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Nonlinear fourth order Taylor expansion of lattice Boltzmann schemes

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Abstract

We propose a formal expansion of multiple relaxation times lattice Boltzmann schemes in terms of a single infinitesimal numerical variable. The result is a system of partial differential equations for the conserved moments of the lattice Boltzmann scheme. The expansion is presented in the nonlinear case up to fourth order accuracy. The asymptotic corrections of the nonconserved moments are developed in terms of equilibrium values and partial differentials of the conserved moments. Both expansions are coupled and conduct to explicit compact formulas. The new algebraic expressions are validated with previous results obtained with this framework. The example of isothermal D2Q9 lattice Boltzmann scheme illustrates the theoretical framework.

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1) Introduction

The lattice Boltzmann schemes in their modern form have been developed with the contributions of d’Humières, Lallemand, Succi [31, 43, 30, 36] and many others. An underlying lattice Boltzmann equation is discretised on a cartesian grid with a finite set of velocities chosen in such a way that during one time step, an exact transport is done between two vertices of the mesh. A lattice Boltzmann scheme is composed with two steps: a nonlinear local relaxation step, followed by a linear advection scheme coupling a given vertex with a given family of neighbours. The relaxation step follows in general the “BGK” approximation introduced by Bhatnagar, Gross and Krook [4]. This numerical method allows the simulation of an important number of physical phenomena as isothermal flows, compressible flows with heat transfer, non-ideal fluids, multiphase and multi-component flows, microscale gas flows, soft-matter flows,... up to quantum mechanics. For the actual status of the method and the various applications, we refer *e.g.* to the books of Guo and Shu [25], Krüger *et al.* [28] and to the prospective article of Succi [48]. The lattice Boltzmann method is founded on a mesoscopic Boltzmann model but is not able in general to solve the Boltzmann equation or associated kinetic models. It is admitted that essentially macroscopic models are approximated with the lattice Boltzmann schemes.

The link between mesoscopic and macroscopic models is never straightforward and an analysis is necessary. The usual method of formal analysis is founded on the Chapman-Enskog [6] expansion in the spirit of the book of Huang [32]. The classical approach for the Boltzmann equation and other mesoscopic models posed in a continuum space-time. The Chapman-Enskog method has been adapted to lattice Boltzmann schemes with discrete space and time equations by Chen and Doolen [7] and by Qian and Zhou [44]. It allows the derivation the equivalent partial differential equations founded on a multiscale time analysis. This classical Chapman Enskog expansion is popular in the lattice Boltzmann community, as reported in the contributions of Lallemand and Luo [36], Philippi and Hegele [41] and Shan *et al.* [46] among others. A main drawback of this approach is the fact that multiscale expansions are used without a clear mathematical signification of the various variables and associated functions.

Independently of this framework, we have proposed in [10, 11] the Taylor expansion method for isothermal fluid problems to obtain formally equivalent partial differential equations at second order accuracy. This work was inspired by the method of equivalent equations for finite difference schemes, in a spirit proposed by Lerat and Peyret [38] and Warming and Hyett [49]. In this approach, the infinitesimal variable is simply the time step (proportional to the space step with the acoustic scaling) and there is only one infinitesimal scale for the analysis. This approach has been experimentally validated with Pierre Lallemand in various contributions [17, 18, 20, 35]. It was extended to third order accuracy for thermal and fluid problems in [12], automated at an arbitrary order in the linear case in [3], extended with an external drift in [21] and to relative velocities in [14, 15]. Our point of view is *a priori* not to consider the third and fourth order terms as approximations of Burnett or super-Burnett equations (see *e.g.* [1, 47]) but simply as errors of the lattice Boltzmann scheme when solving partial differential equations of second order type. Nevertheless, progress in

the approximation of fourth order partial differential equations have been obtained in [40]. Here, we have no particular fluid hypothesis. It can be applied to scalar or to vectorial [13, 23] lattice Boltzmann schemes. This Taylor expansion method has been also revisited with the Maxwell iterations of Yong *et al.* [50].

In this contribution, we recall the framework of multiple relaxation times lattice Boltzmann schemes (Section 2) as initially proposed by d’Humières [30]. Then we present the Taylor expansion method in a very general way and the result is explicit with compact formulas. Our main result (Section 3) concerns the derivation of asymptotic partial differential equations in the nonlinear case, up to fourth order accuracy. The proof for first and second orders is presented in Section 4, with a validation in the isothermal fluid case in the specific case of the D2Q9 scheme. In Section 5, the expansion up to third and fourth orders is detailed, with a confrontation with our previous work [12]. The proofs of these results need specific algebraic developments, presented in this contribution. The linear case with constant coefficients is described in Section 6.

2) Multiple Relaxation Times Lattice Boltzmann schemes

In this contribution, we consider a regular cartesian lattice \mathcal{L} composed by vertices x separated by distances that are simple expressions of the space step Δx . A discrete time t is supposed to be an integer multiple of a time step $\Delta t > 0$. The unknowns of a lattice Boltzmann scheme with q discrete velocities $v_j \in \mathcal{V}$ for a configuration space of dimension d are the particle densities f_j that are functions of discrete space x , discrete time t and discrete velocities v_j for $0 \leq j < q$:

$$f_j = f_j(x, t), \quad x \in \mathcal{L}, t = n \Delta t, n \in \mathbb{N}, v_j \in \mathcal{V}.$$

The discrete velocity set \mathcal{V} does not depend on space or time. We have two steps for one time iteration: nonlinear relaxation and linear advection. In the first relaxation step, the particle distribution f is modified locally into a new distribution f^* . In the second step of advection, the method of characteristics is applied in a case where it is exact. Our framework concerns multi relaxation times : with d’Humières [30], we introduce a constant invertible matrix M called “d’Humières matrix” in this contribution. This matrix defines the moments m by a simple product:

$$(1) \quad m_k \equiv \sum_{0 \leq j < q} M_{kj} f_j.$$

We suppose that the moments are divided into two families:

$$(2) \quad m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}.$$

The conserved moments or macroscopic variables W constitute a linear space of dimension N . The nonconserved moments or microscopic variables Y generate a linear space of dimension $q - N$. After relaxation, the vector of moments m is transformed into a new vector m^* that satisfies

$$(3) \quad m^* \equiv \begin{pmatrix} W^* \\ Y^* \end{pmatrix}.$$

The conserved moments are not modified during this relaxation step:

$$(4) \quad W^* = W .$$

We suppose that the nonconserved moments relax towards an equilibrium vector Y^{eq} equal to a given function of the conserved variables. We have $Y^{\text{eq}} = \Phi(W)$ and

$$(5) \quad Y^* = Y + S(\Phi(W) - Y)$$

after relaxation. In the relation (5) the vector field $W \mapsto Y^{\text{eq}} \equiv \Phi(W)$ is the set of equilibrium values. The relaxation matrix S is a fixed invertible square matrix of dimension $(q - N) \times (q - N)$. Usually [36], it is a diagonal matrix. Then the particle distribution f^* after relaxation is given according to

$$(6) \quad f^* = M^{-1} m^* .$$

The iteration of the lattice Boltzmann scheme is finally given by the relation

$$(7) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad v_j \in \mathcal{V}, \quad x \in \mathcal{L}^0 .$$

Observe that this framework is very general and allows the introduction of two particle distributions [2, 16, 26, 33] or eventually more with the vectorial schemes developed by Graille [23] or a variant proposed in [13]. In this case, the numbering $j \mapsto v_j$ of the velocities is simply non injective.

- **Momentum-velocity operator**

For a linear space of dimension d , we introduce the momentum-velocity operator matrix Λ defined by the relation

$$(8) \quad \Lambda = M \text{diag} \left(\sum_{1 \leq \alpha \leq d} v^\alpha \partial_\alpha \right) M^{-1} .$$

It is a $q \times q$ operator matrix composed by first-order space differential operators. It is obtained by conjugation of the first order advection operator $v \cdot \nabla$ by the d’Humières matrix M . The matrix Λ is nothing else than the advection operator seen in the space of moments. We can concretize this matrix with the popular two-dimensional “D2Q9” scheme. A set of nine velocities is defined by the Figure 1.

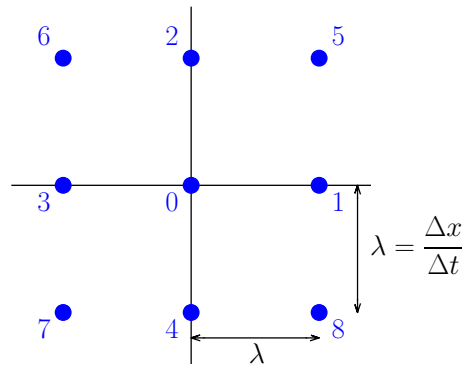


Figure 1: D2Q9

To fix the ideas, we use the moment matrix presented in Lallemand and Luo [36]:

$$(9) \quad M_{D2Q9} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{bmatrix}.$$

Observe that other choices are possible with the Hermite moments developed in [41, 46]. The moments are associated with the lines of the matrix (9). They are denominated (in this order) by $\rho, J_x, J_y, \varepsilon, x_x, x_y, q_x, q_y, h$. The lines of this invertible matrix are chosen orthogonal. For isothermal flows, the conserved moments

$$(10) \quad W = (\rho, J_x, J_y)^t$$

correspond to the three first lines of the d'Humières matrix (9). The non-conserved moments complete the family:

$$(11) \quad Y = (\varepsilon, x_x, x_y, q_x, q_y, h)^t.$$

They are linked to the six last lines of the matrix defined in (9). With the velocities defined in Figure 1 and the moment matrix (9), we construct without difficulty the operator matrix Λ for the thermal D2Q9 scheme:

$$(12) \quad \Lambda_{D2Q9} = \begin{bmatrix} \begin{array}{ccc|ccc} 0 & \partial_x & \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2\lambda^2}{3} \partial_x & 0 & 0 & \frac{1}{6} \partial_x & \frac{1}{2} \partial_x & \partial_y & 0 & 0 & 0 \\ \frac{2\lambda^2}{3} \partial_y & 0 & 0 & \frac{1}{6} \partial_y & -\frac{1}{2} \partial_y & \partial_x & 0 & 0 & 0 \end{array} \\ \hline \begin{array}{ccc|ccc} 0 & \lambda^2 \partial_x & \lambda^2 \partial_y & 0 & 0 & 0 & \partial_x & \partial_y & 0 \\ 0 & \frac{\lambda^2}{3} \partial_x & -\frac{\lambda^2}{3} \partial_y & 0 & 0 & 0 & -\frac{1}{3} \partial_x & \frac{1}{3} \partial_y & 0 \\ 0 & \frac{2}{3} \lambda^2 \partial_y & \frac{2}{3} \lambda^2 \partial_x & 0 & 0 & 0 & \frac{1}{3} \partial_y & \frac{1}{3} \partial_x & 0 \\ 0 & 0 & 0 & \frac{\lambda^2}{3} \partial_x & -\lambda^2 \partial_x & \lambda^2 \partial_y & 0 & 0 & \frac{1}{3} \partial_x \\ 0 & 0 & 0 & \frac{\lambda^2}{3} \partial_y & \lambda^2 \partial_y & \lambda^2 \partial_x & 0 & 0 & \frac{1}{3} \partial_y \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2 \partial_x & \lambda^2 \partial_y & 0 \end{array} \end{bmatrix}.$$

Proposition 1. Exponential form of lattice Boltzmann schemes

Consider a lattice Boltzmann scheme as defined at the previous section by the relations (1) to (7). Then we have an exponential form of the discrete iteration (7):

$$(13) \quad m(x, t + \Delta t) = \exp(-\Delta t \Lambda) m^*(x, t).$$

- Proof of Proposition 1.

We have simply a long sequence of identities:

$$m_k(x, t + \Delta t) = \sum_j M_{kj} f_j(x, t + \Delta t) \quad \text{due to (1)}$$

$$\begin{aligned}
 &= \sum_j M_{kj} f_j^*(x - v_j \Delta t, t) && \text{due to (7)} \\
 &= \sum_{j\ell} M_{kj} (M^{-1})_{j\ell} m_\ell^*(x - v_j \Delta t, t) && \text{due to (6)} \\
 &= \sum_{j\ell} M_{kj} (M^{-1})_{j\ell} \sum_{n=0}^{\infty} \frac{1}{n!} (-\Delta t \sum_{\alpha} v_j^\alpha \partial_\alpha)^n m_\ell^*(x, t) && \text{Taylor expansion} \\
 &= \sum_{\ell} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_j M_{kj} \left(-\Delta t \sum_{\alpha} v_j^\alpha \partial_\alpha \right)^n (M^{-1})_{j\ell} m_\ell^*(x, t) && \text{elementary algebra} \\
 &= \sum_{\ell} \sum_{n=0}^{\infty} \frac{1}{n!} (-\Delta t)^n \left(\left(M \left(\sum_{\alpha} v^\alpha \partial_\alpha \right) M^{-1} \right)_{k\ell}^n \right) m_\ell^*(x, t) \\
 & && \text{because } M \text{ is a constant matrix} \\
 &= \sum_{\ell} \sum_{n=0}^{\infty} \frac{1}{n!} (-\Delta t)^n (\Lambda^n)_{k\ell} m_\ell^*(x, t) && \text{due to (8)} \\
 &= \sum_{\ell} \left[\sum_{n=0}^{\infty} \frac{1}{n!} (-\Delta t \Lambda)_{k\ell}^n \right] m_\ell^*(x, t) && \text{elementary algebra} \\
 &= \sum_{\ell} \exp(-\Delta t \Lambda)_{k\ell} m_\ell^*(x, t) && \text{elementary algebra} \\
 &= \left(\exp(-\Delta t \Lambda) m^*(x, t) \right)_k && \text{elementary algebra}
 \end{aligned}$$

and the proof is completed. \square

We can see the relation (13) as a discrete form of the Duhamel formula for ordinary differential equations. The idea of introducing a formal exponential expansion is also present in the work of Boghosian and Coveney in the BGK case [5].

