ESR 11
Lattice Boltzmann Modelling of Water Transport in Hydrates Agglomerates

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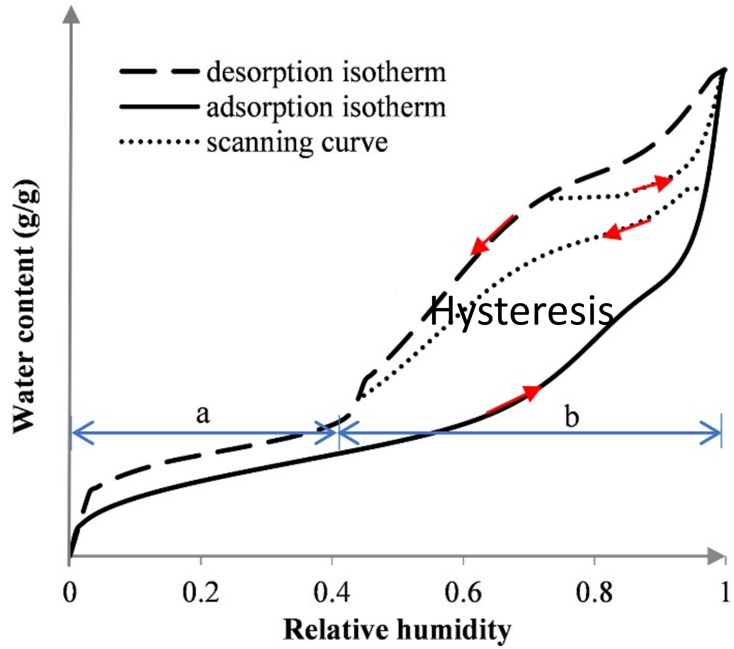
Overview

- Project Aims & Objectives
- The Lattice Boltzmann Methodology
- Multiphase Pseudo-Potential Model
- Moving Solid Boundaries & Simple Bounce-Back
- Results
- Conclusions & Future Work
- Secondments & Outreach

Project Aims & Objectives

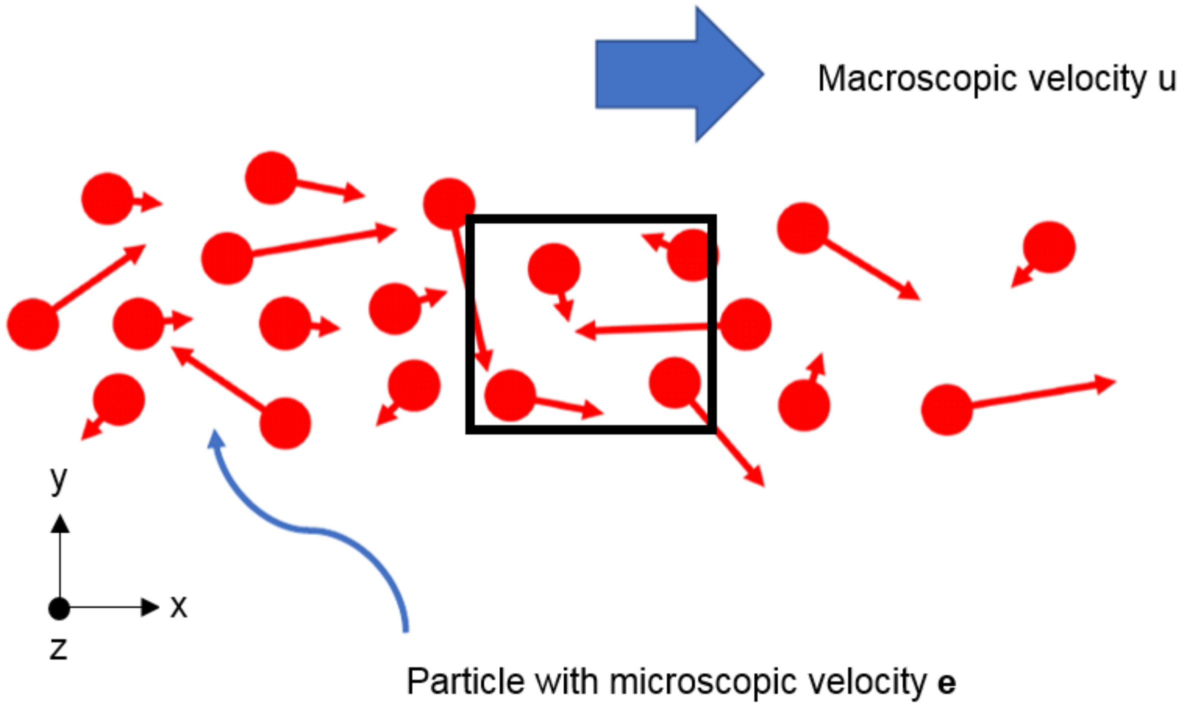
- Aim to simulate water transport in model C-S-H hydrate structures by multiphase (liquid & vapour) and multiscale (effective media) Lattice Boltzmann methods for de/sorption cycles
- Objectives focus on the introduction of:
    1. Moving Boundaries
    2. Swelling
    3. Mechanical Distortion



