Two-phase flow relative permeability determination using lattice Boltzmann method at the pore scale

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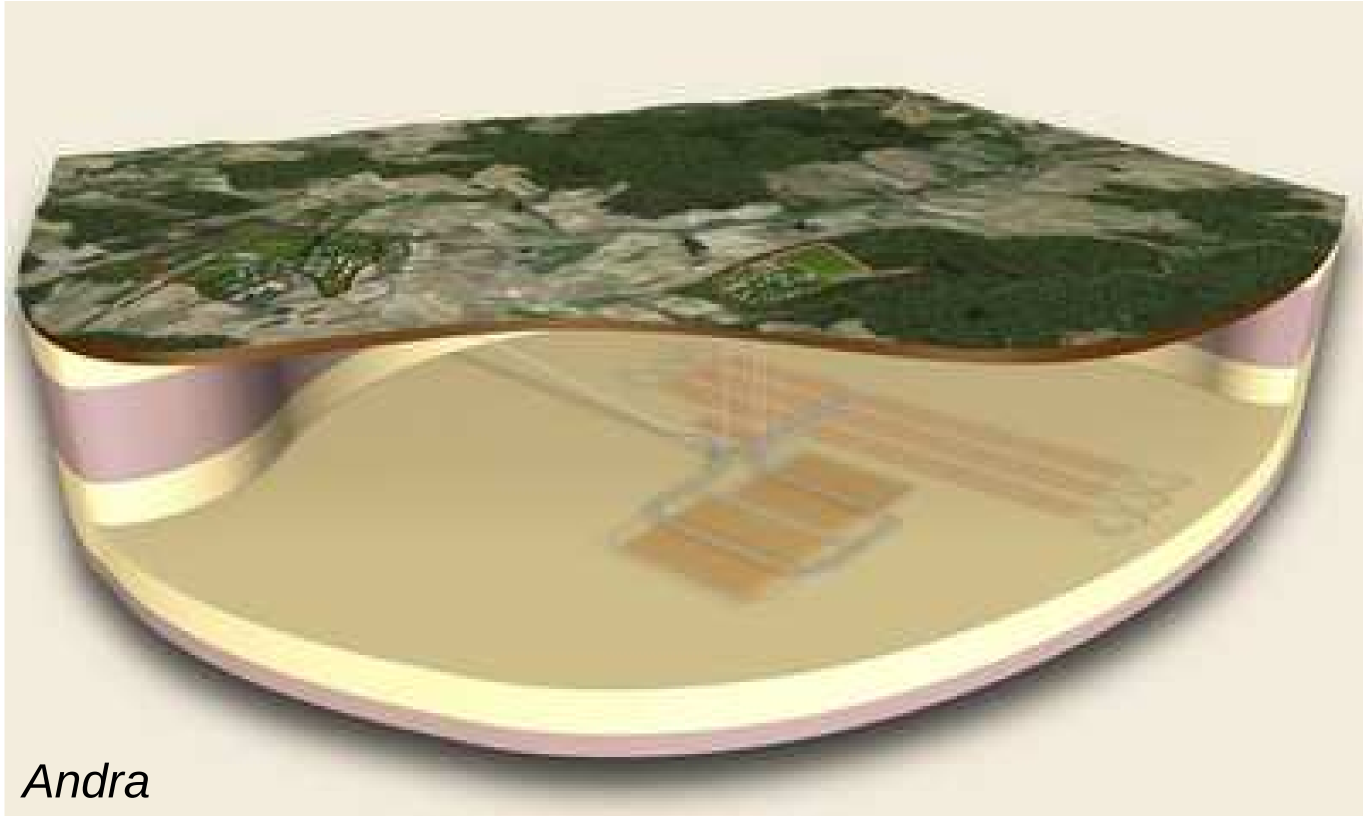
❑ The context : two-phase flow modeling in radioactive waste disposal



CONTEXT

Two-phase flow modeling at the radioactive waste repository scale.

- Anaerobic corrosion of metallic objects introduced inside the radioactive waste repository (canisters) is expected to produce a significant amount of hydrogen.

- The impact on repository behavior must be quantified :
  → Early gas breakthrough (^{14}C)?
  → Degradation of components confinement properties (pressure build-up)?
    → Host-rock fracking?
    → Plugs and sealing / host-rock interface degradation (by-pass)?

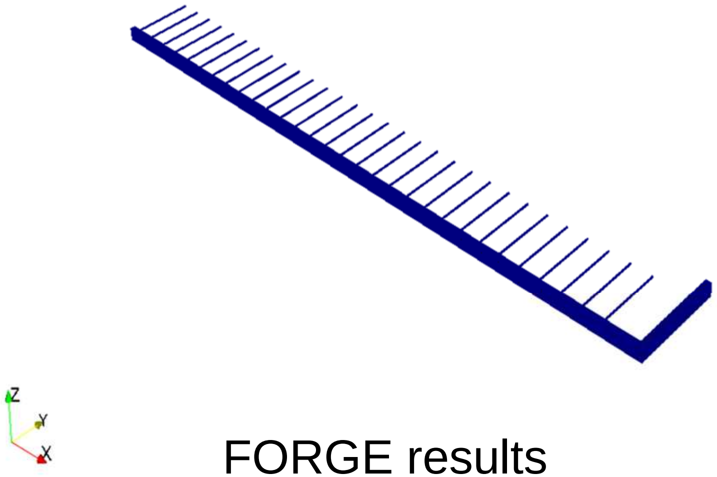
CONTEXT

Two-phase flow modeling at the radioactive waste repository scale.

