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Active Matter

a hydrodynamic approach

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What is active matter?

Active constituents, such as fish in a school, self arrange in ordered patterns.

Such systems have been known with the term active matter.

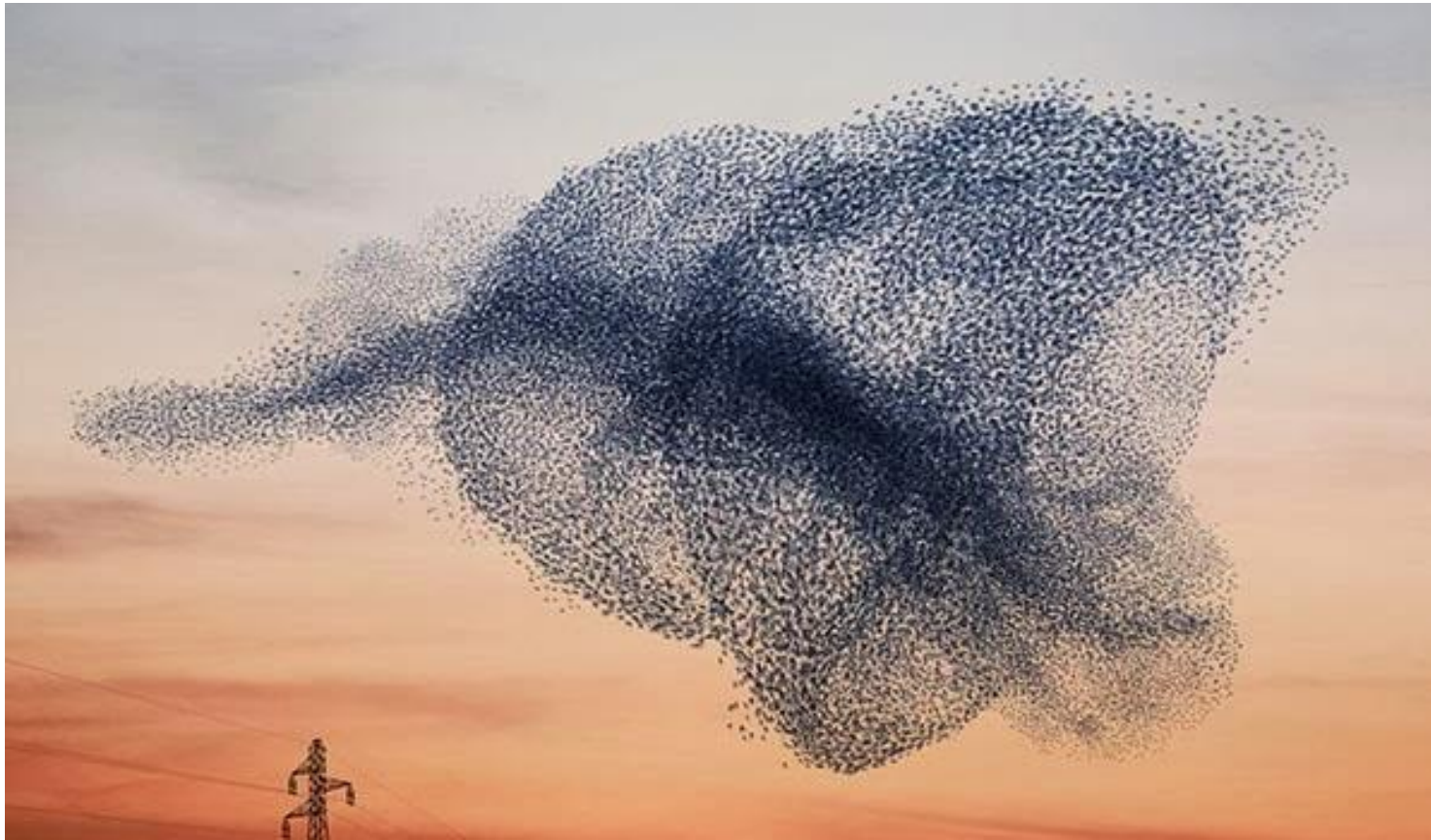
Generally they are condensed matter systems

Energy injection occurs at small lengthscales, on the level of individual constituents.

