Confined active fluids: morphology, topological defects and flow behaviors

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Tutor: Prof. Giuseppe Gonnella, Dr. Antonio Lamura

Summary

Field theory approach for the numerical study of **complex fluids** and **out-of-equilibrium** systems through a continuum approach.

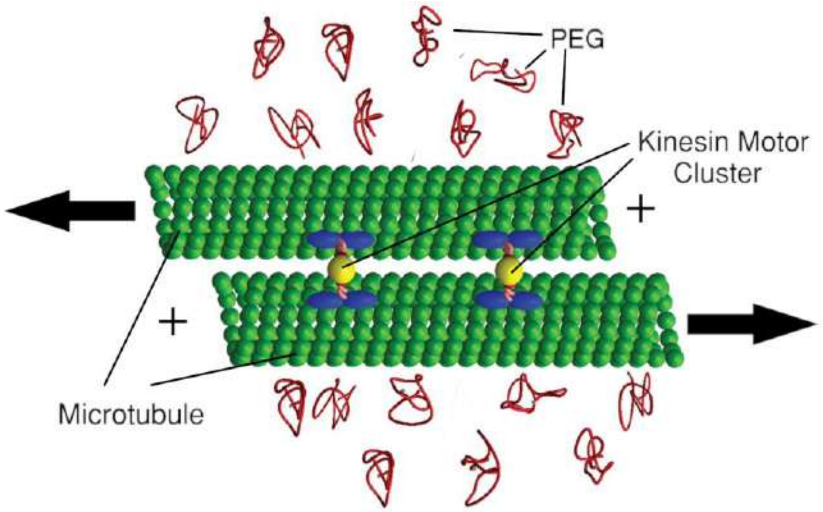
$$\partial_t \mathbf{P} + \mathbf{v} \cdot \nabla \mathbf{P} + \Omega \cdot \mathbf{P} = \xi D \cdot \mathbf{P} - \Gamma \mathbf{h}$$

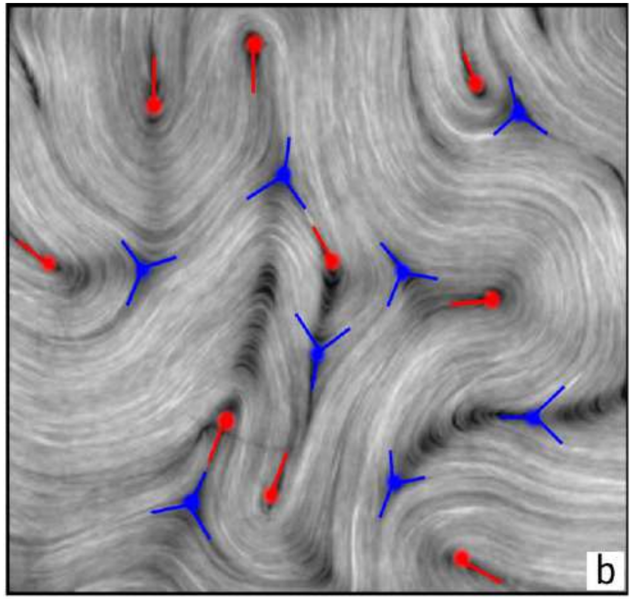
$$\partial_t \phi + \mathbf{v} \cdot \nabla \phi = -D \nabla^2 \mu$$

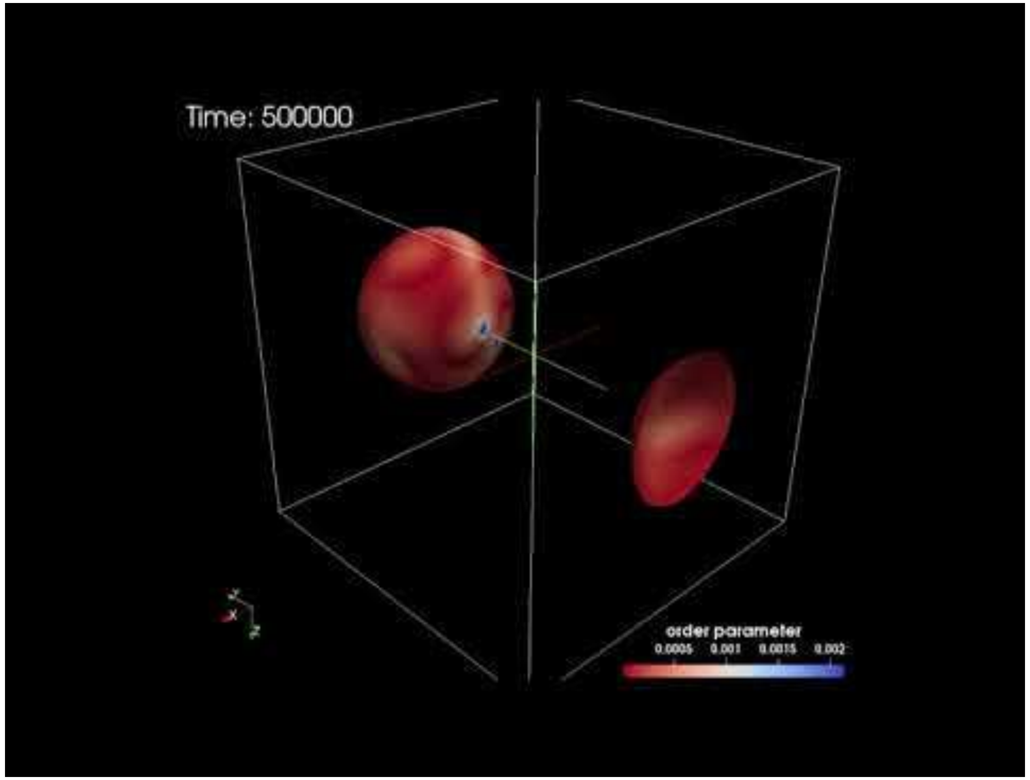
$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \boxed{\nabla \cdot \sigma}$$

<u>In this presentation</u>

- Motivation of the study
- Overview on the research activity
- Characterization of the rheological behavior of some complex fluids
- Conclusions







L. Carenza, G. Gonnella, D. Marenduzzo, and G. Negro, "Rotation and propulsion in 3d active chiral droplets," **Proc. Natl. Acad. Sci.**, vol. 116, no. 44, pp. 22065–22070, 2019.

Self-assembled and bio-inspired materials

- **Self propelled constituents**
- **Self-driven ordering**
- **Local self-sustained flows**
- **Intrinsically non-equilibrium systems**

Topics

Complex Fluids and Liquid Crystals:

- Topology of LC
- Soft Confinement
- Mirror symmetry breaking
- Blue Phases
- Rheology

Active and Biological Matter:

- Self-Motility in Active Droplets
- Morphology of active emulsions
- Negative viscosity sates in active fluids

Turbulence at low Reynolds number

- Spectral analysis of energy transfer in complex fluids

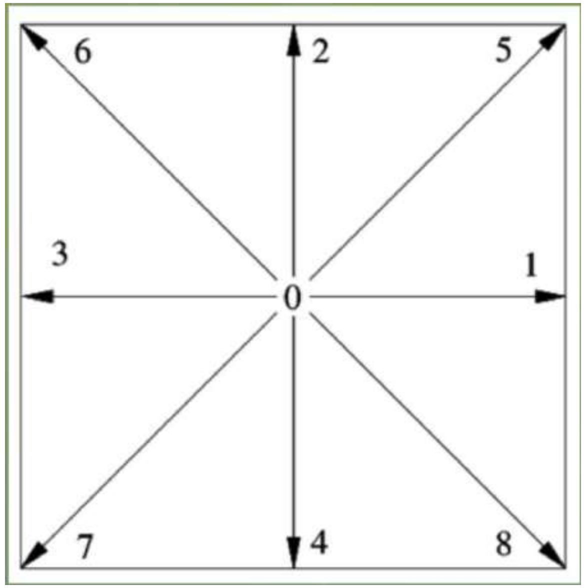
Numerical Schemes for simulations: Lattice Boltzmann and High Performance Computing

Lattice Boltzmann Method

LBMs are a class of computational methods based on a discretized version of the Boltzmann equation.

- Physical space and velocity space are both discretized

$$(\partial_t + \vec{v}\cdot\nabla)f + (\vec{F}\cdot\nabla_v)f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$



D2Q9

$$c = \frac{\Delta x}{\Delta t}$$

Fluid particles can only move in definite directions in space.
Distribution functions are defined on the the descrete lattice on grid points and along lattice velocities.

Assuming the system close to equilibrium the collision operator can be expandend in terms of an equilibrium set of distribution functions:

$$f_i(\vec{x}+\vec{e}_i\Delta t, t+\Delta t) - f_i(\vec{x},t) = -\frac{1}{\tau}(f_i - f_i^{eq})$$

The hydrodynamic limit can be restored in the continuum limit by requiring that the following conditions hold

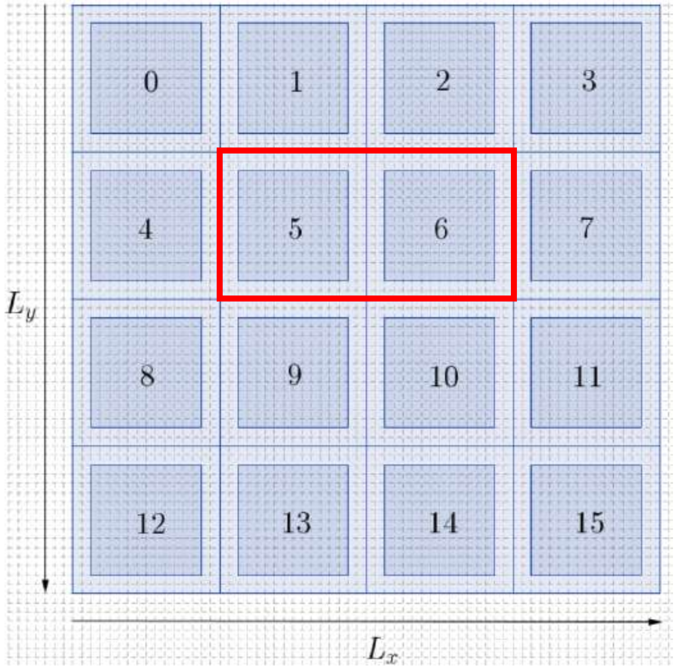
$$\rho = \sum_i f_i \qquad \rho\vec{v} = \sum_i f_i\vec{e}_i \qquad \rho v_\alpha v_\beta + \sigma_{\alpha\beta} = \sum_i f_i^{eq} e_{i,\alpha} e_{i,\beta}$$

