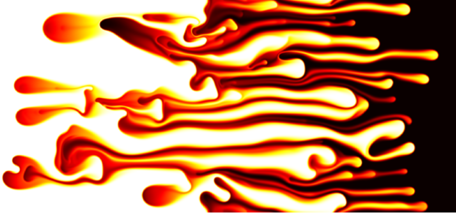

Simulation of multi-component flows by the lattice Boltzmann method and application to the viscous fingering instability

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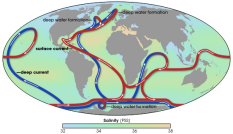
Context

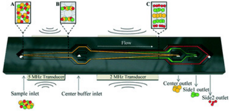
Mass transfer is ubiquitous in natural phenomena and industrial applications



Oceanic (thermohaline) circulation

Combustion, energy production, rocket propulsion

Chemistry, food processing, pharmacy, biology



Microfluidics, lab on a chip (image published by The Royal Society of Chemistry)

large scale → small scale

Mixing in tight space and porous medium

- Difficult (molecular diffusion)
- Mixing with dissimilar viscosities $\hookrightarrow$ viscous fingering instability

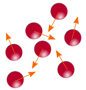
Context

le cnam

Transport phenomena

- transport of momentum
- transport of energy
- transport of mass of various chemical species

From a molecular point of view, all these mechanisms are related to the collision of molecules.



$\hookrightarrow$ Kinetic theory and Lattice Boltzmann method are based on a statistical description and provide a unified way to deal with transport phenomena.

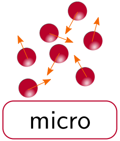
Simulation of multi-component flows by the lattice Boltzmann method and application to the viscous fingering instability

Introduction

Kinetic theory of gas

Fluid $\Longleftrightarrow$ molecules moving around and colliding

- Position $\boldsymbol{x} = (x, y, z)$
- Velocity $\boldsymbol{e} = (e_x, e_y, e_z)$
- Time t



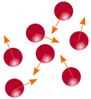
Fluid $\Longleftrightarrow$ molecules moving around and colliding

- Position $\boldsymbol{x} = (x, y, z)$
- Velocity $\boldsymbol{e} = (e_x, e_y, e_z)$
- Time t

Statistical description

$f(\boldsymbol{x}, \boldsymbol{e}, t)$: distribution function
$\hookrightarrow$ density of molecules with a velocity $\boldsymbol{e}$ at position $\boldsymbol{x}$ and time t.
Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{e} \cdot \boldsymbol{\nabla} f + \frac{\boldsymbol{F}_{\mathcal{B}}}{\rho} \cdot \boldsymbol{\nabla}_{\boldsymbol{e}} f = \left(\frac{df}{dt} \right)_{coll}$$



micro

meso

Introduction

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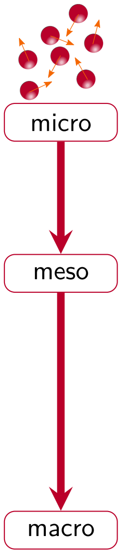
Macroscopic moments

- $\rho(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{e}, t) d\boldsymbol{e}$,
- $\rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \int \boldsymbol{e} f(\boldsymbol{x}, \boldsymbol{e}, t) d\boldsymbol{e}$,
- $\rho(\boldsymbol{x}, t)E(\boldsymbol{x}, t) = \int \frac{1}{2}\boldsymbol{e}^2 f(\boldsymbol{x}, \boldsymbol{e}, t) d\boldsymbol{e}$.



Introduction

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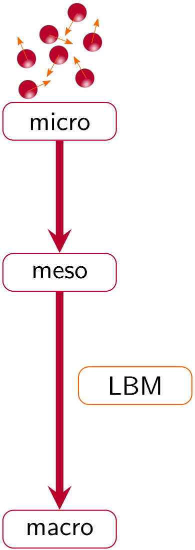


Introduction

Lattice Boltzmann method - LBM (1/3)

1. Bhatnagar-Gross-Krook (BGK) collision operator

$$\left(\frac{df}{dt}\right)_{coll} = -\frac{1}{\tau}\left(f - f^{eq}\right)$$

with $f^{eq}(\boldsymbol{x}, \boldsymbol{e}, t)$ Maxwell-Boltzmann distribution (Gaussian-like).

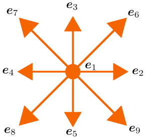
- Capture the relaxation of f toward an equilibrium state according to the relaxation time τ.
- Chapman-Enskog expansion shows that Navier-Stokes equations are recovered, and
- τ is related to the fluid viscosity.

Note: Other more advanced relaxation operators exist to remedy some numerical stability defects.

2. Velocity space discretization

- Macroscopic moments conservation ($\int \cdot d\boldsymbol{e} = \sum_\alpha$ up to a certain order)
- Only a few velocities are required to recover the macroscopic behavior of the fluid (mass and momentum transport)

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \boldsymbol{\nabla} f_\alpha = -\frac{1}{\tau}\left(f_\alpha - f_\alpha^{eq}\right) + S_\alpha$$



$$\alpha = 1, ..., 9 \quad f_\alpha = \begin{pmatrix} f_1 \\ \vdots \\ f_9 \end{pmatrix}$$

$$\rho = \sum_\alpha f_\alpha \qquad f_\alpha^{eq} = \rho \omega_\alpha \left[1 + \frac{\boldsymbol{u} \cdot \boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{u} \cdot \boldsymbol{e}_\alpha)^2}{2 c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2 c_s^2}\right]$$

$$\rho \boldsymbol{u} = \sum_\alpha \boldsymbol{e}_\alpha f_\alpha \qquad S_\alpha = \omega_\alpha \left[\frac{\boldsymbol{e}_\alpha - \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{e}_\alpha \cdot \boldsymbol{u}) \boldsymbol{e}_\alpha}{c_s^4}\right] \cdot \boldsymbol{F}_{\mathcal{B}}$$

