LBM for advection-diffusion systems

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Plan

- LBM introduction
- D1Q3 and magic parameters.
- D2Q9, D3Q15 and D3Q19 and quartic parameters.
- Conlusion

Boltzmann Equation

In the 19th century, Boltzmann :

- Mesoscopic scale to describe the statistical behaviour of a thermodynamic system not in a state of equilibrium.
- The probability density function $f(x, v, t)$ describes the number of molecules (mass) which have position x, velocity v and at time t :

$$\mathrm{d}m = f(x, v, t)\mathrm{d}x\mathrm{d}v.$$

The Boltzmann equation takes the form :

$$\frac{\partial f}{\partial t} + v.\nabla_x f = Q(f, f), \quad x \ in\ \mathbb{R}^3, \quad v \in \mathbb{R}^3, \quad t > 0.$$

where the collision integral $Q(f, f)$ is a quadratic integral operator acting only on the v-argument of the number density f.

Boltzmann equation :

$$\frac{\partial f}{\partial t} + v.\nabla_x f = Q(f, f), \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3, \quad t > 0.$$

Two fundamental steps :

- The transport of the particles (taking $Q(f, f) = 0$), simple advection equation with velocity v.

$$\frac{\partial f}{\partial t}(x, v, t) + v.\nabla_x f(x, v, t) = 0.$$

- The collision represented by $Q(f, f)$.

The collision operator $Q(f, f)$:
• Conserves mass, velocity and energy.

$$\int_{\mathbb{R}^3} Q(f, f)\mathrm{d}v = 0, \quad \int_{\mathbb{R}^3} vQ(f, f)\mathrm{d}v = 0, \quad \int_{\mathbb{R}^3} \frac{|v|^2}{2} Q(f, f)\mathrm{d}v = 0,$$

• The thermodynamic equilibrium which satisfies the global cancellation of collisions :

$$Q(f^{eq}, f^{eq}) = 0,$$

where f^{eq} is Maxwellian distribution function (Gauss distribution).

• Chapman-Enskog theory (1916-1917) :
Navier-Stokes equations can be recovered from Boltzmann equation using asymptotic expansion of density f, for a small Knudsen number, around the equilibrium f^{eq}.

$$
\begin{cases}
\dfrac{\partial \rho}{\partial t} + \mathrm{div} J = 0, \\[2ex]
\dfrac{\partial J_k}{\partial t} + \dfrac{\partial}{\partial x_j} \left\{ \displaystyle\int_{\mathbb{R}^3} v_j \, v_k \, f(x, v, t) \mathrm{d}v \right\} = 0, \quad 1 \leq j \leq 3, \\[2ex]
\dfrac{\partial \rho E}{\partial t} + \mathrm{div} \left\{ \displaystyle\int_{\mathbb{R}^3} \frac{1}{2} |v|^2 v \, f(x, v, t) \mathrm{d}v \right\} = 0.
\end{cases}
$$

Towards the Lattice Boltzmann Method

• Lattice Gas Automata :
Discretize space, time, velocities and the numbers of molecules in a given node at a give time.
• Lattice Boltzmann Method (Mac Namara & Zanetti 1988)
Keep a discrete space (lattice) and determine a continuous variable f which describes the average of population in a given node with a discrete velocity imposed by the geometry.
The evolution of scheme (with time step $\Delta t = 1$)

$$f_i(x + v_i, t + 1) = f_i(x, t) + Q_i(f, f)(x, t),$$

where $Q_i(f, f) = \sum_{j=0}^{b} S_{i,j}(f_j - f_j^{\mathrm{eq}})$.

1. determine the equilibrium distribution f_j^{eq}.
2. the choice of the collision matrix $S_{i,j}$.

Multiple-relaxation-time lattice Boltzmann model

• Qian, D'Humières & Lallemand (1992) : the equilibrium distribution is polynomial function of velocities. This model resolves Navier-Stokes equation, is noise-free, has Galilean invariance and a velocity-independent pressure.

• D'Humières (1992) : the collision operator is diagonal in new variables "moments" which are obtained by a linear transformation of f_j.

Remark The moment representation provides a convenient and effective means by which to incorporate the physics into LBM.

1. The relaxation parameters of the moments are directly related to the various transport coefficients.
2. Allows us to control each mode independently.

LBM Scheme

DdQq lattice Boltzmann scheme (where d is the space dimension and q is the number of discrete velocities) :

- A regular lattice $\mathcal{L}_0$ in $\mathbb{R}^d$ parametrized by Δx.
- A fixed time step Δt.
- A constant $\lambda = \frac{\Delta x}{\Delta t}$ the mesh speed.
- A discrete velocity set $\mathcal{V} = \{v_j = \lambda e_j, 0 \leq j \leq q-1\}$ composed by $q = J + 1$ elements.

The evolution of scheme :

$$f_j(x, t + \Delta t) = f^*(x - v_j \Delta t, t), \quad v_j \in \mathcal{V}, \quad x \in \mathcal{L}_0$$

1. Advection : couples linearly a vertex x with its neighbor $x + v_j \Delta t$, for $0 \leq j \leq J$.
2. Relaxation : $f \mapsto f^*$ local in space and *a priori non linear*

Remark All difficulties are concentrated in the relaxation step.

Collision step

• Bhatnagar-Gross-Krook (BGK) approximation :

$$Q_i(f,f) = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}}),$$

where the constant $\tau > 0$ macroscopique time scale.
• MRT : The "moments" m space : $m_k = \sum_j M_{k\,j} f_j$, where matrix $M = (M_{k\,j})_{1\leq k,j\leq q}$ is invertible.
<u>Conserved moments</u> :
$m_0^* = m_0,\ m_1^* = m_1, \ldots, m_N^* = m_N.$
<u>Non-conserved moments</u> :

$$\frac{dm_k}{dt} + \frac{1}{\tau_k}(m_k - m_k^{eq}) = 0, \quad k \geq N+1,$$

relaxe towards m_k^{eq} where τ_k is a constant. Forward Euler method :

$$m_k^* = (1 - s_k)m_k + s_k m_k^{eq}, \quad k \geq N+1.$$

$s_k = \frac{\Delta t}{\tau_k} < 2$ to keep stability. m_k^{eq} are functions of conserved moments.

The moment Matrix

Let $f_j(x) \in \mathbb{R}, \quad 0 \leq j \leq J, x \in \mathcal{L}_0$, at time step $n\Delta t$.
We introduce conserved moments :

Density $\rho(x) = \sum_{j=0}^{J} f_j(x)$

Velocity $q^\alpha(x) = \sum_{j=0}^{J} v_j^\alpha f_j(x), \qquad$ (e.g. $1 \leq \alpha \leq 2$ if $d = 2$).

Equilibrium distribution $f_j^{eq}(x)$ is function of conserved moments

$$f_j^{eq} = G_j(\rho, q)$$

Main idea of d'Humières : complete vector (ρ, q^1, q^2) in a vector of moments $m \in \mathbb{R}^{J+1}$, where the first composants are conserved moments.

The moments m_k, are obtained by a linear function of f_j :

$$m = M.f$$

The matrix M must be **invertible** and the collision operator ($f \mapsto f^*$) in moments space is **diagonal.**
Collision : $f \mapsto f^* = C.f$ becomes $m \mapsto m^* = MCM^{-1}.m$
Conserved variables still invariants in collision step :
$m_k^* = m_k^{eq} = m_k,\ 0 \leq k \leq 2.$
Non-conserved variables relax to $m_k^{eq} = G(\rho, q^1, q^2)$ with constant τ_k.