In this scope viscosity arises directly from discretization effects $\nu = c^2\Delta t\frac{2\tau - 1}{6}$

High Performance Computing for LBM

Numerical implementation of LBM must face some computational issues:

- <u>Memory resources</u>
- <u>Long processing times</u> (the typical amount of time required to perform 10E7 LB iterations on a squared 256 grid with a C code ~200h of CPU time using proc. Intel® Core™ i7)

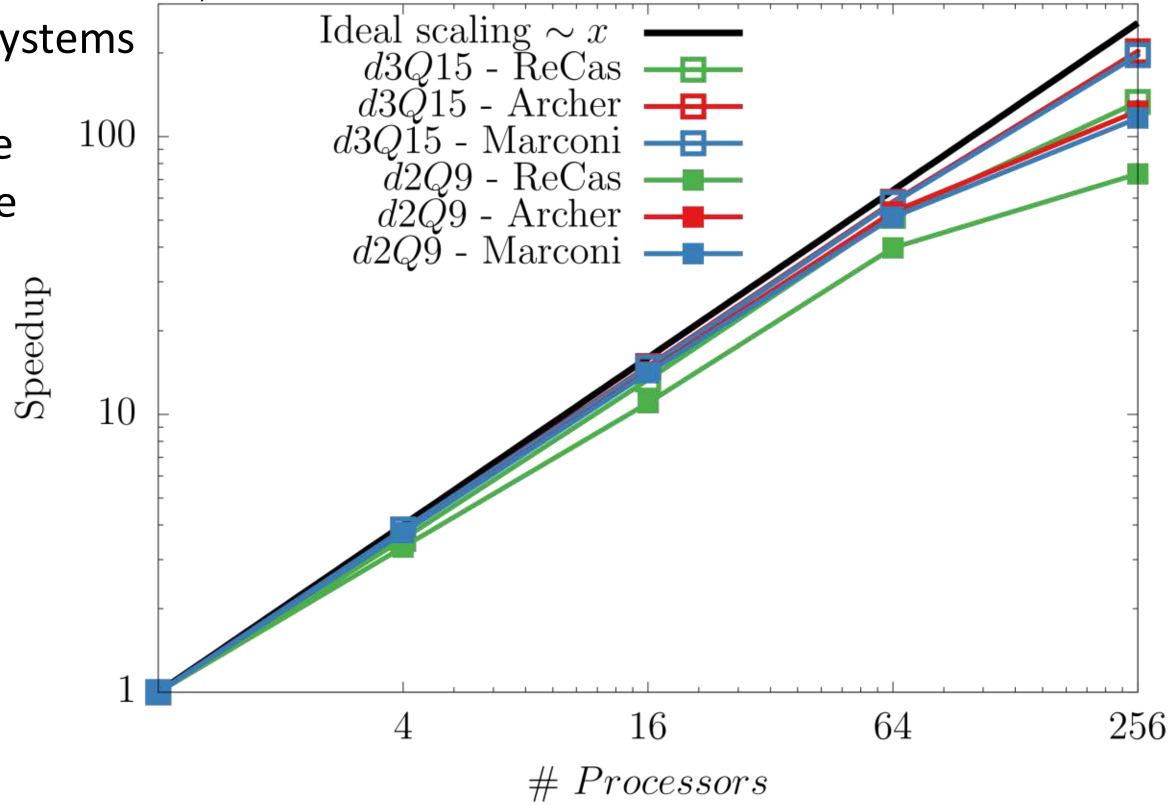


"Be wise... parallelize!"

- MPI protocol
- Distributed memory systems

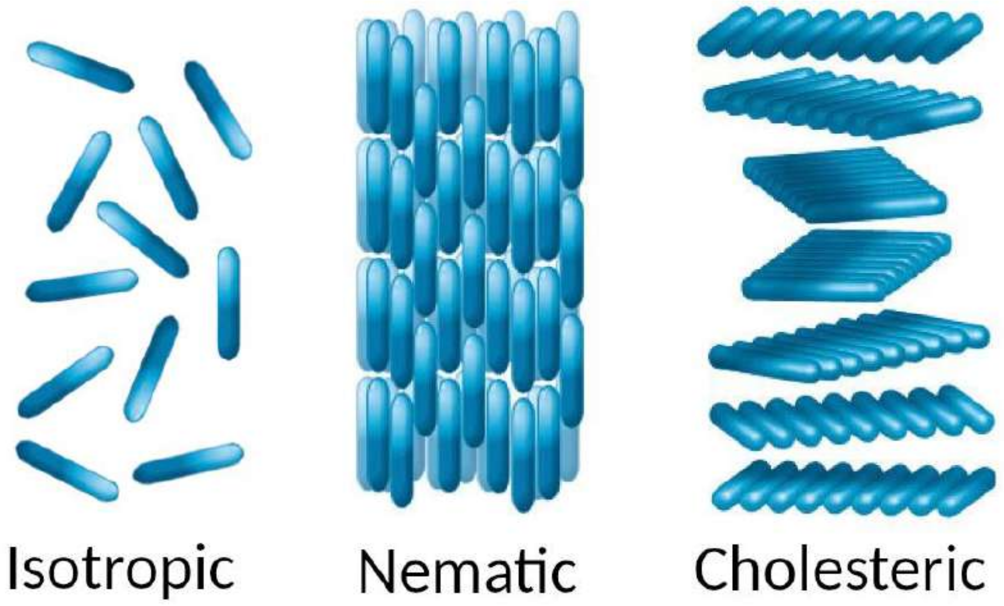
Ghost cell method can be implemented to solve the problem of derivative computation on the boundaries.

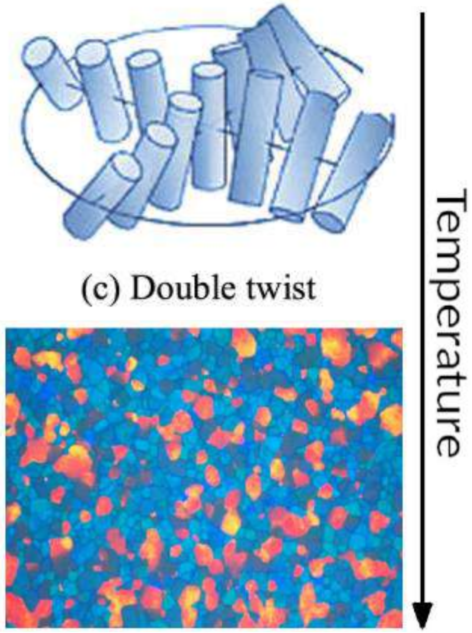
L. Carenza, G. Gonnella, A. Lamura, G. Negro, and A. Tiribocchi, "Lattice boltzmann methods and active fluids," **Eur. Phys. J. E**, vol. 42, no. 6, p. 81, 2019.

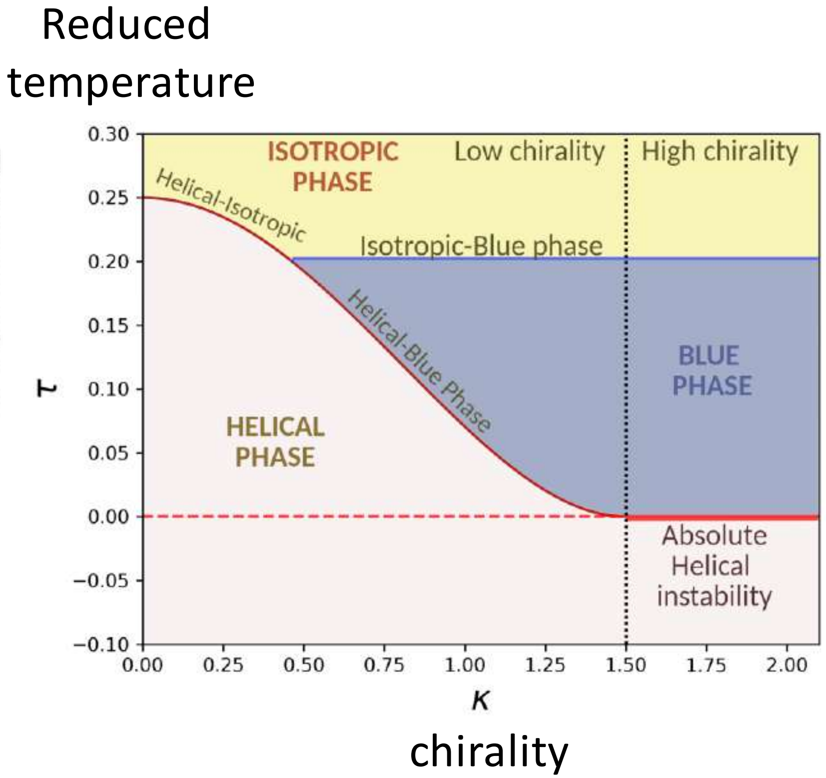


Liquid Crystals

- LC are a phase of matter with properties in the middle between solids and liquid
- LC flows as fluids do as the molecule center of masses are disordered
- LC molecules preserve orientational order







