Numerical Modeling of Liquid-Vapor Interface in Fluid Flows

Institut Henri Poincaré
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Lattice Boltzmann Method (LBM) for two-fluid flows with possibly high density ratio

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Outline

- Non viscous non thermal two-fluids flow (Isentropic Euler equations):

$$\left\{\begin{array}{llll} \partial_t(\alpha\rho_g) & + & \nabla\cdot(\alpha\rho_g\mathbf{u}) & = 0, \\ \partial_t((1-\alpha)\rho_\ell) & + & \nabla\cdot((1-\alpha)\rho_\ell\mathbf{u}) & = 0, \\ \partial_t(\rho\mathbf{u}) & + & \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}+p\mathbf{I}) & = \rho\mathbf{g}, \end{array}\right.$$

with

$$\rho = \alpha\rho_g + (1-\alpha)\rho_\ell$$

$+$ Interface pressure equilibrium

$$p = p_g(\rho_g) = p_\ell(\rho_\ell)$$

- Low Mach number flow
- Compressible fluids
- Two immiscible fluids
- Possibly high density ratio

Examples:

- Bubble flow, sloshing, ...

Why LBM ?

Observation

- Graphics Processing Units (GPU) peu chers et hautement parallélisables

Keywords for high performances

- Single Instruction Multiple Data (SIMD)
- Low memory communication

Appropriated methods: LBM

- Local collision
- Exchange with direct neighbours

Ex : Nvidia Titan X (Pascal)

- 3584 CUDA cores
- Memory 12Go
- 11Tflops SP
- $\sim$ 1300 €

$\rightarrow$ Analysis of LBM for two-fluid flow with possibly high-density ratio

Lattice Boltzmann Method (LBM)

Boltzmann equation

$$\partial_t f + \mathbf{v} \cdot \nabla f = Q(f,f) \overset{BGK}{=} \frac{(f^{eq} - f)}{\tau \Delta t}$$
$$\mathrm{d}\mathcal{N} = f(x, \mathbf{v}, t)\ \mathrm{d}^3 x \mathrm{d}^3 v.$$

In Navier-Stokes[1] case

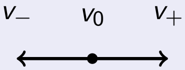
$$\nu = \Delta t\ c_s^2 \left(\tau - \frac{1}{2}\right) \quad \rightarrow \tau \geqslant 1/2$$

[1] [He Luo,1997]

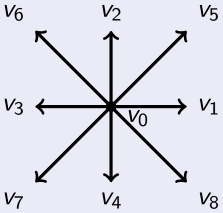
Discrete Boltzmann equation (LBGK[2]-type)

$$\partial_t f_i + \mathbf{v_i} \cdot \nabla f_i = Q(f_i, f_i) \overset{BGK}{=} \frac{(f_i^{eq} - f_i)}{\tau \Delta t} \quad v_i \in \mathcal{L}, i \in [\![0, q-1]\!]$$

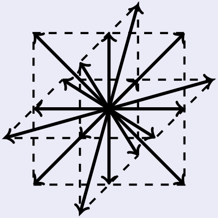
Lattice $\mathcal{L}$ DdQq



D1Q3



D2Q9


D3Q19 = D2Q9 in each direction

[2] [Bhatnagar, Gross et Krook, 1954]

Discrete Boltzmann equation (LBGK-type)

$$\partial_t f_i + \mathbf{v_i} \cdot \nabla f_i = Q(f_i, f_i) \overset{BGK}{=} \frac{(f_i^{eq} - f_i)}{\tau \Delta t} \qquad v_i \in \mathcal{L}, i \in [\![0, q-1]\!]$$

Lattice $\mathcal{L}$ DdQq

v_6 v_2 v_5

Flux consistency:

$$\sum_{i \in \mathcal{I}} (1, v_i, v_i \otimes v_i) f_i^{eq} = (\rho, \rho\mathbf{u}, \rho\mathbf{u} \otimes \mathbf{u} + p\mathbf{I})$$

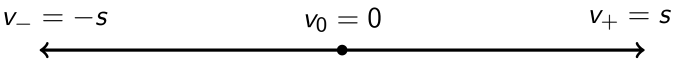
$$\sum_{i \in \mathcal{I}} (1, v_i) f_i = (\rho, \rho\mathbf{u})$$

Notation

$$(f_i)_j^n = f(x_j, v_i, t^n)$$

each direction

D1Q3 lattice



with $s = \dfrac{\Delta x}{\Delta t}$, numerical sound speed

Flux consistency:

$$\sum_{i \in \{-,0,+\}} (1, v_i, v_i^2) f_i^{eq} = (\rho, \rho u, \rho u^2 + p)$$

where

$$p(\rho) = \rho^\gamma + \pi_0$$

$$\begin{cases} f_\pm^{eq} = \dfrac{\rho u(u \pm s) + p}{2s^2}, \\ f_0^{eq} = \rho - \dfrac{\rho u^2 + p}{s^2}. \end{cases}$$

Mass conservativity

$$\rho_j^{n+1} = \sum_i (f_i)_j^{n+1} = \sum_i \widetilde{(f_i)}_{j(i)} = \rho_j^n - \frac{\Delta t}{\Delta x}\left(s\rho_j^n - s\sum_i \widetilde{(f_i)}_{j(i)} \right)$$
$$= \rho_j^n - \frac{\Delta t}{\Delta x}\left(s\rho_j^n - s\left(\widetilde{(f_0)}_j + \widetilde{(f_-)}_{j+1} + \widetilde{(f_+)}_{j-1} \right)\right)$$

As $\rho_j^n = \rho_j^{eq,n}$ then $\widetilde{\rho}_j = (1-\omega)\rho_j^n + \omega\rho_j^{eq,n} = \rho_j^n$.