- Moments :

density $\rho = f_0 + f_1 + f_2$ conserved
velocity $q = \lambda f_1 - \lambda f_2$ conserved
energy $e = \frac{\lambda^2}{2}(f_1 + f_2)$, equilibrium value : $e^{eq} = \alpha \frac{\lambda^2}{2}\rho$.

$$e^* = e - s(e - e^{eq}),$$

$$M = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ 0 & \frac{\lambda^2}{2} & \frac{\lambda^2}{2} \end{pmatrix}, \qquad C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ s\alpha\frac{\lambda^2}{2}\rho & 0 & 1-s \end{pmatrix},$$

- LBM Scheme one time step :

$$f_{new} = A\, M^{-1}\, C\, M\, f_{old}.$$

Equivalent Equation

Macroscopic equation :

$$\frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} - \frac{1}{12}(1-\alpha)\lambda^2 \Delta t^2 \frac{\partial^3 q}{\partial x^3} = O(\Delta t^3)$$

$$\left\{ \begin{aligned} \frac{\partial q}{\partial t} + \alpha\lambda^2 \frac{\partial \rho}{\partial x} - \left(\frac{1}{s} - \frac{1}{2}\right) \lambda^2 \Delta t (1-\alpha) \frac{\partial^2 q}{\partial x^2} - & \\ -\frac{\lambda^4 \Delta t^2}{6} \alpha (1-\alpha)(6(\frac{1}{s} - \frac{1}{2})^2 - 1) \frac{\partial^3 \rho}{\partial x^3} &= O(\Delta t^3) \end{aligned} \right.$$

sound speed : $c_s = \sqrt{\alpha}\lambda$, viscosity : $\nu = \left(\frac{1}{s} - \frac{1}{2}\right) \lambda^2 \Delta t (1-\alpha)$.

Remark : The stability condition $0 < s < 2$ guarantees $\frac{1}{s} - \frac{1}{2} > 0$.

Dispertion equation and numerical stability

In Fourier space : $f_i(x,t) = \phi_i e^{i(\omega t - kx)}$.

$$f(x, t+\Delta t) = e^{i\omega \Delta t} f(x,t) = A(M^{-1}CM) f(x,t)$$

where $A = \mathrm{diag}\left(1, p, \frac{1}{p}\right)$, where $p = e^{ik\Delta x}$.
We take $z = e^{(i\omega \Delta t)}$; we obtain dispertion relation :

$$zf(x,t) = G(p) f(x,t).$$

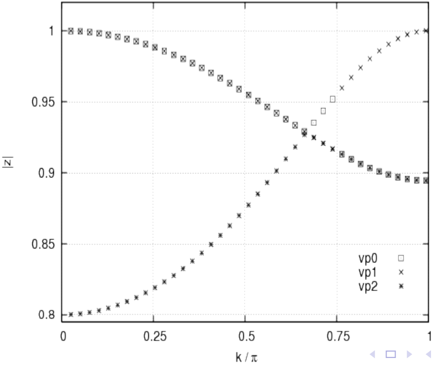
$$\det(G(p) - zId) = 0.$$

Remark The dispertion equation gives a relation between ω and k. (*via* relation between z and p). For a fixed k we have an eigenvalues problems. The eigenvalues will give the expression of transport coeffiecient in function of k. (see [LL2000])

$$Q(z) \equiv \det\left[G(p) - zId\right] = 0,$$

where Q is a polynomial of z with degree 3.

- $z_{0,1} = 1 \pm \mathrm{i}\frac{k}{c_s} + \mathrm{o}(k)$, which corresponds to two hydodynamics (conserved) modes. (see vp0 and vp1 in the above figure).
- $z_2 = (1 - s) + \mathrm{o}(k)$, corresponds to non conserved mode. (see vp2 in the above figure).



Numerical Stability

Stability relies on the eigenvalues problem.
The LBM scheme is stable when all eigenvalues of the matrix $G(p)$ have module less then 1.

$$f^{n+1} = G(p) f^n = G(p)^{n+1} f^0.$$

Stability L^2 occurs if G diagonalizable and eigenvalues

$$|\lambda_i| < 1 \quad \forall i = 1, \ldots J.$$

Proof If G is diagonalisable and all eigenvalues λ_i are less then 1, then it exists $K > 0$, that $\|G^{n+1}\| \leq K \quad \forall n \in \mathbb{N}$.

$$\|f^{n+1}\|_2 \leq \|G^{n+1}\| \|f^0\|_2 \leq K \|f^0\|_2.$$

LBM for diffusion

- For D1Q3 :

1. $m_0 = \rho = f_0 + f_1 + f_2 \equiv \rho$ (density) conserved.
2. $m_1 = \lambda(f_1 + f_2)$, non-conserved $m_1^{eq} = 0$, relax with s_1.
3. $m_2 = \frac{\lambda^2}{2}(f_1 + f_2)$, non-conserved $m_2^{eq} = \alpha\frac{\lambda^2}{2}\rho$, relax with s_2.

Equivalent equation :

$$\frac{\partial \rho}{\partial t} - \mathcal{K}\frac{\partial^2 \rho}{\partial x^2} = \mathrm{O}(\Delta x^3),$$

where $\mathcal{K} = \Delta t \lambda^2 \left(\frac{1}{s_1} - \frac{1}{2}\right)\alpha$.

For notation : let $\sigma_1 = \left(\frac{1}{s_1} - \frac{1}{2}\right)$ and $\sigma_2 = \left(\frac{1}{s_2} - \frac{1}{2}\right)$

1D Diffusion problems and matrix of moments

Let's consider the following 1D Poisson's problem :

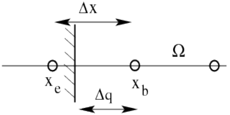
$$\begin{cases} -\mathcal{K}u''(x) & = & c \quad \text{in} \quad]0,1[, \\ u(0) & = & 0, \\ u(1) & = & 0. \end{cases} \tag{1}$$

Anti-bounce back condition at $x = 0$ and $x = 1$:

$$f_1(x_b, t + \Delta t) = -f_2(x_e, t + \Delta t) = -f_2^*(x_b, t),$$

to obtain homogeneous Dirichlet b. c. and a uniform body force (δp) to model c.

Let Δq the solid wall position (where the LB solution vanishes).
x_b boundary node, x_e a fictitious outside node.



First D1Q3 scheme

$$\left\{ \begin{array}{ll} \bullet & \mathbf{m} = M.\mathbf{f} \\ \bullet & \widetilde{\rho} = \rho + \frac{\delta p}{2} \\ \bullet & \text{Evaluate moments} \\ \bullet & \text{Collision } \; m_\ell^* = (1 - s_\ell) m_\ell + s_\ell m_\ell^{eq}, \quad 1 \le \ell \le 2, \\ \bullet & \widetilde{\rho} = \rho + \frac{\delta p}{2} \\ \bullet & \mathbf{f} = M^{-1}.\mathbf{m} \\ \bullet & \text{Advection} \end{array} \right.$$

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

Equilibrium values :
$m_1^{eq} = 0$ and $m_2^{eq} = \zeta \widetilde{\rho}$.