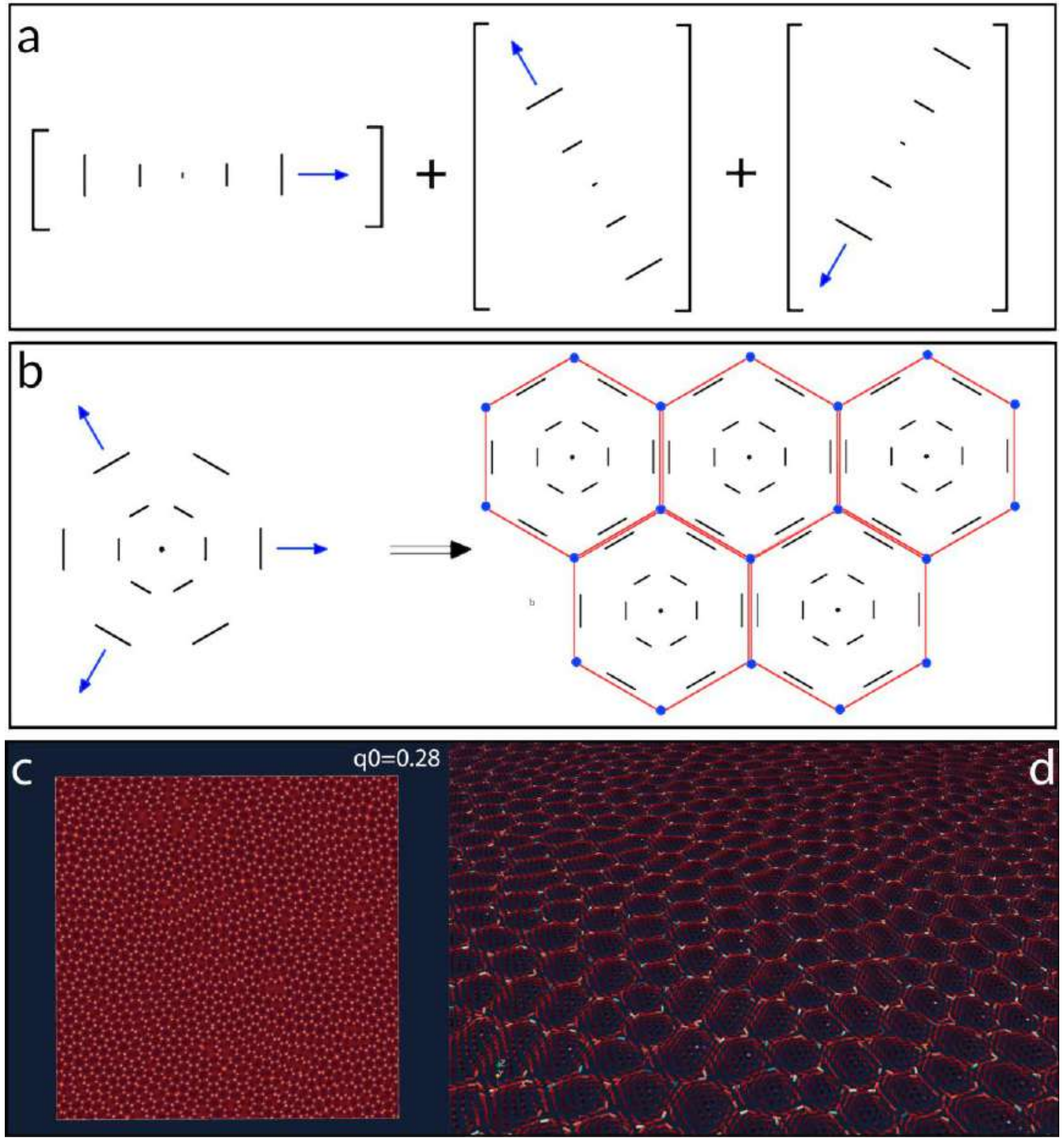
Chiral Liquid Crystals and Blue Phases

$$\mathcal{F} = \mathcal{F}^{bulk} + \mathcal{F}^{el}$$
$$\mathcal{F}^{bulk} = a\mathbf{Q}^2 - \sqrt{6}b\mathbf{Q}^3 + c\mathbf{Q}^4$$
$$\mathcal{F}^{el} = \frac{L}{2}\left[(\nabla\cdot\mathbf{Q})^2 + [\nabla\times\mathbf{Q} + 2q_0\mathbf{Q}]^2\right]$$

$$\mathbf{Q_k} = \sum_S \phi^S_{\mathbf{k}}\sigma^S_{\mathbf{k}}$$

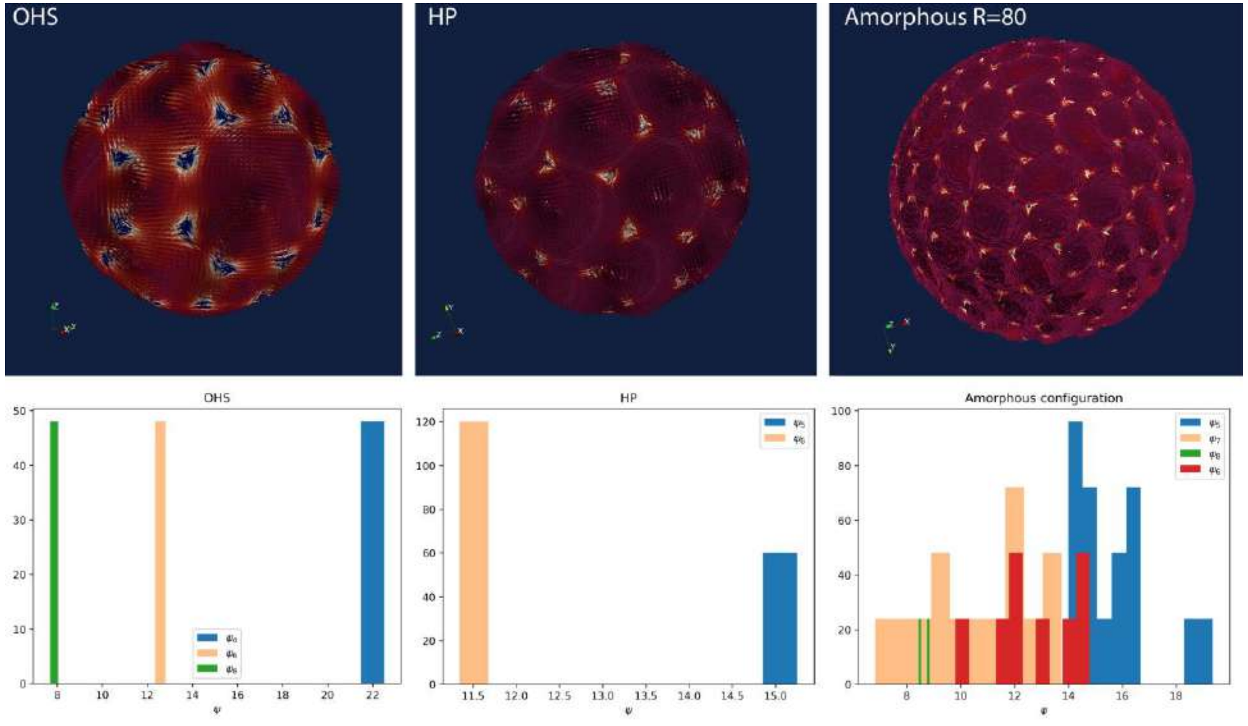
$$F^{hc} = \varepsilon^1_{\mathbf{k}_{q0}}(\phi^1_{\mathbf{k}_{q0}})^2 - 3!\sqrt{6}b\phi^1_{\mathbf{k}_1}\phi^1_{\mathbf{k}_2}\phi^1_{-\mathbf{k}_1-\mathbf{k}_2}Tr\left[\sigma^1_{\mathbf{k}_1}\sigma^1_{\mathbf{k}_2}\sigma^1_{-\mathbf{k}_1-\mathbf{k}_2}\right] + 4c(\phi^1_{\mathbf{k}_{q0}})^4 + 4!c\phi^1_{\mathbf{k}_1}\phi^1_{\mathbf{k}_2}\phi^1_{\mathbf{k}_3}\phi^1_{-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3}Tr\left[\sigma^1_{\mathbf{k}_1}\sigma^1_{\mathbf{k}_2}\sigma^1_{\mathbf{k}_3}\sigma^1_{-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3}\right]$$

$$F^{hc} = \phi^2_{\mathbf{k}_{q0}}\left[a + \frac{81\sqrt{3}}{8}b\phi_{\mathbf{k}_{q0}} + 28c\phi^2_{\mathbf{k}_{q0}}\right].$$



Blue Phases in Curved Geometries

- Topological contraints prevent the formation of a defect free hexagonal lattice
- On a thin shell of blue phase either <u>**quasi-crystal**</u> or <u>**amorphous configuration**</u> (never observed in 2d).

