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General third order Chapman-Enskog expansion of lattice Boltzmann schemes

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08 May 2019 *

The lattice Boltzmann scheme in his actual form has been developed with the contributions of Lallemand, Succi, d'Humières, Luo [HSB91, QHL92, DDH92, LL00] and many others. In order to derive the equivalent partial differential equations, a classical of the Chapman Enskog expansion is popular in the lattice Boltzmann community (see *e.g.* [LL00]) A main drawback of this approach is the fact that multiscale expansions are used without a clear mathematical signification of the various variables and functions. Independently of this framework, we have proposed in [FD07, FD08] the Taylor expansion method to obtain formally equivalent partial differential equations. The infinitesimal variable is simply the time step (proportional to the space step with the acoustic scaling). This approach has been experimentally validated in various contributions [DL10, DL11]. A third order extension for fluid flow has been proposed in [FD09] and an efficient implementation up to fourth order accuracy is presented in [ADGL14].

In this contribution, we consider a regular 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 $\Delta t > 0$.

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A very general lattice Boltzmann scheme with q discrete velocities of the form

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

The distribution f^* after relaxation is defined with moments m such that

$$m_k = \sum_j M_{kj} f_j.$$

The d'Humières matrix [DDH92] M is invertible and we decompose the moments in the following way:

$$m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}.$$

The conserved variables W are not modified after relaxation: $W^* = W$. The microscopic variables Y are changed in a nonlinear way by the relaxation process:

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

The matrix S is invertible, and often chosen as diagonal. It is supposed to be fixed in the asymptotic process presented hereafter. The equilibrium values $Y^{\text{eq}} = \Phi(W)$ are given smooth functions of the conserved variables. When Y^* is evaluated, we have simply

$$f^* = M^{-1} m^*.$$

We introduce the momentum-velocity operator matrix Λ defined by the relation

$$\Lambda_{k\ell} = \sum_{j, \alpha} M_{kj} v_j^\alpha (M^{-1})_{j\ell} \partial_\alpha, \quad 0 \leq k, \ell < q.$$

It is nothing else than the advection operator seen in the space of moments. Then we have an exponential form of the discrete iteration of the lattice Boltzmann scheme:

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

With this general framework, we follow in this contribution the Chapman-Enskog formalism proposed by Chen–Doolen [CD98] and Qian–Zhou [QZ00]. We suppose that $\Delta t \equiv \varepsilon$ is an infinitesimal parameter and we expand the nonconserved moments as differential nonlinear function of the conserved variables:

$$Y = \Phi(W) + \varepsilon S^{-1}(\Psi_1(W) + \varepsilon^2 \Psi_2(W)) + O(\varepsilon^3).$$

Then we suppose that a multi-scale approach is present for the time dynamics:

$$\partial_t = \partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3} + O(\varepsilon^3).$$

Then we prove that the conserved quantities W follow the following multi-time dynamics:

$$\partial_{t_1} W + \Gamma_1(W) = 0, \quad \partial_{t_2} W + \Gamma_2(W) = 0, \quad \partial_{t_3} W + \Gamma_3(W) = 0.$$

The differential operators $\Gamma_1(W)$, $\Psi_1(W)$, $\Gamma_2(W)$, $\Psi_2(W)$ and $\Gamma_3(W)$ of this expansion are recursively determined as a function of the data v_j , M , $\Phi(W)$ and S . We compare our result with the particular third order expansion proposed in [FD19] and the linear approach presented in [ADGL14]. The previous operators $\Gamma_j(W)$ and $\Psi_i(W)$ are of order j and are exactly the ones derived in our fourth order expansion of lattice Boltzmann schemes with the Taylor expansion method [FD19].

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ICMMES 2019 conference
Edinburgh University
23 July 2019

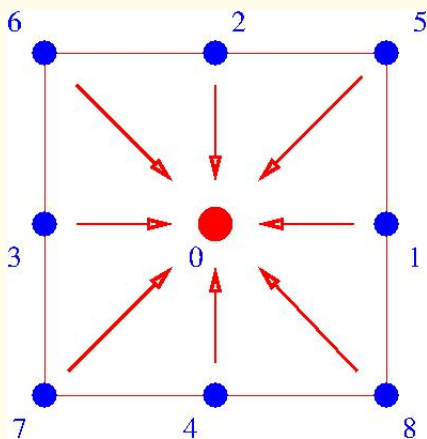
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Lattice Boltzmann scheme

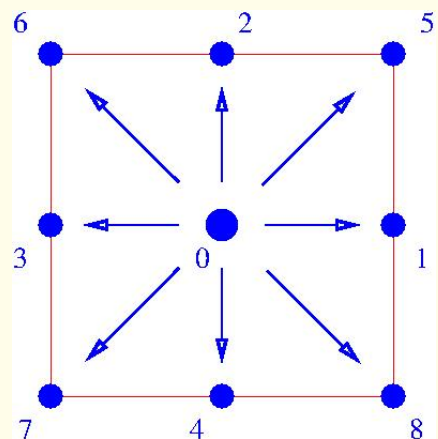
2



advection



collision



advection

- Multiple Relaxation Times Lattice Boltzmann scheme
- Compact expression
- A general expansion result at third order
- Proof for Chapman-Enskog
- Proof for Taylor expansion method
- Link with the previous expansion at third-order
(DCDS-A, 2009)
- Survey

Multiple Relaxation Times Lattice Boltzmann scheme

Two steps for one time iteration

(i) **Nonlinear relaxation**

the particle distribution f is modified **locally**
into a new distribution f^*

(ii) **Linear advection**

method of characteristics when it is **exact** !

Compact description of the lattice Boltzmann scheme:

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

d'Humières matrix M for moments: $m_k \equiv M_{kl} f_l$, $m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}$

Conserved variables W ; after relaxation, $W^* = W$

Non-Conserved moments Y

equilibrium value: $Y^{\text{eq}} = \Phi(W)$

after relaxation: $Y^* = Y + S(Y^{\text{eq}} - Y)$, $m^* = \begin{pmatrix} W \\ Y^* \end{pmatrix}$

Important hypotheses

5

the discrete function $f(x, t)$ for
 x vertex of the lattice
 t discrete time

is supposed to be the **restriction of a very regular function**
denoted in the same way $f(x, t, \Delta t, s_k, \dots)$

but defined for

x a point of the continuous space \mathbb{R}^d

t continuous time

Δt the time step

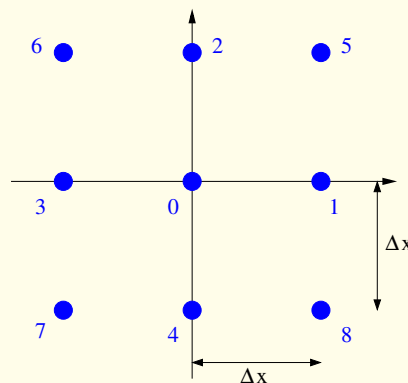
s_k the relaxation parameters

The **numerical velocity** $\lambda \equiv \frac{\Delta x}{\Delta t}$ is fixed

The **relaxation parameters** s_k are fixed

Example of D2Q9

6



$$\lambda = \frac{\Delta x}{\Delta t}$$

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{bmatrix} \begin{matrix} \rho \\ J_x \\ J_y \\ \varepsilon \\ XX \\ XY \\ q_x \\ q_y \\ h \end{matrix}$$

