UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

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DOTTORATO IN FISICA XXXII CICLO
Dipartimento di Fisica ''Michelangelo Merlin''

Dynamics of complex and active fluids

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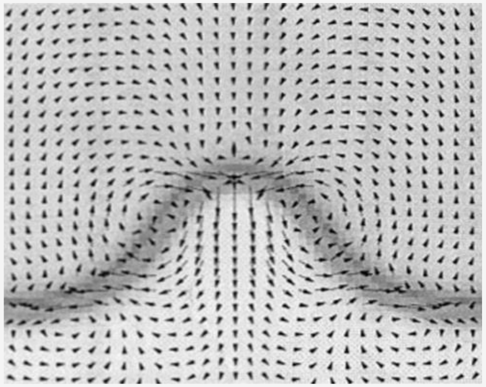
Summary

- Complex and active fluids
- Dynamical model
- Lattice Boltzmann Method
- Activities

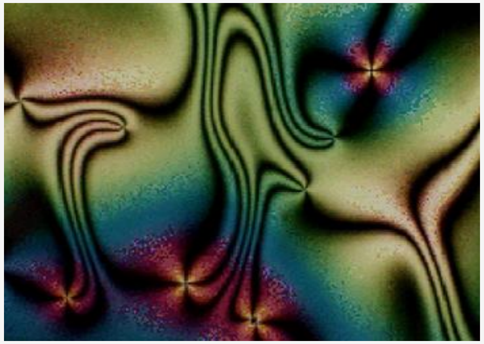
Complex fluids

with focus on the coupling between the velocity field and the defects dynamics.
Examples:



- **Binary mixture**

  velocity fields of different intensity
  and directions at interfaces



- **Liquid crystals**

  coupling between velocity field and
  orientation

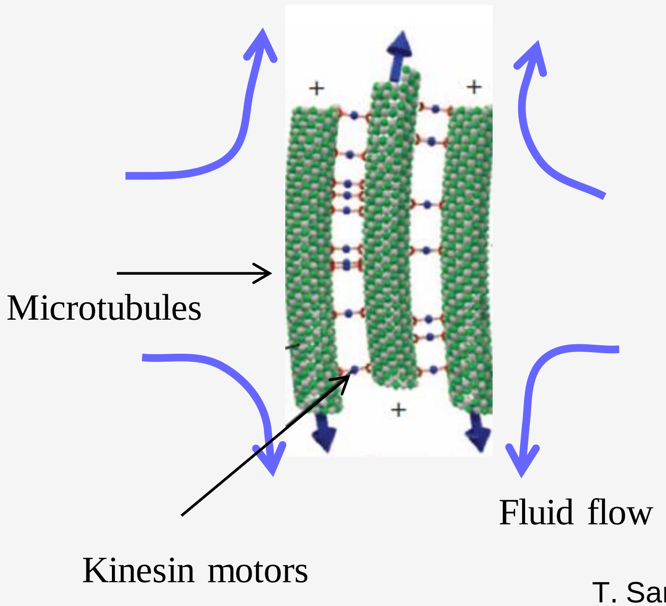
Every defect has a topological charge ⟶ flows of different intensity
(G. Toth, C. Denniston, and J. M. Yeomans, “Hydrodynamics of Topological Defects in Nematic Liquid Crystals”, Phys. Rev. Lett. 88, 105504 (2002).)

Active systems

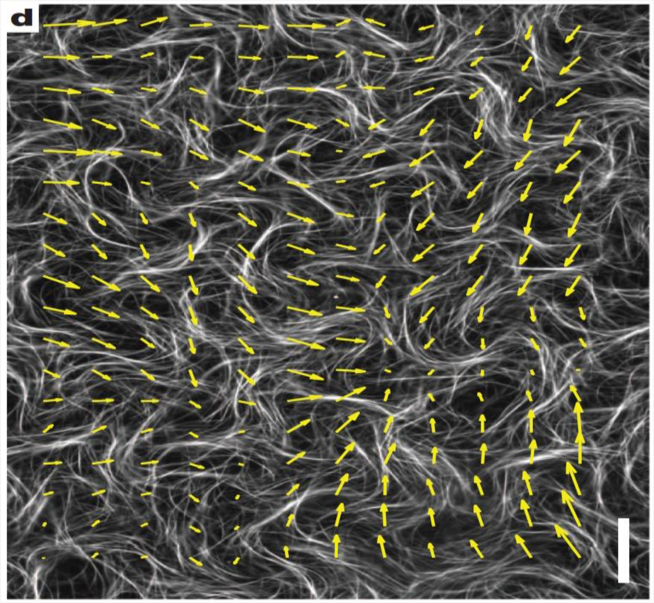
Active matter are self-driven systems which live, or function, far from equilibrium.