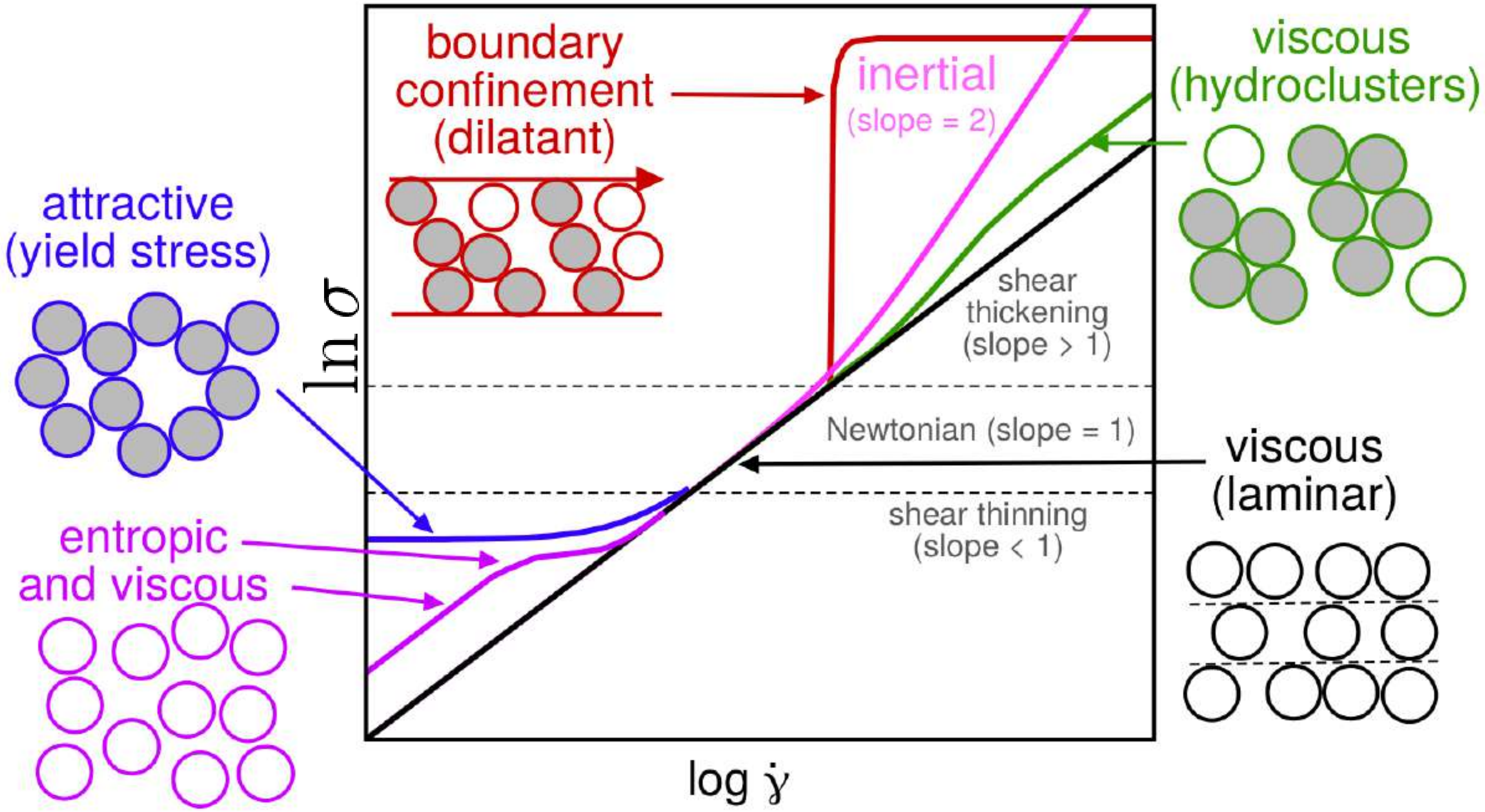


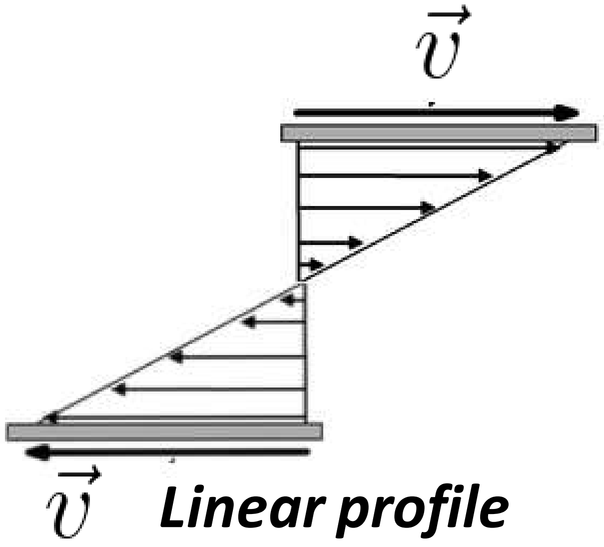
- Curvature by itself may favor the transition to the blue phase.

L. Carenza, G. Gonnella, D. Marenduzzo, G. Negro, and E. Orlandini, "Quasi-crystal and amorphous states of blue phases in non-euclidean geometries," **In preparation**

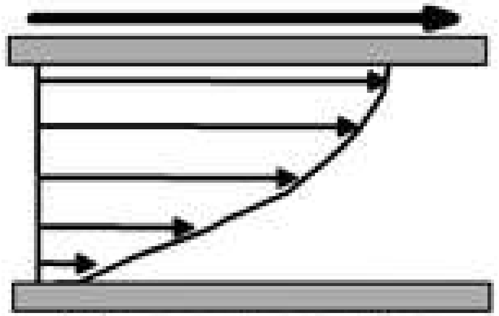
Rheological regimes

$$\eta_{app} = \sigma / \dot{\gamma}$$





Linear profile

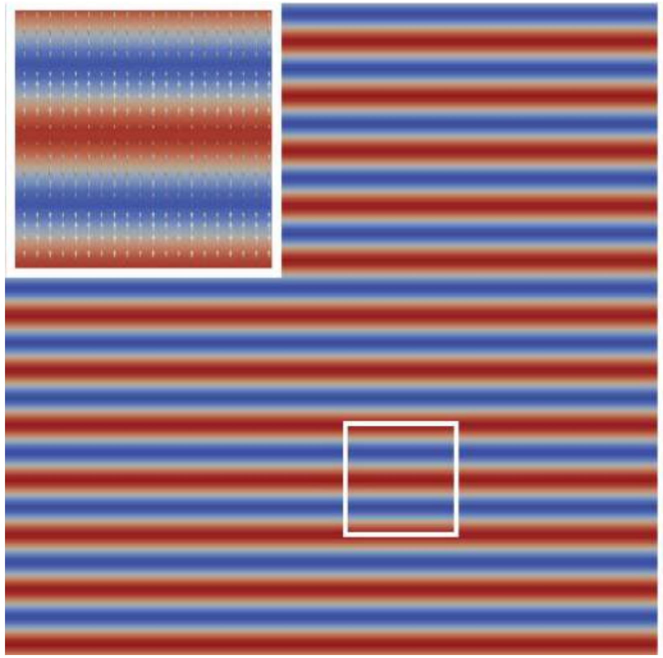


Shear-banding

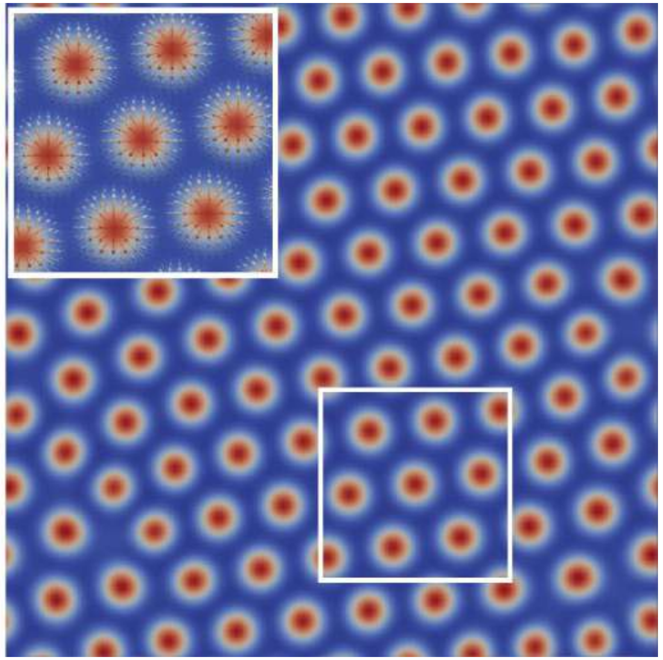
Which is more viscous?

Landau-Brazovskii theory for microphase separation

F. Bonelli, **L. Carenza**, G. Gonnella, D. Marenduzzo, E. Orlandini, and A. Tiribocchi, “Lamellar ordering, droplet formation and phase inversion in exotic active emulsions,” Sci. Rep., vol. 9, p. 2801, 2019.



G. Negro, **L. Carenza**, P. Digregorio, G. Gonnella, and A. Lamura, “Morphology and flow patterns in highly asymmetric active emulsions,” Physica A, vol. 503, pp. 464–475, 2018.



Field theory for microphase separation and lyotropic smectic liquid crystals

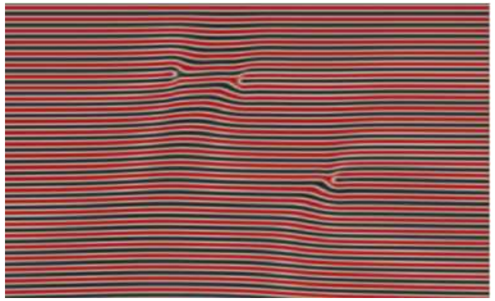
$$\mathcal{F} = \int dV \left[\frac{a}{2}\phi^2(\phi-\phi_0)^2 + \frac{k_\phi}{2}(\nabla\phi)^2 + \frac{c}{2}(\nabla^2\phi)^2 - \frac{\alpha}{2}\frac{\phi-\phi_{cr}}{\phi cr}\vec{P}^2 + \frac{\alpha}{4}\vec{P}^4 + \frac{k_P}{2}(\nabla\vec{P})^2 + \beta\vec{P}\cdot\nabla\phi \right]$$

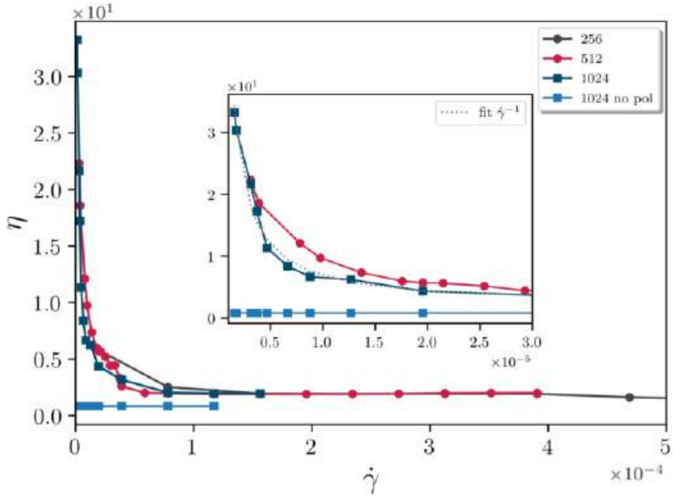
$$a > 0, \quad k_\phi < 0, \quad c > 0$$
$$\alpha > 0, \quad k_P > 0, \quad \beta > 0$$