Advection operator in the basis of moments

7

Momentum-velocity operator matrix $\Lambda \equiv M \text{diag}\left(\sum_{\alpha} v^{\alpha} \partial_{\alpha}\right) M^{-1}$
 $1 \leq \alpha \leq d = \text{space dimension}$

Block decomposition $\Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}$

Example of Λ operator matrix for the thermal D2Q9 scheme

0	∂_x	∂_y	0	0	0	0	0	0	0
$\frac{2\lambda^2}{3} \partial_x$	0	0	$\frac{1}{6} \partial_x$	$\frac{1}{2} \partial_x$	∂_y	0	0	0	0
$\frac{2\lambda^2}{3} \partial_y$	0	0	$\frac{1}{6} \partial_y$	$-\frac{1}{2} \partial_y$	∂_x	0	0	0	0
0	$\lambda^2 \partial_x$	$\lambda^2 \partial_y$	0	0	0	∂_x	∂_y	0	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
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	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	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	0	$\lambda^2 \partial_x$	$\lambda^2 \partial_y$	0	0

Compact expression of the lattice Boltzmann scheme

8

Proposition $m(x, t + \varepsilon) = \exp(-\varepsilon \Lambda) m^*(x, t)$

$$\begin{aligned}
 m_k(x, t + \varepsilon) &= \sum_j M_{kj} f_j^*(x - v_j \varepsilon, t) \\
 &= \sum_{j\ell} M_{kj} (M^{-1})_{j\ell} m_{\ell}^*(x - v_j \varepsilon, t) \\
 &= \sum_{j\ell} M_{kj} (M^{-1})_{j\ell} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\varepsilon \sum_{\alpha} v_j^{\alpha} \partial_{\alpha}\right)^n m_{\ell}^*(x, t) \\
 &= \sum_{\ell} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_j M_{kj} \left(-\varepsilon \sum_{\alpha} v_j^{\alpha} \partial_{\alpha}\right)^n (M^{-1})_{j\ell} m_{\ell}^*(x, t) \\
 &= \sum_{\ell} \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(-\varepsilon \Lambda\right)_{k\ell}^n \right] m_{\ell}^*(x, t) \\
 &= \sum_{\ell} \exp(-\varepsilon \Lambda)_{k\ell} m_{\ell}^*(x, t) \\
 &= \left(\exp(-\varepsilon \Lambda) m^*(x, t) \right)_k
 \end{aligned}$$

Chapman-Enskog framework

9

Introduce a **small parameter** ε . For numerical schemes, $\varepsilon = \Delta t$

$$f = f^{\text{eq}} + \varepsilon f^1 + \varepsilon^2 f^2 + O(\varepsilon^3)$$

Chapman-Enskog hypothesis : the perturbation terms f^ℓ
are only function of the **equilibrium** $f = f^{\text{eq}}$

apply the d'Humières matrix:

$$M f = M f^{\text{eq}} + \varepsilon M f^1 + \varepsilon^2 M f^2 + O(\varepsilon^3)$$

take the first conserved component : $W = W + 0$

take the second nonconserved component :

$$Y = Y^{\text{eq}} + \varepsilon (M f^1)_Y + \varepsilon^2 (M f^2)_Y + O(\varepsilon^3)$$

The perturbation terms $\varepsilon^\ell (M f^\ell)_Y$ depend only
on the conserved moments W .

Then $Y = \Phi(W) + S^{-1} (\varepsilon \Psi_1(W) + \varepsilon^2 \Psi_2(W)) + O(\varepsilon^3)$

Suppose also a **multi-scale** approach for the **time dynamics**:

$$\partial_t = \partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3} + O(\varepsilon^3)$$

Chapman-Enskog expansion

10

The conserved quantities W follow a multi-time dynamics :

$$\partial_{t_1} W + \Gamma_1(W) = 0$$

$$\partial_{t_2} W + \Gamma_2(W) = 0$$

$$\partial_{t_3} W + \Gamma_3(W) = 0$$

The differential operators

$$\Gamma_1(W), \Psi_1(W), \Gamma_2(W), \Psi_2(W) \text{ and } \Gamma_3(W)$$

of this expansion are **recursively determined**

coefficients at first order

$$\Gamma_1 = A W + B \Phi(W)$$

coefficients at second order

$$\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))$$

$$\Gamma_2 = B \Sigma \Psi_1$$

Hénon matrix $\Sigma \equiv S^{-1} - \frac{1}{2} I$

coefficients at third order

$$\Psi_2 = \Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi(W) \cdot \Gamma_2 - D \Sigma \Psi_1$$

$$\Gamma_3 = B \Sigma \Psi_2 + \frac{1}{12} B_2 \Psi_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1$$

Taylor vs Chapman-Enskog expansion methods

11

Asymptotic hypothesis: emerging partial differential equations

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

Γ_j : vector obtained after j space derivations
of the conserved moments W
and the equilibrium vector $\Phi(W)$.

Non-Conserved moments:

$$Y = \Phi(W) + S^{-1} (\Delta t \Psi_1 + \Delta t^2 \Psi_2) O(\Delta t^2)$$

Φ_j analogous to Γ_j but not with the same dimension!

General nonlinear Taylor expansion method

12

Coefficients at first order

$$\Gamma_1 = A W + B \Phi(W)$$

Coefficients at second order

$$\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))$$

$$\Gamma_2 = B \Sigma \Psi_1 \quad \text{with } \Sigma \text{ the Hénon matrix: } \Sigma \equiv S^{-1} - \frac{1}{2} I$$

Coefficients at third order

$$\Psi_2 = d\Phi(W) \cdot \Gamma_2 + \Sigma d\Psi_1 \cdot \Gamma_1 - D \Sigma \Psi_1$$

$$\Gamma_3 = B \Sigma \Psi_2 + \frac{1}{6} B d\Psi_1 \cdot \Gamma_1 - \frac{1}{12} B_2 \Psi_1$$

We find the **same formulas** than with Chapman-Enskog:

the two expansions are equivalent!

