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DROPLETS & EMULSIONS: dynamics & rheology **with LBM numerical simulations**

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DROPLETS & EMULSIONS:

dynamics & rheology with LBM numerical simulations

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Credits:

R. Benzi, M. Lulli (Dept. Physics, University of Rome “Tor Vergata”, Italy)

A. Scagliarini (Helmholtz Institute, Nunberg, Germany)

S. Succi, M. Bernaschi (IAC-CNR, Rome, Italy)



Complex Fluids & Soft Glassy Materials

Emulsions, Foams, Gels, Pastes, etc



Composition

- Multiple Phases
- Multiple Components
- Often Both

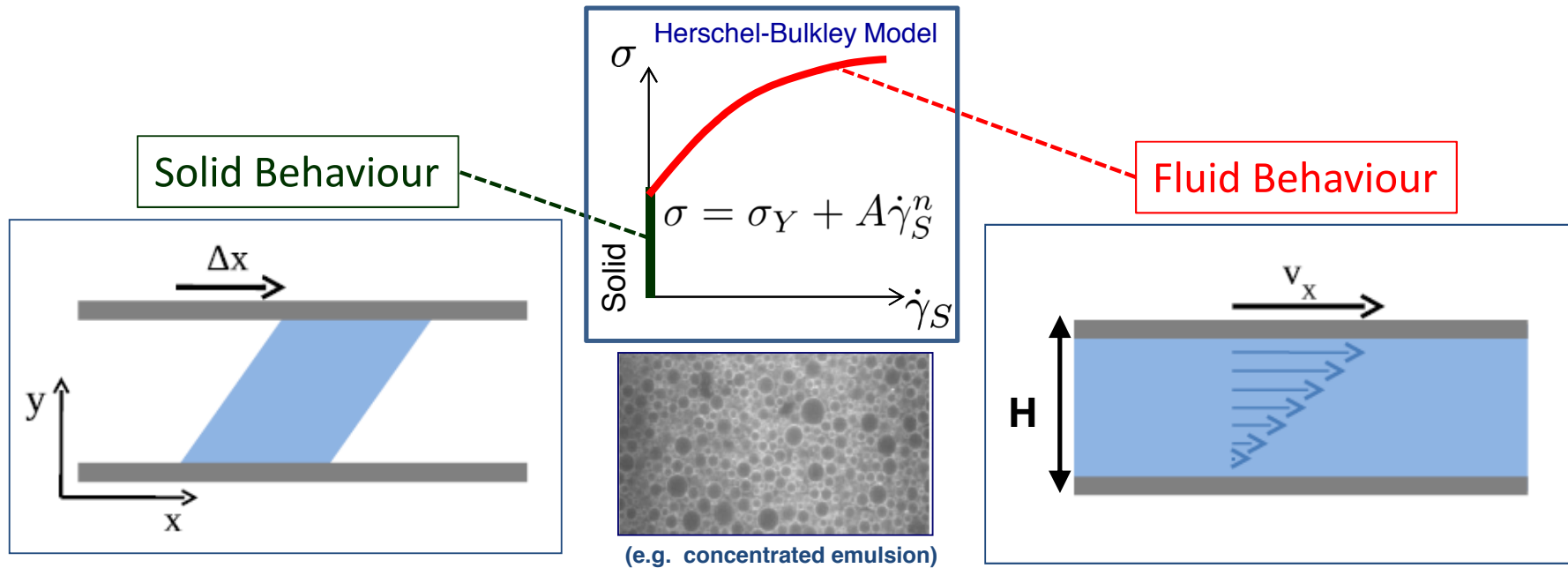
Structural Complexity

- Dynamical Arrest
- Clustering Networks
- Heterogeneities

Rheological Complexity

- Yield Stress Fluids
- Viscoelasticity
- Cooperativity

Flow-Curves of Soft Glassy Materials



Hookean (Elastic) solid displaced by a distance Δx :

The Stress needed to do this is:

$$\sigma = G \frac{\Delta x}{H} = G\gamma_S$$

γ_S : Strain G : Storage Modulus

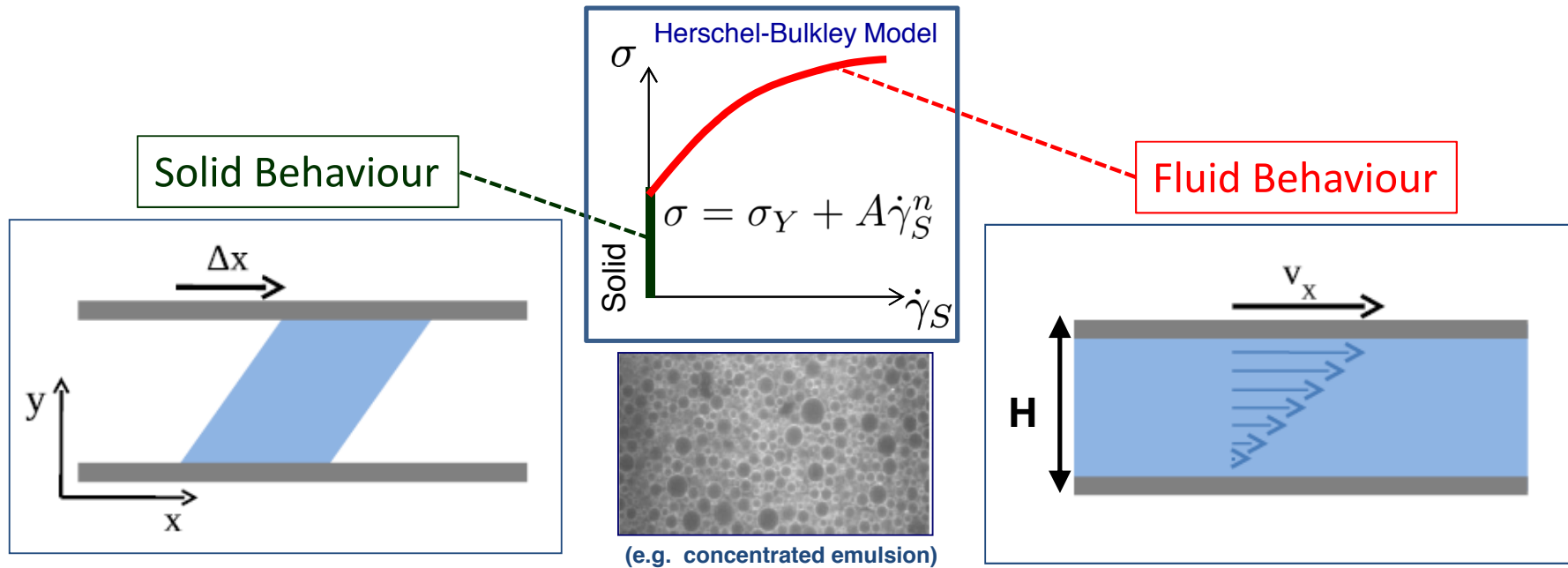
Viscous Fluid driven by a constant velocity :

The Stress needed to do this is:

$$\sigma = \eta \frac{\partial v_x}{\partial y} = \eta \frac{v_x}{H} = \eta\dot{\gamma}_S$$

$\dot{\gamma}_S$: Shear η : Viscosity

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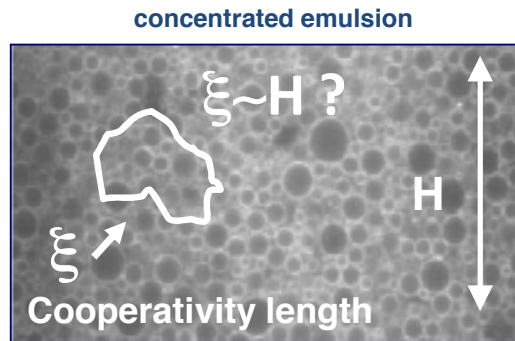
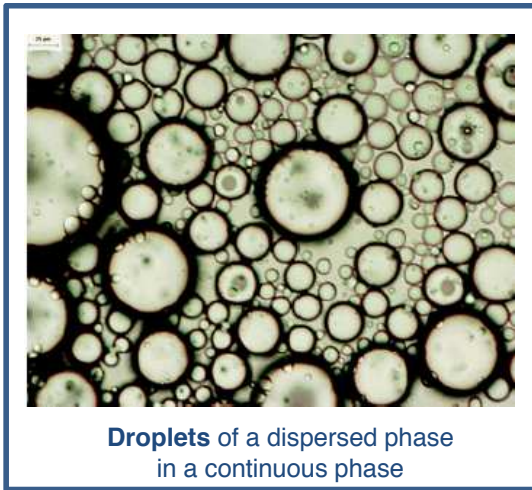
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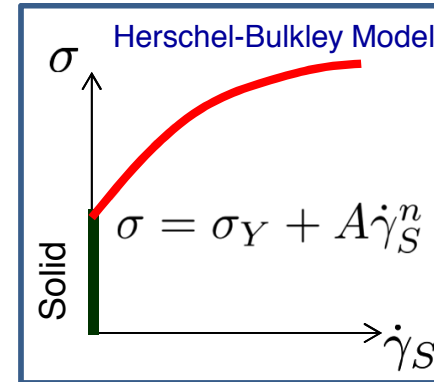
$\dot{\gamma}_S$: Shear η : Viscosity

How does motion take place at the level of **Micro-Structural Constituents** (i.e. Droplets) ?

Soft Glassy Materials & Fluidity Models

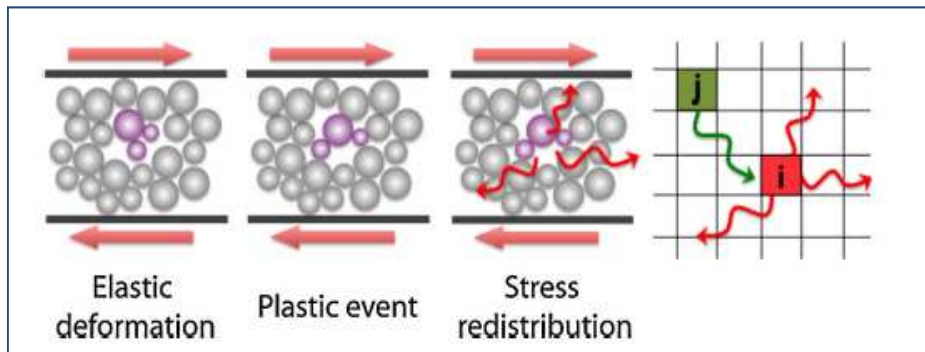


- ✓ Yield Stress (Solid below)
- ✓ Non-Newtonian Fluid (Above Yield)
- ✓ Effects of **Confinement** ?



$\dot{\gamma}_S$: Shear σ : Stress
 σ_Y : Yield Stress
 ξ : **Cooperativity** length
 $f = \frac{\dot{\gamma}_S}{\sigma}$ **Fluidity**

Bocquet, Ajdari, Colin, Phys Rev. Lett **103**, 0360011 (2009)



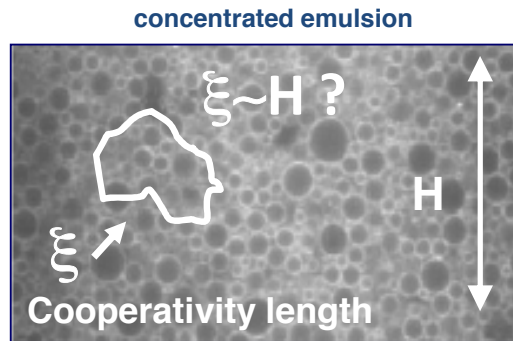
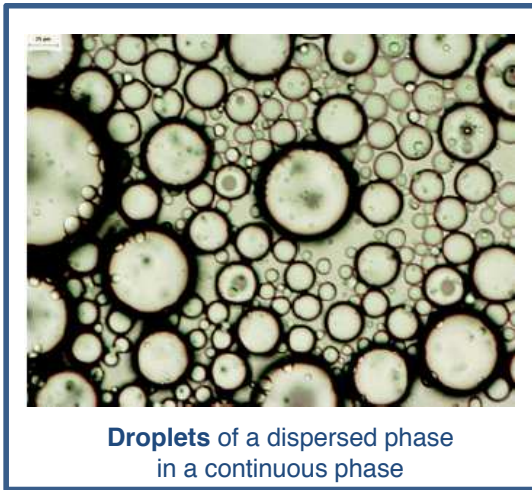
$$\xi^2 \Delta f + (f_b - f) = 0$$

Relaxation-Diffusion equation for the Fluidity

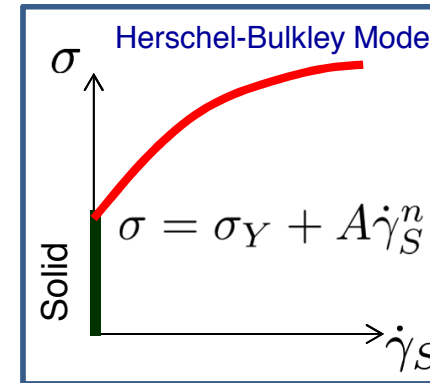
$$f_b = f_b(\sigma(\vec{r}))$$

"Bulk" Fluidity

Soft Glassy Materials & Fluidity Models

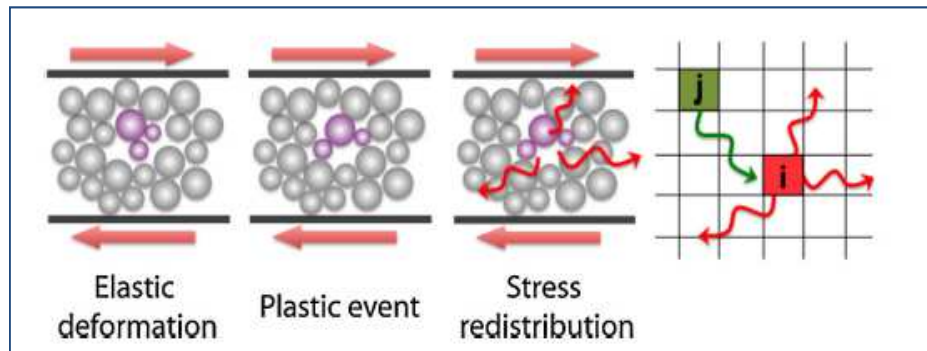


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 ξ : **Cooperativity** length
 $f = \frac{\dot{\gamma}_S}{\sigma}$ **Fluidity**

Bocquet, Ajdari, Colin, Phys Rev. Lett **103**, 0360011 (2009)



- ✓ **Ab Initio** Proof of "Plastic Flows" !?!
- ✓ **Test** Fluidity Models !?!
- ✓ **Extend** the picture of plastic flows !?!

$$\xi^2 \Delta f + (f_b - f) = 0$$

Relaxation-Diffusion equation for the Fluidity

$$f \propto \Gamma$$

Proportionality Between Fluidity and **RATE** of Plastic Events (Γ)

Where to Sit Across the scales?



