Nature convective et diffusive de la méthode de Boltzmann sur réseau

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1. Eléments fondateurs de la LBM
   - Liens avec l'équation de Boltzmann continue
   - Les vitesses discrètes
   - L'algorithme LBM
2. Analyse convective du modèle
   - Modes du modèle NS compressible isotherme
   - Modes LBM
   - Selective and adaptive filtering
   - Adaptive relaxation times
   - Quelques applications
3. Interfaces et Mélanges complexes
   - Interfacial dynamics
   - Multicomponent mixing

Equation de Boltzmann (1872)

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + \frac{F_i}{m} \frac{\partial f}{\partial c_i} = \left(\frac{\partial f}{\partial t} \right)_{coll} \qquad (1)$$

$f(\mathbf{x}, c, t)$ Densité de probabilité qu'une particule de vitesse $\mathbf{c}$ soit en (x_1, x_2, x_3) au temps t.

Les quantités macroscopiques $\rho, \rho U$, ρe sont obtenus par les moments :

$$\int (.) d\mathbf{c}, \quad \int c(.) d\mathbf{c}, \quad \int c^2 (.) d\mathbf{c}$$

En 1954, P.,L. Bhatnagar, E.P. Gross et M. Krook montrent que l'EDP :

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = -\frac{1}{\tau}[f - f^{eq}] \tag{2}$$

Avec la fonction d'équilibre :

$$f^{eq}(\mathbf{x}, \mathbf{c}, t) = \rho \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left[-\frac{m}{2k_B T}(\mathbf{c} - \mathbf{u})^2 \right] \tag{3}$$

Est équivalent à Navier-Stokes pour les faibles nombres de Knundsen. (Chapmann-Enskog)
Problème : $\mathbf{c} \in \mathcal{R}^3$ => Il faut discrétiser l'espace des vitesses pour résoudre numériquement.

Vitesses Discrètes

- 1964 Premier réseaux de vitesses par J. Broadwell puis R. Gatignol.

Gaz sur Réseaux

- 1973 Réseau HPP (Hardy, Pomeau, Pazzis) gaz sur réseau (automates cellulaires)
- 1986 Synthèse des automates cellulaires par S.Wolfram.
- 1988 Premiers réseaux à distributions réelles par McNamara & Zanetti.

Boltzmann sur Réseau

- 1992 D'Humière et Qian propose le modèle D2Q9.
- 1992 Modèle à temps de relaxation multiples (d'Humière, Lallemand)
- 2002 MRT 3D (d'Humière et al.)
- 2006 Cascaded LBM (Geier)
- 2013 Modèle à vitesses relatives (Février,Graille, Dubois)
- 2015 Cumulant Model (Geier)

La discrétisation des vitesses se fait en assurant l'égalité des moments continus et discrets :

- Le nombre de vitesse détermine le nombre de moments conservés.
- L'équilibre est écrit sous forme polynômial.
- Les premiers réseaux compacts conservent les 2 premiers moments. (ρ et ρu). Le moment d'ordre 3 (ρe) possède un terme d'erreur en $\mathcal{O}(Ma^3)$.
- Les réseaux compacts sont donc isothermes et faiblement compressibles.

Lattice Boltzmann Method

Lattice Boltzmann algorithm :

$$g_\alpha^{coll}(\mathbf{x},t) = g_\alpha(\mathbf{x},t) - \frac{1}{\tau_g}[g_\alpha(\mathbf{x},t) - g_\alpha^{eq}(\mathbf{x},t)]$$

MPI communication

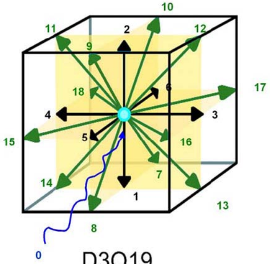
$$g_\alpha(\mathbf{x},t) = g_\alpha^{coll}(\mathbf{x} - \mathbf{c}_\alpha \Delta t, t - \Delta t)$$

Conditions aux limites

$$\rho = \sum_\alpha g_\alpha$$

$$\rho\mathbf{u} = \sum_\alpha \mathbf{c}_\alpha g_\alpha$$

$$g_\alpha^{eq}(\mathbf{x},t) = \rho\omega_\alpha \left(1 + \frac{\mathbf{u}.\mathbf{c}_\alpha}{\tilde{c}_0^2} + \frac{(\mathbf{u}.\mathbf{c}_\alpha)^2}{2\tilde{c}_0^4} - \frac{|\mathbf{u}|^2}{2\tilde{c}_0^2}\right)$$