Chapman-Enskog expansion : order zero

13

$$m(t + \varepsilon) = \exp(-\varepsilon \Lambda) m^*$$

$$m + O(\varepsilon) = m^* + O(\varepsilon)$$

$$\text{first component : } W + O(\varepsilon) = W^* + O(\varepsilon)$$

no more information because $W^* = W$

$$\text{second component : } Y + O(\varepsilon) = Y^* + O(\varepsilon)$$

$$\text{relaxation: } Y^* = Y + S(\Phi(W) - Y)$$

The matrix S is supposed fixed

$$\text{then } Y = \Phi(W) + O(\varepsilon)$$

$$\text{and } Y^* = \Phi(W) + O(\varepsilon)$$

Chapman-Enskog expansion : order one

14

$$m(t + \varepsilon) = \exp(-\varepsilon \Lambda) m^*$$

$$m + \varepsilon \partial_t m + O(\varepsilon^2) = m^* - \varepsilon \Lambda m^* + O(\varepsilon^2)$$

$$\text{with } \partial_t = \partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3} + O(\varepsilon^3)$$

$$\text{then } m + \varepsilon \partial_{t_1} m + O(\varepsilon^2) = m^* - \varepsilon \Lambda m^* + O(\varepsilon^2)$$

first component

$$W + \varepsilon \partial_{t_1} W + O(\varepsilon^2) = W^* - \varepsilon (A W + B Y^*) + O(\varepsilon^2)$$

$$\text{with } W^* = W \quad \text{and} \quad Y^* = \Phi(W) + O(\varepsilon)$$

$$\text{then } \partial_{t_1} W = -(A W + B \Phi(W))$$

$$\partial_{t_1} W + \Gamma_1(W) = 0 \quad \text{with} \quad \Gamma_1 = A W + B \Phi(W)$$

Chapman-Enskog expansion : order one bis

15

second component of $m + \varepsilon \partial_{t_1} m + O(\varepsilon^2) = m^* - \varepsilon \Lambda m^* + O(\varepsilon^2)$

$$Y + \varepsilon \partial_{t_1} Y + O(\varepsilon^2) = Y^* - \varepsilon (C W + D Y^*) + O(\varepsilon^2)$$

known: $Y^* = Y + S(\Phi(W) - Y)$

$$Y = \Phi(W) + O(\varepsilon) \quad \text{and} \quad Y^* = \Phi(W) + O(\varepsilon)$$

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

$$= -\varepsilon \partial_{t_1} (\Phi(W) + O(\varepsilon)) - \varepsilon (C W + D (\Phi(W) + O(\varepsilon))) + O(\varepsilon^2)$$

$$= \varepsilon [-d\Phi(W) \cdot \partial_{t_1} W - (C W + D \Phi(W))] + O(\varepsilon^2)$$

$$= \varepsilon [d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))] + O(\varepsilon^2)$$

Then $Y = \Phi(W) + \varepsilon S^{-1} \Psi_1(W) + O(\varepsilon^2)$

$$\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))$$

$$Y^* = \Phi(W) + \varepsilon (S^{-1} - I) \Psi_1(W) + O(\varepsilon^2)$$

Chapman-Enskog expansion : Hénon's matrix

16

$$\Sigma = S^{-1} - \frac{1}{2} I$$

$$Y = \Phi(W) + \varepsilon S^{-1} \Psi_1(W) + O(\varepsilon^2)$$

Then $Y = \Phi(W) + \varepsilon (\Sigma + \frac{1}{2} I) \Psi_1(W) + O(\varepsilon^2)$

$$Y^* = \Phi(W) + \varepsilon (\Sigma - \frac{1}{2} I) \Psi_1(W) + O(\varepsilon^2)$$

$$\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))$$

Chapman-Enskog expansion : order two

17

$$m + \varepsilon \partial_t m + \frac{1}{2} \varepsilon^2 \partial_t^2 m + O(\varepsilon^3) = m^* - \varepsilon \Lambda m^* + \frac{1}{2} \varepsilon^2 \Lambda^2 m^* + O(\varepsilon^3)$$

then

$$\begin{aligned} m + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2}) m + \frac{1}{2} \varepsilon^2 (\partial_{t_1} + O(\varepsilon))^2 m + O(\varepsilon^3) \\ = m^* - \varepsilon \Lambda m^* + \frac{1}{2} \varepsilon^2 \Lambda^2 m^* + O(\varepsilon^3) \end{aligned}$$

first component

$$\begin{aligned} W + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2}) W + \frac{1}{2} \varepsilon^2 \partial_{t_1}^2 W + O(\varepsilon^3) \\ = W - \varepsilon (A W + B Y^*) + \frac{1}{2} \varepsilon^2 (A_2 W + B_2 Y^*) + O(\varepsilon^3) \\ \text{with } Y^* = \Phi(W) + \varepsilon (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + O(\varepsilon^2) \end{aligned}$$

second order term

$$\partial_{t_2} W + \frac{1}{2} \partial_{t_1}^2 W = -B (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + \frac{1}{2} (A_2 W + B_2 \Phi)$$

Chapman-Enskog expansion : order two (ii)

18

$$\partial_{t_2} W + \frac{1}{2} \partial_{t_1}^2 W = -B \Sigma \Psi_1 + \frac{1}{2} B \Psi_1 + \frac{1}{2} (A_2 W + B_2 \Phi)$$

$$\begin{aligned} \text{with } \partial_{t_1}^2 W &= -\partial_{t_1} (\Gamma_1(W)) = -\partial_{t_1} (A W + B \Phi(W)) \\ &= A \Gamma_1 + B d\Phi(W). \Gamma_1 = A (A W + B \Phi) + B d\Phi(W). \Gamma_1 \end{aligned}$$

$$\begin{aligned} \partial_{t_2} W + \frac{1}{2} (A^2 W + A B \Phi) + \frac{1}{2} B d\Phi(W). \Gamma_1 \\ = -B \Sigma \Psi_1 + \frac{1}{2} B \Psi_1 + \frac{1}{2} (A_2 W + B_2 \Phi) \\ \text{with } A_2 = A^2 + B C, \quad B_2 = A B + B D \end{aligned}$$

$$\begin{aligned} \partial_{t_2} W + B \Sigma \Psi_1 &= -\frac{1}{2} (A^2 W + A B \Phi) - \frac{1}{2} B d\Phi(W). \Gamma_1 \\ &\quad + \frac{1}{2} B \Psi_1 + \frac{1}{2} (A^2 + B C) W + \frac{1}{2} (A B + B D) \Phi \\ &= -\frac{1}{2} B d\Phi(W). \Gamma_1 + \frac{1}{2} B (d\Phi(W). \Gamma_1 - C W - D \Phi) \\ &\quad + \frac{1}{2} B C W + \frac{1}{2} B D \Phi \\ &= 0 \end{aligned}$$

$$\partial_{t_2} W + \Gamma_2(W) = 0 \quad \text{with} \quad \Gamma_2(W) = B \Sigma \Psi_1(W)$$

Chapman-Enskog expansion : order two bis

19

$$\begin{aligned}
m + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2})m + \frac{1}{2} \varepsilon^2 \partial_{t_1}^2 m + O(\varepsilon^3) \\
= m^* - \varepsilon \Lambda m^* + \frac{1}{2} \varepsilon^2 \Lambda^2 m^* + O(\varepsilon^3)
\end{aligned}$$

second component

$$\begin{aligned}
Y + \varepsilon \partial_{t_1} Y + \varepsilon^2 \partial_{t_2} Y + \frac{1}{2} \varepsilon^2 \partial_{t_1}^2 Y + O(\varepsilon^3) \\
= Y^* - \varepsilon (C W + D Y^*) + \frac{1}{2} \varepsilon^2 (C_2 W + D_2 Y^*) + O(\varepsilon^3)
\end{aligned}$$

