambda & -\lambda & \lambda & -\lambda & \lambda & -\lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda & 0 & 0 & -\lambda & 0 & 0 & 0 & 0 & \lambda & \lambda & -\lambda & -\lambda & \lambda & -\lambda & \lambda & -\lambda \\ -30\lambda^2 & -11\lambda^2 & -11\lambda^2 & -11\lambda^2 & -11\lambda^2 & -11\lambda^2 & -11\lambda^2 & 8\lambda^2 \\ 0 & 2\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & -\lambda^2 & -\lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & -2\lambda^2 & -2\lambda^2 & -2\lambda^2 & -2\lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 \\ 0 & 0 & \lambda^2 & -\lambda^2 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & 0 & 0 & 0 & 0 & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & -\lambda^2 & \lambda^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & -\lambda^2 & \lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & -\lambda^2 & \lambda^2 \\ 0 & -4\lambda^3 & 0 & 0 & 4\lambda^3 & 0 & 0 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 & 0 & 0 & 0 & 0 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 0 & 0 & -4\lambda^3 & 0 & 0 & 4\lambda^3 & 0 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -4\lambda^3 & 0 & 0 & 4\lambda^3 & 0 & 0 & 0 & 0 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 \\ 12\lambda^4 & -4\lambda^4 & -4\lambda^4 & -4\lambda^4 & -4\lambda^4 & -4\lambda^4 & -4\lambda^4 & \lambda^4 \\ 0 & -4\lambda^4 & 2\lambda^4 & 2\lambda^4 & -4\lambda^4 & 2\lambda^4 & 2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \\ 0 & 0 & -2\lambda^4 & 2\lambda^4 & 0 & -2\lambda^4 & 2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & 0 & 0 & 0 & 0 & -\lambda^4 & -\lambda^4 & -\lambda^4 & -\lambda^4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 & 0 & 0 & 0 & 0 & -\lambda^3 & -\lambda^3 & \lambda^3 & \lambda^3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda^3 & -\lambda^3 & \lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & \lambda^3 & -\lambda^3 \end{bmatrix}.$$

Due to the important number of moments, we detail in this sub-section the way the previous matrix is obtained. First, velocities v_j^α for $0 \leq j \leq J \equiv 18$ and $1 \leq \alpha \leq 3$ are naturally associated with Figure 22. The four first moments ρ and q^α are determined according to (6) and (7) and the associated elements for matrix M are given in (8) and (9). The construction of other moments uses the tensorial nature of the variety of

moments that can be constructed, as analyzed by Rubinstein and Luo [41]: scalar fields are naturally coupled with one another and similarly for vector fields, and so on. So components of kinetic energy are introduced:

$$(82) \quad \widetilde{M}_{4j} = 19 \sum_{\alpha} |v_j^{\alpha}|^2, \quad 0 \leq j \leq J.$$

The entire set of second-order tensors is completed according to

$$(83) \quad \begin{cases} \widetilde{M}_{5j} &= 2(v_j^1)^2 - (v_j^2)^2 - (v_j^3)^2 \\ \widetilde{M}_{6j} &= (v_j^2)^2 - (v_j^3)^2 \\ \widetilde{M}_{7j} &= v_j^1 v_j^2, \quad \widetilde{M}_{8j} = v_j^2 v_j^3, \quad \widetilde{M}_{9j} = v_j^3 v_j^1, \end{cases} \quad 0 \leq j \leq J.$$

The three components of heat flux are defined by

$$(84) \quad \begin{cases} \widetilde{M}_{10j} = 5 v_j^1 \sum_{\alpha} |v_j^{\alpha}|^2, & \widetilde{M}_{11j} = 5 v_j^2 \sum_{\alpha} |v_j^{\alpha}|^2, & \widetilde{M}_{12j} = 5 v_j^3 \sum_{\alpha} |v_j^{\alpha}|^2, \\ & & 0 \leq j \leq J. \end{cases}$$