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x}\left((\Phi_\rho)_{j+\frac{1}{2}}^n - (\Phi_\rho)_{j-\frac{1}{2}}^n \right)$$

with $(\Phi_\rho)_{j+\frac{1}{2}}^n = \sum_i \left(v_i^+ \widetilde{(f_i)}_j + v_i^- \widetilde{(f_i)}_{j+1} \right)$.

$\rightarrow$ Mass conservative scheme $\forall \tau \in \left] \frac{1}{2}, +\infty \right[$!

Momentum conservativity

$$(\rho u)_j^{n+1} = \sum_i v_i (f_i)_j^{n+1} = \sum_i v_i \widetilde{(f_i)}_{j(i)}$$
$$= (\rho u)_j^n - \frac{\Delta t}{\Delta x}\left(s(\rho u)_j^n - s\left(s\widetilde{(f_+)}_{j-1} - s\widetilde{(f_-)}_{j+1} \right)\right)$$

As $(\rho u)_j^n = (\rho u)_j^{eq,n}$, then $(\rho u)_j^n = \widetilde{(\rho u)}_j$.

$$(\rho u)_j^{n+1} = (\rho u)_j^n - \frac{\Delta t}{\Delta x}\left((\Phi_{\rho u})_{j+\frac{1}{2}}^n - (\Phi_{\rho u})_{j-\frac{1}{2}}^n \right)$$

with $\Phi_{\rho u, j+\frac{1}{2}} = \sum_i \left((v_i^+)^2 \widetilde{(f_i)}_j + (v_i^-)^2 \widetilde{(f_i)}_{j+1} \right)$.

$\rightarrow$ Momentum conservative scheme $\forall \tau \in \left]\frac{1}{2}, +\infty\right[$!

Stability by positivity

We want $f_i^{eq} > 0$ for all $i \in [-, 0, +]$, so:

$$\boxed{\sqrt{u^2 + \frac{p}{\rho}} \leqslant s = \frac{\Delta x}{\Delta t} \leqslant \frac{u^2 + p/\rho}{|u|}}$$

For each point $x \in \Omega$, we have

$$\sqrt{u^2 + \frac{p}{\rho}} \leqslant \frac{u^2 + p/\rho}{|u|}$$

But

$$\max_\Omega \left(\sqrt{u^2 + \frac{p}{\rho}} \right) \overset{?}{\leqslant} \min_\Omega \left(\frac{u^2 + p/\rho}{|u|} \right)$$

Example : in the case where $u(x, t = 0) = 0$, we numerically define,

$$s^2 = \beta \max_\Omega \left(u^2 + \frac{p}{\rho} \right), \quad \beta > 1$$

Presentation of the monodimensional test case

Monodimensionel isentropic Euler equations (one fluid)

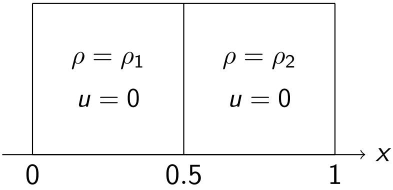
$$\begin{cases} \partial_t \rho & + \quad \partial_x(\rho u) & = 0, \\ \partial_t(\rho u) & + \quad \partial_x(\rho u^2 + p) & = 0. \end{cases}$$

with

$$p = \rho^\gamma + \pi_0, \quad \gamma = 1.4$$

At initial time, $t = 0$,

$$\rho = \rho_1 * (x < 0.5) + \rho_2 * (x >= 0.5).$$

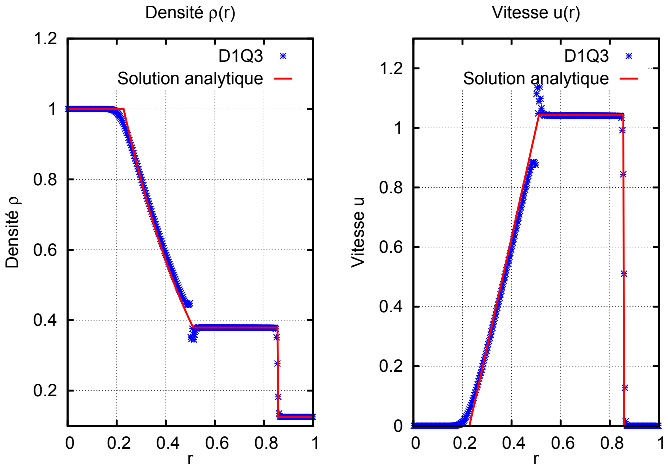


Homogeneous Neumann boundary conditions

Results for the shock tube test case

Isentropic Euler equations solved with the classical LBM D1Q3 scheme

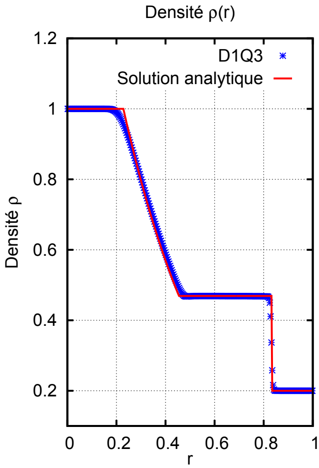
$$\rho = 1.0 * (x < 0.5) + 0.125 * (x >= 0.5),$$
$$\tau = 1,\ \beta = 4,\ \pi_0 = 0 \text{ and } N = 300.$$

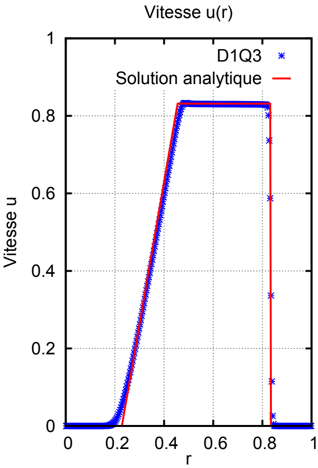


Results for the shock tube test case

Isentropic Euler equations solved with the classical LBM D1Q3 scheme

$$\rho = 1.0 * (x < 0.5) + 0.2 * (x >= 0.5),$$
$$\tau = 1,\ \beta = 4,\ \pi_0 = 0 \text{ and } N = 300.$$