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

$$\begin{aligned}
= -\varepsilon \partial_{t_1} Y - \varepsilon^2 (\partial_{t_2} Y + \frac{1}{2} \partial_{t_1}^2 Y) - \varepsilon (C W + D Y^*) \\
+ \frac{1}{2} \varepsilon^2 (C_2 W + D_2 Y^*) + O(\varepsilon^3)
\end{aligned}$$

$$\text{with } Y = \Phi(W) + \varepsilon (\Sigma \Psi_1 + \frac{1}{2} \Psi_1) + O(\varepsilon^2)$$

$$\begin{aligned}
= -\varepsilon \partial_{t_1} \Phi(W) - \varepsilon^2 (\partial_{t_1} (\Sigma \Psi_1 + \frac{1}{2} \Psi_1) + \partial_{t_2} \Phi(W) + \frac{1}{2} \partial_{t_1}^2 \Phi(W)) \\
- \varepsilon (C W + D Y^*) + \frac{1}{2} \varepsilon^2 (C_2 W + D_2 Y^*) + O(\varepsilon^3)
\end{aligned}$$

Chapman-Enskog expansion : order two bis (ii)

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$$\begin{aligned}
S(Y - \Phi(W)) &= -\varepsilon \partial_{t_1} \Phi(W) \\
&\quad - \varepsilon^2 (\partial_{t_1} (\Sigma \Psi_1 + \frac{1}{2} \Psi_1) + \partial_{t_2} \Phi(W) + \frac{1}{2} \partial_{t_1}^2 \Phi(W)) \\
&\quad - \varepsilon (C W + D Y^*) + \frac{1}{2} \varepsilon^2 (C_2 W + D_2 Y^*) + O(\varepsilon^3) \\
&\quad \text{with } Y^* = \Phi(W) + \varepsilon (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + O(\varepsilon^2)
\end{aligned}$$

we have by definition $S(Y - \Phi(W)) = \varepsilon \Psi_1 + \varepsilon^2 \Psi_2 + O(\varepsilon^3)$

second order term

$$\begin{aligned}
\Psi_2 &= -\Sigma \partial_{t_1} \Psi_1 - \frac{1}{2} \partial_{t_1} \Psi_1 - \partial_{t_2} \Phi(W) - \frac{1}{2} \partial_{t_1}^2 \Phi(W) \\
&\quad - D (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + \frac{1}{2} C_2 W + \frac{1}{2} D_2 \Phi(W) \\
&\quad \text{with } \partial_{t_1} \Psi_1 = d\Psi_1 \cdot \partial_{t_1} W = -d\Psi_1 \cdot \Gamma_1 \\
&\quad \text{and } \partial_{t_1} \Psi_1 = \partial_{t_1} (d\Phi \cdot \Gamma_1 - C W - D \Phi(W)) \\
&\quad = \partial_{t_1} (d\Phi \cdot \Gamma_1) - C \partial_{t_1} W - D d\Phi \cdot \partial_{t_1} W \\
&\quad = \partial_{t_1} (d\Phi \cdot \Gamma_1) + C \Gamma_1 + D d\Phi \cdot \Gamma_1
\end{aligned}$$

$$\begin{aligned}
\Psi_2 &= \Sigma d\Psi_1 \cdot \Gamma_1 - \frac{1}{2} (\partial_{t_1} (d\Phi \cdot \Gamma_1) + C \Gamma_1 + D d\Phi \cdot \Gamma_1) - \partial_{t_2} \Phi(W) \\
&\quad - \frac{1}{2} \partial_{t_1}^2 \Phi(W) - D (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + \frac{1}{2} C_2 W + \frac{1}{2} D_2 \Phi(W)
\end{aligned}$$

Chapman-Enskog expansion : order two bis (iii)

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$$\begin{aligned} \Psi_2 = \Sigma d\Psi_1.\Gamma_1 - \frac{1}{2} (\partial_{t_1}(d\Phi.\Gamma_1) + C\Gamma_1 + D d\Phi.\Gamma_1) - \partial_{t_2}\Phi(W) \\ - \frac{1}{2} \partial_{t_1}^2 \Phi(W) - D(\Sigma\Psi_1 - \frac{1}{2}\Psi_1) + \frac{1}{2} C_2 W + \frac{1}{2} D_2 \Phi(W) \\ \text{with } \partial_{t_2}\Phi(W) = d\Phi(W).\partial_{t_2}W = -\Phi(W).\Gamma_2 \end{aligned}$$

$$\partial_{t_1}^2 \Phi(W) = \partial_{t_1}(\partial_{t_1}\Phi(W)) = \partial_{t_1}(d\Phi.\partial_{t_1}W) = -\partial_{t_1}(d\Phi.\Gamma_1)$$

$$\begin{aligned} \Psi_2 = \Sigma d\Psi_1.\Gamma_1 - \frac{1}{2} (\partial_{t_1}(d\Phi.\Gamma_1) + C\Gamma_1 + D d\Phi.\Gamma_1) + \Phi(W).\Gamma_2 \\ + \frac{1}{2} \partial_{t_1}(d\Phi.\Gamma_1) - D\Sigma\Psi_1 + \frac{1}{2} D\Psi_1 + \frac{1}{2} C_2 W + \frac{1}{2} D_2 \Phi(W) \\ \text{with } C_2 = CA + BD, \quad D_2 = CB + D^2 \end{aligned}$$

$$\begin{aligned} \Psi_2 = \Sigma d\Psi_1.\Gamma_1 - \frac{1}{2} (C\Gamma_1 + D d\Phi.\Gamma_1) + \Phi(W).\Gamma_2 - D\Sigma\Psi_1 + \frac{1}{2} D\Psi_1 \\ + \frac{1}{2} C(AW + B\Phi) + \frac{1}{2} D(CW + B\Phi) \\ \text{with } CW + B\Phi = d\Phi.\Gamma_1 - \Psi_1 \end{aligned}$$

$$\begin{aligned} \Psi_2 = \Sigma d\Psi_1.\Gamma_1 - \frac{1}{2} D d\Phi.\Gamma_1 + \Phi(W).\Gamma_2 - D\Sigma\Psi_1 + \frac{1}{2} D\Psi_1 \\ + \frac{1}{2} D(d\Phi.\Gamma_1 - \Psi_1) \end{aligned}$$

$$\Psi_2 = \Sigma d\Psi_1.\Gamma_1 + d\Phi(W).\Gamma_2 - D\Sigma\Psi_1$$

Chapman-Enskog expansion : order three

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

then

$$\begin{aligned} m + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3}) m + \frac{1}{2} \varepsilon^2 (\partial_{t_1} + \varepsilon \partial_{t_2} + O(\varepsilon^2))^2 m \\ + \frac{1}{6} \varepsilon^3 (\partial_{t_1} + O(\varepsilon))^3 m + O(\varepsilon^4) = m^* - \varepsilon \Lambda m^* \\ + \frac{1}{2} \varepsilon^2 \Lambda^2 m^* - \frac{1}{6} \varepsilon^3 \Lambda^3 m^* + O(\varepsilon^4) \end{aligned}$$

