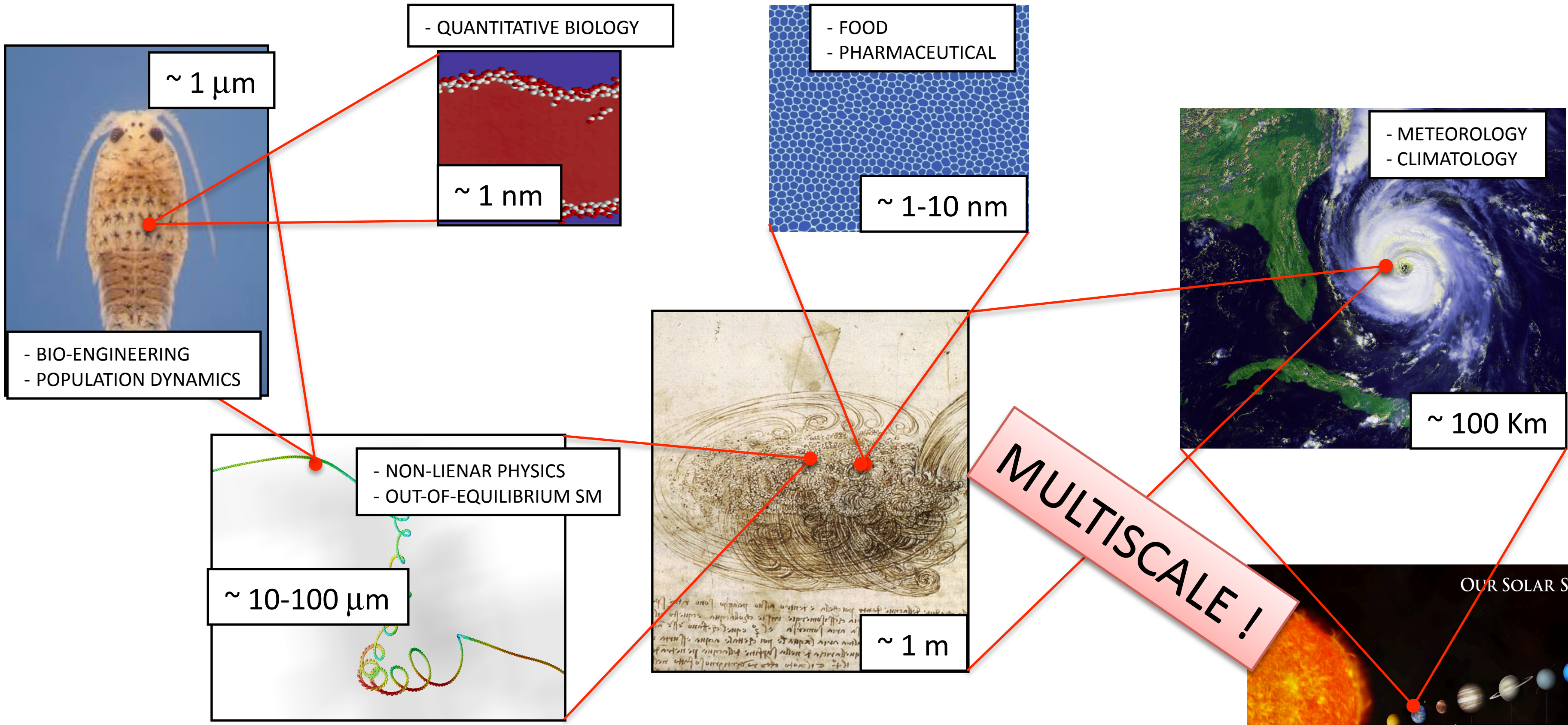
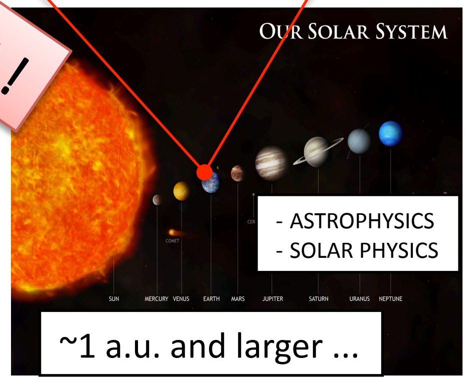
Παντα ρει

inside, outside, above, below and around us





"C'e' molto spazio nel fondo"

Luca Biferale
SIF 2015
Dept. Physics, INFN and CAST, University of Rome 'Tor Vergata'

-A guided short tour around a mesoscopic/kinetic numerical tool:
Lattice Boltzman Equations

-Fluctuating Hydrodynamics
-Softy Glass Material

Credits:

M. Sbragaglia, R. Benzi, A. Gupta, A. Scagliarini (Dept. Physics, University of Rome " Tor Vergata")
S. Succi & M. Bernaschi (IAC-CNR, Rome)
F. Toschi (University of Eindhoven & IAC-CNR, Rome)
M. Pierno, S. Varagnolo, G.P. Mistura (Dept. Physics, University of Padova)

UNIVERSITA' degli STUDI di ROMA TOR VERGATA

INFN Istituto Nazionale di Fisica Nucleare

CINECA

HPC-LEAP EUROPEAN JOINT DOCTORATES

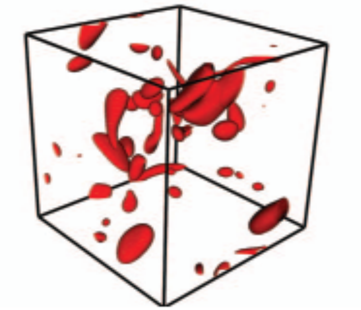
SEVENTH FRAMEWORK PROGRAMME

erc

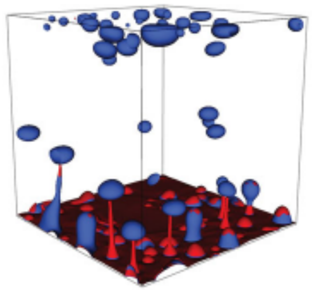
PRACE

LBM for Complex Fluid Dynamics: Why & Where ?

$10^{-3} - 10^{0}m$



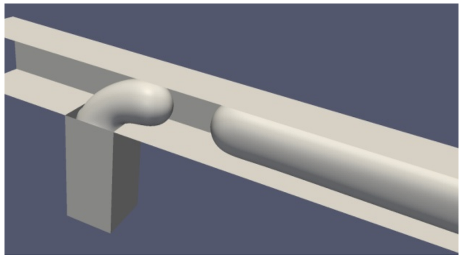
Droplets/Particles in Turbulence



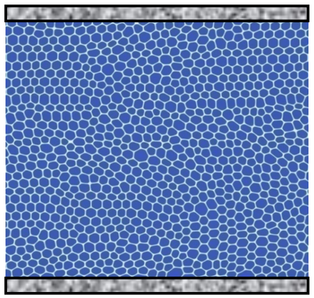
Boiling Fluids

- ✓ How the Heat Transport in a Rayleigh-Bènard Cell is affected by the presence of bubbles ?
- ✓ How Droplets interact with small scales Turbulence ?