D1Q3 for ρ + D1Q3 for ρu = D1Q3Q3 approach[3]

One lattice per equation. Previous D1Q3 for ρ.

$$\begin{array}{rlll} & \sum_i g_i & = \sum_i g_i^{eq} & = \rho u, \\ & \sum_i v_i g_i & = \sum_i v_i g_i^{eq} & = \rho u^2 + p \\ + & \sum_i v_i^2 g_i & = \sum_i v_i^2 g_i^{eq} & = \rho u^3 + 3pu \end{array}$$

$$\begin{cases} g_\pm^{eq} = \dfrac{\rho u^3 + 3pu}{2s^2} \pm \dfrac{\rho u^2 + p}{2s}, \\ g_0^{eq} = \rho u - \dfrac{\rho u^3 + 3pu}{s^2}. \end{cases}$$

Definition:

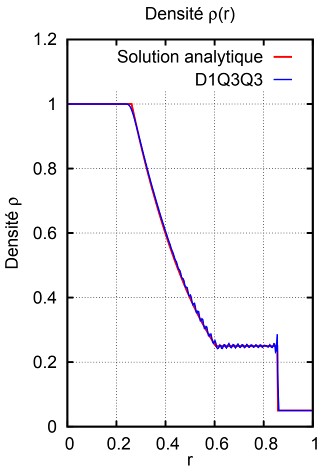
$$\boxed{u = \frac{\sum_i g_i}{\sum_i f_i}}$$

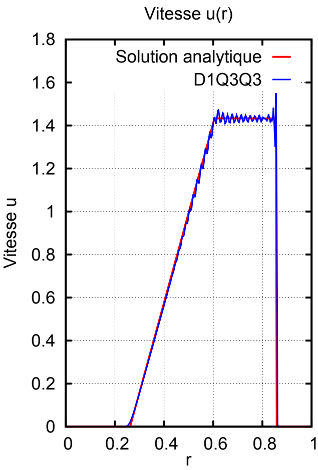
[3] [Parmigiani et al., 2009], [Dubois, Graille, Lallemand, 2016]

Test case $\tau = 0.7$, $\beta = 5$, $N = 300$ and $T_f = 0.2$

$$\rho = 1.0 * (x < 0.5) + 0.05 * (x >= 0.5)$$

$$\pi_0 = 0$$

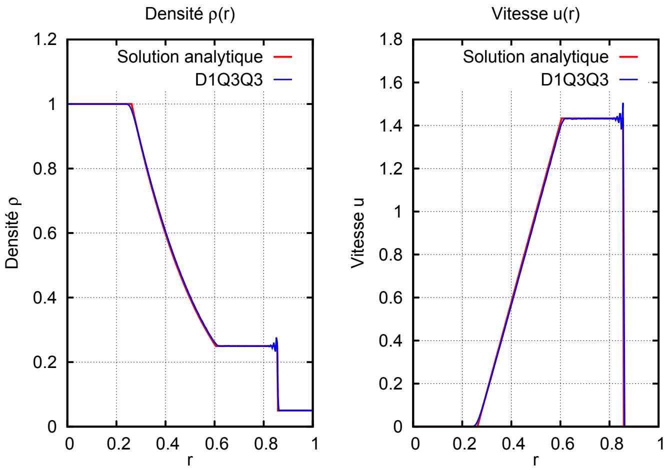




Test case $\tau = 0.7$, $\beta = 5$, $N = 300$ and $T_f = 0.2$

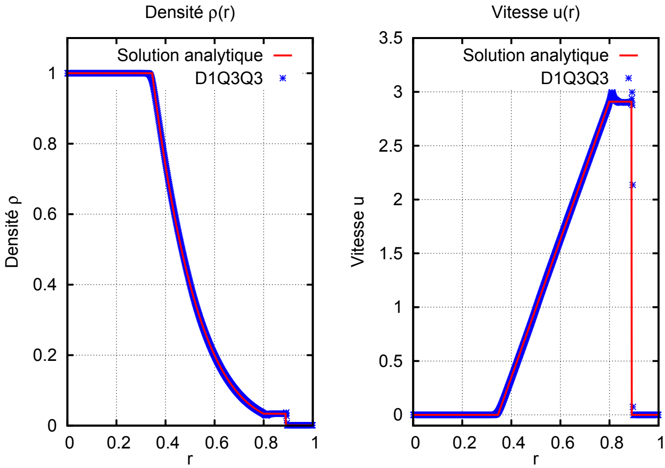
$$\rho = 1.0 * (x < 0.5) + 0.05 * (x >= 0.5)$$

$$\pi_0 = 0.05$$



With a density ratio of 1000

$$\rho = 1.0 * (x < 0.5) + 0.001 * (x >= 0.5)$$
$$\tau = 1,\ \beta = 18,\ N = 800,\ \pi_0 = 0,\ T_f = 0.13.$$



Link with Finite Volume Schemes

Reminder

- Collision

$$\widetilde{(f_i)}_j = \omega \; (f_i^{eq})_j^n + (1-\omega)(f_i)_j^n \quad \text{with } \omega = \tau^{-1}.$$

- Advection

$$(f_i)_j^{n+1} = \widetilde{(f_i)}_{j(i)} \stackrel{\tau=1}{=} (f_i^{eq})_{j(i)}$$