Macroscopic equation :

$$\frac{\partial \rho}{\partial t} - \Delta t \lambda^2 \sigma_1 \zeta \frac{\partial^2 \rho}{\partial x^2} = \mathrm{O}(\Delta t^3), \text{ where } \sigma_1 = (\frac{1}{s_1} - \frac{1}{2}).$$

The exact solution of the problem (1) is : $u(x) = x(1 - x)c/(2\mathcal{K})$.

$$m_1^* = \Delta t \lambda^2 \left(\frac{1}{2} - \sigma_1\right) \zeta \frac{\partial \rho}{\partial x} + \mathrm{O}(\Delta t^3). \quad (2)$$

$$m_2^* = \lambda^2 \frac{\zeta}{2} \rho - \Delta t^2 \lambda^4 \frac{\zeta}{2} \sigma_1 \left(\frac{1}{2} - \sigma_2\right) \frac{\partial \rho}{\partial x^2} + \mathrm{O}(\Delta t^3) \quad (3)$$

With the help of the inverse moments matrix M^{-1}, we have :

$$f_1^* = \frac{1}{2\lambda^2} \left[2m_2^* + \lambda m_1^*\right], \quad f_2^* = \frac{1}{2\lambda^2} \left[2m_2^* - \lambda m_1^*\right]. \quad (4)$$

At the boundary we consider the following quantity :

$$f_1^*(x_e) + f_2^*(x_b) = \frac{1}{2\lambda^2} \left[2(m_2^*(x_e) + m_2^*(x_b)) + \lambda(m_1^*(x_e) - m_1^*(x_b))\right]. \quad (5)$$

Using (3) and (2) we have respectively :

$$\begin{aligned} m_2^*(x_e) + m_2^*(x_b) &= \lambda^2 \frac{\zeta}{2} [\rho(x_e) + \rho(x_b)] - \quad (6) \\ &- \Delta t^2 \lambda^4 \frac{\zeta}{2} \sigma_1 (\frac{1}{2} - \sigma_2) [\frac{\partial^2 \rho}{\partial x^2}(x_e) + \frac{\partial^2 \rho}{\partial x^2}(x_b)] + \mathrm{O}(\Delta t^3), \\ m_1^*(x_e) - m_1^*(x_b) &= \Delta t \lambda^2 \zeta (\frac{1}{2} - \sigma_1) [\frac{\partial \rho}{\partial x}(x_e) - \frac{\partial \rho}{\partial x}(x_b)] + \mathrm{O}(\Delta t^3). \quad (7) \end{aligned}$$

With the help of classical Taylor expansion we have, with the notation $x_i \equiv \frac{1}{2}(x_b + x_e)$:

$$\rho(x_e) + \rho(x_b) = 2\rho(x_i) + \frac{\Delta x^2}{4}\frac{\partial^2 \rho}{\partial x^2}(x_i) + \mathrm{O}(\Delta x^3), \quad (8)$$

$$\frac{\partial \rho}{\partial x}(x_e) - \frac{\partial \rho}{\partial x}(x_b) = -\Delta x \frac{\partial^2 \rho}{\partial x^2}(x_i) + \mathrm{O}(\Delta x^3), \quad (9)$$

$$\frac{\partial^2 \rho}{\partial x^2}(x_e) + \frac{\partial^2 \rho}{\partial x^2}(x_b) = 2\frac{\partial^2 \rho}{\partial x^2}(x_i) + \mathrm{O}(\Delta x^2). \quad (10)$$

Considering equation (5), together with (6), and (7) and taking into account relations (8), (9) and (10) we obtain :

$$f_1^*(x_e) + f_2^*(x_b) = \zeta\rho(x_i) + \Delta t^2 \lambda^2 \zeta \left[\sigma_1\sigma_2 - \frac{1}{8}\right] \frac{\partial^2 \rho}{\partial x^2}(x_i) + \mathrm{O}(\Delta t^3). \quad (11)$$

Thus when

$$\sigma_1\sigma_2 = \tfrac{1}{8}$$

the boundary interface is located at $x = \frac{\Delta x}{2}$.

Second D1Q3 scheme

We change now the following matrix D1Q3 :

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

Equilibrium values : $m_1^{eq} = 0$ and $m_2^{eq} = \lambda^2 \widetilde{\zeta} \rho.$
Macroscopic equation :

$$\frac{\partial \rho}{\partial t} - \Delta t \lambda^2 \sigma_1 \frac{2 + \widetilde{\zeta}}{3} \frac{\partial^2 \rho}{\partial x^2} = \mathrm{O}(\Delta t^3),$$

and thermal diffusion $\mathcal{K}$ is equal to $\Delta t \lambda^2 \sigma_1 \frac{2+\widetilde{\zeta}}{3}$

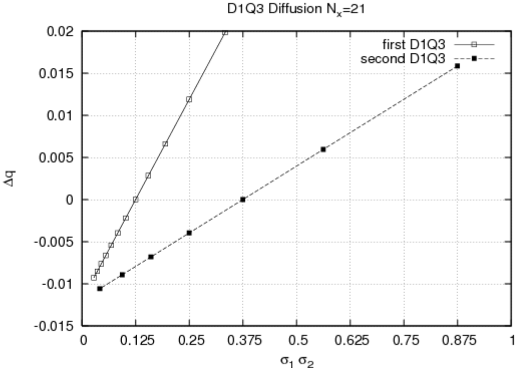
For the above D1Q3 lattice Boltzmann scheme, the Poisson's numerical solution vanishes at $\Delta q = \frac{\Delta x}{2}$ for the following condition :

$$(\frac{1}{s_1} - \frac{1}{2})(\frac{1}{s_2} - \frac{1}{2}) \equiv \sigma_1 \sigma_2 = \frac{3}{8}.$$

• Proof : Similarly to the previous proof, we obtain :

$$f_1^*(x_e) + f_2^*(x_b) = \frac{2+\widetilde{\zeta}}{3}\rho(x_i) + \Delta t^2 \lambda^2 \frac{2+\widetilde{\zeta}}{72}\left[8\sigma_1\sigma_2 - 3\right]\frac{\partial^2 \rho}{\partial x^2}(x_i) + \mathrm{O}(\Delta t^3).$$

Product $\sigma_1 \sigma_2$ *vs.* solid "wall" position Δq.



□ First D1Q3 model : Magic $\sigma_1 \sigma_2 = \frac{1}{8}$.

■ Second D1Q3 model : Magic $\sigma_1 \sigma_2 = \frac{3}{8}$.

D2Q9 scheme

Velocity set

$$\begin{cases} e_0 = (0,0), e_1 = (1,0), e_2 = (0,1), e_3 = (-1,0), e_4 = (0,-1) \\ e_5 = (1,1), e_6 = (-1,1), e_7 = (-1,-1), e_8 = (1,-1) \end{cases}$$

$$v_j = \lambda e_j, j = 0, .., 8$$

LBM scheme

$$f_j(x, t+\Delta t) = f^*(x - v_j \Delta t, t), \quad v_j \in \mathcal{V}, \quad x \in \mathcal{L}_0$$

Matrix moments :

• Conserved moments :

$m_0 = \rho = \sum_{i=0}^{8} f_i$ (density, order zero $x^0 \times y^0 = \mathbf{1}$)

$m_1 = j_x = \sum_{j=0}^{8} v_j^1 f_j = \lambda(f_1 - f_3 + f_5 - f_6 - f_7 + f_8)$ (mass flux,order x^1)

$m_2 = j_y = \sum_{j=0}^{8} v_j^2 f_j = \lambda(f_2 - f_4 + f_5 + f_6 - f_7 - f_8)$,(mass flux, order y^1)

Non conserved moments :

• cinetique energie : $e = \frac{1}{2}\sum_j |v_j|^2 f_j$ (order $x^2 + y^2$)

$$m_3 = \frac{e}{\lambda^2} - \frac{2}{3}\rho = -4f_0 - \sum_{j=1}^{j=4} f_j + 2\sum_{j=5}^{9} f_j, \qquad (-4 + 3(x^2 + y^2))$$