We finally obtain the moments of higher degree: the square of the kinetic energy

$$(85) \quad \widetilde{M}_{13j} = \frac{21}{2} \left(\sum_{\alpha} |v_j^{\alpha}|^2 \right)^2, \quad 0 \leq j \leq J,$$

second-order moments “weighted” by kinetic energy:

$$(86) \quad \begin{cases} \widetilde{M}_{14j} &= 3 \left(2(v_j^1)^2 - (v_j^2)^2 - (v_j^3)^2 \right) \sum_{\alpha} |v_j^{\alpha}|^2 \\ \widetilde{M}_{15j} &= 3 \left((v_j^2)^2 - (v_j^3)^2 \right) \sum_{\alpha} |v_j^{\alpha}|^2, \end{cases} \quad 0 \leq j \leq J,$$

and third-order anti-symmetric moments:

$$(87) \quad \begin{cases} \widetilde{M}_{16j} &= v_j^1 \left((v_j^2)^2 - (v_j^3)^2 \right) \\ \widetilde{M}_{17j} &= v_j^2 \left((v_j^3)^2 - (v_j^1)^2 \right) \\ \widetilde{M}_{18j} &= v_j^3 \left((v_j^1)^2 - (v_j^2)^2 \right), \end{cases} \quad 0 \leq j \leq J.$$

Then matrix M is orthogonalized from relations (8), (9), (82), (83), (84), (85), (86) and (87) with a Gram-Schmidt classical algorithm:

$$M_{ij} = \widetilde{M}_{ij} - \sum_{\ell < i} g_{i\ell} M_{\ell j}, \quad i \geq 4.$$

The coefficients $g_{i\ell}$ are computed recursively in order to force orthogonality:

$$\sum_{j=0}^J M_{ij} M_{kj} = 0 \quad \text{for } i \neq k.$$

Appendix C. Quartic parameters in three dimensions

- We use the equivalent equations of lattice Boltzmann scheme D3Q19 obtained previously in the following way. We consider the vector of conserved variables (5): $W \equiv (\rho, q_x, q_y, q_z)^t$. We write the equivalent partial differential equations under the combined form:

$$(88) \quad \partial_t W_k + \sum_{j,p,q,r} A_{kpqr}^j \partial_x^p \partial_y^q \partial_z^r W_j = O(\Delta t^4).$$

We search dissipative mode solution of (88) under the form $W(t) = e^{-\Gamma t + i(k_x x + k_y y + k_z z)} \widetilde{W}$. Then Γ is an eigenvalue of the matrix A defined by

$$A_k^j = \sum_{p,q,r} A_{kpqr}^j (i k_x)^p (i k_y)^q (i k_z)^r.$$

- We wish to solve this dispersion equation with a high order of accuracy, *id est* in our present case:

$$(89) \quad \Delta \equiv \det [A - \Gamma \text{Id}] = O(\Delta t^7).$$

We impose also that this eigenvalue is **double** as classical for shear waves in three dimensions [32]: $\frac{d}{d\Gamma} (\det [A - \Gamma \text{Id}]) \approx 0$. The first nontrivial term in powers of Δt for this derivative of the determinant is the term of order 3. Then we force

$$(90) \quad \frac{d}{d\Gamma} (\det [A - \Gamma \text{Id}]) = O(\Delta t^4).$$

For Stokes problem (incompressible shear modes) and D3Q19 lattice Boltzmann d'Humières scheme, we have [38]:

$$(91) \quad \Gamma \equiv \nu |k|^2 = \frac{\lambda^2}{3} \Delta t \sigma_5 (k_x^2 + k_y^2 + k_z^2).$$

- We solve the set (89) (90) (91) of equations for all values of the time step Δt . We obtain in this way a set of eight algebraic equations:

$$\left\{ \begin{array}{l} 2 \sigma_5 \sigma_{10} - 4 \sigma_5^2 + 6 \sigma_5 \sigma_{16} = 1 \\ 80 \sigma_5^4 - 32 \sigma_5^3 \sigma_{10} + 24 \sigma_5^2 \sigma_{10} \sigma_{16} + 12 \sigma_{14} \sigma_{16} \sigma_5^2 - 8 \sigma_5^2 - 4 \sigma_5^2 \sigma_{10}^2 \\ \quad + 12 \sigma_5^2 \sigma_{16}^2 - 12 \sigma_5^2 \sigma_{14} \sigma_{10} - 12 \sigma_5 \sigma_{16} \sigma_{14} \sigma_{10} + 6 \sigma_5 \sigma_{14} \sigma_{10}^2 \\ \quad - 8 \sigma_5 \sigma_{16} + 6 \sigma_5 \sigma_{16}^2 \sigma_{14} - \sigma_{14} \sigma_{16} + \sigma_{14} \sigma_{10} + 1 = 0 \\ -48 \sigma_5^5 \sigma_{10} + 44 \sigma_5^4 \sigma_{10}^2 + 2000 \sigma_5^5 \sigma_{16} + 95 \sigma_5^2 - 16 \sigma_5^4 \sigma_{14} \sigma_{10} \\ \quad + 292 \sigma_{14} \sigma_{16} \sigma_5^2 + 68 \sigma_5^2 \sigma_{14} \sigma_{10} - 272 \sigma_5^4 \sigma_{16} \sigma_{14} - 1032 \sigma_5^3 \sigma_{16}^2 \sigma_{14} \\ + 56 \sigma_5^3 \sigma_{14} \sigma_{10}^2 - 320 \sigma_5^6 - 1048 \sigma_5^4 \sigma_{10} \sigma_{16} + \sigma_{14}^2 + 60 \sigma_5^2 \sigma_{16}^2 \sigma_{14}^2 - 16 \sigma_5 \sigma_{16} \sigma_{14}^2 \\ \quad + 72 \sigma_5^2 \sigma_{14}^2 \sigma_{10} \sigma_{16} - 8 \sigma_5 \sigma_{14}^2 \sigma_{10} + 24 \sigma_5^3 \sigma_{14} + 12 \sigma_5^2 \sigma_{14}^2 \sigma_{10}^2 - 248 \sigma_5^4 \\ - 464 \sigma_5^3 \sigma_{16} \sigma_{14} \sigma_{10} + 148 \sigma_5^3 \sigma_{10} - 1284 \sigma_{16} \sigma_5^3 + 4284 \sigma_{16}^2 \sigma_5^4 - 20 \sigma_5 \sigma_{14} = 0 \end{array} \right.$$

$$\left\{ \begin{array}{l}
(-1 + 2\sigma_5\sigma_{10} - 4\sigma_5^2 + 6\sigma_5\sigma_{16})(2\sigma_5\sigma_{10} + 2\sigma_{14}\sigma_{10} \\
\quad - 2\sigma_5^2 - 10\sigma_5\sigma_{16} - 2\sigma_{14}\sigma_{16} + 3) = 0 \\
96\sigma_5^5\sigma_{10} + 24\sigma_5^4\sigma_{10}^2 - 1920\sigma_5^5\sigma_{16} + 98\sigma_5^2 + 24\sigma_5^4\sigma_{14}\sigma_{10} + 350\sigma_{14}\sigma_{16}\sigma_5^2 \\
\quad + 34\sigma_5^2\sigma_{14}\sigma_{10} + 264\sigma_5^4\sigma_{16}\sigma_{14} - 1524\sigma_5^3\sigma_{16}^2\sigma_{14} + 12\sigma_5^3\sigma_{14}\sigma_{10}^2 \\
+ 240\sigma_5^6 - 576\sigma_5^4\sigma_{10}\sigma_{16} + \sigma_{14}^2 + 102\sigma_5^2\sigma_{16}^2\sigma_{14}^2 - 20\sigma_5\sigma_{16}\sigma_{14}^2 + 36\sigma_5^2\sigma_{14}^2\sigma_{10}\sigma_{16} \\
- 4\sigma_5\sigma_{14}^2\sigma_{10} - 24\sigma_5^3\sigma_{14} + 6\sigma_5^2\sigma_{14}^2\sigma_{10}^2 + 240\sigma_5^4 - 216\sigma_5^3\sigma_{16}\sigma_{14}\sigma_{10} + 72\sigma_5^3\sigma_{10} \\
\quad - 1488\sigma_{16}\sigma_5^3 + 5688\sigma_{16}^2\sigma_5^4 - 20\sigma_5\sigma_{14} = 0 \\
\quad - \sigma_5 + 6\sigma_{16}\sigma_5^2 + 2\sigma_5^2\sigma_{10} - 4\sigma_5^3 = 0 \\
\quad 2\sigma_5^2\sigma_{10} - 2\sigma_{16}\sigma_5^2 + \sigma_5 - \sigma_5\sigma_{16}\sigma_{14} + \sigma_5\sigma_{14}\sigma_{10} - 12\sigma_5^3 = 0 \\
10\sigma_5\sigma_{16}\sigma_{14} + 2\sigma_5\sigma_{14}\sigma_{10} + 11\sigma_5 - \sigma_{14} + 8\sigma_5^3 - 82\sigma_{16}\sigma_5^2 + 6\sigma_5^2\sigma_{10} = 0.
\end{array} \right.$$

These equations have only one nontrivial family of solutions given by (68).

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