We introduce a block decomposition of the momentum-velocity operator matrix associated to the decomposition (2) of the moments. We define a $N \times N$ operator matrix A , a $N \times (q-N)$ operator matrix B , a $(q-N) \times N$ operator matrix C and a $(q-N) \times (q-N)$ operator matrix D according to

$$(14) \quad \Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}.$$

In the relation (12), we have put in evidence this block decomposition for the D2Q9 scheme with the conserved moments precised in (10). Even if the space differential operators commute, the matrices that compose the momentum-velocity operator matrix does not commute! We have the very important but elementary structure

$$\Lambda^2 \equiv \begin{pmatrix} A_2 & B_2 \\ C_2 & D_2 \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A^2 + BC & AB + BD \\ CA + DC & CB + D^2 \end{pmatrix}$$

and to fix the ideas

$$\Lambda^3 \equiv \begin{pmatrix} A_3 & B_3 \\ C_3 & D_3 \end{pmatrix} = \begin{pmatrix} A_2 & B_2 \\ C_2 & D_2 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A_2 A + B_2 C & A_2 B + B_2 D \\ C_2 A + D_2 C & C_2 B + D_2 D \end{pmatrix}.$$

3) Taylor expansion method

In this section, we revisit the Taylor expansion method: we specify the hypotheses, express our general result and begin the proof with the order zero.

- **Hypotheses for a formal expansion**

The formal Taylor expansion supposes some precise hypotheses. First, we adopt the acoustic scaling: the ratio $\lambda \equiv \frac{\Delta x}{\Delta t}$ is supposed to be constant in all this work. In consequence, the Hénon [29] matrix

$$(15) \quad \Sigma \equiv S^{-1} - \frac{1}{2} \mathbf{I}$$

remains fixed. Secondly, we suppose also that we can differentiate all the expansions relative to space and/or time. This hypothesis is mathematically absolutely non trivial and expresses that all the formal expansions should take place in very regular functional spaces. Thirdly, we use the notation $d\Psi(W).\xi$ for the action of the differential of some regular function $W \mapsto \Psi(W)$ against a test vector ξ . In particular,

$$(16) \quad \gamma_j(W) \equiv d\Phi(W).\Gamma_j(W), \quad 1 \leq j \leq 3.$$

For second order derivatives, we introduce

$$(17) \quad \partial^2 \Psi.\Gamma_1 \equiv d(d\Psi(W).\Gamma_1).\Gamma_1 = d^2 \Psi(W).(\Gamma_1, \Gamma_1) + d\Psi(W).d\Gamma_1(W).\Gamma_1.$$

The asymptotic analysis occurs for a time step Δt (or a space step Δx) tending to zero. Emerging partial differential equations for the conserved variables are denoted as

$$(18) \quad \partial_t W + \Gamma_1(W) + \Delta t \Gamma_2(W) + \Delta t^2 \Gamma_3(W) + \Delta t^3 \Gamma_4(W) = O(\Delta t^4).$$

The vector $\Gamma_j(W)$ belongs in \mathbb{R}^N . It is obtained after j space derivations of the conserved moments W and of the equilibrium vector $\Phi(W)$. For this reason, we will speak in the following of *e.g.* $\Gamma_1(W)$ as “first order term”, even if it is a term of order zero relative to the infinitesimal Δt . For non-conserved moments (or microscopic variables), we suppose

$$(19) \quad \begin{cases} Y = \Phi(W) + S^{-1} (\Delta t \Phi_1(W) + \Delta t^2 \Phi_2(W) + \Delta t^3 \Phi_3(W)) + O(\Delta t^4) \\ Y^* = \Phi(W) + (\Sigma - \frac{1}{2} \mathbf{I}) (\Delta t \Phi_1(W) + \Delta t^2 \Phi_2(W) + \Delta t^3 \Phi_3(W)) + O(\Delta t^4) \end{cases}$$

where \mathbf{I} is the identity matrix of dimension $q - N$. Observe that the two lines of (19) are equivalent thanks to (5) and (15). The vectors $\Phi_j(W)$ are analogous to $\Gamma_j(W)$ but not with the same dimension: $\Gamma_j(W) \in \mathbb{R}^N$ and $\Phi_j(W) \in \mathbb{R}^{q-N}$.

- **Main result. Recurrence formulas for fourth order expansion**

We prove in this contribution that we have the following recurrence formulas for the explicitation of the vectors $\Gamma_j(W)$ and $\Phi_j(W)$ up to fourth order accuracy:

$$(20) \quad \left\{ \begin{array}{l} \Gamma_1(W) = A W + B \Phi(W) \\ \Phi_1(W) = d\Phi(W).\Gamma_1(W) - (C W + D \Phi(W)) \\ \Gamma_2(W) = B \Sigma \Phi_1(W) \\ \Phi_2(W) = \Sigma d\Phi_1(W).\Gamma_1(W) + d\Phi(W).\Gamma_2(W) - D \Sigma \Phi_1(W) \\ \Gamma_3(W) = B \Sigma \Phi_2(W) + \frac{1}{12} B_2 \Phi_1(W) - \frac{1}{6} B d\Phi_1(W).\Gamma_1(W) \\ \Phi_3(W) = \Sigma d\Phi_1(W).\Gamma_2(W) + d\Phi(W).\Gamma_3(W) - D \Sigma \Phi_2(W) + \Sigma d\Phi_2(W).\Gamma_1(W) \\ \quad + \frac{1}{6} D d\Phi_1(W).\Gamma_1(W) - \frac{1}{12} D_2 \Phi_1(W) - \frac{1}{12} \partial^2 \Phi_1(W).\Gamma_1(W) \\ \Gamma_4(W) = B \Sigma \Phi_3(W) + \frac{1}{4} B_2 \Phi_2(W) + \frac{1}{6} B D_2 \Sigma \Phi_1(W) - \frac{1}{6} A B \Phi_2(W) \\ \quad - \frac{1}{6} B (d\gamma_1(W).\Gamma_2(W) + d\gamma_2(W).\Gamma_1(W)) - \frac{1}{6} B \Sigma \partial^2 \Phi_1(W).\Gamma_1(W). \end{array} \right.$$

Observe that the order of the relations in (20) is mandatory. Each step has to be explicitated before the evaluation of the next expression. At second order accuracy, the three first lines of the relations (20) summarizes what is needed for a lot of applications with only first and second order partial differential equations. Observe that the compact form $\Gamma_2 = B \Sigma \Phi_1$ for the second order term put in evidence the important choice of a Hénon matrix “as small as possible”.

Proposition 2. Equilibrium state and zero order expansion

When Δt tends to zero, the microscopic moments are close to their equilibrium value:

$$(21) \quad Y = \Phi(W) + O(\Delta t), \quad Y^* = \Phi(W) + O(\Delta t).$$

- Proof of Proposition 2.

We expand one iteration of the scheme (13) at order zero:

$$(22) \quad m + O(\Delta t) = m^* + O(\Delta t^3).$$

Then we deduce from (22):

$$Y - Y^* = O(\Delta t).$$

Then due to the iteration (5) and the fact that the matrix S is supposed fixed, we have

$$(23) \quad Y = \Phi(W) + O(\Delta t).$$

The first relation of (21) is satisfied. It is then immediate to deduce from the scheme iteration (5) the second relation of (21). The proposition is established. \square

In the following, we detail all the ingredients that conduct to the main result (18) to (20).

4) Taylor expansion method at first and second order accuracy

In this section, we prove the two first orders of the expansion (18)(19)(20). We make the link with the Taylor expansion as presented in [10, 11] and we apply the result for the isothermal D2Q9 scheme.

Proposition 3. First order expansion

When Δt tends to zero, the macroscopic moments W satisfy asymptotically the following system of N first order equations:

$$(24) \quad \partial_t W + \Gamma_1(W) = O(\Delta t).$$

Moreover, the vector $\Gamma_1(W)$ for the first order dynamics satisfy

$$(25) \quad \Gamma_1(W) = A W + B \Phi(W).$$

- Proof of Proposition 3.

We expand one iteration of the scheme (13) at first order:

$$(26) \quad m + \Delta t \partial_t m + O(\Delta t^2) = m^* - \Delta t \Lambda m^* + O(\Delta t^2).$$

We can replace the vector m by its two components W and Y . We have for the first line

$$W + \Delta t \partial_t W + O(\Delta t^2) = W - \Delta t (A W + B Y^*) + O(\Delta t^2).$$

We simplify by the constant W term, divide by Δt and take into account the expansion (21):

$$\partial_t W + O(\Delta t) = -(A W + B \Phi(W)) + O(\Delta t).$$

This relation is exactly the expansion (24) with the first order dynamics $\Gamma_1(W)$ evaluated according to the relation (25).

• **Example of the D2Q9 fluid scheme**

The results presented here are essentially a reformulation of the classic work of Lallemand and Luo [36]. With the moments introduced in (9), (10) and (11), we denote by Φ_ε , Φ_{xx} and Φ_{xy} the equilibrium values of the three first non conserved moments (11). The dynamics at first order is given by (25). We have in this D2Q9 case,

$$\Gamma_1 = \begin{pmatrix} \partial_x J_x + \partial_y J_y \\ \frac{2}{3} \lambda^2 \partial_x \rho + \frac{1}{6} \partial_x \Phi_\varepsilon + \frac{1}{2} \partial_x \Phi_{xx} + \partial_y \Phi_{xy} \\ \frac{2}{3} \lambda^2 \partial_y \rho + \frac{1}{6} \partial_y \Phi_\varepsilon - \frac{1}{2} \partial_y \Phi_{xx} + \partial_x \Phi_{xy} \end{pmatrix}.$$

These relations can be easily fitted with the Euler equations of gas dynamics in two space dimensions

$$\begin{cases} \partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \\ \partial_t J_x + \partial_x \left(\frac{1}{\rho} J_x^2 + p \right) + \partial_y \left(\frac{1}{\rho} J_x J_y \right) = 0 \\ \partial_t J_y + \partial_x \left(\frac{1}{\rho} J_x J_y \right) + \partial_y \left(\frac{1}{\rho} J_y^2 + p \right) = 0. \end{cases}$$

We identify the two expressions with $J_x \equiv \rho u$ and $J_y \equiv \rho v$:

$$\frac{2}{3} \lambda^2 \rho + \frac{1}{6} \Phi_\varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p, \quad \Phi_{xy} = \rho u v \quad \frac{2}{3} \lambda^2 \rho + \frac{1}{6} \Phi_\varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p,$$

and we deduce the expression for the three first nonconserved moments:

$$\Phi_\varepsilon = 6p - 4\lambda^2 \rho + 3\rho(u^2 + v^2), \quad \Phi_{xx} = \rho(u^2 - v^2), \quad \Phi_{xy} = \rho u v.$$

The other nonequilibrium moments q_x , q_y and h does not play any role in the first order partial equivalent equations.

Proposition 4. Taylor expansion method at second order accuracy

An essential result for the applications is the second order asymptotic analysis for a time step Δt (or a space step Δx) tending to zero. The expansion of the microscopic variables takes the form

$$(27) \quad Y = \Phi(W) + \Delta t S^{-1} \Phi_1(W) + O(\Delta t^2)$$

and the vector $\Phi_1(W)$ satisfies the relation

$$(28) \quad \Phi_1(W) = d\Phi(W) \cdot \Gamma_1(W) - (C W + D \Phi(W)).$$

A set of second order partial differential equations emerges

$$(29) \quad \partial_t W + \Gamma_1(W) + \Delta t \Gamma_2(W) = O(\Delta t^2).$$

The vector $\Gamma_1(W)$ has been precised in (25) the vector $\Gamma_2(W)$ is obtained after two derivations of the conserved moments W and the equilibrium vector $\Phi(W)$:

$$(30) \quad \Gamma_2(W) = B \Sigma \Phi_1(W).$$

The expression of the second order term puts in evidence the importance of taking over-relaxation in the applications where Σ should also be as small as possible.

- Proof of Proposition 4.