$10^{-6} - 10^{-3}m$



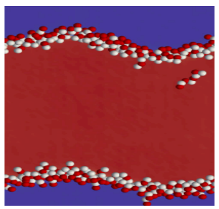
Droplets in Microfluidics



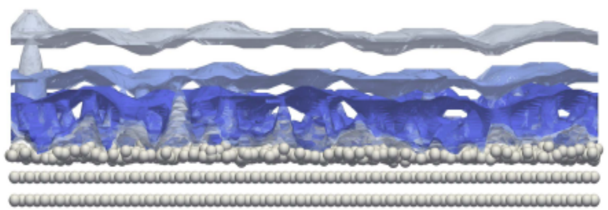
Soft-Glassy Materials

- ✓ Dynamics of Single Droplets: bounded *vs* unbounded geometries ?
- ✓ How The Rheology of a Collection of Droplets is affected by confinement?

$10^{-9} - 10^{-6}m$



Membranes



Nanofluids

- ✓ How to correcty control surfactant dynamics at the interfaces?
- ✓ How the slip at the liquid-solid interfaces is affected by roughness and wettability ?

Where to Sit Across the scales?


MACROSCOPIC

(NAVIER-STOKES)

$$\vec{\nabla} \cdot \vec{u} = 0$$

$$\rho D_t \vec{u} = -\vec{\nabla} p + \eta \Delta \vec{u}$$

....

Continuum Description

Chapman-Enskog

(Multi-Scale Lattice Theory)

MESOSCOPIC

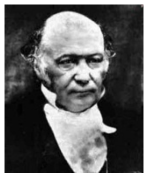
(LATTICE BOLTZMANN)

$$\partial_t f(\vec{x},\vec{v}) + \vec{v} \cdot \vec{\partial}_x f(\vec{v},\vec{x}) = -\frac{1}{\tau}(f(\vec{x},\vec{v}) - f^{eq}(\vec{u},\rho))$$

Kinetic ‘*Inspired*’ Equations

Supra-molecular

Framework for lattice interactions



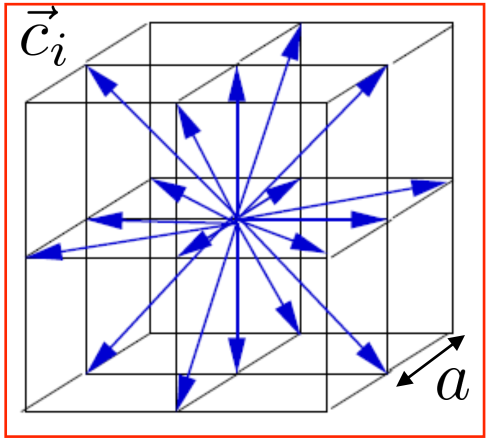
MICROSCOPIC

(MOLECULAR DYNAMICS)

$$\mathcal{H} = \sum_k \frac{p_k^2}{2m} + \sum_{i,k} V_{i,k}$$

$$\dot{q}_k = \frac{\partial \mathcal{H}}{\partial p_k} \qquad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k}$$

Lattice Boltzmann: Basics & Conservation Laws



$$\partial_t f(\vec{x},\vec{v}) + \vec{v}\cdot\vec{\partial}_x f(\vec{v},\vec{x}) = -\frac{1}{\tau}\left(f(\vec{x},\vec{v}) - f^{eq}(\vec{u},\rho)\right)$$

$$\vec{v} \longrightarrow c_i$$

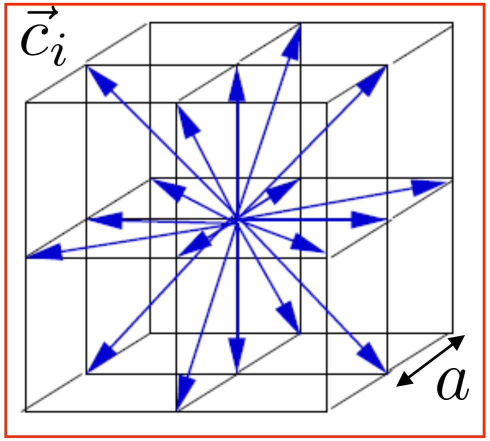
$$f(\vec{v},\vec{x}) \rightarrow n_i(\vec{x})$$

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

- $\vec{c}_i$ **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 $(\vec{r},t)$

How to access coarse grained variables?

Lattice Boltzmann: Basics & Conservation Laws



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

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

Coarse Grained Fields:

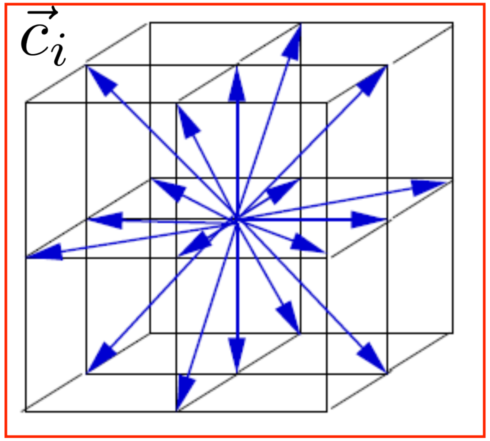
$$\rho(\vec{r}, t) = \sum_i n_i(\vec{r}, t)$$ (Density)

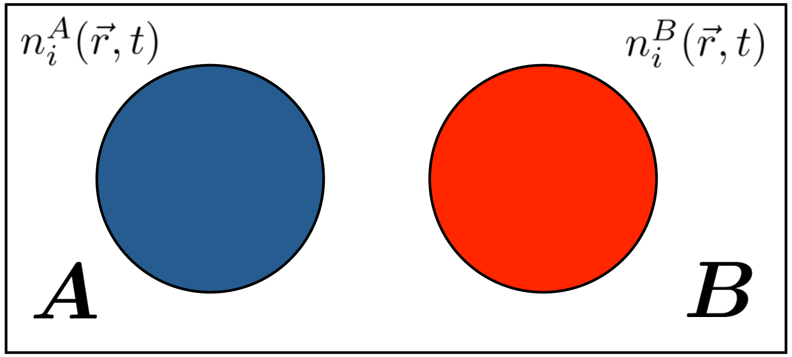
$$\vec{j}(\vec{r}, t) = \sum_i \vec{c}_i n_i(\vec{r}, t)$$ (Momentum)

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

Mass Conservation!
Momentum Conservation!!
Locality !!!

Increasing Complexity: Multicomponent LBM





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

$n_i^{\sigma}(\vec{r},t)$ Real Number: particle pdf on space-time location $(\vec{r},t)$ for component σ

<u>Coarse Grained Fields:</u>

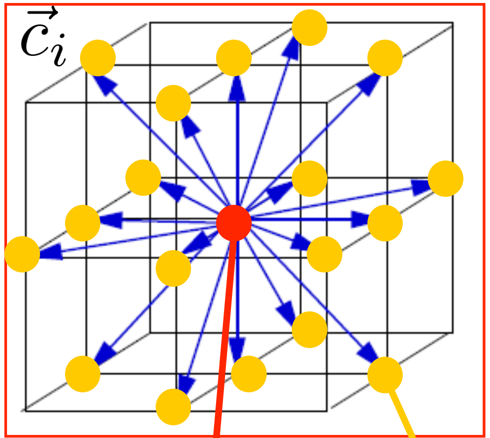
$\rho_{\sigma}(\vec{r},t) = \sum_i n_i^{\sigma}(\vec{r},t)$ (Density)

$\vec{j}_{\sigma}(\vec{r},t) = \sum_i \vec{c}_i n_i^{\sigma}(\vec{r},t)$ (Momentum)

Mass Conservation!
Global Momentum Conservation
Locality !!!