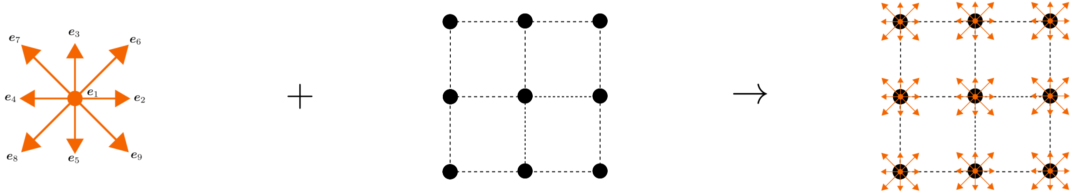
Introduction

Lattice Boltzmann method - LBM (3/3)

3. Physical space and time discretization

- Integration along the characteristics $\boldsymbol{e}_\alpha$: space, time, and kinetic velocities $\boldsymbol{e}_\alpha$ coupling.

$$f_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t, t + \delta_t) = f_\alpha(\boldsymbol{x}, t) - \frac{\delta_t}{\tau}\left[f_\alpha(\boldsymbol{x}, t) - f_\alpha^{eq}(\boldsymbol{x}, t)\right] + \delta_t\left(1 - \frac{\delta_t}{2\tau}\right) S_\alpha$$



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$$f_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t, t + \delta_t) = f_\alpha(\boldsymbol{x}, t) - \frac{\delta_t}{\tau}\left[f_\alpha(\boldsymbol{x}, t) - f_\alpha^{eq}(\boldsymbol{x}, t)\right] + \delta_t(1 - \frac{\delta_t}{2\tau})S_\alpha$$

↪ Collide and Stream algorithm

$$f_\alpha(\boldsymbol{x}+\boldsymbol{e}_\alpha\delta_t, t+\delta_t) = f_\alpha(\boldsymbol{x},t) - \frac{\delta_t}{\tau}\left[f_\alpha(\boldsymbol{x},t) - f_\alpha^{eq}(\boldsymbol{x},t)\right] + \delta_t\left(1-\frac{\delta_t}{2\tau}\right)S_\alpha$$

$\hookrightarrow$ Collide and Stream algorithm

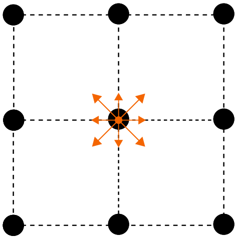
init

$$f_\alpha\left(\boldsymbol{x}, t=0\right) = f_\alpha^{eq}\left(\rho(\boldsymbol{x},0), \boldsymbol{u}(\boldsymbol{x},0)\right)$$

$$f_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t, t + \delta_t) = \boxed{f_\alpha(\boldsymbol{x}, t) - \frac{\delta_t}{\tau}\left[f_\alpha(\boldsymbol{x}, t) - f_\alpha^{eq}(\boldsymbol{x}, t)\right] + \delta_t\left(1 - \frac{\delta_t}{2\tau}\right)S_\alpha}$$

↪ Collide and Stream algorithm

init → collide



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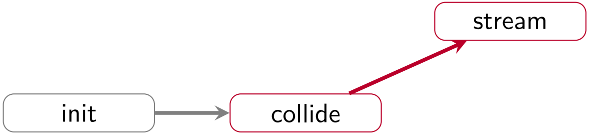

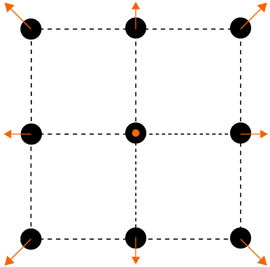

Introduction

Lattice Boltzmann method - LBM algorithm

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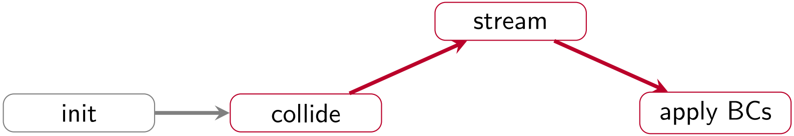

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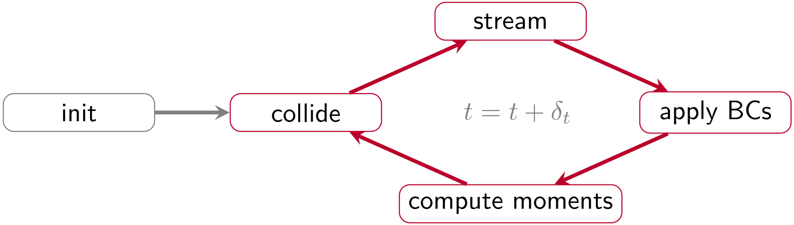

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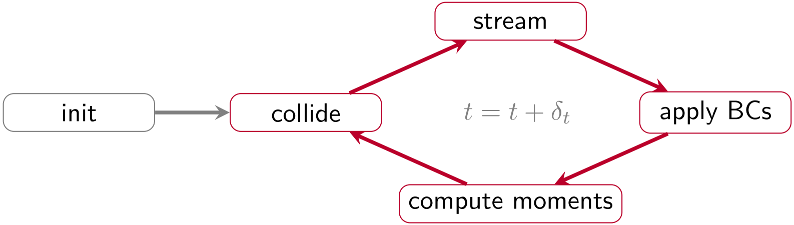

Advantages

- simple yet physically based on the Boltzmann equation
- 2nd order accurate for the weakly compressible NS equations
- efficient and HPC ready (parallel architectures and GPU)

