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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 “DDH” lattice Boltzmann scheme 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 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 and compare our results with analytical references.

**Keywords:** lattice Boltzmann, Taylor formula, thermics, acoustics, linearized Navier–Stokes, 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 to conservation laws of physics. The principle is to mimic at a discrete level the dynamics of the Boltzmann equation. In such a 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 [6]):

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

- 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 momenta 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  $f^{\text{eq}}$  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  $\Delta t$  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  $\Delta t$ .

• In the pioneering work of cellular automata introduced by Hardy, Pomeau and De Pazzis [21], Frisch, Hasslacher and Pomeau [16] and developed by D’Humières, Lallemand and Frisch [12], the distribution  $f_j(x, t)$  was chosen as boolean. Since the so-called lattice Boltzmann equation of Mac Namara and Zanetti [31], Higuera, Succi and Benzi [24], Chen, Chen and Matthaeus [7], Higuera and Jimenez [23], 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 [3]. With Qian, D’Humières and Lallemand [33], the equilibrium distribution  $f^{\text{eq}}$  is determined with a polynomial in velocity.

• The numerical scheme is defined by 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. With the lattice Boltzmann DDH scheme, proposed by D’Humières [10] in the form that we use here, we introduce an invertible matrix  $M$  with  $(J + 1)$  lines and  $(J + 1)$  columns. We define so-called momenta  $m$  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  $N$  momenta 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 by the  $W_i$ ’s for  $0 \leq i \leq N - 1$ . 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 (Lallemand-Luo [27]) 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 momenta, 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 momenta  $m_k^{\text{eq}}$  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* [32]) for modelling of liquid crystals.

- With D'Humières [10], we introduce relaxation parameters (also named as  $s$ -parameters in the following)  $s_k$  ( $N \leq k \leq J$ ) satisfying for stability constraints (see *e.g.* Lallemand and Luo [26]) the conditions

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

Then the nonconserved momentum  $m_k^*$  after collision 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 coefficient 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. 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 reflexion:

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

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

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

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

- The asymptotic analysis of cellular automata (see *e.g.* Hénon [22]) puts in evidence asymptotic partial differential equation 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 DDH scheme (4) to (15) has been analyzed by D’Humières [10] with a Chapman Enskog method coming from statistical physics. This method is classical for an analysis at second order of accuracy but is more complex for higher orders (Qian-Zhou [34]). It puts in evidence derivation operators with noncommutative algebraic rules. Recently, Junk and Rheinländer [25] developed a Hilbert type expansion for the analysis of lattice Boltzmann schemes at high order of accuracy. We have proposed in previous works [13, 14] an extension to lattice Boltzmann DDH scheme of the so-called method of equivalent partial differential equation proposed by Lerat and Peyret [29] and independently by Warming and Hyett [40]. In this framework, the parameter  $\Delta t$  is considered as the only infinitesimal variable and we introduce a (constant) velocity ratio  $\lambda$  between space step and time step:

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

Then shear viscosity coefficients  $\mu$  is recovered according to

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

for a particular value of label  $k$ . The coefficient  $\zeta$  is equal to  $\frac{1}{3}$  for the simplest DDH models that are considered hereafter. The extension to third order of accuracy [15] is possible and puts in evidence the tensor of momentum-velocity defined by

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

The general extension to higher orders seems to be too complex for present studies and we simplify the problem as a first approach in the present contribution.

- The relaxation process is related with the linearized collision operator introduced at relation (3). In particular for 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 [6]) and the eigenvectors are known. Moreover, the discrete model is highly constrained by symmetry and exchanges of coordinates. In what follows, we suppose that the collision process is **linear** *i.e.* that the  $G_k$

functions introduced in (10) (11) have been linearized around some reference state. With this hypothesis, we can write:

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

Precisely, there exists an  $(J+1) \times (J+1)$  matrix  $\Psi$  such that the collided momentum  $m^*$  defined in (12) is a linear combination of the momenta 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  $\Psi$  has a structure of the type

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

The top left block 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 contains the coefficients  $1 - s_k$  ( $k \geq N$ ) related to relaxation (13). From this hypothesis, we develop in section 2 a formal calculus in order to write the lattice Boltzmann DDH scheme at an arbitrary order of accuracy. In section 3, we apply the previous development to some classical linear problems of mathematical physics, from one space dimension to three space dimensions. In section 4, a simple but fundamental observation allows us to specify some parameters of matrix  $\Psi$  of (19) in order to improve the accuracy of the scheme for very particular waves.

## 2 A formal development of lattice Boltzmann DDH scheme

- We start from relation (15) 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, with Einstein convention for indices  $k, \ell, p, r$ , running from 0 to  $J$ ,

$$(22) \quad m_k(x, t + \Delta t) = M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} m_r(x - v_\ell \Delta t, t), \quad 0 \leq k \leq J.$$

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

$$(23) \quad m_r(x - v_\ell \Delta t, t) = \sum_{q=0}^{+\infty} \frac{(\Delta t)^q}{q!} \left( - \sum_{\alpha=1}^d M_{\alpha\ell} \partial_\alpha \right)^q m_r(x, t).$$

We introduce multi-indices  $\gamma, \delta, \varepsilon$  in  $\{1, \dots, d\}^q$  in order to represent multiple derivation 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  $\gamma$ :

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

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

$$(24) \quad \left( - \sum_{\alpha=1}^d M_{\alpha\ell} \partial_\alpha \right)^q \equiv \sum_{|\gamma|=q} P_{\ell\gamma} \partial_\gamma.$$

Then due to (22), (23) and (24), we have

$$(25) \quad m_k(x, t + \Delta t) = \sum_{\gamma} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} \frac{\Delta t^{|\gamma|}}{|\gamma|!} P_{\ell\gamma} \partial_\gamma m_r, \quad 0 \leq k \leq J.$$

We can also expand the left hand side of (25) and we have finally

$$(26) \quad \sum_{q=0}^{\infty} \frac{\Delta t^q}{q!} \partial_t^q m_k = \sum_{\gamma} M_{k\ell} M_{\ell p}^{-1} \Psi_{pr} \frac{\Delta t^{|\gamma|}}{|\gamma|!} P_{\ell\gamma} \partial_\gamma m_r, \quad 0 \leq k \leq J.$$

- We consider relation (26) 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 (26) is equal to  $m_i + O(\Delta t)$



and we have

$$\begin{aligned}
W_i + O(\Delta t) &= M_{il} M_{lp}^{-1} \Psi_{pr} m_r + O(\Delta t) \\
&= \delta_{ip} \Psi_{pr} m_r + O(\Delta t) \\
&= \Psi_{ir} m_r + O(\Delta t) \quad \text{with } 0 \leq i \leq N \\
&= \delta_{ir} m_r + O(\Delta t) \quad \text{due to (18)} \\
&= m_i + O(\Delta t)
\end{aligned}$$

and no information is contained at this first step. Consider now the same development for  $k \geq N$ :

$$\begin{aligned}
m_k + O(\Delta t) &= M_{kl} M_{lp}^{-1} \Psi_{pr} m_r + O(\Delta t) \\
&= \sum_{j=0}^{N-1} M_{kl} M_{lp}^{-1} \Psi_{pj} m_j + \sum_{r \geq N} M_{kl} M_{lp}^{-1} \Psi_{pr} m_r + O(\Delta t) \\
&= \sum_{j=0}^{N-1} \delta_{kp} \Psi_{pj} W_j + \sum_{r \geq N} M_{kl} M_{lp}^{-1} \delta_{pr} (1 - s_p) m_r + O(\Delta t) \\
&\hspace{20em} \text{due to (18) and (20)} \\
&= \sum_{j=0}^{N-1} \Psi_{kj} W_j + M_{kl} M_{lp}^{-1} (1 - s_p) m_p + O(\Delta t) \\
&= \delta_{kp} (1 - s_p) m_p + \sum_{j=0}^{N-1} \Psi_{kj} W_j + O(\Delta t) \\
&= (1 - s_k) m_k + \sum_{j=0}^{N-1} \Psi_{kj} W_j + O(\Delta t).
\end{aligned}$$

With the Einstein implicit summation convention for “conservative indices”  $i$  and  $j$  ( $0 \leq i, j \leq N - 1$ ), we deduce from the previous calculus:

$$(27) \quad m_k = \frac{1}{s_k} \Psi_{kj} W_j + O(\Delta t), \quad k \geq N.$$

The nonconserved momenta  $m_k$  for  $k \geq N$  are completely explicited as function of the conserved ones (the  $W$ 's). We set

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

and relation (27) can be re-written under the form

$$(28) \quad m_k = B_{kj}^0 W_j + O(\Delta t), \quad k \geq N.$$

We can go now one step further.

- At first order, relation (26) becomes

$$(29) \quad m_k + \Delta t \frac{\partial m_k}{\partial t} + O(\Delta t^2) = M_{kl} M_{lp}^{-1} \Psi_{pr} \left( m_r - \sum_{\alpha=1}^d \Delta t M_{\alpha l} \partial_{\alpha} m_r \right) + O(\Delta t^2).$$

For conserved variables (5) (*id est*  $0 \leq k \equiv i \leq N-1$ ), we have from previous considerations and after dividing by  $\Delta t$ :

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

For an index  $\gamma$  between 1 and  $d$ , we set

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

and the previous calculus can be written as a conservation law at first order

$$(30) \quad \frac{\partial W_i}{\partial t} + \sum_{|\gamma|=1} A_{ij}^{\gamma} \partial_{\gamma} W_j = O(\Delta t), \quad 0 \leq i \leq N-1.$$

We start again from relation (29) with nonconservative indices  $k$  ( $k \geq N$ ):

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

Then due to (27) and (18),

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

We set

$$B_{kj}^\gamma \equiv \frac{1}{s_k^2} \Psi_{kj} A_{ij}^\gamma - \frac{1}{s_k s_r} \Lambda_{\alpha k}^p \Psi_{pr} \Psi_{rj}, \quad |\gamma|=1, \quad k \geq N, \quad 0 \leq j \leq N-1$$

and due to previous calculus, relation (28) can be extended as

$$(31) \quad m_k = \sum_{0 \leq |\gamma| \leq 1} \Delta t^{|\gamma|} B_{kj}^\gamma \partial_\gamma W_j + O(\Delta t^2).$$

• We generalize the relations (30) and (31) at the order  $\sigma$  through a recurrence hypothesis

$$(32) \quad \frac{\partial W_i}{\partial t} + \sum_{1 \leq |\gamma| \leq \sigma} \Delta t^{|\gamma|-1} A_{ij}^\gamma \partial_\gamma W_j = O(\Delta t^\sigma), \quad 0 \leq i \leq N-1,$$

$$(33) \quad m_k = \sum_{0 \leq |\gamma| \leq \sigma} \Delta t^{|\gamma|} B_{kj}^\gamma \partial_\gamma W_j + O(\Delta t^{\sigma+1}), \quad k \geq N.$$

In order to treat the left hand side of relation (26), 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

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

we have for the second time derivative a relation quite analogous to (32):

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

This relation can be generalized at an arbitrary order according to

$$(34) \quad \partial_t^q W_i + \sum_{q \leq |\gamma| \leq \sigma+q-1} \Delta t^{|\gamma|-q} A_{ij}^{q,\gamma} \partial_\gamma W_j = O(\Delta t^\sigma), \quad 0 \leq i \leq N-1.$$

If relation (34) is true at order  $q$ , we have by derivation according to time,

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

and relation (34) is satisfied at the order  $q + 1$  with  $A_{ij}^{q+1,\gamma}$  given by the recurrence relation

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

In an analogous way, we have

$$(35) \quad \partial_t^q m_k = \sum_{q \leq |\gamma| \leq \sigma + q} \Delta t^{|\gamma| - q} B_{kj}^{q,\gamma} \partial_\gamma W_j + O(\Delta t^{\sigma+1}), \quad k \geq N.$$

If relation (35) is satisfied at order  $q$ , we have by derivation relative to time,

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

with coefficients  $B_{kj}^{q+1,\gamma}$  determined according to

$$B_{kj}^{q+1,\gamma} = - \sum_{|\delta| \geq q, |\varepsilon| \geq 1, \delta + \varepsilon = \gamma} B_{k\ell}^{q,\delta} A_{\ell j}^{\varepsilon}, \quad q + 1 \leq |\gamma| \leq \sigma + q + 1, \quad k \geq N, \quad 0 \leq j \leq N - 1.$$

- We verify now by induction that the recurrence relations (32) and (33) are satisfied.