D3Q19

$$\begin{aligned} p &= \tilde{c}_0^2 \rho \\ \tilde{c}_0^2 &= 1/3 \\ \omega_0 &= 1/3 \\ \omega_{1-6} &= 1/18 \\ \omega_{7-18} &= 1/36 \end{aligned}$$

Multiple relaxation times :

$$\mathbf{m}_\alpha^* = \mathbf{m}_\alpha - S\left(\mathbf{m}_\alpha - \mathbf{m}_\alpha^{eq}\right)$$

MPI communication

$$g_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = M^{-1}\mathbf{m}_\alpha^*(\mathbf{x}, t)$$

Conditions aux limites

$$\rho = \sum_\alpha g_\alpha$$

$$\rho\mathbf{u} = \sum_\alpha \mathbf{c}_\alpha g_\alpha$$

$$g_\alpha^{eq}(\mathbf{x}, t) = S\mathbf{m}_\alpha^{\mathbf{eq}}$$

$$(m_1, \cdots, m_9) = (\rho, e, \epsilon, \rho u_x, q_x, \rho u_y, q_y, p_{xx}, p_{xy})$$

$$S = diag\left(0, s_e, s_\epsilon, 0, s_q, 0, s_q, s_\nu, s_\nu\right) \tag{4}$$

Stabilité linéaire du modèle de Navier-Stokes isotherme :

$$\frac{\partial \mathbf{U}'}{\partial t} + \mathbf{M_1}\frac{\partial \mathbf{U}'}{\partial x_1} + \mathbf{M_2}\frac{\partial \mathbf{U}'}{\partial x_2} + \mathbf{M_3}\frac{\partial \mathbf{U}'}{\partial x_3} = 0 \tag{5}$$

$$\omega \mathbf{U}' = \mathbf{M}^{\mathrm{NS}}\mathbf{U}' \tag{6}$$

Solution : 3 modes convectifs (Shu & Kovasnay)

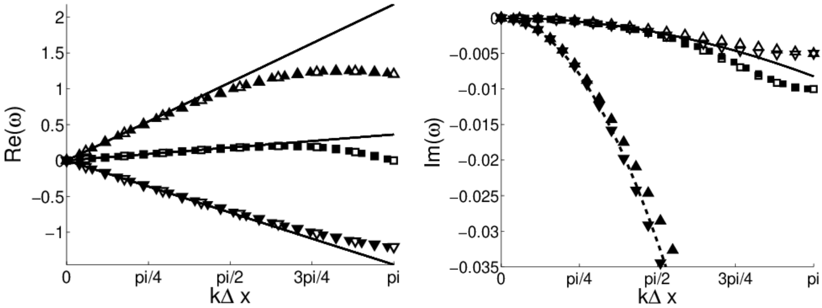
$$\left\{\begin{array}{lcl} \omega_1 & = & \mathbf{k}\cdot\mathbf{u}_0 - i|\mathbf{k}|^2\mathcal{N} + |\mathbf{k}|c_0\sqrt{1-\left(\frac{|\mathbf{k}|\mathcal{N}}{c_0}\right)^2} \\ \omega_2 & = & \mathbf{k}\cdot\mathbf{u}_0 - i|\mathbf{k}|^2\mathcal{N} - |\mathbf{k}|c_0\sqrt{1-\left(\frac{|\mathbf{k}|\mathcal{N}}{c_0}\right)^2} \\ \omega_3 & = & \mathbf{k}\cdot\mathbf{u}_0 - i|\mathbf{k}|^2\nu \\ \omega_4 & = & \omega_3 \\ \omega_5 & = & \mathbf{k}\cdot\mathbf{u}_0 \end{array}\right. \tag{7}$$

Stabilité linéaire de la LBM-BGK : Linéarisation de la fonction d'équilibre :

$$f^{eq}(f_\alpha^{(0)} + f'_\alpha) = f_\alpha^{eq,(0)} + \frac{\partial f_\alpha^{eq}}{\partial f_\beta}\bigg|_{f_\beta = f_\beta^{(0)}} f'_\alpha + o(f'^2_\alpha) \tag{8}$$

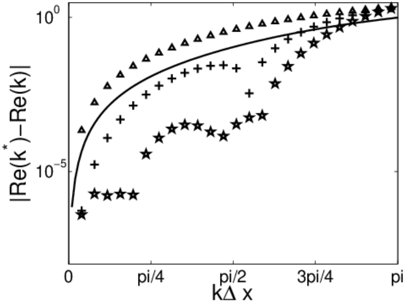
Problème aux valeurs propres :