Limitations

- uniform grid
- low Mach number flow (< 0.3)
- isothermal flow

Multi-species using LBM

Species distribution functions

$$f_\alpha^m(\boldsymbol{x}, t)$$

$\hookrightarrow$ Each species m has its own distribution function which is governed by its own kinetic equation.

$$\rho_m = \sum_\alpha f_\alpha^m,$$

$$\rho_m \boldsymbol{u}_m = \sum_\alpha f_\alpha^m \boldsymbol{e}_\alpha$$

- Mixture: no unique/well-established relaxation collision operator
- Different LB models depending on the underlying kinetic theory: *Luo and Girimaji 2003; Asinari 2006-2008; Arcidiacono et al. 2007*

Limitations: mixture-averaged transport coefficient, free parameters, collision is greatly modified.

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Limitations: mixture-averaged transport coefficient, free parameters, collision is greatly modified.

Solution

↪ Diffusion interaction among species is taken into account by means of a force.

↪ Since collision is not altered, this method can easily be introduced in any existing LB algorithm.

Multi-species using LBM

Part 1: viscous species dissipation

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

$\hookrightarrow$ Each species m has its own distribution function which is governed by its own kinetic equation.

$$\rho_m = \sum_\alpha f_\alpha^m, \qquad \rho_m \boldsymbol{u}_m = \sum_\alpha f_\alpha^m \boldsymbol{e}_\alpha$$

$$f_\alpha^{m(eq)} = \rho_m \omega_\alpha \left[1 + \frac{\boldsymbol{u}_m\cdot\boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{u}_m\cdot\boldsymbol{e}_\alpha)^2}{2c_s^4} - \frac{\boldsymbol{u}_m\cdot\boldsymbol{u}_m}{2c_s^2}\right]$$

How to choose the relaxation time τ_m?

$\hookrightarrow$ From the kinetic theory of gases!
Hirschfelder, Curtiss, and Bird 1954; *Kerkhof and Geboers 2004*

$$\mu_m = \frac{x_m \mu_{0,m}}{\sum_n^N x_n \Phi_{mn}}, \qquad \mu_m = \rho_m c_s^2 (\tau_m - \frac{\delta_t}{2})$$

Multi-species using LBM

Part 2: molecular species diffusion

$$f_\alpha^m(\boldsymbol{x}+\boldsymbol{e}_\alpha\delta_t, t+\delta_t) = f_\alpha^m(\boldsymbol{x},t) - \frac{\delta_t}{\tau_m}\left[f_\alpha^m(\boldsymbol{x},t) - f_\alpha^{m(eq)}(\boldsymbol{x},t)\right] + \delta_t(1-\frac{\delta_t}{2\tau_m})S_\alpha^m(\boldsymbol{x},t)$$

↪ Each species m has its own distribution function which is governed by its own kinetic equation.

$\rho_m = \sum_\alpha f_\alpha^m$,

$\rho_m \boldsymbol{u}_m = \sum_\alpha f_\alpha^m \boldsymbol{e}_\alpha + \frac{1}{2}\boldsymbol{F}_{\mathcal{D},m}$

$$f_\alpha^{m(eq)} = \rho_m \omega_\alpha \left[1 + \frac{\boldsymbol{u}_m\cdot\boldsymbol{e}_\alpha}{c_s^2} + \frac{(\boldsymbol{u}_m\cdot\boldsymbol{e}_\alpha)^2}{2c_s^4} - \frac{\boldsymbol{u}_m\cdot\boldsymbol{u}_m}{2c_s^2}\right]$$

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

Inter-molecular friction force

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

$\mathcal{D}_{mn}$: Maxwell-Stefan diffusion coefficient

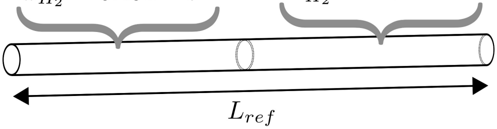
Maxwell 1867; *Chapman and Cowling 1932*; *Hirschfelder, Curtiss, and Bird 1954*; *Kerkhof and Geboers 2004*

Numerical validation

- A-Decay of a density wave ($\hookrightarrow$ molar mass ratio up to 86)
- B-Equimolar counter-diffusion
- C-Loschmidt's tube
- D-Opposed jets flow

Loschmidt's experiment: a ternary mixture exhibiting complex diffusion.

$$x_{Ar} = 0.509 - \delta \qquad x_{Ar} = 0.485 - \delta$$
$$x_{CH_4} = 0 + 2\delta \qquad x_{CH_4} = 0.515 - \delta$$
$$x_{H_2} = 0.491 - \delta \qquad x_{H_2} = 0 + 2\delta$$



Sketch of the experimental apparatus. $\delta = 5 \times 10^{-4}$.

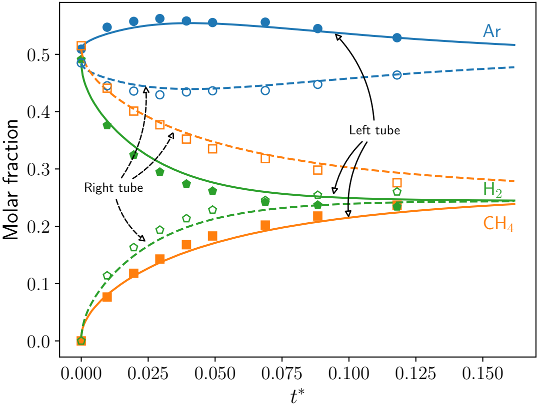
L_{ref}	[m]	$2\pi\sqrt{1/60}$		
p	[Pa]	101325		
T	[K]	307.15		
m		Ar	CH_4	H_2
M_m	[g/mol]	39.948	16.0425	2.01588
$\mathcal{D}_{\mathrm{Ar}\,m}$	[mm^2/s]	–	21.57	83.35
$\mathcal{D}_{\mathrm{CH_4}\,m}$	[mm^2/s]	21.57	–	77.16
$\mathcal{D}_{\mathrm{H_2}\,m}$	[mm^2/s]	83.35	77.16	–
$\mu_{0,m}$	[μPa/s]	22.83	11.35	9.18

Physical parameters of the experiment.