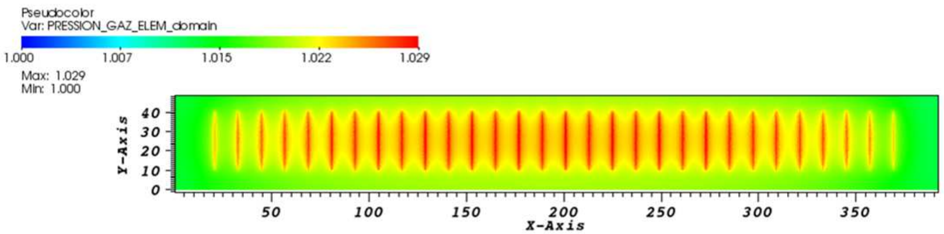
- Part of quantification is made through computation
- Two-phase flow (mass balance)

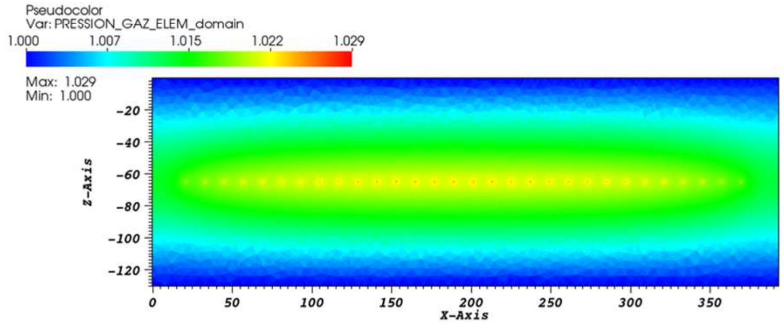
$$\theta \frac{\partial}{\partial t} S_{e,w} - \nabla \left(\frac{\kappa_{\text{int}} k_w}{\eta_w} \nabla (p_w + \rho_w g z) \right) = Q_w$$

$$\theta \frac{\partial}{\partial t} S_{e,nw} - \nabla \left(\frac{\kappa_{\text{int}} k_{nw}}{\eta_{nw}} \nabla (p_{nw} + \rho_{nw} g z) \right) = Q_{nw}$$



FORGE results





CONTEXT

Two-phase flow modeling at the radioactive waste repository scale.

- Relative permeability (Kr(S)) has a strong impact on the results but is not well known

$$\theta \frac{\partial}{\partial t} S_{e,w} - \nabla\left(\frac{\kappa_{\text{int}} k_w}{\eta_w} \nabla(p_w + \rho_w g z)\right) = Q_w$$

$$\theta \frac{\partial}{\partial t} S_{e,nw} - \nabla\left(\frac{\kappa_{\text{int}} k_{nw}}{\eta_{nw}} \nabla(p_{nw} + \rho_{nw} g z)\right) = Q_{nw}$$

- Determination of Kr through experimental measurements is very difficult in argillaceous rocks because of their very small permeability (PhD. Yang 2008).
  → Indirect determination through capillary curve and Mualem theory.

CONTEXT

Two-phase flow modeling at the pore scale.

- We decided to quantify Kr(S) through pore scale modeling
  → like for permeability, effective diffusion …

- What is the pore scale to consider ?
  → Small fractures of few microns in thickness are of major concern for two-phase flow (gas do not enter smallest pores).

- What is the best numerical approach ?
  → Lattice Boltzmann methods were extensively used for pore scale modeling purpose.

- ❑ The context : two-phase flow modeling inside radioactive waste disposal

- ❑ Lattice Boltzmann approach

- ❑ Application : two-phase flow at the pore scale

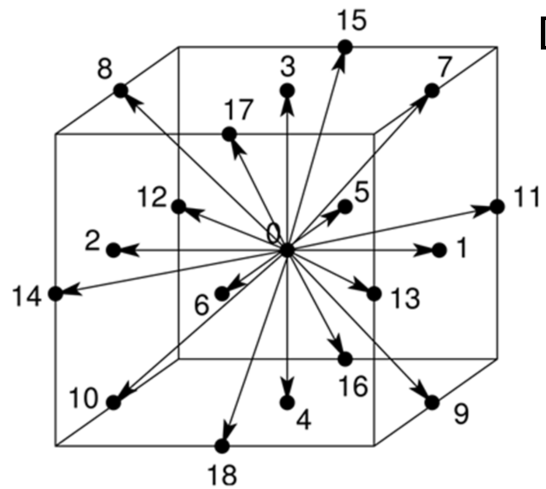
The lattice Boltzmann approach.

