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

1. Context and introduction to Lattice Boltzmann Method
2. LBM 1D for one fluid
3. LBM ALE+R 1D for one fluid
4. LBM ALE+R 2D for one fluid
5. Two-fluid extension
6. Conclusions and outlook
1. Context and introduction to Lattice Boltzmann Method

2. LBM 1D for one fluid

3. LBM ALE+R 1D for one fluid

4. LBM ALE+R 2D for one fluid

5. Two-fluid extension

6. Conclusions and outlook
Non viscous non thermal two-fluids flow (Isentropic Euler equations):

\[
\begin{align*}
\partial_t (\alpha \rho_g) + \nabla \cdot (\alpha \rho_g \mathbf{u}) &= 0, \\
\partial_t ((1 - \alpha) \rho_\ell) + \nabla \cdot ((1 - \alpha) \rho_\ell \mathbf{u}) &= 0, \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{l}) &= \rho \mathbf{g},
\end{align*}
\]

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

→ Analysis of LBM for two-fluid flow with possibly high-density ratio
Lattice Boltzmann Method (LBM)

**Boltzmann equation**

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

**In Navier-Stokes\(^1\) case**

\[
\nu = \Delta t \, c_s^2 \left( \tau - \frac{1}{2} \right) \quad \rightarrow \tau \geq 1/2
\]

\(^1\)He Luo, 1997
Discrete Boltzmann equation (LBGK\textsuperscript{2}-type)

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

Lattice \( \mathcal{L} \) DdQq

D1Q3

D2Q9

D3Q19 = D2Q9 in each direction

\footnote{Bhatnagar, Gross et Krook, 1954}
Discrete Boltzmann equation (LBGK-type)

\[ \partial_t f_i + v_i \cdot \nabla f_i = Q(f_i, f_i) \overset{\text{BGK}}{=} \frac{(f_i^{\text{eq}} - f_i)}{\tau \Delta t} \]

\( v_i \in \mathcal{L}, i \in [0, q - 1] \)

Lattice \( \mathcal{L} \) DdQq

Flux consistency:

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

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

Notation

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

each direction
1. Context and introduction to Lattice Boltzmann Method

2. LBM 1D for one fluid
   - D1Q3 lattice
   - Multi-distributions approach
   - Limitations

3. LBM ALE+R 1D for one fluid

4. LBM ALE+R 2D for one fluid

5. Two-fluid extension

6. Conclusions and outlook
D1Q3 lattice

\[ v_- = -s \quad v_0 = 0 \quad v_+ = s \]

with \( s = \frac{\Delta x}{\Delta t} \), 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

\[
p(\rho) = \rho^\gamma + \pi_0
\]

\[
\begin{align*}
    f_{\pm}^{eq} &= \frac{\rho u (u \pm s) + p}{2s^2}, \\
    f_0^{eq} &= \rho - \frac{\rho u^2 + p}{s^2}.
\end{align*}
\]
Mass conservativity

\[
\rho_j^{n+1} = \sum_i (f_i)_j^{n+1} = \sum_i (\tilde{f}_i)_{j(i)} = \rho_j^n - \frac{\Delta t}{\Delta x} \left( s \rho_j^n - s \sum_i (\tilde{f}_i)_{j(i)} \right)
\]

\[
= \rho_j^n - \frac{\Delta t}{\Delta x} \left( s \rho_j^n - s \left( (f_0)_j + (f_-)_{j+1} + (f_+)_j \right) \right)
\]

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

\[
\rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x} \left( (\Phi_\rho)_j^{n+\frac{1}{2}} - (\Phi_\rho)_j^{n-\frac{1}{2}} \right)
\]

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

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

\[ (\rho u)_j^{n+1} = \sum_i v_i (f_i)_j^{n+1} = \sum_i \tilde{v}_i(f_i)_{j(i)} \]

\[ = (\rho u)_j^n - \frac{\Delta t}{\Delta x} \left( s(\rho u)_j^n - s\left( s(f_+)_j^{n-1} - s(f_-)_j^{n+1} \right) \right) \]

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

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

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

\[ \rightarrow \text{Momentum conservative scheme } \forall \tau \in \left] \frac{1}{2}, +\infty \right[. \]
Stability by positivity

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

\[
\sqrt{u^2 + \frac{p}{\rho}} \leq s = \frac{\Delta x}{\Delta t} \leq \frac{u^2 + p/\rho}{|u|}
\]