$\sum_i \Delta_i^{\sigma} = 0 \qquad \sum_i \vec{c}_i \Delta_i^{\sigma} \neq 0 \qquad \sum_{\sigma} \sum_i \vec{c}_i \Delta_i^{\sigma} = 0$

Non Ideal Lattice Fluids: Basic Ideas



$$\sigma = A, B$$

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

$$\Delta_i^\sigma = \sum_j L_{ij}^\sigma n_i^{\sigma,neq} + \Delta_i^{F,\sigma}$$

Relax to Equilibrium+Forcing

Lattice Mean-Field Interactions (Shan-Chen)

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

Coupling Strength Parameter regulates the Force intensity

A Few Reference Works:

X. Shan & H. Chen, *Physical Review E* **47**, 1815 (1993)

X. Shan & H. Chen, *Physical Review E* **49**, 2941 (1994)

X. Shan, *Physical Review E* **77**, 066702 (2008)

M. Sbragaglia & X. Shan, *Physical Review E* **84**, 036703 (2011)

R. Benzi, *J. Chem. Phys.* **131**, 104903 (2009)

How to rationalize the outcome of numerical simulations ?

Equilibrium Properties: Bulk Densities

$$\mathcal{L}(\rho_A, \rho_B, \nabla\rho_A, \nabla\rho_B) = f_b(\rho_A, \rho_B) - \frac{g_{AB}}{2}\boldsymbol{\nabla}\rho_A \cdot \boldsymbol{\nabla}\rho_B - \lambda_A\rho_A - \lambda_B\rho_B$$

Lagrange Multipliers

$$f_b(\rho_A, \rho_B) = c_s^2\rho_A \log\rho_A + c_s^2\rho_B \log\rho_B + g_{AB}\rho_A\rho_B$$

Bulk Free Energy

$$f_b(\phi, \rho) = \frac{c_s^2}{2}(\rho+\phi)\log\left(\frac{\rho+\phi}{2}\right) + \frac{c_s^2}{2}(\rho-\phi)\log\left(\frac{\rho-\phi}{2}\right) + \frac{1}{4}g_{AB}(\rho^2 - \phi^2)$$

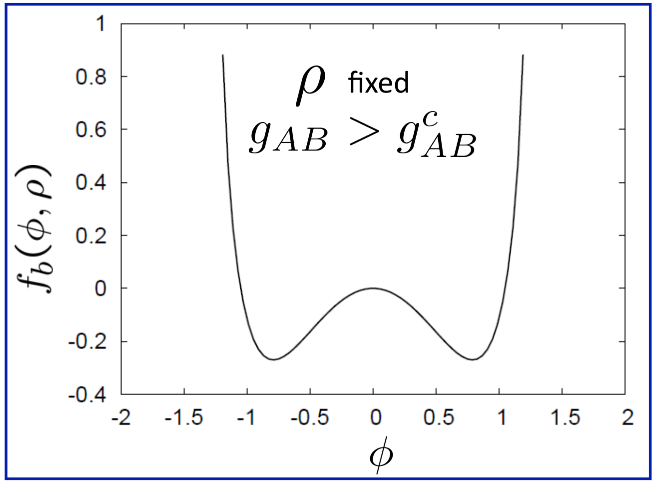
$$\rho = \rho_A + \rho_B$$

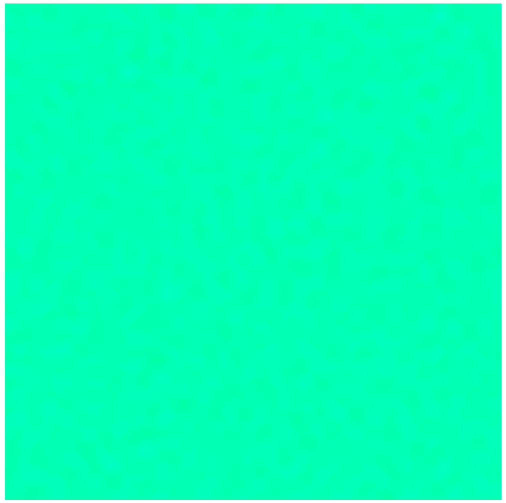
Total Density

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

Order Parameter

Double well structure





R. Benzi, *J. Chem. Phys.* **131**, 104903 (2009)

Fluctuating Multicomponent Lattice Boltzmann

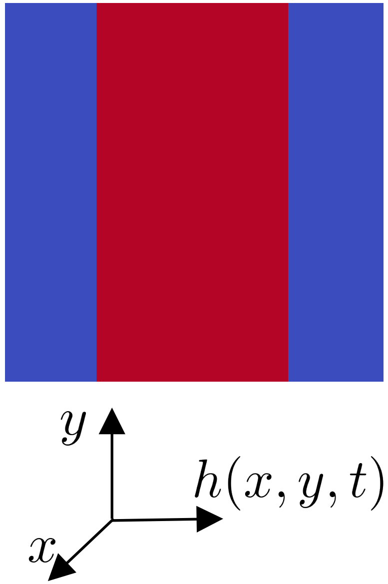
Fluctuating Multicomponent Lattice Boltzmann

$$n_i^\sigma(\vec{r}+\vec{c}_i, t+1) = n_i^\sigma(\vec{r}, t) + \Delta_i^\sigma + \Delta_{i,F}^\sigma + \hat{\Delta}_i^\sigma$$

$$\rho\left(\frac{\partial}{\partial t}\boldsymbol{u} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}\right) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot(\boldsymbol{\sigma}+\hat{\boldsymbol{\sigma}}) + \sum_\sigma \boldsymbol{g}_\sigma,$$

$$\frac{\partial}{\partial t}\rho_\sigma + \boldsymbol{\nabla}\cdot(\rho_\sigma\boldsymbol{u}) = \boldsymbol{\nabla}\cdot(\boldsymbol{d}_\sigma + \hat{\boldsymbol{d}}_\sigma)$$

Fluctuating (Stress/Flux)

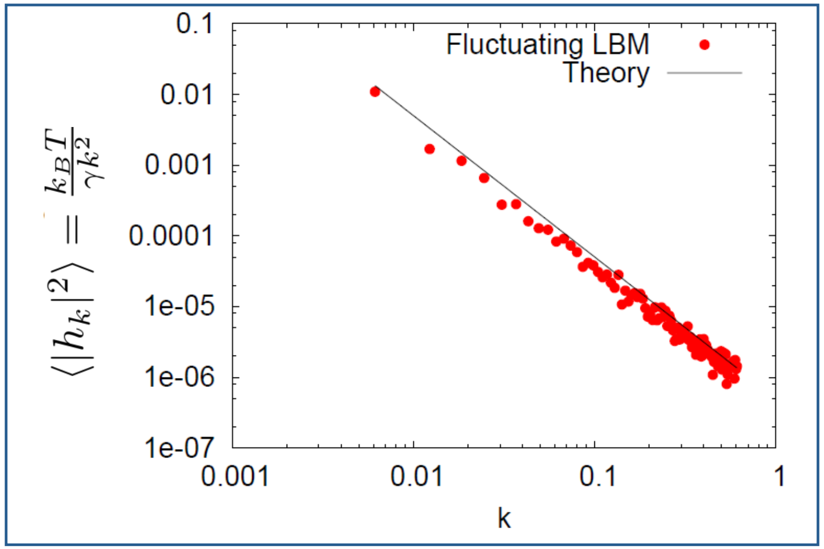


$$E = \gamma\int dxdy\left[\sqrt{1+|\nabla h|^2}-1\right]$$

$$\approx \frac{\gamma}{2}\int dxdy|\nabla h|^2 = \frac{\gamma}{2}\sum_k k^2|h_k|^2$$

Normal Modes Decomposition of Surface distortions

$$\langle|h_k|^2\rangle = \frac{kT}{\gamma k^2}$$



Fluctuating Multicomponent Lattice Boltzmann

$$n_i^\sigma(\vec{r}+\vec{c}_i, t+1) = n_i^\sigma(\vec{r}, t) + \Delta_i^\sigma + \Delta_{i,F}^\sigma + \hat{\Delta}_i^\sigma$$

How to Properly Formulate the Noise terms?