Into a *Shan-Chen Lattice Boltzmann* (LB) methodology and apply to a very simplified hydrate sheet model, with subsequent validation

Source: M. Liu, Z. Yu, T. Wang, J. Wang, L. Fan, **65**, 5615-5623 (2010)

The Lattice Boltzmann - Method



Change in number of particles in a specified volume having a :

- position *r*
- microscopic velocity **e**
- time *t*

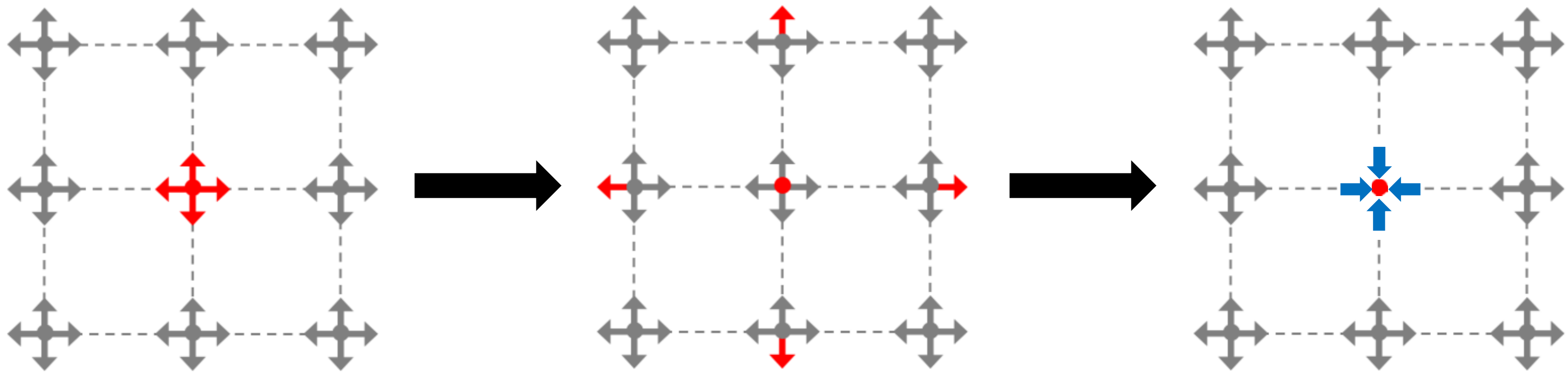
=

Change in number due to **Streaming** process in and out of the specified volume, known as the macroscopic flow

+

Change in number with **e** due to **Collision** of particles amongst one another within the specified volume

The Lattice Boltzmann - Equation



Amount of fluid moving in direction i where i =1:9

Equilibrium function

$$\frac{f_i(r+\delta r, t+\delta t) - f_i(r,t)}{\delta t} = \frac{f_i^{\,eq}(r,t) - f_i(r,t)}{\tau}$$

Relaxation Time ~ $\frac{1}{viscosity}$

Lattice Boltzmann equates to Navier Stoke's equation of fluid dynamics

Source: M. Zalzale, 'Water Dynamics in Cement Paste: Insights from Lattice Boltzmann Modelling', PhD Thesis, EPFL (2014)