It is the case at the order 1 as we have shown in (30) and (31). We first consider a label  $i$  such that  $0 \leq i \leq N - 1$ . Then according to (26), we have at the order  $\sigma + 2$ :

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

We use relation (34) for the left hand side of previous relation. We get after dividing by  $\Delta t$ ,

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

and the relation (32) is extended one step further with a coefficient  $A_{ij}^\gamma$  defined for  $|\gamma| = q + 1$  by the recurrence relation

$$A_{ij}^\gamma = - \sum_{2 \leq q \leq |\gamma|} \frac{1}{q!} A_{ij}^{q,\gamma} - \sum_{1 \leq |\delta| \leq \sigma+1, 0 \leq |\varepsilon| \leq \sigma, \delta+\varepsilon=\gamma} \frac{1}{|\delta|!} M_{i\ell} M_{\ell p}^{-1} \Psi_{pr} P_{\ell\delta} B_{rj}^\varepsilon, \\ |\gamma| = q + 1, \quad 0 \leq i, j \leq N - 1.$$

For the nonconserved momenta ( $k \geq N$ ), the relation (26) can be written at the order  $\sigma + 2$  as:

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

We use the relation (35) and we deduce:

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

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

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

and the relation (33) is established by induction.

### 3 Some theoretical results

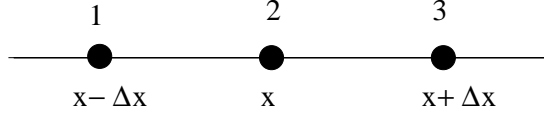


Figure 1: Stencil for the D1Q3-DDH lattice Boltzmann scheme

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

Recall first that D1Q3-DDH 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 1). We introduce  $\lambda$  as in (17) and adopt a labelling for matrix  $M$  of relation (4) as in Figure 1:

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

For thermics problem, we have only one conserved quantity. Then  $N = 1$  in relation (5). The two nonconserved momenta (momentum  $q^{\text{eq}}$  and energy  $\epsilon^{\text{eq}}$ ) at equilibrium are supposed to be **linear** functions of the conserved momentum  $\rho$ :

$$(36) \quad q^{\text{eq}} = u \lambda \rho, \quad \epsilon^{\text{eq}} = \alpha \frac{\lambda^2}{2} \rho.$$

Due to (21) and (36), matrix  $\Psi$  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 can now 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  $\sigma_i$  from relaxation time  $s_i$  according to relation (16). When a drift on velocity  $u$  is present, note that the diffusion coefficient is a function of mean value velocity. We have

$$(37) \quad \frac{\partial \rho}{\partial t} + u \lambda \frac{\partial \rho}{\partial x} - \sigma_1 \Delta t \lambda^2 (\alpha - u^2) \frac{\partial^2 \rho}{\partial x^2} + \kappa_3 \frac{\Delta t^2 \lambda^3}{12} \frac{\partial^3 \rho}{\partial x^3} + \kappa_4 \frac{\Delta t^3 \lambda^4}{12} \frac{\partial^4 \rho}{\partial x^4} = O(\Delta t^4)$$

with parameters  $\kappa_3$  and  $\kappa_4$  given according to

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

If  $u = 0$ , then  $\kappa_3 = 0$  and the DDH scheme is third order accurate. In this particular case, the scheme is fourth order accurate if we set

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

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

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

$$(38) \quad \epsilon^{\text{eq}} = \alpha \frac{\lambda^2}{2} \rho.$$

Due to (21) and (38), matrix  $\Psi$  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  $\sigma$  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 (37). We have precisely:

$$(39) \quad \begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} - \frac{\lambda^2 \Delta t^2}{12} (1 - \alpha) \frac{\partial^3 q}{\partial x^3} - \frac{\lambda^4 \Delta t^3}{12} \alpha (1 - \alpha) \sigma \frac{\partial^4 \rho}{\partial x^4} \\ + \frac{\lambda^4 \Delta t^4}{120} (1 - \alpha) (1 + \alpha + 10(1 - 2\alpha)\sigma^2) \frac{\partial^5 q}{\partial x^5} = O(\Delta t^5). \end{cases}$$

Conservation of momentum takes the form:

$$(40) \quad \begin{cases} \frac{\partial q}{\partial t} + \alpha \lambda^2 \frac{\partial \rho}{\partial x} - \lambda^2 \Delta t (1 - \alpha) \sigma \frac{\partial^2 q}{\partial x^2} + \zeta_3 \frac{\lambda^4 \Delta t^2}{6} \frac{\partial^3 \rho}{\partial x^3} \\ + \zeta_4 \frac{\lambda^4 \Delta t^3}{12} \frac{\partial^4 q}{\partial x^4} + \zeta_5 \frac{\lambda^6 \Delta t^4}{120} \frac{\partial^5 \rho}{\partial x^5} = O(\Delta t^5) \end{cases}$$

with parameters  $\zeta_3$  to  $\zeta_5$  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  $\zeta_3$  of relation (40) is null. In this case, the lattice Boltzmann scheme is formally third order accurate for the momentum equation. But, as we remarked in [15], the mass conservation (39) remains formally second order accurate, except for the case  $\alpha = 1$ , without any practical interest.

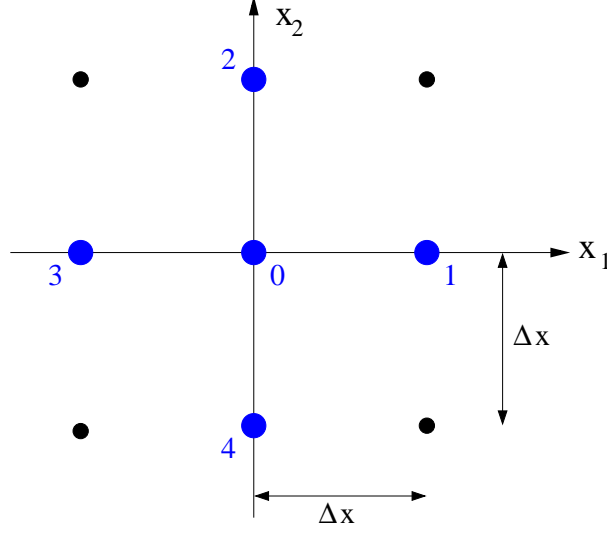


Figure 2: Stencil for the D2Q5-DDH lattice Boltzmann scheme

- **D2Q5-DDH for classical thermics at fourth order**

We have now four nontrivial possible directions for propagation of particles (Figure 2). We adopt for the  $M$  matrix of relation (4) the following choice:

$$(41) \quad M = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 \\ 0 & 0 & \lambda & 0 & -\lambda \\ -4 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 1 & -1 \end{pmatrix}.$$

We have  $J = 4$  and  $N = 1$ . The equilibrium energy (momentum  $m_3$  in (41) with the labelling conventions of Section 1) is the only one to be non equal to zero. The matrix  $\Psi$  of relation (19) is now given by the relation

$$(42) \quad \Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 - s_1 & 0 & 0 & 0 \\ 0 & 0 & 1 - s_1 & 0 & 0 \\ \alpha s_3 & 0 & 0 & 1 - s_3 & 0 \\ 0 & 0 & 0 & 0 & 1 - s_4 \end{pmatrix}.$$

We have developed the conservation law up to fourth order:

$$(43) \quad \frac{\partial \rho}{\partial t} - \frac{\lambda^2 \Delta t}{10} \sigma_1 (4 + \alpha) \left( \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) + \frac{\Delta t^3 \lambda^4}{1200} \sigma_1 (4 + \alpha) \left( \kappa_{40} \left( \frac{\partial^4 \rho}{\partial x^4} \frac{\partial^4 \rho}{\partial y^4} \right) + \kappa_{22} \frac{\partial^4 \rho}{\partial x^2 \partial y^2} \right) = O(\Delta t^4)$$



and the  $\kappa$  coefficients are explicited as follows:

$$(44) \quad \kappa_{40} = 8 - 3\alpha + 12(\alpha + 4)\sigma_1^2 - 12(1 - \alpha)\sigma_1\sigma_3 - 60\sigma_1\sigma_4$$

$$(45) \quad \kappa_{22} = -6(\alpha + 4) + 24(\alpha + 4)\sigma_1^2 - 24(1 - \alpha)\sigma_1\sigma_3 + 120\sigma_1\sigma_4.$$

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

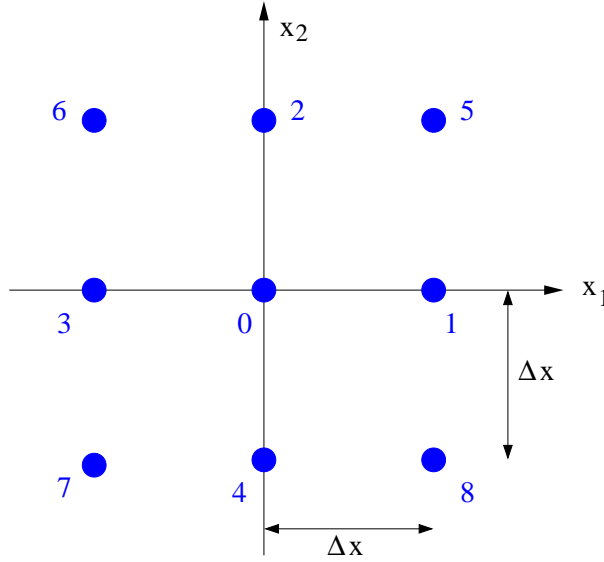


Figure 3: Stencil for the D2Q9-DDH lattice Boltzmann scheme

The lattice Boltzmann model D2Q9-DDH is obtained from the D2Q5-DDH model by adding four velocities along the diagonals (Figure 3). The evaluation of matrix  $M$  is absolutely nontrivial. We refer to Lallemand-Luo [26] and the reader can consult our introduction [13]. We have:

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

Dynamics is given by

$$(46) \quad \Psi = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u \lambda s_1 & 1-s_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v \lambda s_1 & 0 & 1-s_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_3 s_3 & 0 & 0 & 1-s_3 & 0 & 0 & 0 & 0 & 0 \\ a_4 s_4 & 0 & 0 & 0 & 1-s_4 & 0 & 0 & 0 & 0 \\ a_5 u s_5 & 0 & 0 & 0 & 0 & 1-s_5 & 0 & 0 & 0 \\ a_6 v s_5 & 0 & 0 & 0 & 0 & 0 & 1-s_5 & 0 & 0 \\ a_7 s_7 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_7 & 0 \\ a_8 s_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1-s_8 \end{pmatrix}.$$

The coefficients  $a_3$  to  $a_8$  in relation (46) are chosen in order to obtain the advection diffusion equation at order 2:

$$(47) \quad \frac{\partial \rho}{\partial t} + \lambda \left( u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} \right) - \lambda^2 \xi \sigma_1 \Delta t \left( \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) = O(\Delta t)^2.$$

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 our contribution [15]. When  $u = v = 0$ , the equation (47) 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  $\kappa_{40}$  and  $\kappa_{22}$  evaluated according to

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

When we make the ‘‘BGK hypothesis’’ *id est* that all the coefficients  $\sigma$ ’s are equal :

$$(48) \quad \sigma_1 = \sigma_3 = \sigma_4 = \sigma_5 = \sigma_7 = \sigma_8,$$

a first possibility to kill the coefficients  $\kappa_{40}$  and  $\kappa_{22}$  is given by:

$$\sigma_1 = \frac{1}{6}, \quad \xi = 0.$$

We observe that this choice of parameters is without any practical interest because the diffusion term in (47) 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” (48) by the weaker one associated to “Two Relaxation Times” as suggested by Ginzburg, Verhaeghe and D’Humières in [19] and [20], *id est*

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

we can achieve fourth order accuracy for

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

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

The D2Q9-DDH 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  $\Psi$  of (46) 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:

$$(49) \quad \frac{\partial \rho}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - \frac{1}{18} \lambda^2 \Delta t^2 \Delta \left( \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) + \frac{\lambda^4 \Delta t^3}{108} (\sigma_3 + \sigma_7) \Delta^2 \rho = O(\Delta t^4)$$

and conservation of two components of momentum:

$$(50) \quad \left\{ \begin{array}{l} \frac{\partial q_x}{\partial t} + \frac{\lambda^2}{3} \frac{\partial \rho}{\partial x} - \frac{\lambda^2}{3} \Delta t \left[ \sigma_3 \frac{\partial}{\partial x} \left( \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) + \sigma_7 \Delta q_x \right] \\ - \frac{\lambda^4 \Delta t^2}{27} \left( 3(\sigma_3^2 + \sigma_7^2) - 1 \right) \frac{\partial}{\partial x} \Delta \rho - \frac{\lambda^4 \Delta t^3}{108} \left( \zeta_{40} \frac{\partial^4 q_x}{\partial x^4} + \zeta_{31} \frac{\partial^4 q_y}{\partial x^3 \partial y} \right. \\ \left. + \zeta_{22} \frac{\partial^4 q_x}{\partial x^2 \partial y^2} + \zeta_{13} \frac{\partial^4 q_y}{\partial x \partial y^3} + \zeta_{04} \frac{\partial^4 q_x}{\partial y^4} \right) = O(\Delta t^4) \end{array} \right.$$

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

where the coefficients  $\zeta$  are given by

$$(52) \quad \left\{ \begin{array}{l} \zeta_{40} = \eta_{04} = -\sigma_3 - \sigma_7 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 + 18\sigma_3^2\sigma_5 \\ \quad + 6\sigma_5\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 - 24\sigma_3\sigma_5\sigma_7 + 12\sigma_4\sigma_5\sigma_7 \\ \zeta_{31} = \eta_{13} = -4\sigma_3 - 7\sigma_7 + 18\sigma_3^2\sigma_5 + 18\sigma_5\sigma_7^2 - 12\sigma_3^2\sigma_7 \\ \quad - 12\sigma_3\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 + 12\sigma_3\sigma_5\sigma_7 + 12\sigma_4\sigma_5\sigma_7 + 12\sigma_7^3 \\ \zeta_{22} = \eta_{22} = -13\sigma_3 + 6\sigma_4 - 10\sigma_7 + 18\sigma_3^2\sigma_5 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 \\ \quad + 30\sigma_5\sigma_7^2 - 12\sigma_3\sigma_4\sigma_5 + 120\sigma_3\sigma_5\sigma_7 - 60\sigma_4\sigma_5\sigma_7 - 12\sigma_7^3 \\ \zeta_{13} = \eta_{31} = -10\sigma_3 + 6\sigma_4 - 7\sigma_7 + 18\sigma_3^2\sigma_5 - 12\sigma_3^2\sigma_7 - 12\sigma_3\sigma_7^2 \\ \quad + 18\sigma_5\sigma_7^2 + 12\sigma_3\sigma_4\sigma_5 + 84\sigma_3\sigma_5\sigma_7 - 60\sigma_4\sigma_5\sigma_7 + 12\sigma_7^3 \\ \zeta_{04} = \eta_{40} = -3\sigma_7 + 24\sigma_5\sigma_7^2 - 12\sigma_7^3. \end{array} \right.$$

- D3Q7-DDH for pure thermics

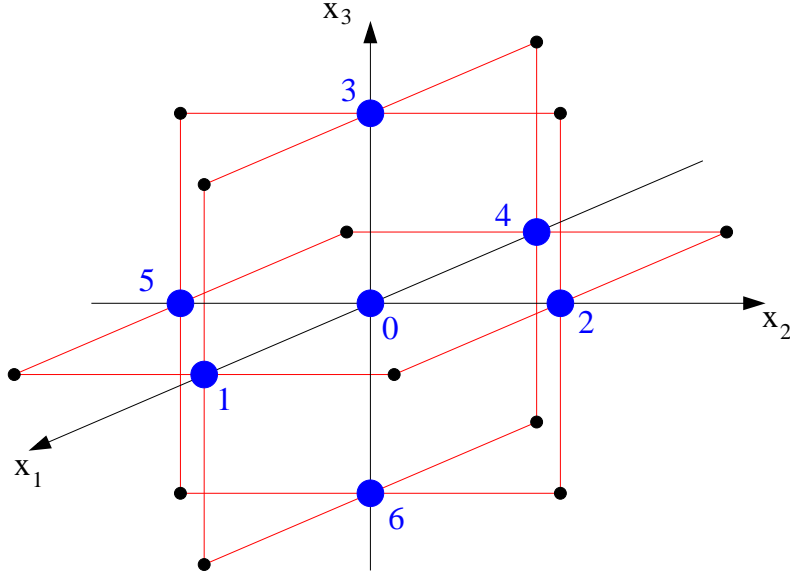


Figure 4: Stencil for the D3Q7-DDH lattice Boltzmann scheme

For three-dimensional thermics, one only needs a seven point scheme and use the so-called D3Q7-DDH lattice Boltzmann scheme whose stencil is described in Figure 4. The matrix

is not very difficult to construct. We follow Lallemand and Luo [27]:

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

The dynamics of DDH Boltzmann scheme uses the following matrix for computation of out of equilibrium momenta, according to relation (19):

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

Thermal scalar conservation law takes now the following form at fourth order of accuracy:

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

where the  $\kappa$  coefficients are given by

$$(53) \quad \kappa_{400} = 8 - \alpha + 4\sigma_1^2(\alpha + 6) - 56\sigma_1\sigma_4 - 4(1 - \alpha)\sigma_1\sigma_6$$

$$(54) \quad \kappa_{220} = -2(\alpha + 6) + 8\sigma_1^2(\alpha + 6) + 56\sigma_1\sigma_4 - 8(1 - \alpha)\sigma_1\sigma_6.$$

- D3Q19-DDH for linearized Navier–Stokes

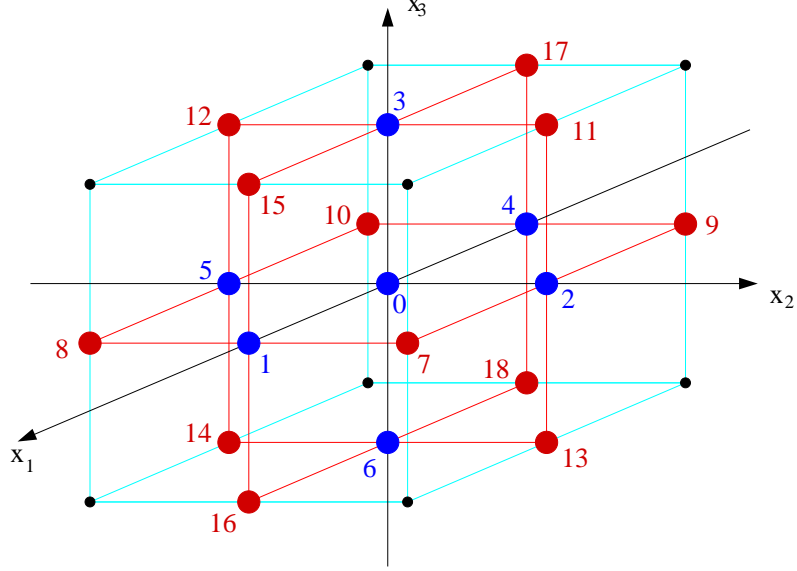


Figure 5: Stencil for the D3Q19-DDH lattice Boltzmann scheme

The D3Q19 Lattice Boltzmann scheme is described with details *e.g.* in J. Tölke *et al* [38]. The matrix  $M$  that parametrizes 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 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\lambda^2 & 8\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 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^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 momenta, we detail in this sub-section the way the previous matrix is obtained. First, velocities  $v_j^\alpha$  for  $0 \leq j \leq J \equiv 18$  and  $1 \leq \alpha \leq 3$  are naturally associated with Figure 5. The four first momenta  $\rho$  and  $q^\alpha$  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 is founded on the respect of tensorial nature of the variety of moments that can be constructed, as analyzed by Rubinstein and Luo [36]: scalar fields are naturally with the equilibrium scalar field, that is density, vector fields are related to momentum, and so on. So components of kinetic energy are introduced:

$$(55) \quad \widetilde{M}_{4j} = 19 \sum_{\alpha} |v_j^\alpha|^2, \quad 0 \leq j \leq J.$$

The entire set of second order tensors is completed according to

$$(56) \quad \begin{cases} \widetilde{M}_{5j} &= 2(v_j^1)^2 - (v_j^2)^2 - (v_j^3)^2 \\ \widetilde{M}_{6j} &= (v_j^2)^2 - (v_j^3)^2 \\ \widetilde{M}_{7j} &= v_j^1 v_j^2 \\ \widetilde{M}_{8j} &= v_j^2 v_j^3 \\ \widetilde{M}_{9j} &= v_j^3 v_j^1, \end{cases} \quad 0 \leq j \leq J.$$