first component

$$\begin{aligned} W + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3}) W + \frac{1}{2} \varepsilon^2 (\partial_{t_1}^2 + \varepsilon \partial_{t_1} \partial_{t_2} + \varepsilon \partial_{t_2} \partial_{t_1}) W \\ + \frac{1}{6} \varepsilon^3 \partial_{t_1}^3 W + O(\varepsilon^4) = W - \varepsilon (AW + BY^*) \\ + \frac{1}{2} \varepsilon^2 (A_2 W + B_2 Y^*) - \frac{1}{6} \varepsilon^3 (A_3 W + B_3 Y^*) + O(\varepsilon^4) \end{aligned}$$

$$\text{with } Y^* = \Phi(W) + \varepsilon (\Sigma\Psi_1 - \frac{1}{2}\Psi_1) + \varepsilon^2 (\Sigma\Psi_2 - \frac{1}{2}\Psi_2) + O(\varepsilon^3)$$

Chapman-Enskog expansion : order three (ii)

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$$\begin{aligned}
& W + \varepsilon (\partial_{t_1} + \varepsilon \partial_{t_2} + \varepsilon^2 \partial_{t_3}) W + \frac{1}{2} \varepsilon^2 (\partial_{t_1}^2 + \varepsilon \partial_{t_1} \partial_{t_2} + \varepsilon \partial_{t_2} \partial_{t_1}) W \\
& \quad + \frac{1}{6} \varepsilon^3 \partial_{t_1}^3 W + O(\varepsilon^4) = W - \varepsilon A W \\
& \quad - \varepsilon B (\Phi(W) + \varepsilon (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + \varepsilon^2 (\Sigma \Psi_2 - \frac{1}{2} \Psi_2)) + \frac{1}{2} \varepsilon^2 A_2 W \\
& \quad + \frac{1}{2} \varepsilon^2 B_2 (\Phi(W) + \varepsilon (\Sigma \Psi_1 - \frac{1}{2} \Psi_1)) - \frac{1}{6} \varepsilon^3 (A_3 W + B_3 \Phi) + O(\varepsilon^4)
\end{aligned}$$

third order term

$$\begin{aligned}
& \partial_{t_3} W + \frac{1}{2} (\partial_{t_1} \partial_{t_2} W + \partial_{t_2} \partial_{t_1} W) + \frac{1}{6} \partial_{t_1}^3 W \\
& \quad = -B (\Sigma \Psi_2 - \frac{1}{2} \Psi_2) + \frac{1}{2} B_2 (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) - \frac{1}{6} (A_3 W + B_3 \Phi)
\end{aligned}$$

with

$$\begin{aligned}
\partial_{t_1} \partial_{t_2} W &= \partial_{t_1} (-B \Sigma \Psi_1) = -B \Sigma d\Psi_1 \cdot \partial_{t_1} W = B \Sigma d\Psi_1 \cdot \Gamma_1 \\
\partial_{t_2} \partial_{t_1} W &= \partial_{t_2} (-A W - B \Phi) = A \Gamma_2 - B d\Phi \cdot \partial_{t_2} W \\
& \quad = A B \Sigma \Gamma_1 + B d\Phi \cdot \Gamma_2
\end{aligned}$$

$$\begin{aligned}
& \partial_{t_3} W + \frac{1}{2} B \Sigma d\Psi_1 \cdot \Gamma_1 + \frac{1}{2} (A B \Sigma \Gamma_1 + B d\Phi \cdot \Gamma_2) + \frac{1}{6} \partial_{t_1}^3 W \\
& \quad = -B (\Sigma \Psi_2 - \frac{1}{2} \Psi_2) + \frac{1}{2} B_2 (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) - \frac{1}{6} (A_3 W + B_3 \Phi)
\end{aligned}$$

Chapman-Enskog expansion : order three (iii)

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$$\begin{aligned}
& \partial_{t_3} W + \frac{1}{2} (B \Sigma d\Psi_1 \cdot \Gamma_1 + A B \Sigma \Gamma_1 + B d\Phi \cdot \Gamma_2) + \frac{1}{6} \partial_{t_1}^3 W \\
& \quad = -B (\Sigma \Psi_2 - \frac{1}{2} \Psi_2) + \frac{1}{2} B_2 (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) - \frac{1}{6} (A_3 W + B_3 \Phi)
\end{aligned}$$

with

$$\begin{aligned}
\partial_{t_1}^3 W &= \partial_{t_1} (A \Gamma_1 + B d\Phi \cdot \Gamma_1) = \partial_{t_1} (A (A W + B \Phi) + B d\Phi \cdot \Gamma_1) \\
& \quad = -A (A \Gamma_1 - B d\Phi \cdot \Gamma_1) - B d(d\Phi \cdot \Gamma_1) \cdot \Gamma_1 \\
& \quad = -A^2 \Gamma_1 - A B d\Phi \cdot \Gamma_1 - B d(d\Phi \cdot \Gamma_1) \cdot \Gamma_1
\end{aligned}$$

$$\text{and } A_3 = A_2 A + B_2 C, \quad B_3 = A_2 B + B_2 D$$

$$\begin{aligned}
A_3 W + B_3 \Phi &= A_2 (A W + B \Phi) + B_2 (C W + D \Phi) \\
& \quad = (A^2 + B C) \Gamma_1 + (A B + B D) (d\Phi \cdot \Gamma_1 - \Psi_1) \\
& \quad = A (A \Gamma_1 + B d\Phi \cdot \Gamma_1) + B (C \Gamma_1 + D d\Phi \cdot \Gamma_1) - B_2 \Psi_1 \\
& \quad = A (A \Gamma_1 + B d\Phi \cdot \Gamma_1) + B (d(d\Phi \cdot \Gamma_1) \cdot \Gamma_1 - d\Psi_1 \cdot \Gamma_1) - B_2 \Psi_1 \\
& \quad = -\partial_{t_1}^3 W - B d\Psi_1 \cdot \Gamma_1 - B_2 \Psi_1
\end{aligned}$$

Chapman-Enskog expansion : order three (iv)