When $\tau = 1$

$$\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x}\left(\Phi_{j+1/2}^n - \Phi_{j-1/2}^n\right)$$

with

$$\Phi_{j+1/2}^n = \frac{(\rho u)_j^n + (\rho u)_{j+1}^n}{2} - \frac{1}{2s}\left[(\rho u^2 + p)_{j+1}^n - (\rho u^2 + p)_j^n\right]$$

Contact discontinuities behaviour when $\tau = 1$

$$\Phi^n_{j+1/2} = \frac{(\rho u)^n_j + (\rho u)^n_{j+1}}{2} - \frac{1}{2s}\left[(\rho u^2 + p)^n_{j+1} - (\rho u^2 + p)^n_j\right]$$

Let's assume $u^n_j = u^n_{j+1} = u$, $p^n_j = p^n_{j+1} = p$

$$\Longrightarrow \quad \Phi^n_{j+1/2} = \frac{\rho^n_j + \rho^n_{j+1}}{2}\, u - \frac{1}{2} m \,|u|\, \left(\rho^n_{j+1} - \rho^n_j\right)$$

Upwind scheme iif $m = \frac{|u|}{s} = 1$, $\rightarrow |u| = s$ (sonic state).
If $|m| < 1$, the scheme is less diffusive than the upwind one.

$\Longrightarrow$ Lack of numerical diffusion $\rightarrow$ Oscillations

Euler Equations in ALE formalism

Reynolds transport theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}_t} q(x,t)\,\mathrm{d}x = \int_{\mathcal{V}_t} \left[\partial_t q + \nabla \cdot (\mathbf{w} q)\right] \mathrm{d}x$$

where $\mathbf{w}$ is the speed of the moving referential $\mathcal{V}_t$.[1]

So ALE Euler equations are

$$\begin{cases} \partial_t(\rho) & +\nabla \cdot (\rho(\mathbf{u}-\mathbf{w})) & = 0, \\ \partial_t(\rho\mathbf{u}) & +\nabla \cdot (\rho\mathbf{u} \otimes (\mathbf{u}-\mathbf{w}) + p) & = \mathbf{0}, \\ \partial_t(\rho E) & +\nabla \cdot (\rho E(\mathbf{u}-\mathbf{w}) + p\mathbf{u}) & = 0. \end{cases}$$

where $2\rho E = \rho|\mathbf{u}|^2 + p$.

[1] [Donea] Encyclopedia of Computational Mechanics Vol. 1: Fundamentals., Chapter 14: Arbitrary Lagrangian-Eulerian Methods, 2004

ALE step - Material

- Mass:

$$\begin{aligned}\sum_i f_i &= \sum_i f_i^{eq} &&= \rho,\\ \sum_i v_i f_i &= \sum_i v_i f_i^{eq} &&= \rho(u-w),\\ \sum_i v_i^2 f_i &= \sum_i v_i^2 f_i^{eq} &&= \rho u(u-w)+p.\end{aligned}$$

$$\begin{cases} f_{\pm}^{eq} &= \dfrac{\rho(u-w)(u\pm s)+p}{2s^2},\\ f_0^{eq} &= \rho - \dfrac{\rho u(u-w)+p}{s^2}.\end{cases}$$

- Momentum:

$$\begin{aligned}\sum_i g_i &= \sum_i g_i^{eq} &&= \rho u,\\ \sum_i v_i g_i &= \sum_i v_i g_i^{eq} &&= \rho u(u-w)+p,\\ \sum_i v_i^2 g_i &= \sum_i v_i^2 g_i^{eq} &&= \rho u^2(u-w)+p(3u-w).\end{aligned}$$

$$\begin{cases} g_{\pm}^{eq} &= \dfrac{\rho u(u-w)(u\pm s)+p(3u-w\pm s)}{2s^2},\\ g_0^{eq} &= \rho u - \dfrac{\rho u^2(u-w)+p(3u-w)}{s^2}.\end{cases}$$

Properties (1/2)

- Conservativity of the ALE step

$$U_j^{n+1/2} = U_j^n - \frac{\Delta t}{\Delta x}\left(\Phi^{ALE}_{j+1/2} - \Phi^{ALE}_{j-1/2}\right)$$

where $U = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}$. If $\tau = 1$,

$$\Phi^{ALE}_{j+1/2} = \frac{F_j^n + F_{j+1}^n}{2} - \frac{1}{2s}\left(G_{j+1}^n - G_j^n\right),$$

with

$$F = \begin{pmatrix} \rho(u-w) \\ \rho u(u-w) + p \end{pmatrix} \text{ and } G = \begin{pmatrix} \rho u(u-w) + p \\ \rho u^2(u-w) + p(3u-w) \end{pmatrix}$$

ALE benefit for contact discontinuities, if $w = u$

$$\Phi^{ALE}_{j+1/2} = \frac{F_j^n + F_{j+1}^n}{2} - \frac{1}{2s}\left(G_{j+1}^n - G_j^n\right) = \begin{pmatrix} 0 \\ p \end{pmatrix}$$

Properties (2/2)

- Conservativity of the remapping step

$$U_j^{n+1} = U_j^{n+1/2} - \frac{\Delta t}{\Delta x}\left(\Phi_{j+1/2}^{Rem} - \Phi_{j-1/2}^{Rem}\right)$$

with

$$\Phi_{j+1/2}^{Rem} = \frac{U_j^{n+1/2} + U_{j+1}^{n+1/2}}{2} w_{j+\frac{1}{2}} - \frac{|w_{j+\frac{1}{2}}|}{2}(U_{j+1}^{n+1/2} - U_j^{n+1/2})$$

where

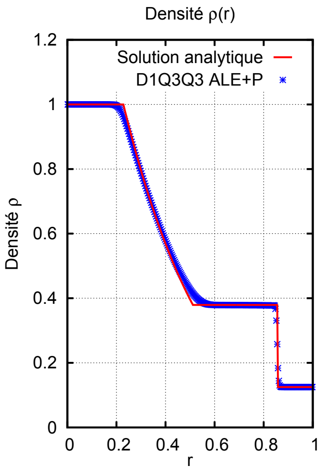
$$w_{j+\frac{1}{2}} = \frac{w_j + w_{j+1}}{2}$$