- **Interplay between interaction and activity**
- **High level of collective organization**

Extensile/pusher swimmer



Active microtubule network

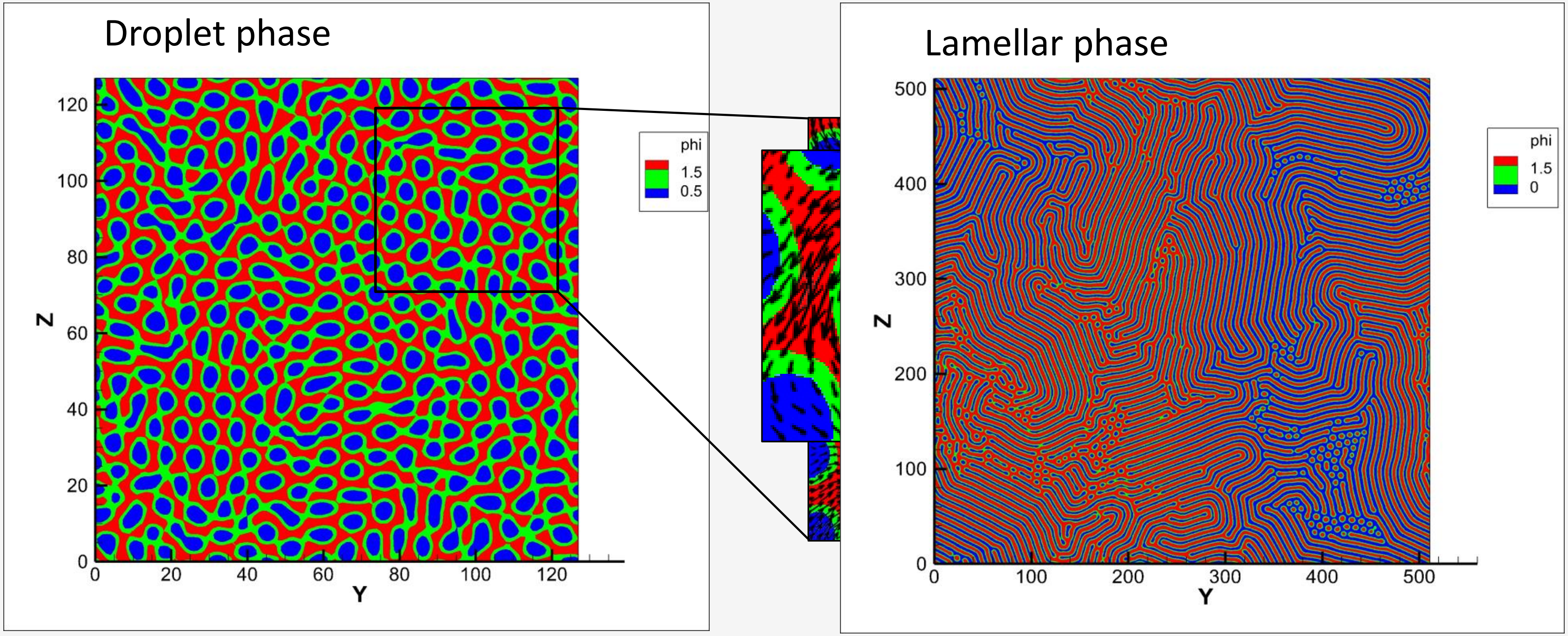


T. Sanchez et al., Nature, 491, 431 (2012)

A new class of complex fluids:
mixtures of active and passive components

Examples:

- Active droplets(M Blow et al.,PRL 2014)
- Exotic emulsions(Gonnella, Tiribocchi, Bonelli, Orlandini, in



Dynamical model

Free energy based model (Ginzburg-Landau)

$$\mathcal{F} = \int dV \left(\frac{a}{2}\phi^2 + \frac{b}{2}\phi^4 + \frac{K}{2} |\nabla\phi|^2 \right)$$

K linked to surface tension $\tilde{\sigma} = \int dy \left(\frac{K}{2} \left(\frac{\partial\phi}{\partial y} \right)^2 + \psi(\phi, T) - \psi_{\pm}(\phi, \mathrm{T}) \right)$