The three components of heat flux are defined by

$$(57) \quad \begin{cases} \widetilde{M}_{10j} &= 5 v_j^1 \sum_{\alpha} |v_j^\alpha|^2 \\ \widetilde{M}_{11j} &= 5 v_j^2 \sum_{\alpha} |v_j^\alpha|^2 \\ \widetilde{M}_{12j} &= 5 v_j^3 \sum_{\alpha} |v_j^\alpha|^2, \end{cases} \quad 0 \leq j \leq J.$$

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

$$(58) \quad \widetilde{M}_{13j} = \frac{21}{2} \left( \sum_{\alpha} |v_j^\alpha|^2 \right)^2, \quad 0 \leq j \leq J,$$

second order momenta of kinetic energy:

$$(59) \quad \begin{cases} \widetilde{M}_{14j} &= 3 \left( 2(v_j^1)^2 - (v_j^2)^2 - (v_j^3)^2 \right) \sum_{\alpha} |v_j^\alpha|^2 \\ \widetilde{M}_{15j} &= 3 \left( (v_j^2)^2 - (v_j^3)^2 \right) \sum_{\alpha} |v_j^\alpha|^2, \end{cases} \quad 0 \leq j \leq J,$$

and third order antisymmetric momenta

$$(60) \quad \begin{cases} \widetilde{M}_{16j} &= v_j^1 \left( (v_j^2)^2 - (v_j^3)^2 \right) \\ \widetilde{M}_{17j} &= v_j^2 \left( (v_j^3)^2 - (v_j^1)^2 \right) \\ \widetilde{M}_{18j} &= v_j^3 \left( (v_j^1)^2 - (v_j^2)^2 \right), \end{cases} \quad 0 \leq j \leq J.$$

Then matrix  $M$  is orthogonalized from relations (8), (9), (55), (56), (57), (58), (59) and (60) with a Gram-Schmidt classical algorithm:

$$(61) \quad M_{ij} = \widetilde{M}_{ij} - \sum_{\ell < i} g_{i\ell} M_{\ell j}, \quad i \geq 4.$$

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

$$(62) \quad \sum_{j=0}^J M_{ij} M_{kj} = 0 \quad \text{for } i \neq k$$

The associated matrix  $\Psi$  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 momenta. We have taken for this D3Q19 DDH scheme

$$(63) \quad \left\{ \begin{array}{l} m_4^{\text{eq}} = \theta \lambda^2 \\ m_5^{\text{eq}} = m_6^{\text{eq}} = m_7^{\text{eq}} = m_8^{\text{eq}} = m_9^{\text{eq}} = 0 \\ m_{10}^{\text{eq}} = m_{11}^{\text{eq}} = m_{12}^{\text{eq}} = 0 \\ m_{13}^{\text{eq}} = \beta \lambda^4 \\ m_{14}^{\text{eq}} = m_{15}^{\text{eq}} = 0 \\ m_{16}^{\text{eq}} = m_{17}^{\text{eq}} = m_{18}^{\text{eq}} = 0. \end{array} \right.$$

In order to obtain physical equations at first order of accuracy with a sound velocity  $c_0$  given by

$$(64) \quad c_0 = \alpha \lambda$$

the relation

$$\theta = 57 \alpha^2 - 30$$

must be imposed to obtain correct fluid second order partial differential equations and the parameter  $\beta$  remains free.

- 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 Numerical results for shear waves and fourth order schemes

- **D2Q5-DDH lattice Boltzmann scheme for thermal problem**

We obtain the order 4 by setting  $\kappa_{40} = 0$  and  $\kappa_{22} = 0$  in relations (44) and (45) respectively. We obtain :

$$(65) \quad \sigma_3 = \sigma_1 \frac{\alpha + 4}{1 - \alpha} - \frac{1}{12 \sigma_1} \frac{2 + 3\alpha}{1 - \alpha}, \quad \sigma_4 = \frac{1}{6 \sigma_1}.$$

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 [19] and [20] supposes simply  $\sigma_3 = \sigma_4$ . If we insert this constraint inside relations (65), we get

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

to enforce fourth order accuracy. Then the DDH 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-DDH 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), (41) and (42), as proposed in Lallemand-Luo [26]. Introduce a wave in the DDH scheme, *id est*

$$f(x, t) = \hat{f}(k_x, k_y) \exp(i k_x x + i k_y y).$$

Then we have

$$f(x, t + \Delta t) = G f(x, t)$$

with the so-called amplification matrix (see *e.g.* Richtmyer and Morton [35]) obtained without difficulty from matrices  $M$ ,  $\Psi$  and  $W$  defined by

$$W = \text{diag} \left( 1, e^{i k_x \Delta x}, e^{i k_y \Delta x}, e^{-i k_x \Delta x}, e^{-i k_y \Delta x} \right)$$

for the D2Q5-DDH scheme displayed in Figure 2. Then

$$G = W M^{-1} \Psi M.$$

Then if  $\frac{\partial}{\partial t}$  is formally given by relation (43) and operators  $\frac{\partial}{\partial x}$  and  $\frac{\partial}{\partial y}$  replaced by  $i k_x$  and  $i k_y$  respectively, the number  $z$  defined by

$$z = \exp \left( \Delta t \frac{\partial}{\partial t} \right)$$

is an eigenvalue of matrix  $G$  at fourth order of accuracy. The numerical experiment 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  $m$  lattice points (and  $(J + 1) \times m$  degrees of freedom), one can study the time evolution starting from some initial state. An other approach for linear situations considers that the state  $X(t)$  that belongs to  $\mathbb{R}^{(J+1) \times m}$  can be decomposed as a sum of eigenmodes of the operator  $A$  defined by the discrete evolution scheme:

$$(66) \quad X(t + \Delta t) \equiv A \bullet X(t).$$

The matrix  $A$  being of very large size, one can look for part of its eigenmodes using for instance the method proposed by Arnoldi [2]. To accelerate the Arnoldi computations, following a suggestion by L. Tuckerman, we replace the determination of the eigenvalues of equation (66) by the determination of the eigenvalues of

$$(67) \quad X(t + (2\ell + 1) \Delta t) \equiv A^{2\ell+1} \bullet X(t)$$

using the fact that the lattice Boltzmann scheme is very fast compared to the inner “working” of the Arnoldi procedure. Replacing problem (66) by problem (67) not only increases the splitting between various eigenmodes it also helps to discriminate against the acoustic modes by multiplying 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.

- Results for “internal” DDH lattice. We first test this method for a periodic  $N_x \times N_y (\equiv m)$  situation and find the same results as those derived from the “one-point” analysis (see Figure 6) with very good accuracy. For this periodic situation, the eigenmodes are plane waves for the following wavevector:

$$k_x = 2\pi \frac{I_x}{N_x}, \quad k_y = 2\pi \frac{I_y}{N_y}.$$

where  $I_x$  and  $I_y$  are integers. We compare the relaxation rates  $\Gamma(I_x, I_y, N_x, N_y)$  to  $\kappa(k_x^2 + k_y^2)$  and show in Figure 7 the relative difference between those two quantities (called “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 7 for D3Q7-DDH.

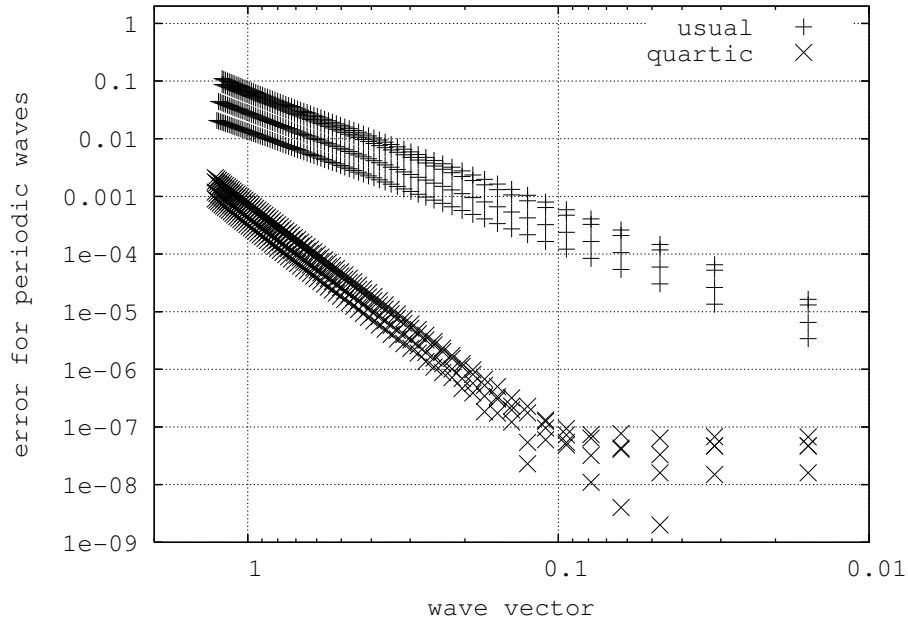


Figure 6: Precision of D2Q5-DDH scheme for thermic test case, “one point” simulation. Different curves correspond to different orientation of the wave-vector with respect to the axis, showing the angular dependence of the next order.

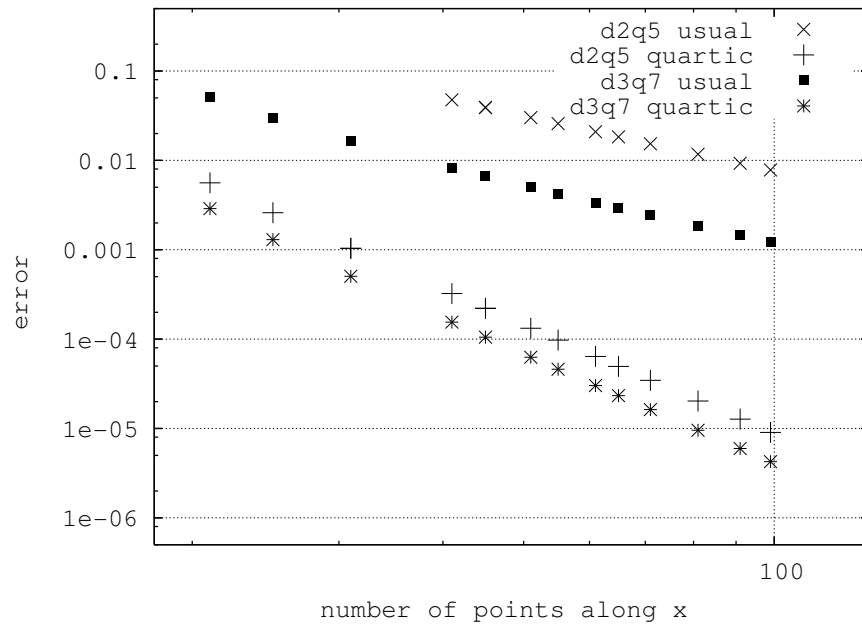


Figure 7: Arnoldi test case for periodic thermics,  $I_x = 5$ ,  $I_y = 0$ . Various parameters for lattice Boltzmann schemes D2Q5-DDH and D3Q7-DDH.