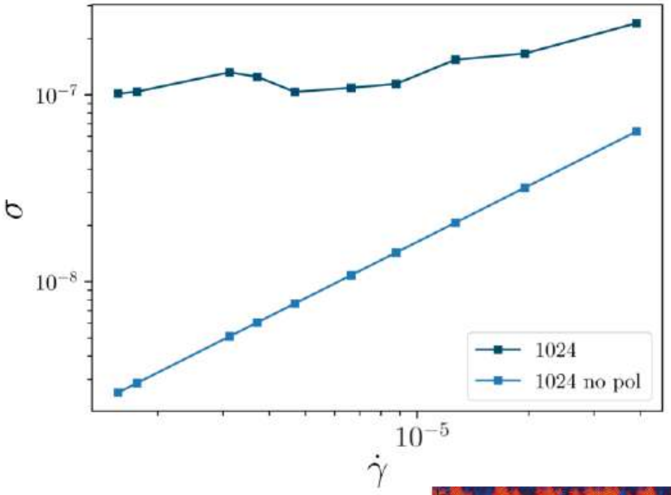
$$\lambda = 2\pi\sqrt{2c/|k_\phi|}$$

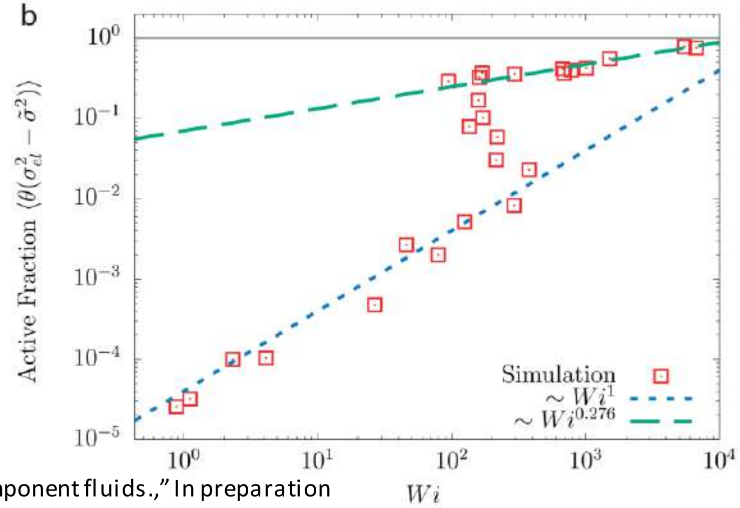
Yield percolation transition

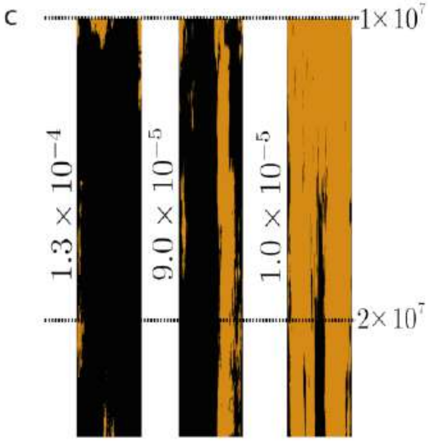
- Optimal model to describe the yielding transition in Smectic LC
- The viscosity diverges as the external forcing is reduced.
- This is signalled by a 1+1 stress percolation transition

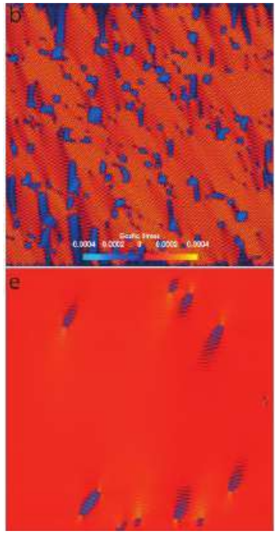












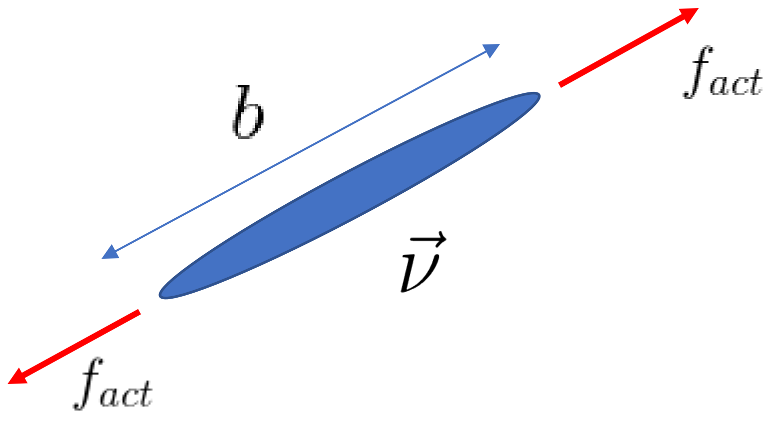
- **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, "Yielding transition occurs in multicomponent fluids.," In preparation
- **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, "Shear yielding and percolation transition is smectics," In preparation

Active Stress

We consider a system of identical swimmers with cylindrical symmetry.

Assuming that the intensity of the forcing on the surrounding fluid is the same at both sides we write for a collection of swimmers:

$$\vec{F}_{act}(\vec{r}) = f\sum_i \vec{\nu}_i \left[\delta\left(\vec{r}-\vec{r}_i-\frac{b}{2}\vec{\nu}_i\right)-\delta\left(\vec{r}-\vec{r}_i+\frac{b}{2}\vec{\nu}_i\right)\right]$$



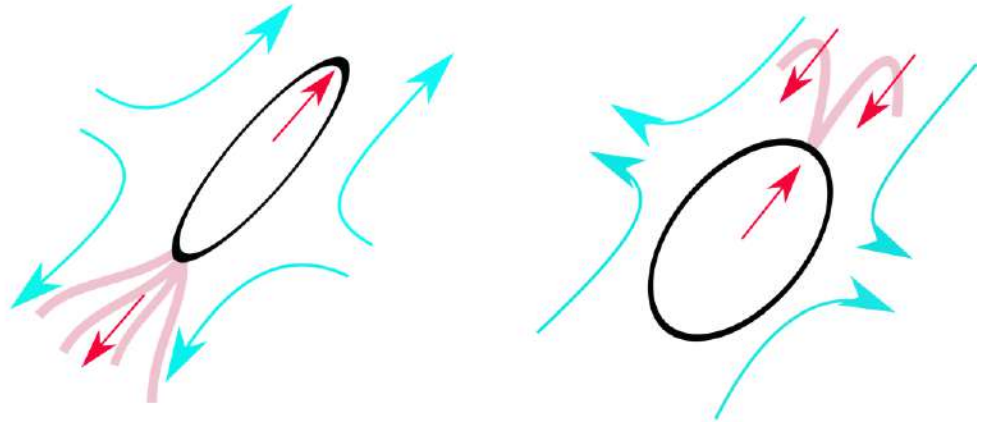
Expanding we can derive an expression for the active force exerted by a collection of swimmers as the divergence of a stress tensor:

$$\vec{F}_{act}(\vec{r}) = -bf\nabla\cdot\sum_i \vec{\nu}_i\otimes\vec{\nu}_i = \nabla\cdot\underline{\underline{\sigma}}^{active}$$

In general we can write:

$$\underline{\underline{\sigma}}^{active} = -\zeta\phi\left(\vec{P}\otimes\vec{P}-\frac{P^2}{d}\underline{\underline{I}}\right)$$

Where we introduced ζ the activity parameter.