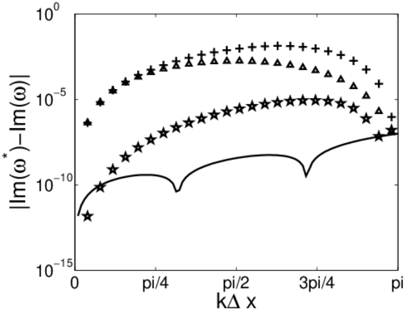
$$\omega \mathbf{f}' = \mathbf{M}^{\mathrm{LBM}} \mathbf{f}' \tag{9}$$



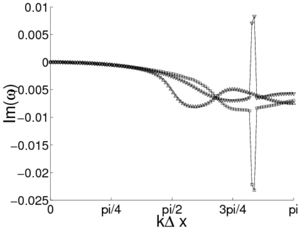
Comparaison avec différences finies :

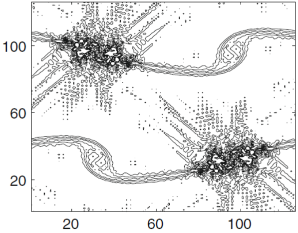
Espace	Temps	Mach	Mode Acoustique
Ordre 2	3-pas	0.2	$\triangle$
DRP	3-pas	0.2	$+$
Ordre 6 optimisé	6-pas opt.	0.2	$\star$





- La dissipation intrinsèque de LBGK est faible.
- Nature compressible du schéma : chaque perturbations se propage de façon isotrope sans être dissipée.
- Problème pour les écoulements haut Reynolds => Instabilités
- Beaucoup de solutions existent pour stabiliser et permettre la simulation des grands voir très grands Reynolds. Beaucoup se font au détriment de la dissipation des ondes acoustiques.
- Application d'un filtrage explicite due à la nature hautes fréquences des instabilités. (Ricot et al. 2009)

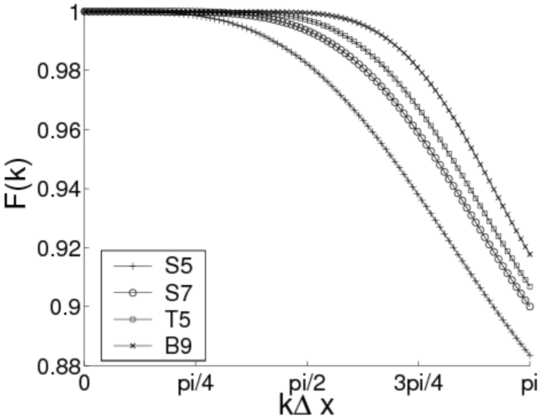




Basic spatial filtering of a given quantity Q is performed as follow :

$$\langle Q(\mathbf{x})\rangle = Q(\mathbf{x}) - \sigma \sum_{j=1}^{D} \sum_{n=-N}^{N} d_n Q(\mathbf{x} + n\Delta x_j) \tag{10}$$

$0 < \sigma = Cste < 1$ and coefficients d_n depending on the filter stencil.



Adaptive filtering :

Le rôle du filtre passe-bas est double :

1. Supprimmer les oscillations hautes fréquences.
2. Apporter la dissipation numérique consistante avec un modèle de sous-maille. (Implicit SGS model)

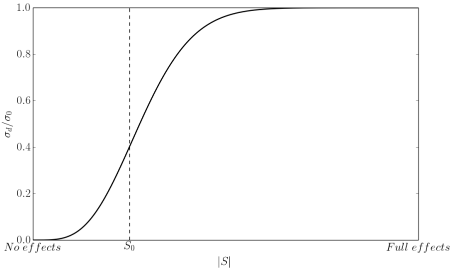
Comme le filtrage est nécessaire surtout dans les zones cisaillé, on fait dépendre le coefficient σ du taux de cisaillement local :

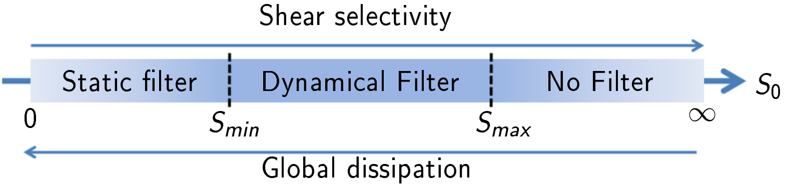
$$\sigma_a(\mathbf{x}) = \sigma_0 \xi(|S|) \tag{11}$$

$$\xi(|S|) = \left(1 - e^{-(|S(\mathbf{x})|/S_0)^2}\right)^2 \tag{12}$$

$|S| = \sqrt{2 S_{ij} S_{ij}}$, S_0 is a threshold to be determined.