**MACROSCOPIC
(NAVIER-STOKES)**

$$\begin{aligned}\vec{\nabla} \cdot \vec{u} &= 0 \\ \rho D_t \vec{u} &= -\vec{\nabla} p + \eta \Delta \vec{u} \\ &\dots\end{aligned}$$

Plastic Flows of Emulsions Live – by definition - at Mesoscales

Can we handle the Problem with a **Mesoscopic Method**?

YES !!! A possibility is the **Lattice Boltzmann Method**



**MICROSCOPIC
(MOLECULAR DYNAMICS)**

$$\begin{aligned}\mathcal{H} &= \sum_k \frac{p_k^2}{2m} + \sum_{i,k} V_{i,k} \\ \dot{q}_k &= \frac{\partial \mathcal{H}}{\partial p_k} \quad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k}\end{aligned}$$

Where to Sit Across the scales?



MACROSCOPIC
(NAVIER-STOKES)

Continuum Description



MESOSCOPIC
(LATTICE BOLTZMANN)

Kinetic '*Inspired*' Equations



MICROSCOPIC
(MOLECULAR DYNAMICS)

$$\begin{aligned}\vec{\nabla} \cdot \vec{u} &= 0 \\ \rho D_t \vec{u} &= -\vec{\nabla} p + \eta \Delta \vec{u} \\ &\dots\end{aligned}$$



Chapman-Enskog
(Multi-Scale Lattice Theory)

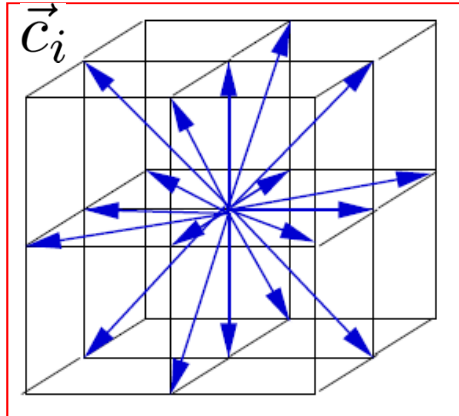
$$n_i(\vec{r} + \vec{c}_i, t + 1) = n_i(\vec{r}, t) + \Delta_i$$



Supra-molecular
Framework for lattice
interactions

$$\begin{aligned}\mathcal{H} &= \sum_k \frac{p_k^2}{2m} + \sum_{i,k} V_{i,k} \\ \dot{q}_k &= \frac{\partial \mathcal{H}}{\partial p_k} \quad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k}\end{aligned}$$

Lattice Boltzmann: Basics & Conservation Laws



- Linearized Boltzmann Equation
- Fully Discretized (time and space)
- Sites \vec{r} , and Lattice Velocities \vec{c}_i
- Time t , time step $\Delta t = 1$

$$n_i(\vec{r} + \vec{c}_i, t + 1) = n_i(\vec{r}, t) + \Delta_i \{n_i(\vec{r}, t)\}$$

"Streaming"

"Local **Relaxation** towards equilibrium"

Example: single time (τ) relaxation

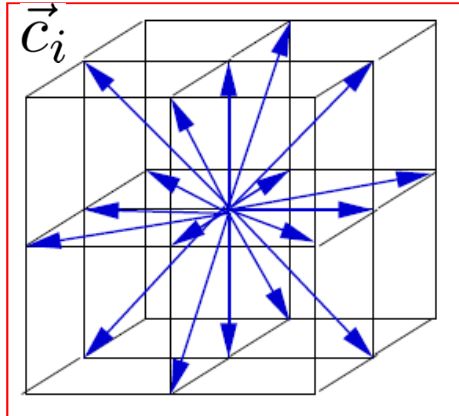
$$\Delta_i \{n_i(\vec{r}, t)\} \propto -\frac{1}{\tau} (n_i - n_i^{(eq)})$$

- \vec{c}_i **Small Set** of Velocities
- \vec{c}_i Connects 2 sites...**exact streaming** preserved
- $n_i(\vec{r}, t)$ Real Number: particle pdf on space-time location (\vec{r}, t)

Succi, "The Lattice Boltzmann Equation: for fluid dynamics and beyond" (2001)
 Wolf Gladrow, "Lattice Gas Cellular Automata and LBM: an introduction" (2000)

How to access coarse grained variables?

Lattice Boltzmann: Basics & Conservation Laws



- Linearized Boltzmann Equation
- Fully Discretized (time and space)
- Sites \vec{r} , and Lattice Velocities \vec{c}_i
- Time t , time step $\Delta t = 1$

$$n_i(\vec{r} + \vec{c}_i, t + 1) = n_i(\vec{r}, t) + \Delta_i \{n_i(\vec{r}, t)\}$$

$$\sum_i \Delta_i = \sum_i \vec{c}_i \Delta_i = 0$$

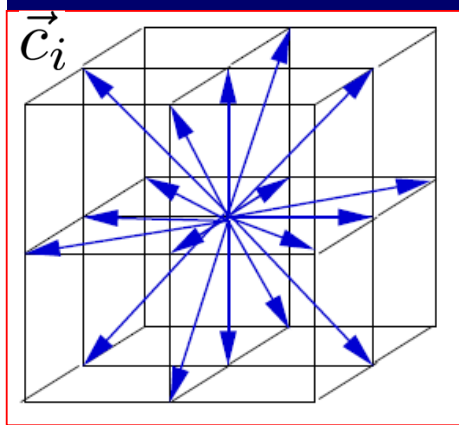
Mass Conservation!
Momentum Conservation!!
Locality !!!

Coarse Grained Fields \longrightarrow Hydrodynamic Equations

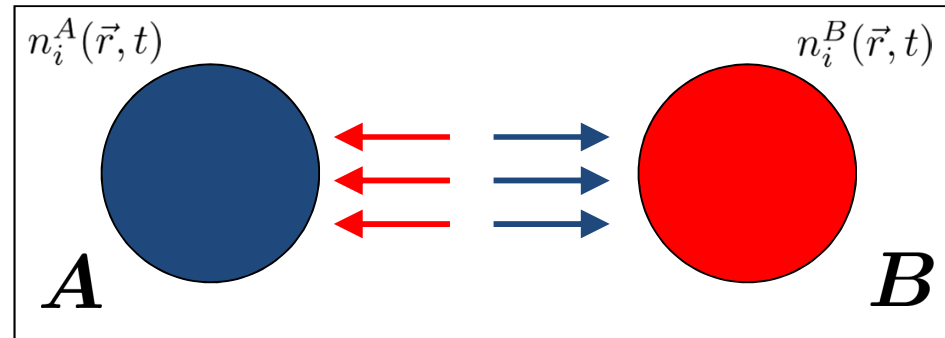
$$\rho(\vec{r}, t) = \sum_i n_i(\vec{r}, t) \quad (\text{Density})$$

$$\vec{u}(\vec{r}, t) = \frac{1}{\rho(\vec{r}, t)} \sum_i \vec{c}_i n_i(\vec{r}, t) \quad (\text{Velocity})$$

Non Ideal Lattice Fluids: Phase Segregation



How ?



$$\vec{F}(\vec{r}) = -g_{AB}\rho_A(\vec{r})\sum_i w_i\rho_B(\vec{r} + \vec{c}_i)\vec{c}_i + (A \leftrightarrow B)$$

LBM Phase Segregating Interactions
(g_{AB} is a coupling strength)

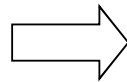
Interaction Range **Crucial** for OUR Application

$$\rho = \rho_A + \rho_B$$

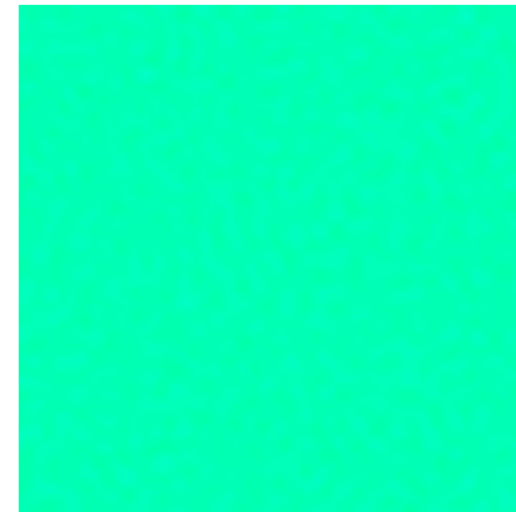
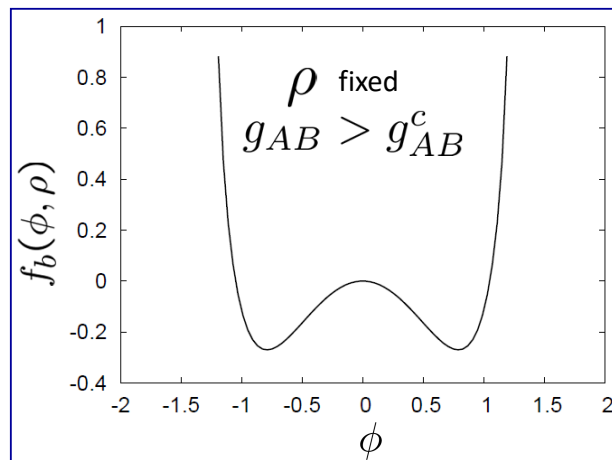
Total Density

$$\phi = \rho_A - \rho_B$$

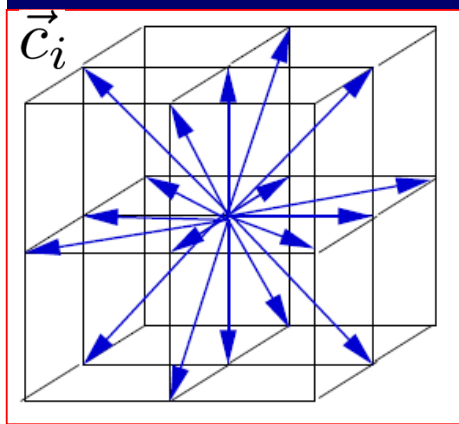
Order Parameter



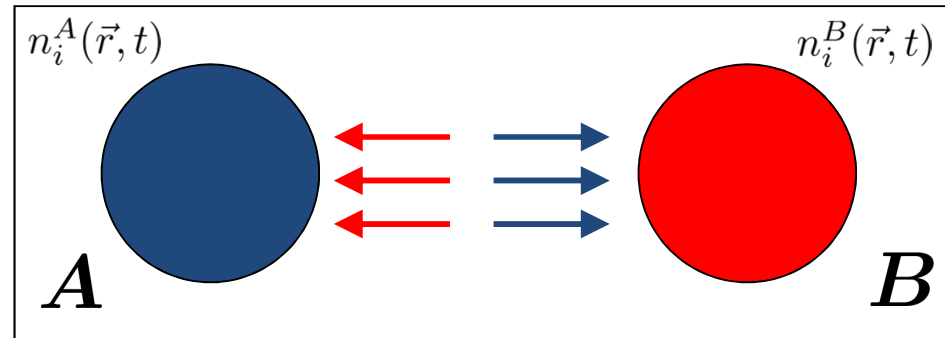
Model (bulk) Free Energy



Non Ideal Lattice Fluids: Phase Segregation



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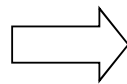
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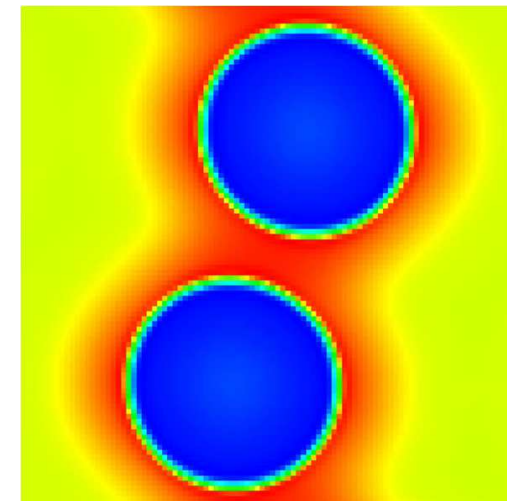
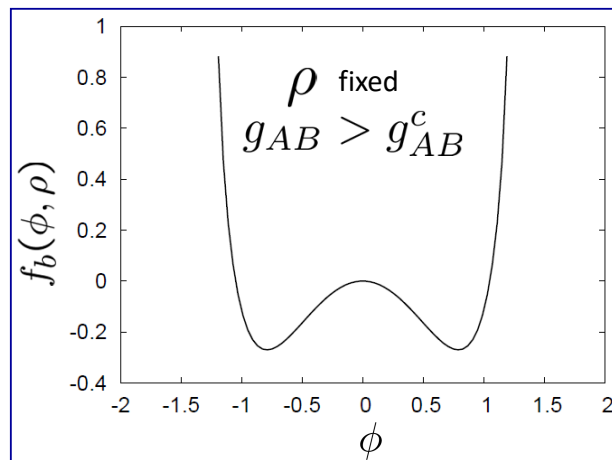
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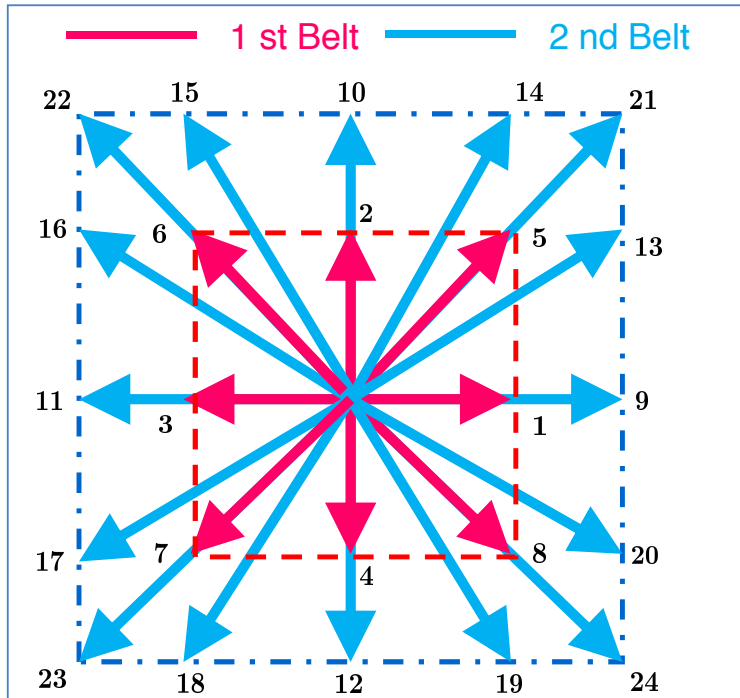
Model (bulk) Free Energy



(Lattice) Disjoining Pressure (Π): How ?