We first consider the first order expansion of microscopic moments. From the expansion (26) of one iteration of the scheme at first order, we can extract relations for the second component. We have for the microscopic moments

$$Y + \Delta t \partial_t Y + O(\Delta t^2) = Y^* - \Delta t (C W + D Y^*) + O(\Delta t^2).$$

Then

$$Y - Y^* = -\Delta t \left(\partial_t Y + (C W + D \Phi(W)) \right) + O(\Delta t^2).$$

The explicitation of $\partial_t Y$ is given by the chain rule from the expansion (23):

$$\begin{aligned} \partial_t Y &= \partial_t (\Phi(W) + O(\Delta t)) \\ &= d\Phi(W) \cdot \partial_t W + O(\Delta t) \\ &= d\Phi(W) \cdot (-\Gamma_1) + O(\Delta t). \end{aligned}$$

Then

$$S (Y - \Phi(W)) = \Delta t (d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi)) + O(\Delta t^2).$$

The relation (27) is established, and the expression of $\Phi_1(W)$ is obtained by the relation (28). Before using the expansion (27), we must expand the microscopic moments Y^* after relaxation up to first order accuracy. We have the following calculus

$$\begin{aligned} Y^* &= Y + S (\Phi(W) - Y) \\ &= Y - (\Delta t \Phi_1 + O(\Delta t^2)) && \text{due to (27)} \\ &= \Phi(W) + \left(\Sigma + \frac{1}{2} \text{I} \right) (\Delta t \Phi_1(W) + O(\Delta t^2)) - (\Delta t \Phi_1 + O(\Delta t^2)) && \text{due to (15) and (27)} \\ &= \Phi(W) + \left(\Sigma - \frac{1}{2} \text{I} \right) \Delta t \Phi_1(W) + O(\Delta t^2) \end{aligned}$$

and we have the relation

$$(31) \quad Y^* = \Phi(W) + \left(\Sigma - \frac{1}{2} \text{I} \right) \Delta t \Phi_1(W) + O(\Delta t^2).$$

The two relations (27) and (31) are nothing else that the first order terms of the general expansion (19).

- Second order partial differential equations

We expand now one iteration of the scheme (13) at second order accuracy:

$$(32) \quad m + \Delta t \partial_t m + \frac{1}{2} \Delta t^2 \partial_t^2 m + O(\Delta t^3) = m^* - \Delta t \Lambda m^* + \frac{1}{2} \Delta t^2 \Lambda^2 m^* + O(\Delta t^3).$$

We replace the vector m by its two components W and Y . We use the decomposition (14) of the momentum-velocity operator matrix Λ . We have for the first component

$$(33) \quad \begin{cases} W + \Delta t \partial_t W + \frac{1}{2} \Delta t^2 \partial_t^2 W + O(\Delta t^3) = \\ W - \Delta t (A W + B Y^*) + \frac{1}{2} \Delta t^2 (A_2 W + B_2 Y^*) + O(\Delta t^3). \end{cases}$$

We explicit some terms present in the relation (33). We have

$$\partial_t W = -\Gamma_1(W) + O(\Delta t) = -(A W + B \Phi(W)) + O(\Delta t)$$

Then, using the formal rule stated at the beginning of Section 3, we keep the order of accuracy after derivation:

$$\begin{aligned}\partial_t^2 W &= -\partial_t(\Gamma_1 + O(\Delta t)) \\ &= -d\Gamma_1 \cdot \partial_t W + O(\Delta t) \\ &= d\Gamma_1 \cdot \Gamma_1 + O(\Delta t) \\ &= A\Gamma_1 + B d\Phi \cdot \Gamma_1 + O(\Delta t).\end{aligned}$$

We deduce from (33):

$$\partial_t W = -\frac{1}{2} \Delta t \partial_t^2 W - (AW + BY^*) + \frac{1}{2} \Delta t (A_2 W + B_2 Y^*) + O(\Delta t^2).$$

We order the various terms by powers of Δt :

$$\begin{aligned}\partial_t W &= -AW - B \left(\Phi + (\Sigma - \frac{1}{2}I) \Delta t \Phi_1 \right) - \frac{1}{2} \Delta t (A\Gamma_1 + B d\Phi \cdot \Gamma_1) \\ &\quad + \frac{1}{2} \Delta t ((A^2 + BC)W + (AB + BD)\Phi) + O(\Delta t^2) \\ &= -AW - B\Phi + \Delta t \left[-B\Sigma\Phi_1 + \frac{1}{2}B(d\Phi \cdot \Gamma_1 - CW - D\Phi) - \frac{1}{2}A(AW + B\Phi) \right. \\ &\quad \left. - \frac{1}{2}B d\Phi \cdot \Gamma_1 + \frac{1}{2}(A^2 + BC)W + \frac{1}{2}(AB + BD)\Phi \right] + O(\Delta t^2) \\ &= -\Gamma_1(W) - \Delta t B \Sigma \Phi_1(W) + O(\Delta t^2)\end{aligned}$$

and the relation (29) is proven with $\Gamma_2(W) = B \Sigma \Phi_1$ as proposed in (30). \square

- **Link with the original Taylor expansion method**

In [10, 11], the moments at equilibrium are denoted m_ℓ^{eq} :

$$m_\ell^{\text{eq}}(W) = \begin{cases} W_\ell & \text{if } 0 \leq \ell < N \\ (\Phi(W))_{\ell-N} & \text{if } \ell \geq N, \end{cases}$$

the coefficients $\tilde{\Lambda}_{i\ell}^\beta$ are given according to

$$(34) \quad \tilde{\Lambda}_{i\ell}^\beta = \sum_j M_{ij} v_j^\beta (M^{-1})_{j\ell}, \quad 1 \leq \beta \leq d, 0 \leq i, \ell < q,$$

are closely related to the operator matrix Λ introduced in (8). The coefficients of the Hénon's matrix (15) have a shifted numbering

$$(35) \quad \tilde{\sigma}_\ell = \sigma_{\ell-N} \equiv \frac{1}{s_{\ell-N}} - \frac{1}{2}, \quad \ell \geq N$$

and the defect of conservation $\tilde{\theta}_k$ is defined according to

$$(36) \quad \tilde{\theta}_k(W) \equiv \partial_t m_k^{\text{eq}} + \sum_{0 \leq \ell < q} \sum_{1 \leq \beta \leq d} \tilde{\Lambda}_{k\ell}^\beta \partial_\beta m_\ell^{\text{eq}}(W), \quad k \geq N.$$

Proposition 5. Equivalence at second order accuracy

The second order expansion (29), (27), (25), (28) and (30) is equivalent to the expansion proposed in [10, 11]:

$$(37) \quad \partial_t W_i + \tilde{\Lambda}_{i\ell}^\beta \partial_\beta m_\ell^{\text{eq}}(W) = \Delta t \sum_{k \geq N} \tilde{\Lambda}_{ik}^\beta \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k(W) + O(\Delta t^2).$$

- Proof of Proposition 5.

Remark first that

$$\Lambda_{ik} = \sum_{j=0}^{q-1} M_{ij} \left(\sum_{1 \leq \beta \leq d} v_j^\beta \partial_\beta \right) (M^{-1})_{jk} = \sum_{1 \leq \beta \leq d} \left(\sum_{j=0}^{q-1} M_{ij} v_j^\beta (M^{-1})_{jk} \right) \partial_\beta = \sum_{1 \leq \beta \leq d} \tilde{\Lambda}_{ik}^\beta \partial_\beta.$$

Then on one hand, the component number i of the first order term $(AW + B\Phi(W))$ can be expanded in the following way:

$$\begin{aligned} (AW + B\Phi(W))_i &= \sum_{k < N} \tilde{\Lambda}_{ik}^\beta \partial_\beta W_k + \sum_{k \geq N} \tilde{\Lambda}_{ik}^\beta \partial_\beta \Phi_k \\ &= \sum_{k < N} \tilde{\Lambda}_{ik}^\beta \partial_\beta m_k^{\text{eq}} + \sum_{k \geq N} \tilde{\Lambda}_{ik}^\beta \partial_\beta m_k^{\text{eq}} \\ &= \sum_{0 \leq k < q} \tilde{\Lambda}_{ik}^\beta \partial_\beta m_k^{\text{eq}} \end{aligned}$$

and the first order terms of (29) and (37) are identical. Secondly, due to (36), we have for $k \geq N$

$$\begin{aligned} \tilde{\theta}_k &= \partial_t m_k^{\text{eq}} + \sum_{\ell \beta} \tilde{\Lambda}_{k\ell}^\beta \partial_\beta m_\ell^{\text{eq}} \\ &= \partial_t \Phi_{k-N} + (\Lambda \cdot m^{\text{eq}})_k \\ &= (d\Phi \cdot \partial_t W)_{k-N} + (\Lambda \cdot m^{\text{eq}})_k \\ &= (d\Phi \cdot (\Gamma_1 + O(\Delta t)))_{k-N} - (CW + D\Phi)_{k-N} \end{aligned}$$

and due to (28),

$$\tilde{\theta}_k = -(\Phi_1)_{k-N} + O(\Delta t), \quad k \geq N.$$

We deduce that for second order terms with $0 \leq i < N$:

$$\begin{aligned} (B\tilde{\sigma}\Phi_1)_i &= \sum_{0 \leq \ell < q-N} B_{i\ell} \tilde{\sigma}_{\ell+N} (\Phi_1(W))_\ell \\ &= \sum_{k \geq N} \sum_{0 \leq \beta \leq d} \tilde{\Lambda}_{ik}^\beta \partial_\beta \left(\sigma_k (-\tilde{\theta}_k + O(\Delta t)) \right) \quad \text{with } k = \ell + N \\ &= - \sum_{k \geq N} \sum_{0 \leq \beta \leq d} \tilde{\Lambda}_{ik}^\beta \tilde{\sigma}_k (\partial_\beta \tilde{\theta}_k) + O(\Delta t) \end{aligned}$$

because the coefficients $\tilde{\sigma}_k$ are supposed constant. Then the relation (37) is established. \square

- **Fluid D2Q9 diffusive tensor**

If we compute the second order term Γ_2 for the D2Q9 scheme introduced previously, the holy grail would be to recover the viscous terms of the compressible Navier Stokes equations in two space dimensions. More recisely, with a given shear viscosity μ and a given bulk viscosity ζ , we write the viscous terms of the lattice Boltzmann expansion as

$$(38) \quad -\Delta t \Gamma_2 = \begin{pmatrix} 0 \\ \partial_j \tau_{xj} \equiv \partial_x (2\mu \partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y (\mu(\partial_x v + \partial_y u)) \\ \partial_j \tau_{yj} \equiv \partial_x (\mu(\partial_x v + \partial_y u)) + \partial_y ((\zeta - \mu)(\partial_x u + \partial_y v) + 2\mu \partial_y v) \end{pmatrix} + \begin{pmatrix} 0 \\ \Psi_x \\ \Psi_y \end{pmatrix},$$

with the notation Ψ_x, Ψ_y for the error for the dissipation of momentum.

The problem to enforce $\Psi_x = \Psi_y = 0$ is ill-posed, as recognized by Dellar [8, 9], HÁZI and KÁVRÁN [27] and PRASIANAKIS *at al.* [42] among others. Nevertheless, it can be proven that the unphysical terms involving second order space derivatives involving the density can be removed with a pressure law of the type

$$p(\rho) = \frac{\lambda^2}{3} \rho,$$

id est a sound velocity equal to $\frac{1}{\sqrt{3}}$ in the velocity unit of the lattice Boltzmann scheme. Nevertheless, with the notation Φ_{qx} and Φ_{qy} for the equilibrium functions of the moments q_x and q_y and the coefficients of the Hénon matrix Σ fixed as

$$\Sigma = \text{diag}(\sigma_e, \sigma_x, \sigma_x, \sigma_q, \sigma_q \sigma_h),$$

the choice

$$\begin{cases} \Phi_{qx} = -\rho \lambda^2 u + 3 \rho (u^2 + v^2) u \\ \Phi_{qy} = -\rho \lambda^2 v + 3 \rho (u^2 + v^2) v, \end{cases}$$

conducts to the relation (38) with associated viscosities fixed in a very classical way:

$$\mu = \frac{\lambda}{3} \rho \sigma_x \Delta x, \quad \zeta = \frac{\lambda}{3} \rho \sigma_e \Delta x.$$

The equilibrium value Φ_h of the last fourth order moment h (see the relation (11)) has no incidence on the value of the diffusive term Γ_2 . The error is then reduced to third order terms relative to the velocity and we have precisely

$$\begin{cases} \Psi_x = \sigma_x \Delta t \left[\partial_x (u^3 \partial_x \rho - v^3 \partial_y \rho + 3 \rho (u^2 \partial_x u - v^2 \partial_y v)) \right. \\ \quad \left. + \partial_y (-v^3 \partial_x \rho - u^3 \partial_y \rho - 3 \rho (u^2 \partial_y u + v^2 \partial_x v)) \right] \\ \Psi_y = \sigma_x \Delta t \left[\partial_x (-v^3 \partial_x \rho - u^3 \partial_y \rho - 3 \rho (u^2 \partial_y u + v^2 \partial_x v)) \right. \\ \quad \left. + \partial_y (-u^3 \partial_x \rho + v^3 \partial_y \rho + 3 \rho (-u^2 \partial_x u + v^2 \partial_y v)) \right]. \end{cases}$$

5) Taylor expansion method at third and fourth order accuracy

The two following orders of the Taylor expansion does not set any theoretical difficulty, except the care of algebra with not so short formal expressions...