The left and right mean compositions are measured in time during the mixing.

Multi-species using LBM

C-Loschmidt's tube



▬ (lines) simulation ;

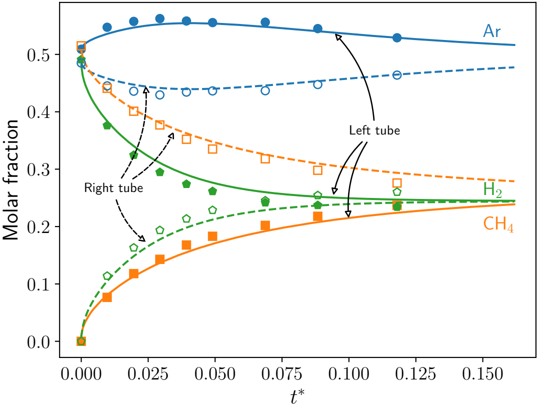
• (symbols) experimental data extracted from *Krishna 2015*

$t^* = t \times \mathcal{D}_{\mathrm{ArCH}_4} / L_{ref}^2$.

Diffusion of Argon

- $t^* < 0.04$ left $\longleftarrow$ right tubes
- $0.04 < t^* < 0.05$ left $\longleftrightarrow$ right tubes
- $t^* > 0.05$ left $\longrightarrow$ right tubes

Is something wrong?
$\mathcal{D}_{\text{Ar}\,\text{H}_2} = 83.35\ \text{mm}^2/\text{s}$
$\mathcal{D}_{\text{Ar}\,\text{CH}_4} = 21.57\ \text{mm}^2/\text{s}$



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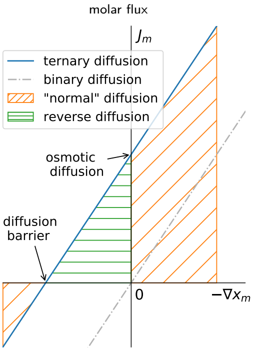
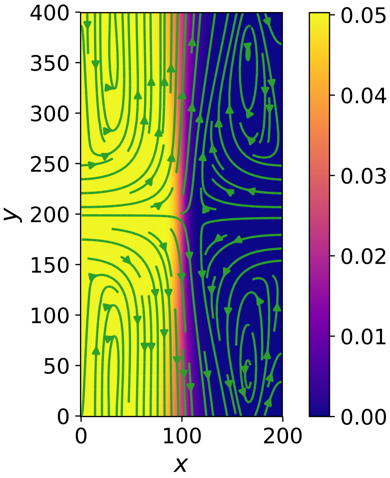
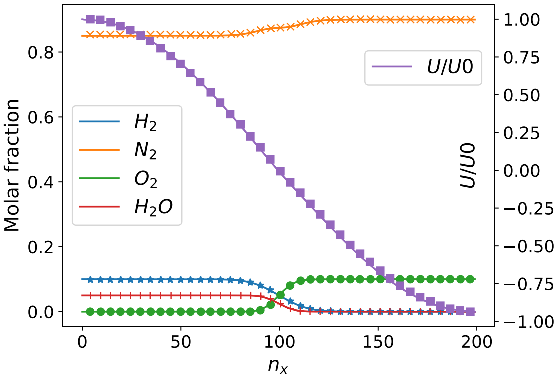


Multi-component diffusion effects

Two opposed jets of a quaternary mixtures: a convection-diffusion competing mechanism.



Molar fraction and velocity streamline plot of H_2O.



▬ (lines) present method;
• (symbols) LBM from *Arcidiacono et al. 2007* at $y = n_y/2$.

Multi-species using LBM

Synthesis

- Each species has its own distribution function which is governed by its own kinetic equation.
- Viscous dissipation is related to the relaxation toward the equilibrium.
- Molecular diffusion is associated with the inter-molecular diffusion force.
- Transport coefficients are calculated from the kinetic theory of gases.
- Species with dissimilar molecular masses are simulated by using an artificial force.

↪ Multi-component diffusion effects are recovered.

↪ The simple structure of the collide and stream algorithm is preserved.

↪ Proposed model is independent of the collision operator.

↪ Only a few modifications are needed to upgrade an existing single-fluid code to take into account diffusion between multiple species.

Introduction

Kinetic theory of gas

Lattice Boltzmann method (LBM)

Multi-component flows using LBM

Proposed model

Numerical validation

Viscous fingering instability using LBM

Porous medium model

Viscous fingering: binary mixture

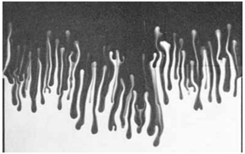
Viscous fingering: ternary mixture

Viscous fingering using LBM

Viscous fingering

This instability occurs when a less viscous fluid displaces a more viscous fluid in a porous medium.
Improve the mixing efficiency in porous media or be detrimental in

- oil recovery
- CO_2 sequestration
  - ↪ *Nijjer et al. 2018* after a shutdown time of 150 years: mixing zone of 50km long with fingering / 5m long with only pure diffusion
- chromatography column
- soil contamination



Viscous fingering in a Hele-Shaw cell.
Homsy 1987

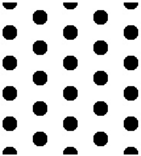
Viscous fingering in an opaque medium visualized by X-ray absorption.