- 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. Recall that density follows the so-called heat equation

$$(68) \quad \frac{\partial \rho}{\partial t} - \kappa \Delta \rho = 0$$

with  $\kappa = \frac{\lambda^2 \Delta t}{10} \sigma_1 (4 + \alpha)$  due to (43) and homogeneous boundary conditions at  $r = R$ :

$$(69) \quad \rho(r \equiv R, t) = 0.$$

We search an exponentially decaying function relative to time

$$(70) \quad \rho(\bullet, t) = \widehat{\rho}(\bullet) \exp(-\Gamma t)$$

then  $\mu \equiv \frac{\Gamma}{\kappa}$  is an eigenvalue of the Laplace operator in the disc of radius  $R$ . We search  $\widehat{\rho}(\bullet)$  under the Fourier form introducing the polar angle  $\theta$ :

$$\widehat{\rho}(r, \theta) = e^{i \ell \theta} f\left(\sqrt{\frac{\Gamma}{\kappa}} r\right).$$

Then  $f$  satisfies the so-called Bessel equation:

$$(71) \quad x^2 \frac{d^2 f(x)}{dx^2} + x \frac{df(x)}{dx} + (x^2 - \ell^2) f = 0$$

whose unique regular solution at the origin is called the Bessel function  $J_\ell$  (see for example Abramowitz and Stegun [1]). We denote by  $\zeta_\ell^n$  the  $n^{\text{th}}$  zero of the Bessel function  $J_\ell$ :

$$(72) \quad J_\ell(\zeta_\ell^n) = 0.$$

We deduce from the previous arguments that  $\Gamma$  can be chosen of the form

$$(73) \quad \Gamma = \kappa \left(\frac{\zeta_\ell^n}{R}\right)^2$$

We admit here that all the eigenvalues follow relation (73).

- The effect of fourth order accuracy Boltzmann scheme in computing the eigenfunction is spectacular: just compare Figures 8 and 9. Nevertheless, the effect of boundary conditions cannot be neglected. In Figure 10, 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 numerical boundary conditions introduced by Bouzidi *et al* [4]. 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.

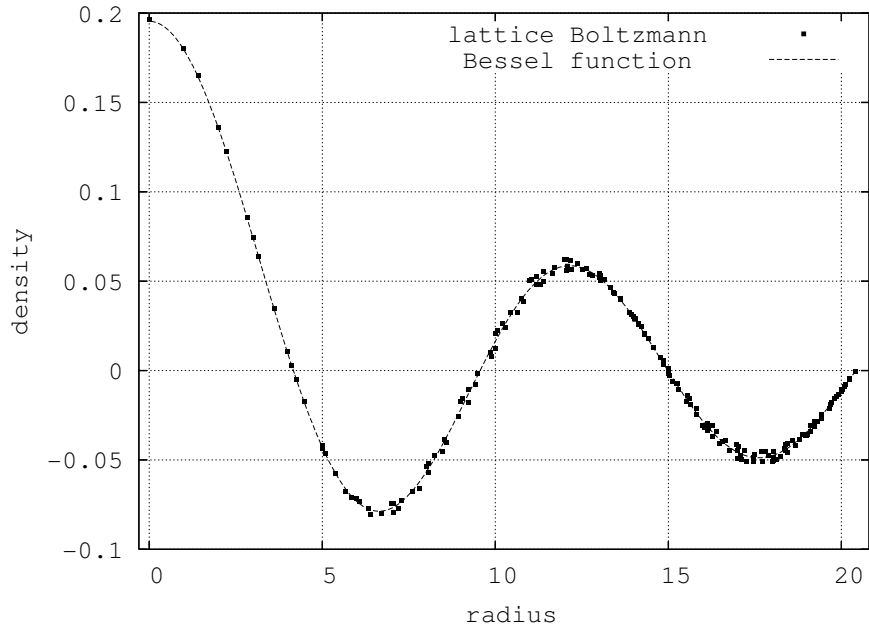


Figure 8: D2Q5-DDH scheme for thermics in a circle. Eigenmode  $n = 4$ ,  $\ell = 0$  for heat equation with Dirichlet boundary conditions. Usual parameters for second order lattice Boltzmann scheme.

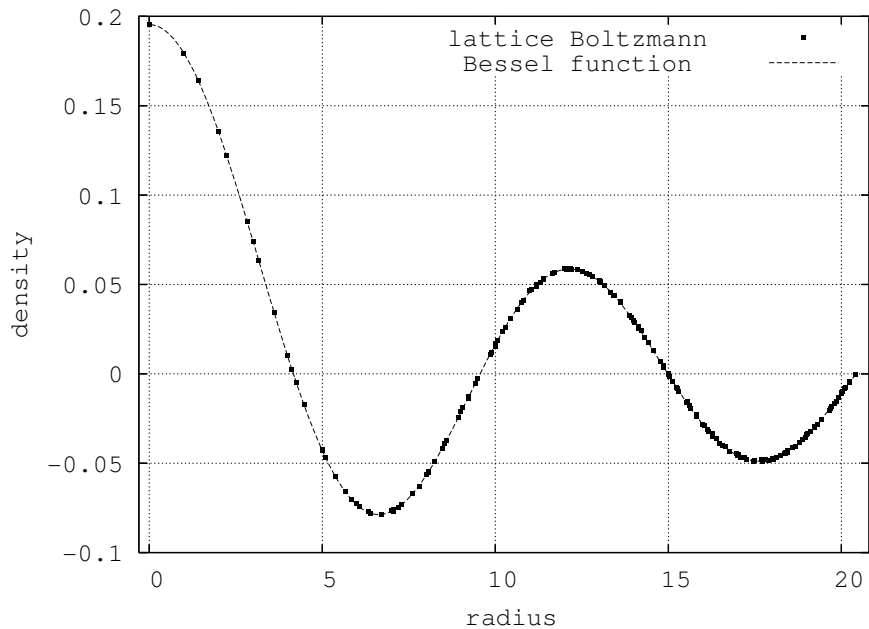


Figure 9: D2Q5-DDH scheme for thermics in a circle. Eigenmode  $n = 4$ ,  $\ell = 0$ . Quartic parameters for fourth order lattice Boltzmann scheme.

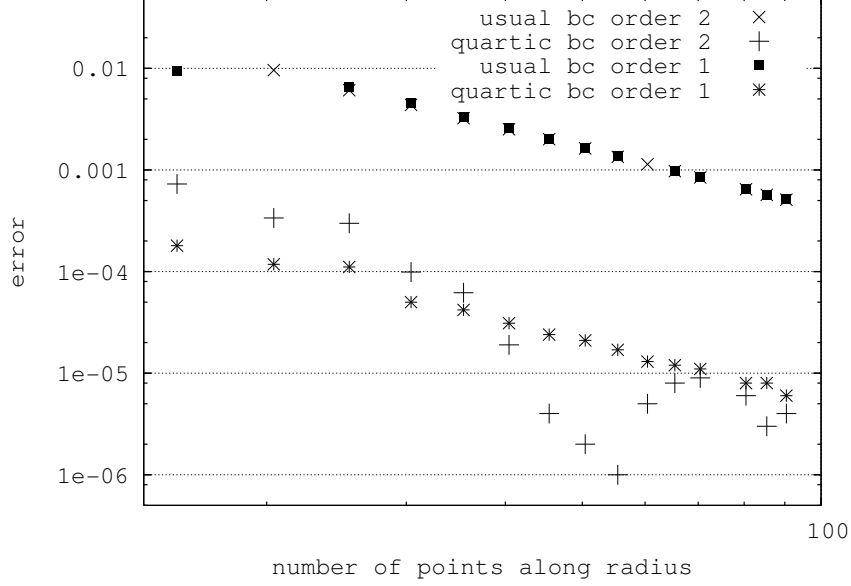


Figure 10: D2Q5-DDH scheme for thermics in a circle. Eigenmode  $n = 1$ ,  $\ell = 5$ . Errors for various parameters for lattice Boltzmann and boundary schemes.

- **D3Q7-DDH lattice Boltzmann scheme for thermal problem**

We obtain the order 4 by setting  $\kappa_{400} = 0$  and  $\kappa_{220} = 0$  in relations (53) and (54). We obtain :

$$\begin{aligned}\sigma_4 &= \frac{1}{6\sigma_1} \\ \sigma_6 &= \frac{\alpha + 6}{1 - \alpha} \sigma_1 - \frac{4 + 3\alpha}{12(1 - \alpha)} \frac{1}{\sigma_1}\end{aligned}$$

As for D2Q5-DDH, 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 can be obtained without difficulty by using the so-called spherical harmonics  $Y_\ell^m$ . First introduce the Laplace-Beltrami operator  $\Delta_{\text{LB}}$  on the unit sphere (see *e.g.* Carslaw and Jaeger [5]):

$$\Delta \equiv \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Delta_{\text{LB}}.$$

Observe that the spherical harmonics  $Y_\ell^m$  are eigenfunctions of the Laplace-Beltrami operator with eigenvalue  $\ell(\ell + 1)$  :

$$-\Delta_{\text{LB}} Y_\ell^m = \ell(\ell + 1) Y_\ell^m, \quad \ell, m \in \mathbb{N}, \quad -\ell \leq m \leq \ell.$$

Then an harmonic solution of the time dependent heat equation (68) (69) of the form (70) can be searched as

$$\widehat{\rho}(r, \theta) = Y_\ell^m(\theta) f\left(\sqrt{\frac{\Gamma}{\kappa}} r\right)$$

and function  $f$  is solution of the ‘‘spherical’’ Bessel equation

$$x^2 \frac{d^2 f(x)}{dx^2} + 2x \frac{df(x)}{dx} + (x^2 - \ell(\ell + 1)) f = 0$$

obtained from classical Bessel functions by

$$f(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x).$$

As in the two-dimensional case, we introduce the  $n^{\text{th}}$  zero  $\eta_{\ell+1/2}^n$  of semi-integer Bessel function:

$$(74) \quad J_{\ell+1/2}(\eta_{\ell+1/2}^n) = 0.$$

Then the eigenvalue  $\Gamma$  is given by the expression

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

- Results of Figures 11 and 12 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  $\pi n$ ). We have used the following parameters for the usual computations:

$$s_1 = 1.26795, \quad s_4 = 1.2, \quad s_6 = 1.3$$

The quartic parameters have been chosen as

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

From results presented in Figure 13, 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 14 the ratio  $\Gamma R^2 / (\kappa \pi^2)$ . We use Bouzidi *et al* [4] 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

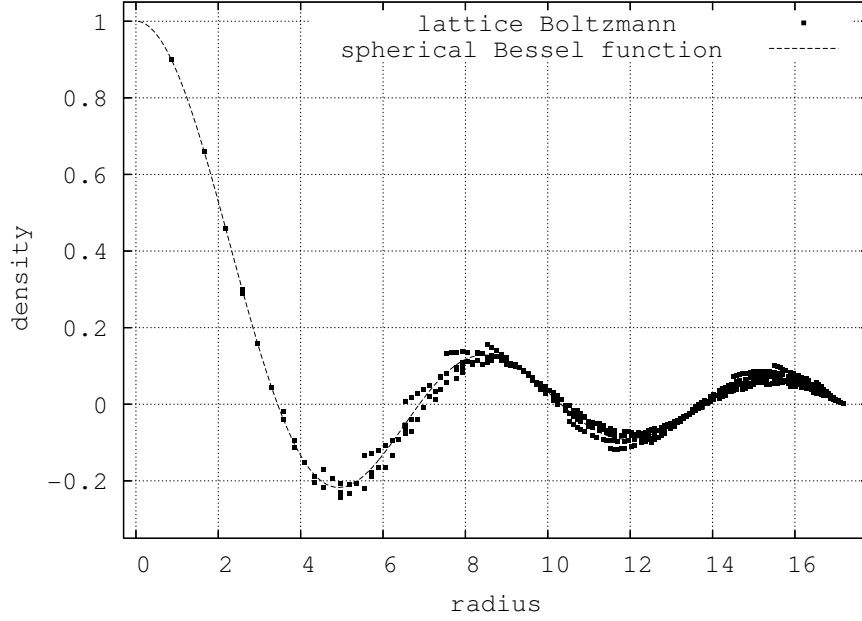


Figure 11: D3Q7-DDH lattice Boltzmann scheme for thermics in a sphere. Eigenmode  $n = 5$ ,  $\ell = 1$ ,  $m = 0$  with usual parameters.