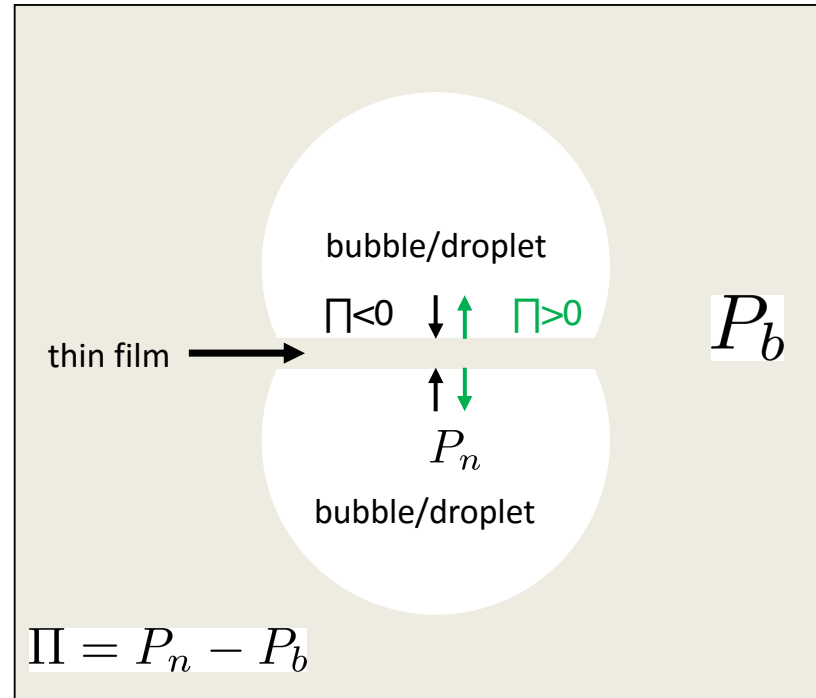
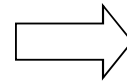
"Multirange" Potentials in LBM:

Competing Nearest Neighbours (NN) +
Next to Nearest Neighbours (NNN) interactions



"Frustration" Mechanism :

"Frustrate" the tendency of the interface to
minimize the area...**does it work ?**



$$\vec{F}(\vec{r}) = -\mathcal{G}_1 \psi(\vec{r}) \sum_{i \in NN} \psi(\vec{r} + \vec{c}_i) \vec{c}_i - \mathcal{G}_2 \psi(\vec{r}) \sum_{i \in NNN} \psi(\vec{r} + \vec{c}_i) \vec{c}_i \quad \psi(\vec{r}) = \psi[\rho(\vec{r})]$$

Pseudo-Potential

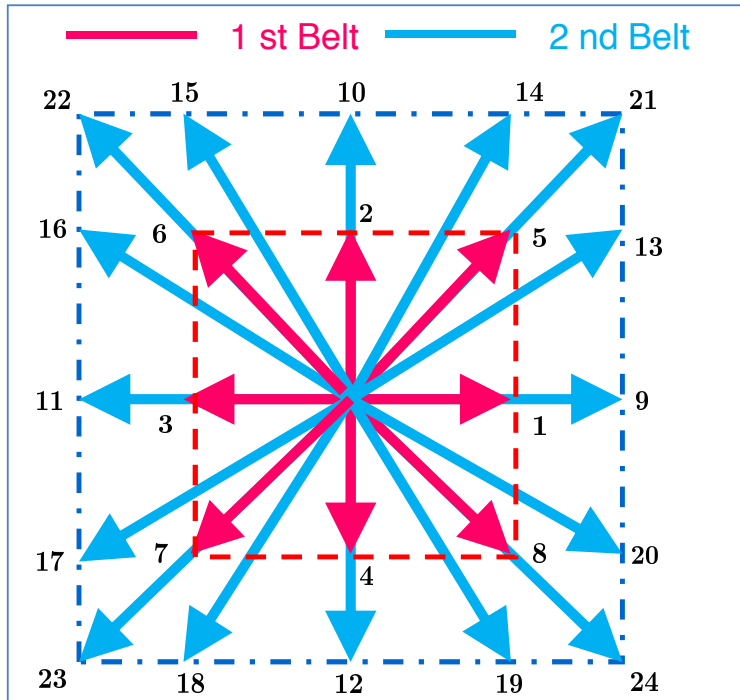
J.D. Shore, M. Holzer, J.P. Sethna, *Phys. Rev. B* **46**, 11376 (1992)

M. Sbragaglia, R. Benzi, M. Bernaschi & S. Succi, *Soft Matter* **8**, 10773-10782 (2012)

(Lattice) Disjoining Pressure (Π): How ?

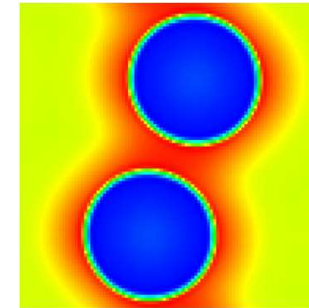
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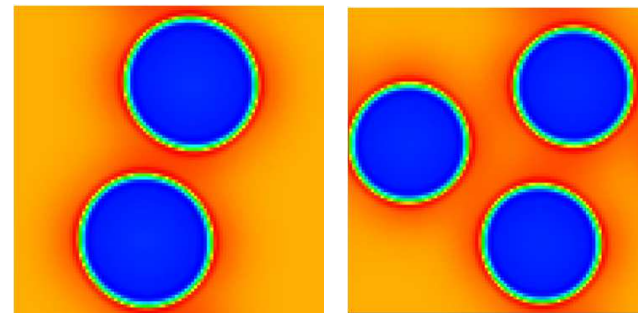


"Frustration" Mechanism :

"Frustrate" the tendency of the interface to
minimize the area... **YES!!!!**



Droplets Coalescence (**Traditional LBM** implementation)



Inhibition of Coalescence (**Multirange LBM**)

$$\vec{F}(\vec{r}) = -\mathcal{G}_1 \psi(\vec{r}) \sum_{i \in NN} \psi(\vec{r} + \vec{c}_i) \vec{c}_i - \mathcal{G}_2 \psi(\vec{r}) \sum_{i \in NNN} \psi(\vec{r} + \vec{c}_i) \vec{c}_i \quad \psi(\vec{r}) = \psi[\rho(\vec{r})]$$

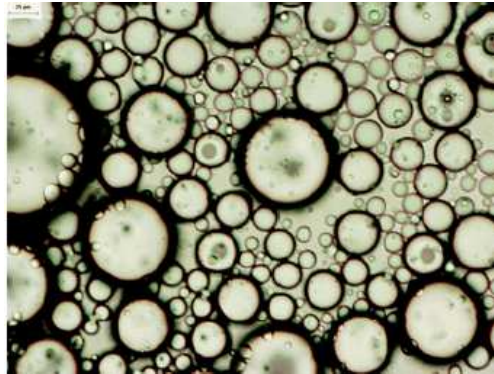
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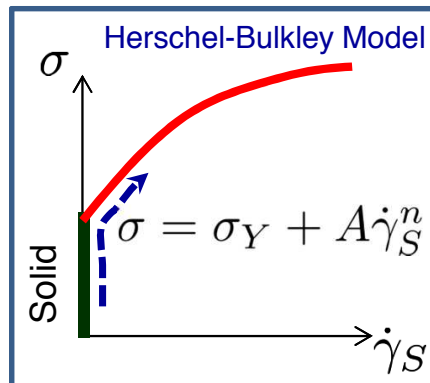
M. Sbragaglia, R. Benzi, M. Bernaschi & S. Succi, *Soft Matter* **8**, 10773-10782 (2012)

Yield Stress Fluids & Plastic Rearrangements

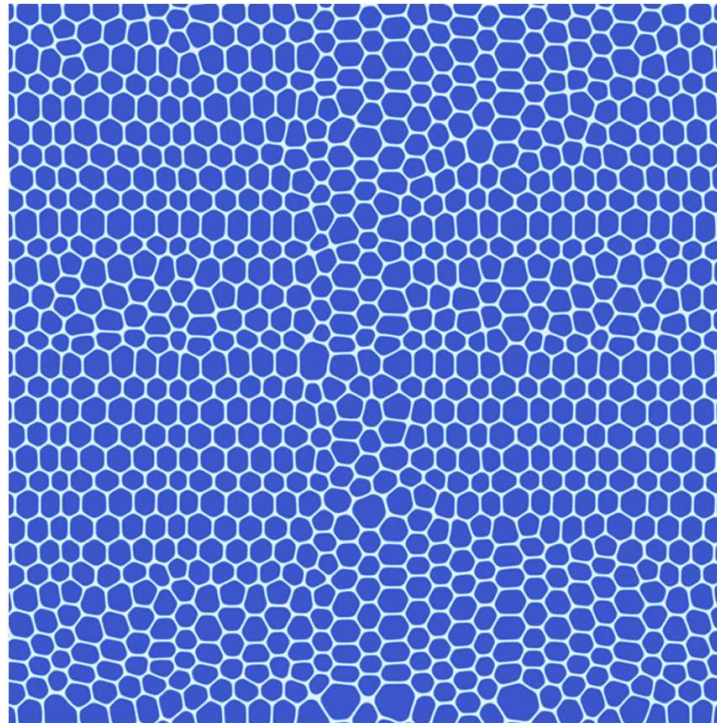
R. Benzi, M. Sbragaglia, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4615-4624 (2014)



Droplets of a dispersed phase
in a continuous phase



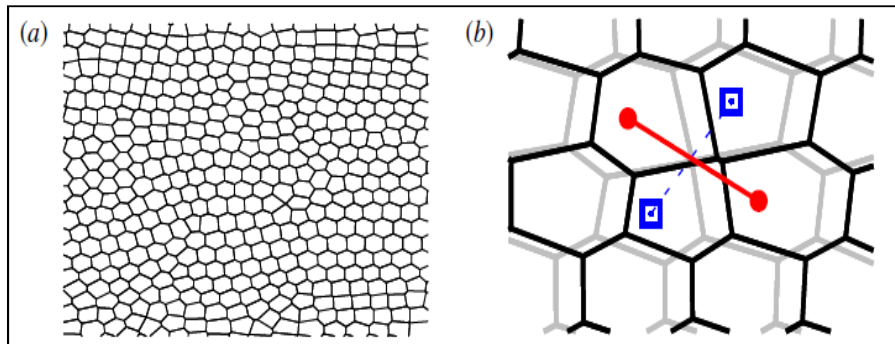
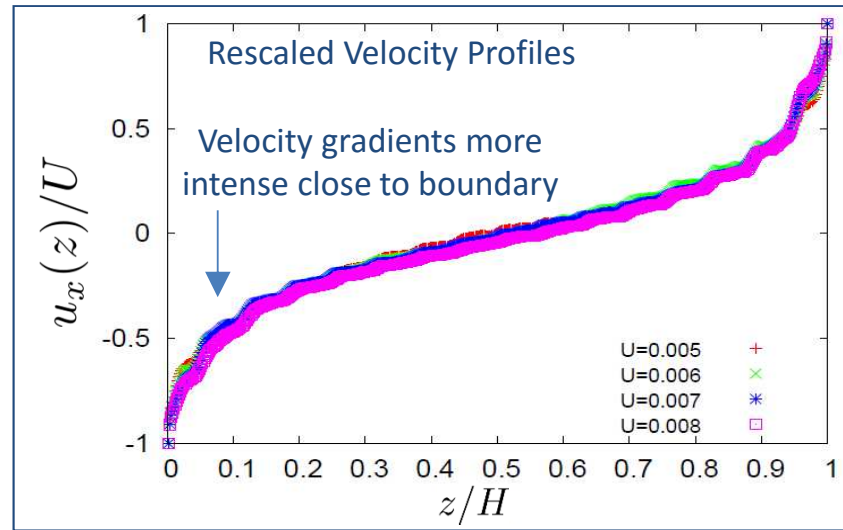
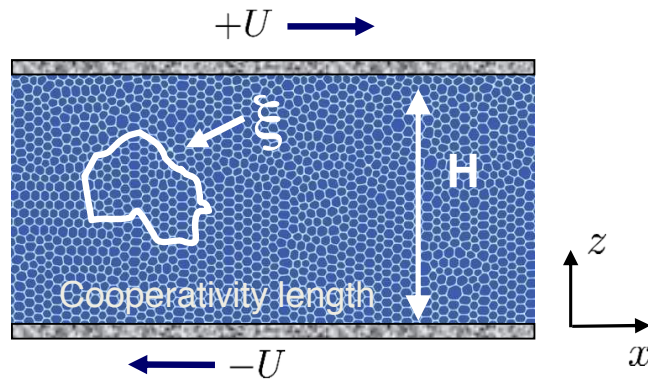
- ✓ Yield Stress (Solid below)
- ✓ Non-Newtonian (above yield)
- ✓ Cooperativity Effects & Plastic Rearrangements



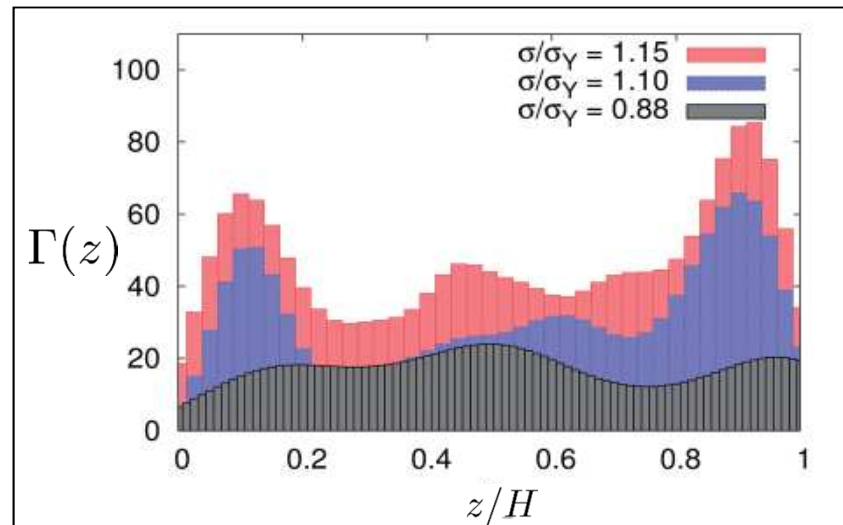
Kolmogorov Flow (full periodic system)
step-by-step increase of the driving force (**solid to liquid transition**)