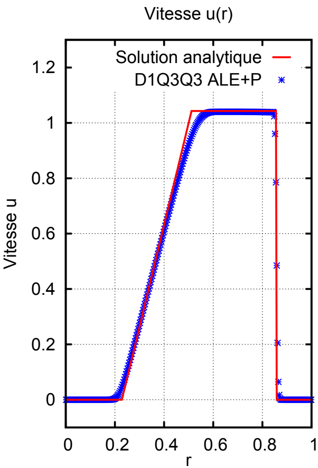
- Stability by positivity

$$\begin{cases} \sqrt{(u-w)^2 + \frac{p}{\rho}} \leqslant s \leqslant \frac{(u-w)^2 + p/\rho}{|u-w|} & \text{if } |u-w| \neq 0 \\ \sqrt{\frac{p}{\rho}} \leqslant s & \text{otherwise} \end{cases}$$

Test case with $\tau = 1$, $\beta = 3$, $\pi_0 = 0.35$ and $N = 300$

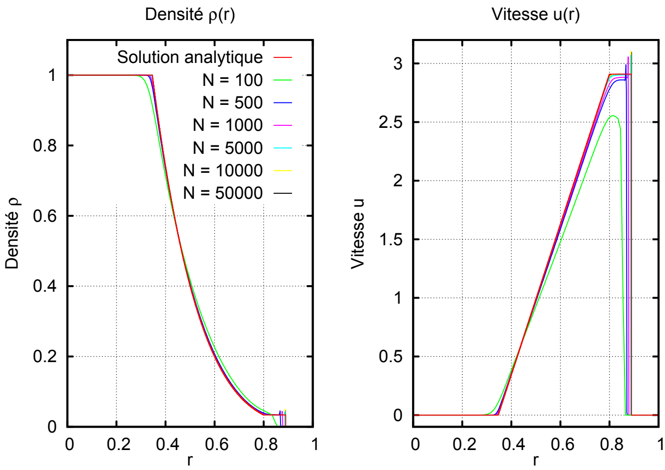
$$\rho = 1.0 * (x < 0.5) + 0.125 * (x >= 0.5)$$





Test case with $\tau = 1$, $\beta = 3$, $\pi_0 = 0$, $N = 100$ to 50000

$$\rho = 1.0 * (x < 0.5) + 0.001 * (x >= 0.5)$$



LBM ALE + R, 2D extension

$$\begin{cases} \partial_t(\rho) & +\partial_x(\rho(u_x - w_x)) & +\partial_y(\rho(u_y - w_y)) & = 0, \\ \partial_t(\rho u_x) & +\partial_x(\rho u_x(u_x - w_x) + p) & +\partial_y(\rho u_x(u_y - w_y)) & = 0, \\ \partial_t(\rho u_y) & +\partial_x(\rho u_y(u_x - w_x)) & +\partial_y(\rho u_y(u_y - w_y) + p) & = 0, \\ \partial_t(\rho E) & +\partial_x(\rho E(u_x - w_x) + p u_x) & +\partial_y(\rho E(u_y - w_y) + p u_y) & = 0. \end{cases}$$

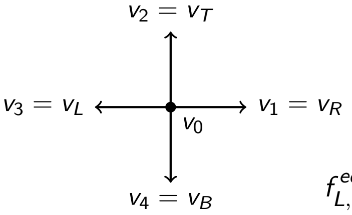


Figure : D2Q5 lattice

$$\sum_i (v_i)_x (v_i)_y f_i^{eq} = \rho(u_x - w_x)(u_y - w_y)$$

$$\Rightarrow \quad w_x = u_x, \quad w_y = u_y$$

$$\begin{aligned} f_{L,R,B,T}^{eq} &= \frac{p}{2s^2}, & f_0^{eq} &= \rho - 4 f_{L,R,B,T} \\ g_{L,R}^{eq} &= \frac{p(2u_x \pm s)}{2s^2}, & g_0^{eq} &= \rho u_x - \frac{p u_x}{s^2} \\ k_{B,T}^{eq} &= \frac{p(2u_y \pm s)}{2s^2}, & k_0^{eq} &= \rho u_y - \frac{p u_y}{s^2} \end{aligned}$$

Properties (1/2)

- f^{eq} positivity is assured by $s \geqslant \sqrt{2p/\rho}$.
- When $\tau = 1$, ALE part becomes:

$$U_{i,j}^{n+1/2} = U_{i,j}^{n} - \frac{\Delta t}{\Delta x}\left(\Phi^{ALE}_{i+\frac{1}{2},j} - \Phi^{ALE}_{i-\frac{1}{2},j}\right) - \frac{\Delta t}{\Delta x}\left(\Phi^{ALE}_{i,j+\frac{1}{2}} - \Phi^{ALE}_{i,j-\frac{1}{2}}\right)$$

$$\text{with} \quad \Phi^{ALE}_{i+\frac{1}{2},j} = \begin{pmatrix} -\dfrac{p^n_{i+1,j} - p^n_{i,j}}{2s} \\ \dfrac{p_{i+1,j} + p_{i,j}}{2} - \dfrac{(pu_x)_{i+1,j} - (pu_x)_{i,j}}{2s} \\ 0 \end{pmatrix}$$

$$\text{and} \quad \Phi^{ALE}_{i,j+\frac{1}{2}} = \begin{pmatrix} -\dfrac{p^n_{i,j+1} - p^n_{i,j}}{2s} \\ 0 \\ \dfrac{p_{i,j+1} + p_{i,j}}{2} - \dfrac{(pu_y)_{i,j+1} - (pu_y)_{i,j}}{2s} \end{pmatrix}$$