$\psi(\phi, T)$ free energy density

$$\mu = \frac{\delta\mathcal{F}}{\delta\phi} = a\phi + b\phi^3 - K\nabla^2\phi$$

$$\Pi_{\alpha\beta} = \left\{ \rho\frac{\delta\mathcal{F}}{\delta\rho} + \phi\frac{\delta\mathcal{F}}{\delta\phi} - \psi(\rho, \phi, T) \right\} \delta_{\alpha\beta} + D_{\alpha\beta}(\phi)$$

Dynamical model

η dynamic viscosity
ξ second viscosity coefficient

Continuity equation $\partial_t \rho = -\partial_\alpha(\rho\, u_\alpha)$

Navier-Stokes $\partial_t(\rho u_\alpha) + \partial_\beta\left(\rho u_\alpha u_\beta\right) = -\partial_\beta(\Pi_{\alpha\beta} - \sigma_{\alpha\beta})$

Viscous stress tensor
$$\sigma_{\alpha\beta} = \eta\left(\partial_\alpha u_\beta + \partial_\alpha u_\beta - \frac{2\delta_{\alpha\beta}}{d}\right) + \xi\delta_{\alpha\beta}\partial_\gamma u_\gamma$$
$$+\zeta\ (P_\alpha P_\beta - \frac{1}{3}P^2\delta_{\alpha\beta})$$

Convection-diffusion $\partial_t\phi + \partial_\alpha(\phi\, u_\alpha) = -2\partial_\alpha\, J_\alpha^d$

For liquid crystals
- Tensorial order parameter

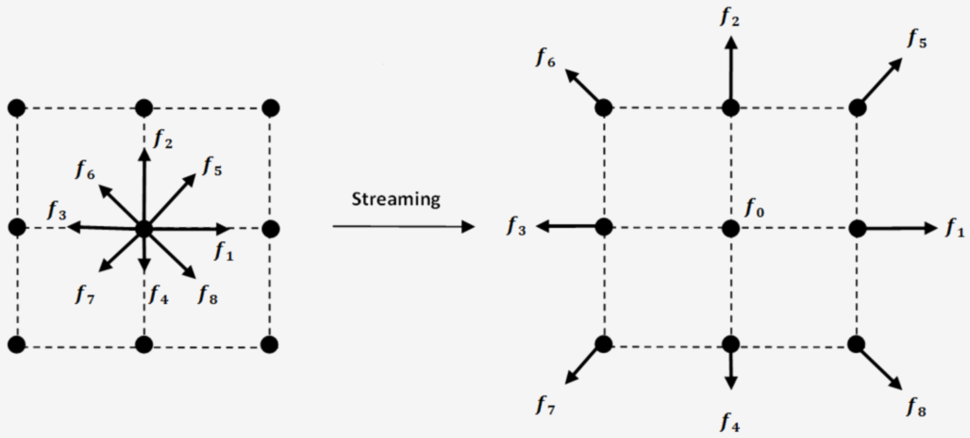
For active fluids
- Active stress tensor
  Ramaswamy et al PRL (2004)

Lattice Boltzmann methods

Boltzmann transport equation

$$\frac{\partial f(\vec{x},t)}{\partial t} + \vec{u} \cdot \nabla f(\vec{x},t) = \Omega$$

''be wise, discretize!'' $$f_i(\vec{x} + c\,\vec{e_i}\Delta t, t + \Delta t) - f_i(\vec{x},t) = -\Delta t \frac{[\, f_i(\vec{x},t) - f_i^{eq}(\vec{x},t\,)]}{\tau}$$



Lattice Boltzmann methods

$$\rho(\vec{x},t) = \sum_{i=0}^{8} f_i(\vec{x}\,,t) \qquad \vec{u}(\vec{x},t) = \frac{1}{8}\sum_{i=0}^{8} c\, f_i(\vec{x}\,,t)\,\vec{e_i}$$

The algorithm can be summarized as follows

1. Initialize $\rho, \vec{u}, f_i$ and f_i^{eq}
2. Streaming step: move $f_i \rightarrow f_i^*$ in the direction of $\vec{e_i}$
3. Compute macroscopic ρ and $\vec{u}$ from f_i^*
4. Compute f_i^{eq} in BGK approximation
5. Collision step: calculate the update distribution $f_i = f_i^* - \frac{1}{\tau}(f_i^* - f_i^{eq})$
6. Repeat from step 2.