Multiphase Pseudo-Potential Model

- Shan-Chen introduce a fluid potential:

$$\psi(r) = \psi_0 \exp\left[\frac{-\rho_0}{\rho(\boldsymbol{r})}\right]$$

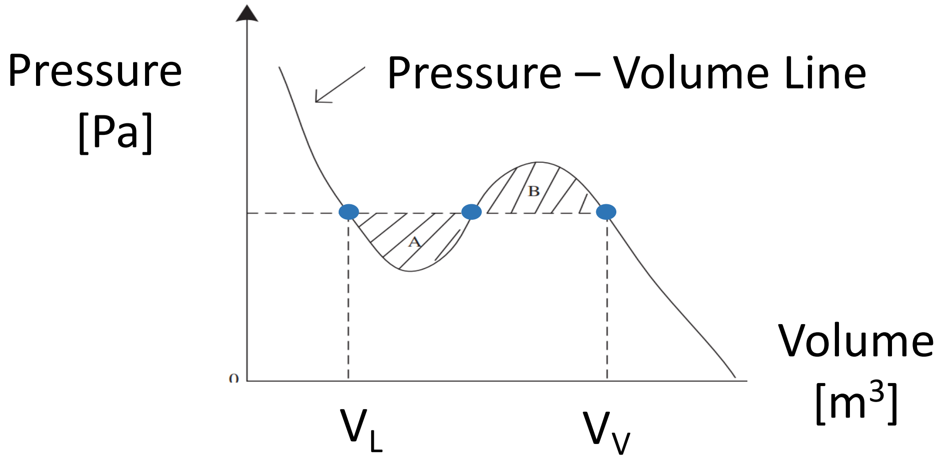
- Fluid-Fluid force:

$$F = G\psi(r)\sum_{i=1}^{Q} \omega_i^a \boldsymbol{e}_i \psi(\boldsymbol{r} + \boldsymbol{e}_i \Delta t)$$

- Fluid-Solid interaction:

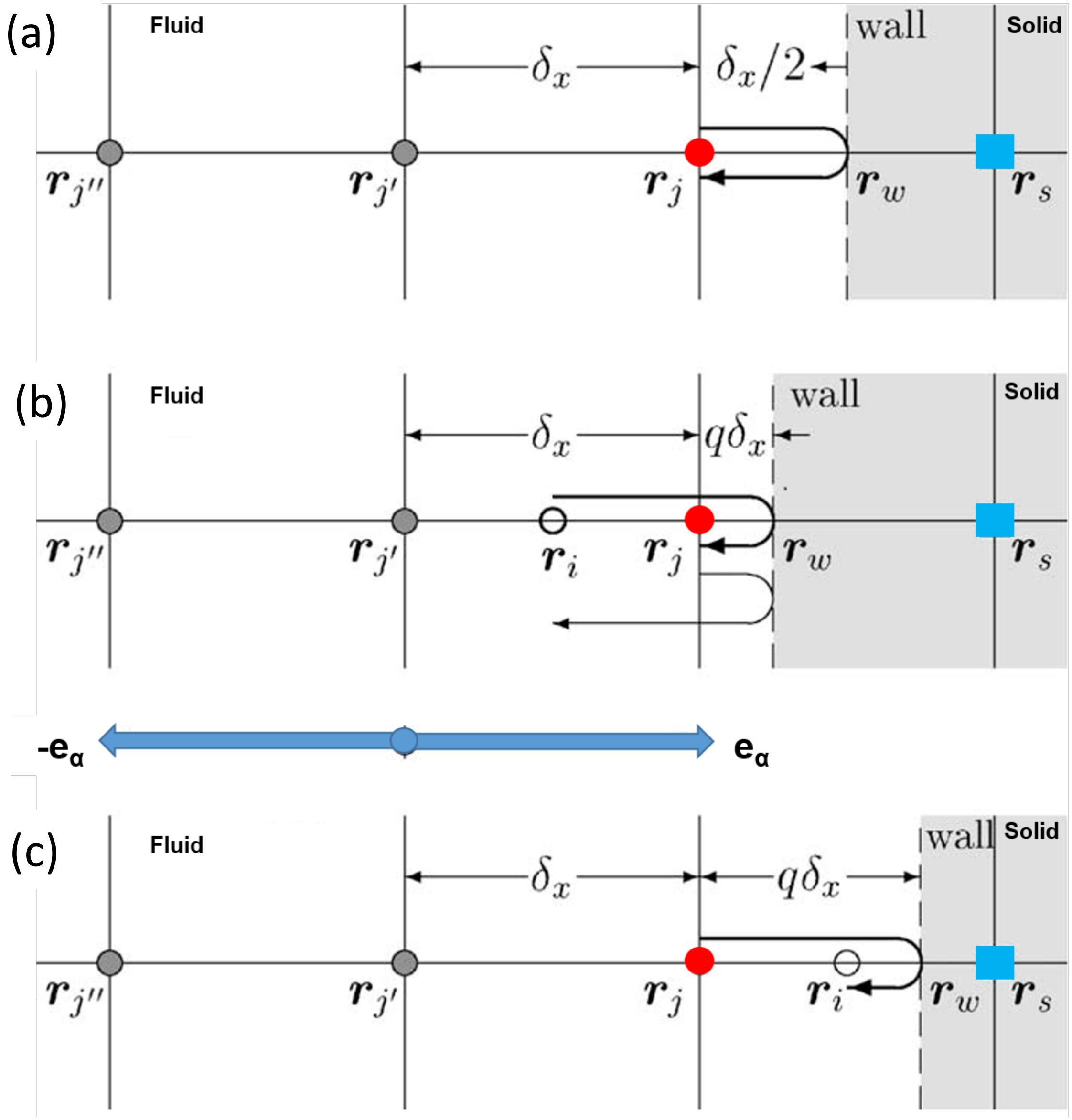
$$\psi(s) = \psi_{0S} \exp\left[\frac{-\rho_0}{\rho_S}\right]$$