Proposition 6. Nonlinear third-order expansion

When the time step Δt has an infinitesimal value, the expansion of the microscopic variables takes the form

$$(39) \quad Y = \Phi(W) + \Delta t S^{-1} \Phi_1(W) + \Delta t^2 S^{-1} \Phi_2(W) + O(\Delta t^3).$$

The vector $\Phi_1(W)$ is evaluated at the relation (28) and $\Phi_2(W)$ satisfies the relation

$$(40) \quad \Phi_2(W) = \Sigma d\Phi_1(W). \Gamma_1(W) + d\Phi(W). \Gamma_2(W) - D \Sigma \Phi_1(W).$$

It is possible to precise a system of third order partial differential equations

$$(41) \quad \partial_t W + \Gamma_1(W) + \Delta t \Gamma_2(W) + \Delta t^2 \Gamma_3(W) = O(\Delta t^3).$$

The vectors $\Gamma_1(W)$ and $\Gamma_2(W)$ have been precised at the relations (25) and (30) respectively. We have moreover

$$(42) \quad \Gamma_3(W) = B \Sigma \Phi_2(W) + \frac{1}{12} B_2 \Phi_1(W) - \frac{1}{6} B d\Phi_1(W). \Gamma_1(W).$$

- Proof of Proposition 6.

We first establish the relations (39) and (40). We start by the expansion of the scheme (32) at order 2. For the second component of nonconserved moments, we have

$$Y + \Delta t \partial_t Y + \frac{1}{2} \Delta t^2 \partial_t^2 Y + O(\Delta t^3) = Y^* - \Delta t (C W + D Y^*) + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^*) + O(\Delta t^3)$$

and, due to the relaxation process $Y - Y^* \equiv S(Y - \Phi(W))$, we have

$$(43) \quad S(Y - \Phi(W)) = -\Delta t (C W + D Y^* + \partial_t Y) + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^* - \partial_t^2 Y) + O(\Delta t^3).$$

We can precise the two first time derivatives of the non-conserved moments. The relation (27) can also be written as

$$Y = \Phi(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t \Phi_1(W) + O(\Delta t^2).$$

We differentiate this previous relation relative to time:

$$\begin{aligned} \partial_t Y &= d\Phi. \partial_t W + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t d\Phi_1. \partial_t W + O(\Delta t^2) \\ &= -d\Phi. (\Gamma_1(W) + \Delta t \Gamma_2(W) + O(\Delta t^2)) + \Delta t \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1. (-\Gamma_1 + O(\Delta t)) + O(\Delta t^2) \end{aligned}$$

and

$$(44) \quad \partial_t Y = -d\Phi(W). \Gamma_1(W) - \Delta t \left[d\Phi(W). \Gamma_2(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1(W). \Gamma_1(W) \right] + O(\Delta t^2).$$

Because we need the second time derivative $\partial_t^2 Y$ in the right hand side of (43), we differentiate the relation (44) relative to time. Using the notation (16), we deduce

$$(45) \quad \partial_t^2 Y = d\gamma_1. \Gamma_1 + O(\Delta t).$$

We precise now the expansions of $C W + D Y^*$ and $C_2 W + D_2 Y^*$. We have

$$C W + D Y^* = C W + D \left[\Phi(W) + \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Delta t \Phi_1 \right] + O(\Delta t^2)$$

and

$$(46) \quad C W + D Y^* = \gamma_1(W) - \Phi_1(W) + \Delta t D \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Phi_1(W) + O(\Delta t^2).$$

With a new set of operator matrices,

$$\begin{aligned} C_2 W + D_2 Y^* &= C_2 W + D_2 (\Phi(W) + O(\Delta t)) \\ &= (C A + D C) W + (C B + D^2) \Phi(W) + O(\Delta t) \\ &= C \Gamma_1 + D (d\Phi. \Gamma_1 - \Phi_1) + O(\Delta t) \end{aligned}$$

and because $d\Phi. \Gamma_1 = d\gamma_1. \Gamma_1 - (C \Gamma_1 + D d\Phi. \Gamma_1)$,

$$(47) \quad C_2 W + D_2 Y^* = d(\gamma_1 - \Phi_1). \Gamma_1(W) - D \Phi_1(W) + O(\Delta t).$$

Then due to (43), (44), (45), (46) and (47), we have

$$\begin{aligned} S(Y - \Phi(W)) &= -\Delta t (C W + D Y^* + \partial_t Y) + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^* - \partial_t^2 Y) + O(\Delta t^3) \\ &= -\Delta t \left(\gamma_1 - \Phi_1 + \Delta t D \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Phi_1 \right) - \Delta t \left(-d\Phi. \Gamma_1 - \Delta t [d\Phi. \Gamma_2 + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1. \Gamma_1] \right) \\ &\quad + \frac{1}{2} \Delta t^2 (d(\gamma_1 - \Phi_1). \Gamma_1 - D \Phi_1) - \frac{1}{2} \Delta t^2 d\gamma_1. \Gamma_1 + O(\Delta t^3) \\ &= \Delta t \Phi_1 + \Delta t^2 \left(-D \Sigma \Phi_1 + \frac{1}{2} D \Phi_1 + d\Phi. \Gamma_2 + \Sigma d\Phi_1. \Gamma_1 - \frac{1}{2} D \Phi_1 \right) + O(\Delta t^3) \\ &= \Delta t \Phi_1 + \Delta t^2 \left(-D \Sigma \Phi_1 + d\Phi. \Gamma_2 + \Sigma d\Phi_1. \Gamma_1 \right) + O(\Delta t^3) \end{aligned}$$

and the relations (39) and (40) are established.

- Third order partial differential equations

We consider now the Taylor expansion of the relation (13) at third order:

$$(48) \quad \begin{cases} m + \Delta t \partial_t m + \frac{1}{2} \Delta t^2 \partial_t^2 m + \frac{1}{6} \Delta t^3 \partial_t^3 m + O(\Delta t^4) = \\ m^* - \Delta t \Lambda m^* + \frac{1}{2} \Delta t^2 \Lambda^2 m^* - \frac{1}{6} \Delta t^3 \Lambda^3 m^* + O(\Delta t^4). \end{cases}$$

We consider the first conserved components of the moments:

$$\begin{cases} W + \Delta t \partial_t W + \frac{1}{2} \Delta t^2 \partial_t^2 W + \frac{1}{6} \Delta t^3 \partial_t^3 W + O(\Delta t^4) = W - \Delta t (A W + B Y^*) \\ \quad + \frac{1}{2} \Delta t^2 (A_2 W + B_2 Y^*) - \frac{1}{6} \Delta t^3 (A_3 W + B_3 Y^*) + O(\Delta t^4). \end{cases}$$

We simplify the constant term W and divide by Δt . We deduce

$$(49) \quad \begin{cases} \partial_t W = -A W - B Y^* + \frac{1}{2} \Delta t (A_2 W + B_2 Y^* - \partial_t^2 W) \\ \quad - \frac{1}{6} \Delta t^2 (A_3 W + B_3 Y^* + \partial_t^3 W) + O(\Delta t^3). \end{cases}$$

We explicit the partial derivatives $\partial_t^2 W$ and $\partial_t^3 W$ at orders one and zero respectively. From the relation

$$\partial_t W + \Gamma_1 + \Delta t \Gamma_2 = O(\Delta t^2)$$

we have

$$\begin{aligned} \partial_t^2 W &= \partial_t (-\Gamma_1 - \Delta t \Gamma_2 + O(\Delta t^2)) \\ &= d(-\Gamma_1 - \Delta t \Gamma_2 + O(\Delta t^2)) \cdot (\partial_t W) \\ &= d(-\Gamma_1 - \Delta t \Gamma_2 + O(\Delta t^2)) \cdot (-\Gamma_1 - \Delta t \Gamma_2 + O(\Delta t^2)) \end{aligned}$$

and

$$(50) \quad \partial_t^3 W = d\Gamma_1 \cdot \Gamma_1 + \Delta t (d\Gamma_1 \cdot \Gamma_2 + d\Gamma_2 \cdot \Gamma_1) + O(\Delta t^2).$$

Then

$$\begin{aligned} \partial_t^3 W &= \partial_t (\partial_t^2 W) \\ &= \partial_t (d\Gamma_1 \cdot \Gamma_1) + O(\Delta t) \\ &= d(d\Gamma_1 \cdot \Gamma_1) \cdot \partial_t W + O(\Delta t) \\ &= -d(d\Gamma_1 \cdot \Gamma_1) \cdot \Gamma_1 + O(\Delta t) \end{aligned}$$

$$(51) \quad \partial_t^3 W = -\partial^2 \Gamma_1 \cdot \Gamma_1 + O(\Delta t).$$

In order to compute the coefficient Γ_3 , we precise now the expansions of the quantities $A_j W + B_j Y^*$ for $j = 1, 2$ and 3 . We have

$$\begin{aligned} A W + B Y^* &= A W + B (\Phi(W) + (\Sigma - \frac{1}{2} \mathbf{I}) (\Delta t \Phi_1 + \Delta t^2 \Phi_2) + O(\Delta t^3)) \\ &= A W + B \Phi + \Delta t B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + O(\Delta t^3) \\ A_2 W + B_2 Y^* &= A_2 W + B_2 (\Phi(W) + (\Sigma - \frac{1}{2} \mathbf{I}) \Delta t \Phi_1) + O(\Delta t^2) \\ &= (A^2 + B C) W + (A B + B D) \Phi + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + O(\Delta t^2) \\ &= A \Gamma_1 + B (\gamma_1 - \Phi_1) + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + O(\Delta t^2) \\ &\quad \text{because } C W + D \Phi_1 = \gamma_1 - \Phi_1 \\ &= d\Gamma_1 \cdot \Gamma_1 - B \Phi_1 + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + O(\Delta t^2) \\ &\quad \text{because } d\Gamma_1 \cdot \Gamma_1 = A \Gamma_1 + B \gamma_1, \end{aligned}$$

$$\begin{aligned} A_3 W + B_3 Y^* &= A_3 W + B_3 \Phi(W) + O(\Delta t) \\ &= (A_2 A + B_2 C) W + (A_2 B + B_2 D) \Phi + O(\Delta t) \end{aligned}$$

$$\begin{aligned}
 &= A_2 \Gamma_1 + B_2 (\gamma_1 - \Phi_1) + O(\Delta t) \\
 &= (A^2 + B C) \Gamma_1 + (A B + B D) \gamma_1 - B_2 \Phi_1 + O(\Delta t) \\
 &= A (A \Gamma_1 + B \gamma_1) + B (C \Gamma_1 + D \gamma_1) - B_2 \Phi_1 + O(\Delta t) \\
 &= A d\Gamma_1 \cdot \Gamma_1 + B (C \Gamma_1 + D \gamma_1) - B_2 \Phi_1 + O(\Delta t) \\
 &\hspace{15em} \text{because } d\Gamma_1 \cdot \Gamma_1 = A \Gamma_1 + B \gamma_1 \\
 &= A d\Gamma_1 \cdot \Gamma_1 + B d(\gamma_1 - \Phi_1) \cdot \Gamma_1 - B_2 \Phi_1 + O(\Delta t) \\
 &\hspace{15em} \text{because } C \Gamma_1 + D \gamma_1 = d(\gamma_1 - \Phi_1) \cdot \Gamma_1 \\
 &= \partial^2 \Gamma_1 \cdot \Gamma_1 - B d\Phi_1 \cdot \Gamma_1 - B_2 \Phi_1 + O(\Delta t) \\
 &\hspace{15em} \text{because } \partial^2 \Gamma_1 \cdot \Gamma_1 \equiv d(d\Gamma_1 \cdot \Gamma_1) \cdot \Gamma_1 = A d\Gamma_1 \cdot \Gamma_1 + B d\gamma_1 \cdot \Gamma_1.
 \end{aligned}$$

We deduce now from (49), (50), (51) and the previous expressions:

$$\begin{aligned}
 \partial_t W &= -A W - B Y^* + \frac{1}{2} \Delta t (A_2 W + B_2 Y^* - \partial_t^2 W) - \frac{1}{6} \Delta t^2 (A_3 W + B_3 Y^* + \partial_t^3 W) + O(\Delta t^3) \\
 &= -(A W + B \Phi + \Delta t B (\Sigma - \frac{1}{2} I) \Phi_1 + \Delta t^2 B (\Sigma - \frac{1}{2} I) \Phi_2) \\
 &\quad + \frac{1}{2} \Delta t (d\Gamma_1 \cdot \Gamma_1 - B \Phi_1 + \Delta t B_2 (\Sigma - \frac{1}{2} I) \Phi_1 - d\Gamma_1 \cdot \Gamma_1 - \Delta t (d\Gamma_1 \cdot \Gamma_2 + d\Gamma_2 \cdot \Gamma_1)) \\
 &\quad - \frac{1}{6} \Delta t^2 (\partial^2 \Gamma_1 \cdot \Gamma_1 - B d\Phi_1 \cdot \Gamma_1 - B_2 \Phi_1 - \partial^2 \Gamma_1 \cdot \Gamma_1) + O(\Delta t^3) \\
 &= -\Gamma_1 - \Delta t B \Sigma \Phi_1 + \Delta t^2 (-B \Sigma \Phi_2 + \frac{1}{2} B \Phi_2 + \frac{1}{2} B_2 \Sigma \Phi_1 - \frac{1}{4} B_2 \Phi_1 - \frac{1}{2} (d\Gamma_1 \cdot \Gamma_2 + d\Gamma_2 \cdot \Gamma_1) \\
 &\quad + \frac{1}{6} B d\Phi_1 \cdot \Gamma_1 + \frac{1}{6} B_2 \Phi_1) + O(\Delta t^3) \hspace{2em} \text{because } \partial^2 \Gamma_1 \cdot \Gamma_1 = A d\Gamma_1 \cdot \Gamma_1 + B d\gamma_1 \cdot \Gamma_1 \\
 &= -\Gamma_1 - \Delta t B \Sigma \Phi_1 + \Delta t^2 (-B \Sigma \Phi_2 + \frac{1}{2} B (\Sigma d\Phi_1 \cdot \Gamma_1 + \gamma_2 - D \Sigma \Phi_1) + \frac{1}{2} (A B + B D) \Sigma \Phi_1 \\
 &\quad - \frac{1}{12} B_2 \Phi_1 - \frac{1}{2} (A \Gamma_2 + B \gamma_2) - \frac{1}{2} B \Sigma d\Phi_1 \cdot \Gamma_1 + \frac{1}{6} B d\Phi_1 \cdot \Gamma_1) + O(\Delta t^3) \\
 &= -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 (B \Sigma \Phi_2 + \frac{1}{12} B_2 \Phi_1 - \frac{1}{6} B d\Phi_1 \cdot \Gamma_1) + O(\Delta t^3)
 \end{aligned}$$

and the relations (41) and (42) are established. \square

In [12], we have proposed a third order expansion of nonlinear lattice Boltzmann schemes for two specific applications: scalar advection diffusion ($N = 1$) and fluid system ($N = d + 1$) with mass and momentum conservation. In the following proposition, we show that our previous result at third order accuracy can be reformulated with the compact formulation (41) (42) of Proposition 6.