Properties (2/2)

- Flux associated with projection avec convective upwind fluxes

$$U_{i,j}^{n+1} = U_{i,j}^{n+1/2} - \frac{\Delta t}{\Delta x}\left(\Phi^{proj}_{i+\frac{1}{2},j} - \Phi^{proj}_{i-\frac{1}{2},j}\right) - \frac{\Delta t}{\Delta x}\left(\Phi^{proj}_{i,j+\frac{1}{2}} - \Phi^{proj}_{i,j-\frac{1}{2}}\right)$$

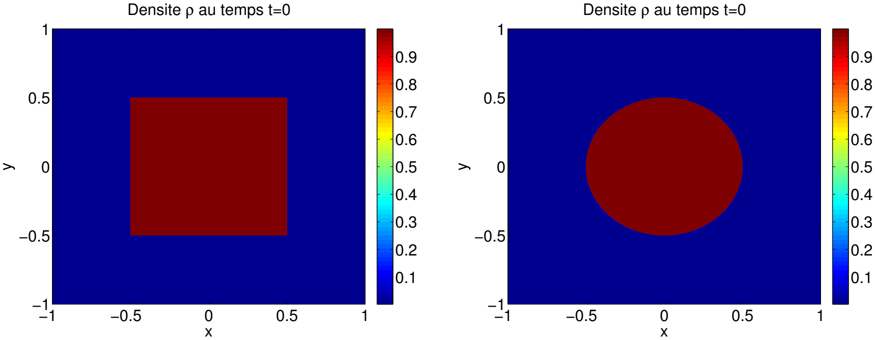
$$\Phi^{proj}_{i+\frac{1}{2},j} = \begin{pmatrix} \left((w_x)_{i+\frac{1}{2},j}\right)_+ \rho_{i,j}^{n+1/2} + \left((w_x)_{i+\frac{1}{2},j}\right)_- \rho_{i+1,j}^{n+1/2} \\ \left((w_x)_{i+\frac{1}{2},j}\right)_+ (\rho u_x)_{i,j}^{n+1/2} + \left((w_x)_{i+\frac{1}{2},j}\right)_- (\rho u_x)_{i+1,j}^{n+1/2} \\ 0 \end{pmatrix}$$

$$\Phi^{proj}_{i,j+\frac{1}{2}} = \begin{pmatrix} \left((w_y)_{i,j+\frac{1}{2}}\right)_+ \rho_{i,j}^{n+1/2} + \left((w_y)_{i,j+\frac{1}{2}}\right)_- \rho_{i,j+1}^{n+1/2} \\ 0 \\ \left((w_y)_{i,j+\frac{1}{2}}\right)_+ (\rho u_y)_{i,j}^{n+1/2} + \left((w_y)_{i,j+\frac{1}{2}}\right)_- (\rho u_y)_{i,j+1}^{n+1/2} \end{pmatrix}$$

Test case with $\tau = 1$, $\beta = 12$, $\pi_0 = 0$, $N_x = N_y = 512$

$$\rho = 1 * \mathbb{1}_{int} + 0.001 * \mathbb{1}_{ext}$$

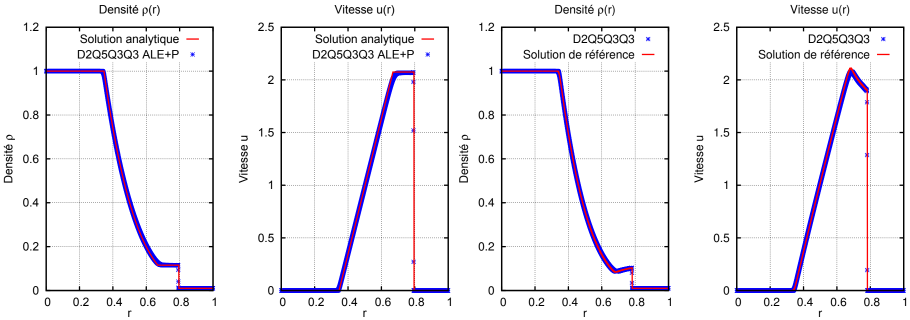
Periodic boundary conditions



Test case with $\tau = 1$, $\beta = 12$, $\pi_0 = 0$, $N = 1500$

$$\rho = 1 * \mathbb{1}_{int} + 0.01 * \mathbb{1}_{ext}$$

Homogeneous Neumann boundary conditions



Complete ALE two-fluid system

Two-fluid ALE Euler equations:

$$\begin{cases} \partial_t(\alpha\rho_g) & + \quad \nabla\cdot(\alpha\rho_g(\mathbf{u}-\mathbf{w})) & = 0, \\ \partial_t((1-\alpha)\rho_\ell) & + \quad \nabla\cdot((1-\alpha)\rho_\ell(\mathbf{u}-\mathbf{w})) & = 0, \\ \partial_t(\rho\mathbf{u}) & + \quad \nabla\cdot(\rho\mathbf{u}\otimes(\mathbf{u}-\mathbf{w})+p\mathbf{I}) & = \rho\mathbf{g}, \end{cases}$$

$$\rho = \alpha\rho_g + (1-\alpha)\rho_\ell, \quad p = p_g(\rho_g) = p_\ell(\rho_\ell)$$

$$\iff \begin{cases} \partial_t\rho & + \quad \nabla\cdot(\rho(\mathbf{u}-\mathbf{w})) & = 0, \\ \partial_t(\rho\mathbf{u}) & + \quad \nabla\cdot(\rho\mathbf{u}\otimes(\mathbf{u}-\mathbf{w})+p\mathbf{I}) & = \rho\mathbf{g}, \\ \partial_t(\rho Y) & + \quad \nabla\cdot(\rho Y(\mathbf{u}-\mathbf{w})) & = 0, \end{cases}$$

where

$$Y = \frac{\alpha\rho_g}{\rho}$$

Treatment of additionnal equation

Transport equation on $Y \Leftrightarrow$ Maximum principle

Two possibilities:

- Larrouturou[2], Upwind flux with mass fluxes already calculated

$$\Phi_{\rho Y,j+1/2} = \left(\Phi_{\rho,j+1/2}\right)_+ Y_j + \left(\Phi_{\rho,j+1/2}\right)_- Y_{j+1}$$

- New equation = New distributions
  Which constraint(s) add ? $\sum_i v_i^2 y_i^{eq} = \rho u^2 Y$? $(\rho u^2 + p)Y$?

$$\Phi_{\rho Y,j+1/2} = \frac{(\rho u Y)_{j+1} + (\rho u Y)_j}{2} - \frac{((\rho u^2 + p)Y)_{j+1} - ((\rho u^2 + p)Y)_j}{2s}$$

[2] [Larrouturou] How to preserve the mass fractions positivity when computing compressible multi-component flows, 1991

Equations of state

- For gas:

$$p_g(\rho_g) = \frac{p_0}{(\rho_g^0)^\gamma}\ \rho_g^\gamma$$

- For liquid:

$$p_\ell(\rho_\ell) = \frac{p_0}{1 - \frac{\rho_\ell^0 c_\ell^2}{p_0}\left(1 - \frac{\rho_\ell^0}{\rho_\ell}\right)} \quad \text{with} \quad K = \frac{\rho_\ell^0 c_\ell^2}{p_0}$$

Pressure equilibrium at interface

- Gas-gas:

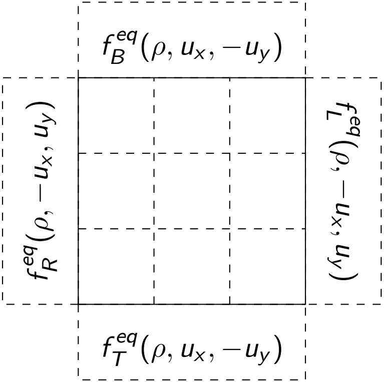
$$\alpha = \frac{m_1 \rho_2^0}{m_2 \rho_1^0 + m_1 \rho_2^0}, \quad \text{and} \quad p(\rho, Y) = p_0 \rho^\gamma \left(\frac{Y}{\rho_1^0} + \frac{1-Y}{\rho_2^0}\right)^\gamma$$

- Gas-liquid:

$$\alpha = 1 - \frac{(K-1)m_g + \rho_g^0}{m_\ell \rho_g^0 + K m_g \rho_\ell^0} m_\ell \quad \text{and} \quad p(\rho, Y) = \frac{\rho(Y c_g^2 + (1-Y)c_\ell^2/K^2)}{1 - (1 - \frac{1}{K})\frac{\rho(1-Y)}{\rho_\ell^0}}$$

Wall boundary conditions for our LBM approach

- Mirror cells as in Finite Volumes
- Distributions chosen at equilibrium[3]



- D2Q5 $\Rightarrow$ no coins problem

[3] [Inamuro] A non-slip boundary condition for lattice Boltzmann simulations, 1995

Gravity treatment

Splitting ALE + Projection

1. $\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes(\mathbf{u}-\mathbf{w}) + p\mathbf{I}) = \rho\mathbf{g}$

   Solved with LBM ! → Only g_i in 1D and k_i in 2D will be modified.

2. $\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{w}) = 0$

En LBM, les termes sources sont traités durant la collision[a].

$$\partial_t f + \mathbf{v}\cdot\nabla_x f = \Omega(f) + \rho\mathbf{g}$$

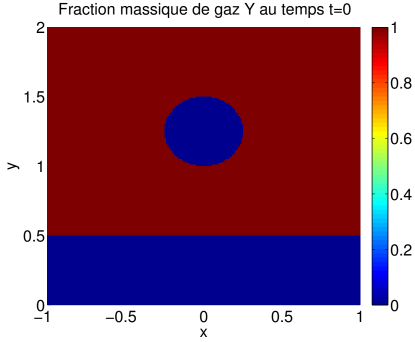
1. Collision $\partial_t f = \Omega(f) + \rho\mathbf{g}$
2. Transport $\partial_t f + \mathbf{v}\cdot\nabla_x f = 0$

$$\partial_t k_i = \frac{\widetilde{k}_i - k_i^n}{\Delta t} = -\frac{k_i^n - k_i^{eq,n}}{\tau\Delta t} - \rho g$$
$$\Rightarrow \widetilde{k}_{B,T} = k_{B,T}^n + \omega(k_{B,T}^{eq,n} - k_{B,T}^n) - 0.5\ \Delta t\ \rho g$$

[a] [Buick, 2000]

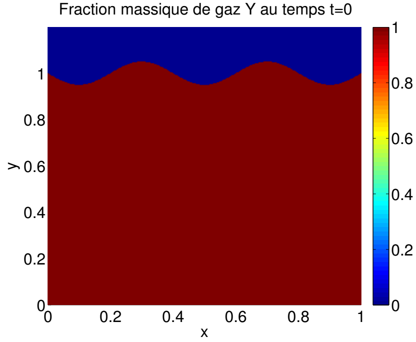
First results (order 1)

Free fall of a drop (ratio=1000)



$\tau = 1,\ \beta = 6,\ \pi_0 = 2,$
$g = 9.81,\ N_x = N_y = 200$

Rayleigh-Taylor instabilities (rt=20)