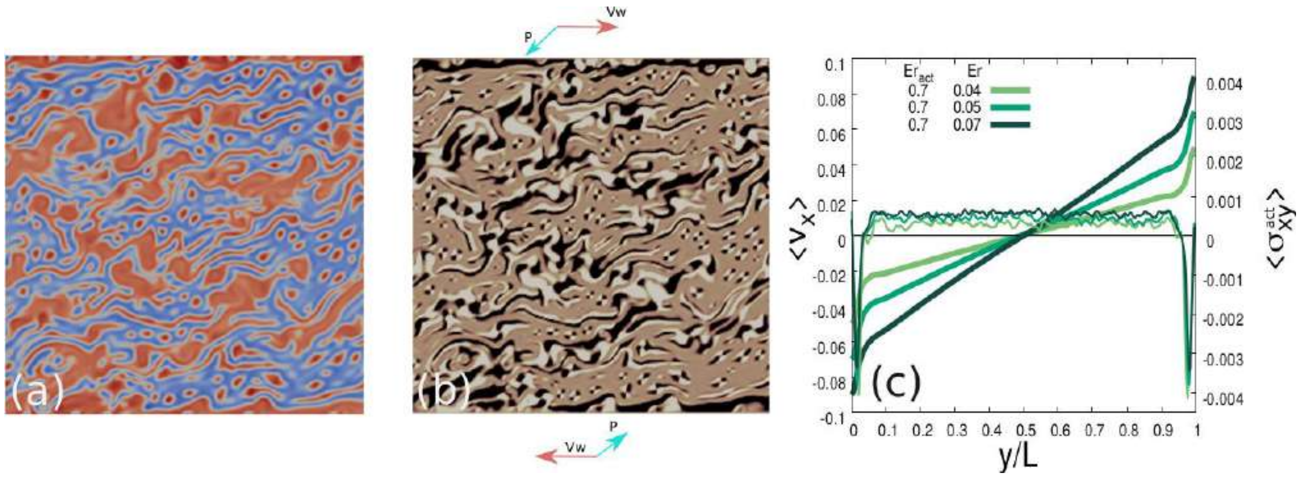


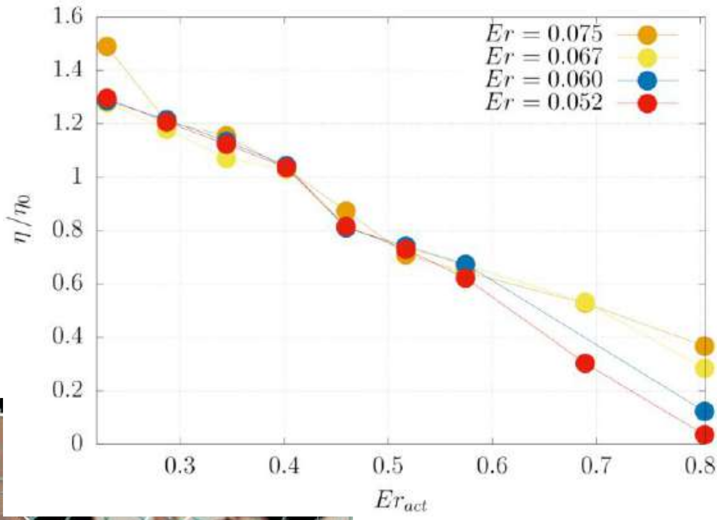
Pusher/Extensile

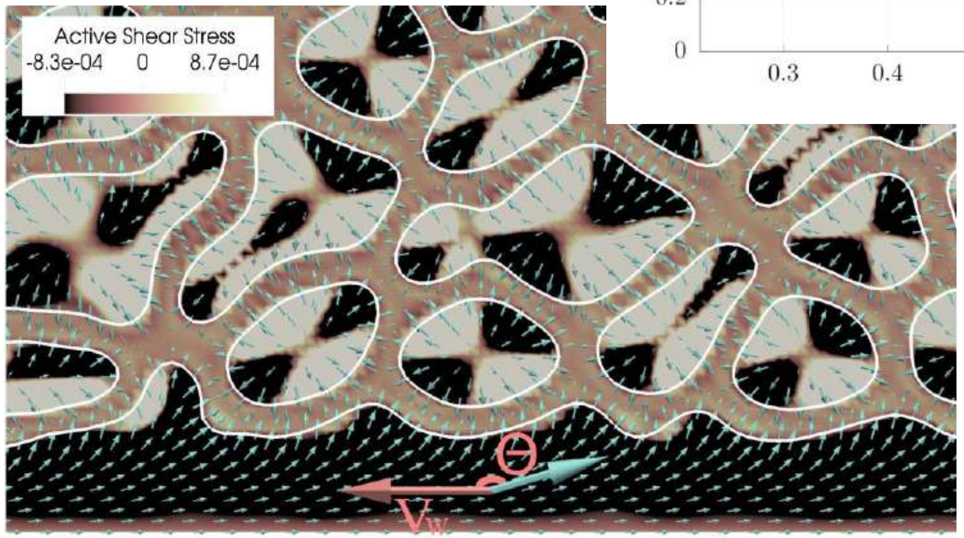
Puller/Contractile

Rheology of active Liquid Crystals

- Activity has important effects on the rheology of fluidic suspensions.
- The lamellar phase is lost and large rotating domains populate the system.
- The polarization field adheres at the walls in a homogeneous fashion either reinforcing or opposing the imposed velocity.
- As internal forcing is increased, the apparent viscosity of the fluid drops and eventually reaches an almost superfluid state.



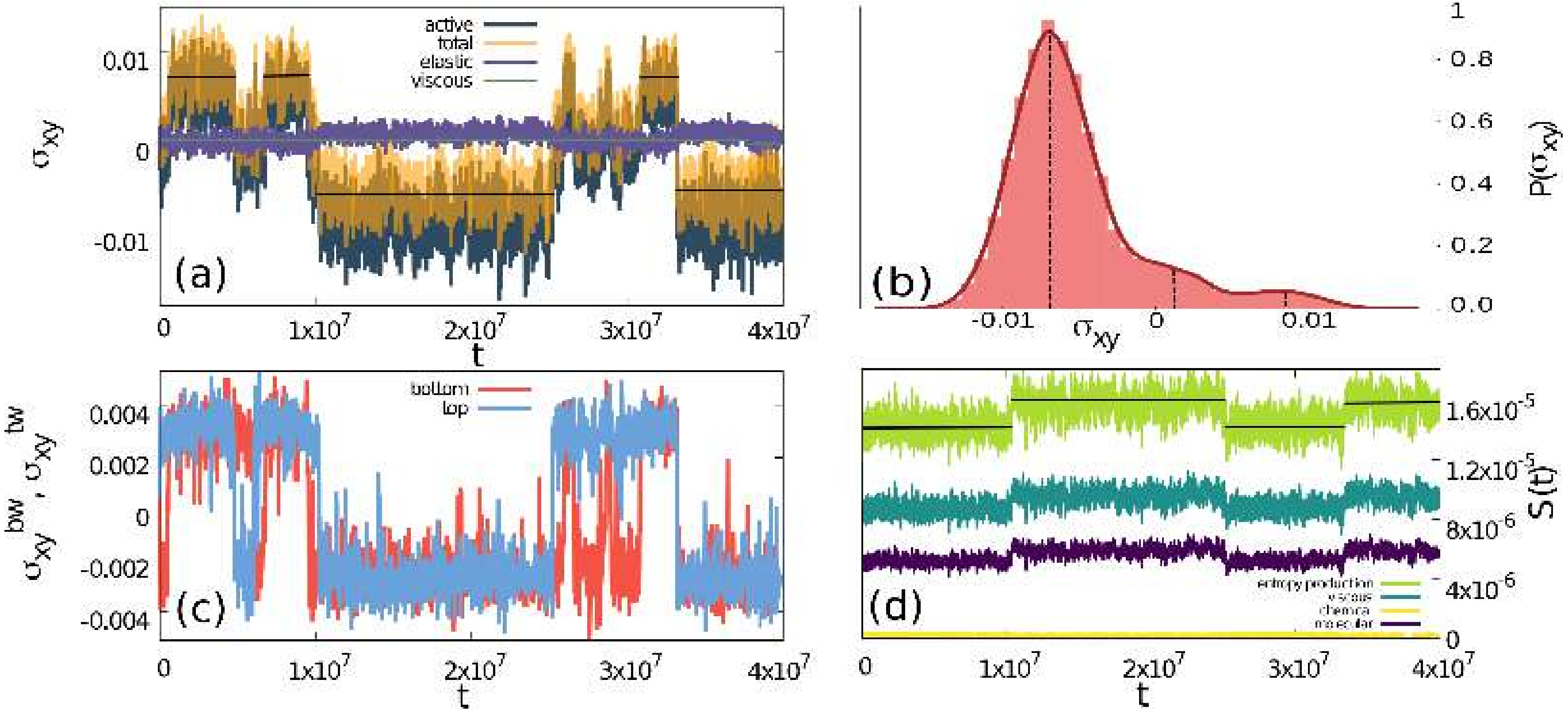




G. Negro, **L. Carenza**, A. Lamura, A. Tiribocchi, and G. Gonnella, “Rheology of active polar emulsions: from linear to unidirectional and unviscid flow, and intermittent viscosity,” **Soft Matter,** vol. 15, 8251, 2019.

Negative viscosity and superfluidic regimes in active fluids

- Active fluids are able to perform work on the walls
- Hydrodynamic instabilities driven by energy supply lead to intermittent dynamics
- A MaxEPP helps to determine the most favorable state.

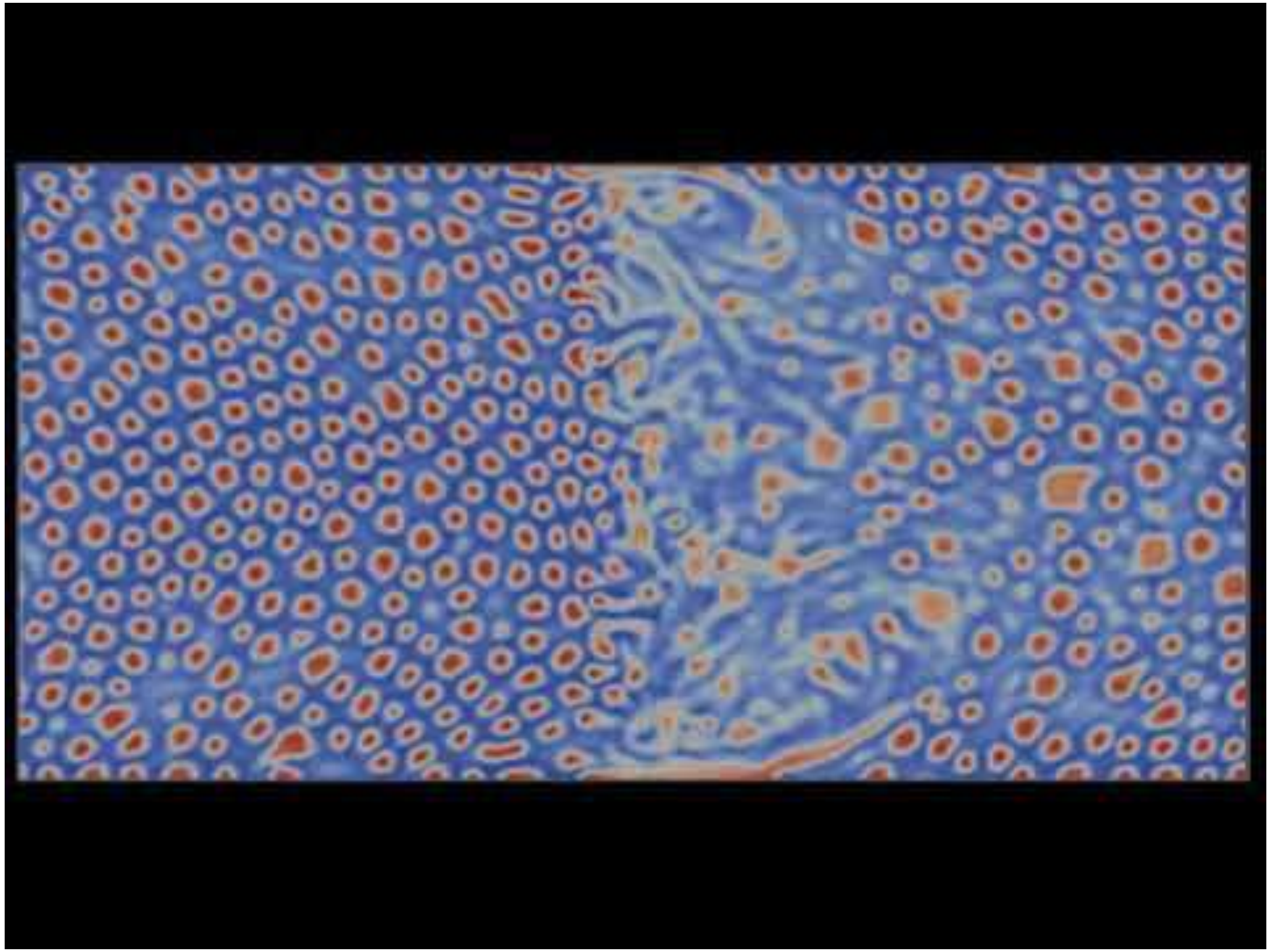


$$\partial_t \Sigma + \nabla \cdot (\Sigma \vec{v}) = s,$$

$$Ts = 2\eta \mathbf{D} : \mathbf{D} + \Gamma \mathbf{h} \cdot \mathbf{h} + M(\nabla \phi)^2,$$