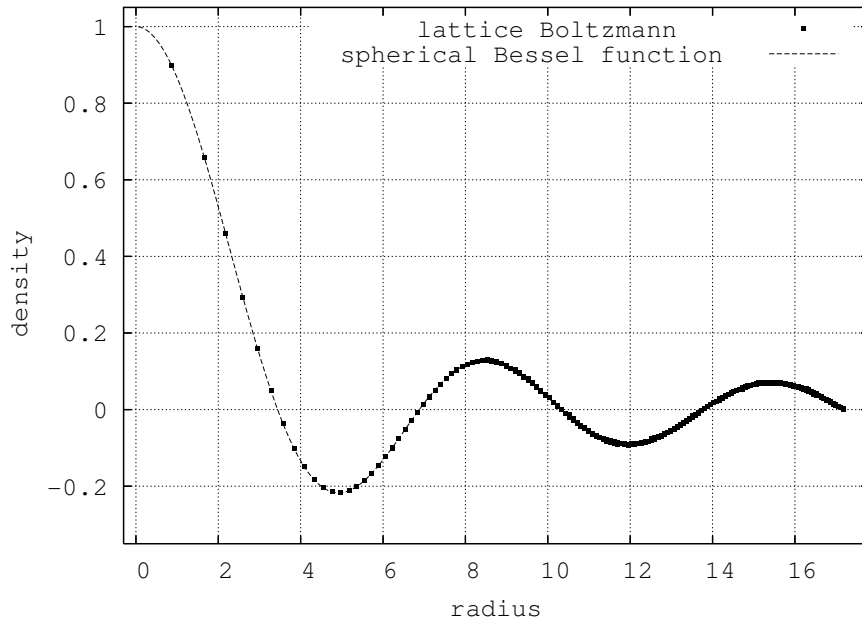


Figure 12: D3Q7-DDH lattice Boltzmann scheme for thermics in a sphere. Eigenmode  $n = 5$ ,  $\ell = 1$ ,  $m = 0$  with quartic parameters.



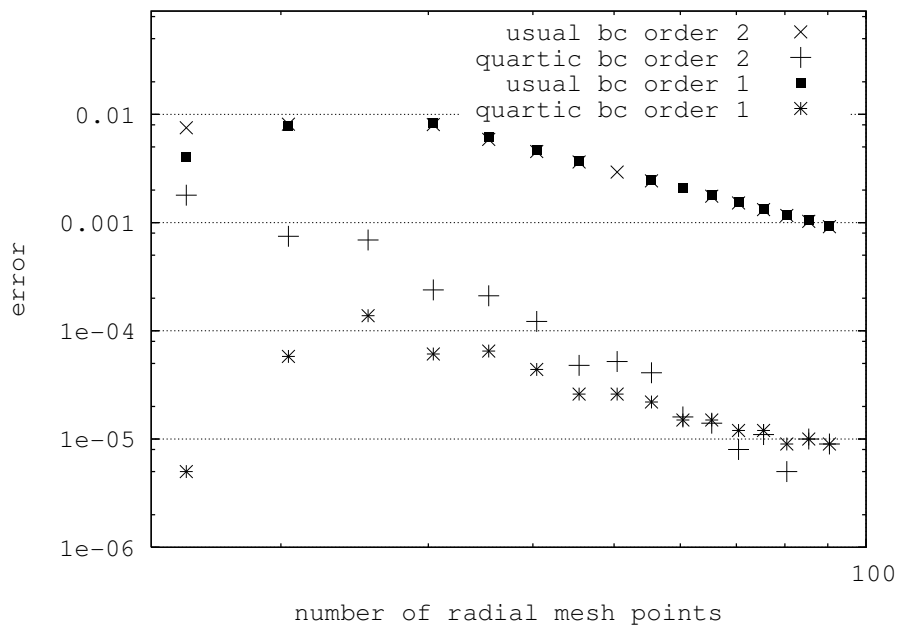


Figure 13: D3Q7-DDH scheme for thermics in a sphere with Dirichlet boundary conditions. Eigenmode  $n = 1$ ,  $\ell = 0$ . Errors for various parameters for lattice Boltzmann and boundary schemes.

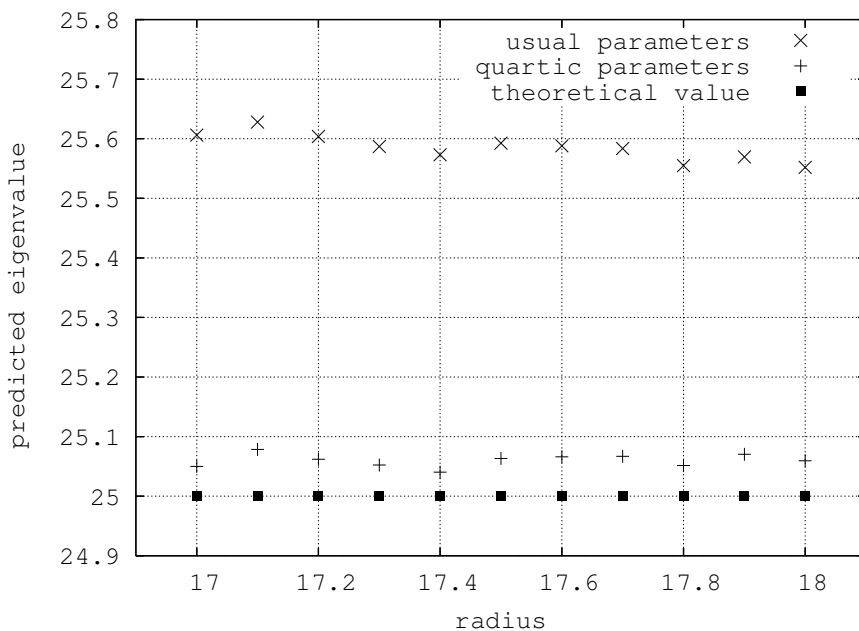


Figure 14: D3Q7-DDH for thermics in a sphere. Eigenmode (in units  $\kappa\pi^2/R^2$ ) for  $n = 5$  and  $\ell = 0$ . Variation of the location of the boundary between  $R = 17$  and  $R = 18$ .

order of 2%. We observe that this gap is one magnitude larger than the error due to the choice of the boundary condition estimated from the fluctuations with the imposed radius.

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

We consider now the linear fluid model obtained by a D2Q9-DDH lattice Boltzmann scheme. The equivalent partial differential equations are given at the order 4 by relations (50) to (52). 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 (49). Recall notation (5) for conservative variables:

$$W \equiv (\rho, q_x, q_y)^t$$

and write the equivalent equations (50)-(52) under the synthetic form:

$$(75) \quad \partial_t W_k + \sum_{j,p,q} A_{kpq}^j \partial_x^p \partial_y^q W_j = O(\Delta t^4).$$

We search a dissipative mode, *id est* a mode for linear incompressible Stokes problem under the form

$$W(t) = e^{-\Gamma t} + i(k_x x + k_y y) \widetilde{W}.$$

Then  $\Gamma$  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 [28]) that for Stokes problem (incompressible shear modes), the relation

$$(76) \quad \Gamma = \nu (k_x^2 + k_y^2)$$

is classical. Moreover, as a consequence of (50) and (51)

$$(77) \quad \nu = \frac{\lambda^2}{3} \Delta t \sigma_7$$

for a DDH Lattice Boltzmann scheme. We propose here to tune the DDH parameters  $s_\ell$  in such a way that the relation (76) is enforced for the modes of (75). Precisely, we search  $s_\ell$  such that

$$(78) \quad \Delta_m \equiv \det \left[ A - \left( \frac{\lambda^2}{3} \Delta t \sigma_7 \right) (k_x^2 + k_y^2) \text{Id} \right] = O(\Delta t^7).$$

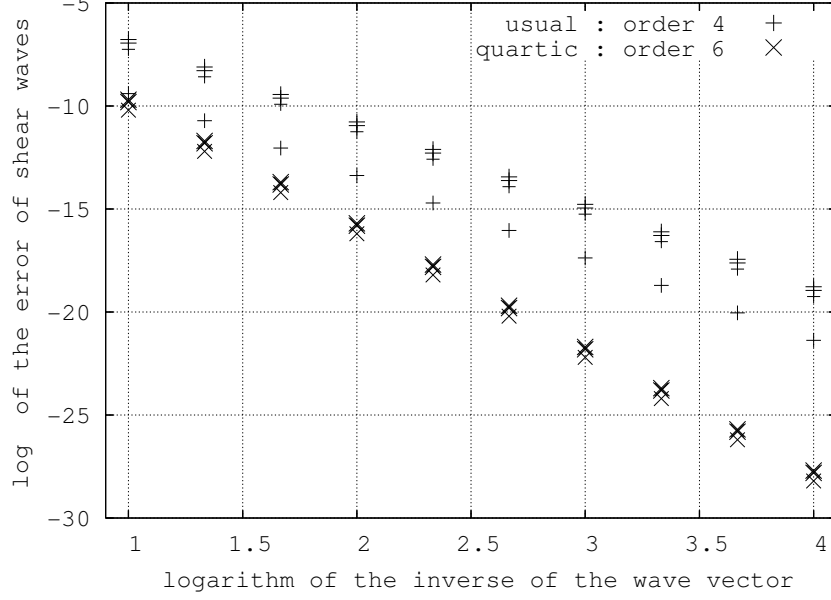


Figure 15: D2Q9 “one point” test case of shear waves for different angles of the wave vector.

With an elementary formal computation, the third order term  $\Delta_m^3$  of  $\Delta_m$  relative to  $\Delta t$  is equal to

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

It is then clear that this term is identically null for parameters  $\sigma_5$  and  $\sigma_7$  chosen according to

$$(79) \quad \sigma_5 = \frac{\sqrt{3}}{3}, \quad \sigma_7 = \frac{\sqrt{3}}{6}.$$

With this particular choice of parameters, so-called quartic in what follows, the viscosity  $\nu$  in relation (77) has the following particular value:

$$(80) \quad \nu = \frac{\lambda^2 \Delta t}{\sqrt{108}} \approx 0.096225 \lambda^2 \Delta t.$$

Then it is very simple to verify that the determinant  $\Delta_m$  is null up to terms of order seven and relation (78) is satisfied.