Proposition 7. Third-order formal expansion for thermics and fluids

With the notations (34), (35) and (36) introduced at Proposition 5, we suppose moreover

$$M_{0j} = 1, \quad M_{\alpha j} = v_j^\alpha, \quad 0 \leq j < q, \quad 1 \leq \alpha \leq d.$$

The first moments are denoted by $\rho \equiv \sum_j f_j$ and $J_\alpha \equiv \sum_j v_j^\alpha f_j$. For the scalar advection diffusion ($N = 1$), the third order equivalent partial differential equation (41) (42) can be written

$$(52) \quad \partial_t \rho + \partial_\alpha J_\alpha^{\text{eq}} - \Delta t \tilde{\sigma}_\alpha \partial_\alpha \tilde{\theta}_\alpha + \Delta t^2 \left[\Lambda_{\beta\ell}^\gamma \left(\tilde{\sigma}_\beta \tilde{\sigma}_\ell - \frac{1}{12} \right) \partial_\beta \partial_\gamma \tilde{\theta}_\ell + \left(\tilde{\sigma}_\beta^2 - \frac{1}{6} \right) \partial_t (\partial_\beta \tilde{\theta}_\beta) \right] = O(\Delta t^3)$$

with $J_\alpha^{\text{eq}} \equiv \Phi_\alpha(\rho)$ and the defects of conservation $\tilde{\theta}_k(W)$ defined in (36). For the fluid system ($N = d + 1$), we have

$$(53) \quad \left\{ \begin{array}{l} \partial_t \rho + \partial_\alpha J_\alpha - \frac{1}{12} \Delta t^2 \Lambda_{\beta\ell}^\gamma \partial_\beta \partial_\gamma \tilde{\theta}_\ell = O(\Delta t^3) \\ \partial_t J_\alpha + \Lambda_{\alpha k}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{\alpha k}^\beta \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k \\ \quad + \Delta t^2 \left[\Lambda_{\alpha k}^\beta \Lambda_{k\ell}^\gamma \left(\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12} \right) \partial_\beta \partial_\gamma \tilde{\theta}_\ell + \Lambda_{\alpha k}^\beta \left(\tilde{\sigma}_k^2 - \frac{1}{6} \right) \partial_\beta \partial_t \tilde{\theta}_k \right] = O(\Delta t^3). \end{array} \right.$$

The relations (52) and (53) are exactly the ones proposed with numbers (35), (40) and (41) in the reference [12].

- Proof of Proposition 7.

We first consider the conservation defect $\tilde{\theta}_k(W) \equiv \partial_t m_k^{\text{eq}} + \sum_{\ell\beta} \tilde{\Lambda}_{k\ell}^\beta \partial_\beta m_\ell^{\text{eq}}$ introduced in (36). We define a vector conservation defect θ of dimension $q - N$ just obtained by a shift of component numbering:

$$\theta_k = \tilde{\theta}_{k+N}(W), \quad 0 \leq k < q - N.$$

We have for $0 \leq k < q - N$:

$$\begin{aligned} \theta_k &= (\text{d}\Phi \cdot \partial_t W)_k + (\tilde{\Lambda} \cdot m^{\text{eq}})_{k+N} \\ &= (\text{d}\Phi \cdot \partial_t W)_k + (C W + D \Phi(W))_k \\ &= (\text{d}\Phi \cdot (-\Gamma_1 - \Delta t \Gamma_2))_k + (C W + D \Phi(W))_k + O(\Delta t^2) && \text{due to the expansion (18)} \\ &= -(\Phi_1 + \Delta t \text{d}\Phi \cdot \Gamma_2)_k + O(\Delta t^2) && \text{due to the relation (20)} \end{aligned}$$

and

$$\theta = -\Phi_1 - \Delta t \text{d}\Phi \cdot \Gamma_2 + O(\Delta t^2).$$

In particular, $\partial_t \theta = -\partial_t \Phi_1 + O(\Delta t) = -\text{d}\Phi_1 \cdot (-\Gamma_1) + O(\Delta t)$ and

$$\partial_t \theta = \text{d}\Phi_1 \cdot \Gamma_1 + O(\Delta t).$$

Due to (30) and (42), we have the following calculus:

$$\begin{aligned} \Gamma_2 + \Delta t \Gamma_3 &= B \Sigma \Phi_1 + \Delta t (B \Sigma \Phi_2 - \frac{1}{12} B_2 \Phi_1 + \frac{1}{6} B \text{d}\Phi_1 \cdot \Gamma_1) \\ &= B \Sigma (-\theta + \Delta t \text{d}\Phi \cdot \Gamma_2 + O(\Delta t^2)) + \Delta t B \Sigma (D \Sigma \Phi_1 - \text{d}\Phi \cdot \Gamma_2 - \Sigma \text{d}\Phi_1 \cdot \Gamma_1) \\ &\quad - \frac{1}{12} \Delta t B_2 \Phi_1 + \frac{1}{6} \Delta t B \text{d}\Phi_1 \cdot \Gamma_1 \\ &= -B \Sigma \theta + \Delta t [(B \Sigma D \Sigma - \frac{1}{12} B_2) \Phi_1 + B (\frac{1}{6} - \Sigma^2) \text{d}\Phi_1 \cdot \Gamma_1] + O(\Delta t^2) \\ &= -B \Sigma \theta + \Delta t [- (B \Sigma D \Sigma - \frac{1}{12} B_2) \theta + B (\Sigma^2 - \frac{1}{6}) \partial_t \theta] + O(\Delta t^2). \end{aligned}$$

The third-order partial equivalent equations (41) can be written under the form

$$\partial_t W + \tilde{\Lambda} m^{\text{eq}} + \Delta t B \Sigma \theta + \Delta t^2 \left[\left(B \Sigma D \Sigma - \frac{1}{12} B_2 \right) \theta - B \left(\Sigma^2 - \frac{1}{6} \right) \partial_t \theta \right] = O(\Delta t^3).$$

- We explicit now the following cartesian components:

$$(B \Sigma D \Sigma \theta)_i = -\tilde{\Lambda}_{ik}^\beta \tilde{\sigma}_k (-\tilde{\Lambda}_{k\ell}^\gamma) \tilde{\sigma}_\ell \partial_\beta \partial_\gamma \tilde{\theta}_\ell = \tilde{\Lambda}_{ik}^\beta \tilde{\sigma}_k \tilde{\Lambda}_{k\ell}^\gamma \tilde{\sigma}_\ell \partial_\beta \partial_\gamma \tilde{\theta}_\ell,$$

$$(B_2 \theta)_i = (\tilde{\Lambda}_{ik}^\beta \partial_\beta) (\tilde{\Lambda}_{k\ell}^\gamma \partial_\gamma) \tilde{\theta}_\ell = \tilde{\Lambda}_{ik}^\beta \tilde{\Lambda}_{k\ell}^\gamma \partial_\beta \partial_\gamma \tilde{\theta}_\ell,$$

$$((B \Sigma D \Sigma - \frac{1}{12} B_2) \tilde{\theta})_i = \tilde{\Lambda}_{ik}^\beta \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \tilde{\theta}_\ell$$

$$\text{and } -(B (\Sigma^2 - \frac{1}{6}) \partial_t \tilde{\theta})_i = \tilde{\Lambda}_{ik}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \tilde{\theta}_k.$$

We deduce a new form of the third-order partial equivalent equations for $0 \leq i < N$:

$$(54) \quad \begin{cases} \partial_t W_i + \tilde{\Lambda}_{ik}^\alpha \partial_\alpha m_k^{\text{eq}} - \Delta t \tilde{\Lambda}_{ik}^\beta \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k \\ \quad + \Delta t^2 [\tilde{\Lambda}_{ik}^\beta \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \tilde{\theta}_\ell + \tilde{\Lambda}_{ik}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \tilde{\theta}_k] = O(\Delta t^3). \end{cases}$$

- We focus on the mass conservation ($i = 0$). We have

$$\tilde{\Lambda}_{0\ell}^\alpha = M_{0j} v_j^\alpha (M^{-1})_{j\ell} = M_{\alpha j} (M^{-1})_{j\ell} = \delta_{\alpha\ell}.$$

Then

$$\tilde{\Lambda}_{0k}^\beta \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k = \delta_{\beta k} \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k = \tilde{\sigma}_\beta \partial_\beta \tilde{\theta}_\beta.$$

In the thermal case, we have only one conservation law and $\tilde{\sigma}_\beta \neq 0$. Thus we have enlightened the second order term of the left hand side of the relation (52). In the fluid case, the momentum (*id est* moments numbered from 1 to d) are conserved. In consequence, $\tilde{\sigma}_\beta = 0$ and we have no second order term in the mass conservation (53).

Now for the first term relative to third order term of (54), we have

$$\tilde{\Lambda}_{0k}^\beta \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell = \delta_{\beta k} \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell = \tilde{\Lambda}_{\beta\ell}^\gamma (\tilde{\sigma}_\beta \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell.$$

In the thermal case, $\tilde{\sigma}_\beta \neq 0$ and this term is exactly the first of the two third order terms of the relation (52). In the fluid case, $\tilde{\sigma}_\beta = 0$ and this term has a more compact expression. Finally,

$$(55) \quad \tilde{\Lambda}_{0k}^\beta \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell = \begin{cases} \tilde{\Lambda}_{\beta\ell}^\gamma (\tilde{\sigma}_\beta \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell & \text{thermics} \\ -\frac{1}{12} \tilde{\Lambda}_{\beta\ell}^\gamma \partial_\beta \partial_\gamma \theta_\ell & \text{fluid.} \end{cases}$$

For the second term relative to third order, we have

$$\tilde{\Lambda}_{0k}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = (\tilde{\sigma}_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta)$$

In the thermal case, $\tilde{\sigma}_\beta \neq 0$ and $\tilde{\Lambda}_{0k}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = (\tilde{\sigma}_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta)$. In the fluid case, the momentum is conserved and $\theta_\beta = O(\Delta t)$ and $\tilde{\Lambda}_{0k}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = O(\Delta t)$. In a synthetic way,

$$(56) \quad \tilde{\Lambda}_{0k}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = \begin{cases} (\tilde{\sigma}_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta) & \text{thermics} \\ O(\Delta t) & \text{fluid.} \end{cases}$$

We deduce from (55) and (56) the expansion (52) in the thermal case and the first relation of (53) in the fluid case.

- For the momentum equation of the fluid case, $1 \leq i = \alpha \leq d$ and the relation (54) can be rewritten as

$$\begin{cases} \partial_t J_\alpha + \tilde{\Lambda}_{\alpha k}^\alpha \partial_\alpha m_k^{\text{eq}} - \Delta t \tilde{\Lambda}_{\alpha k}^\beta \tilde{\sigma}_k \partial_\beta \tilde{\theta}_k \\ + \Delta t^2 [\tilde{\Lambda}_{\alpha k}^\beta \tilde{\Lambda}_{k\ell}^\gamma (\tilde{\sigma}_k \tilde{\sigma}_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \tilde{\theta}_\ell + \tilde{\Lambda}_{\alpha k}^\beta (\tilde{\sigma}_k^2 - \frac{1}{6}) \partial_\beta \partial_t \tilde{\theta}_k] = O(\Delta t^3). \end{cases}$$

This relation is exactly the second relation of (53). \square

Proposition 8. Nonlinear expansion at fourth order

When the time step Δt has an infinitesimal value, the expansion of the microscopic variables takes the form

$$(57) \quad Y = \Phi(W) + \Delta t S^{-1} \Phi_1(W) + \Delta t^2 S^{-1} \Phi_2(W) + \Delta t^3 S^{-1} \Phi_3(W) + O(\Delta t^4).$$

The vectors $\Phi_1(W)$ and $\Phi_2(W)$ have been evaluated at the relations (28) and (40). We have

$$(58) \quad \begin{cases} \Phi_3(W) = d\Phi(W). \Gamma_3(W) + \Sigma d\Phi_1(W). \Gamma_2(W) + \Sigma d\Phi_2(W). \Gamma_1(W) - D \Sigma \Phi_2(W) \\ + \frac{1}{6} D d\Phi_1(W). \Gamma_1(W) - \frac{1}{12} D_2 \Phi_1(W) - \frac{1}{12} \partial^2 \Phi_1(W). \Gamma_1(W). \end{cases}$$

A system of fourth order partial differential equations is asymptotically satisfied by the lattice Boltzmann scheme:

$$(59) \quad \partial_t W + \Gamma_1(W) + \Delta t \Gamma_2(W) + \Delta t^2 \Gamma_3(W) + \Delta t^3 \Gamma_4(W) = O(\Delta t^4).$$

The vectors $\Gamma_1(W)$, $\Gamma_2(W)$ and $\Gamma_3(W)$ have been precised at the relations (25), (30) and (42) respectively. We have now

$$(60) \quad \begin{cases} \Gamma_4(W) = B \Sigma \Phi_3(W) + \frac{1}{4} B_2 \Phi_2(W) + \frac{1}{6} B D_2 \Sigma \Phi_1 - \frac{1}{6} A B \Phi_2(W) \\ -\frac{1}{6} B d\gamma_1(W) \cdot \Gamma_2(W) - \frac{1}{6} B d\gamma_2(W) \cdot \Gamma_1(W) - \frac{1}{6} B \Sigma \partial^2 \Phi_1(W) \cdot \Gamma_1(W). \end{cases}$$

- Proof of Proposition 8.