$$\sigma_a(\mathbf{x}) = \sigma_0 \left(1 - e^{-(|S|/S_0)^2}\right)^2$$





$$\sigma_d(\mathbf{x}) = \sigma_0 \left(1 - e^{-(|S|/S_0)^2}\right)^2$$

Threshold estimation :

S_0 could be linked with the maximum amount of shear stress S_{max} :
$S_0 = \epsilon S_{max}$

- S_{max} imposed to a constant.
- S_{max} computed from mean field.
- S_{max} based on g_α positivity.

LBM shear computation :

From a LBM framework, the shear stress can be obtained with :

$$2\rho\nu S_{ij} = -\sum_{\alpha} c_{\alpha,i} c_{\alpha,j} (g_\alpha - g_\alpha^{eq})) \tag{13}$$

Assuming the positivity of g_α and $\sum_{\alpha} c_{\alpha,i} c_{\alpha,j} g_\alpha^{eq} = \rho u_i u_j$

$$|S| = \frac{\mathbf{Q_f}}{2\rho\nu} = \frac{\sqrt{2\sum_\alpha c_{\alpha,i} c_{\alpha,j} g_\alpha^{eq} \sum_\alpha c_{\alpha,i} c_{\alpha,j} g_\alpha^{eq}}}{2\rho\nu} \leq \frac{\sqrt{2} u_i u_j}{2\nu}$$

Then :

$$S_{max} = \frac{\sqrt{2} U_0^2}{2\nu} \sim \frac{Re_\delta U_0}{\delta}$$

Choosing the filtered quantity

3 different possibilities with increasing computational cost :

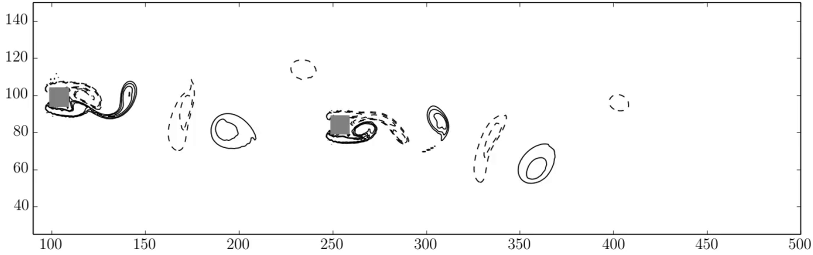
1. Filtering momenta : ρ, u_x, u_y, u_z (4 tables).
2. Filtering distribution functions : g_α (19 tables).
3. Filtering collision operator : $-\frac{1}{\tau_g}(g_\alpha - g_\alpha^{eq})$ (19 tables).

Then the overall algorithm becomes :

Modified algorithm for moments filtering :

- Estimation of S_0.
- Compute $|S|$ with (13) and update σ_d
- Collision Step
- (Collision Filtering)
- Propagation Step
- Update moments
- (Moments filtering)
- Update g_α^{eq}

An example of adaptivity :



Taylor Green Vortex

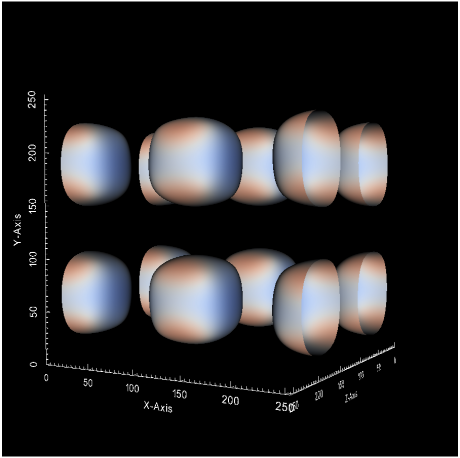
Initialization of the Taylor-Green vortex is done by setting velocity and pressure in a cubic and fully periodic domain of size 2π :

$$\begin{cases} p &= p_\infty + \dfrac{\rho_\infty U_\infty^2}{16}[\cos(2z)+2][\cos(2x)+\cos(2y)] \\ u &= U_\infty \sin(x)\cos(y)\cos(z) \\ v &= -U_\infty \cos(x)\sin(y)\cos(z) \\ w &= 0 \end{cases} \tag{14}$$