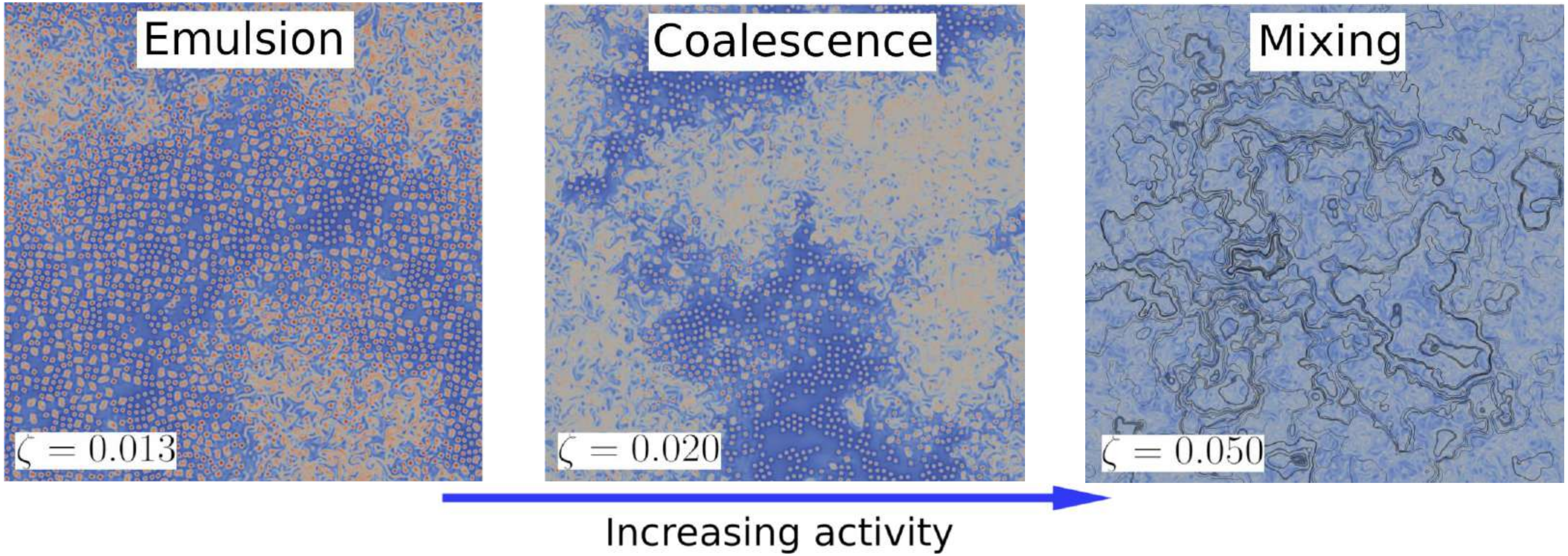
Drug delivery?

Rheological properties of active fluids may be exploited for the development of novel smart materials, capable of reacting to external stimula.



L. Carenza, L. Biferale, and G. Gonnella, "Multiscale control of active emulsion dynamics," Phys. Rev. Fluids, vol. 5, p. 011302, Jan 2020.

Coalescence – Mixing Transition



- As activity is increased a morphological transition occurs from the rotating droplet regime towards coalescence of active domains
- In the high-activity regime a mixed phase appears, characterized by fully developed chaotic flows spanning all the system

<u>Need a hydrodynamic characterization of the flow field!</u>

Flows and energy injection

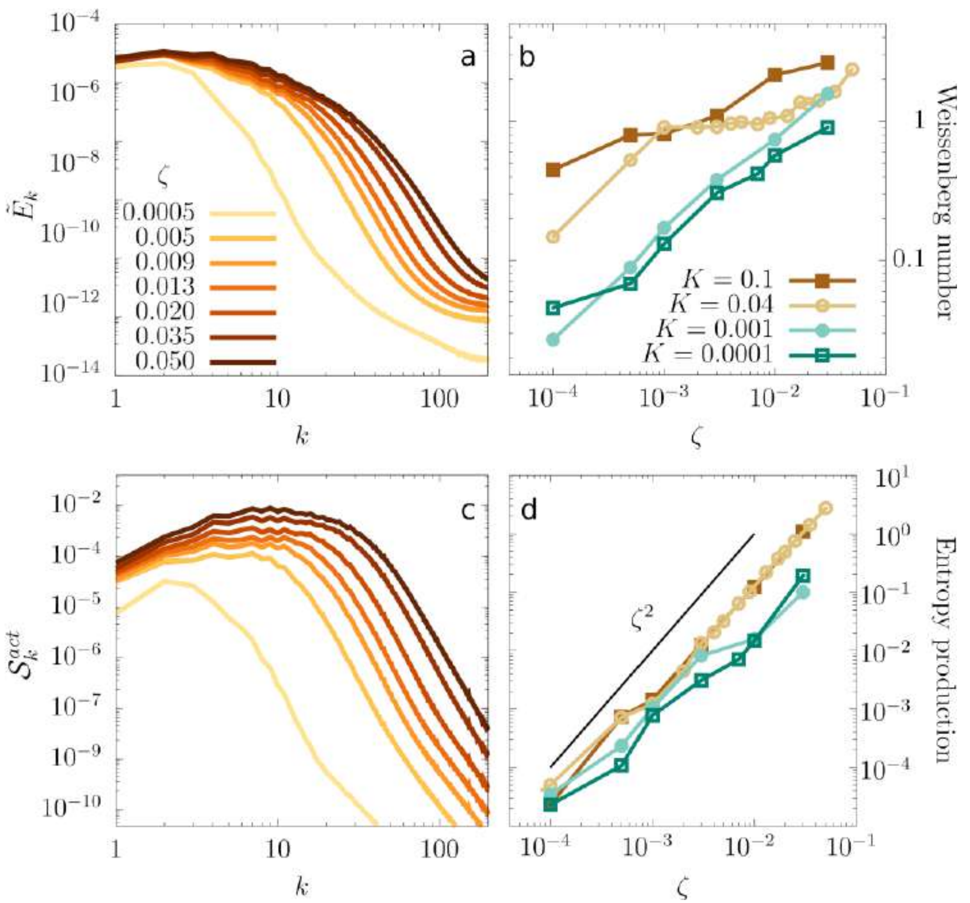
$$E(k) = \frac{1}{2}\langle|\mathbf{v}(\mathbf{k})|^2\rangle$$

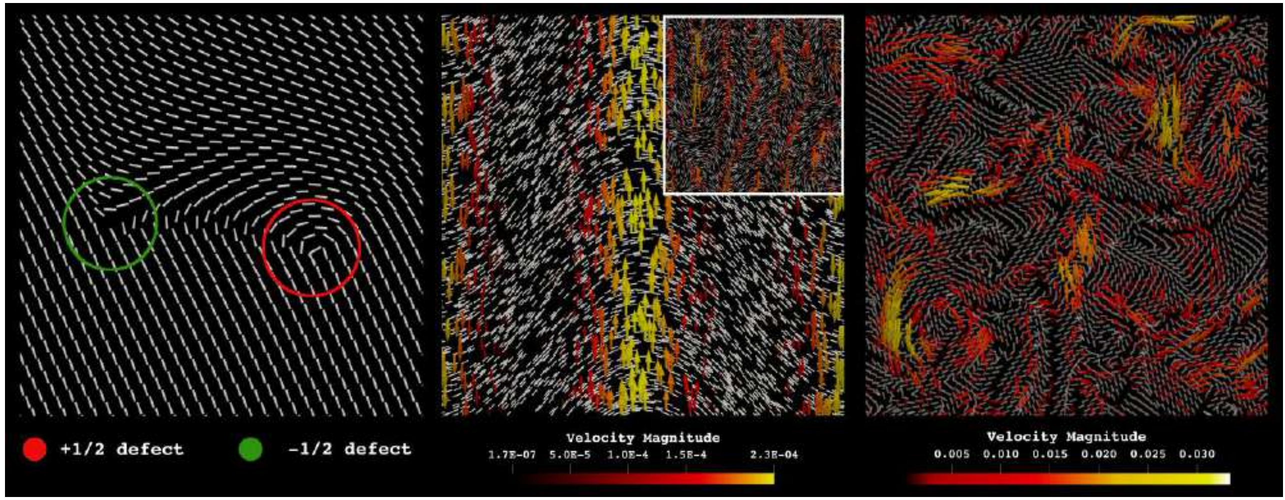
$$\mathcal{S}^{act}(k,t) = \langle \mathbf{v}^*(\mathbf{k},t)\cdot\mathbf{F}^{act}(\mathbf{k},t)\rangle$$

$$\mathbf{F}^{act}(k,t) = \frac{2\pi i}{L}\mathbf{k}\cdot\tilde{\sigma}^{act}(\mathbf{k},t)$$