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$$\partial_{t_3} W + \frac{1}{2} (B \Sigma d\Psi_1 \cdot \Gamma_1 + AB \Sigma \Gamma_1 + B d\Phi \cdot \Gamma_2) = -B \Sigma \Psi_2$$

$$+ \frac{1}{2} B \Psi_2 + \frac{1}{2} B_2 (\Sigma \Psi_1 - \frac{1}{2} \Psi_1) + \frac{1}{6} (B d\Psi_1 \cdot \Gamma_1 + B_2 \Psi_1)$$

with $\Psi_2 = \Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi \cdot \Gamma_2 - D \Sigma \Psi_1$

$$\partial_{t_3} W + \frac{1}{2} (B \Sigma d\Psi_1 \cdot \Gamma_1 + AB \Sigma \Gamma_1 + B d\Phi \cdot \Gamma_2) = -B \Sigma \Psi_2$$

$$+ \frac{1}{2} B (\Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi \cdot \Gamma_2 - D \Sigma \Psi_1) + \frac{1}{2} B_2 \Sigma \Psi_1$$

$$- (\frac{1}{4} - \frac{1}{6}) B_2 \Psi_1 + \frac{1}{6} B d\Psi_1 \cdot \Gamma_1$$

then $\partial_{t_3} W + B \Sigma \Psi_2 + \frac{1}{12} B_2 \Psi_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1 = 0$

$$\Gamma_3 = B \Sigma \Psi_2 + \frac{1}{12} B_2 \Psi_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1$$

Taylor second-order expansion

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$$m + \Delta t \partial_t m + \frac{1}{2} \Delta t^2 \partial_t^2 m + O(\Delta t^3) =$$

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

We replace the vector m by its two components W and Y

$$W + \Delta t \partial_t W + \frac{1}{2} \Delta t^2 \partial_t^2 W + O(\Delta t^3) =$$

$$= W - \Delta t (A W + B Y^*) + \frac{1}{2} \Delta t^2 (A_2 W + B_2 Y^*) + O(\Delta t^3)$$

$$Y + \Delta t \partial_t Y + \frac{1}{2} \Delta t^2 \partial_t^2 Y + O(\Delta t^3) =$$

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

At zero-order: $Y - Y^* = O(\Delta t)$ and $Y^* \equiv Y + S(\Phi(W) - Y)$

The matrix S is supposed fixed

then $Y = \Phi(W) + O(\Delta t)$ and $Y^* = \Phi(W) + O(\Delta t)$

Taylor second-order expansion (ii)

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$$Y^* = \Phi(W) + O(\Delta t)$$

Second-order partial differential equations:

$$\begin{aligned} \partial_t W + \frac{1}{2} \Delta t \partial_t^2 W + O(\Delta t^2) &= \\ &= -(A W + B Y^*) + \frac{1}{2} \Delta t (A_2 W + B_2 Y^*) + O(\Delta t^2) \end{aligned}$$

at first-order:

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

$$\text{then } \partial_t W = -\Gamma_1 \quad \text{with} \quad \Gamma_1 = A W + B \Phi(W)$$

$$\text{then } \partial_t Y = d\Phi(W) \cdot \partial_t W + O(\Delta t) = -d\Phi(W) \cdot \Gamma_1 + O(\Delta t)$$

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

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

$$Y = \Phi + \Delta t S^{-1} (d\Phi(W) \cdot \Gamma_1 - C W - D \Phi) + O(\Delta t^2)$$

$$\text{and} \quad \Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi)$$

Taylor second-order expansion (iii)

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

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

Second-order partial differential equations:

$$\begin{aligned} \partial_t W + \frac{1}{2} \Delta t \partial_t^2 W + O(\Delta t^2) &= \\ &= -(A W + B Y^*) + \frac{1}{2} \Delta t (A_2 W + B_2 Y^*) + O(\Delta t^2) \end{aligned}$$

$$\begin{aligned} \partial_t W &= -A W - B (\Phi + (\Sigma - \frac{1}{2}I) \Delta t \Psi_1) - \frac{1}{2} \Delta t (A \Gamma_1 + B d\Phi \cdot \Gamma_1) \\ &\quad + \frac{1}{2} \Delta t ((A^2 + B C) W + (A B + B D) \Phi) + O(\Delta t^2) \\ &= -A W - B \Phi + \Delta t (-B \Sigma \Psi_1 + \frac{1}{2} B (d\Phi \cdot \Gamma_1 - C W - D \Phi)) \\ &\quad - \frac{1}{2} (A (A W + B \Phi)) - \frac{1}{2} B d\Phi \cdot \Gamma_1 + \frac{1}{2} (A^2 + B C) W \\ &\quad + \frac{1}{2} (A B + B D) \Phi + O(\Delta t^2) \end{aligned}$$

$$\partial_t W = -\Gamma_1 - \Delta t B \Sigma \Psi_1 + O(\Delta t^2) \quad \text{and} \quad \Gamma_2 = B \Sigma \Psi_1$$

Link with the original Taylor expansion method (2007) 29

$$\text{First-order } \partial_t W = -\Gamma_1 + O(\Delta t) = -A W - B \Phi(W) + O(\Delta t)$$

$$\text{id est } \partial_t W_i + \Lambda_{ij}^\beta \partial_\beta W_j + \Lambda_{i\ell}^\beta \partial_\beta \Phi(W)_\ell = O(\Delta t)$$

$$\text{or } \partial_t W_i + \Lambda_{i\ell}^\beta \partial_\beta m_\ell^{\text{eq}} = O(\Delta t)$$

$$\text{with the notation } m_k^{\text{eq}} \equiv \Phi(W)_k$$

$$\text{Defect of conservation } \theta_k \equiv \partial_t m_k^{\text{eq}} + \sum_{\ell\beta} \Lambda_{k\ell}^\beta \partial_\beta m_\ell^{\text{eq}}$$

vector of conservation defect

$$\theta = \partial_t \Phi(W) + \Lambda \cdot m^{\text{eq}}$$

$$= d\Phi \cdot (-\Gamma_1 - \Delta t \Gamma_2 + \dots) + (C W + D \Phi(W))$$

$$= (-d\Phi \cdot \Gamma_1 + O(\Delta t)) + (C W + D \Phi(W))$$

$$= -\Psi_1 + O(\Delta t)$$

$$\theta = -\Psi_1 + O(\Delta t)$$

Second-order term

$$(B \Sigma \Psi_1)_i = \sum_k B_{ik} \sigma_k (-\theta_k + O(\Delta t)) = \sum_k \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + O(\Delta t)$$

$$\text{and } \partial_t W_i + \Lambda_{i\ell}^\beta \partial_\beta m_\ell^{\text{eq}} = \Delta t \sum_k \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + O(\Delta t^2)$$