• energie square $\epsilon = \sum \left(\frac{1}{2}|v_j|^2\right)^2 f_j$, (order $(x^2 + y^2)^2$)

$$m_4 = 4f_0 - 2\sum_{j=1}^{j=4} f_j + \sum_{j=5}^{j=8} f_j$$

• energy flux $\varphi = \sum_j \frac{1}{2}|v_j|^2 v_j f_j$ (order $x * (x^2 + y^2)$ et $y * (x^2 + y^2)$)

$$m_5 = \frac{6}{\lambda^3}\varphi^1 - 5\frac{j_x}{\lambda} = -2f_1 + 2f_3 + f_5 - f_6 - f_7 + f_8$$
$$m_6 = \frac{6}{\lambda^2}\varphi^2 - 5\frac{j_y}{\lambda} = -2f_1 + 2f_3 + f_5 - f_6 - f_7 + f_8$$

• diagonal component of the stress tensor (order $x^2 - y^2$)

$$m_7 = \frac{1}{\lambda^2}\left(\sum_j v_j^1 v_j^1 f_j - \sum_j v_j^2 v_j^2 f_j\right) = f_1 - f_2 + f_3 - f_4$$

• off-diagonal component of the stress tensor (order $x * y$)

$$m_8 = \frac{1}{\lambda^2}\sum_j v_j^1 v_j^2 f_j = f_5 - f_6 + f_7 - f_8$$

Relaxation and Equilibrium

- Relaxation of moments : $m_j^* = m_j - s_j(m_j - m_j^{eq})$

	m_j	m_j^{eq}	relaxation rates
energy	e	$\alpha\rho + \frac{\gamma_3}{\lambda^2}(j_x^2 + j_y^2)$	s_3
energy square	ϵ	$\beta\rho + \frac{\gamma_4}{\lambda^2}(j_x^2 + j_y^2)$	s_4
energy flux	q_x	$c_1 \frac{j_x}{\lambda}$	s_5
energy flux	q_y	$c_2 \frac{j_y}{\lambda}$	s_5
stress tensor	$p_x x$	$\frac{\gamma_7}{\lambda^2}\left(j_x^2 - j_y^2\right)$	s_7
stress tensor	$p_x y$	$\frac{\gamma_8}{\lambda^2} j_x j_y$	s_8

• Linear case

$c_1 = c_2 = -1, \gamma_3 = \gamma_4 = \gamma_7 = \gamma_8 = 0$

$$\left\{ \begin{array}{lcl} \partial_t \rho + \partial_x j_x + \partial_y j_y & = & \mathrm{O}(\Delta t^2), \\ \partial_t j_x + c_0^2 \partial_x \rho - \zeta \left(\partial_x^2 j_x + \partial_{xy} j_y \right) - \nu \left(\partial_x^2 j_x + \partial_y^2 j_x \right) & = & \mathrm{O}(\Delta t^2), \\ \partial_t j_y + c_0^2 \partial_y \rho - \zeta \left(\partial_{yx} j_x + \partial_y^2 j_y \right) - \nu \left(\partial_x^2 j_y + \partial_y^2 j_y \right) & = & \mathrm{O}(\Delta t^2). \end{array} \right.$$

$$c_0^2 = \lambda^2 \frac{4+\alpha}{6},$$

Isotropic viscosity : $c_1 = c_2 = -1$ and $s_7 = s_8$.

$$\begin{array}{rcl} \zeta & = & -\alpha \frac{\lambda^2 \Delta t}{6} \left(\frac{1}{s_3} - \frac{1}{2} \right), \\ \nu & = & \frac{\lambda^2 \Delta t}{3} \left(\frac{1}{s_8} - \frac{1}{2} \right). \end{array}$$

• Non linear case (Navier-Stokes)
$\gamma_3 = 3, \gamma_7 = 1$ and $\gamma_8 = 1$

$$\begin{aligned}
\partial_t \rho + \partial_x j_x + \partial_y j_y &= \mathrm{O}(\Delta t^2), \\
\partial_t j_x + \partial_x j_x^2 + \partial_y \left(j_x j_y \right) + c_0^2 \partial_x \rho &- \zeta \left(\partial_x^2 j_x + \partial_{xy} j_y \right) - \\
&- \nu \left(\partial_x^2 j_x + \partial_y^2 j_x \right) = \mathrm{O}(\Delta t^2), \\
\partial_t j_y + \partial_x \left(j_x j_y \right) + \partial_y j_y^2 + c_0^2 \partial_y \rho &- \zeta \left(\partial_{yx} j_x + \partial_y^2 j_y \right) - \\
&- \nu \left(\partial_x^2 j_y + \partial_y^2 j_y \right) = \mathrm{O}(\Delta t^2).
\end{aligned}$$

β and γ_4 remain adjustable.

Equilibrium distribution is given by :

$$\mathbf{f} = M^{-1}\mathbf{m}^{\mathbf{eq}}$$

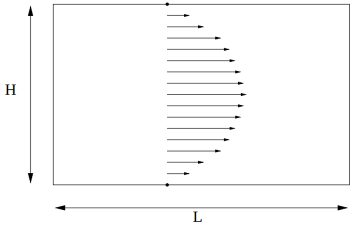
$$f_j^{eq} = w_j\left[\rho + \frac{3}{\lambda}(e_j.\mathbf{j}) + \frac{9}{2\lambda^2}(e_j.\mathbf{j}) - \frac{3}{2\lambda^2}|\mathbf{j}|^2\right],$$

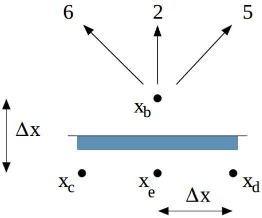
where $w_0 = \frac{4}{9}$, $w_1 = w_2 = w_3 = w_4 = \frac{1}{9}$ and $w_5 = w_6 = w_7 = w_8 = \frac{1}{36}$.
The same equilibrium distribution for BGK model.

Remarks

• Take the same relaxation time for odd moments and another one for even moments the above MRT model degenerates to the TRT model.

• If $s_3 = s_4 = \cdots = s_8 = \frac{1}{\tau}$, $\beta = 4$ and $\gamma_4 = -18$ the above MRT model degenerates to the LBGK model.





$$\begin{cases} -\nu\Delta\mathbf{u} + \frac{1}{\rho}\nabla p &= 0, \\ p(0,y) = -p(L,y) &= \delta p, \text{ for } 0 \leq y \leq H, \\ \mathbf{u}(x,0) = \mathbf{u}(x,H) &= 0 \text{ for } 0 \leq y \leq H \end{cases}$$

The solution is :

$$\mathbf{u}(x,y) \equiv (u(y) = Ky(H-y), v(x,y) = 0),$$
$$p(x,y) = 2\rho\nu Kx + P_0,$$

where P_0 is a given constants.