We first establish the relations (57) and (58). We start by the expansion of the scheme (48) at order 3. For the second component of nonconserved moments, we have

$$\begin{cases} Y + \Delta t \partial_t Y + \frac{1}{2} \Delta t^2 \partial_t^2 Y + \frac{1}{6} \Delta t^3 \partial_t^3 Y + O(\Delta t^4) = Y^* - \Delta t (C W + D Y^*) \\ + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^*) - \frac{1}{6} \Delta t^3 (C_3 W + D_3 Y^*) + O(\Delta t^4). \end{cases}$$

The relaxation process can be written $Y - Y^* \equiv S(Y - \Phi(W))$. We deduce

$$(61) \quad \begin{cases} S(Y - \Phi(W)) = -\Delta t (C W + D Y^* + \partial_t Y) + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^* - \partial_t^2 Y) \\ -\frac{1}{6} \Delta t^3 (C_3 W + D_3 Y^* + \partial_t^3 Y) + O(\Delta t^4). \end{cases}$$

We have to precise the three first time derivatives of the non-conserved moments. The relation (57) can also be written at second order accuracy:

$$Y = \Phi(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t \Phi_1(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t^2 \Phi_2(W) + O(\Delta t^3).$$

We differentiate this previous relation relative to time:

$$\begin{aligned} \partial_t Y &= d\Phi \cdot \partial_t W + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t d\Phi_1 \cdot \partial_t W + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \Delta t^2 d\Phi_2 \cdot \partial_t W + O(\Delta t^3) \\ &= -d\Phi \cdot (\Gamma_1(W) + \Delta t \Gamma_2(W) + \Delta t^2 \Gamma_3(W) + O(\Delta t^3)) \\ &\quad - \Delta t \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1 \cdot (\Gamma_1 + \Delta t \Gamma_2 + O(\Delta t^2)) + \Delta t^2 \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_2 \cdot (-\Gamma_1 + O(\Delta t)) + O(\Delta t^3) \end{aligned}$$

and

$$(62) \quad \begin{cases} \partial_t Y = -d\Phi(W) \cdot \Gamma_1(W) - \Delta t [d\Phi(W) \cdot \Gamma_2(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1(W) \cdot \Gamma_1(W)] \\ -\Delta t^2 [d\Phi(W) \cdot \Gamma_3(W) + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_1(W) \cdot \Gamma_2(W) \\ + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) d\Phi_2(W) \cdot \Gamma_1(W)] + O(\Delta t^3). \end{cases}$$

We need the second time derivative $\partial_t^2 Y$ and third order time derivative $\partial_t^3 Y$ in the right hand side of (61). We differentiate the relation (62) relative to time. Using the notation (16), we deduce

$$\partial_t^2 Y = -d\gamma_1 \cdot (-\Gamma_1 - \Delta t \Gamma_2) - \Delta t [-d\gamma_2 \cdot \Gamma_1 - \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \partial^2 \Phi(W) \cdot \Gamma_1(W)] + O(\Delta t^2)$$

and

$$(63) \quad \partial_t^2 Y = d\gamma_1 \cdot \Gamma_1 + \Delta t [d\gamma_1 \cdot \Gamma_2 + d\gamma_2 \cdot \Gamma_1 + \left(\Sigma + \frac{1}{2} \mathbf{I} \right) \partial^2 \Phi_1(W) \cdot \Gamma_1(W)] + O(\Delta t^2).$$

Finally,

$$(64) \quad \partial_t^3 Y = -\partial^2 \gamma_1(W) \cdot \Gamma_1(W) + O(\Delta t).$$

We precise now the expansions of $C W + D Y^*$, $C_2 W + D_2 Y^*$ and $C_3 W + D_3 Y^*$. We have

$$C W + D Y^* = C W + D [\Phi(W) + \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Delta t \Phi_1 + \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Delta t^2 \Phi_2] + O(\Delta t^2)$$

and

$$(65) \quad \begin{cases} C W + D Y^* = \gamma_1(W) - \Phi_1(W) + \Delta t D \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Phi_1(W) \\ + \Delta t^2 D \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Phi_2(W) + O(\Delta t^3). \end{cases}$$

For the second order term,

$$C_2 W + D_2 Y^* = C_2 W + D_2 [\Phi(W) + \Delta t (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1] + O(\Delta t^2)$$

and due to (47),

$$(66) \quad C_2 W + D_2 Y^* = d(\gamma_1 - \Phi_1) \cdot \Gamma_1(W) - D \Phi_1(W) + \Delta t D_2 \left(\Sigma - \frac{1}{2} \mathbf{I} \right) \Phi_1 + O(\Delta t^2).$$

We have finally for the third order terms

$$\begin{aligned} C_3 W + D_3 Y^* &= C_3 W + D_3 \Phi(W) + O(\Delta t) \\ &= (C_2 A + D_2 C) W + (C_2 B + D_2 D) \Phi(W) + O(\Delta t) \\ &= C_2 \Gamma_1 + D_2 (\gamma_1 - \Phi_1) + O(\Delta t) \\ &= (C A + D C) \Gamma_1 + (C B + D^2) \gamma_1 - D_2 \Phi_1 + O(\Delta t) \\ &= C d\gamma_1 \cdot \Gamma_1 + D d(\gamma_1 - \Phi_1) \cdot \Gamma_1 - D_2 \Phi_1 + O(\Delta t) \\ &= C d\gamma_1 \cdot \Gamma_1 + D d\gamma_1 \cdot \Gamma_1 - D d\Phi_1 \cdot \Gamma_1 - D_2 \Phi_1 + O(\Delta t) \end{aligned}$$

and

$$(67) \quad C_3 W + D_3 Y^* = \partial^2(\gamma_1 - \Phi_1) \cdot \Gamma_1 - D d\Phi_1 \cdot \Gamma_1 - D_2 \Phi_1 + O(\Delta t)$$

Then due to (61), (62), (63), (64), (65), (66) and (67), we have

$$\begin{aligned} S(Y - \Phi(W)) &= -\Delta t (C W + D Y^* + \partial_t Y) + \frac{1}{2} \Delta t^2 (C_2 W + D_2 Y^* - \partial_t^2 Y) \\ &\quad - \frac{1}{6} \Delta t^3 (C_3 W + D_3 Y^* + \partial_t^3 Y) + O(\Delta t^4) \\ &= -\Delta t (\gamma_1 - \Phi_1 + \Delta t D (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 D (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2) \\ &\quad - \Delta t [-d\Phi \cdot \Gamma_1 - \Delta t (d\Phi \cdot \Gamma_2 + (\Sigma + \frac{1}{2} \mathbf{I}) d\Phi_1 \cdot \Gamma_1) \\ &\quad \quad - \Delta t^2 (d\Phi \cdot \Gamma_3 + (\Sigma + \frac{1}{2} \mathbf{I}) d\Phi_1 \cdot \Gamma_2 + (\Sigma + \frac{1}{2} \mathbf{I}) d\Phi_2 \cdot \Gamma_1)] \\ &\quad + \frac{1}{2} \Delta t^2 (d(\gamma_1 - \Phi_1) \cdot \Gamma_1 - D \Phi_1 + \Delta t D_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1) \\ &\quad - \frac{1}{2} \Delta t^2 (d\gamma_1 \cdot \Gamma_1 + \Delta t [d\gamma_1 \cdot \Gamma_2 + d\gamma_2 \cdot \Gamma_1 + (\Sigma + \frac{1}{2} \mathbf{I}) \partial^2 \Phi_1 \cdot \Gamma_1]) \\ &\quad - \frac{1}{6} \Delta t^3 (\partial^2(\gamma_1 - \Phi_1) \cdot \Gamma_1 - D d\Phi_1 \cdot \Gamma_1 - D_2 \Phi_1) - \frac{1}{6} \Delta t^3 (-\partial^2 \gamma_1 \cdot \Gamma_1) + O(\Delta t^4) \\ &= \Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 [-D (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + d\Phi \cdot \Gamma_3 + (\Sigma + \frac{1}{2} \mathbf{I}) d\Phi_1 \cdot \Gamma_2 + (\Sigma + \frac{1}{2} \mathbf{I}) d\Phi_2 \cdot \Gamma_1 \\ &\quad + \frac{1}{2} D_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 - \frac{1}{2} d\gamma_1 \cdot \Gamma_2 - \frac{1}{2} d\gamma_2 \cdot \Gamma_1 - \frac{1}{2} (\Sigma + \frac{1}{2} \mathbf{I}) \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{6} \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{6} D d\Phi_1 \cdot \Gamma_1 \\ &\quad + \frac{1}{6} D_2 \Phi_1] + O(\Delta t^4) \\ &= \Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 [-D \Sigma \Phi_2 + \frac{1}{2} D (\Sigma d\Phi_1 \cdot \Gamma_1 + \gamma_2 - D \Sigma \Phi_1) + d\Phi \cdot \Gamma_3 + \Sigma d\Phi_1 \cdot \Gamma_2 \\ &\quad + \frac{1}{2} d\Phi_1 \cdot \Gamma_2 + \Sigma d\Phi_2 \cdot \Gamma_1 + \frac{1}{2} (\Sigma \partial^2 \Phi_1 \cdot \Gamma_1 + d\gamma_2 \cdot \Gamma_1 - D \Sigma d\Phi_1 \cdot \Gamma_1) + \frac{1}{2} (C B + D^2) \Sigma \Phi_1 \\ &\quad - \frac{1}{4} D_2 \Phi_1 - \frac{1}{2} d\gamma_1 \cdot \Gamma_2 - \frac{1}{2} d\gamma_2 \cdot \Gamma_1 - \frac{1}{2} \Sigma \partial^2 \Phi_1 \cdot \Gamma_1 - \frac{1}{12} \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{6} D d\Phi_1 \cdot \Gamma_1 + \frac{1}{6} D_2 \Phi_1] + O(\Delta t^4) \\ &= \Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 [d\Phi \cdot \Gamma_3 - D \Sigma \Phi_2 + \frac{1}{2} D \gamma_2 + \Sigma d\Phi_1 \cdot \Gamma_2 + \frac{1}{2} d\Phi_1 \cdot \Gamma_2 + \Sigma d\Phi_2 \cdot \Gamma_1 \\ &\quad + \frac{1}{2} C B \Sigma \Phi_1 - \frac{1}{12} D_2 \Phi_1 - \frac{1}{2} d\gamma_1 \cdot \Gamma_2 - \frac{1}{12} \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{6} D d\Phi_1 \cdot \Gamma_1] + O(\Delta t^4) \\ &= \Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 [d\Phi \cdot \Gamma_3 - D \Sigma \Phi_2 + \frac{1}{2} D \gamma_2 + \Sigma d\Phi_1 \cdot \Gamma_2 + \frac{1}{2} (-C \Gamma_2 - D \gamma_2 + d\gamma_1 \cdot \Gamma_2) \\ &\quad + \Sigma d\Phi_2 \cdot \Gamma_1 + \frac{1}{2} C B \Sigma \Phi_1 - \frac{1}{12} D_2 \Phi_1 - \frac{1}{2} d\gamma_1 \cdot \Gamma_2 - \frac{1}{12} \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{6} D d\Phi_1 \cdot \Gamma_1] + O(\Delta t^4) \\ &= \Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 [d\Phi \cdot \Gamma_3 - D \Sigma \Phi_2 + \Sigma d\Phi_1 \cdot \Gamma_2 + \Sigma d\Phi_2 \cdot \Gamma_1 - \frac{1}{12} D_2 \Phi_1 - \frac{1}{12} \partial^2 \Phi_1 \cdot \Gamma_1 \\ &\quad + \frac{1}{6} D d\Phi_1 \cdot \Gamma_1] + O(\Delta t^4). \end{aligned}$$

The relations (57) and (58) are established.