Taylor third-order expansion

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

We replace the vector m by its two components W and Y

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

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

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

and

$$Y - Y^* \equiv S(Y - \Phi)$$

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

Computation of the coefficient Ψ_2

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

with [see Annex -1- page (iii)]

$$C W + D Y^* = -\Psi_1 + d\Phi \cdot \Gamma_1 + \Delta t D (\Sigma - \frac{1}{2} I) \Psi_1 + O(\Delta t^2)$$

$$C_2 W + D_2 Y^* = d(d\Phi \cdot \Gamma_1 - \Psi_1) \cdot \Gamma_1 - D \Psi_1 + O(\Delta t)$$

and [see Annex -2- pages (iii) and (iv)]

$$\partial_t Y = -d\Phi \cdot \Gamma_1 - \Delta t \left(d\Phi \cdot \Gamma_2 + (\Sigma + \frac{1}{2} I) d\Psi_1 \cdot \Gamma_1 \right) + O(\Delta t^2)$$

$$\partial_t^2 Y = d(d\Phi \cdot \Gamma_1) \cdot \Gamma_1 + O(\Delta t)$$

Then

$$S(Y - \Phi) = \Delta t \Psi_1 + \Delta t^2 \left(-D (\Sigma - \frac{1}{2} I) \Psi_1 + d\Phi \cdot \Gamma_2 + (\Sigma + \frac{1}{2} I) d\Psi_1 \cdot \Gamma_1 - \frac{1}{2} (d\Psi_1 \cdot \Gamma_1 + D \Psi_1) \right) + O(\Delta t^3)$$

$$= \Delta t \Psi_1 + \Delta t^2 (\Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi \cdot \Gamma_2 - D \Sigma \Psi_1) + O(\Delta t^3)$$

$$\Psi_2 = \Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi \cdot \Gamma_2 - D \Sigma \Psi_1$$

Computation of the coefficient Γ_3

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

with [see Annex -1- pages (i) and (ii)]

$$A W + B Y^* = A W + B \Phi + \Delta t B (\Sigma - \frac{1}{2} I) \Psi_1 + \Delta t^2 B (\Sigma - \frac{1}{2} I) \Psi_2 + O(\Delta t^3)$$

$$A_2 W + B_2 Y^* = A \Gamma_1 + B (d\Phi \cdot \Gamma_1 - \Psi_1) + \Delta t B_2 (\Sigma - \frac{1}{2} I) \Psi_1 + O(\Delta t^2)$$

$$A_3 W + B_3 Y^* = \partial^2 \Gamma_1 \cdot \Gamma_1 - B d\Psi_1 \cdot \Gamma_1 - B_2 \Psi_1 + O(\Delta t)$$

and [see Annex -2- pages (i) and (ii)]

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

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

$$\partial_t W = -\Gamma_1 - \Delta t B \Sigma \Psi_1$$

$$+ \Delta t^2 \left(-B (\Sigma - \frac{1}{2} I) \Psi_2 + \frac{1}{2} (B_2 (\Sigma - \frac{1}{2} I) \Psi_1 - d\Gamma_1 \cdot \Gamma_2 - d\Gamma_2 \cdot \Gamma_1) + \frac{1}{6} (B d\Psi_1 \cdot \Gamma_1 + B_2 \Psi_1) \right) + O(\Delta t^3)$$

Computation of the coefficient Γ_3 (ii)

$$\partial_t W + \Gamma_1 + \Delta t \Gamma_2 = \Delta t^2 \left(-B \left(\Sigma - \frac{1}{2} I \right) \Psi_2 + \frac{1}{2} (B_2 \left(\Sigma - \frac{1}{2} I \right) \Psi_1 - d\Gamma_1 \cdot \Gamma_2 - d\Gamma_2 \cdot \Gamma_1) + \frac{1}{6} (B d\Psi_1 \cdot \Gamma_1 + B_2 \Psi_1) \right) + O(\Delta t^3)$$

and the coefficient of Δt^2 is given by

$$\begin{aligned} \Gamma_3 &= B \Sigma \Psi_2 - \frac{1}{2} B \Psi_2 + \frac{1}{2} (AB + BD) \Sigma \Psi_1 + \left(\frac{1}{4} - \frac{1}{6} \right) B_2 \Psi_1 \\ &\quad - \frac{1}{2} (A\Gamma_2 + B d\Phi \cdot \Gamma_2) - \frac{1}{2} B \Sigma d\Psi_1 \cdot \Gamma_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1 \\ &\hspace{15em} \text{because } \Gamma_2 = B \Sigma \Psi_1 \\ &= B \Sigma \Psi_2 - \frac{1}{2} B (D \Sigma \Psi_1 - d\Phi \cdot \Gamma_2 - \Sigma d\Psi_1 \cdot \Gamma_1) + \frac{1}{2} B D \Sigma \Psi_1 \\ &\quad \frac{1}{12} B_2 \Psi_1 - \frac{1}{2} B d\Phi \cdot \Gamma_2 - \frac{1}{2} B \Sigma d\Psi_1 \cdot \Gamma_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1 \end{aligned}$$

Finally,

$$\Gamma_3 = B \Sigma \Psi_2 + \frac{1}{12} B_2 \Psi_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1$$

Link with the previous formal expansion at third-order 34

$$\text{Defect of conservation } \theta_k \equiv \partial_t m_k^{\text{eq}} + \sum_{\ell\beta} \Lambda_{k\ell}^\beta \partial_\beta m_\ell^{\text{eq}}$$

$$\text{vector of conservation defect } \theta = \partial_t \Phi(W) + \Lambda \cdot m^{\text{eq}}$$

$$\text{then } \theta = -\Psi_1 - \Delta t d\Phi \cdot \Gamma_2 + O(\Delta t)$$

$$\text{and } \partial_t \theta = -\partial_t \Psi_1 + O(\Delta t) = d\Psi_1 \cdot \Gamma_1 + O(\Delta t)$$

We have the following calculus:

$$\begin{aligned} \Gamma_2 + \Delta t \Gamma_3 &= B \Sigma \Psi_1 + \Delta t (B \Sigma \Psi_2 + \frac{1}{12} B_2 \Psi_1 - \frac{1}{6} B d\Psi_1 \cdot \Gamma_1) \\ &= B \Sigma (-\theta - \Delta t d\Phi \cdot \Gamma_2 + O(\Delta t^2)) + \Delta t B \Sigma (\Sigma d\Psi_1 \cdot \Gamma_1 + d\Phi \cdot \Gamma_2 \\ &\quad - D \Sigma \Psi_1) + \frac{1}{12} \Delta t B_2 \Psi_1 - \frac{1}{6} \Delta t B d\Psi_1 \cdot \Gamma_1 \\ &= -B \Sigma \theta + \Delta t \left(- (B \Sigma D \Sigma - \frac{1}{12} B_2) \Psi_1 \right. \\ &\quad \left. + B (\Sigma^2 - \frac{1}{6}) d\Psi_1 \cdot \Gamma_1 \right) + O(\Delta t^2) \\ &= -B \Sigma \theta + \Delta t \left((B \Sigma D \Sigma - \frac{1}{12} B_2) \theta \right. \\ &\quad \left. + B (\Sigma^2 - \frac{1}{6}) \partial_t \theta \right) + O(\Delta t^2) \end{aligned}$$

Link with the previous formal expansion at third-order (ii)

$$\Gamma_2 + \Delta t \Gamma_3 = -B \Sigma \theta + \Delta t \left((B \Sigma D \Sigma - \frac{1}{12} B_2) \theta + B (\Sigma^2 - \frac{1}{6}) \partial_t \theta \right) + O(\Delta t^2)$$

Third-order partial equivalent equations:

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

Explicitation with the cartesian components:

$$(B \Sigma D \Sigma \theta)_i = \Lambda_{ik}^\beta \sigma_k (\Lambda_{kl}^\gamma) \sigma_l \partial_\beta \partial_\gamma \theta_l = \Lambda_{ik}^\beta \sigma_k \Lambda_{kl}^\gamma \sigma_l \partial_\beta \partial_\gamma \theta_l$$

$$(B_2 \theta)_i = (\Lambda_{ik}^\beta \partial_\beta) (\Lambda_{kl}^\gamma \partial_\gamma) \theta_l = \Lambda_{ik}^\beta \Lambda_{kl}^\gamma \partial_\beta \partial_\gamma \theta_l$$

$$((B \Sigma D \Sigma - \frac{1}{12} B_2) \theta)_i = \Lambda_{ik}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l$$

$$(B (\Sigma^2 - \frac{1}{6}) \partial_t \theta)_i = \Lambda_{ik}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k$$

Other form of the third-order partial equivalent equations:

$$\partial_t W_i + \Lambda_{ik}^\alpha \partial_\alpha m_k^{\text{eq}} - \Delta t \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + \Delta t^2 \left(\Lambda_{ik}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l + \Lambda_{ik}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3)$$

Link with the previous formal expansion at third-order (iii)

$$\partial_t W_i + \Lambda_{ik}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + \Delta t^2 \left(\Lambda_{ik}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l + \Lambda_{ik}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3)$$

Classical lattice Boltzmann scheme : $M_{0j} = 1$ and $M_{\alpha j} = v_j^\alpha$

then $\Lambda_{0\ell}^\alpha = M_{0j} v_j^\alpha (M^{-1})_{j\ell} = M_{\alpha j} (M^{-1})_{j\ell} = \delta_{\alpha\ell}$

$$\text{and } \Lambda_{0k}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l = \delta_{\beta k} \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l = \Lambda_{\beta l}^\gamma (\sigma_\beta \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l$$

Thermal case: $\sigma_\beta \neq 0$ and

$$\Lambda_{0k}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l = \Lambda_{\beta l}^\gamma (\sigma_\beta \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l$$

Fluid case; the momentum is conserved: $\sigma_\beta = 0$. Then

$$\Lambda_{0k}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_l - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_l = -\frac{1}{12} \Lambda_{\beta l}^\gamma \partial_\beta \partial_\gamma \theta_l$$

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = \delta_{\beta k} (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = (\sigma_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta)$$

Link with the previous formal expansion at third-order (iv)

$$\partial_t W_i + \Lambda_{ik}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + \Delta t^2 \left(\Lambda_{ik}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell + \Lambda_{ik}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3)$$

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = \begin{cases} \Lambda_{\beta\ell}^\gamma (\sigma_\beta \sigma_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell & \text{thermics} \\ -\frac{1}{12} \Lambda_{\beta\ell}^\gamma \partial_\beta \partial_\gamma \theta_\ell & \text{fluid} \end{cases}$$

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = (\sigma_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta)$$

Thermal case: $\sigma_\beta \neq 0$ and

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = (\sigma_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta)$$

Fluid case; the momentum is conserved: $\theta_\beta = O(\Delta t)$. Then

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = O(\Delta t)$$

Link with the previous formal expansion at third-order (v)

$$\partial_t W_i + \Lambda_{ik}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k + \Delta t^2 \left(\Lambda_{ik}^\beta \Lambda_{kl}^\gamma (\sigma_k \sigma_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell + \Lambda_{ik}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3)$$

Classical notations: $W_0 = \rho \equiv \sum_j f_j$, $W_\alpha = J_\alpha = \sum_j v_j^\alpha f_j$

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = \begin{cases} \Lambda_{\beta\ell}^\gamma (\sigma_\beta \sigma_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell & \text{thermics} \\ -\frac{1}{12} \Lambda_{\beta\ell}^\gamma \partial_\beta \partial_\gamma \theta_\ell & \text{fluid} \end{cases}$$

$$\Lambda_{0k}^\beta (\sigma_k^2 - \frac{1}{6}) \partial_\beta \partial_t \theta_k = \begin{cases} (\sigma_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta) & \text{thermics} \\ 0 & \text{fluid} \end{cases}$$

Mass conservation in the thermal case :

$$\partial_t \rho + \partial_\alpha J_\alpha^{\text{eq}} - \Delta t \sigma_\alpha \partial_\alpha \theta_\alpha + \Delta t^2 \left(\Lambda_{\beta\ell}^\gamma (\sigma_\beta \sigma_\ell - \frac{1}{12}) \partial_\beta \partial_\gamma \theta_\ell + (\sigma_\beta^2 - \frac{1}{6}) \partial_t (\partial_\beta \theta_\beta) \right) = O(\Delta t^3)$$

[relation (35) of DCDS-A, 2009].

Mass conservation in the fluid case :

$$\partial_t \rho + \partial_\alpha J_\alpha - \frac{1}{12} \Delta t^2 \Lambda_{\beta\ell}^\gamma \partial_\beta \partial_\gamma \theta_\ell = O(\Delta t^3)$$

[relation (40) of DCDS-A, 2009].

Link with the previous formal expansion at third-order (vi)

$$\begin{aligned} & \partial_t W_i + \Lambda_{ik}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{ik}^\beta \sigma_k \partial_\beta \theta_k \\ & + \Delta t^2 \left(\Lambda_{ik}^\beta \Lambda_{kl}^\gamma \left(\sigma_k \sigma_l - \frac{1}{12} \right) \partial_\beta \partial_\gamma \theta_l + \Lambda_{ik}^\beta \left(\sigma_k^2 - \frac{1}{6} \right) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3) \end{aligned}$$

Momentum conservation for the fluid case: $i = \alpha$

$$\begin{aligned} & \partial_t J_\alpha + \Lambda_{\alpha k}^\beta \partial_\beta m_k^{\text{eq}} - \Delta t \Lambda_{\alpha k}^\beta \sigma_k \partial_\beta \theta_k \\ & + \Delta t^2 \left(\Lambda_{\alpha k}^\beta \Lambda_{kl}^\gamma \left(\sigma_k \sigma_l - \frac{1}{12} \right) \partial_\beta \partial_\gamma \theta_l \right. \\ & \quad \left. + \Lambda_{\alpha k}^\beta \left(\sigma_k^2 - \frac{1}{6} \right) \partial_\beta \partial_t \theta_k \right) = O(\Delta t^3) \end{aligned}$$

[relation (41) of *DCDS-A*, 2009].

- **Compact iteration** of lattice Boltzmann schemes
- Block decomposition of the moment-velocity operator matrix
- Asymptotic expansion of the equivalent partial differential equations and of the non conserved moments
- Explication of the coefficients up to **order 3** with **recursive formulas containing less than 3 terms**
- Intensive use of differential calculus
- **Validation** of the nonlinear expansion for fluid flow and thermal problems up to the order 3
- **Validation** of the non linear expansion at second order for Navier Stokes flows with two or three space dimensions [Icmmes 2018, ICIAM 2019, ...]
- New applications soon !