Viscous fingering a complex convection-diffusion mechanism.
We need a

- binary miscible flow $\rightarrow$ inter-molecular friction force
- with a disparity in viscosity $\rightarrow$ partial viscosities
- in a porous medium $\rightarrow$?

Porous medium

Explicit: model the pores of the porous medium (computationally expensive)



Implicit: use a model

- Average view of the porous medium: permeability K
- Less computationally expensive
- Comparison with the literature (Darcy's law)

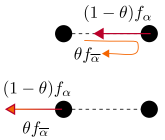
Gray lattice Boltzmann (GLBM)

Porous medium effect $\sim$ partial bounce-back.
Yoshida and Hayashi 2014: Post-collision distribution functions are reflected.

- θ is the amount of reflection

$\theta_m = 0 \Rightarrow$ standard streaming

$\theta_m = 1 \Rightarrow$ bounce-back condition



Streaming step with GLBM

Brinkman forcing scheme (BF)

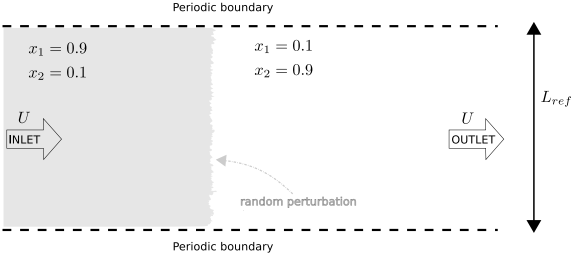
Porous medium effect $\sim$ global drag effect.
Martys 2001, *Guo and Zhao 2002*, *Ginzburg 2008*

$$\boldsymbol{F}_{porous,m} = -\frac{\mu_m}{K}\boldsymbol{u}_m$$

$$\frac{2\theta_m}{(1-\theta_m)\delta_t} = \frac{\mu_m}{K\rho_m}$$

Viscous fingering using LBM

Numerical configuration



Initial conditions

$$f_\alpha^m(t=0) = f_\alpha^{m(eq)}(\rho_m, u_{x,m} = U, u_{y,m} = 0)$$

Grid resolution

Resolution corresponding to

- $n_y = 4000$ to study the early times
- $n_y = 2000$ to study the intermediate times

Dimensionless numbers

$$R = \ln\left(\mu_{0,2}/\mu_{0,1}\right) = 3$$
$$\text{Pe} = U L_{ref}/\mathcal{D}_{12} = [500 \ldots 5000]$$
$$\text{Re}_{0,1} = \rho_{ref} U L_{ref}/\mu_{0,1} = 10$$
$$\text{Da} = K/L_{ref}^2 = 6.25 \times 10^{-8}$$
$$\text{Ma} = U/c_s = \sqrt{3} \times 10^{-3}$$

Viscous fingering using LBM

Global dynamics

BF scheme, Pe=2000.

Fingers development

- Coarsening of the fingers in the transverse direction.
- Growth of the fingers in the streamwise direction

Early times: linear interactions

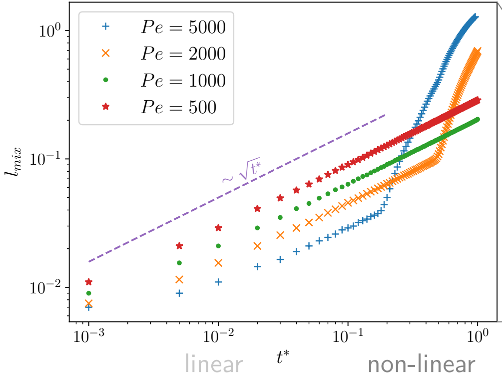
- Initial planar interface starts to deform
- Small fingers develop

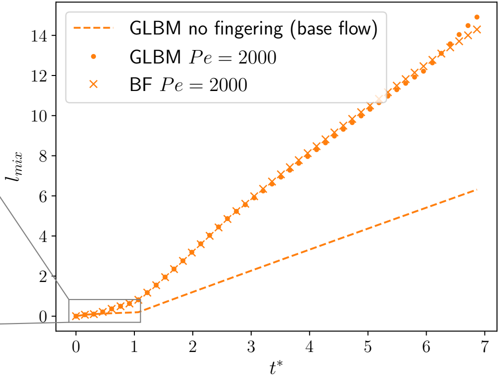
Intermediate times: non-linear interactions

- spreading, shielding, fading, coalescence
- tip splitting, and side branching

Viscous fingering using LBM

Intermediate times: mixing length





linear — non-linear

early times — intermediate times

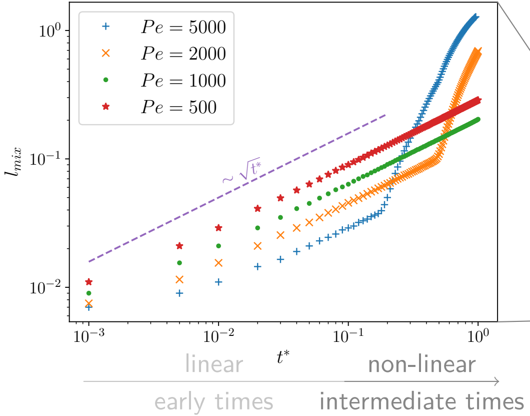
Mixing length

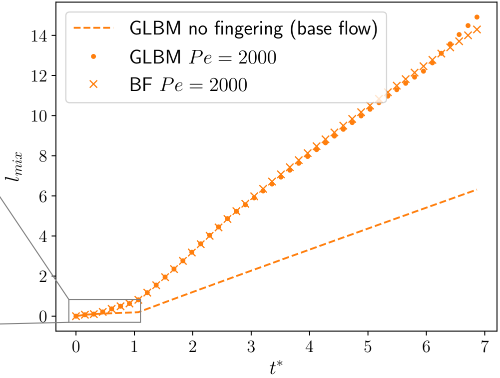
$$l_{mix}(t) = ||\bar{X}_{x_1=0.89}(t) - \bar{X}_{x_1=0.11}(t)||$$

$$t^* = tU/L_{ref}$$

Viscous fingering using LBM

Intermediate times: mixing length





- Diffusion-dominated regime $l_{mix} \sim \sqrt{t^*}$
- Advection-dominated regime $l_{mix} \sim t^*$
- No difference between GLBM and BF schemes