Perturbation around equilibrium state at rest

$$\rho^\sigma(\vec{r}, t) = \rho_0^\sigma(\vec{r}) + \delta\rho^\sigma(\vec{r}, t)$$

$$\vec{v}(\vec{r}, t) = \vec{0} + \delta\vec{v}(\vec{r}, t)$$

Mode decomposition of the fluctuations in the number density

$$\delta n_i^\sigma(\vec{r}, t) = n_i^\sigma(\vec{r}, t) - n_i^{\sigma, eq}(\rho_0^\sigma(\vec{r}), \vec{0}) \longrightarrow \delta m_a^\sigma(\vec{r}, t) = \sum_i e_{ai} \delta n_i^\sigma(\vec{r}, t)$$

$$\partial_t \delta\hat{m}_a^\sigma(\vec{k}, t) = \sum_{b,\zeta} \int d\vec{k}' \mathcal{L}_{ab}^{\sigma\zeta} \delta\hat{m}_b^\zeta(\vec{k}', t) + \hat{\zeta}_a^\sigma(\vec{k}, t)$$

Belardinelli et al., *Phys. Rev. E* **91**, 023313 *(2015)*

$$\partial_t a_i(t) = -\sum_j L_{ij} a_j(t) + \zeta_i(t)$$ Linear Langevin Equation !!!

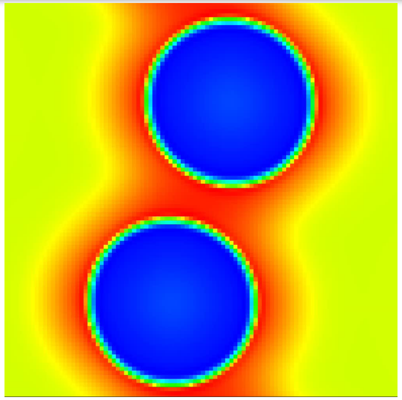
$$G_{ij} = \langle a_i a_j^* \rangle$$ Equilibrium Correlations (Entropy Matrix) ⟵ Input for the Theory

$$\langle \zeta_i(t) \zeta_j^*(t) \rangle = \sum_k (G_{ik} L_k^* + L_{ik} G_{kj})$$ ⟵ Fixed by FDT (Fluctuation Dissipation Theorem)

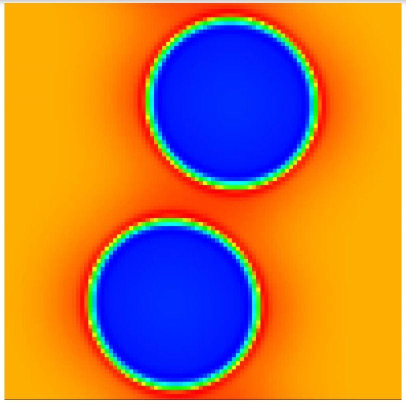
Modelling Soft-Glassy Materials

Frustration Mechanism at the interface

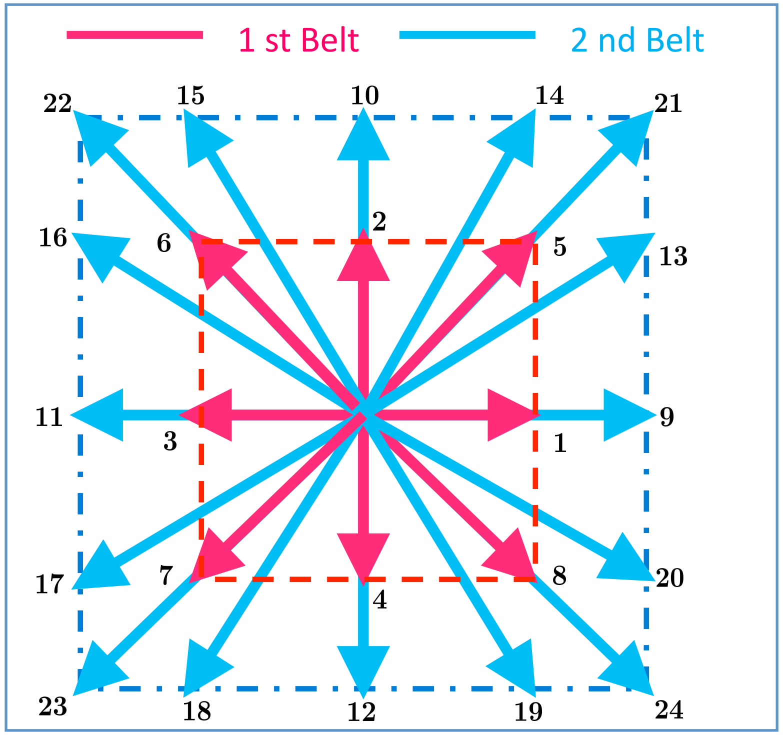
- ✓ "Simple" Lattice (competing) Interactions
- ✓ A variety of Rich Effects
- ✓ Control over these effects ?



Droplets Coalescence



Inhibition of Coalescence



Idea: Multirange Potentials NN & NNN

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

$$\psi(\vec{r}) = \psi[\rho(\vec{r})]$$ Pseudo-Potential

A Few Reference Works:

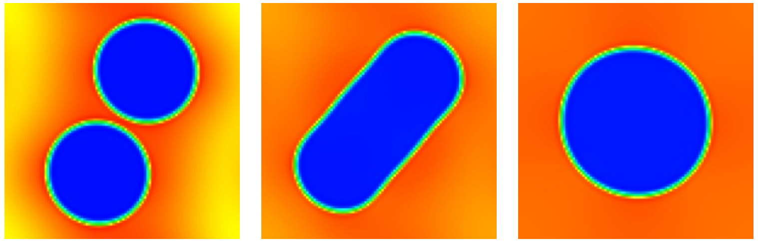
-R. Benzi et al, *J. Chem. Phys.* 131, 104903 (2009)

-R. Benzi et al, *Europhys. Lett*. 91, 14003 (2010)