- <u>NO universal behavior</u>
- <u>Active injection lenght-scales differ from typical flow scales (SMALL SCALE PUMPING)</u>
- <u>Kinetic energy increases as active pumping is reduced at increasing activity</u>

ANALYSIS OF FLUXES TO DISENTAGLE TRANSFER MECHANISM





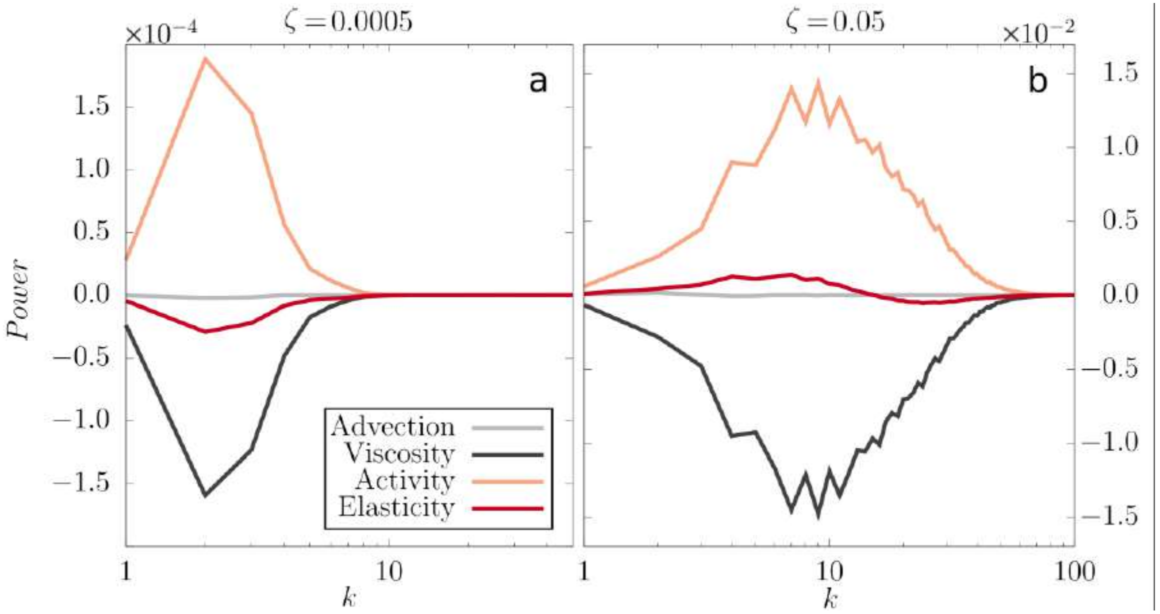
L. Carenza, L. Biferale, and G. Gonnella, "Cascade or not cascade? Energy Transfer and Elastic Effects in Active Nematics," EPL (On press) 2020.

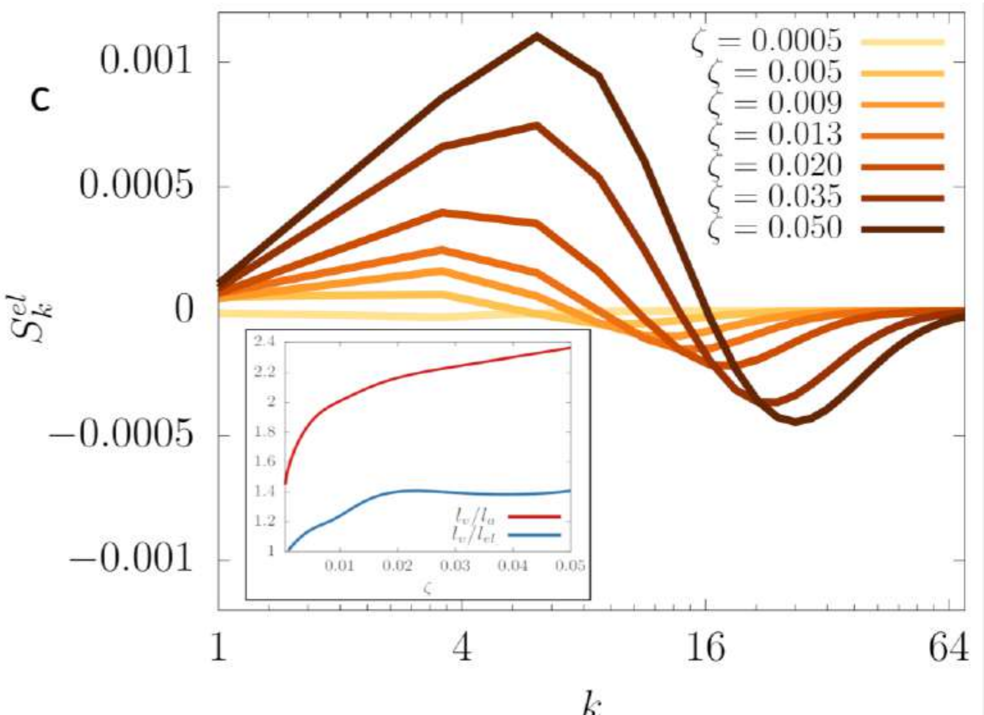
Scale-to-scale balance

$$\rho \partial_t E(k,t) + \mathcal{T}(k,t) = \sum_i \mathcal{S}^{(i)}(k,t)$$

- All terms are energy sinks except for the active stress that drive the system out of equilibrium
- NO HYDRODYNAMIC TRANSFER : the advective term is negligible, as expect ed for low-Re flows
- Elastic terms may give rise to weak energy transfer for large enough active forcing

Absence of hydrodynamic turbulence





Schools

- Summer school on Parallel Computing 2017 – Cineca (Bologna)
- Advanced School on Parallel Computing 2018 – Cineca (Bologna)
- XXX National Seminar of Nuclear and Subnuclear Physics "Francesco Romano" Otranto

Conferences

- SM&FT - Bari 2018;
- APS - Division of Fluid Mechanics 2018; Atlanta (USA)
- XXIII National Conference on Statistical Physics and Complex Systems; Parma
- FisMat2019 - Catania
- APS - Division of Fluid Mechanics 2019; Seattle (USA)
- Workshop INFN FieldTurb; Roma 2020
- Italian Soft Days 2020; Virtual Edition
- ESCI 2020; Virtual Edition

Offsite periods

- November 2018, Visit to prof. Biferale, Tor Vergata.
- March-April 2019 HPC Europa3 grant, Edinburgh, under the supervision of Prof. D. Marenduzzo.
- May 2019, Visit to prof. Biferale, Tor Vergata.
- July 2019, Visit to prof. Sagues, Barcelona.
- December 2019 - January 2020 HPC Europa3 grant, Edinburgh, under the supervision of Prof. D. Marenduzzo.

Pubblications

1. G. Negro, **L. Carenza**, P. Digregorio, G. Gonnella, and A. Lamura, “Morphology and flow patterns in highly asymmetric active emulsions,” Physica A, vol. 503, pp. 464 – 475, 2018.
2. F. Bonelli, **L. Carenza**, G. Gonnella, D. Marenduzzo, E. Orlandini, and A. Tiribocchi, “Lamellar ordering, droplet formation and phase inversion in exotic active emulsions,” Sci. Rep., vol. 9, p. 2801, 2019.
3. **L. Carenza**, G. Gonnella, A. Lamura, and G. Negro, “Dynamically asymmetric and bicontinuous morphologies in active emulsions,” Int. J. Mod. Phys. C, vol. 30, no. 10, p. 1941002, 2019.
4. G. Negro, **L. Carenza**, P. Digregorio, G. Gonnella, and A. Lamura, “In silico characterization of asymmetric active polar emulsions,” vol. 2071, p. 020012, 2019.
5. **L. Carenza**, G. Gonnella, A. Lamura, G. Negro, and A. Tiribocchi, “Lattice boltzmann methods and active fluids,” Eur. Phys. J. E, vol. 42, no. 6, p. 81, 2019.
6. G. Negro, **L. Carenza**, A. Lamura, A. Tiribocchi, and G. Gonnella, “Rheology of active polar emulsions: from linear to unidirectional and unviscid flow, and intermittentviscosity,” Soft Matter, vol. 15, 8251, 2019.
7. **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, “Rotation and propulsion in 3d active chiral droplets,” Proc. Natl. Acad. Sci., vol. 116, no. 44, pp. 22065–22070, 2019.
8. **L. Carenza**, L. Biferale, and G. Gonnella, “Multiscale control of active emulsion dynamics,” Phys. Rev. Fluids, vol. 5, p. 011302, Jan 2020.
9. **L. Carenza**, G. Gonnella, A. Lamura, D. Marenduzzo, and G. Negro, “Soft channel formation and symmetry breaking in exotic active emulsions,” Sci. Rep., vol. 10, 2020.
10. **L. Carenza**, G. Gonnella, and G. Negro, Lattice Boltzmann simulations of selfpropelling chiral active droplets. Gangemi Editore, 2020.
11. **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, “Chaotic and periodical dynamics of active chiral droplets,” Physica A, vol. 559, p. 125025, 2020.
12. **L. Carenza**, L. Biferale, and G. Gonnella, “Cascade or not cascade? Energy Transfer and Elastic Effects in Active Nematics,” EPL (On press) 2020.
13. **L. Carenza**, M. Giordano, G. Gonnella, and G. Negro, “Activity induced isotropic-polar transition in active liquid crystals,” Under Review, 2020.

In preparation

- **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, “Yielding transition occurs in multicomponent fluids.,” In preparation
- **L. Carenza**, G. Gonnella, D. Marenduzzo, and G. Negro, “Shear yielding and percolation transition is smectics,” In preparation
- **L. Carenza**, G. Gonnella, D. Marenduzzo, G. Negro, and E. Orlandini, “Quasi-crystal and amorphous states of blue phases in non-euclidean geometries,” In preparation
- **L. Carenza**, F. Corberi, G. Gonnella, and G. Negro, “Stable negative viscosities in active emulsions.,” In preparation