We note that the above problem is equivalent to :

$$\begin{cases} -\nu\Delta \mathbf{u} & = & \mathbf{F}, \\ \mathbf{u}(x,0) = \mathbf{u}(x,H) & = & 0, \end{cases}$$

where $\mathbf{F} = (F_x, 0)$ is the external force. The solution is given by :

$$\mathbf{u}(x,y) = \left(u(y) = \frac{F_x}{2\nu} y(H-y), v(x,y) = 0 \right).$$

LBM scheme :

- Equilibrium values :
  $m_3^{eq} = \alpha\rho,\ m_4^{eq} = \beta\rho,\ m_5^{eq} = -\frac{j_x}{\lambda},\ m_6^{eq} = -\frac{j_y}{\lambda},\ m_7^{eq} = 0,\ m_8^{eq} = 0.$
- Relaxation rates : $s_7 = s_8 = \left(\frac{1}{2} + \frac{3\nu}{\lambda^2 \Delta t}\right)^{-1}$

$$
\begin{cases}
\mathbf{m}=M\mathbf{f} \\
\widetilde{J}_x = j_x + \frac{\Delta t}{2} F_x \\
\text{evaluate moments} \\
\text{collision (relaxation of moments)} \\
\widetilde{J}_x = j_x + \frac{\Delta t}{2} F_x \\
\mathbf{f} = M^{-1}\mathbf{m} \\
\text{advection and boundary conditions}
\end{cases}
$$

Boundary condition (bounce back) :

$$
f_2(x_b, t+\Delta t) = f_4^*(x_e, t+\Delta t) = f_4^*(x_b, t)
$$
$$
f_5(x_b, t+\Delta t) = f_7^*(x_c, t+\Delta t) = f_7^*(x_b, t)
$$
$$
f_6(x_b, t+\Delta t) = f_8^*(x_d, t+\Delta t) = f_8^*(x_b, t)
$$

Proposition

For the above D2Q9 scheme the bounce-back numerical boundary condition is of order 3 at location $\Delta q = \frac{\Delta x}{2}$ for the Dirichlet boundary condition $\mathbf{u} = 0$ if and only if

$$\sigma_5 \sigma_8 = \frac{3}{8},$$

where $\sigma_l = \left(\frac{1}{s_l} - \frac{1}{2}\right)$.

Proof

We evaluate the non conserved moments. We compute moements at the "external nodes". Using matrix M^{-1} we evaluate $f^*(x_b)$, $f^*(x_c)$, $f^*(x_d)$, and $f^*(x_e)$. We obtain :

$$f_5^*(x_c) - f_7^*(x_b) = \frac{1}{6} j_x(x_i) + \frac{\Delta x^2}{144}\left(8\sigma_5\sigma_8 - 3\right)\frac{\partial^2 j_x}{\partial y^2}(x_i) + \mathrm{O}(\Delta t^3).$$

Remark if we perform the body force as follows :

$$\begin{cases} \mathbf{m}\text{=M } \mathbf{f} \\ \text{collision} \\ \mathbf{f} = M^{-1}\mathbf{m} \\ \text{advection} \\ \text{apply the body force} \quad \begin{cases} f_1 = f_1 + \frac{F_x}{3\lambda}, & f_2 = f_2 \\ f_3 = f_3 - \frac{F_x}{3\lambda}, & f_4 = f_4 \\ f_5 = f_5 + \frac{F_x}{12\lambda}, & f_6 = f_6 - \frac{F_x}{12\lambda} \\ f_7 = f_7 - \frac{F_x}{12\lambda}, & f_8 = f_8 + \frac{F_x}{12\lambda} \end{cases} \end{cases}$$

which is equivalent in moments space to

$$\widetilde{j}_x = j_x + F_x, \quad \widetilde{m}_5 = m_5 - \frac{F_x}{\lambda} \text{ and } \widetilde{m}_k = m_k \text{ for others moments,}$$

the solid wall for the Poiseuille is exactly located at $\Delta q = \frac{\Delta x}{2}$ for the following value of relaxation parameters

$$\sigma_5 \sigma_8 = \frac{3}{16}$$

as proposed by I. Ginzburg and D. d'Humières (2003).

D2Q9 for advection-diffusion problems

Conserved moment : $\rho = T$.
Non-conserved moments :

m_j	m_j^{eq}	relaxation rates
j_x	$\lambda U \rho$	s_x
j_y	$\lambda V \rho$	s_y
e	$\alpha\rho + \gamma_3(U^2 + V^2)$	s_3
ϵ	$\beta\rho$	s_4
q_x	$U\rho[c_1 + \gamma_5(U^2 + V^2)]$	s_5
q_y	$V\rho[c_2 + \gamma_6(U^2 + V^2)]$	s_5
$p_x x$	$a_x\rho + \gamma_7(U^2 - V^2)$	s_7
$p_x y$	$a_y\rho + \gamma_8 UV$	s_8

• Equivalent Equation :

$$\frac{\partial T}{\partial t} + \lambda\left(U\frac{\partial T}{\partial x} + V\frac{\partial T}{\partial y}\right) - \lambda^2\Delta t\Big[\frac{1}{6}(\frac{1}{2} - \frac{1}{s_x})(\alpha + 3a_x + 4)\frac{\partial^2 T}{\partial x^2}$$

$$+ \frac{1}{6}(\frac{1}{2} - \frac{1}{s_y})(\alpha - 3a_x + 4)\frac{\partial^2 T}{\partial y^2}$$

$$+ a_y(\frac{1}{s_x} + \frac{1}{s_y} - 1)\frac{\partial^2 T}{\partial xy}\Big] = 0.$$

where

$$c_1 = c_2 = -1, \gamma_3 = 3, \gamma_5 = \gamma_6 = 3, \gamma_7 = \gamma_8 = 1$$

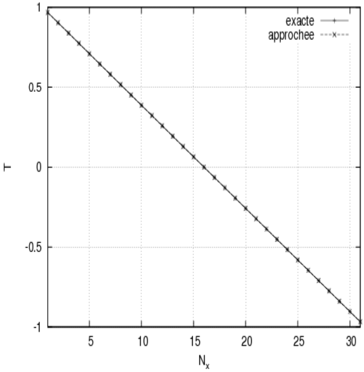
to kill the dependency of the diffusivity to the advection velocity (U, V).

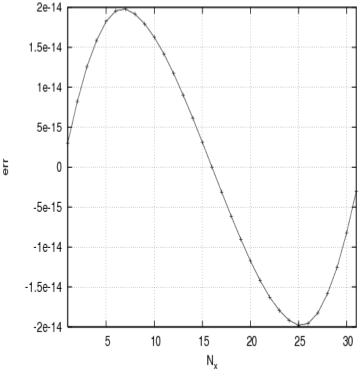
Numerical tests

- 1-D test case, affine solution $u(x) = -2x + 1$.

$$\left\{ \begin{array}{rcl} -k.u''(x) & = & 0 \quad \text{on} \quad]0,1[, \\ u(0) & = & 1, u(1) = -1. \end{array} \right.$$

LB coefficients :
$\alpha = -2$, $\beta = 1$, $U = V = 0$, $s_x = s_y$ and $a_x = a_y = 0$.
Periodic boundary conditions in y and anti-bounce back in x.





Solutions : exact and approximate　　　　Error : $(u_{\mathrm{ex}} - u_{\mathrm{app}})$,

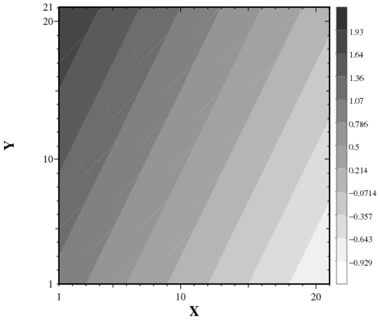
Coefficient of diffusion $k = 0.11$ and nember of nodes $N_x = 31$.

Error l^2=$\left(\frac{\sum_{K\in\mathcal{T}}|K|(u(x_K)-u_K)^2}{\sum_{K\in\mathcal{T}}|K|u(x_K)^2}\right)^{\frac{1}{2}} = 2.41606899.10^{-14}$, where $h = 0.032$.

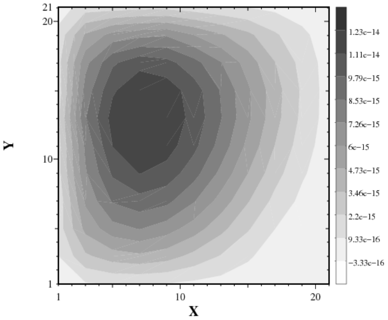
Case test : solution affine in 2-D $u(x,y) = 1 - 2x + y$.

$$\begin{cases} -k.\Delta u & = & 0 \quad \text{sur} \quad \Omega, \\ \overline{u} & = & u_{|\Gamma_D = \partial\Omega} \end{cases}$$

LB Coefficients :
$\alpha = -2$, $\beta = 1$, $U = V = 0$, $s_x = s_y$ and $a_x = a_y = 0$.
Boundaries Conditions : Anti-Bounce Back in x and y.