Assuming a perturbation

$$x'_m(\mathbf{x}, t) = x'_m(\mathbf{x}) \exp(\sigma t)$$

Growth rate of the perturbation σ

$$x'_m(\mathbf{x}, t) = x^0_m(\mathbf{x}, t) - x_m(\mathbf{x}, t)$$

$$\hat{x}(x, k, t) = \mathsf{FFT}_y\left(x'_m(\mathbf{x}, t)\right)$$

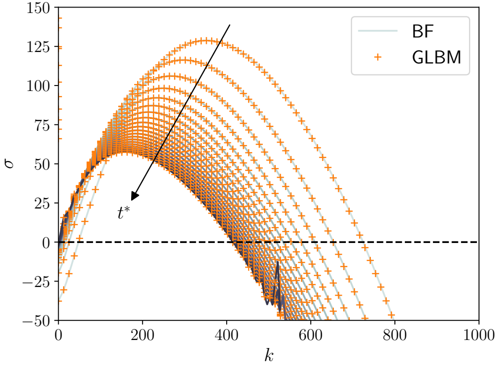
$$a(k, t) = ||\hat{x}(x, k, t)||_2 = \sqrt{\int \hat{x} \cdot \hat{x}^\dagger dx}$$

$$\sigma(k, t) = \frac{d \ln\left(a(k, t)\right)}{dt}$$

x^0_m: base state $\Longleftrightarrow$ non-perturbed simulation.

Viscous fingering using LBM

Early times: influence of the porous model

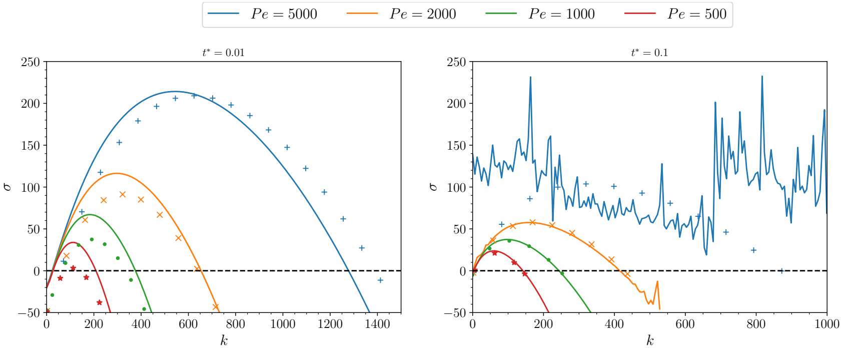


Dispersion curve for Pe $= 2000$ at various times from $t^* = 0.005$ to $t^* = 0.1$ with a time step $\Delta t^* = 0.05$.

- GLBM and BF schemes leads to equivalent growth rates.
- Growth rate decreases in time.
- Most dangerous, threshold and cutoff wave numbers are reduced as the instability progresses.

Viscous fingering using LBM

Early times: influence of the Péclet number Pe$= U L_{ref}/\mathcal{D}_{12}$

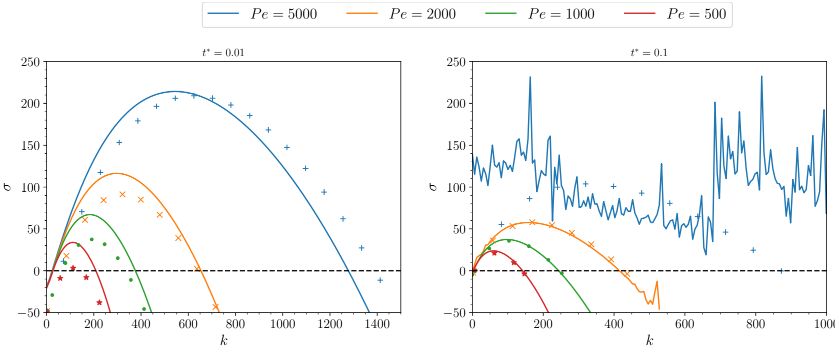


▬ (lines) simulation;
• (symbols) linear stability analysis from *Pramanik and Mishra 2015*.

- High Péclet numbers lead to a more intense instability.
- The range of unstable wave numbers and the growth rate increase with Pe.
- The Péclet number influences the transition from linear to non-linear interactions.

Viscous fingering using LBM

Early times: influence of the Péclet number Pe$= U L_{ref}/\mathcal{D}_{12}$



▬ (lines) simulation;
● (symbols) linear stability analysis from *Pramanik and Mishra 2015*.

- Symbols: linear stability analysis with quasi-steady-state approximation (QSSA).
- QSSA is known to have some flaws for very short times (compared to IVP, non-modal analysis) *Hota et al. 2015*.
- Excellent agreement for $t^* = 0.1$.

What are the differences between two and three species?