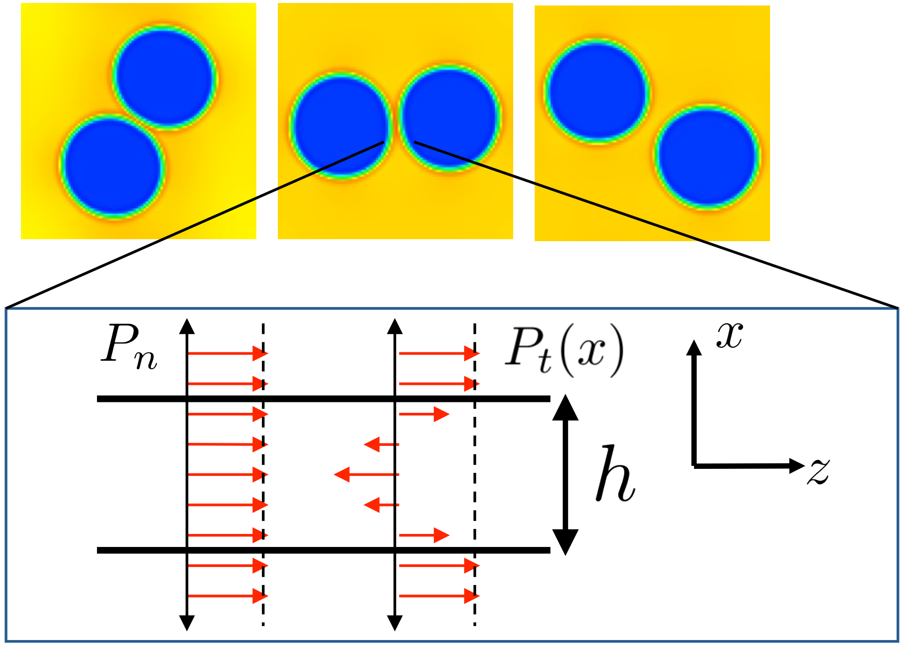
-M. Sbragaglia et al, *Soft Matter* 8, 10773-10782 (2012)

Modelling of Disjoining Pressure

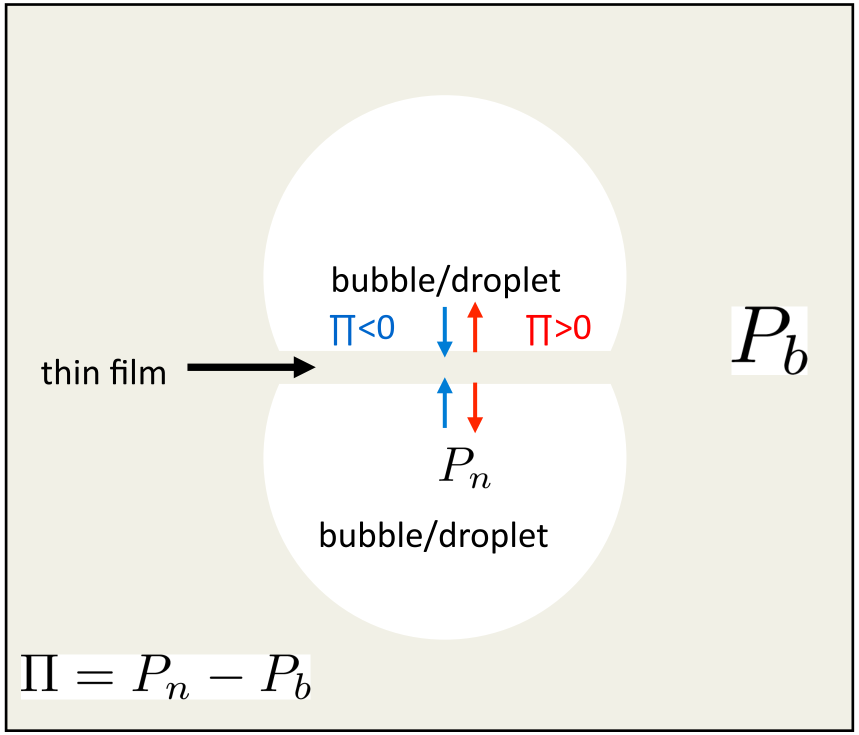
Droplets Coalescence



No Coalescence...why?

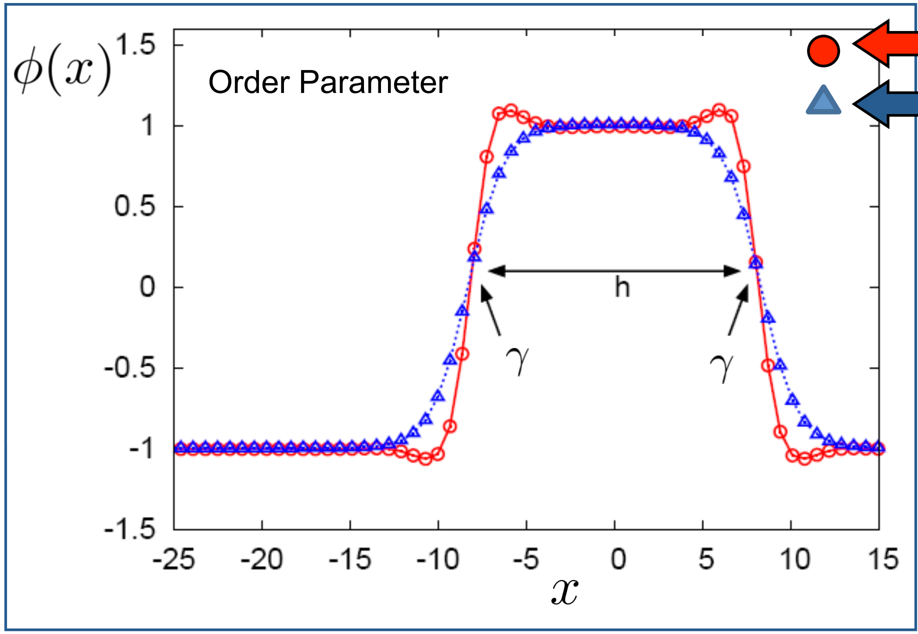


Derjaguin & Churaev, J. Colloid. Interface Sci. 66, 389 (1978)



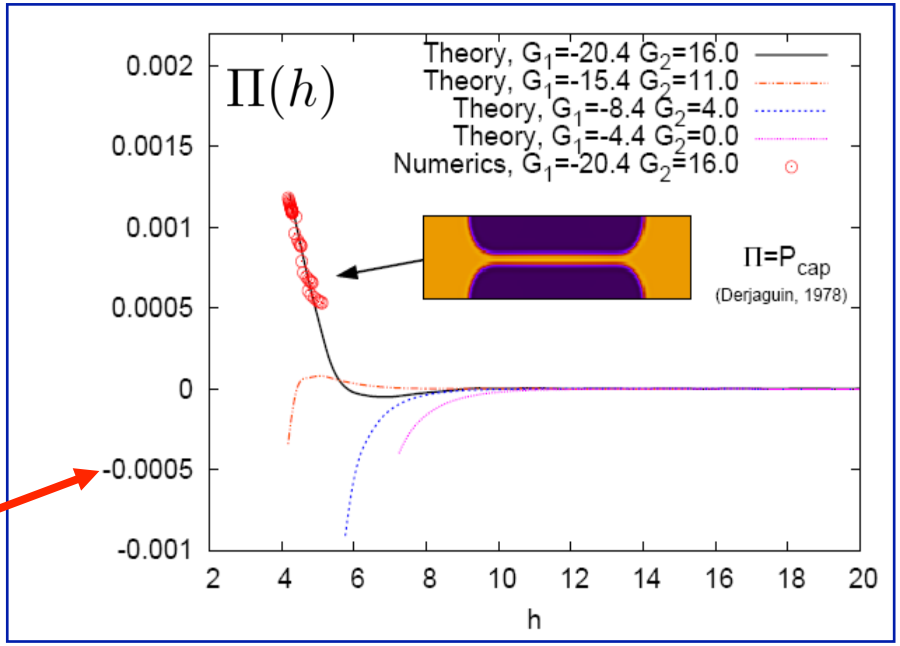
.....Because you have a Positive disjoining pressure