Approximate Solution



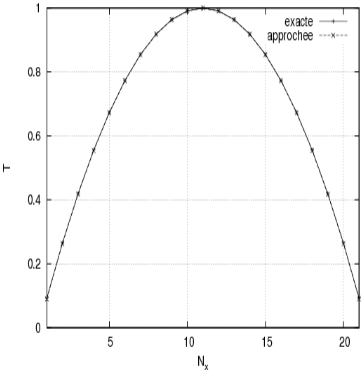
Erreur : $(u_{\text{ex}} - u_{\text{app}})$,

Coefficient of diffusion $k = 0.11$ and number of nodes $N_x = N_y = 21$.
Error $l^2 = 7.55994542.10^{-15}$, where $h = \Delta x = \Delta y = 0.047$.

Case test : Polynomial solution in 1-D $u(x) = 4x(x-1)$.

$$\begin{cases} -k.\Delta u & = & f \quad \text{on} \quad \Omega, \\ \overline{u} & = & u_{|\Gamma_D = \partial\Omega} \end{cases}$$

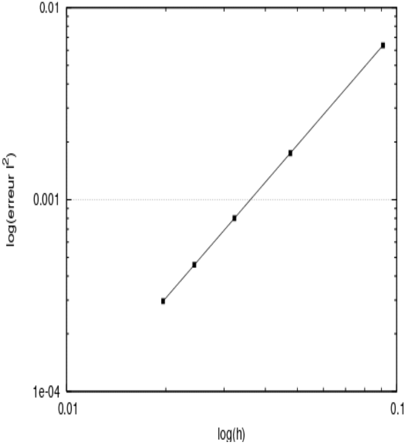
where $f = -4k$.
LB Coefficients :
$\alpha = -2$, $\beta = 1$, $U = V = 0$, $s_x = s_y$ and $a_x = a_y = 0$.
Boundaries Conditions : Anti-Bouce Back in x and periodique in y.



Approximate solution

Diffusion Coefficient $k = 0.11$ and number of nodes $N_x = 21$.
Error $l^2 = 0.0017$, where $h = \Delta x = 0.047$.

• Ordre accuracy.



The ℓ^2 error between analytical solution and approximate one. It shows second order accuracy.

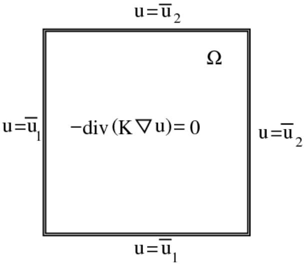
D2Q9 for anisotropic diffusion problem

- Using LBM for anisotropic diffusion problem. Let $\Omega =]0,1[\times]0,1[$.

$$\left\{\begin{array}{ccccc} -\nabla.(K\nabla u) & = & f & \text{dans} & \Omega, \\ u & = & \overline{u} & \text{sur} & \Gamma_D, \\ K\nabla u.n & = & g & \text{sur} & \Gamma_N, \end{array}\right.$$

where $\Gamma_D \cap \Gamma_N = \partial\Omega$,
$K = \begin{pmatrix} k_{1,1} & k_{1,2} \\ k_{2,1} & k_{2,2} \end{pmatrix}$ diffusion tensor,
f source term,
$\overline{u}$ and g Dirichlet and Neumann boundary conditions.

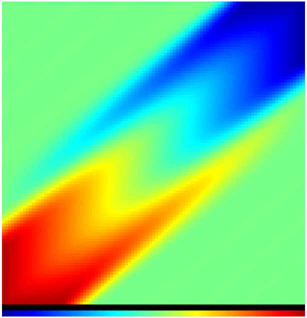
2-D anisotropic diffusion problem with Dirichlet boundaries conditions.
Let $\Omega =]0,1[\times]0,1[$,
$\mathbf{K} = R_\theta \,\mathrm{diag}(1, 10^{-3})\, R_\theta^{-1}$, R_θ is matrix of rotation with $\theta = 40$ degrees.



The givens functions $\overline{u}_i$ are continuous and linear on $\partial\Omega$:

$$\overline{u}_1 = \begin{cases} 1 & , \quad x \in [0, 0.2] \\ \frac{1}{2} & , \quad x \in [0.3, 1] \end{cases}, \quad \overline{u}_2 = \begin{cases} \frac{1}{2} & , \quad x \in [0, 0.7] \\ 0 & , \quad x \in [0.8, 1] \end{cases}$$

• Approximation of the solution computed by D2Q9 after convergence (*i.e.* 5.10^6 times steps) with $s_1 = 1.3$, $s_2 = 1.8$ and $\beta = 1$.



Approximation of solution on regular lattice (151×151 nodes).

Higher order LB scheme for advection diffusion

• D2Q9, Equivalent Equation :

$$\frac{\partial T}{\partial t} + \lambda\Big(U\frac{\partial T}{\partial x} + V\frac{\partial T}{\partial y}\Big) - \frac{\lambda^2 \Delta t}{6}(\frac{1}{2} - \frac{1}{s})(\alpha + 4)\Delta T + \Delta t^2 A + \Delta t^3 B = 0.$$

where $s_x = s_y = s$, $a_x = a_y = 0$.
Free parameters : s_3, s_4, s_5, s_7, s_8, α and β.
Quantity A : involves third order space derivatives of T and depends on the advection velocity.
Quantity B : involves fourth order space derivatives of T.
is it possible to get $A = 0$?
is it possible to get $B = 0$ at least for pure diffusion ?

Let recall that $\sigma_k = \left(\frac{1}{s_k} - \frac{1}{2}\right)$. By taking the following configuration :

$$\sigma_1 = \sigma_3 = \sigma_4 = \sigma_5 = \frac{1}{\sqrt{12}}$$

the quantity A becomes null.
Thus the LB scheme is exact up to order 3.
Remark : The LB parameters β, s_4 and s_5 remain free.

Numerical Validation of third order accuracy

Initial condition : $T(\vec{x}, 0) = \sin\left(2\pi \vec{k}^T \cdot \vec{x}\right), \forall \vec{x} \in \Omega$;

Analytic solution : $T^{th}(\vec{x}, t) = \sin\left(2\pi \vec{k}^T \cdot \left(\vec{x} - \vec{w}t\right)\right) \mathrm{e}^{-\|2\pi\vec{k}\|\kappa t}, \forall \vec{x} \in \Omega, \forall t > 0$;

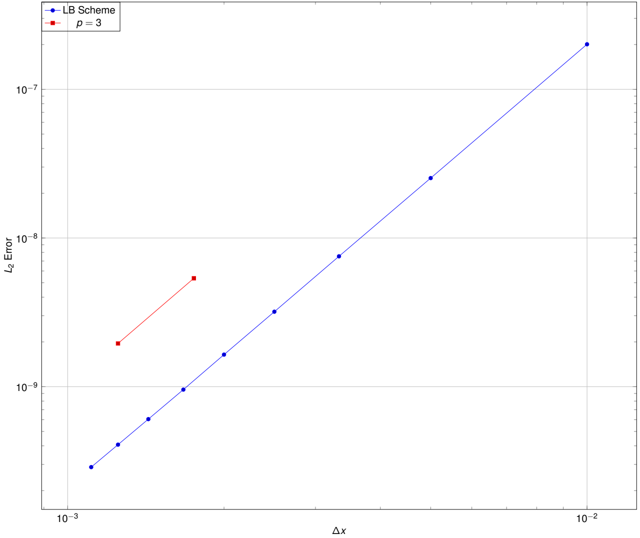
Boundaries Conditions : Periodic for all boundaries (avoid boundary accuracy);