For each point \( x \in \Omega \), we have

\[
\sqrt{u^2 + \frac{p}{\rho}} \leq \frac{u^2 + p/\rho}{|u|}
\]

But

\[
\max_\Omega \left( \sqrt{u^2 + \frac{p}{\rho}} \right)^2 \leq \min_\Omega \left( \frac{u^2 + p/\rho}{|u|} \right)
\]

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)

\[
\begin{align*}
\frac{\partial t}{\partial t} \rho &+ \frac{\partial}{\partial x} (\rho u) = 0, \\
\frac{\partial t}{\partial t} (\rho u) &+ \frac{\partial}{\partial x} (\rho u^2 + p) = 0.
\end{align*}
\]

with

\[ p = \rho^\gamma + \pi_0, \quad \gamma = 1.4 \]

At initial time, \( t = 0 \),

\[ \rho = \rho_1 \ast (x < 0.5) + \rho_2 \ast (x \geq 0.5). \]

\[
\begin{array}{|c|c|}
\hline
\rho = \rho_1 & \rho = \rho_2 \\
0 & 0.5 & 1 \\
\hline
\end{array}
\]

Homogeneous Neumann boundary conditions
Results for the shock tube test case

Isentropic Euler equations solved with the classical LBM D1Q3 scheme

\[
\rho = 1.0 \times (x < 0.5) + 0.125 \times (x \geq 0.5),
\]

\[
\tau = 1, \quad \beta = 4, \quad \pi_0 = 0 \text{ and } N = 300.
\]
Results for the shock tube test case

Isentropic Euler equations solved with the classical LBM D1Q3 scheme

\[
\rho = 1.0 \times (x < 0.5) + 0.2 \times (x \geq 0.5),
\]
\[
\tau = 1, \ \beta = 4, \ \pi_0 = 0 \text{ and } N = 300.
\]
D1Q3 for $\rho$ + D1Q3 for $\rho u = \text{D1Q3Q3 approach}^3$

One lattice per equation. Previous D1Q3 for $\rho$.

$$\sum_i g_i = \sum_i g_i^{eq} = \rho u,$$
$$\sum_i v_i g_i = \sum_i v_i g_i^{eq} = \rho u^2 + p$$
$$+ \sum_i v_i^2 g_i = \sum_i v_i^2 g_i^{eq} = \rho u^3 + 3pu$$

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

Definition:

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

$^3$[Parmigiani et al., 2009], [Dubois, Graille, Lallemand, 2016]
Test case $\tau = 0.7$, $\beta = 5$, $N = 300$ and $T_f = 0.2$

$$\rho = 1.0 \ast (x < 0.5) + 0.05 \ast (x \geq 0.5)$$

$$\pi_0 = 0$$
Test case $\tau = 0.7$, $\beta = 5$, $N = 300$ and $T_f = 0.2$

$$\rho = 1.0 \times (x < 0.5) + 0.05 \times (x \geq 0.5)$$

$$\pi_0 = 0.05$$
With a density ratio of 1000

\[ \rho = 1.0 \ast (x < 0.5) + 0.001 \ast (x \geq 0.5) \]

\[ \tau = 1, \quad \beta = 18, \quad N = 800, \quad \pi_0 = 0, \quad T_f = 0.13. \]
Link with Finite Volume Schemes

Reminder

- Collision

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

- Advection

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

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 $\tau = 1$

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

Let’s assume $u_j^n = u_{j+1}^n = u$, $p_j^n = p_{j+1}^n = p$

$$\implies \Phi_{j+1/2} = \frac{\rho_j^n + \rho_{j+1}^n}{2} u - \frac{1}{2} m |u| (\rho_{j+1}^n - \rho_j^n)$$

Upwind scheme iif $m = \frac{|u|}{s} = 1$, $\implies |u| = s$ (sonic state).

If $|m| < 1$, the scheme is less diffusive than the upwind one.

$$\implies$$ Lack of numerical diffusion $\rightarrow$ Oscillations
1. Context and introduction to Lattice Boltzmann Method

2. LBM 1D for one fluid

3. LBM ALE+R 1D for one fluid
   - ALE formalism
   - Scheme
   - Properties
   - Results

4. LBM ALE+R 2D for one fluid

5. Two-fluid extension

6. Conclusions and outlook
Euler Equations in ALE formalism

Reynolds transport theorem:

\[
\frac{d}{dt} \int_{\mathcal{V}_t} q(x, t) \, dx = \int_{\mathcal{V}_t} [\partial_t q + \nabla \cdot (w q)] \, dx
\]

where \( w \) is the speed of the moving referential \( \mathcal{V}_t \).