- Lattice Boltzmann approach originates from cellular automaton approach that mimic fluid behavior through "particles" propagation and collision.

- In the lattice Boltzmann approach, mass, time and space are discretized.
  Space is discretized using a regular grid and velocity space is discretized in Q directions.

- A "population function" f is associated to each node x for each direction q that evolves through a "collision step" and a "propagation step".

D3Q19



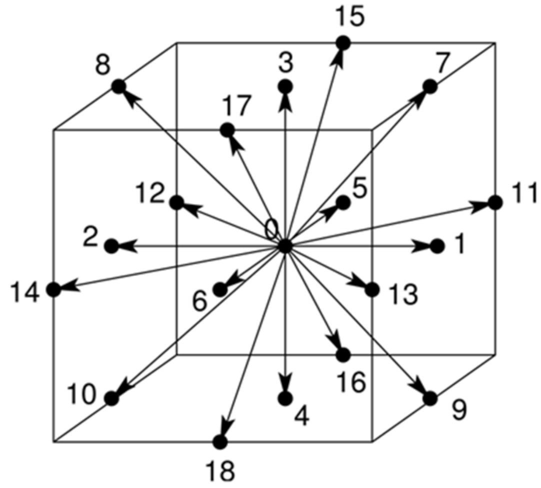
The lattice Boltzmann approach.

- "Collision step"

$$f_q(x,t+dt) = f_q(x,t) + (f_q^{eq} - f_q(x,t))/\tau$$

- "Propagation step"

$$f_q(x+e_i,t+dt) = f_q(x,t+dt)$$



D3Q19

Modeled physic depend on the choice of f_q^{eq}
(for fluid flow $\rho = \sum f_q$ and $\rho u = \sum f_q.e_i$)
τ is a relaxation time parameter (BGK, TRT, MRT)

- Note that equivalence of LBM scheme and finite difference Du Fort-Frankel scheme was shown for 1D heat transfer equation (Dellacherie, *Acta Applicandae Mathematicae*, 2014)

Lattice Boltzmann model

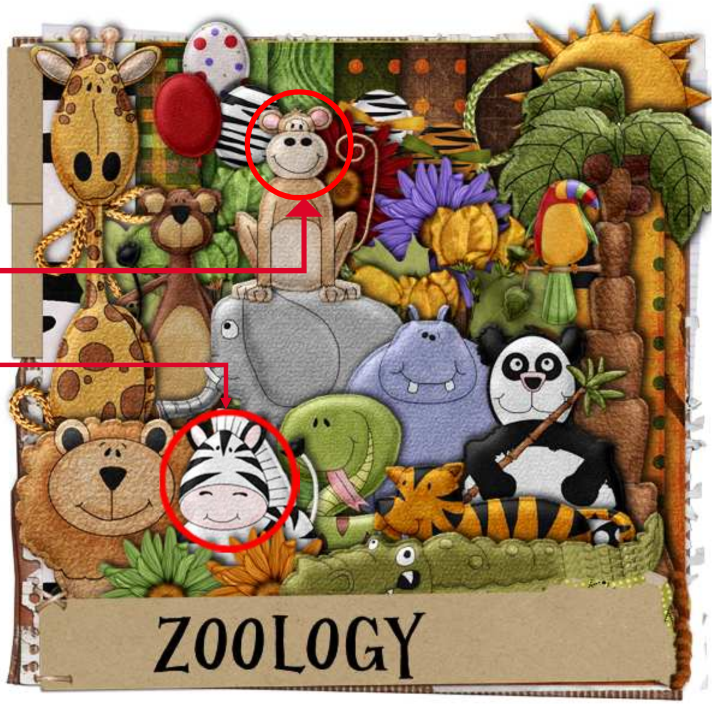
- Lattice Boltzmann models used to simulate two-phase flow are very numerous.

- Among the LBM zoology we use the two color RK model (color gradient model, Rothman & Keller 1988) with a Two Relaxation Time scheme (TRT)(Ginzburg *et al.* 2008)

  → one collision step

  → one re-coloration step

  → one propagation step



Lattice Boltzmann model

RK model in detail

Collision

$$\Omega^1(f_q) = f_q + \lambda_{even}\,(f_q^+ - f_q^{eq,+}) + \lambda_{odd}\,(f_q^- - f_q^{eq,-}) + S_q$$

- f_q^-, f_q^+ : odd and even parts of the distributions
- λ_{even}, λ_{odd} : TRT relaxation parameters
- S_q : source term