Disjoining Pressure From Lattice Kinetic models



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

(bare NN) $\mathcal{G}_1 < 0; \mathcal{G}_2 = 0$



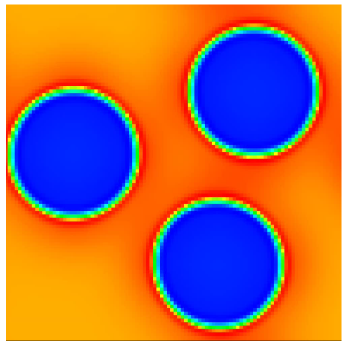
$$\gamma_f = 2\gamma + \int_{\Pi(h=\infty)}^{\Pi(h)} h \, d\Pi$$

Disjoining Pressure definition based on 'film tension'

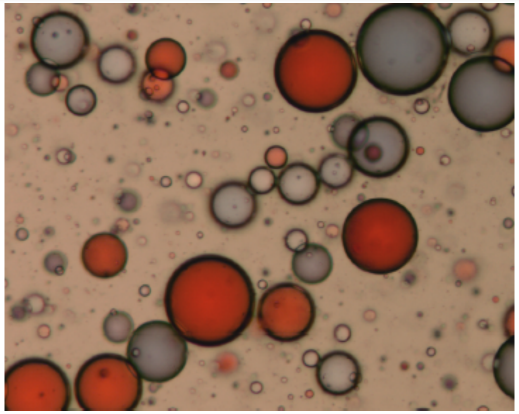
Exactly computed on the lattice

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

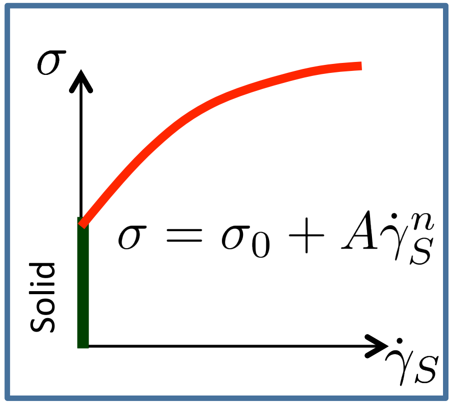
Analytical with the exact pressure tensor
(differential equation-> Profile)



Rheology of Soft Glassy "Materials"



Oil in water Emulsion

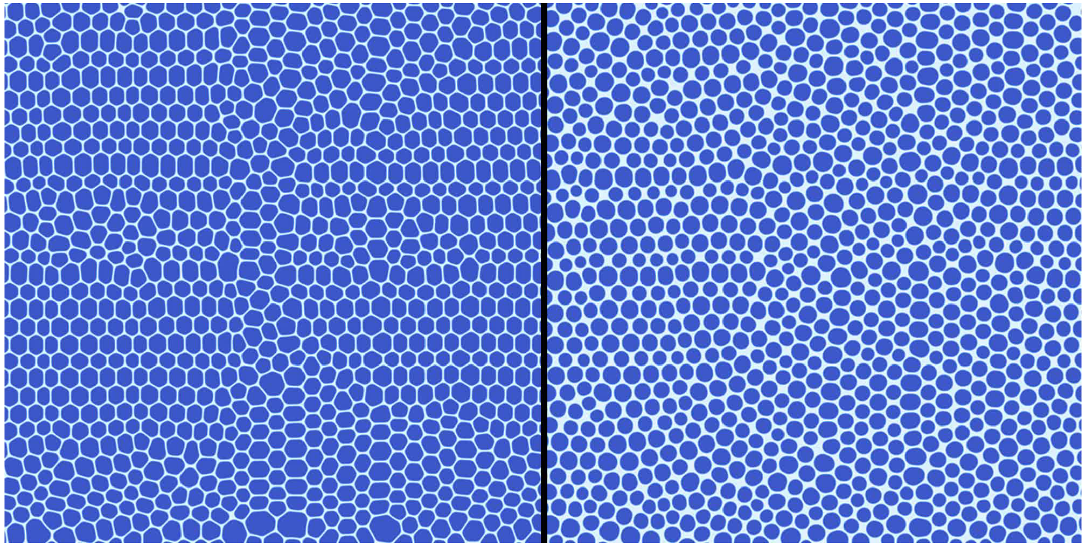


Herschel-Bulkley Model

✓Yield Stress (Solid below)

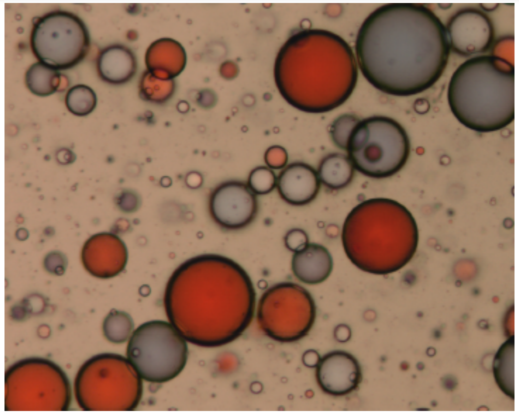
✓Non-Newtonian (above yield Stress)

✓Effect of Confinement (Cooperativity Effects)

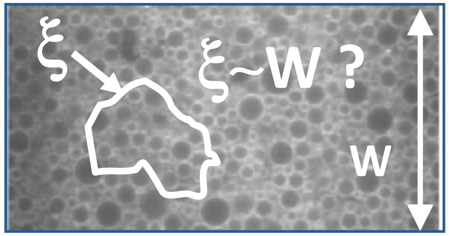


High Packing Fraction | Lower Packing Fraction

Rheology of Soft Glassy “Materials”



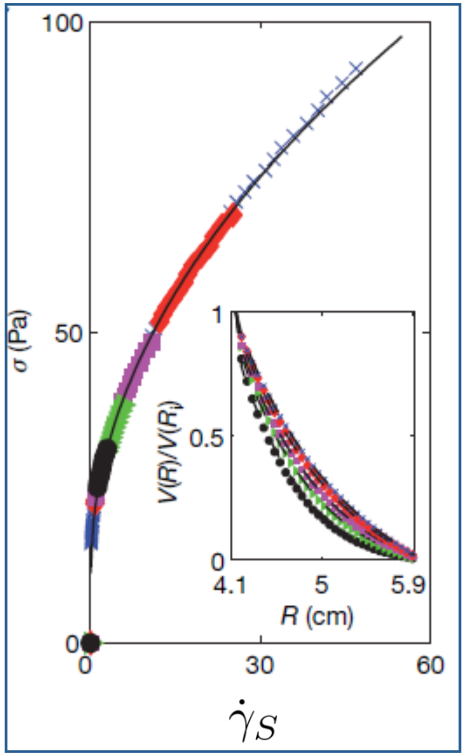
Oil in water Emulsion

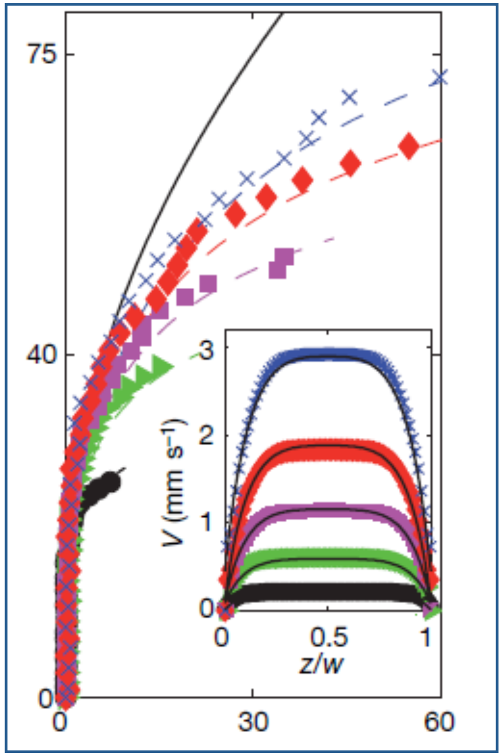


✓Yield Stress (Solid below)