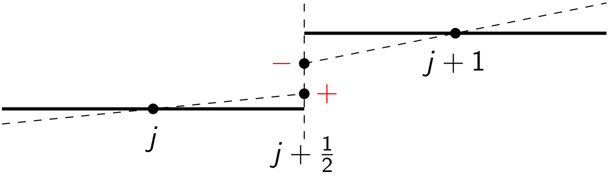
$\tau = 1,\ \beta = 12,\ \pi_0 = 0.5,$
$g = 0.2,\ N_x = 256,\ N_y = 307$

Order 2 for the projection, case 1D (1/2)

1) Definition of $Y = \dfrac{\alpha\rho_g}{\rho}$, $z_i = \dfrac{f_i}{\rho}$ and $a_i = \dfrac{g_i}{\rho}$

2) MUSCL reconstruction of pressure p, gas mass fraction Y, z_i and a_i

- $p_+ = p_j + \frac{1}{2}(\partial_x p)_j$ and $p_- = p_{j+1} - \frac{1}{2}(\partial_x p)_{j+1}$
- $Y_+ = Y_j + \frac{1}{2}(\partial_x Y)_j$ and $Y_- = Y_{j+1} - \frac{1}{2}(\partial_x Y)_{j+1}$
- $(z_i)_+ = (z_i)_j + \frac{1}{2}(\partial_x z_i)_j$ and $(z_i)_- = (z_i)_{j+1} - \frac{1}{2}(\partial_x z_i)_{j+1}$
- $(a_i)_+ = (a_i)_j + \frac{1}{2}(\partial_x a_i)_j$ and $(a_i)_- = (a_i)_{j+1} - \frac{1}{2}(\partial_x a_i)_{j+1}$



3) Calculation of $(\rho_g)_\pm$ and $(\rho_\ell)_\pm$ at interface $j+\frac{1}{2}$

- $(\rho_g)_\pm = \rho_g(p_\pm)$
- $(\rho_\ell)_\pm = \rho_\ell(p_\pm)$

Order 2 for the projection, case 1D (1/2)

4)

$$\rho = \alpha\rho_g + (1-\alpha)\rho_\ell \quad \Leftrightarrow \quad \tau = Y\tau_g + (1-Y)\tau_\ell \quad \text{with} \quad \tau = \frac{1}{\rho}$$

5) $(f_i)_\pm = (z_i)_\pm * \rho_\pm$
$(g_i)_\pm = (a_i)_\pm * \rho_\pm$

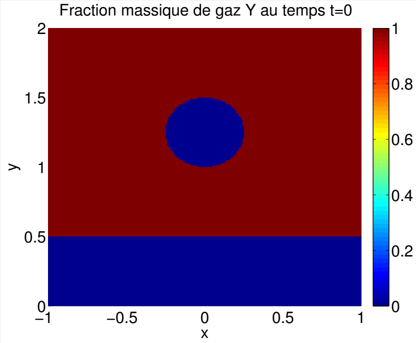
6) Calculation of upwind fluxes

- $\phi_{\rho,j+\frac{1}{2}} = (u_{j+\frac{1}{2}})_+ * \rho_+ + (u_{j+\frac{1}{2}})_- * \rho_-$
- $\phi_{f_i,j+\frac{1}{2}} = (u_{j+\frac{1}{2}})_+ * (f_i)_+ + (u_{j+\frac{1}{2}})_- * (f_i)_-$
- $\phi_{g_i,j+\frac{1}{2}} = (u_{j+\frac{1}{2}})_+ * (g_i)_+ + (u_{j+\frac{1}{2}})_- * (g_i)_-$
- $\phi_{m_g,j+\frac{1}{2}} = (u_{j+\frac{1}{2}})_+ * \rho_+ * Y_+ + (u_{j+\frac{1}{2}})_- * \rho_- * Y_-$
- $\phi_{\rho u,j+\frac{1}{2}} = (\phi_{\rho,j+\frac{1}{2}})_+ * (u_j + \frac{1}{2}(\partial_x u)_j) + (\phi_{\rho,j+\frac{1}{2}})_- * (u_{j+1} - \frac{1}{2}(\partial_x u)_{j+1})$

7) Update of f_i, g_i, ρ, ρu and m_g

Results (order 2)

Free fall of a drop (ratio=1000)



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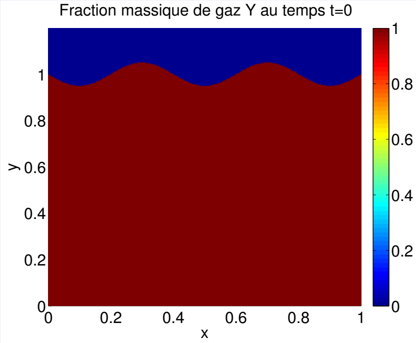

$$\tau = 1,\ \beta = 12,\ \pi_0 = 0.5,$$
$$g = 0.2,\ N_x = 256,\ N_y = 307$$

Conclusions

- Presentation of a scheme family $\mathcal{S}_{\tau,\beta,\pi_0}$
- Links between LBM and FV when $\tau = 1$
- Need of an ALE approach to stabilize contact discontinuities
- To calculate u in a quasi-Lagrangian case
  $\rightarrow$ Multi-distribution approach
- More stable for big density ratio
- 1^{st} results very promising for two-fluid flow

Outlook

- Asymptotic study for Navier-Stokes equations
- Implement gas-liquid interface + add surface tension
- Analysis of parameters and their interactions for stability
  $\rightarrow$ link π_0 / entropy ?
- "MRT", for now same τ for each distribution
- Implement other boundary conditions
- 3D extension (D3Q7Q3Q3Q3 ?)

Thank you for your attention
Questions ?

PhD defense tomorrow afternoon
ENS Cachan 14h30