So ALE Euler equations are

\[
\begin{aligned}
\partial_t (\rho) + \nabla \cdot (\rho (u - w)) &= 0, \\
\partial_t (\rho u) + \nabla \cdot (\rho u \otimes (u - w) + p) &= 0, \\
\partial_t (\rho E) + \nabla \cdot (\rho E (u - w) + p u) &= 0.
\end{aligned}
\]

where \( 2\rho E = \rho |u|^2 + p \).

---

ALE step - Material

- **Mass:**
  \[
  \sum_i f_i = \sum_i f_i^{eq} = \rho,
  \sum_i v_i f_i = \sum_i v_i f_i^{eq} = \rho(u - w),
  \sum_i v_i^2 f_i = \sum_i v_i^2 f_i^{eq} = \rho u(u - w) + p.
  \]

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

- **Momentum:**
  \[
  \sum_i g_i = \sum_i g_i^{eq} = \rho u,
  \sum_i v_i g_i = \sum_i v_i g_i^{eq} = \rho u(u - w) + p,
  \sum_i v_i^2 g_i = \sum_i v_i^2 g_i^{eq} = \rho u^2(u - w) + p(3u - w).
  \]

\[
\begin{cases}
  g_{\pm}^{eq} = \frac{\rho u(u - w)(u \pm s) + p(3u - w \pm s)}{2s^2}, \\
  g_0^{eq} = \rho u - \frac{\rho u^2(u - w) + p(3u - w)}{s^2}.
\end{cases}
\]
Properties (1/2)

- Conservativity of the ALE step

\[
U_{j}^{n+1/2} = U_{j}^{n} - \frac{\Delta t}{\Delta x} \left( \Phi_{j+1/2}^{ALE} - \Phi_{j-1/2}^{ALE} \right)
\]

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

\[
\Phi_{j+1/2}^{ALE} = \frac{F_{j}^{n} + F_{j+1}^{n}}{2} - \frac{1}{2s} \left( G_{j+1}^{n} - G_{j}^{n} \right),
\]

with

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

ALE benefit for contact discontinuities, if \( w = u \)

\[
\Phi_{j+1/2}^{ALE} = \frac{F_{j}^{n} + F_{j+1}^{n}}{2} - \frac{1}{2s} \left( G_{j+1}^{n} - G_{j}^{n} \right) = \begin{pmatrix} 0 \\ p \end{pmatrix}
\]
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

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

where

\[ w_{j+1/2} = \frac{w_{j} + w_{j+1}}{2} \]

- Stability by positivity

\[
\begin{cases}
\sqrt{(u - w)^2 + \frac{p}{\rho}} \leq s \leq \frac{(u - w)^2 + p/\rho}{|u - w|} & \text{if } |u - w| \neq 0 \\
\sqrt{\frac{p}{\rho}} \leq s & \text{otherwise}
\end{cases}
\]
Test case with $\tau = 1$, $\beta = 3$, $\pi_0 = 0.35$ and $N = 300$

$$\rho = 1.0 \times (x < 0.5) + 0.125 \times (x \geq 0.5)$$
Test case with $\tau = 1, \beta = 3, \pi_0 = 0, N = 100$ to $50000$

$$
\rho = 1.0 \times (x < 0.5) + 0.001 \times (x \geq 0.5)
$$
1. Context and introduction to Lattice Boltzmann Method

2. LBM 1D for one fluid

3. LBM ALE+R 1D for one fluid

4. LBM ALE+R 2D for one fluid
   - Developments
   - Validation on test case

5. Two-fluid extension

6. Conclusions and outlook
\[
\begin{align*}
\partial_t(\rho) + \partial_x(\rho(u_x - w_x)) + \partial_y(\rho(u_y - w_y)) &= 0, \\
\partial_t(\rho u_x) + \partial_x(\rho u_x(u_x - w_x) + p) + \partial_y(\rho u_x(u_y - w_y)) &= 0, \\
\partial_t(\rho u_y) + \partial_x(\rho u_y(u_x - w_x)) + \partial_y(\rho u_y(u_y - w_y) + p) &= 0, \\
\partial_t(\rho E) + \partial_x(\rho E(u_x - w_x) + \rho u_x) + \partial_y(\rho E(u_y - w_y) + \rho u_y) &= 0.
\end{align*}
\]

\[v_2 = v_T\]

\[v_3 = v_L\]

\[v_1 = v_R\]

\[v_4 = v_B\]