Testing Fluidity Models with LBM

M. Sbragaglia, R. Benzi, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4514-4524 (2014)

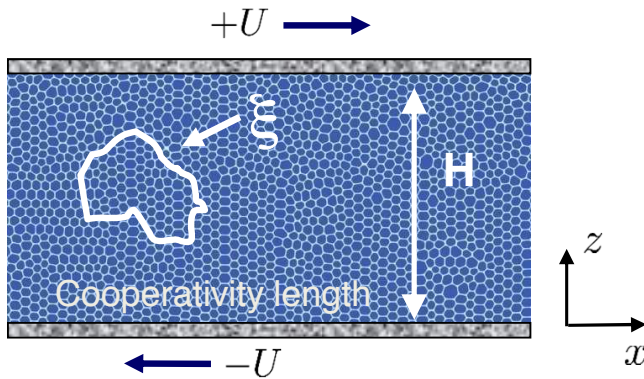


Rate (Γ) of plastic rearrangements estimated from Voronoi Tessellation



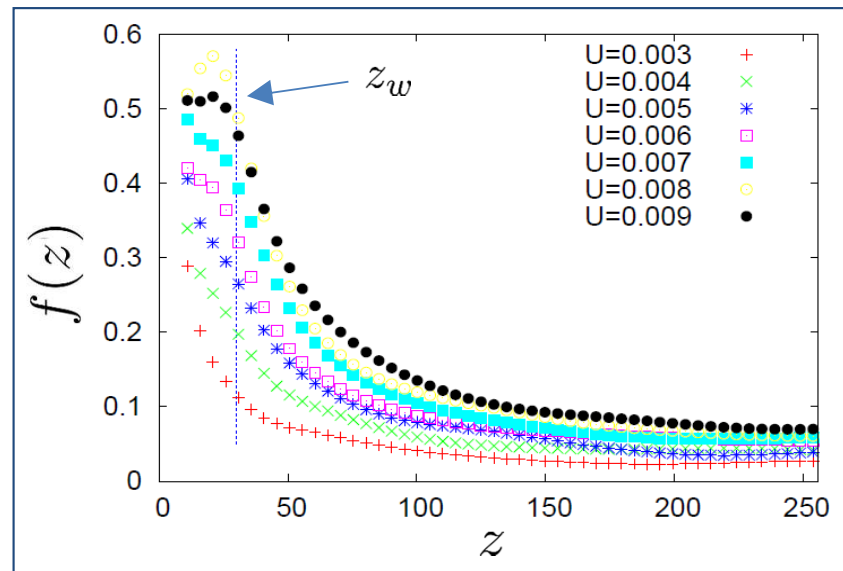
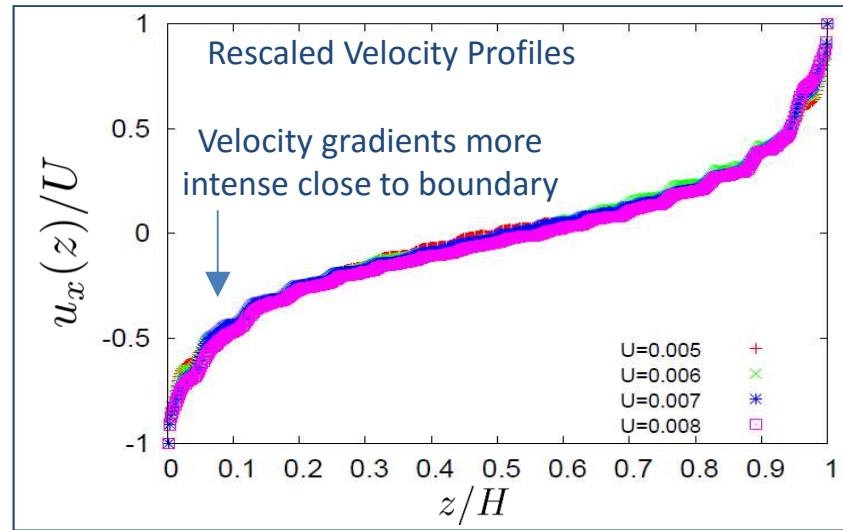
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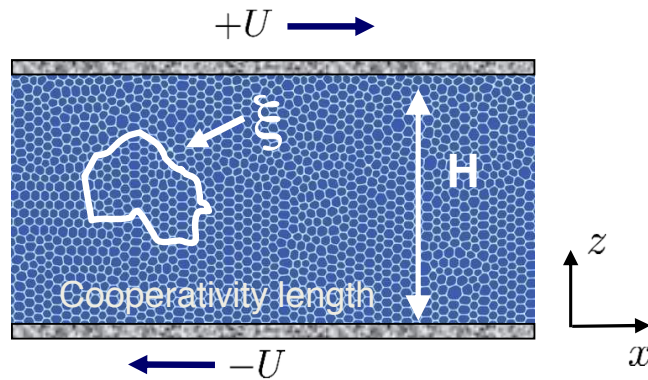
$$f = \frac{\dot{\gamma}S}{\sigma} \quad \xi^2 \frac{d^2 f(z)}{dz^2} + (f_b - f(z)) = 0$$

Fluidity Relaxation-Diffusion equation for the Fluidity



Testing Fluidity Models with LBM

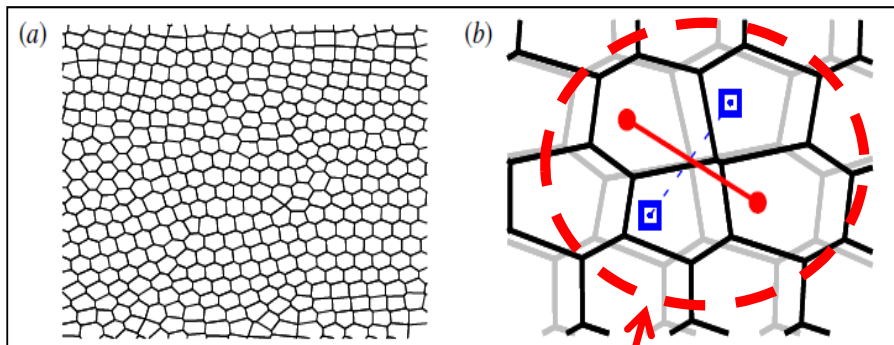
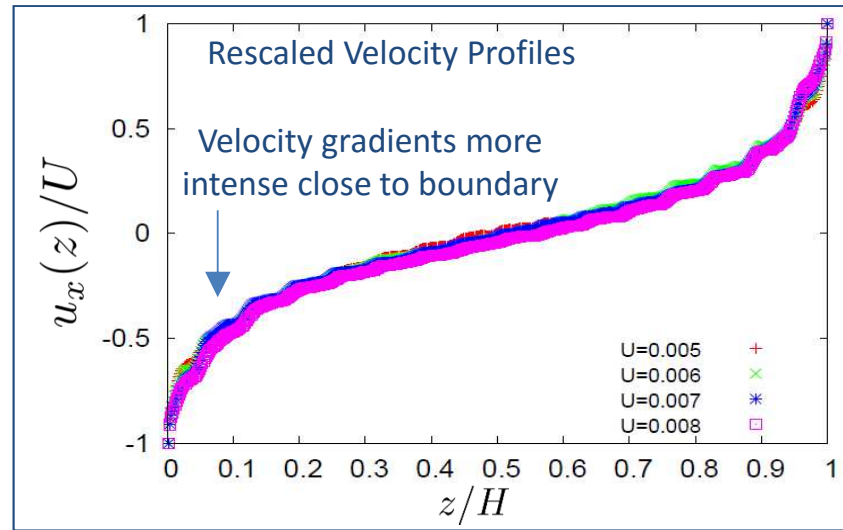
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$$f = \frac{\dot{\gamma} S}{\sigma} \quad \frac{(f(z) - f_b)}{(f_w - f_b)} = e^{-(z - z_w)/\xi}$$

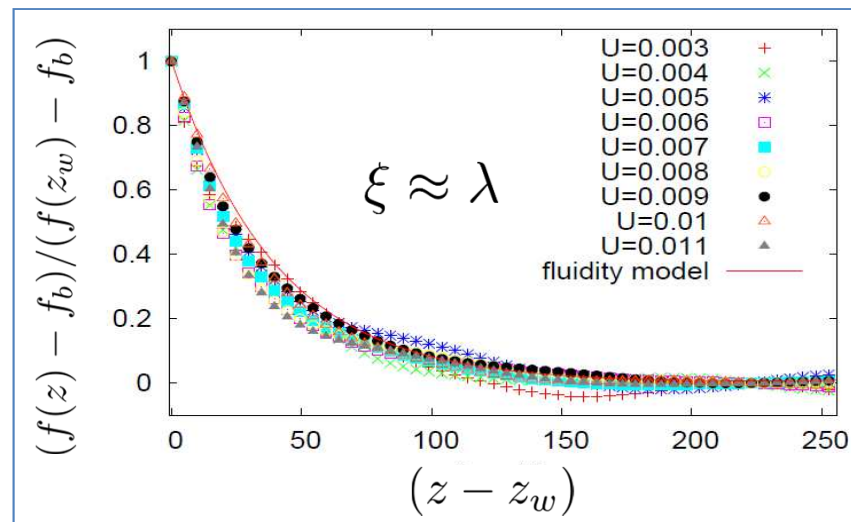
Fluidity

Exact Solution for Couette Flow
(f_b is constant)



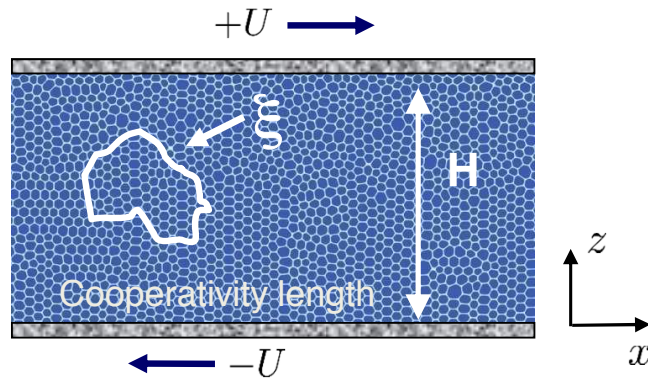
Characteristic size of plastic rearrangements estimated from Voronoi Tessellation

$$A \sim \pi \lambda^2$$



Testing Fluidity Models with LBM

M. Sbragaglia, R. Benzi, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4514-4524 (2014)



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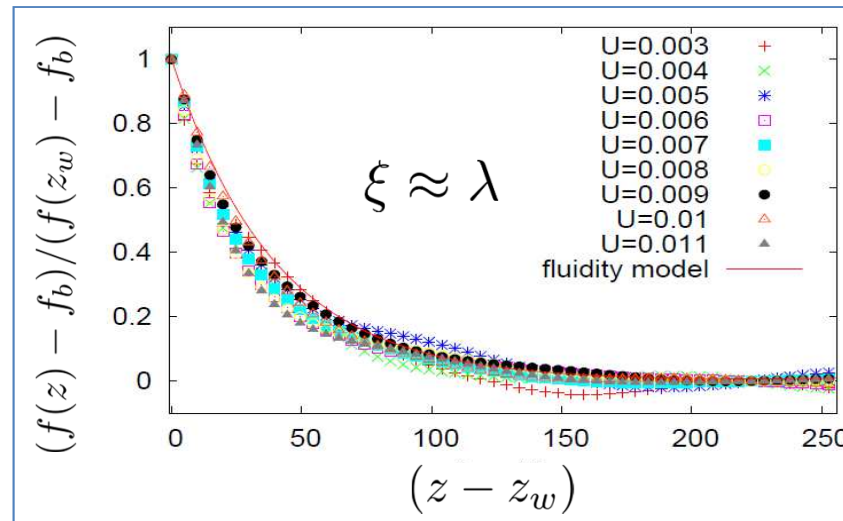
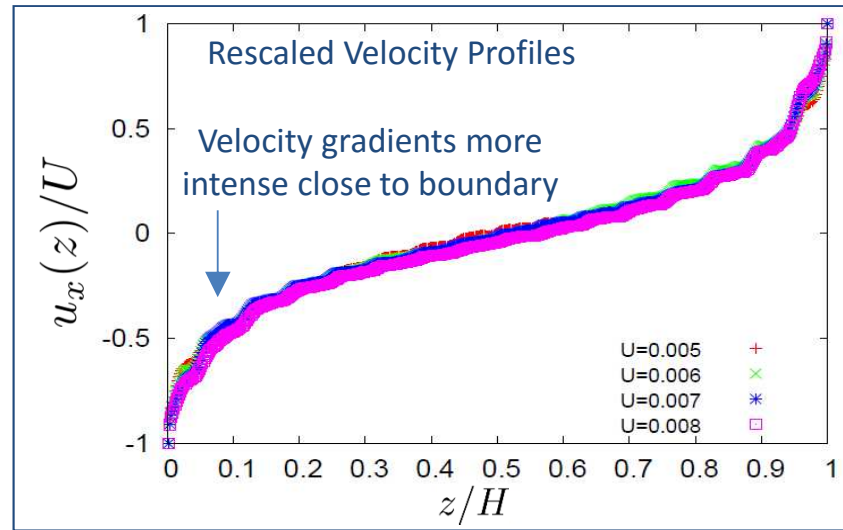
Fluidity Exact Solution for Couette Flow
(f_b is constant)

f_w ← Wall Fluidity

- ✓ **Wall Fluidity:** "Phenomenological" Parameter
- ✓ **Importance:** Engineering appropriate surface
- ✓ **Quantify** the Impact of:

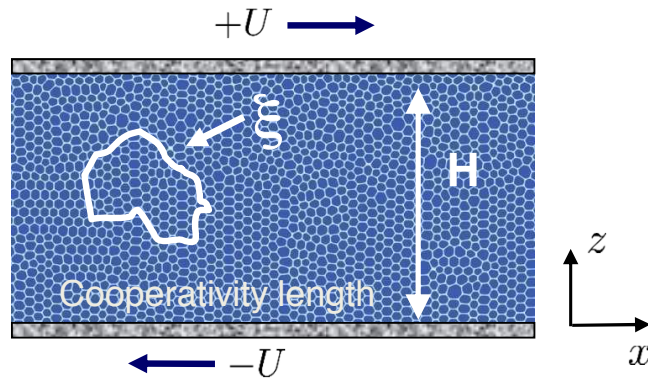
1) Wettability J. Paredes, *Phys. Rev. E* **95**, 042313 (2015)

2) Roughness M. Sbragaglia et al., *Europhys. Lett.* **114**, 64003 (2016)



Testing Fluidity Models with LBM

M. Sbragaglia, R. Benzi, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4514-4524 (2014)



$$f = \frac{\dot{\gamma}S}{\sigma} \quad \frac{(f(z) - f_b)}{(f_w - f_b)} = e^{-(z - z_w)/\xi}$$