Binary mixture

- $\mathcal{D}_{12} = \mathcal{D}_{21}$
- $x_1 = 1 - x_2$
- $\boldsymbol{\nabla} x_1 = -\boldsymbol{\nabla} x_2$

Ternary mixture

- $\mathcal{D}_{12} \neq \mathcal{D}_{13} \neq \mathcal{D}_{23}$
- $x_1 + x_2 + x_3 = 1$
- $\boldsymbol{\nabla} x_1 + \boldsymbol{\nabla} x_2 + \boldsymbol{\nabla} x_3 = \mathbf{0}$

$\hookrightarrow$ Multi-component diffusion effects

Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion

Molar fractions	Invading fluid	Displaced fluid
x_1 (R)	0.1	0.45
x_2 (G)	0.45	0.1
x_3 (B)	0.45	0.45
RGB color		

$$\text{Pe} = 5000$$

$$\text{Re}_{0,1} = 10$$

$$R_{12} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,2}}\right) = 0$$

$$R_{13} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,3}}\right) = 3$$

$$\mathcal{D}_{mn} = \frac{L_{ref}U}{\text{Pe}} \begin{pmatrix} 0 & 1 & 0.1 \\ 1 & 0 & 1 \\ 0.1 & 1 & 0 \end{pmatrix}$$

Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion

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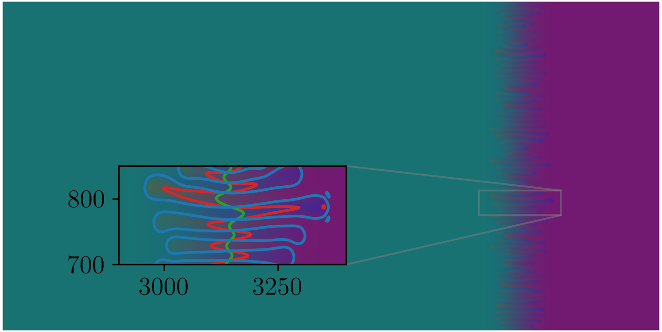
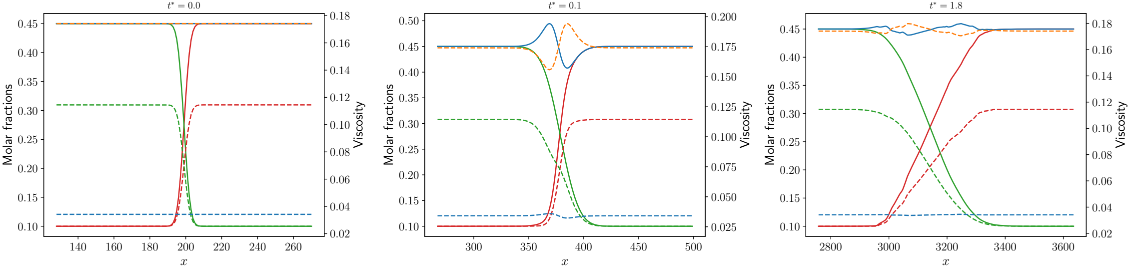


Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion



▬ (continuous lines) mean molar fraction over the transverse direction

‒ ‒ (dashed lines) mean partial viscosity over the transverse direction normalized by the pure viscosity $\mu_{0,1}$

species 1, species 2; species 3, mixture viscosity

Causes

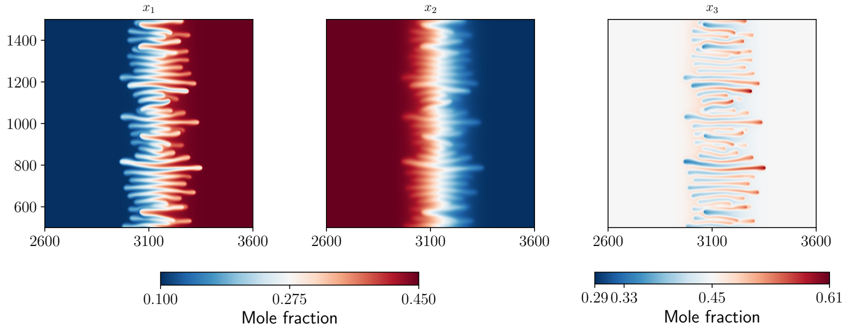
- multicomponent effects: osmotic & reverse diffusion
- result in a localised less viscous slice of fluid

Consequences

- viscous fingering in spite of an initial stable configuration
- fingers mostly composed of the third species

Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion



Color-map of the molar fraction at $t^* = 1.8$ for each species

Species fingering

- Third species: interface significantly deformed.
  Reverse diffusion tends to accentuate the fingering.
- Second species: $\mathcal{D}_{12} = \mathcal{D}_{23} \hookrightarrow$ almost symmetric interface.
- First species: $\mathcal{D}_{13} < \mathcal{D}_{12} \hookrightarrow$ fingers of low concentration are dragged along the third species.

Viscous fingering using LBM

Synthesis

- The physics of the binary viscous fingering instability is recovered
  - for early times (growth rates)
  - for intermediate times (diffusive then advective regimes).
- Both BF and GLBM schemes lead to equivalent results for the observed case.
- Behavior of the instability can dramatically change for three and more species.
- Viscous fingering could be induced by reverse diffusion despite having an initial stable flow configuration.

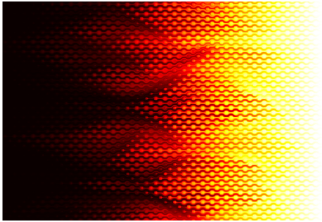
Conclusion

Conclusion

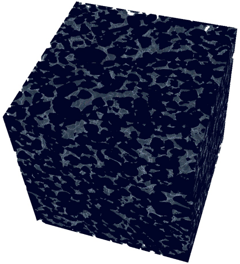
- A lattice Boltzmann method for multi-component flows is proposed.
- Standard relaxation process $\rightarrow$ viscous dissipation (partial viscosities).
- Inter-molecular-friction force $\rightarrow$ molecular diffusion (Maxwell-Stefan diffusion coefficient).
- Basic features of the model are validated.
- The physics of the binary viscous fingering instability is recovered.
- The influence of reverse diffusion on the instability is highlighted.