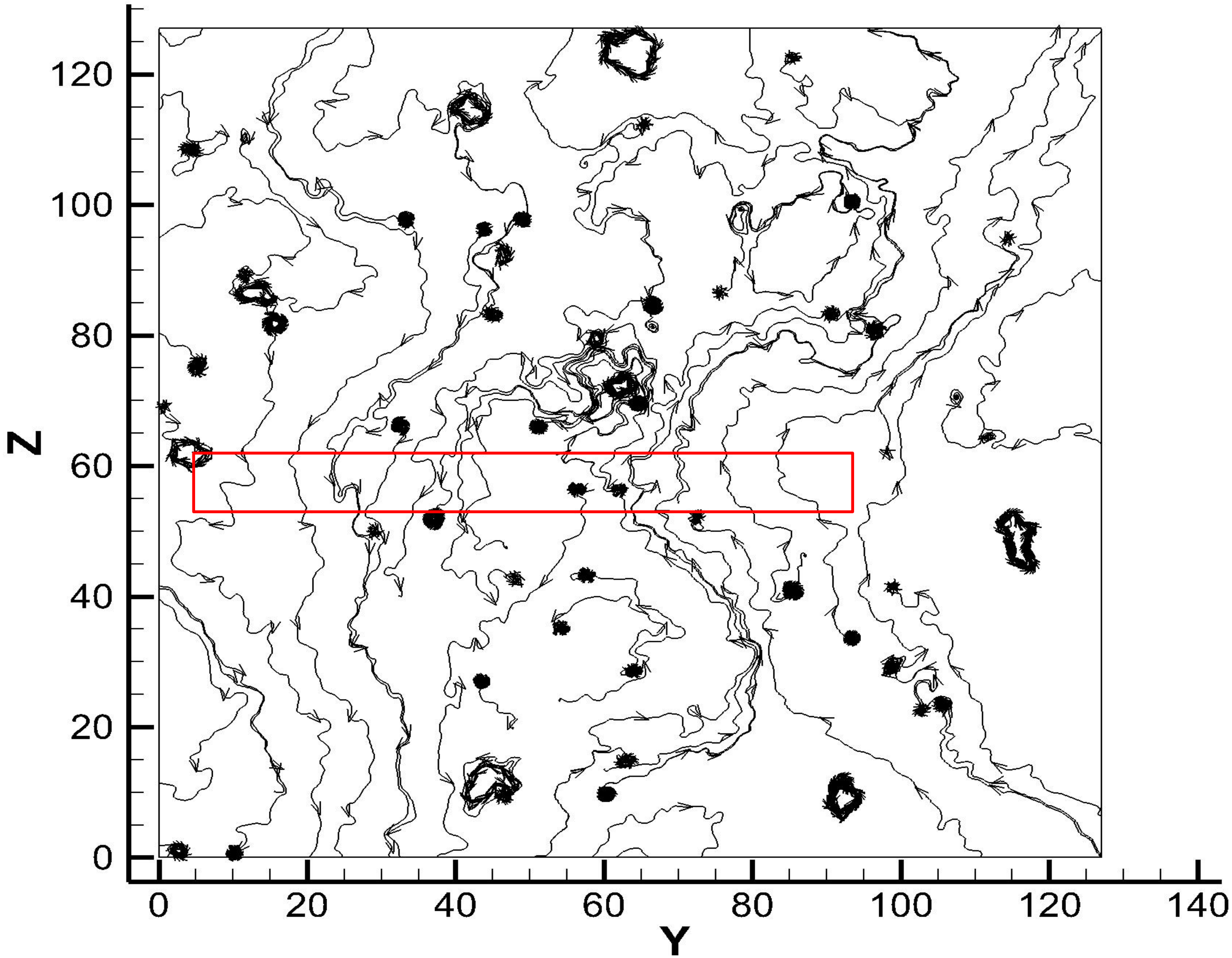
In the continuum limit it is possible to derive Navier-Stokes equations from LBE

Activities

- **Extend previous work on single component systems with phase transition**
  - Extend recent work[1] on liquid-vapor systems
    to systems of real dimensionality
  - Parallelization
  - Calculation of domain growth exponents in phase separation dynamics
  - Study of the Rayleigh-Plesset equation in d=3

- **Mixtures of active and passive fluids (2d)**
  - Characterization of different phases and dynamics of
    transition
  - Response to external flows

[1]Pattern formation in liquid-vapor systems under periodic potential and shear
A Coclite, G Gonnella, A Lamura - Physical Review E, 2014



Z
Y
0
20
40
60
80
100
120
140