Physical variables : $\mathcal{K} = 2 \cdot 10^{-2}$ and $\vec{w} = (U, V) = \left(10^{-1}, -5 \cdot 10^{-2}\right)^T$;

LB variable : $\lambda = 5 \cdot 10^3$, $\Delta x = \frac{1}{\ell 10^2}, \forall \ell \in \{1, 2, \ldots, 10\}$, $\Delta t = \frac{\Delta x}{\lambda}$, $\alpha = \frac{-6\kappa}{\sigma_1 \Delta t \lambda^2}$, $\beta = 0$, $s_4 = 2$ and $s_5 = 1.2$;

Error between numerical and analytic solution :

$$Err\left(T^{LB} - T^{th}\right) = \sqrt{\Delta x^2 \sum_{\vec{x} \in \mathcal{L}} \left(T^{LB}(\vec{x}) - T^{th}(\vec{x})\right)^2}.$$



LB scheme : $p \simeq 2.98$

Fourth order accuracy for pur diffusion scheme

In this case the advection diffusion $U = V = 0$.
The D2Q9, Equivalent Equation :

$$\frac{\partial T}{\partial t} - \frac{\lambda^2 \Delta t}{6}(\frac{1}{s} - \frac{1}{2})(\alpha + 4)\Delta T + \Delta t^3 B = 0.$$

With this configuration :

$$\sigma_7 = \sigma_8 = \frac{1}{12\sigma}, \sigma_3 = -\frac{2(\alpha+4)\sigma}{\alpha} + \frac{8+3\alpha}{12\alpha\sigma}$$

$$4 + 3\alpha + 2\beta = 0$$

$$\sigma_5 = \sigma_6 = \frac{2\sigma(\alpha-2)(1-(3\alpha+12)\sigma^2)}{(1-12\sigma^2)(\alpha+4)}$$

the quantity B is equal zero and the scheme is fourth order accuracy.

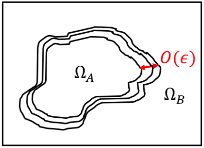
3D Image processing using LBM

Objective : Investigate **a phase field segmentation** method using multiple relaxation time LBM for 3D ultrasound images.

- Cahn-Hilliard Energy : $E_\epsilon^{CH}(u) = \int_\Omega \left(\epsilon \frac{|\nabla u|^2}{2} + \frac{1}{\epsilon} W(u) \right) d\mathbf{x}$

  where $W(u) = 1/2u^2(1-u)^2$
- Allen-Cahn Equation (minimize Cahn-Hilliard energy by a gradient descent) :

$$\frac{\partial u}{\partial t} = \epsilon \Delta u - \frac{1}{\epsilon} W'(u)$$



- $\Omega_A = \{\mathbf{x} \ : \ u(\mathbf{x}, t) > 1/2, t \geq 0\}$
- $\Omega_B = \{\mathbf{x} \ : \ u(\mathbf{x}, t) < 1/2, t \geq 0\}$
- $\Gamma_t = \{\mathbf{x} \ : \ u(\mathbf{x}, t) = 1/2, t \geq 0\}$

Application to segmentation process

- A log-likelihood distance

$$LL = -(S_A + S_B)$$

$$S_A = -|\Omega_A| \sum_I \hat{P}_A(I) \log \hat{P}_A(I)$$

$$S_B = -|\Omega_B| \sum_I \hat{P}_B(I) \log \hat{P}_B(I)$$

- Parzen estimation

$$\hat{P}_A(I) = \frac{\int u^2 \delta(I_{\mathbf{x}} - I) d\mathbf{x}}{\int u^2 d\mathbf{x}}$$

$$\hat{P}_B(I) = \frac{\int (u-1)^2 \delta(I_{\mathbf{x}} - I) d\mathbf{x}}{\int (u-1)^2 d\mathbf{x}}$$

- Minimize the following energy

$$E_\epsilon(u) = LL(u) + \frac{\alpha}{c_W} E_\epsilon^{CH}(u)$$

- Using a gradient descent of the above energy

$$\frac{\partial u}{\partial t} = 2u \log \hat{P}_A(I_{\mathbf{x}}) + 2(u-1) \log \hat{P}_B(I_{\mathbf{x}}) + \frac{\alpha}{c_W}\left(\epsilon \Delta u - \frac{1}{\epsilon} W'(u)\right)$$

- Thus, the following diffusion equation is obtained :

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathcal{K} \nabla u) + F,$$

where diffusion coefficient

$$\mathcal{K} = \frac{\varepsilon \mu}{c_W},$$

and the source term

$$F = 2u \log \hat{P}_A(I(x)) + 2(u-1) \log \hat{P}_B(I(x)) - \frac{\mu}{c_W}\frac{1}{\varepsilon} W'(u).$$

The D3Q7 scheme, have 7 discrete velocities :

$e_0 = (0, 0, 0)$
$e_1 = (1, 0, 0)$, $e_2 = (-1, 0, 0)$
$e_3 = (0, 1, 0)$, $e_4 = (0, -1, 0)$
$e_5 = (0, 0, 1)$, $e_6 = (0, 0, -1)$

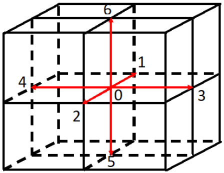
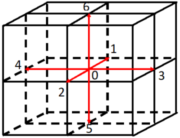


FIGURE – D3Q7 stencil

- Only one conserved moment : $\rho = \bar{u} = \sum_i u_i$
- Non-conserved moments :

m_j	m_j^{eq}	relaxation rate
j_x	0	s_x
j_y	0	s_y
j_z	0	s_z
e	$\beta\rho$	s_4
p_{xx}	0	s_5
p_{yy}	0	s_5

The evolution of the population u_i :



$$u_i(x, t+\Delta t) = u_i^*(x - v_i\Delta t, t), \quad 0 \leq i \leq 6$$

where superscript $*$ describe quantities after collision.
Algorithm :

$$\begin{cases} \mathbf{m}=M\mathbf{u} \\ \widetilde{\mathbf{m}} = \mathbf{m} + \Delta t \frac{\mathbf{F}^{mo}}{2} \\ \text{Collision (relaxation of moments)} \\ \mathbf{m} = \widetilde{\mathbf{m}} + \Delta t \frac{\mathbf{F}^{mo}}{2} \\ \mathbf{u} = M^{-1}\mathbf{m} \\ \text{Advection and boundary condtions (Anti-bounce back)} \end{cases}$$

where $\mathbf{m} = [m_0, ..., m_i, ..., m_6]^T$, $\mathbf{F}^{mo} = [{F_0}^{mo}, ..., {F_i}^{mo}, ..., {F_6}^{mo}]^T$ and $F_i^{mo} = \mathbf{M} t_i S$

$$S = 2\bar{u} \sum_I \hat{P}_{\bar{\mathbf{x}}}(I) \log \hat{P}_A(I_\mathbf{x}) + 2(\bar{u} - 1) \sum_I \hat{P}_{\bar{\mathbf{x}}}(I) \log \hat{P}_B(I_\mathbf{x})$$

MRT D3Q7

- Macroscopic equation, where $s = s_x = s_y = s_z$:

$$\frac{\partial u}{\partial t} - \mathcal{K}\Delta u + \Delta t^2 A + \Delta t^3 B = O(\Delta t^4)$$

where the diffusion coefficient is :

$$\mathcal{K} = \frac{\lambda^2}{21}\Delta t(6+\beta)\left(\frac{1}{s} - \frac{1}{2}\right)$$

- $\mathcal{K}$ is fixed by Δt, Δx, s et β.
- With the following choice :

$$s_4 = \left[\frac{6+\beta}{1-\beta}\left(\frac{1}{s} - \frac{1}{2}\right) + \frac{3\beta+4}{12(\beta-1)\left(\frac{1}{s} - \frac{1}{2}\right)} + \frac{1}{2}\right]^{-1}$$

$$s_5 = \left[\frac{1}{6\left(\frac{1}{s} - \frac{1}{2}\right)} + \frac{1}{2}\right]^{-1}$$

The LB scheme is exact up to order 4, *i. e.* terms $A = B = 0$.