Perspectives

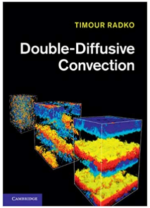
- Further studies are required on the multi-component model
- Parametric study of the ternary viscous fingering
  (passive control of viscous fingering).
- Explicit model of the porous medium

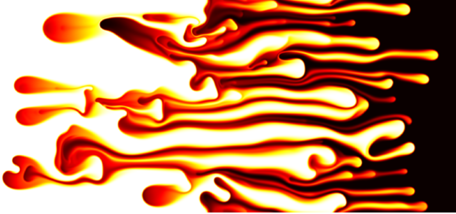


- 3D simulations



- Gravity currents and double-diffusive convection problems in oceans





Thank you for your attention.

Any questions?

Why not an advection-diffusion equation?

Diffusion equation is postulated, and a kinetic scheme is taylored to solve it.
$\hookrightarrow$ Loss of physical molecular meaning (collision of molecules).
$\partial_t c_m + \boldsymbol{\nabla} \cdot (c_m \boldsymbol{u}) = -\boldsymbol{J}_m$

Generalized Fick's law (ternary mixture)

$$\boldsymbol{J}_1 = -c_t D_{11} \boldsymbol{\nabla} x_1 - c_t D_{12} \boldsymbol{\nabla} x_2$$

$$\boldsymbol{J}_2 = -c_t D_{21} \boldsymbol{\nabla} x_1 - c_t D_{22} \boldsymbol{\nabla} x_2$$

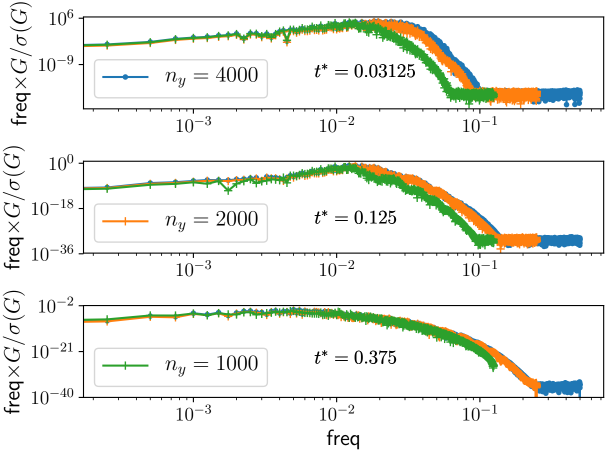
$$\text{and } \boldsymbol{J}_3 = -\boldsymbol{J}_1 - \boldsymbol{J}_2$$

Not as practical as the Maxwell-Stefan approach ($\boldsymbol{\nabla} x_m = \sum_{n=1}^{N} \frac{x_m \boldsymbol{J}_n - x_n \boldsymbol{J}_m}{c_t \mathcal{D}_{mn}}$) to mass transfer

- 4 Fick diffusion coefficients for a ternary mixture.
- D may be positive, negative, are usually non-symmetric and vary according to the mixture composition.
- D_{mn} do not reflect the $m - n$ interaction (collision). Its value depends on the component numbering.

Convergence study

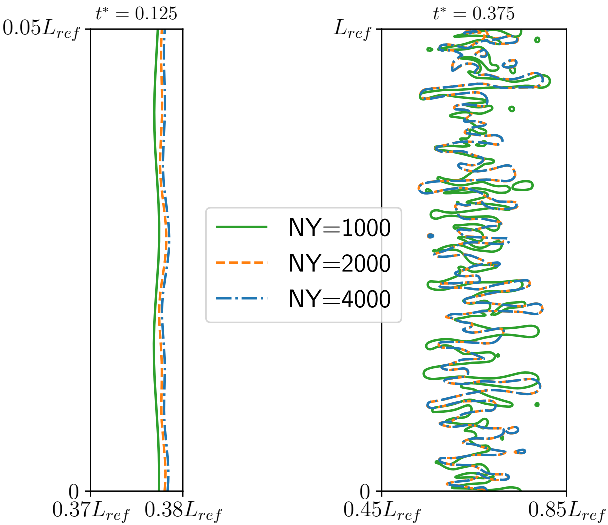
PSD



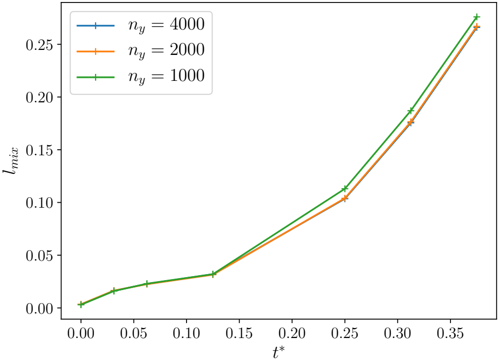
Power spectral density at different times t^* for different resolutions equivalent to blue, $n_y = 4000$; orange, $n_y = 2000$; green, $n_y = 1000$. $G = \hat{x}\hat{x}^\dagger$ where $\hat{x}^\dagger$ is the conjugate of the Fourier coefficients $\hat{x}$. G is normalized by its variance: $\sigma(G)$.

Convergence study

Contour-plots and mixing length



Contour plot for $x_1 = 0.4$ at $t^* = 0.125$ and $t^* = 0.375$.



Mixing length according to t^*.