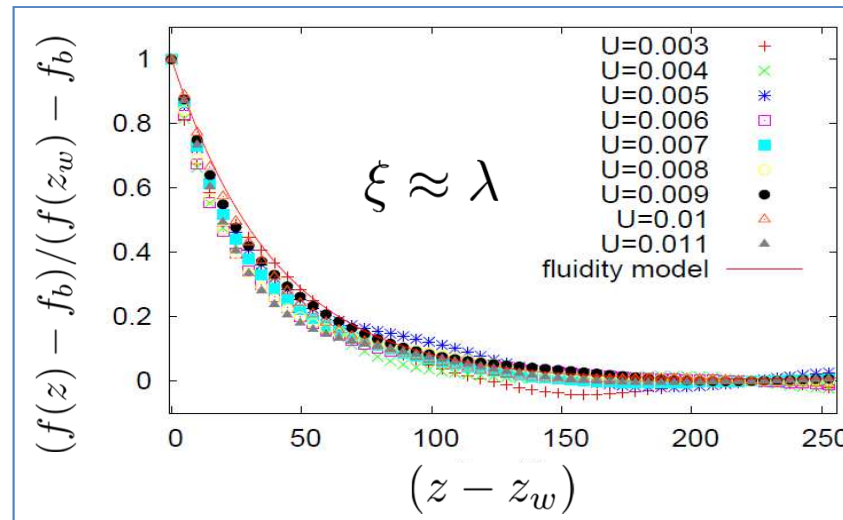
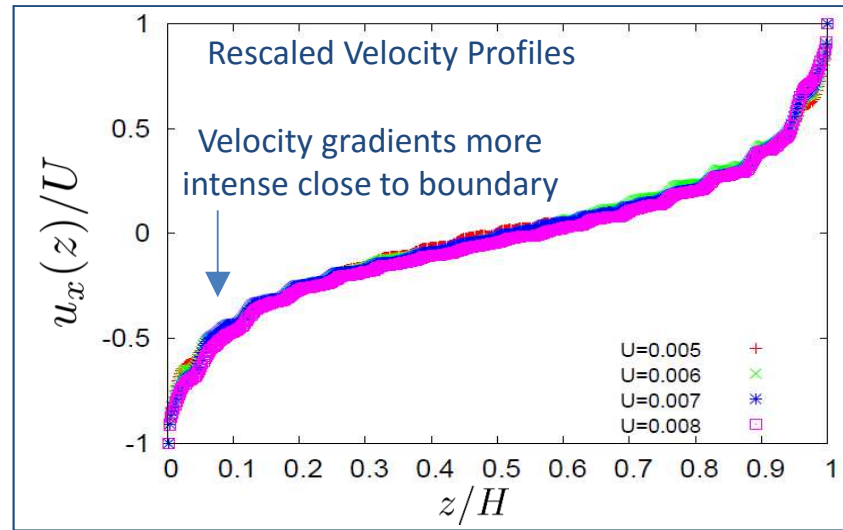
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- ✓ **Quantify** the Impact of:

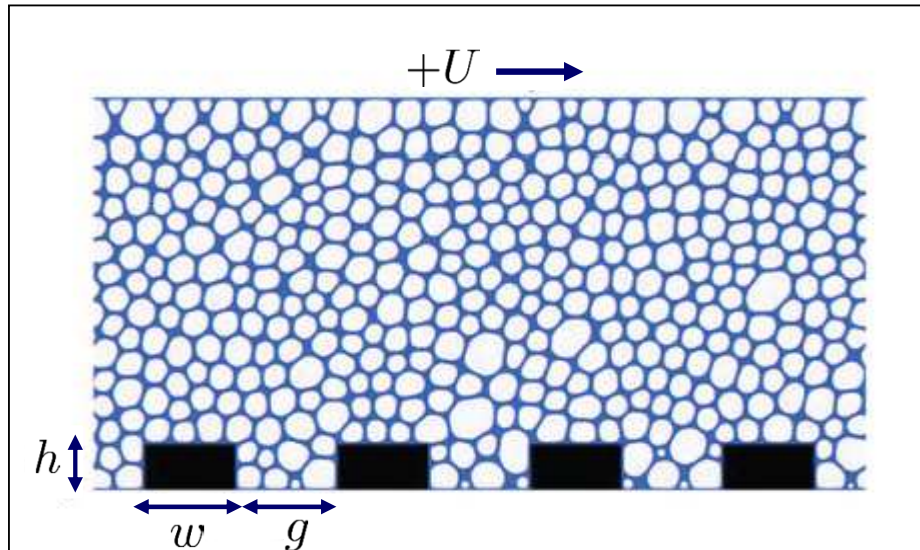
1) Wettability J. Paredes, *Phys. Rev. E* **95**, 042313 (2015)

→ 2) Roughness M. Sbragaglia et al., *Europhys. Lett.* **114**, 64003 (2016)



Rough Channels: Study of Boundary Fluidity

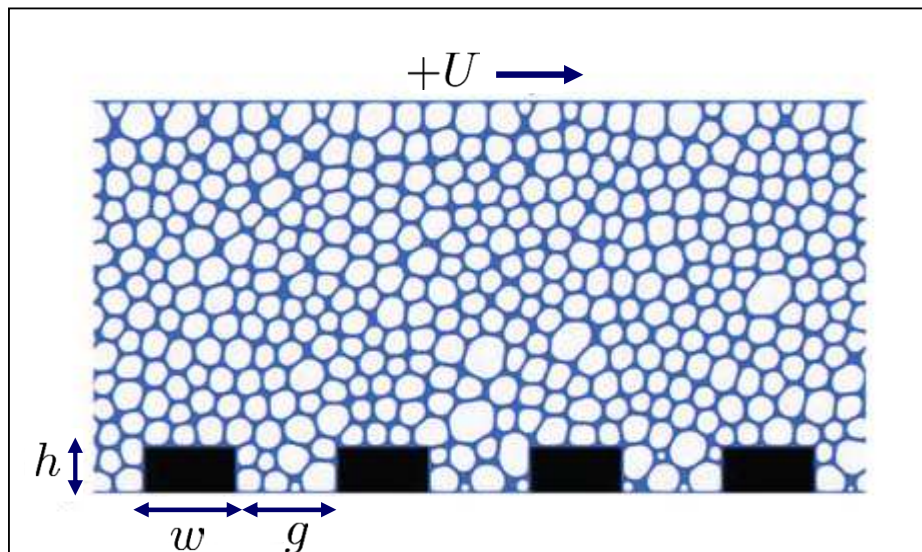
A. Scagliarini, M. Lulli, M. Sbragaglia and M. Bernaschi, *Europhys. Lett.* **114**, 64003 (2016)



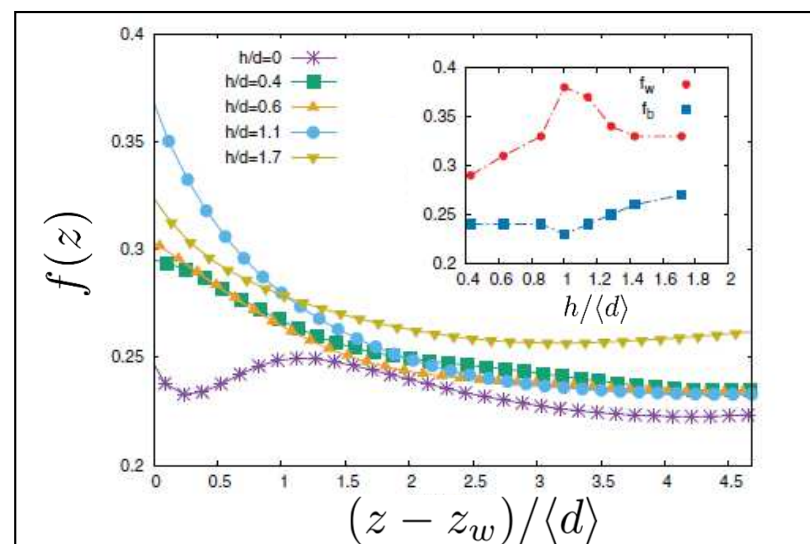
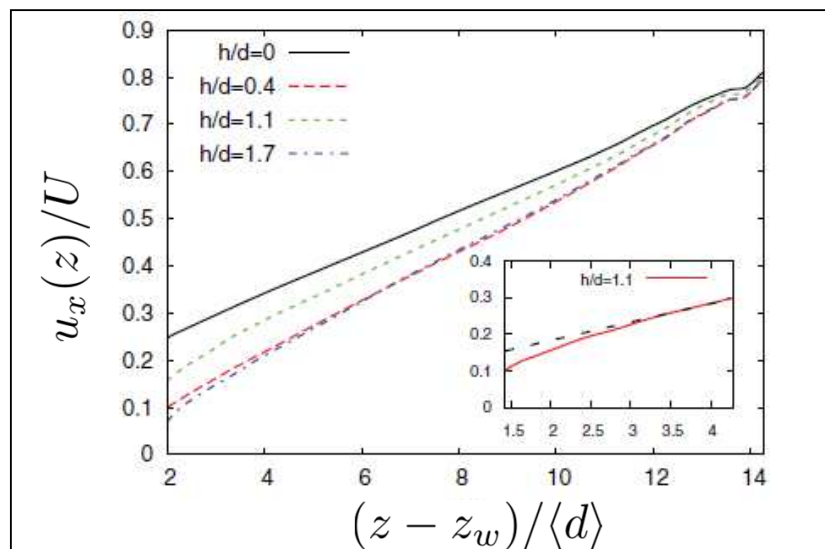
- ✓ Couette Cell with **controlled** Roughness
- ✓ **Fixed** Gap (g) and Width (w)
- ✓ **Variable** height (h)
- ✓ Interplay between h and droplet diameter $\langle d \rangle$

Rough Channels: Study of Boundary Fluidity

A. Scagliarini, M. Lulli, M. Sbragaglia and M. Bernaschi, *Europhys. Lett.* **114**, 64003 (2016)

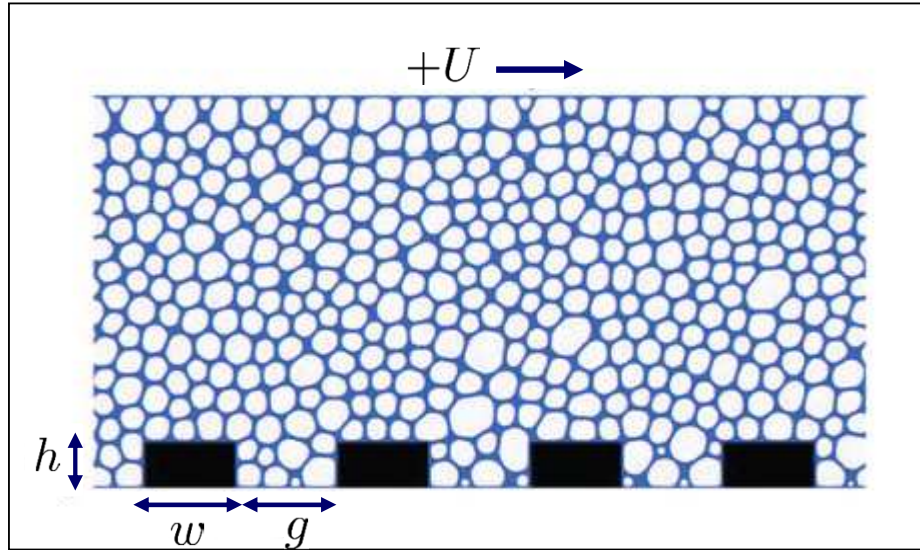


- ✓ Couette Cell with **controlled** Roughness
- ✓ **Fixed** Gap (g) and Width (w)
- ✓ **Variable** height (h)
- ✓ Interplay between h and droplet diameter $\langle d \rangle$



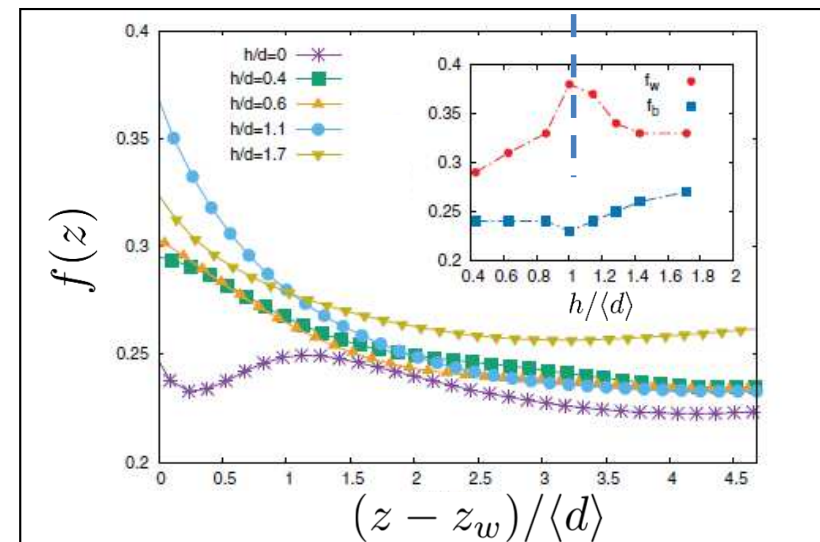
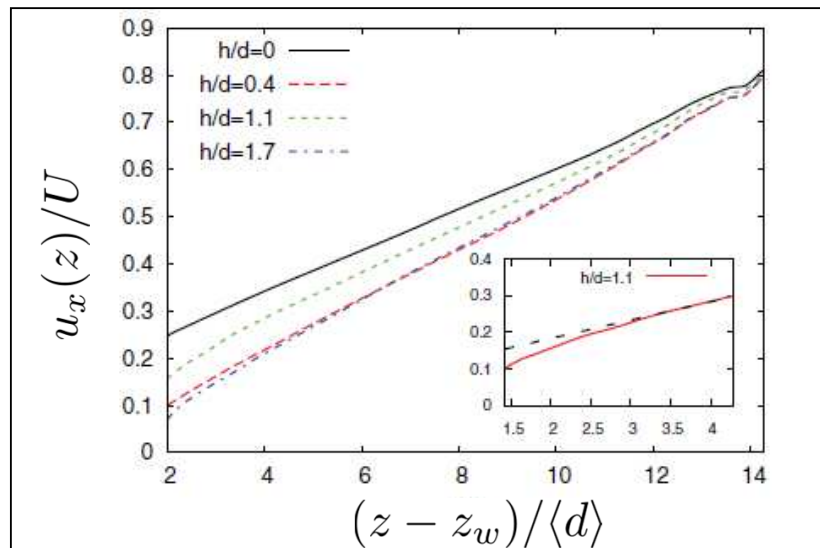
Rough Channels: Study of Boundary Fluidity