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

\[\Rightarrow w_x = u_x, \quad w_y = u_y\]

\[f^{eq}_{L,R,B,T} = \frac{p}{2s^2}, \quad f_0^{eq} = \rho - 4f_{L,R,B,T}\]

\[g^{eq}_{L,R} = \frac{p(2u_x \pm s)}{2s^2}, \quad g_0^{eq} = \rho u_x - \frac{pu_x}{s^2}\]

\[k^{eq}_{B,T} = \frac{p(2u_y \pm s)}{2s^2}, \quad k_0^{eq} = \rho u_y - \frac{pu_y}{s^2}\]
Properties (1/2)

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

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

with

$$\Phi_{i+\frac{1}{2},j}^{ALE} = \begin{pmatrix} 0 \\ \frac{p_{i+1,j}^n - p_{i,j}^n}{2} \\ \frac{p_{i+1,j} + p_{i,j}}{2} - \frac{2s}{(pu_x)_{i+1,j} - (pu_x)_{i,j}} \\ 0 \end{pmatrix}$$

and

$$\Phi_{i,j+\frac{1}{2}}^{ALE} = \begin{pmatrix} \frac{2s}{(pu_y)_{i,j+1} - (pu_y)_{i,j}} \\ 0 \\ \frac{p_{i,j+1} + p_{i,j}}{2} - \frac{2s}{(pu_y)_{i,j+1} - (pu_y)_{i,j}} \end{pmatrix}$$
Properties (2/2)

- Flux associated with projection avec convective upwind fluxes

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

\[
\Phi_{i+1/2,j}^{proj} = \begin{pmatrix}
\left( (w_x)_{i+1/2,j} + \rho_{i,j} \right)^{n+1/2} + \left( (w_x)_{i+1/2,j} - \rho_{i+1,j} \right) \\
0
\end{pmatrix}
\]

\[
\Phi_{i,j+1/2}^{proj} = \begin{pmatrix}
\left( (w_y)_{i,j+1/2} + \rho_{i,j} \right)^{n+1/2} + \left( (w_y)_{i,j+1/2} - \rho_{i,j+1} \right) \\
0
\end{pmatrix}
\]
Test case with $\tau = 1$, $\beta = 12$, $\pi_0 = 0$, $N_x = N_y = 512$

$$\rho = 1 \times 1_{\text{int}} + 0.001 \times 1_{\text{ext}}$$

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

$$\rho = 1 \times 1_{\text{int}} + 0.01 \times 1_{\text{ext}}$$

Homogeneous Neumann boundary conditions
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4. LBM ALE+R 2D for one fluid

5. Two-fluid extension
   - Possible treatments
   - Equations of state
   - Validation on test case

6. Conclusions and outlook
Complete ALE two-fluid system

Two-fluid ALE Euler equations:

\[
\begin{align*}
\partial_t(\alpha \rho g) &+ \nabla \cdot (\alpha \rho g (u - w)) = 0, \\
\partial_t((1 - \alpha) \rho \ell) &+ \nabla \cdot ((1 - \alpha) \rho \ell (u - w)) = 0, \\
\partial_t(\rho u) &+ \nabla \cdot (\rho u \otimes (u - w) + pI) = \rho g,
\end{align*}
\]

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

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

- 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:
  \[ p_g(\rho_g) = \frac{p_0}{(\rho_g^0)^\gamma} \rho_g \]

- For liquid:
  \[ p_l(\rho_l) = \frac{p_0}{1 - \frac{\rho_l^0 c_l^2}{p_0}} \left( 1 - \frac{\rho_l}{\rho_l^0} \right) \]
  with \( K = \frac{\rho_l^0 c_l^2}{p_0} \)

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:
  \[ \alpha = 1 - \frac{(K - 1) m_g + \rho_g^0}{m_l \rho_g^0 + K m_g \rho_l^0} m_l \quad \text{and} \quad p(\rho, Y) = \frac{\rho (Y c_g^2 + (1 - Y) c_l^2 / K^2)}{1 - (1 - \frac{1}{K}) \frac{\rho (1 - Y)}{\rho_l^0}} \]
Wall boundary conditions for our LBM approach