Perturation – Recoloring

$$\Omega^2(f_q) = f_q + \frac{A_{r,b}}{2}\,\overrightarrow{\nabla C}\left(\frac{(\overrightarrow{\nabla C}\cdot\vec{c_q})^2}{||\overrightarrow{\nabla C}||^2\,||\vec{c_q}||^2} - B_q\right)$$

$$\Omega^3(f_q) = \beta\,\frac{\rho_r\rho_b}{\rho^2}\,cos(\theta_q)\ f_q^{eq}\Big|_{\vec{u}=0}$$

$$r_q = \frac{\rho_r}{\rho}\,\Omega^2(f_q) + \Omega^3(f_q),\quad b_q = \frac{\rho_b}{\rho}\,\Omega^2(f_q) + \Omega^3(f_q)$$

- r, b, ρ_r, and ρ_b designate the two phase distributions and densities
- $\overrightarrow{\nabla C}$: Color or phase gradient
- β, $A_{r,b}$: Interface parameters
- θ_q : angle formed by $(\overrightarrow{\nabla C}, \vec{c_q})$

Propagation

$$f_q^{temp} = r_q + b_q,\quad f_q(\vec{r} + \vec{c_q}, t + \Delta t) = f_q^{temp}(\vec{r}, t)$$

- Propagation is done in a second temporary array f^{temp}

Bounceback

When the q direction neighbor is a solid site, the distribution is "bounced back" in the $\overline{q}$ direction,

$$f_q(\vec{r} + \vec{c_{\overline{q}}}, t + \Delta t) = f_{\overline{q}}^{temp}(\vec{r}, t)$$

- q and $\overline{q}$ are velocity opposite directions

Lattice Boltzmann model advantages and drawbacks

- Advantages

  Porous geometries like the ones obtained through computed tomography (voxels) are naturally integrated (LBM node).
  → No meshing work needed.

  Structure of the LBM (node by node description with no matrix inversion) allow efficient parallelism implementation.

- Drawback

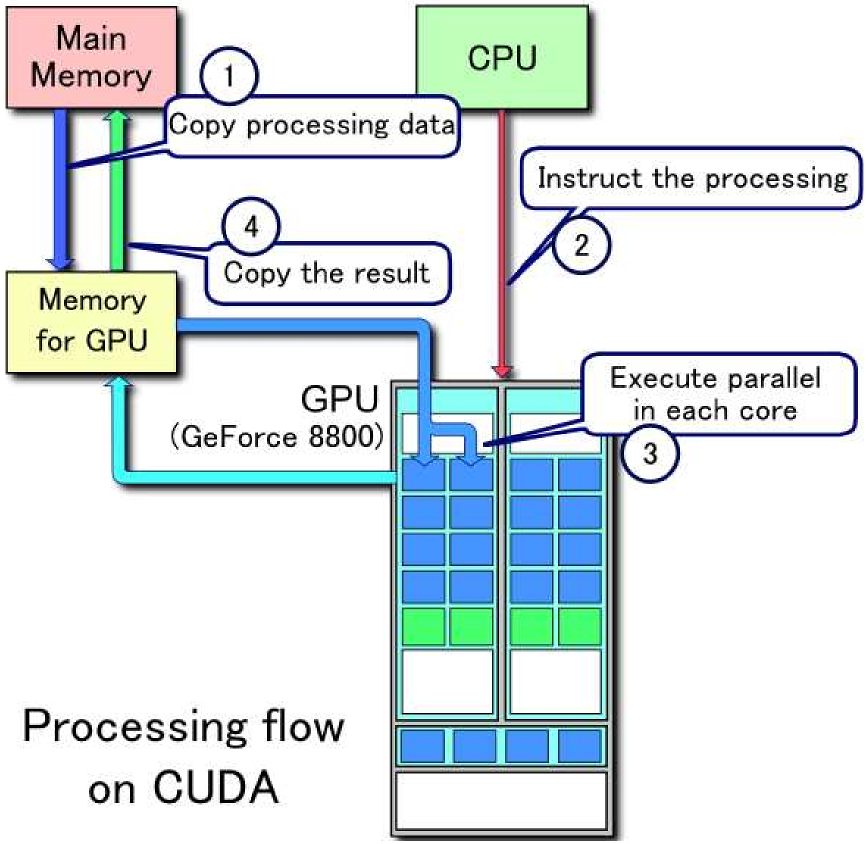
  Computations are conducted using “LBM fluids parameters” which are “different” from the fluids physical parameters (density, viscosity).
  → dimensional scaling is mandatory.