Source: X. Shan, H. Chen, **49**, 2941-2948 (1994)



Symbol	Definition
$\psi_{(\boldsymbol{r})}$	Fluid Potential
ψ_0, ρ_0	Numerical Constants
$\rho(\boldsymbol{r})$	Fluid Density at Lattice Position
$\boldsymbol{r}$	Lattice Position
F	Fluid-Fluid Force
G	Interaction Strength Constant
ω_i^a	Force Weight Coefficients
$\boldsymbol{e}_i$	Velocity Vector
Δt	Time Increment
$\psi(s)$	Solid Potential
ψ_{0S}, ρ_0	Numerical Constants
ρ_S	Fictitious Fluid (Solid) Density

Moving Solid Boundaries & Simple Bounce Back



Source: P. Lallemand, L. Luo, **184**, 406-421 (2003)

(a) q = ½

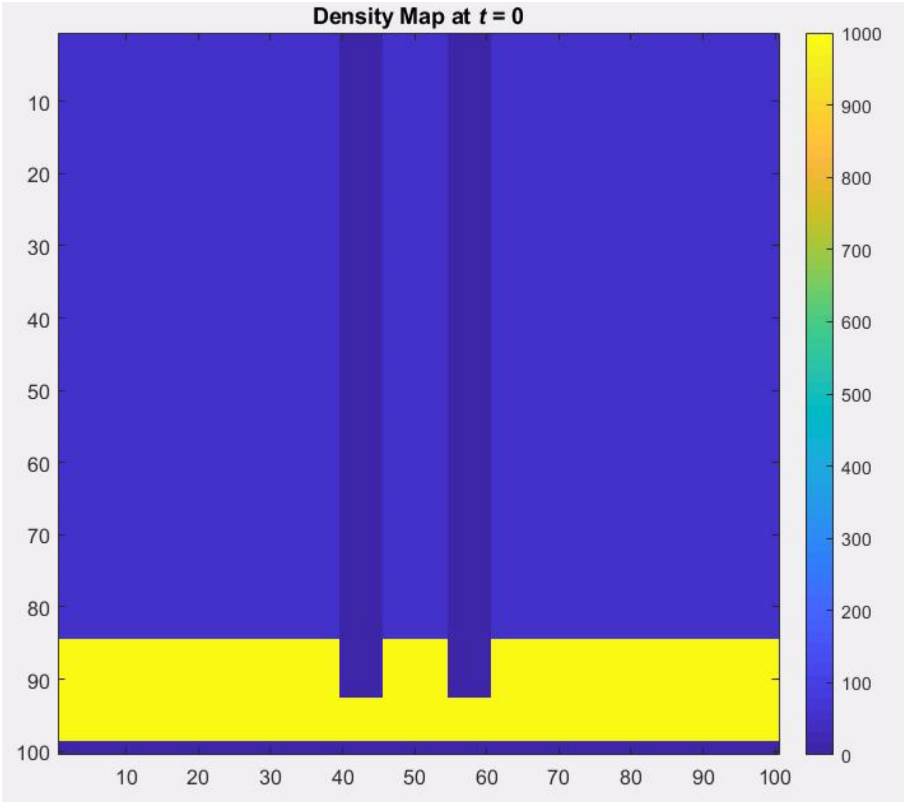
(b) q < ½

(c) q ≥ ½

Symbol	Definition
q	Grid spacing beyond the last fluid node
δx	Singular Grid Spacing
r_w	Location of Boundary Wall
r_s	Location of Solid Node
r_i	Location of Fluid Particle following Simple Bounce Back
r_j $r_{j'}$ $r_{j''}$	Location of Fluid Nodes
e_α	Particle Velocity Vector

Results: Capillary Action in a Capillary Tube

- Liquid capillary rise in a capillary tube without damping
- Liquid front advances proportional to the square root of time