- Mirror cells as in Finite Volumes
- Distributions chosen at equilibrium\(^3\)

\[
\begin{align*}
    f_{R}^{eq}(\rho, -u_x, u_y) \\
    f_{T}^{eq}(\rho, u_x, -u_y) \\
    f_{B}^{eq}(\rho, u_x, -u_y) \\
    (\eta n\cdot n - \eta d)_{bb}^{eq}
\end{align*}
\]

- D2Q5 ⇒ no coins problem

\(^3\)Inamuro A non-slip boundary condition for lattice Boltzmann simulations, 1995
Gravity treatment

Splitting ALE + Projection

1. \( \partial_t (\rho u) + \nabla \cdot (\rho u \otimes (u - w)) + pl) = \rho g \)

Solved with LBM ! \( \rightarrow \) Only \( g_i \) in 1D and \( k_i \) in 2D will be modified.

2. \( \partial_t (\rho u) + \nabla \cdot (\rho u \otimes w) = 0 \)

En LBM, les termes sources sont traités durant la collision\(^a\).

\[
\partial_t f + v \cdot \nabla_x f = \Omega(f) + \rho g 
\]

1. Collision \( \partial_t f = \Omega(f) + \rho g \)

2. Transport \( \partial_t f + v \cdot \nabla_x f = 0 \)

\[
\partial_t k_i = \frac{\widetilde{k}_i - k_i^n}{\Delta t} = -\frac{k_i^n - k_i^{eq,n}}{\tau \Delta t} - \rho g 
\]

\[\Rightarrow \kappa_{B, T} = k_{B, T}^n + \omega(k_{B, T}^{eq,n} - k_{B, T}^n) - 0.5 \Delta t \rho g \]

\(^a[\text{Buick, 2000}]\)
Free fall of a drop (ratio=1000)

\[ \tau = 1, \beta = 6, \pi_0 = 2, \quad g = 9.81, \quad N_x = N_y = 200 \]

Rayleigh-Taylor instabilities (rt=20)

\[ \tau = 1, \beta = 12, \pi_0 = 0.5, \quad g = 0.2, \quad N_x = 256, \quad N_y = 307 \]
Order 2 for the projection, case 1D (1/2)

1) Definition of \( Y = \frac{\alpha \rho g}{\rho}, \ z_i = \frac{f_i}{\rho} \) and \( a_i = \frac{g_i}{\rho} \)

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

\[
\begin{align*}
\n\n\n(\rho g)_+ &= \rho g(p_+), \quad \text{and} \quad (\rho g)_- = \rho g(p_-) \\
(\rho \ell)_+ &= \rho \ell(p_+), \quad \text{and} \quad (\rho \ell)_- = \rho \ell(p_-)
\end{align*}
\]

3) Calculation of \((\rho g)_\pm\) and \((\rho \ell)_\pm\) at interface \( j + \frac{1}{2} \)
Order 2 for the projection, case 1D (1/2)

4)
\[\rho = \alpha \rho_g + (1 - \alpha) \rho_\ell \quad \Rightarrow \quad \tau = Y \tau_g + (1 - Y) \tau_\ell \quad \text{with} \quad \tau = \frac{1}{\rho}\]

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

6) Calculation of upwind fluxes

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

7) Update of \(f_i, g_i, \rho, \rho u\) and \(m_g\)
Results (order 2)

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)

- \( \tau = 1, \beta = 12, \pi_0 = 0.5, \)
- \( g = 0.2, N_x = 256, N_y = 307 \)
1. Context and introduction to Lattice Boltzmann Method

2. LBM 1D for one fluid

3. LBM ALE+R 1D for one fluid

4. LBM ALE+R 2D for one fluid

5. Two-fluid extension

6. Conclusions and outlook
Conclusions

- Presentation of a scheme family $S_{\tau,\beta,\pi_0}$
- 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 → link $\pi_0$ / entropy ?
- ”MRT”, for now same $\tau$ for each distribution
- Implement other boundary conditions
- 3D extension (D3Q7Q3Q3Q3 ?)
Thank you for your attention

Questions ?

PhD defense tomorrow afternoon
ENS Cachan 14h30