A. Scagliarini, M. Lulli, M. Sbragaglia and M. Bernaschi, *Europhys. Lett.* **114**, 64003 (2016)

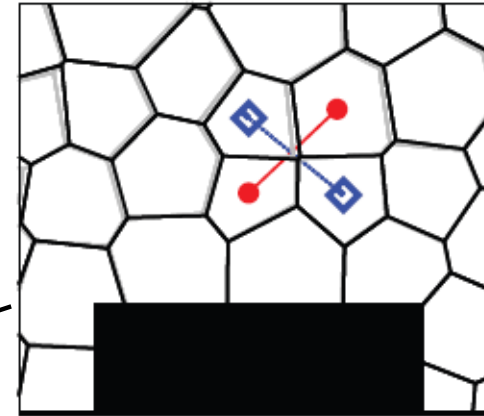
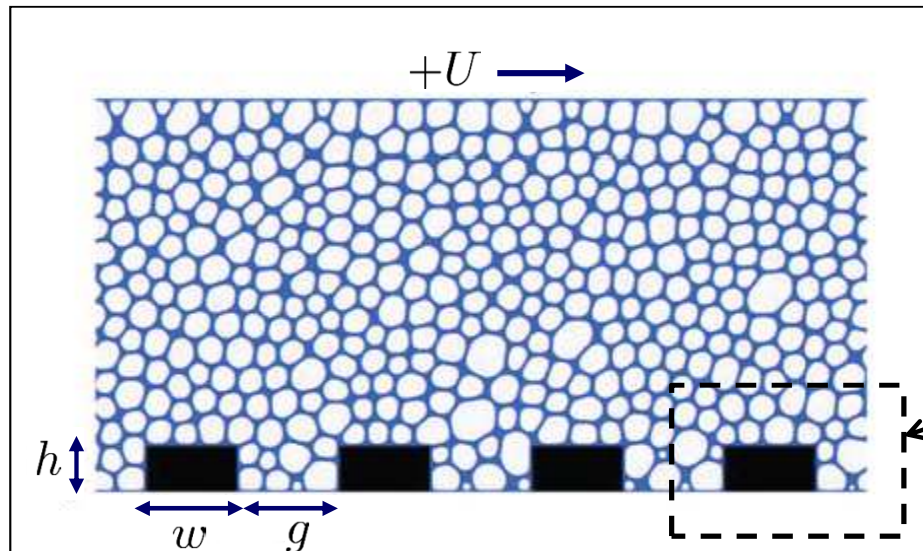


- ✓ Couette Cell with **controlled** Roughness
- ✓ **Fixed** Gap (g) and Width (w)
- ✓ **Variable** height (h)
- ✓ Interplay between h and droplet diameter $\langle d \rangle$

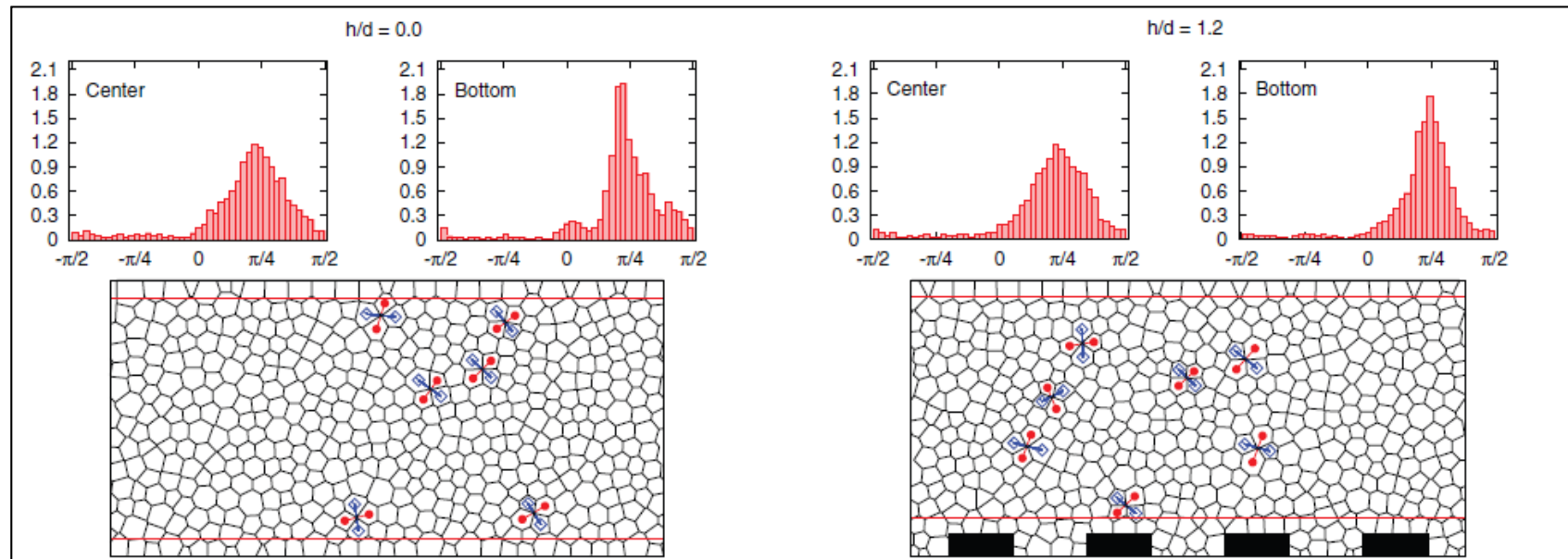
Optimal Height $h \approx \langle d \rangle$



Orientational Statistics



M. Lulli, M. Sbragaglia *et al.*, *arXiv1607.00908* (2016)



Conclusions & Perspectives

LBM For Complex Hydrodynamics at Mesoscales

- ✓ Direct Link with Hydrodynamics (Chapman-Enskog Analysis)
- ✓ Flexibility in modelling Non-Ideal interactions
- ✓ Easy Handling of Boundary Conditions

Applications: Plastic Flows of Foams and Emulsions

- ✓ **Plastic Activity** of Jammed Systems and (corr)relation to hydrodynamics
- ✓ Impact of **Boundary Conditions**
- ✓ Impact of **Orientation** of Plastic Events (Quadrupoles not just "points")
- ✓ Importance of **Heterogeneities** within Fluidity Models (not shown...but see refs.)

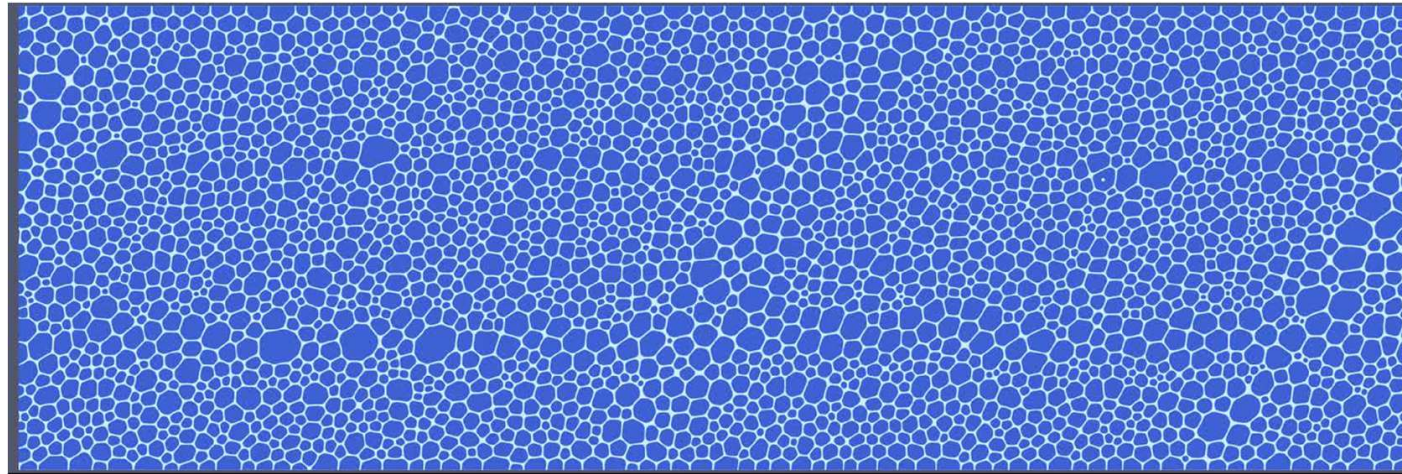
References:

- M. Sbragaglia, R. Benzi, M. Bernaschi & S. Succi, *Soft Matter* **8**, 10773-10782 (2012)
- M. Sbragaglia, R. Benzi, M. Bernaschi & S. Succi, *Europhys. Lett.* **104**, 48006 (2013)
- M. Sbragaglia, R. Benzi, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4514-4524 (2014)
- B. Dollet, A. Scagliarini & M. Sbragaglia, *Jour. Fluid Mech.* **766**, 556-589 (2015)
- R. Benzi, M. Sbragaglia, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **12**, 514-530 (2016)
- A. Scagliarini, M. Lulli, M. Sbragaglia and M. Bernaschi, *Europhys. Lett.* **114**, 64003 (2016)
- M. Lulli, M. Sbragaglia and M. Bernaschi, *arXiv1607.00908* (2016)

Plastic Events: LBM with Different Load Conditions

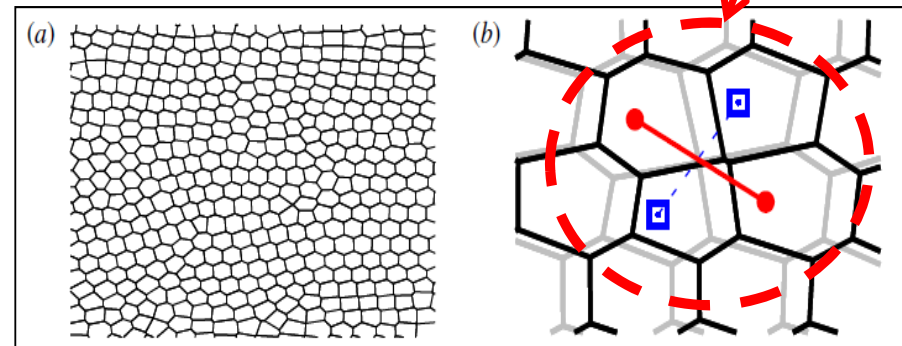
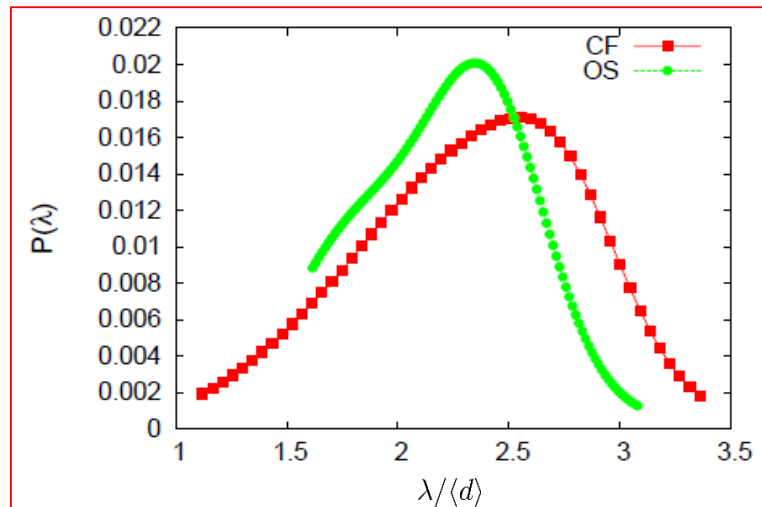
M. Sbragaglia, R. Benzi, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4514-4524 (2014)

Oscillating Strain (OS) Boundary Conditions



Characteristic size of plastic rearrangements estimated from Voronoi Tessellation

$$\sim \pi \lambda^2$$



Benzi R., Sbragaglia M., Perlekar P., Bernaschi M., Succi S. Toschi F. *Soft Matter* **10**, 4615-4624 (2014)

Probability Distribution of size of Plastic Rearrangement
(Different Flow Conditions: **CF** (Couette Flow); **OS** (Oscillatory Strain))

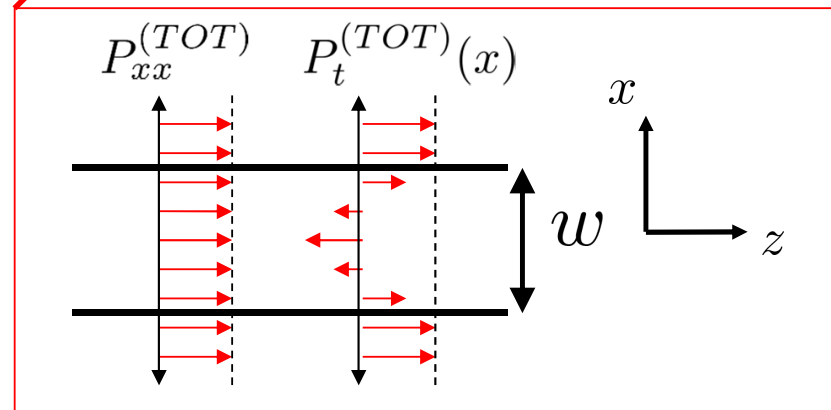
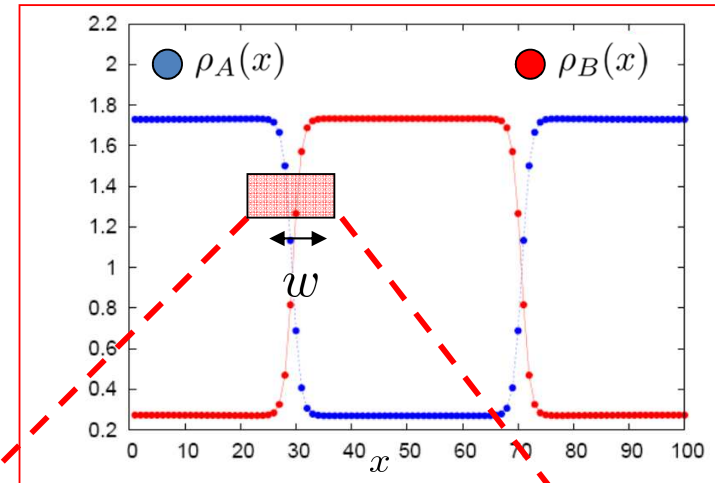
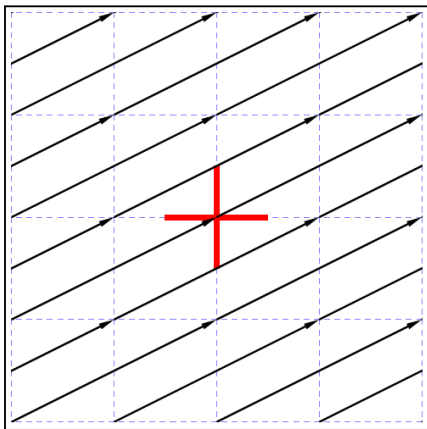
Mechanical Pressure Tensor: How?