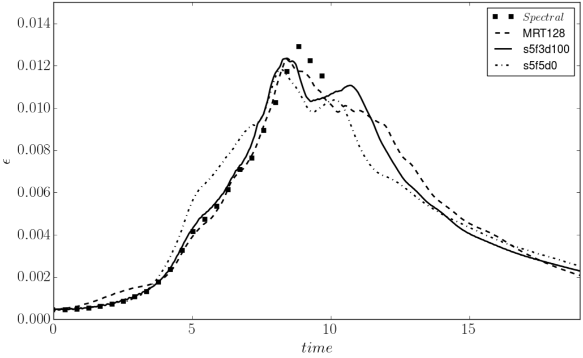
Parameters :

- Imposing $Re = 1600$, $M_\infty = 0.085$, $\rho_\infty = 1$, $dx = 2\pi/n_x$
- Induces : $U_\infty = 0.049$, $p_\infty = 1/3$, $\tau_g = 0.5 + 1.46 n_x 10^{-5}$

Taylor-Green vortex at $R_e = 1600$:



Dissipation rate of kinetic energy



Comparison between Adaptive and classical techniques.

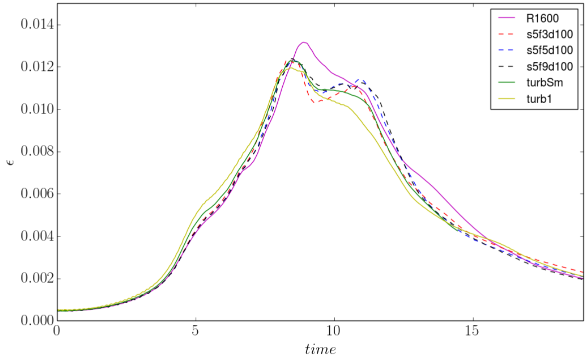
- Results on a 128^3 grid
- MRT results from P.Lallemand
- Adaptive filtering give similar results than the MRT model.
- Adaptive filtering with 3-point stencil gives better results than static 5-point.

Comparison to subgrid scale model

- Adaptive filtering gives better results than SGS model.
- SGS describes poorly the laminar-turbulent transition region.
- SGS strategy gives similar results as adaptive filtering with a low shear stress sensitivity S_0.

— 3-point filter, — 5-point filter, — 9-point filter

— Smagorinsky ($C_s = 0.18$), — Smagorinsky ($C_s = 0.1$)



Comparison between adaptive filtering and subgrid-scale model

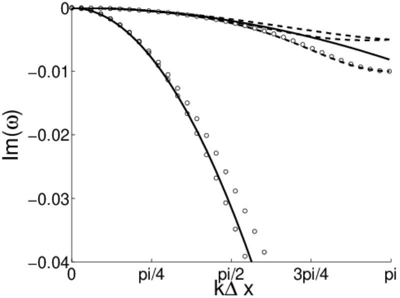
Adaptive Relaxation Times (ART)

MRT Collision

$$\mathbf{m}_\alpha^* = \mathbf{m}_\alpha - S\left(\mathbf{m}_\alpha - \mathbf{m}_\alpha^{eq}\right)$$

$$g_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = M^{-1}\mathbf{m}_\alpha^*(\mathbf{x}, t)$$

In the MRT framework, the filtering step is not needed.



$$(m_1, \cdots, m_9) = (\rho, e, \epsilon, \rho u_x, q_x, \rho u_y, q_y, p_{xx}, p_{xy})$$

The function $\xi(|S|)$ is used to switch from MRT in sheared region to BGK in uniform flow region :

$$S' = diag\left(0, s_e', s_\epsilon', 0, s_q', 0, s_q', s_\nu, s_\nu\right) \tag{15}$$

where $s' = s + (1 - \xi)(s_\nu - s)$

Then the overall algorithm becomes :

Modified algorithm for adaptive relaxation times :

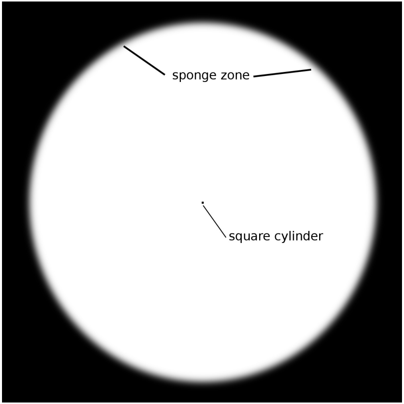
- Compute $|S|$ with (13) and update ξ
- Update relaxation time matrix S'
- Collision Step in the momentum space
- Propagation Step
- Update moments
- Update equilibrium