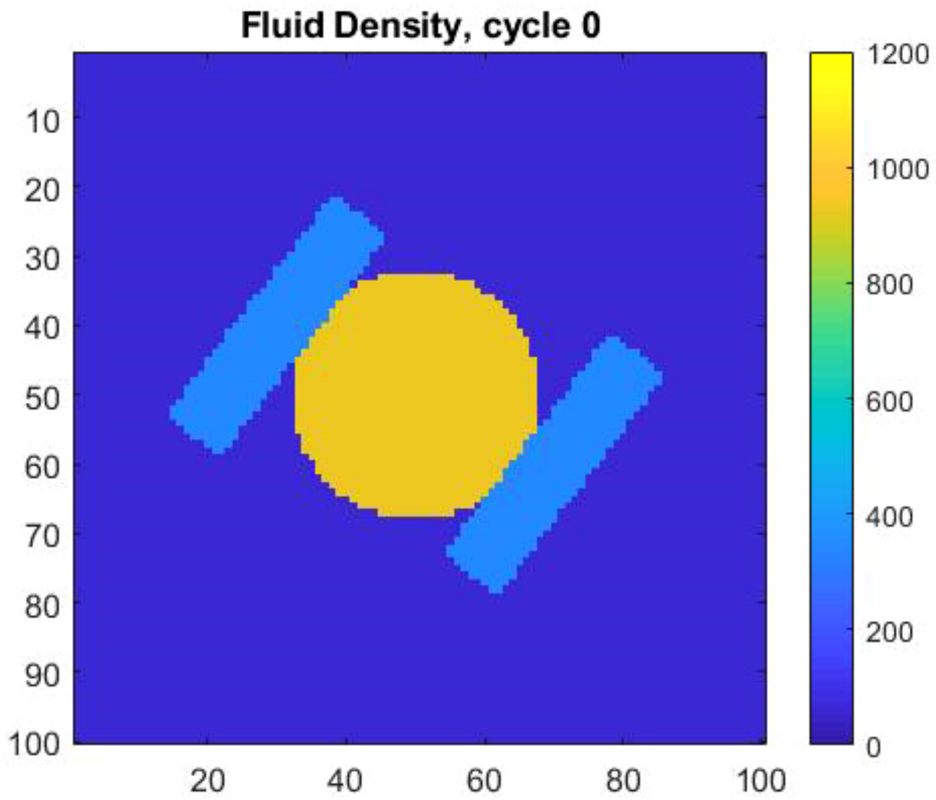
Solid

Liquid

Vapour

Results: Capillary Action with Wetting Solids

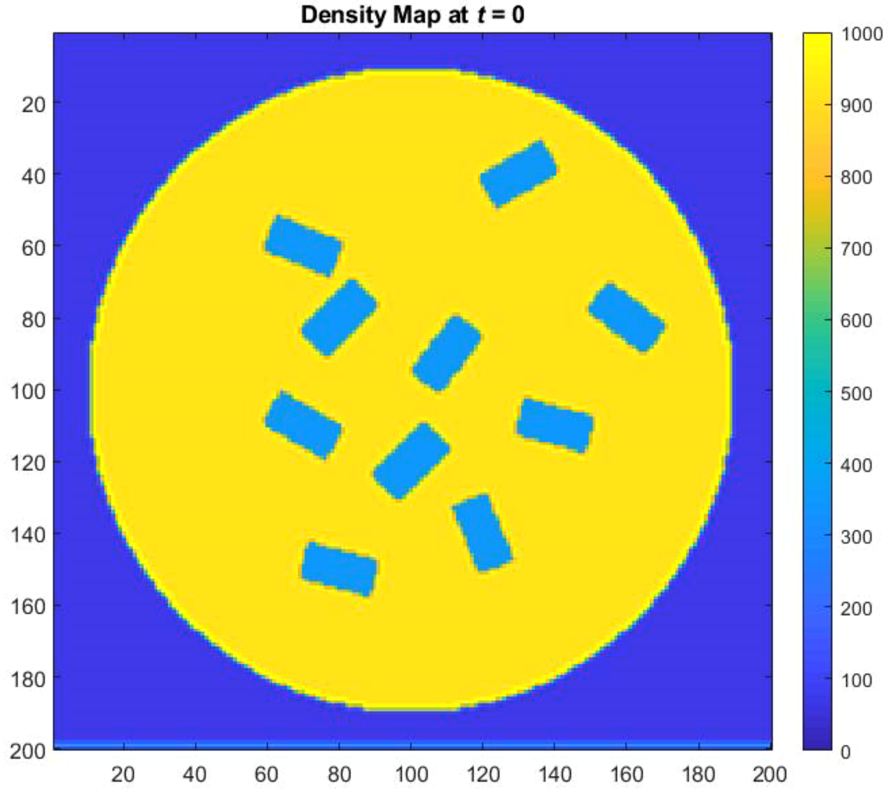
- Liquid droplet interaction between solid wetting particles without damping
- Control of contact angle between liquid-vapour-solid phases