Dimensional analysis

- Two phase flow physics in porous media is defined through 4 dimensional numbers Re, M, Ca, Bo
- $L = 10^{-6}$ m ; $V = 10^{-7}$ m/s
- $Re = \rho_w V L / \mu_w = 1000 \times 10^{-7} \times 2\ 10^{-6} / 10^{-3} = 2\ 10^{-7}$
- $M = \mu_w / \mu_g = 10^{-3} / 10^{-5} = 100$
- $Ca = \mu_w V / \sigma = 10^{-3} \times 10^{-7} / 75\ 10^{-3} = 1.3\ 10^{-10}$
- $Bo = \Delta\rho\ g\ L^2 / \sigma = 1000 \times 10 \times (2\ 10^{-6})^2 / 75\ 10^{-3} = 5\ 10^{-7}$

Cuda (*Compute Unified Device Architecture*)

- CPU use GPU as a set of multi-processors units :
  NVS 5200M : 2 x 48 = 96
  Tesla C2050 : 14 x 32 = 448



wikipedia

- ++++ Equivalent to parallelism.
- \- Slight programming changes
  → sequential functions
- \- Small memory for elementary operation
- \- Don’t like conditional operation

- The context : two-phase flow modeling inside radioactive waste disposal

- Lattice Boltzmann approach

- Application : two-phase flow at the pore scale

Two-phase flow at the pore scale : preliminary computations

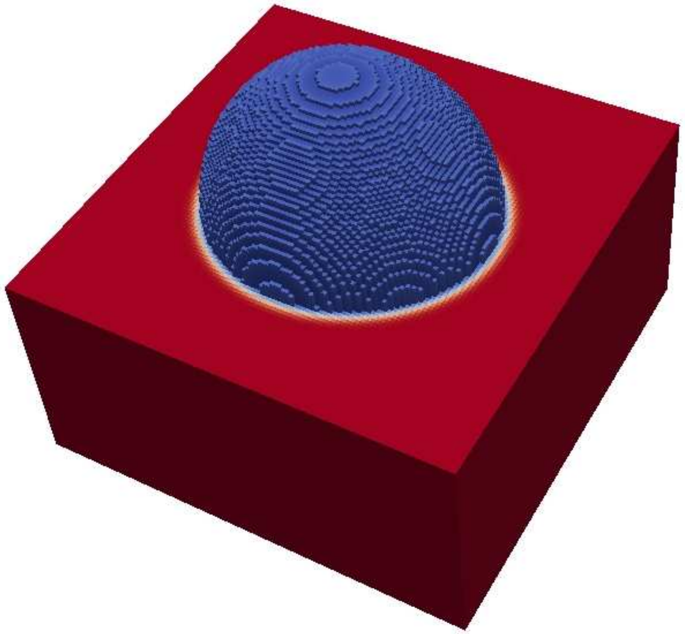
- Free numerical parameters of the model were adjusted in order to fit the relevant dimensional numbers describing two-phase flow in fractures when gravity effects are neglected (capillary number, mobility ratio).

  LBM parameters → LBM fluids properties → Ca, M

- The resulting RK model was tested against analytical solutions for static (Laplace law) and dynamic (Poiseuille flow) conditions.

Two-phase flow at the pore scale : static test

- We tested our LBM against the Laplace law and verified that the pressure difference in fluids ΔP for a bubble is linearly dependent in 2σ/R (with σ the surface tension and R the radius of the bubble).



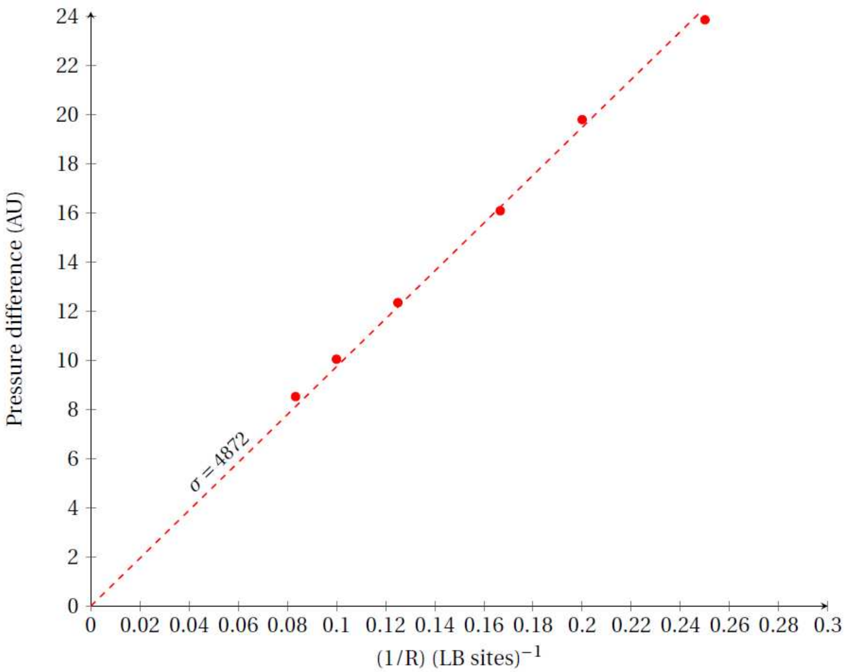
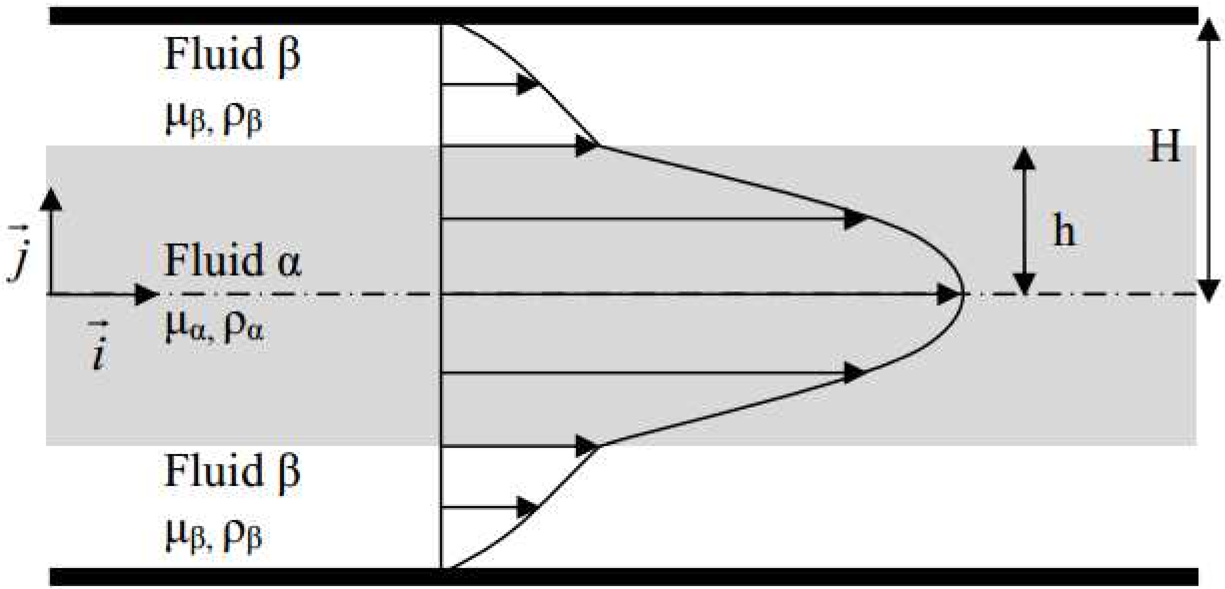