Sound radiated by a square cylinder

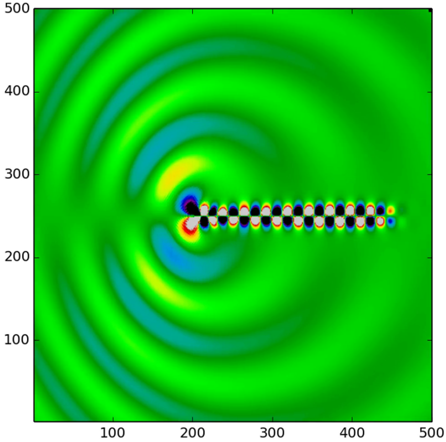
Parameters

- Reynolds $R_D = 500$
- Mach number $M_a = 0.3$
- the square size is $D = 5$
- the domain size is $300D \times 300D$
- The domain is initialized with a uniform flow and periodic boundary conditions.
- A circular sponge zone is defined at the domain boundary to damp the outgoing structures.

Case setup



- Details about LBM sponge zone from Hui et al 2011.
- Here the filter coefficient σ and the relaxation time τ_ν are set to high values in the sponge zone.
- For ART model, the switcher is set to 1 in the sponge zone.


500
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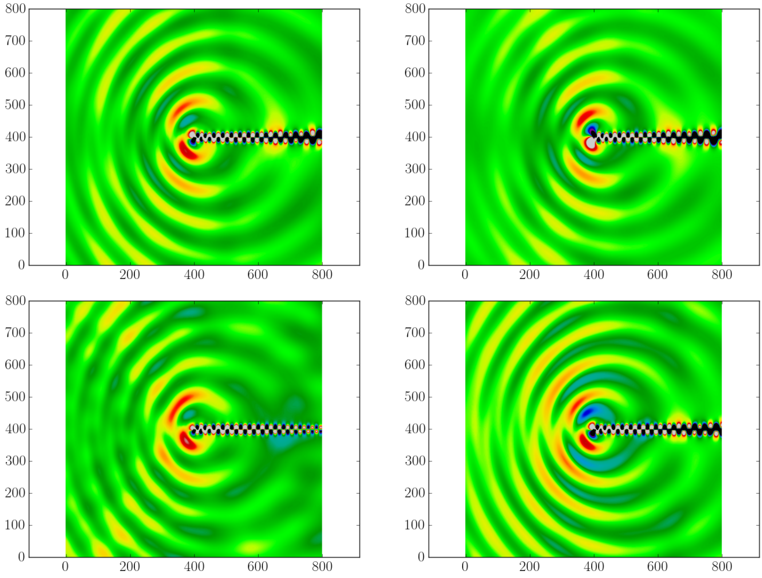
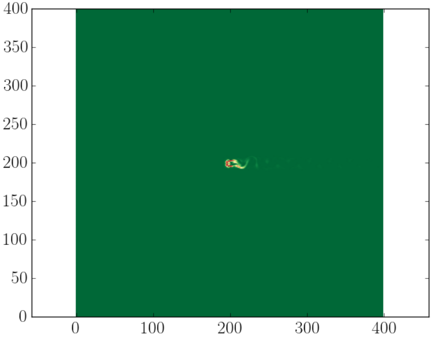
500

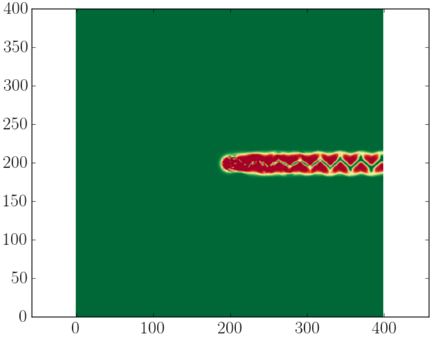
	BGK	MRT
Standard		
Adaptive $S_0 = 1.0$		



Maps of $\xi(|S|)$



$S_0 = 0.1$



$S_0 = 1.0$

Perspectives

- Traitement de paroi optimisé pour les modèles adaptatifs.
- Etude d'un couplage NS/LBM
- Etude des modèles Cascaded et Cumulant
- Etude d'un cas acoustique hautes fréquences.
- Comparaison avec les approches lagrangiennes.