- Fourth order partial differential equations

We consider now the Taylor expansion of the relation (13) at fourth order:

$$\begin{aligned} m + \Delta t \partial_t m + \frac{1}{2} \Delta t^2 \partial_t^2 m + \frac{1}{6} \Delta t^3 \partial_t^3 m + \frac{1}{24} \Delta t^4 \partial_t^4 m + O(\Delta t^5) \\ = m^* - \Delta t \Lambda m^* + \frac{1}{2} \Delta t^2 \Lambda^2 m^* - \frac{1}{6} \Delta t^3 \Lambda^3 m^* + \frac{1}{24} \Delta t^4 \Lambda^4 m^* + O(\Delta t^5). \end{aligned}$$

For the first components (conserved moments):

$$\begin{aligned} W + \Delta t \partial_t W + \frac{1}{2} \Delta t^2 \partial_t^2 W + \frac{1}{6} \Delta t^3 \partial_t^3 W + \frac{1}{24} \Delta t^4 \partial_t^4 W + O(\Delta t^5) = W - \Delta t (A W + B Y^*) \\ + \frac{1}{2} \Delta t^2 (A_2 W + B_2 Y^*) - \frac{1}{6} \Delta t^3 (A_3 W + B_3 Y^*) + \frac{1}{24} \Delta t^4 (A_4 W + B_4 Y^*) + O(\Delta t^5). \end{aligned}$$

We simplify the constant term W and divide by Δt . We deduce

$$(68) \quad \begin{cases} \partial_t W = -(A W + B Y^*) + \frac{1}{2} \Delta t (A_2 W + B_2 Y^* - \partial_t^2 W) \\ \quad - \frac{1}{6} \Delta t^2 (A_3 W + B_3 Y^* + \partial_t^3 W) + \frac{1}{24} \Delta t^3 (A_4 W + B_4 Y^* - \partial_t^4 W) + O(\Delta t^4). \end{cases}$$

We explicit the partial derivatives $\partial_t^2 W$, $\partial_t^3 W$ and $\partial_t^4 W$ at orders two, one and zero respectively. We start with the relation

$$\partial_t W + \Gamma_1 + \Delta t \Gamma_2 + \Delta t^2 \Gamma_3 = O(\Delta t^3)$$

where Γ_1 , Γ_2 and Γ_3 have been evaluated previously. We have

$$\begin{aligned} \partial_t^2 W &= \partial_t (-\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 + O(\Delta t^3)) \\ &= d(-\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 + O(\Delta t^3)).(\partial_t W) \\ &= d(-\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 + O(\Delta t^2)).(-\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3) + O(\Delta t^3) \end{aligned}$$

and

$$(69) \quad \partial_t^2 W = d\Gamma_1.\Gamma_1 + \Delta t (d\Gamma_1.\Gamma_2 + d\Gamma_2.\Gamma_1) + \Delta t^2 (d\Gamma_1.\Gamma_3 + d\Gamma_2.\Gamma_2 + d\Gamma_3.\Gamma_1) + O(\Delta t^2).$$

Then

$$\begin{aligned} \partial_t^3 W &= \partial_t(\partial_t^2 W) \\ &= \partial_t(d\Gamma_1.\Gamma_1 + \Delta t (d\Gamma_1.\Gamma_2 + d\Gamma_2.\Gamma_1)) + O(\Delta t^2) \\ &= d(d\Gamma_1.\Gamma_1 + \Delta t (d\Gamma_1.\Gamma_2 + d\Gamma_2.\Gamma_1)).\partial_t W + O(\Delta t^2) \\ &= d(d\Gamma_1.\Gamma_1 + \Delta t (d\Gamma_1.\Gamma_2 + d\Gamma_2.\Gamma_1)).(-\Gamma_1 - \Delta t \Gamma_2) + O(\Delta t^2) \\ &= -d(d\Gamma_1.\Gamma_1).\Gamma_1 - \Delta t [d(A\Gamma_2 + B\gamma_2 + B\Sigma d\Phi_1).\Gamma_1 + d(A\Gamma_1 + B\gamma_1).\Gamma_2] + O(\Delta t^2) \\ &= -\partial^2 \Gamma_1.\Gamma_1 - \Delta t [A d\Gamma_2.\Gamma_1 + B d\gamma_2.\Gamma_1 + B\Sigma \partial^2 \Phi_1.\Gamma_1 + A d\Gamma_1.\Gamma_2 + B d\gamma_1.\Gamma_2] + O(\Delta t^2) \end{aligned}$$

and we have at first order for this third order derivative

$$(70) \quad \begin{cases} \partial_t^3 W = -\partial^2 \Gamma_1.\Gamma_1 - \Delta t [A (d\Gamma_2.\Gamma_1 + d\Gamma_1.\Gamma_2) \\ \quad + B (d\gamma_2.\Gamma_1 + d\gamma_1.\Gamma_2 + \Sigma \partial^2 \Phi_1.\Gamma_1)] + O(\Delta t^2). \end{cases}$$

Last but not least, we have

$$\begin{aligned} \partial_t^4 W &= \partial_t(-\partial^2 \Gamma_1.\Gamma_1 + O(\Delta t)) \\ &= -\partial_t(A d\Gamma_1.\Gamma_1 + B d\gamma_1.\Gamma_1) + O(\Delta t) \\ &= d(A d\Gamma_1.\Gamma_1 + B d\gamma_1.\Gamma_1).(\Gamma_1 + O(\Delta t)) \end{aligned}$$

and finally

$$(71) \quad \partial_t^4 W = A \partial^2 \Gamma_1.\Gamma_1 + B \partial^2 \gamma_1.\Gamma_1 + O(\Delta t).$$

For the determination of the coefficient Γ_4 , we precise the expansions of the quantities $A_j W + B_j Y^*$ for $j = 1$ to $j = 4$. We use the previous evaluations done in the proof of the previous propositions:

$$\begin{aligned}
 A W + B Y^* &= A W + B [\Phi(W) + (\Sigma - \frac{1}{2} \mathbf{I}) (\Delta t \Phi_1 + \Delta t^2 \Phi_2 + \Delta t^3 \Phi_3)] + O(\Delta t^4) \\
 &= A W + B \Phi + \Delta t B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + \Delta t^3 B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_3 + O(\Delta t^4) \\
 A_2 W + B_2 Y^* &= A_2 W + B_2 [\Phi(W) + (\Sigma - \frac{1}{2} \mathbf{I}) (\Delta t \Phi_1 + \Delta t^2 \Phi_2)] + O(\Delta t^3) \\
 &= (A^2 + B C) W + (A B + B D) \Phi + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + O(\Delta t^3) \\
 &= d\Gamma_1. \Gamma_1 - B \Phi_1 + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + O(\Delta t^3) \\
 A_3 W + B_3 Y^* &= A_3 W + B_3 [\Phi(W) + \Delta t (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1] + O(\Delta t^2) \\
 &= (A_2 A + B_2 C) W + (A_2 B + B_2 D) \Phi + \Delta t B_3 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + O(\Delta t^2) \\
 &= \partial^2 \Gamma_1. \Gamma_1 - B d\Phi_1. \Gamma_1 - B_2 \Phi_1 + \Delta t B_3 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + O(\Delta t^2) \\
 A_4 W + B_4 Y^* &= A_4 W + B_4 \Phi(W) + O(\Delta t) \\
 &= (A_3 A + B_3 C) W + (A_3 B + B_3 D) \Phi + O(\Delta t) \\
 &= A_3 \Gamma_1 + B_3 (\gamma_1 - \Phi_1) + O(\Delta t) \\
 &= (A_2 A + B_2 C) \Gamma_1 + (A_2 B + B_2 D) \gamma_1 - B_3 \Phi_1 + O(\Delta t) \\
 &= A_2 d\Gamma_1. \Gamma_1 + B_2 d(\gamma_1 - \Phi_1). \Gamma_1 - B_3 \Phi_1 + O(\Delta t) \\
 &= (A^2 + B C) d\Gamma_1. \Gamma_1 + (A B + B D) d\gamma_1. \Gamma_1 - B_2 d\Phi_1. \Gamma_1 - B_3 \Phi_1 + O(\Delta t) \\
 &= A \partial^2 \Gamma_1. \Gamma_1 + B \partial^2 (\gamma_1 - \Phi_1). \Gamma_1 - B_2 d\Phi_1. \Gamma_1 - B_3 \Phi_1 + O(\Delta t) \\
 &= A \partial^2 \Gamma_1. \Gamma_1 + B \partial^2 \gamma_1. \Gamma_1 - B \partial^2 \Phi_1. \Gamma_1 - B_2 d\Phi_1. \Gamma_1 - B_3 \Phi_1 + O(\Delta t).
 \end{aligned}$$

We deduce now from (68), (69), (70), (71) and the previous expressions:

$$\begin{aligned}
 \partial_t W &= -(A W + B Y^*) + \frac{1}{2} \Delta t (A_2 W + B_2 Y^* - \partial_t^2 W) - \frac{1}{6} \Delta t^2 (A_3 W + B_3 Y^* + \partial_t^3 W) \\
 &\quad + \frac{1}{24} \Delta t^3 (A_4 W + B_4 Y^* - \partial_t^4 W) + O(\Delta t^4) \\
 &= -(A W + B \Phi + \Delta t B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 + \Delta t^3 B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_3) \\
 &\quad + \frac{1}{2} \Delta t [d\Gamma_1. \Gamma_1 - B \Phi_1 + \Delta t B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + \Delta t^2 B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 \\
 &\quad - (d\Gamma_1. \Gamma_1 + \Delta t (d\Gamma_1. \Gamma_2 + d\Gamma_2. \Gamma_1) + \Delta t^2 (d\Gamma_1. \Gamma_3 + d\Gamma_2. \Gamma_2 + d\Gamma_3. \Gamma_1))] \\
 &\quad - \frac{1}{6} \Delta t^2 [\partial^2 \Gamma_1. \Gamma_1 - B d\Phi_1. \Gamma_1 - B_2 \Phi_1 + \Delta t B_3 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 \\
 &\quad - \partial^2 \Gamma_1. \Gamma_1 - \Delta t (A (d\Gamma_2. \Gamma_1 + d\Gamma_1. \Gamma_2) + B (d\gamma_2. \Gamma_1 + d\gamma_1. \Gamma_2 + \Sigma \partial^2 \Phi_1. \Gamma_1))] \\
 &\quad + \frac{1}{24} \Delta t^3 [A \partial^2 \Gamma_1. \Gamma_1 + B \partial^2 \gamma_1. \Gamma_1 - B \partial^2 \Phi_1. \Gamma_1 - B_2 d\Phi_1. \Gamma_1 - B_3 \Phi_1 \\
 &\quad - (A \partial^2 \Gamma_1. \Gamma_1 + B \partial^2 \gamma_1. \Gamma_1)] + O(\Delta t^4) \\
 &= -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 + \Delta t^3 [-B (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_3 + \frac{1}{2} B_2 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_2 \\
 &\quad - \frac{1}{2} (d\Gamma_1. \Gamma_3 + d\Gamma_2. \Gamma_2 + d\Gamma_3. \Gamma_1) + \frac{1}{6} (-B_3 (\Sigma - \frac{1}{2} \mathbf{I}) \Phi_1 + A (d\Gamma_2. \Gamma_1 + d\Gamma_1. \Gamma_2) \\
 &\quad + B (d\gamma_2. \Gamma_1 + d\gamma_1. \Gamma_2 + \Sigma \partial^2 \Phi_1. \Gamma_1)) + \frac{1}{24} (A \partial^2 \Gamma_1. \Gamma_1 + B \partial^2 \gamma_1. \Gamma_1 \\
 &\quad - B \partial^2 \Phi_1. \Gamma_1 - B_2 d\Phi_1. \Gamma_1 - B_3 \Phi_1 - A \partial^2 \Gamma_1. \Gamma_1 - B \partial^2 \gamma_1. \Gamma_1)] + O(\Delta t^4) \\
 &= -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 - \Delta t^3 [B \Sigma \Phi_3 - \frac{1}{2} B (\gamma_3 + \Sigma d\Phi_1. \Gamma_2 + \Sigma d\Phi_2. \Gamma_1 - D \Sigma \Phi_2 \\
 &\quad + \frac{1}{6} D d\Phi_1. \Gamma_1 - \frac{1}{12} D_2 \Phi_1 - \frac{1}{12} \partial^2 \Phi_1. \Gamma_1) - \frac{1}{2} (A B + B D) \Sigma \Phi_2 + \frac{1}{4} B_2 \Phi_2 \\
 &\quad + \frac{1}{2} (A \Gamma_3 + B \gamma_3 + B \Sigma d\Phi_1. \Gamma_1 + d\Gamma_3. \Gamma_1) + \frac{1}{6} B_3 \Sigma \Phi_1 - \frac{1}{12} B_3 \Phi_1 - \frac{1}{6} A B \Sigma d\Phi_1. \Gamma_1
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{1}{6} A (A \Gamma_2 + B \gamma_2) - \frac{1}{6} B (d\gamma_2 \cdot \Gamma_1 + d\gamma_1 \cdot \Gamma_2 + \Sigma \partial^2 \Phi_1 \cdot \Gamma_1) + \frac{1}{24} B \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{24} B_2 d\Phi_1 \cdot \Gamma_1 \\
 & + \frac{1}{24} B_3 \Phi_1] + O(\Delta t^4) \\
 = & -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 - \Delta t^3 [B \Sigma \Phi_3 - \frac{1}{2} B \Sigma d\Phi_2 \cdot \Gamma_1 - \frac{1}{12} B D d\Phi_1 \cdot \Gamma_1 + \frac{1}{24} B D_2 \Phi_1 \\
 & + \frac{1}{24} B \partial^2 \Phi_1 \cdot \Gamma_1 - \frac{1}{2} A B \Sigma \Phi_2 + \frac{1}{4} B_2 \Phi_2 + \frac{1}{2} A (B \Sigma \Phi_2 - \frac{1}{6} B d\Phi_1 \cdot \Gamma_1 + \frac{1}{12} B_2 \Phi_1) \\
 & + \frac{1}{2} (B \Sigma d\Phi_2 \cdot \Gamma_1 - \frac{1}{6} B \partial^2 \Phi_1 \cdot \Gamma_1 + \frac{1}{12} B_2 d\Phi_1 \cdot \Gamma_1) + \frac{1}{6} B_3 \Sigma \Phi_1 - \frac{1}{24} B_3 \Phi_1 - \frac{1}{6} A B \Sigma d\Phi_1 \cdot \Gamma_1 \\
 & - \frac{1}{6} A^2 \Gamma_2 - \frac{1}{6} A B \gamma_2 - \frac{1}{6} B (d\gamma_2 \cdot \Gamma_1 + d\gamma_1 \cdot \Gamma_2 + \Sigma \partial^2 \Phi_1 \cdot \Gamma_1) + \frac{1}{24} B \partial^2 \Phi_1 \cdot \Gamma_1 \\
 & + \frac{1}{24} B_2 d\Phi_1 \cdot \Gamma_1] + O(\Delta t^4) \\
 = & -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 - \Delta t^3 [B \Sigma \Phi_3 - \frac{1}{12} B_2 d\Phi_1 \cdot \Gamma_1 + \frac{1}{24} B D_2 \Phi_1 + \frac{1}{4} B_2 \Phi_2 + \frac{1}{24} A B_2 \Phi_1 \\
 & + \frac{1}{6} B_3 \Sigma \Phi_1 - \frac{1}{24} B_3 \Phi_1 - \frac{1}{6} A B \Sigma d\Phi_1 \cdot \Gamma_1 - \frac{1}{6} A^2 B \Sigma \Phi_1 - \frac{1}{6} A B \gamma_2 \\
 & - \frac{1}{6} B (d\gamma_2 \cdot \Gamma_1 + d\gamma_1 \cdot \Gamma_2 + \Sigma \partial^2 \Phi_1 \cdot \Gamma_1) + \frac{1}{12} B_2 d\Phi_1 \cdot \Gamma_1] + O(\Delta t^4) \\
 = & -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 - \Delta t^3 [B \Sigma \Phi_3 + \frac{1}{4} B_2 \Phi_2 + \frac{1}{6} B_3 \Sigma \Phi_1 - \frac{1}{6} A B \Sigma d\Phi_1 \cdot \Gamma_1 - \frac{1}{6} A^2 B \Sigma \Phi_1 \\
 & - \frac{1}{6} A B (\Phi_2 - \Sigma d\Phi_1 \cdot \Gamma_1 + D \Sigma \Phi_1) - \frac{1}{6} B (d\gamma_2 \cdot \Gamma_1 + d\gamma_1 \cdot \Gamma_2 + \Sigma \partial^2 \Phi_1 \cdot \Gamma_1)] + O(\Delta t^4) \\
 & \text{because } A B_2 + B D_2 = B_3 \\
 = & -\Gamma_1 - \Delta t \Gamma_2 - \Delta t^2 \Gamma_3 - \Delta t^3 [B \Sigma \Phi_3 + \frac{1}{4} B_2 \Phi_2 + \frac{1}{6} B D_2 \Sigma \Phi_1 - \frac{1}{6} A B \Phi_2 \\
 & - \frac{1}{6} B (d\gamma_2 \cdot \Gamma_1 + d\gamma_1 \cdot \Gamma_2 + \Sigma \partial^2 \Phi_1 \cdot \Gamma_1)] + O(\Delta t^4)
 \end{aligned}$$