✓Non-Newtonian (above yield Stress)

✓Effect of Confinement (Cooperativity Effects)





$W/\xi \gg 1$

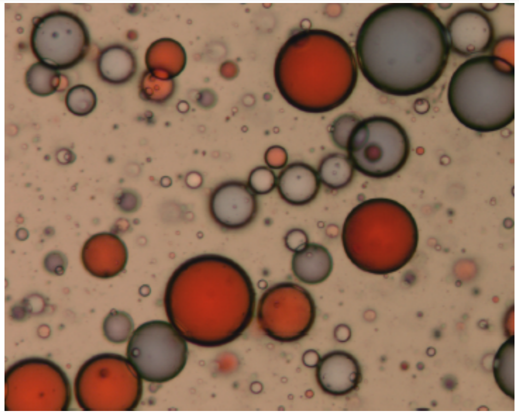
cooperativity does not matter

$W/\xi \sim 1$

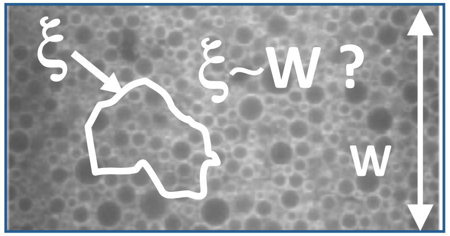
cooperativity matters

Goyon et al, Nature (**2008**)

Rheology of Soft Glassy "Materials"



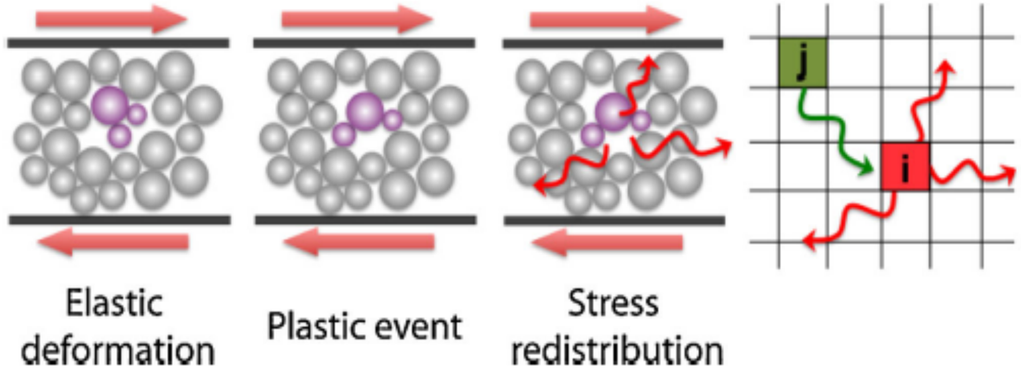
Oil in water Emulsion



✓Yield Stress (Solid below)

✓Non-Newtonian (above yield Stress)

✓Effect of Confinement (Cooperativity Effects)



$$f = \frac{\dot{\gamma}_S}{\sigma}$$

Fluidity

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

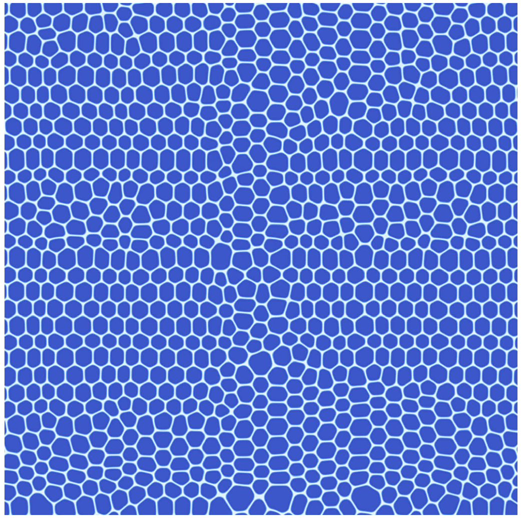
Diffusion equation for the Fluidity

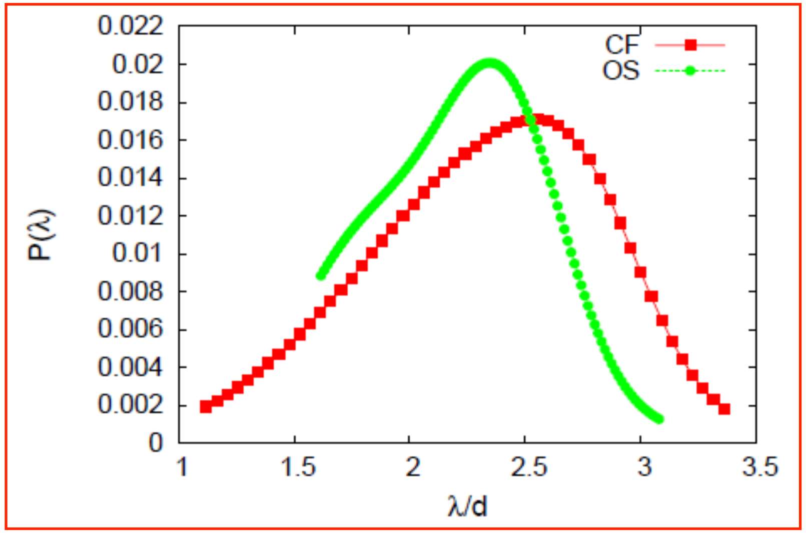
$$f_b = f_b(\sigma(\boldsymbol{x}))$$

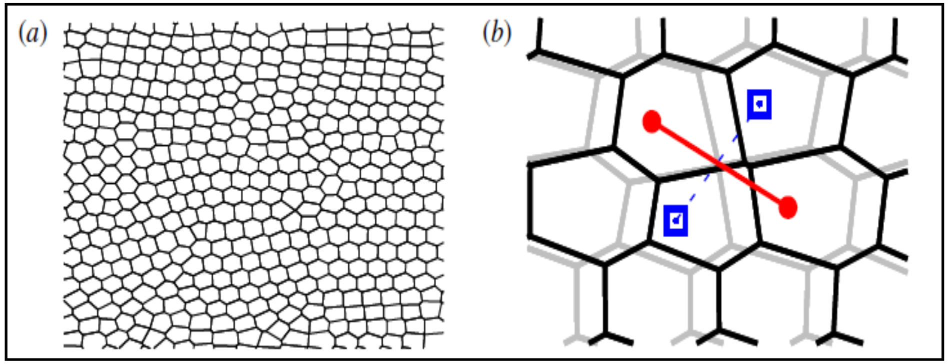
"Bulk" Fluidity

Plastic Events: LBM with Different Load Conditions

Oscillating Strain (OS) Boundary Conditions







Dollet, Scagliarini & Sbragaglia, Jour. Fluid. Mech **776**, 556 (2015)