He-Chen-Zhang model

1 additional distribution function to track index function ϕ :

BGK on a D2Q9 lattice with force terms :

$$f_\alpha^+ = \mathbf{BGK}(f_\alpha) - \frac{2\tau - 1}{2\tau}(\mathbf{c}_\alpha - \mathbf{u}).\frac{\nabla\psi(\phi)}{RT}\Gamma_\alpha(\mathbf{u})$$

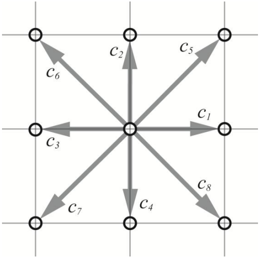
$$g_\alpha^+ = \mathbf{BGK}(g_\alpha) - \frac{2\tau - 1}{2\tau}(\mathbf{c}_\alpha - \mathbf{u}).\left[\nabla\psi(\rho)(\Gamma_\alpha(\mathbf{u}) - \Gamma_\alpha(0)) - \Gamma_\alpha(\mathbf{u})(\mathbf{F_s} + \mathbf{G})\right]$$

Equilibrium state :

$$\Gamma_\alpha(\mathbf{u}) = \omega_\alpha\left(1 + \frac{\mathbf{u.c}_\alpha}{RT} + \frac{(\mathbf{u.c}_\alpha)^2}{2(RT)^2} - \frac{|\mathbf{u}|^2}{2RT}\right)$$

$$f_\alpha^{eq} = \phi\Gamma_\alpha(\mathbf{u})$$

$$g_\alpha^{eq} = \omega_\alpha\left[p + \rho RT\left(\frac{\mathbf{u.c}_\alpha}{RT} + \frac{(\mathbf{u.c}_\alpha)^2}{2(RT)^2} - \frac{|\mathbf{u}|^2}{2RT}\right)\right]$$



He-Chen-Zhang model

Moments :

$$\begin{aligned}\phi &= \sum_\alpha f_\alpha \\ p_h &= \sum_\alpha g_\alpha - \frac{1}{2}\mathbf{u}.\nabla\psi(\rho) \\ \rho RT\mathbf{u} &= \sum_\alpha \mathbf{c}_\alpha g_\alpha + \frac{RT}{2}(\mathbf{F_s} + \mathbf{G})\end{aligned}$$

Thermodynamics :

$$\begin{aligned}\psi(\rho) &= p_h - \rho RT \\ \psi(\phi) &= p_{th} - \phi RT\end{aligned}$$

Equation d'état : Carnahan-Starling

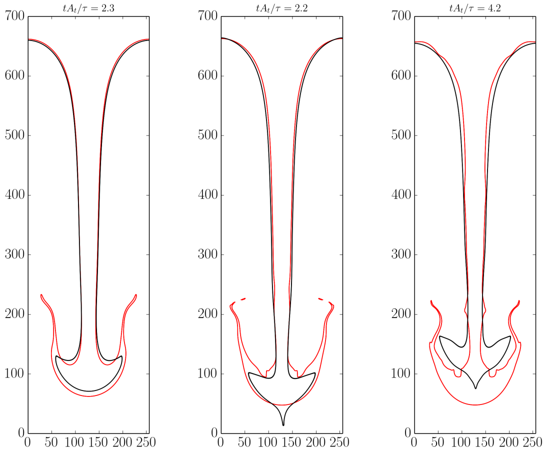
$$p_{th} = \phi RT\frac{1+\phi+\phi^2-\phi^3}{(1-\phi)^3} - a\phi^2$$

Défauts de stabilité dans les zones à fort gradient de densité => Utilisation du filtrage adaptatif basé sur $\nabla\rho$.

Rayleigh-Taylor Instability $A_t = 0.9$

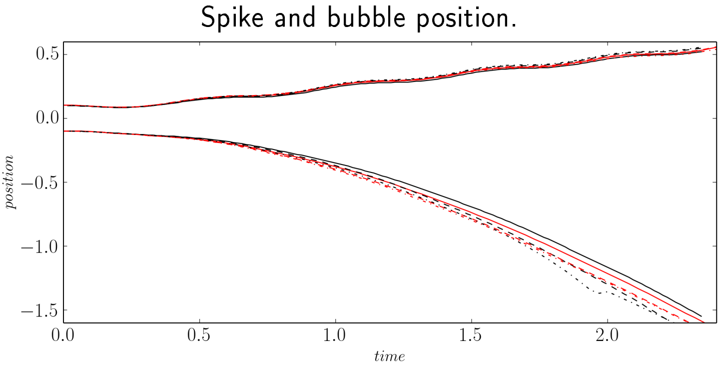
NS Results from V.Daru (2nd order TVD + SuperBee limiter)