Forces

$$\vec{F} = -g_{AB}\rho_A(\vec{r}) \sum_i w_i \rho_B(\vec{r} + \vec{c}_i) \vec{c}_i + (A \leftrightarrow B)$$

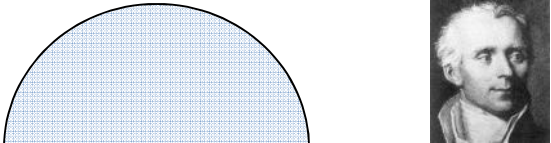
Non-ideal **Lattice** Pressure Tensor

$$\mathbf{P}^{(NI)} = \frac{g_{AB}}{2} \rho_A(\vec{r}) \sum_i w_i \rho_B(\vec{r} + \vec{c}_i) \vec{c}_i \vec{c}_i + (A \leftrightarrow B)$$



- X. Shan, Physical Review E 77, 066702 (2008)
- M. Sbragaglia & X. Shan, Physical Review E 84, 036703 (2011)
- M. Sbragaglia & D. Belardinelli, Physical Review E 91, 023313 (2013)

Surface Tension at the non ideal interfaces



Laplace Law

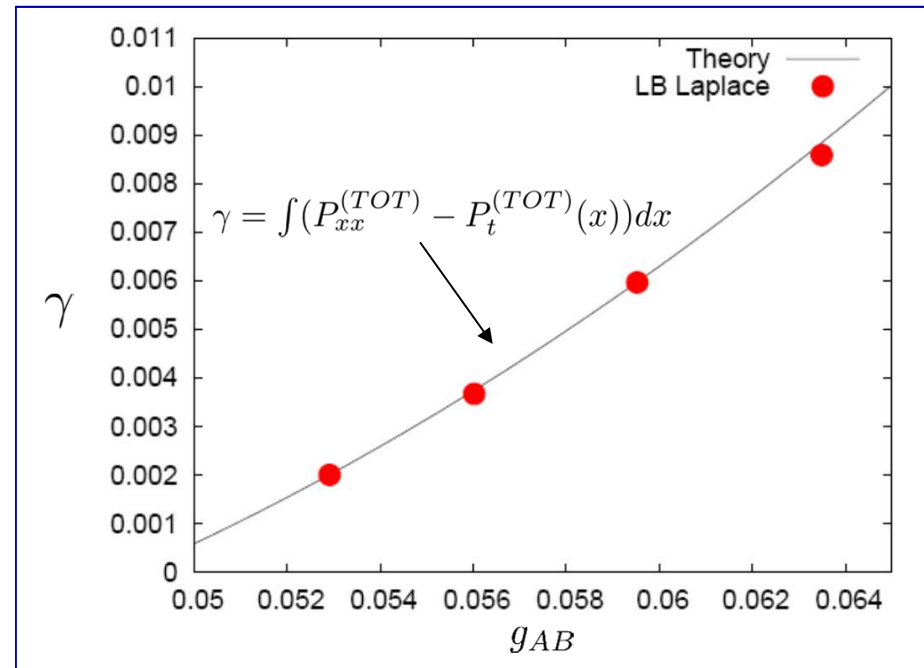
$$\Delta P = P_{bulk,in}^{(TOT)} - P_{bulk,out}^{(TOT)} = \frac{\gamma}{R}$$

Inner-Outer pressures for equilibrium droplets

↕ YES! →

$$\gamma = \int (P_{xx}^{(TOT)} - P_t^{(TOT)}(x)) dx$$

**Surface Tension
(Mechanical Definition)**



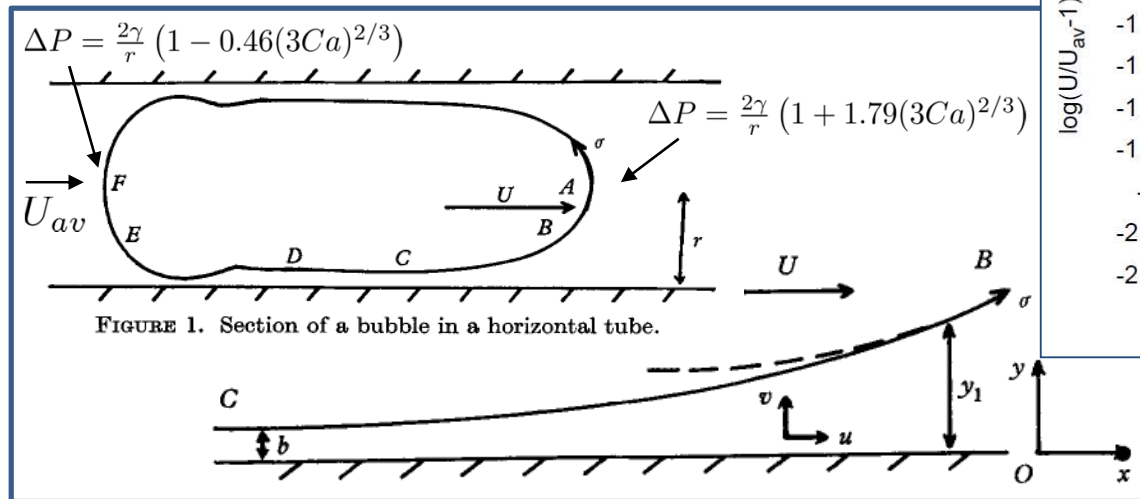
Benchmark Computation: Motion of "Long" Droplets in a Tube



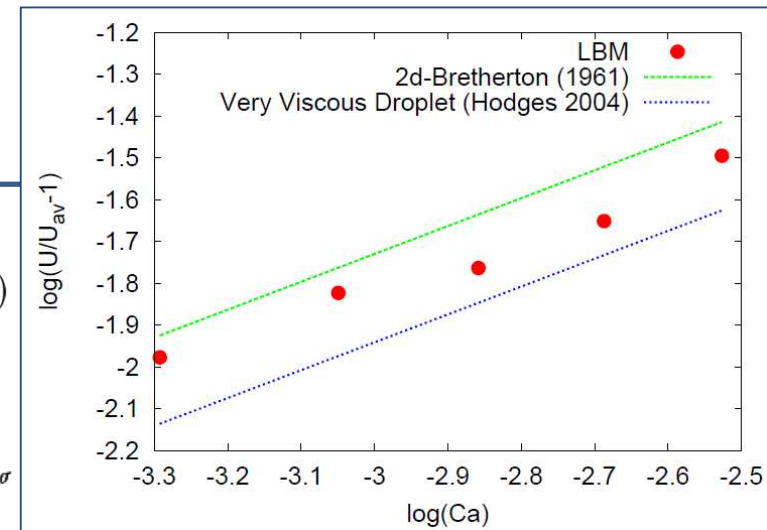
$Ca = \eta U / \gamma$
 Capillary number
 (viscous/surface)

$$U/U_{av} = 1 + 0.643 Ca^{2/3}$$

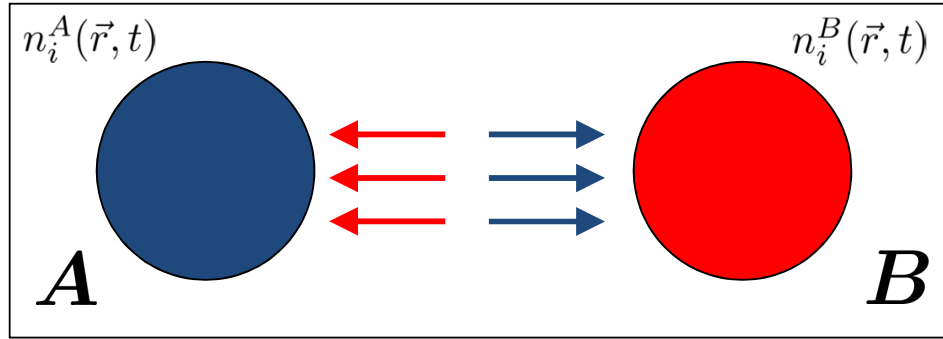
Bretherton Scaling



Bretherton, *Jour. Fluid Mech.* (1961)

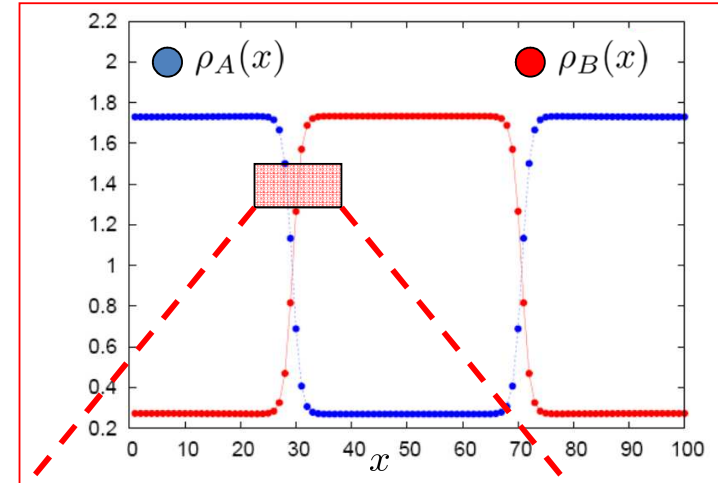
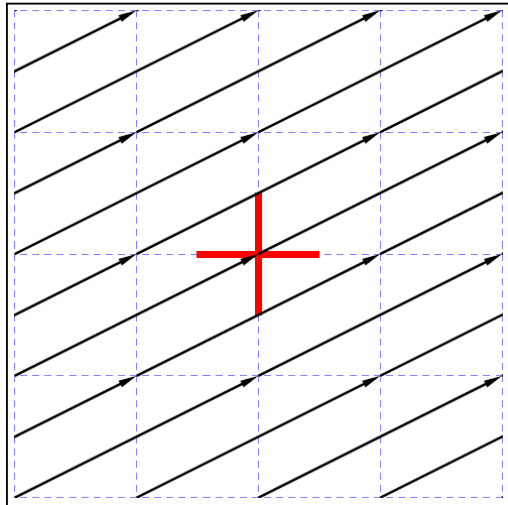


Non Ideal Forces & Coalescence

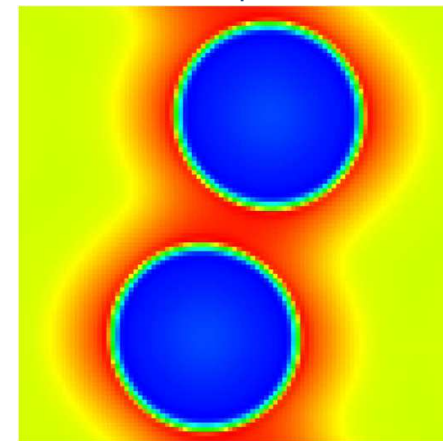


Non-ideal (NI) Lattice Pressure Tensor

$$P_{jk}^{(NI)} = \frac{g_{AB}}{2} \rho_A(\vec{r}) \sum_i w_i \rho_B(\vec{r} + \vec{c}_i) c_i^j c_i^k + (A \leftrightarrow B)$$

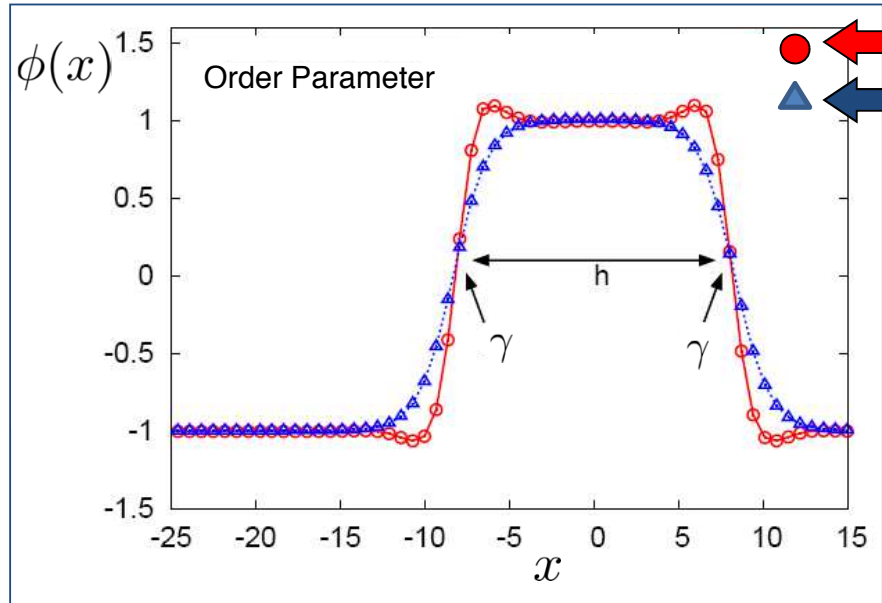


Minimization of interface Free-Energy leads to film rupture

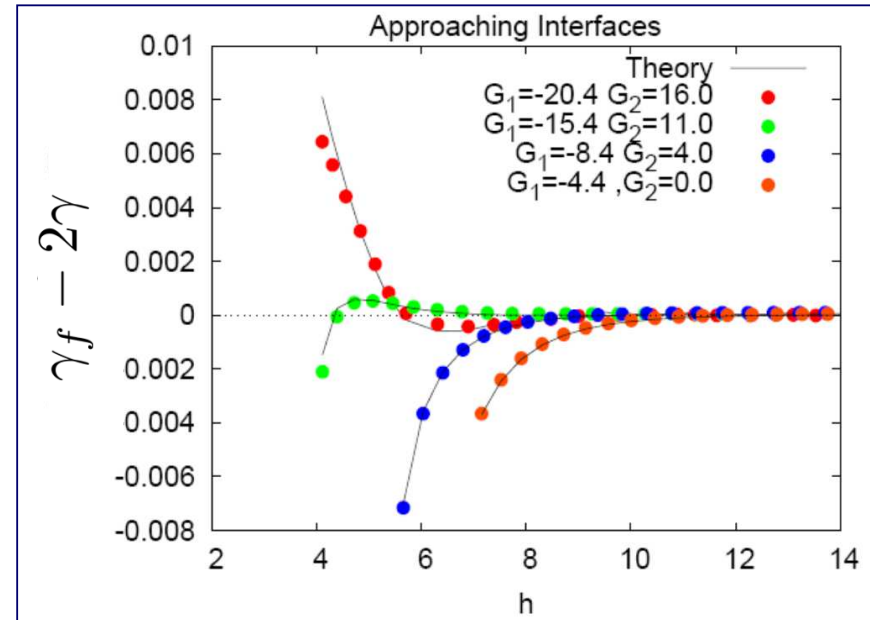


Droplets Coalescence

Disjoining Pressure From Lattice Kinetic models



● ← (Competing NN & NNN) $\mathcal{G}_1 < 0; \mathcal{G}_2 > 0$
▲ ← (bare NN) $\mathcal{G}_1 < 0; \mathcal{G}_2 = 0$



M. Sbragaglia et al., *Soft Matter* 8, 10773-10782 (2012)

$$\gamma_f = \int_{-\infty}^{+\infty} (P_n - P_t(x)) dx$$

'film tension'