Solid
Liquid
Vapour

Results: Capillary Action with Multiple Solids

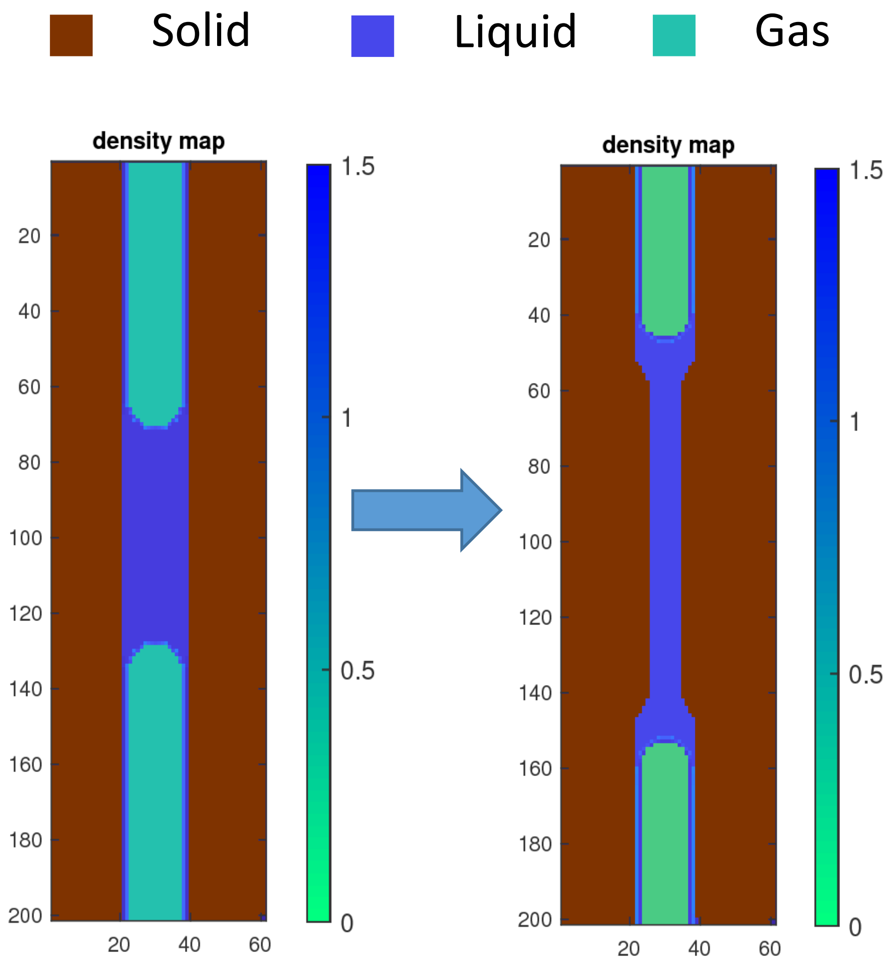
- Multiple wetting solid particles in a liquid droplet during drying and rewetting of a super saturated vapour with damping