$\eta = 20$ −−LBM −−NS

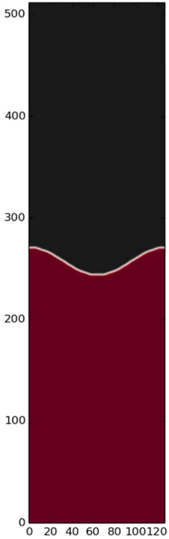


$Re = 256$ $Re = 1024$ $Re = 4096$

$A_t = 0.9$



$-Re = 256, \; - - \; Re = 1024, \; -.Re = 4096$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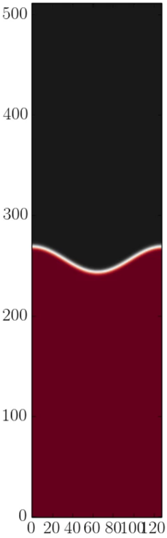
$A_t = 0.5$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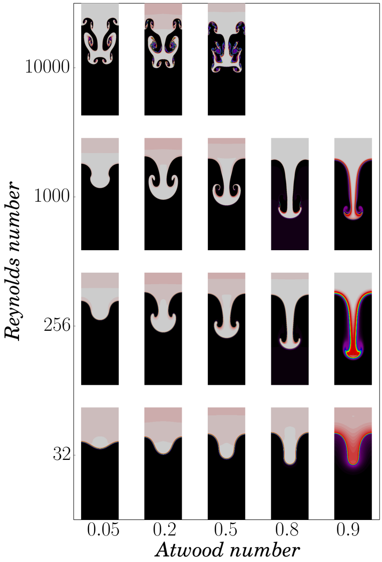
$A_t = 0.9$


Reynolds number
10000
1000
256
32
0.05
0.2
0.5
0.8
0.9
Atwood number

- Work from PhD student L.Vienne ending in 2019.
- Build a LBM model for mixing simulation of miscible gas.
- Independent of the collision operator.
- Taking diffusion into acount through forcing term.

Multicomponent LBM :

$$f_\alpha^m\left(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t\right) = f_\alpha^m\left(\mathbf{x}, t\right) - \frac{1}{\tau_m}\left[f_\alpha^m\left(\mathbf{x}, t\right) - f_\alpha^{m(eq)}\left(\mathbf{x}, t\right)\right] + S_\alpha^m\left(\mathbf{x}, t\right)$$

Forcing term :

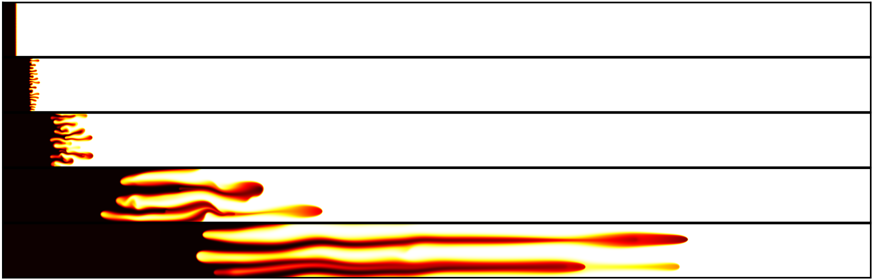
$$S_\alpha^m = \left(1-\frac{\delta_t}{2\tau_m}\right)\omega_\alpha\left[\frac{\mathbf{e}_\alpha - \mathbf{u}_m}{c_s^2} + \frac{(\mathbf{e}_\alpha\cdot\mathbf{u}_m)\mathbf{e}_\alpha}{c_s^4}\right]\cdot\mathcal{F}_m$$

Diffusion term between species : Kerkhof & Geboers

$$F_m = -p\sum_{n=1}^{N}\frac{x_m x_n}{\mathcal{D}_{mn}}(\mathbf{u}_m - \mathbf{u}_n),$$

Application to the viscous fingering instability (Saffman-Taylor)

Porous medium is modeled with Gray Lattice Boltzmann (I.Ginzburg).



Perspectives

- Etude de l'instabilité de ST à l'échelle du pore.
- Etude d'une couche de mélange transitoire multiespèces.
- Caractérisation numérique de la diffusion dans les approches LBM-multiespèces.
- Etudes des faibles nombres de Schmidt.