- As in the particular case of D2Q5-DDH scheme, we have verified with periodic boundary conditions that the relaxation rate of a transverse wave is determined with error of

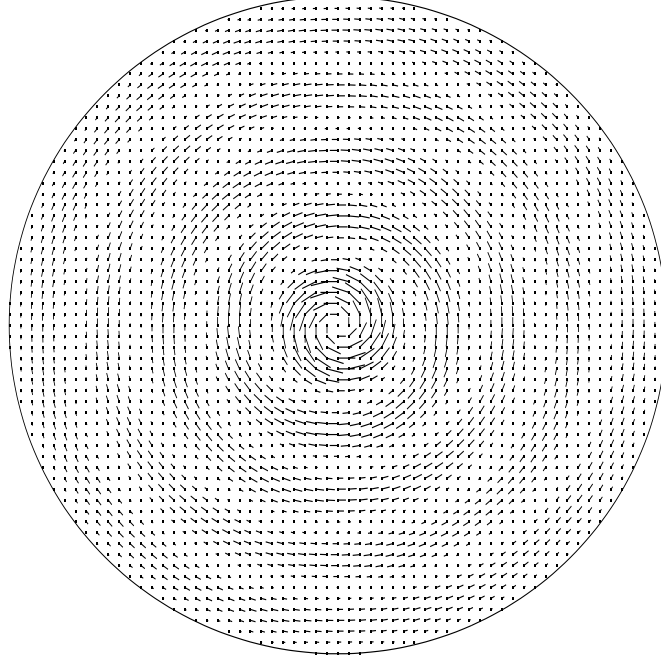


Figure 16: D2Q9-DDH scheme for linear Navier–Stokes. Eigenmode  $n = 5$   $\ell = 1$  for the Stokes problem in a circle.

order 6 and relative fourth order precision, as shown in Figure 15. The detailed numerical convergence plot is very similar to Figure 7.

- We have also validated our results for eigenmodes of the Stokes problem in a circle. We set  $\Omega = D(0, R)$  and  $R = 30.07$ . We search a nontrivial velocity field  $\mathbf{u}$  with null divergence such that there exists a pressure field  $p$  and an eigenvalue  $\Gamma$  such that

$$(81) \quad \begin{cases} -\nu \Delta \mathbf{u} + \nabla p = \Gamma \mathbf{u} & \text{in } \Omega \\ \operatorname{div} \mathbf{u} = 0 & \text{in } \Omega \\ \mathbf{u} = 0 & \text{on } \partial\Omega. \end{cases}$$

We look for a simple velocity field without radial component:

$$u_\theta = -\frac{d\psi}{dr}, \quad \frac{\partial\psi}{\partial\theta} = 0$$

and after an elementary calculus (see *e.g.* [28]), we find that  $u_\theta$  is solution of the Bessel equation (71) with  $\ell \geq 1$ . Then with notation introduced in (72), we have

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

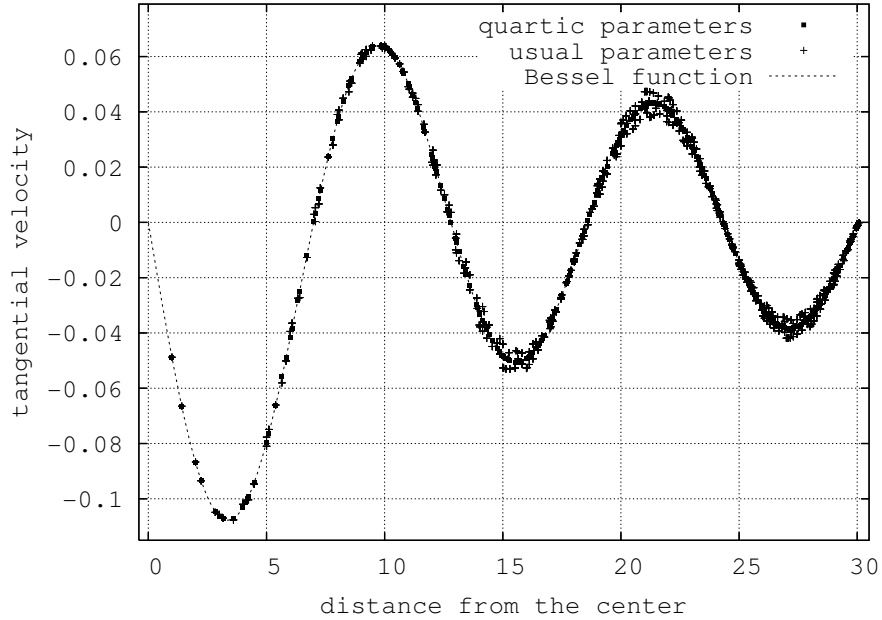


Figure 17: D2Q9-DDH scheme for linear Navier–Stokes in a circle. Eigenmode  $n = 5$ ,  $\ell = 1$  for the Stokes problem. Usual parameters.

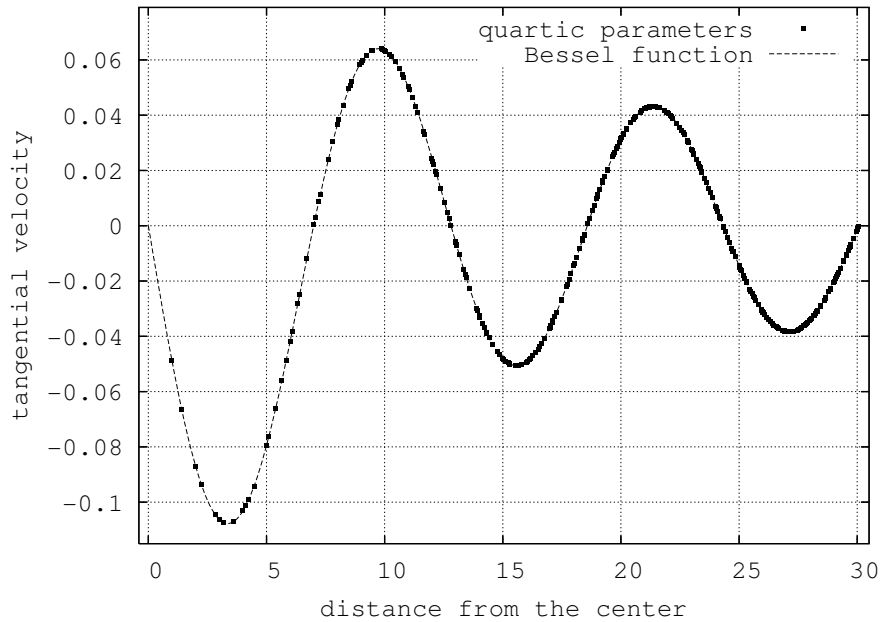


Figure 18: D2Q9-DDH scheme for linear Navier–Stokes in a circle. Eigenmode  $n = 5$ ,  $\ell = 1$  for the Stokes problem. Quartic parameters.

- The result for  $R = 30.07$ ,  $\ell = 1$  and  $n = 5$  is presented in Figure 16 for the velocity field with a mesh included in a square of size  $61 \times 61$ . The alternance of directions for vector field is clearly visible on the figure. We have compared with the same mesh the results obtained with DDH lattice Boltzmann scheme with usual parameters that does not satisfy relation (79) but such that

$$\nu = \frac{\lambda^2 \Delta t}{10}$$

which is very close to (80) and quartic parameters. The radial profile of the tangential velocity is shown in Figures 17 to 19. The difference is visually spectacular. As for the thermics case, we observe that simple boundary conditions, here we use Bouzidi *et al.* [4], prevent fourth order convergence for the Stokes problem. Use of more sophisticated boundary conditions (see Ginzburg and D’Humières [18]) 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”.

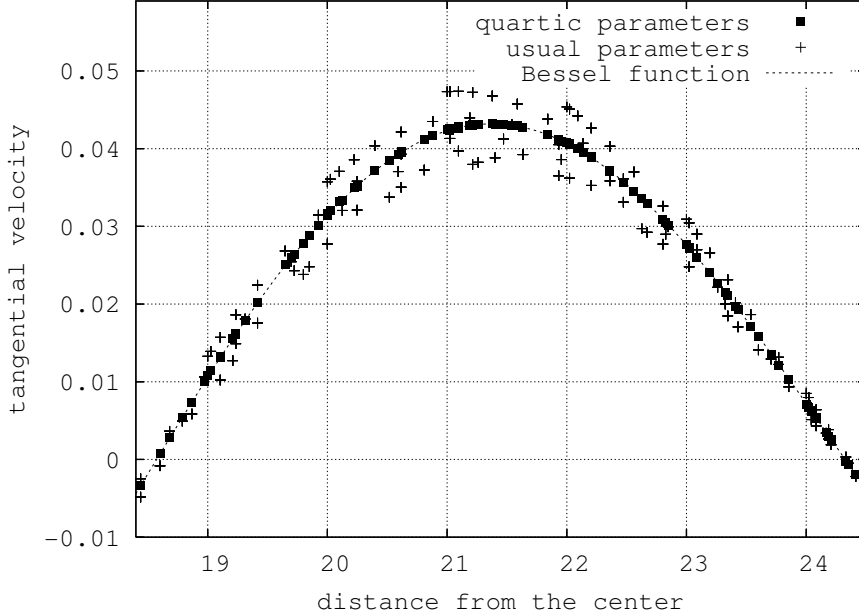


Figure 19: D2Q9-DDH scheme for linear Navier–Stokes in a circle. Eigenmode  $n = 5$ ,  $\ell = 1$  for the Stokes problem. Zoom of the figures 17 and 18.

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

The D3Q19-DDH model (we refer for our notations to the previous work of D’Humières *et al* [11]) is analyzed as done above for the D2Q9-DDH model. We use the equivalent

equations of lattice Boltzmann scheme D3Q19 obtained previously in the following way. We consider the vector of conserved variables (5):

$$(82) \quad W \equiv (\rho, q_x, q_y, q_z)^{\text{t}}.$$

We write the equivalent partial differential equations under the synthetic form:

$$(83) \quad \partial_t W_k + \sum_{j,p,q,r} A_{kpqr}^j \partial_x^p \partial_y^q \partial_y^r W_j = O(\Delta t^4).$$

We search dissipative mode solution of (83) under the form

$$W(t) = e^{-\Gamma t + i(k_x x + k_y y + k_z z)} \cdot \widetilde{W}$$

Then  $\Gamma$  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:

$$(84) \quad \Delta \equiv \det \left[ A - \Gamma \text{Id} \right] = O(\Delta t^7).$$

We impose also that this eigenvalue is **double** as classical for shear waves in three dimensions [28]:

$$(85) \quad \frac{d}{d\Gamma} \left( \det \left[ A - \Gamma \text{Id} \right] \right) \approx 0.$$

The first nontrivial term in powers of  $\Delta t$  for this derivative of the determinant is the term of order 3. Then we force

$$(86) \quad \frac{d}{d\Gamma} \left( \det \left[ A - \Gamma \text{Id} \right] \right) = O(\Delta t^4).$$

For Stokes problem (incompressible shear modes) and D3Q19 lattice Boltzmann DDH scheme, we have [33]:

$$(87) \quad \Gamma \equiv \nu |k|^2 = \frac{\lambda^2}{3} \Delta t \sigma_5 (k_x^2 + k_y^2 + k_z^2).$$