FIGURE 19 – Young-Laplace equation $\rho = 10^5$, $\mu = 10$, $A = 10^{-2}$

Two-phase flow at the pore scale : dynamic test

- We tested our LBM against the Poiseuille flow analytical solution 2 fluids / 3 layers) and verified that the velocity profile match the analytical one for our viscosity ratio.



Rannou, 2008

Two-phase flow at the pore scale : dynamic test

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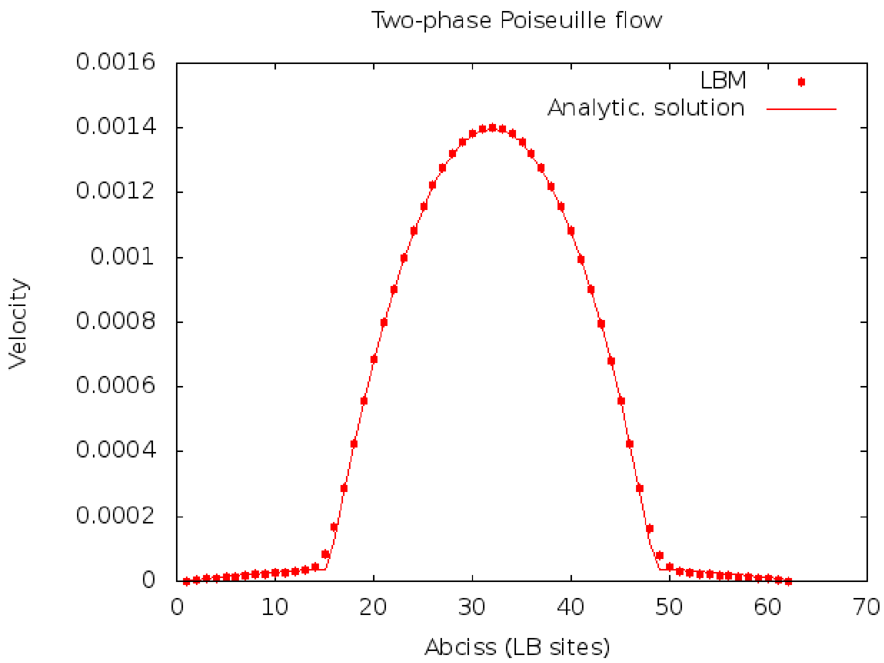
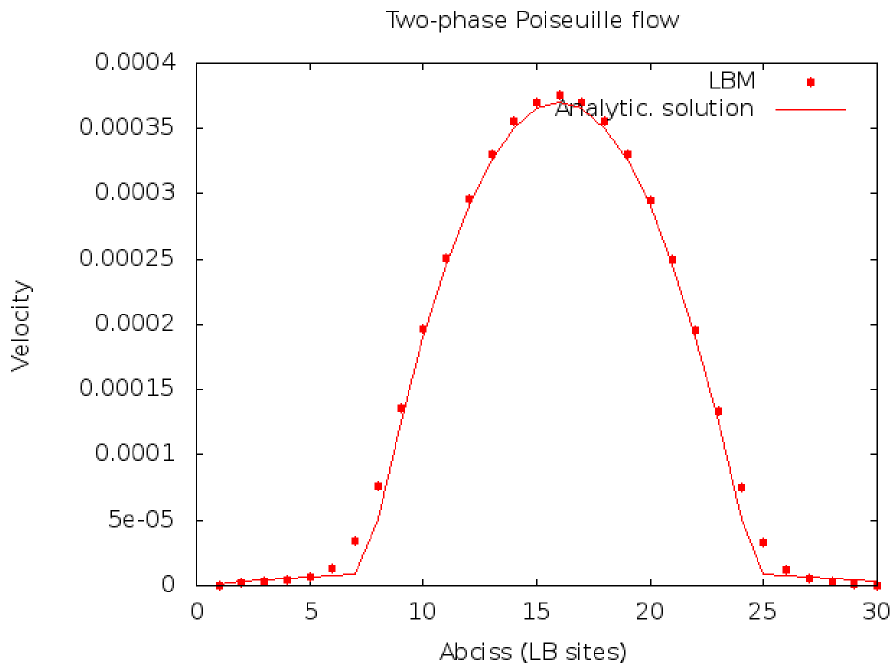
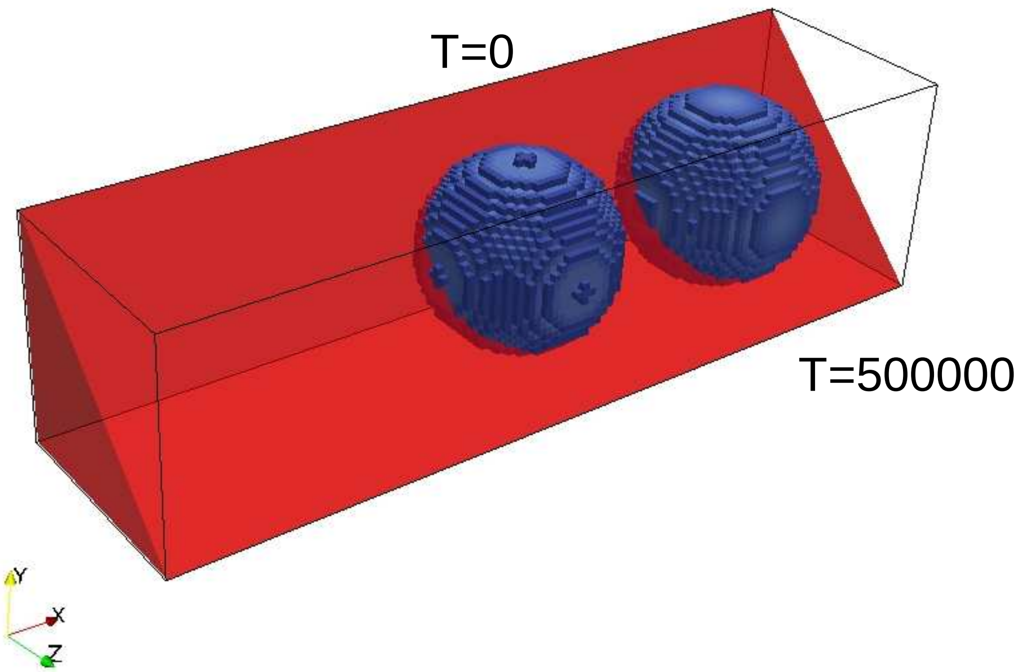




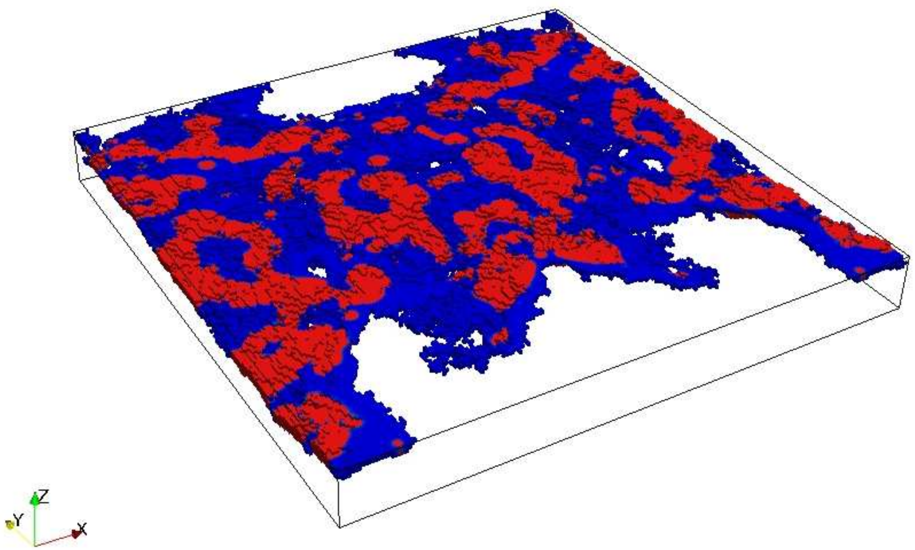
Two-phase flow at the pore scale : dynamic test