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

Conclusions

✓**Lattice Boltzmann:**

✓ Direct Link with Hydrodynamics (Chapman Enskog)

✓Easy Handling of Boundary Conditions

✓Flexibility in modelling Non-Ideal interactions (Shan-Chen, Free-Energy, Lee-Fisher, Color Models, approaches)

✓Solid Background (at least Single-Phase with/without Thermal Fluctuations …see Shan et al. *Jour. Fluid. Mech.* (2006);Dunweg, Shiller, Ladd, *Phys. Rev. E* (2007))

✓**Useful in Revealing Interesting Physics of Complex Fluid Dynamics problem…and Beyond:**

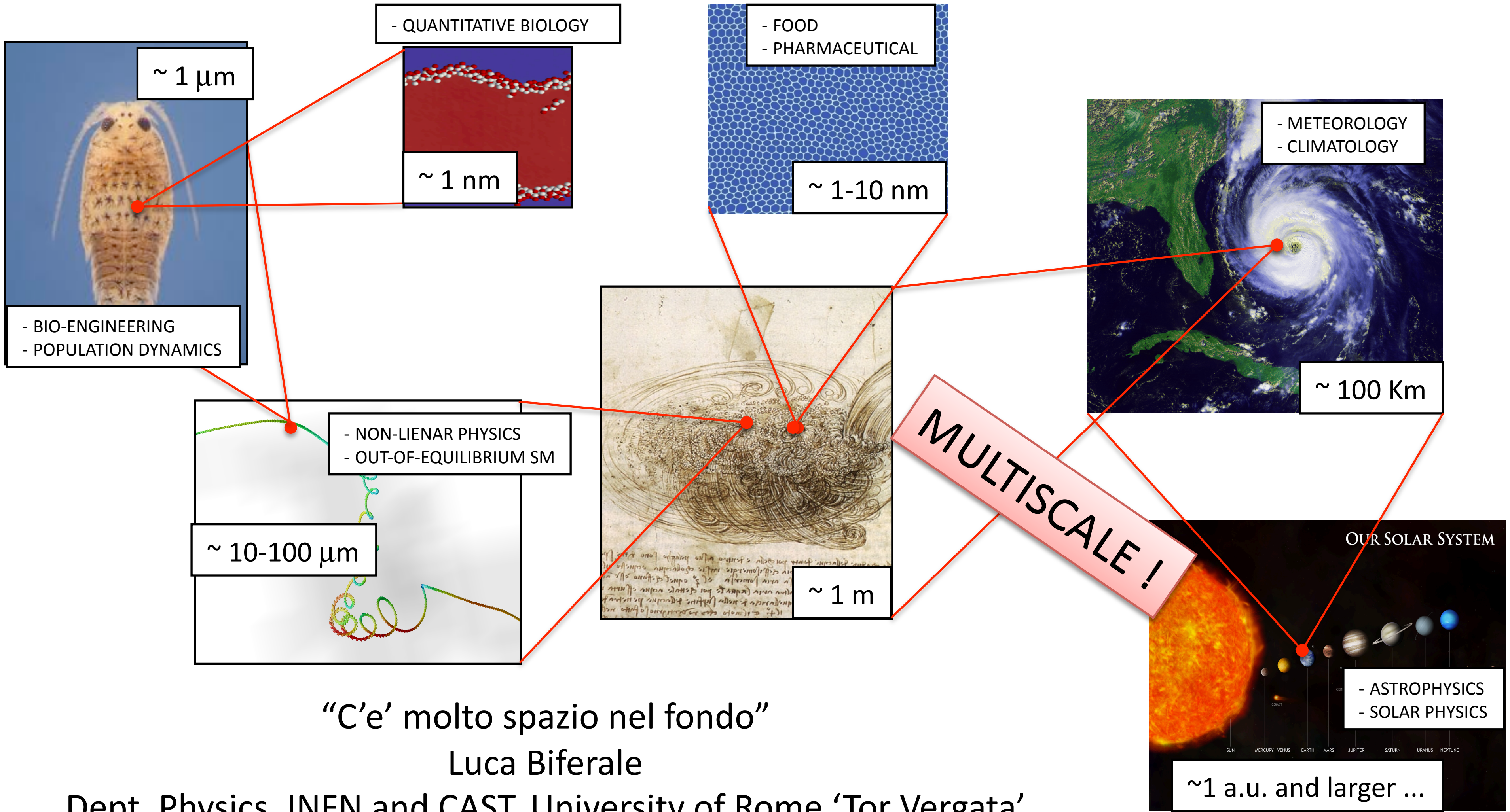
✓Microfluidics Droplets (Surface tension, wettaibility Gradients, strong Confinement, Boundary Conditions, etc etc)

✓Soft-Glassy Rheology (Onset of Motion, Fluidity, Spatial Stress Correlations, etc etc)

✓Coupling with Atomistic Scales (Fluctuating Hydrodynamics)

Παντα ρει

inside, outside, above, below and around us



"C'e' molto spazio nel fondo"

Luca Biferale
Dept. Physics, INFN and CAST, University of Rome 'Tor Vergata'

A simple (textbook) example on how to set Noise

Motion of particle with mass m in a fluid: **total Force** due to the **other particles** in the fluid

$$m\frac{dv(t)}{dt} = F_{tot}(t) \approx -\zeta v(t)$$

Dominated by Friction: Is this the whole Story ?

$$v(t) = e^{-\zeta t/m} v(0) \to 0 \qquad (t \to \infty)$$

$$\langle v^2 \rangle_{eq} \neq \frac{kT}{m}$$

Mean Squared Velocity at equilibrium (t >>0) is not reproduced !! **Modify above picture !!**

Observed Randomness in the individual trajectory: **add Random Force**

$$m\frac{dv(t)}{dt} = F_{tot}(t) = -\zeta v(t) + \delta F(t)$$

Langevin Equation fot Brownian Particle

$$\langle \delta F(t) \rangle = 0 \qquad \langle \delta F(t) \delta F(t') \rangle = 2B\delta(t - t')$$

More commonly presented view

Both **Friction** and **Random Force** come from the bath: **Any fundamental relation ?**

$$\langle v^2(t) \rangle = e^{-2\zeta t/m} v^2(0) + \frac{B}{\zeta m}\left(1 - e^{-2\zeta t/m}\right)$$

$$\langle v^2(t) \rangle \to \langle v^2(t) \rangle_{eq} = \frac{kT}{m} \qquad (t \to \infty)$$

$$\boxed{B = \zeta kT}$$

Fluctuation Dissipation Relation

Where to Sit Across the scales?


MACROSCOPIC

(NAVIER-STOKES)

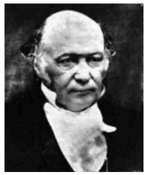
$$\vec{\nabla} \cdot \vec{u} = 0$$

$$\rho D_t \vec{u} = -\vec{\nabla} p + \eta \Delta \vec{u}$$

....

✓Can we explore “Complex Hydrodynamics“ with **Capillarity Phenomena** via a **Coarse grained** description?

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



MICROSCOPIC

(MOLECULAR DYNAMICS)

$$\mathcal{H} = \sum_k \frac{p_k^2}{2m} + \sum_{i,k} V_{i,k}$$

$$\dot{q}_k = \frac{\partial \mathcal{H}}{\partial p_k} \qquad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k}$$