We solve the set (84), (86), (87) of equations for all values of the time step  $\Delta t$ . We obtain in this way a set of 8 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 \\ + 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 \\ - 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} \\ + 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 \\ + 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 \\ (-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} \\ - 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 \\ + 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} \\ - 1488\sigma_{16}\sigma_5^3 + 5688\sigma_{16}^2\sigma_5^4 - 20\sigma_5\sigma_{14} = 0 \\ -\sigma_5 + 6\sigma_{16}\sigma_5^2 + 2\sigma_5^2\sigma_{10} - 4\sigma_5^3 = 0 \\ 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 :

$$(88) \quad \left\{ \begin{array}{ll} \text{energy} & \sigma_4 = \frac{1}{s_4} - \frac{1}{2} \quad s_4 = \textit{ad libitum} \\ \text{stress tensor} & \sigma_5 = 1/\sqrt{12} \quad s_5 = 3 - \sqrt{3} \\ \text{energy flux} & \sigma_{10} = 1/\sqrt{3} \quad s_{10} = 4\sqrt{3} - 6 \\ \text{square of energy} & \sigma_{13} = \frac{1}{s_{13}} - \frac{1}{2} \quad s_{13} = \textit{ad libitum} \\ \text{other momenta of kinetic energy} & \sigma_{14} = 1/\sqrt{12} \quad s_{14} = 3 - \sqrt{3} \\ \text{third order antisymmetric} & \sigma_{16} = 1/\sqrt{3} \quad s_{16} = 4\sqrt{3} - 6. \end{array} \right.$$

Note these results are incompatible with BGK hypothesis (all  $\sigma$  equal) but are compatible with the “two relaxation times” hypothesis which enforces equality of even moments  $\sigma_4 = \sigma_5 = \sigma_{13} = \sigma_{14}$  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  $\nu$  takes the value  $1/\sqrt{108}$  as in (80). As for D2Q9-DDH 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.



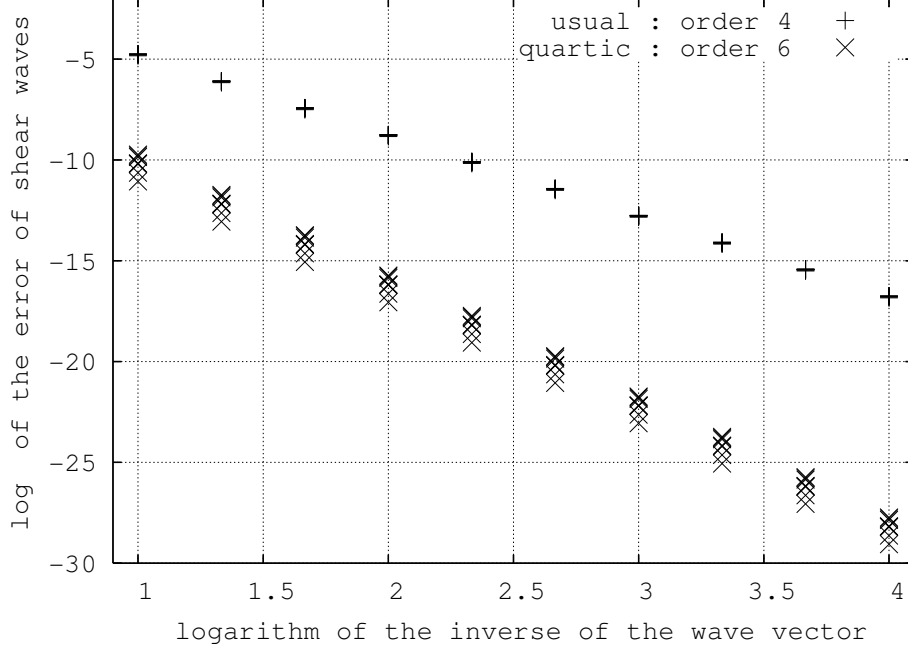


Figure 20: D3Q19-DDH for “one point” experiment and various directions of the wave vector.

- We have performed the same kind of numerical analysis as for the 2-D D2Q9-DDH 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 in matrix (82) and compute numerically the eigenmodes. The shear mode is close to  $\frac{\lambda^2}{3} \sigma_5 |k|^2$  and we plot in Figure 20 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 (81) searches for solutions of Stokes equations 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

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

with  $\zeta_{\ell+1/2}^n$  equal to the  $n^{\text{th}}$  zero of the Bessel function  $J_{\ell+1/2}$  as defined in (74). Using the Arnoldi technique, we can determine a few eigenvalues and verify that they are close to the theoretical formula. 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

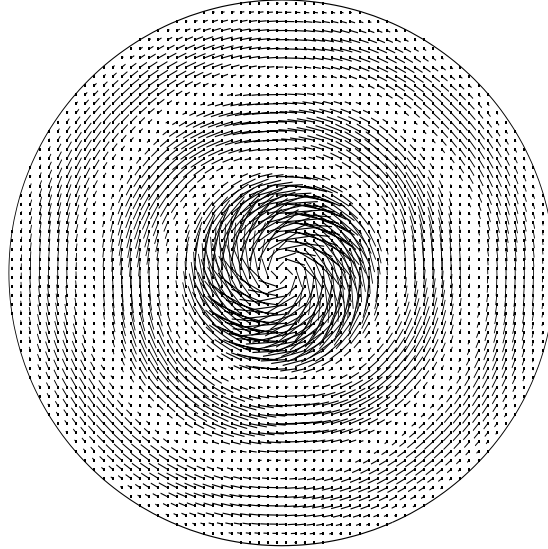


Figure 21: D3Q19-DDH for linear Navier–Stokes in a sphere. Eigenmode  $n = 3$ ,  $\ell = 1$  for Stokes problem with Dirichlet boundary conditions. Tangential velocity vector field for a plane through the center of the sphere.

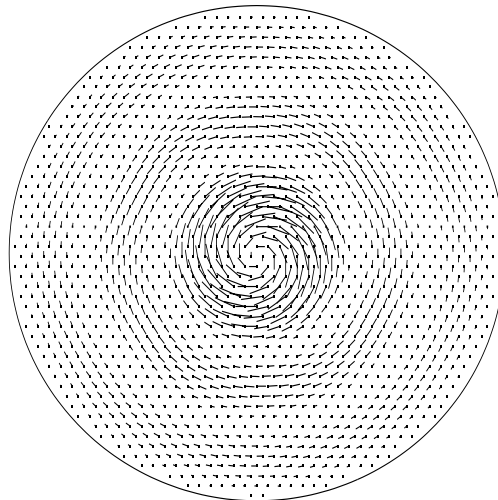


Figure 22: D3Q19-DDH for linear Navier–Stokes in a sphere. Eigenmode  $n = 3$ ,  $\ell = 1$  for Stokes problem with Dirichlet boundary conditions. Tangent vector field for a plane orthogonal to vector  $(1, 1, 1)$ .

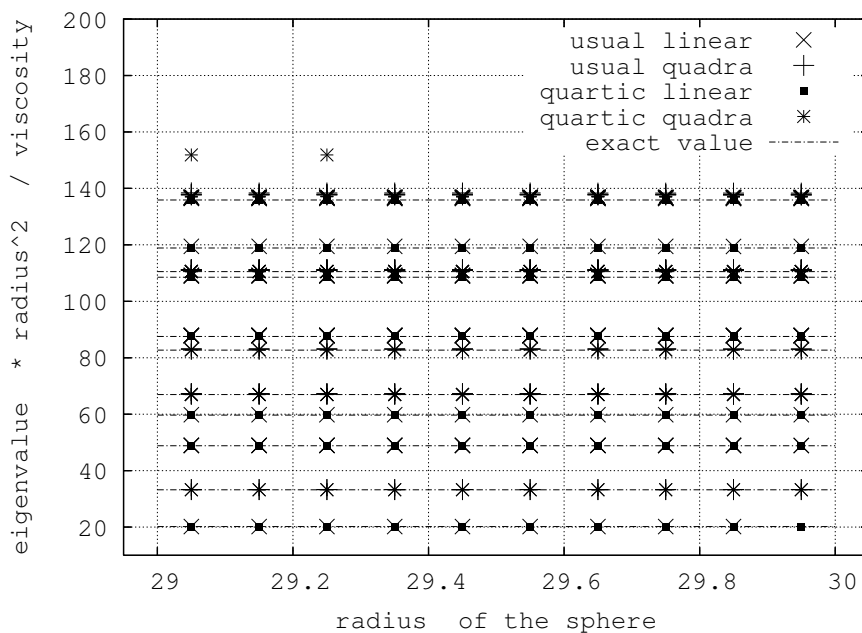


Figure 23: D3Q19-DDH for linear Navier–Stokes in a sphere. First eigenmodes for stationary Stokes problem with Dirichlet boundary conditions.

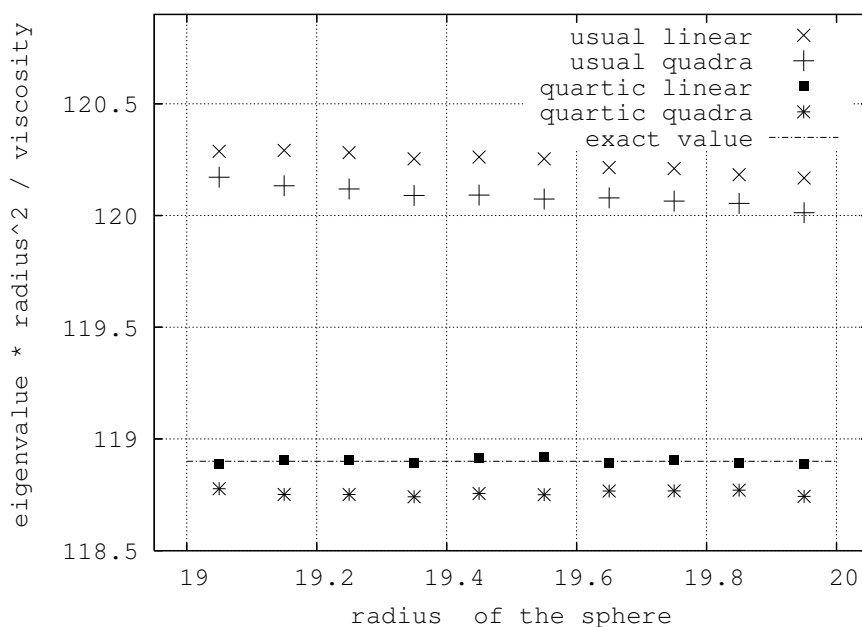


Figure 24: D3Q19-DDH for linear Navier–Stokes in a sphere. Eigenmode for stationary Stokes problem. Zoom of various schemes for Dirichlet eigenmode close to 118.8998692.

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  $1/8$  of 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 4 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 two orders of magnitude reduction in computer time.

- We present in Figure 23 the effect of boundary conditions for a number of values of the radius from 29 to 30. We give in Figure 24 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 preceedingly in (88) with

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

Similar work has been done for a cube. The results are published by Leriche, Lallemand and Labrosse in [30].

## 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 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 10 times as much computer time as the preceding one.
- 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 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”.

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