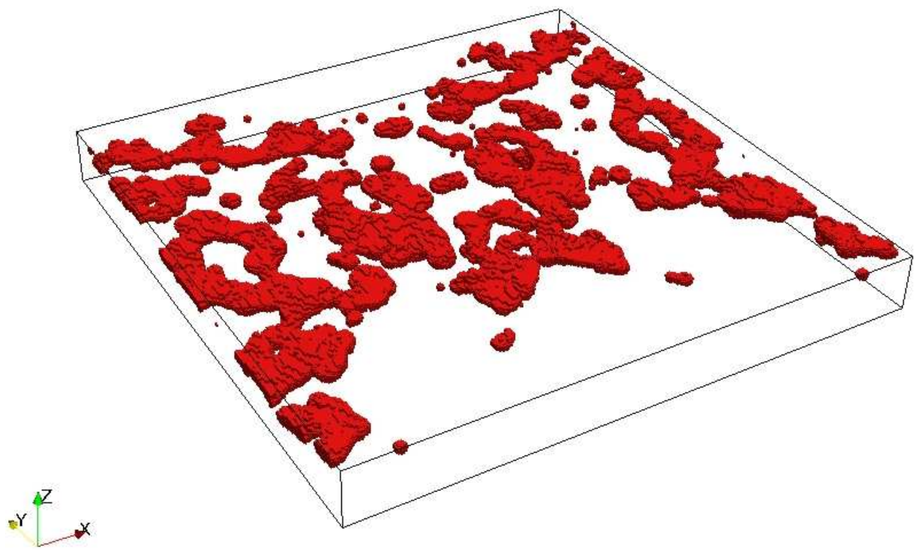
- Bubble flow (Channel = 32x32x120 sites; Bubble diameter = 24 sites)



Two-phase flow at the pore scale

- Two-phase flow in fracture (system = 40x400x400)



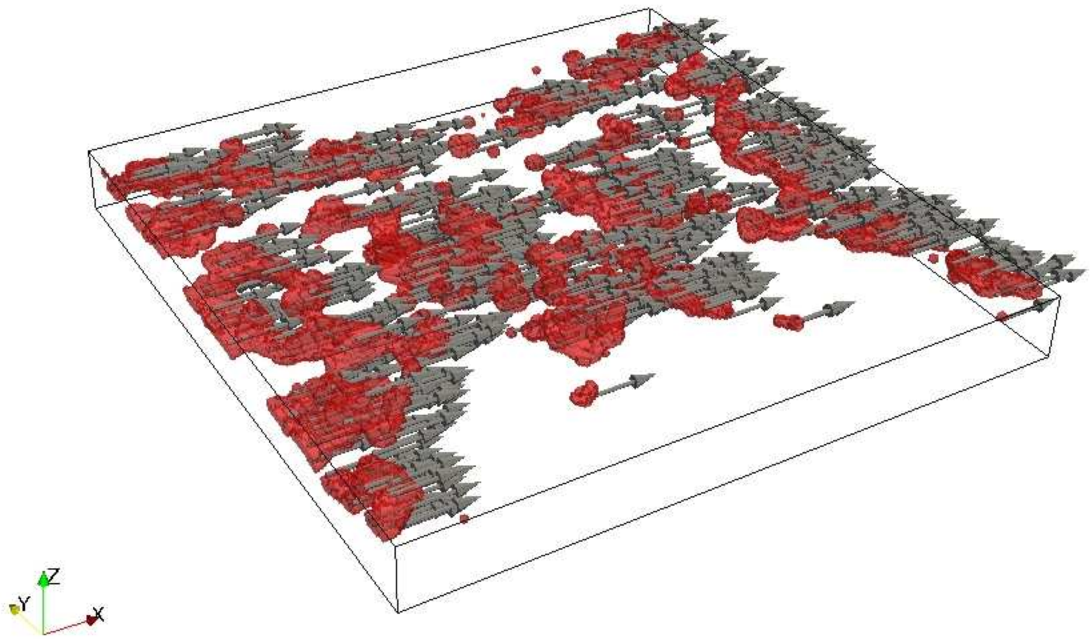


Two-phase flow at the pore scale : Kr computation

- Two-phase flow in fracture

V_{sat} = - K_i grad H
V_S = $-K_i$ Kr(S) grad H

→ Kr(S) = V_S/V_{sat}



CONCLUSION

- Rothman and Keller LBM (TRT) was selected and implemented on GPU using CUDA (x64 performance // CPU)

- Verification tests were successfully performed on static and dynamic problems with analytic solutions.

- First two-phase flow computations in argillite micro-fractures are promising.