Solid
Liquid
Vapour

Future Objectives: Introducing Swelling & Distortion in LB

- Based on LB work in softwoods, having swelling and distortion in elongated softwood cells
- Observing a bubble of liquid inside a gas filled cylinder
- Capillary collapse due to solid matrix swelling and capillary forces crushing the bubble of liquid



Source: S. Henderson, R. Adey-Johnson, 'Multi-Scale MRI/X-ray CT characterisation and Lattice Boltzmann modelling study of moisture movement in wood', Forest Research (In Progress)

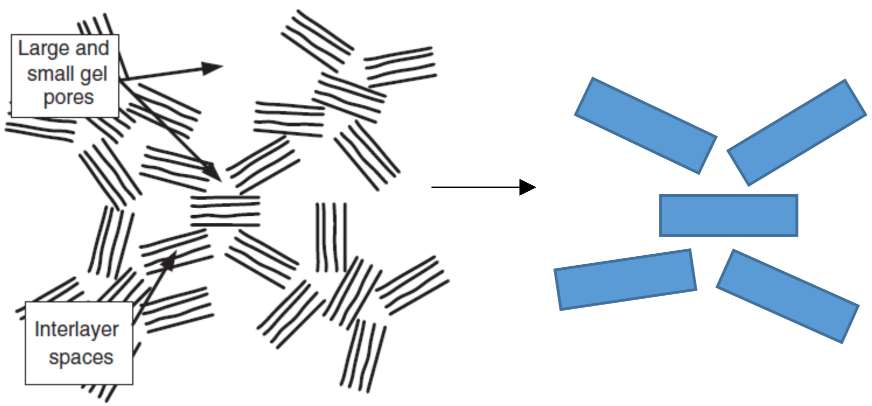
Conclusions & Future Work

Conclusions:

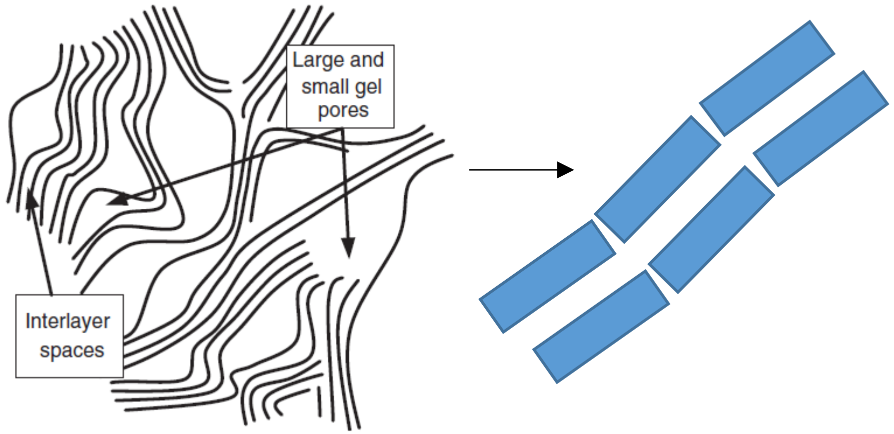
- Lattice Boltzmann model depicts capillary action in a multiphase environment with moving solid boundaries

Future Work:

- Build an understanding of sorption isotherms by analysing the effect of repetitive de/wetting cycles
- Introduce swelling and mechanical distortion



Colloidal Model



Quasi-Continuous Sheet Model

Source: M. Etzold, P. J. McDonald, A. F. Routh, **63**, 137-142 (2014)

Secondments & Outreach

Secondments:

- Nov ‘19 - 1 week visit to LafargeHolcim:
  discuss the implementation of LB in cement industry
- Nov ’20 - Extended stay at LafargeHolcim

Outreach:

- July ’19 – University of Surrey
- Collective UOS ESR summer school activity promoting and disseminating the knowledge of cementitious materials for 26 school students
- 1 hr lecture / 2 hr lab work

Thank you
for your attention