MRT D3Q19

The D3Q19 scheme, have 19 discrete velocities :

$$\mathbf{e}_i = \begin{cases} (0,0,0), & \alpha = 0 \\ (\pm 1,0,0), \quad (0,\pm 1,0), \quad (0,0,\pm 1) & \alpha = 1,2,...,6 \\ (\pm 1,\pm 1,0), \quad (\pm 1,0,\pm 1), \quad (0,\pm 1,\pm 1) & \alpha = 7,8,...,18 \end{cases}$$

Only one conserved moment : $\rho = \bar{u} = \sum_i u_i$

18 non conserved moments :

m_j	m_j^{eq}	relaxation rate	m_j	m_j^{eq}	Coeff. de relaxation
e	$\beta\rho$	ω_e	π_{xx}	0	$\omega_{\mathcal{K}}$
ϵ	$\gamma\rho$	$\omega_{\mathcal{K}}$	$p_{\omega\omega}$	0	ω_e
j_x	0	$\omega_{\mathcal{K}}$	$\pi_{\omega\omega}$	0	$\omega_{\mathcal{K}}$
q_x	0	$\omega_{\mathcal{K}}$	p_{xy}	0	ω_e
j_y	0	$\omega_{\mathcal{K}}$	p_{yz}	0	ω_e
q_y	0	$\omega_{\mathcal{K}}$	p_{xz}	0	ω_e
j_z	0	$\omega_{\mathcal{K}}$	m_x	0	ω_e
q_z	0	$\omega_{\mathcal{K}}$	m_y	0	ω_e
p_{xx}	0	ω_e	m_z	0	ω_e

- Macroscopic equation up to order 4 :

$$\frac{\partial u}{\partial t} - \mathcal{K}\Delta u + \Delta t^2 A + \Delta t^3 B = O(\Delta t^4)$$

where the diffusion coefficient is :

$$\mathcal{K} = \frac{\lambda^2}{57}\Delta t(\beta + 30)\left(\frac{1}{\omega_{\mathcal{K}}} - \frac{1}{2}\right)$$

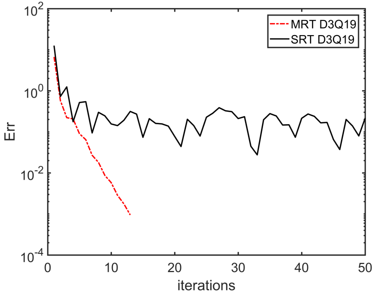
- $\mathcal{K}$ is fixed by Δt, Δx, $\omega_{\mathcal{K}}$ and β.
- With the following choice :

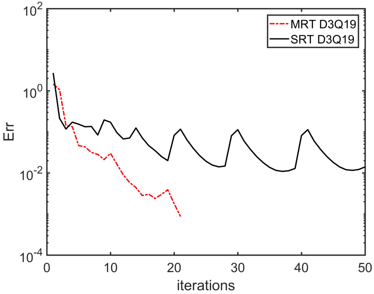
$$\omega_e = \frac{1}{\frac{1}{\sqrt{3}} + \frac{1}{2}}; \qquad \omega_{\mathcal{K}} = \frac{1}{\sqrt{3}}$$

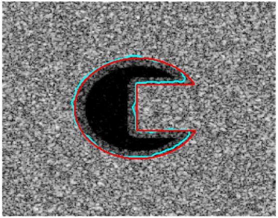
The LB scheme is exact up to order 4, *i. e.* terms $A = B = 0$

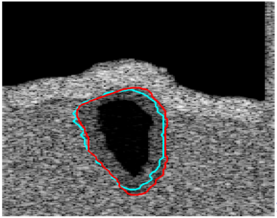
Results for synthetic image

- BGK *vs* MRT (D3Q19) for synthetic image :
  Left : 256^3 voxels and Right : $322 \times 142 \times 172$ voxels.



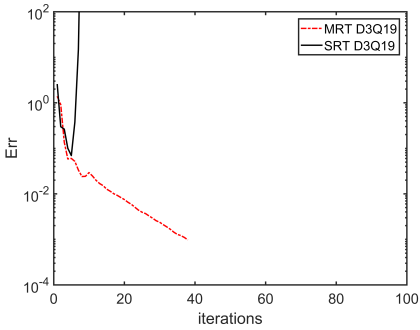


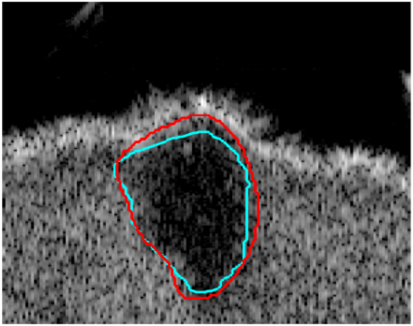




Results for ultrasound 3D image

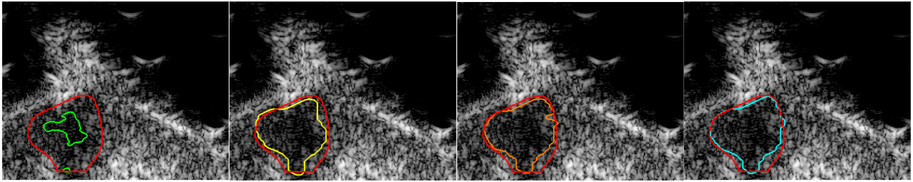
- BGK *vs* MRT (D3Q19)





Left : Convergence test, MRT D3Q19 (black), BGK D3Q19 (red).
Right : Contour of tumor obtained by MRT D3Q19 (cyan) and reference contour (red, given by a doctor).

- Comparison between ADLL, LLCH-exact and MRT LBM.



	ADLL(green)	LLCH-exact (yellow)	MRT D3Q7 (orange)	MRT D3Q19 (cyan)
Dice	0.748 $\pm$ 0.081	**0.861** $\pm$ 0.051	**0.860** $\pm$ 0.048	**0.858** $\pm$ 0.048
S	0.634 $\pm$ 0.122	**0.849** $\pm$ 0.052	**0.858** $\pm$ 0.068	**0.848** $\pm$ 0.064
P	0.937 $\pm$ 0.071	0.876 $\pm$ 0.071	0.868 $\pm$ 0.072	0.873 $\pm$ 0.069
MAD (μm)	341 $\pm$ 110	**197** $\pm$ 83	**197** $\pm$ 71	**200** $\pm$ 70
Times (s)	**19**	23.1	211.2	461

Conclusion

- LB can model advection diffusion problems.
- MRT has some free parameters which have no physical effect (no effect up to order two).
- Free parameters can be chosen either to enhance stability or to enhance boundary condition or to enhance the accuracy of the scheme.
- Magic parameters are related to the way how the scheme is performed, to the choice of the matrix moments and to the numerical problem.
- In 3D, MRT LB scheme has many free parameters and find a stable configuration is difficult. One answer is to chose the parameters which enhance the accuracy of the scheme.

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Thank you for your attention