because $B_3 - A(A B + B D) = B D_2$. The relations (59) and (60) are established and the proposition is proven. \square

6) Revisiting the ‘‘Berlin algorithm’’ in the linear case

In [3], we have presented the Berlin explicit algorithm in order to determine, with the help of formal calculus, the equivalent partial differential equations if a linear lattice Boltzmann scheme. We do not enter here into the details of our previous contribution because the linearized version of the present algorithm is much more simple.

Proposition 9. Linearized general expansion at fourth order

We suppose that the equilibrium value of the nonconserved moments is a linear function:

$$\Phi(W) = E W$$

with a given fixed $(q - N) \times N$ rectangle matrix E . Then the nonequilibrium moments can be expanded as

$$Y = [E + S^{-1}(\Delta t \beta_1 + \Delta t^2 \beta_2 + \Delta t^3 \beta_3)] W + O(\Delta t^4).$$

The $(q - N) \times N$ matrices β_j are linear operators of order j . The equivalent partial equivalent equations are linear and can be written as

$$\partial_t W + [\alpha_1 + \Delta t \alpha_2 + \Delta t^2 \alpha_3 + \Delta t^3 \alpha_4] W + O(\Delta t^4),$$

and α_j is a $N \times N$ differential matrix of order j . In other terms, $\Phi_j(W) = \beta_j W$ and $\Gamma_j(W) = \alpha_j W$ are linear functions of the conserved moments. The coefficient matrices α_j

and β_j are computed according to a linearized version of (20):

$$(72) \quad \begin{cases} \alpha_1 = A + B E \\ \beta_1 = E \alpha_1 - C - D E \\ \alpha_2 = B \Sigma \beta_1 \\ \beta_2 = \Sigma \beta_1 \alpha_1 + E \alpha_2 - D \Sigma \beta_1 \\ \alpha_3 = B \Sigma \beta_2 + \frac{1}{12} B_2 \beta_1 - \frac{1}{6} B \beta_1 \alpha_1 \\ \beta_3 = \Sigma \beta_1 \alpha_2 + E \alpha_3 - D \Sigma \beta_2 + \Sigma \beta_2 \alpha_1 + \frac{1}{6} D \beta_1 \alpha_1 - \frac{1}{12} D_2 \beta_1 - \frac{1}{12} \beta_1 \alpha_1^2 \\ \alpha_4 = B \Sigma \beta_3 + \frac{1}{4} B_2 \beta_2 + \frac{1}{6} B D_2 \Sigma \beta_1 - \frac{1}{6} A B \beta_2 \\ \quad - \frac{1}{6} B E \alpha_1 \alpha_2 - \frac{1}{6} B E \alpha_2 \alpha_1 - \frac{1}{6} B \Sigma \beta_1 \alpha_1^2. \end{cases}$$

- Proof of Proposition 9.

First observe that $d\Phi.\xi = E\xi$ for any test vector ξ . Due to the relation (25), we have

$\Gamma_1 = A W + B \Phi(W) = A W + B E W = (A + B E) W$ and $\alpha_1 = A + B E$. Due to (28), we have moreover

$$\begin{aligned} \Phi_1 &= d\Phi(W).\Gamma_1(W) - (C W + D \Phi(W)) \\ &= E \alpha_1 W - C W - D E W \\ &= (E \alpha_1 - C - D E) W \end{aligned}$$

and the second relation of (72) is established. Due to (30),

$$\begin{aligned} \Gamma_2(W) &= B \Sigma \Phi_1(W) \\ &= B \Sigma \beta_1 W. \end{aligned}$$

Then $\alpha_2 = B \Sigma \beta_1$ and the third line of (72) is proven. We have now from (40),

$$\begin{aligned} \Phi_2(W) &= \Sigma d\Phi_1(W).\Gamma_1(W) + d\Phi(W).\Gamma_2(W) - D \Sigma \Phi_1(W) \\ &= \Sigma \beta_1 \alpha_1 W + E \alpha_2 W - D \Sigma \beta_1 W \\ &= (\Sigma \beta_1 \alpha_1 + E \alpha_2 - D \Sigma \beta_1) W \end{aligned}$$

and $\beta_2 = \Sigma \beta_1 \alpha_1 + E \alpha_2 - D \Sigma \beta_1$ as suggested in the fourth line of (72). From the relation (42), we have now

$$\begin{aligned} \Gamma_3(W) &= B \Sigma \Phi_2(W) + \frac{1}{12} B_2 \Phi_1(W) - \frac{1}{6} B d\Phi_1(W).\Gamma_1(W) \\ &= B \Sigma \beta_2 W + \frac{1}{12} B_2 \beta_1 W - \frac{1}{6} B \beta_1 \alpha_1 W \\ &= (B \Sigma \beta_2 + \frac{1}{12} B_2 \beta_1 - \frac{1}{6} B \beta_1 \alpha_1) W. \end{aligned}$$

Then $\alpha_3 = B \Sigma \beta_2 + \frac{1}{12} B_2 \beta_1 - \frac{1}{6} B \beta_1 \alpha_1$ as proposed in the fifth line of (72). Observe now that due to (17), we have

$$\begin{aligned} \partial^2 \Phi_1.\Gamma_1(W) &= d^2 \Phi_1(W).(\Gamma_1, \Gamma_1) + d\Phi_1(W).d\Gamma_1(W).\Gamma_1 \\ &= d\Phi_1(W).d\Gamma_1(W).\Gamma_1 && \text{because } \Phi_1 \text{ is linear} \\ &= \beta_1 \alpha_1^2 W. \end{aligned}$$

Then due to (58), we have in this linear case,

$$\begin{aligned} \Phi_3(W) &= d\Phi(W).\Gamma_3(W) + \Sigma d\Phi_1(W).\Gamma_2(W) + \Sigma d\Phi_2(W).\Gamma_1(W) - D \Sigma \Phi_2(W) \\ &\quad + \frac{1}{6} D d\Phi_1(W).\Gamma_1(W) - \frac{1}{12} D_2 \Phi_1(W) - \frac{1}{12} \partial^2 \Phi_1(W).\Gamma_1(W) \\ &= E \alpha_3 W + \Sigma \beta_1 \alpha_2 W + \Sigma \beta_2 \alpha_1 W - D \Sigma \beta_2 W + \frac{1}{6} D \beta_1 \alpha_1 W \end{aligned}$$

$$-\frac{1}{12} D_2 \beta_1 W - \frac{1}{12} \beta_1 \alpha_1^2 W$$

$$= (E \alpha_3 + \Sigma \beta_1 \alpha_2 + \Sigma \beta_2 \alpha_1 - D \Sigma \beta_2 + \frac{1}{6} D \beta_1 \alpha_1 - \frac{1}{12} D_2 \beta_1 - \frac{1}{12} \beta_1 \alpha_1^2) W$$

and $\beta_3 = E \alpha_3 + \Sigma \beta_1 \alpha_2 + \Sigma \beta_2 \alpha_1 - D \Sigma \beta_2 + \frac{1}{6} D \beta_1 \alpha_1 - \frac{1}{12} D_2 \beta_1 - \frac{1}{12} \beta_1 \alpha_1^2$. We have finally, due to (60),

$$\begin{aligned} \Gamma_4(W) &= B \Sigma \Phi_3(W) + \frac{1}{4} B_2 \Phi_2(W) + \frac{1}{6} B D_2 \Sigma \Phi_1 - \frac{1}{6} A B \Phi_2(W) - \frac{1}{6} B d\gamma_1(W). \Gamma_2(W) \\ &\quad - \frac{1}{6} B d\gamma_2(W). \Gamma_1(W) - \frac{1}{6} B \Sigma \partial^2 \Phi_1(W). \Gamma_1(W) \\ &= B \Sigma \beta_3 W + \frac{1}{4} B_2 \beta_2 W + \frac{1}{6} B D_2 \Sigma \beta_1 W - \frac{1}{6} A B \beta_2 W - \frac{1}{6} B E \alpha_2 W \\ &\quad - \frac{1}{6} B E \alpha_1 W - \frac{1}{6} B \Sigma \beta_1 \alpha_1^2 W \\ &= (B \Sigma \beta_3 + \frac{1}{4} B_2 \beta_2 + \frac{1}{6} B D_2 \Sigma \beta_1 - \frac{1}{6} A B \beta_2 - \frac{1}{6} B E \alpha_2 - \frac{1}{6} B E \alpha_1 - \frac{1}{6} B \Sigma \beta_1 \alpha_1^2) W \end{aligned}$$

and the proposition is established. \square

7) Conclusion

In this paper, we have extended the Taylor expansion method of a multiple relaxation times lattice Boltzmann scheme up to fourth order accuracy. With this expansion, nonlinear partial differential equations for the conserved variables and various differential expressions for the nonconserved moments emerge naturally. This expansion has been validated with previous works on the subject.

Observe that the main result is implemented with this framework in the “pyLBM” software [24]. The next step is the introduction of source terms, in the spirit proposed in [21], and other geometries like triangles, in a way suggested in [19]. The adaptation of the Taylor expansion method to other variants of lattice Boltzmann schemes as recentered schemes [22, 15], regularized lattice Boltzmann [37, 41, 46] or entropic lattice Boltzmann schemes [34] are also into study. After a first step in [40], the link between the single scale Taylor expansion and the multiple scale Chapman-Enskog is also a project for the near future.

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