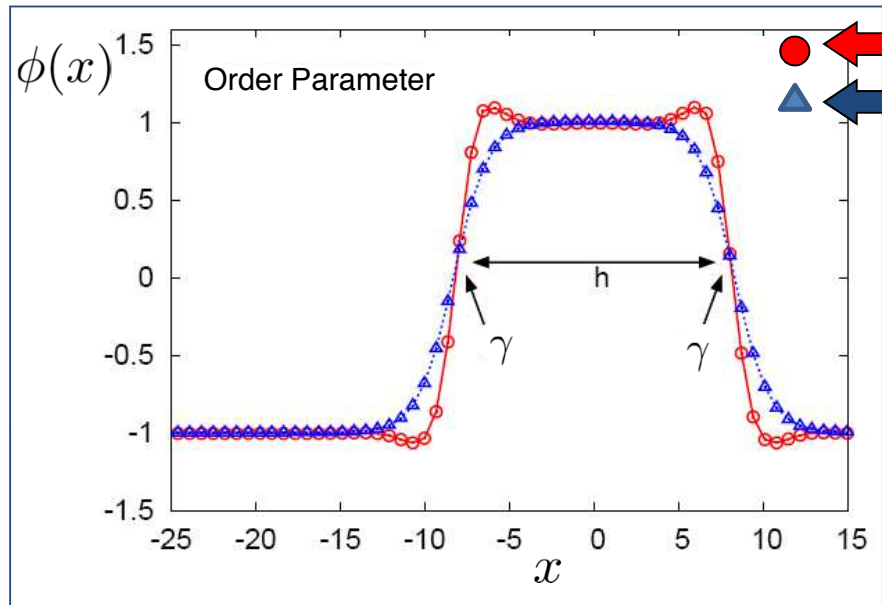


Exactly computed on the lattice

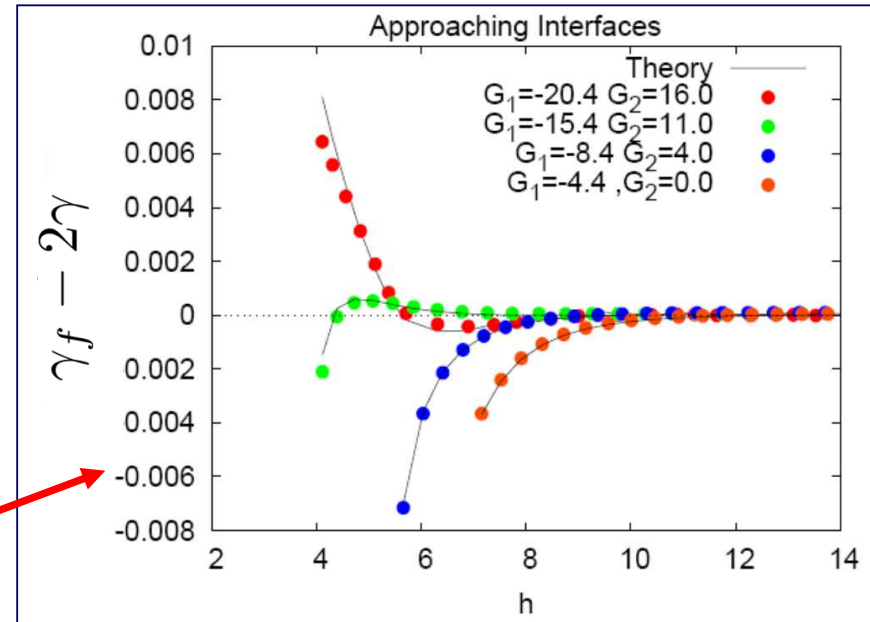
$$P_n = P_b(x) + C_1 \psi \frac{d^2 \psi}{dx^2} + \dots = \text{const}$$

Analytical with the exact pressure tensor
(differential equation -> Profile)

Disjoining Pressure From Lattice Kinetic models



● ← (Competing NN & NNN) $\mathcal{G}_1 < 0; \mathcal{G}_2 > 0$
▲ ← (bare NN) $\mathcal{G}_1 < 0; \mathcal{G}_2 = 0$



$$\gamma_f = 2\gamma + \int_{\Pi(h=\infty)}^{\Pi(h)} h d\Pi$$

Disjoining Pressure definition based on 'film tension'



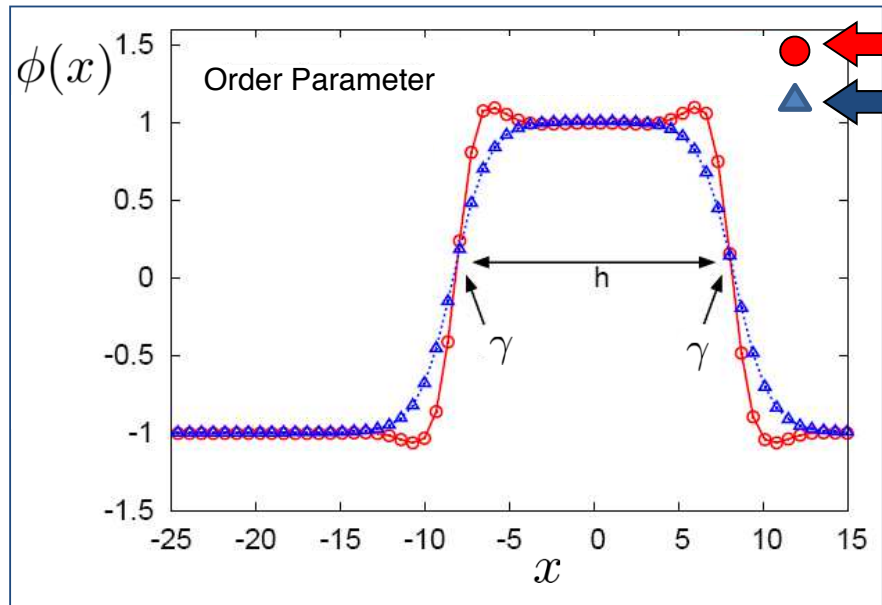
Exactly computed on the lattice

$$P_n = P_b(x) + C_1 \psi \frac{d^2 \psi}{dx^2} + \dots = \text{const}$$

Analytical with the exact pressure tensor
(differential equation -> Profile)

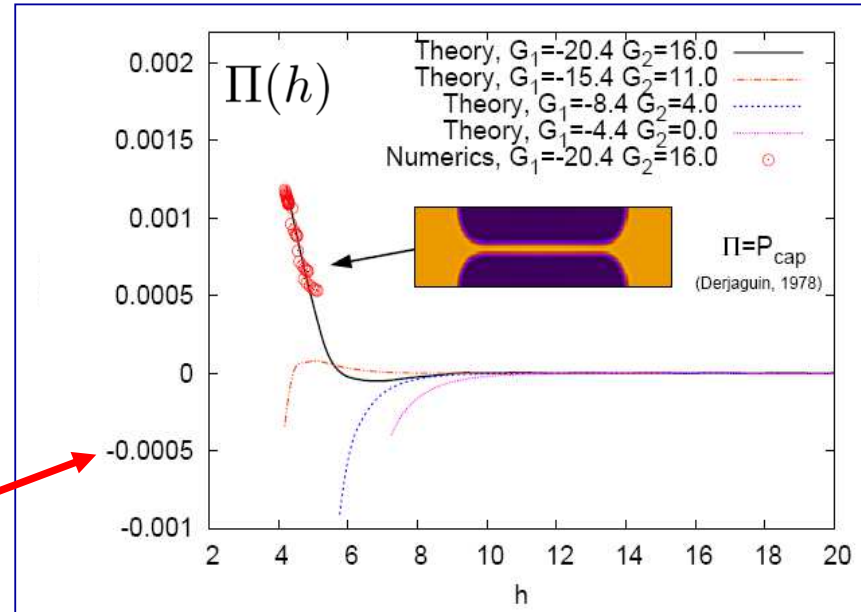
M. Sbragaglia et al., *Soft Matter* 8, 10773-10782 (2012)

Disjoining Pressure From Lattice Kinetic models



● (Competing NN & NNN) $\mathcal{G}_1 < 0; \mathcal{G}_2 > 0$

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$$\gamma_f = 2\gamma + \int_{\Pi(h=\infty)}^{\Pi(h)} h d\Pi$$

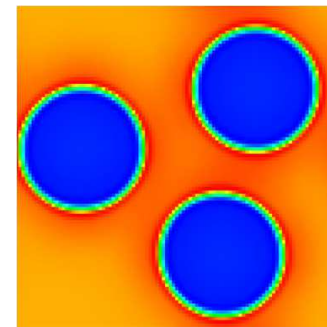
Disjoining Pressure definition based on 'film tension'



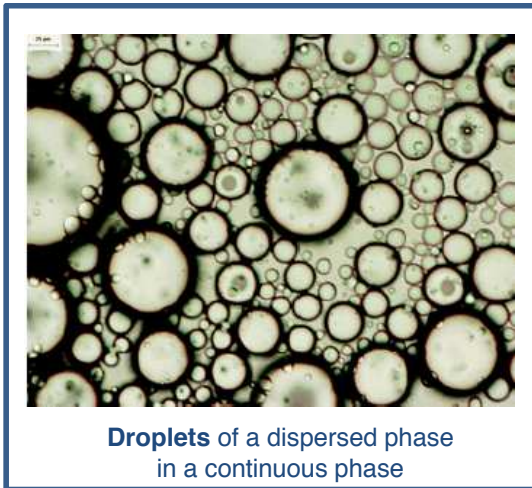
Exactly computed on the lattice

$$P_n = P_b(x) + C_1 \psi \frac{d^2 \psi}{dx^2} + \dots = \text{const}$$

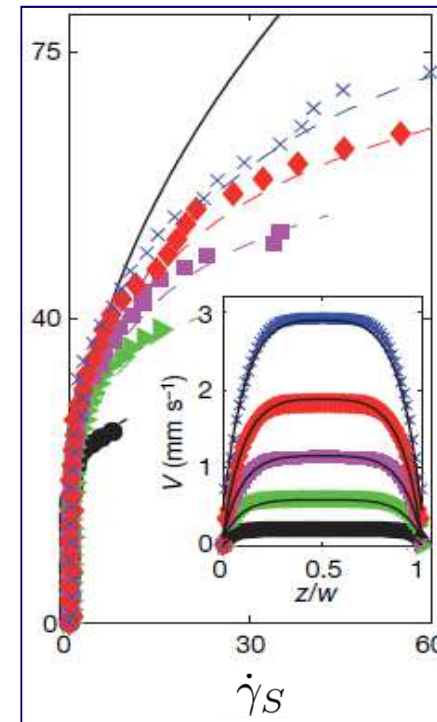
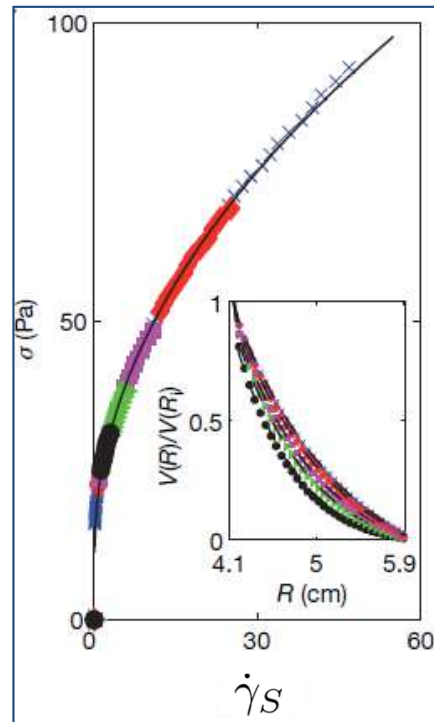
Analytical with the exact pressure tensor
(differential equation -> Profile)



Universality Under Confinement ?



- ✓ Yield Stress (Solid below)
- ✓ Non-Newtonian (above yield Stress)
- ✓ Effect of Confinement (Cooperativity Effects)

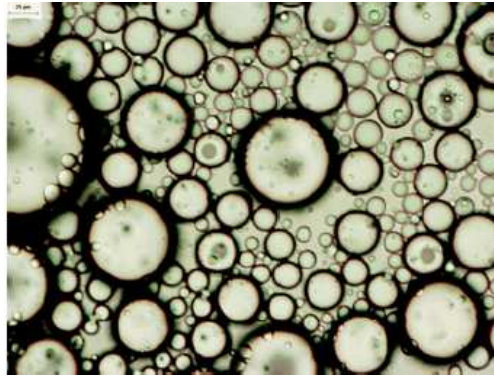


Rheology in a **wide** Rheometer Rheology in **thin** Rheometer

Goyon et al, Nature (2008)

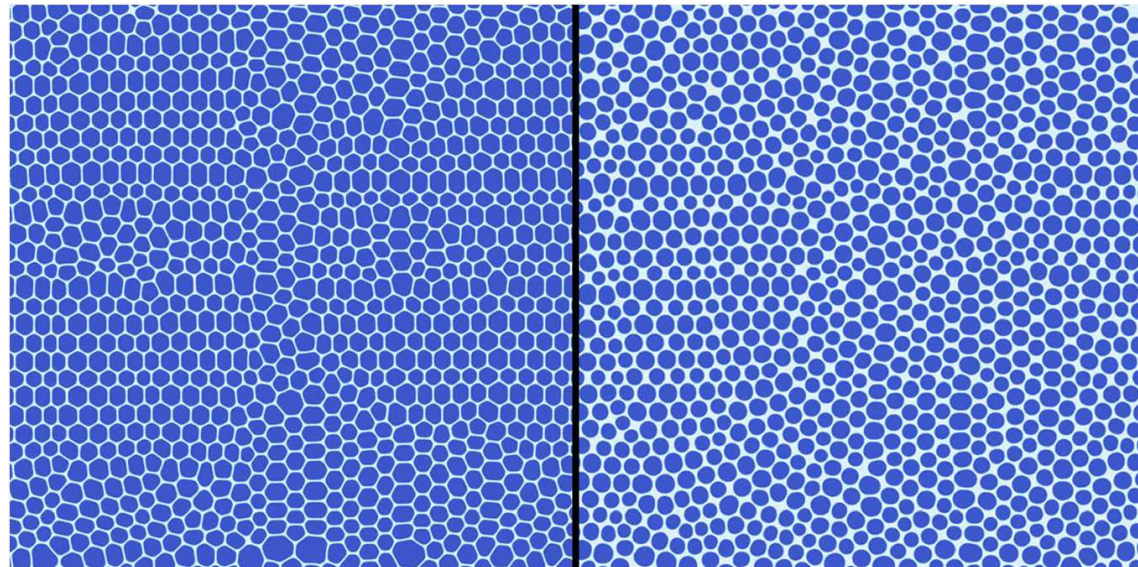
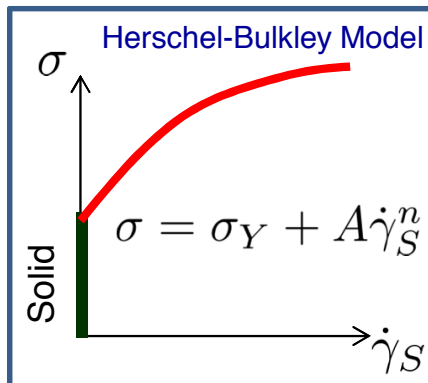
Yield Stress Fluids & Plastic Rearrangements

R. Benzi, M. Sbragaglia, P. Perlekar, M. Bernaschi, S. Succi & F. Toschi, *Soft Matter* **10**, 4615-4624 (2014)



Droplets of a dispersed phase
in a continuous phase

- ✓ Yield Stress (Solid below)
- ✓ Non-Newtonian (above yield)
- ✓ Cooperativity Effects & Plastic Rearrangements



High Packing Fraction

Lower Packing Fraction