They are inherently out-of-equilibrium.

Their origin can be both biological or artificial

Typical lengthscales may range from a few micrometers up to some hundreds of meters.



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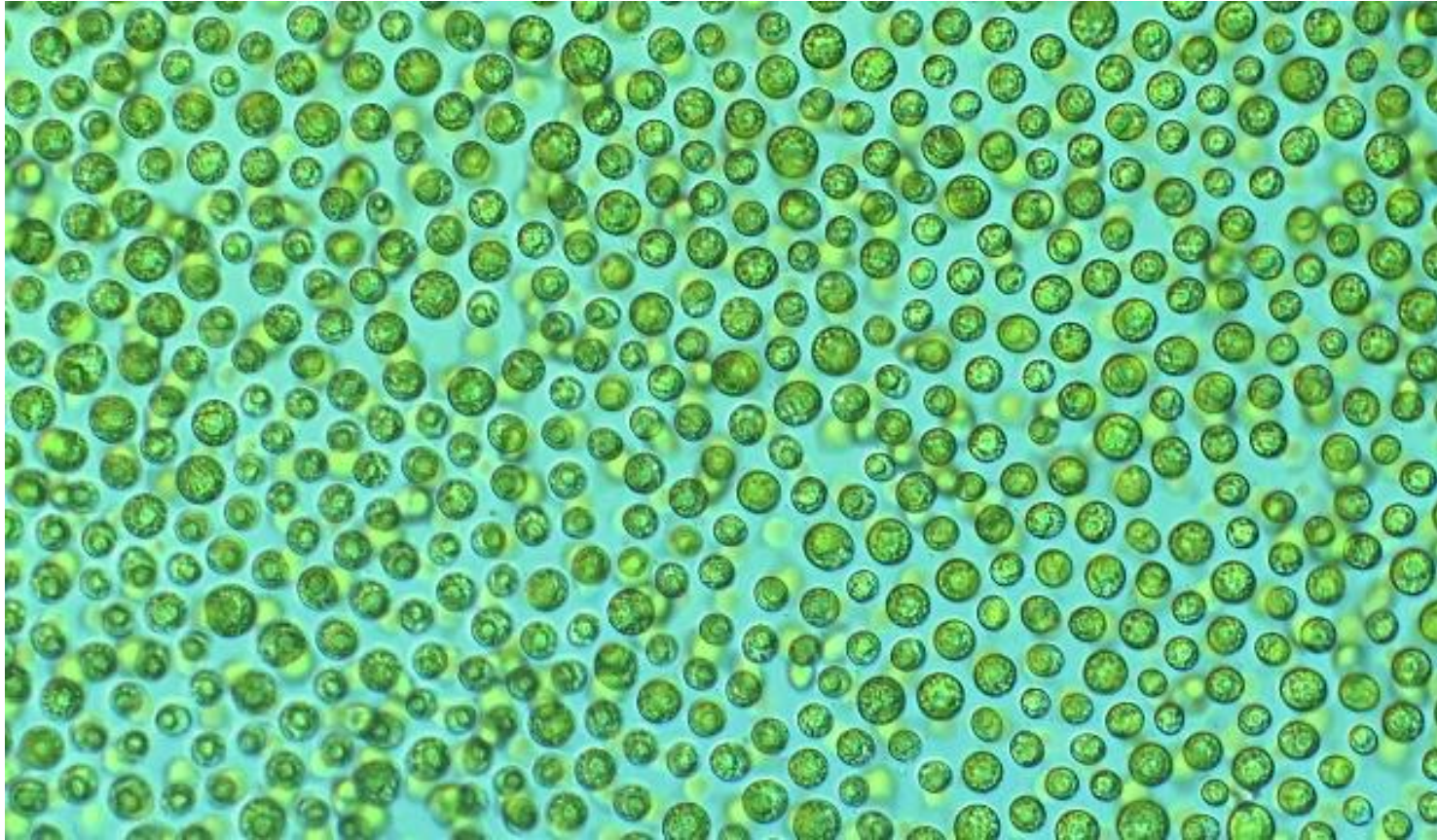
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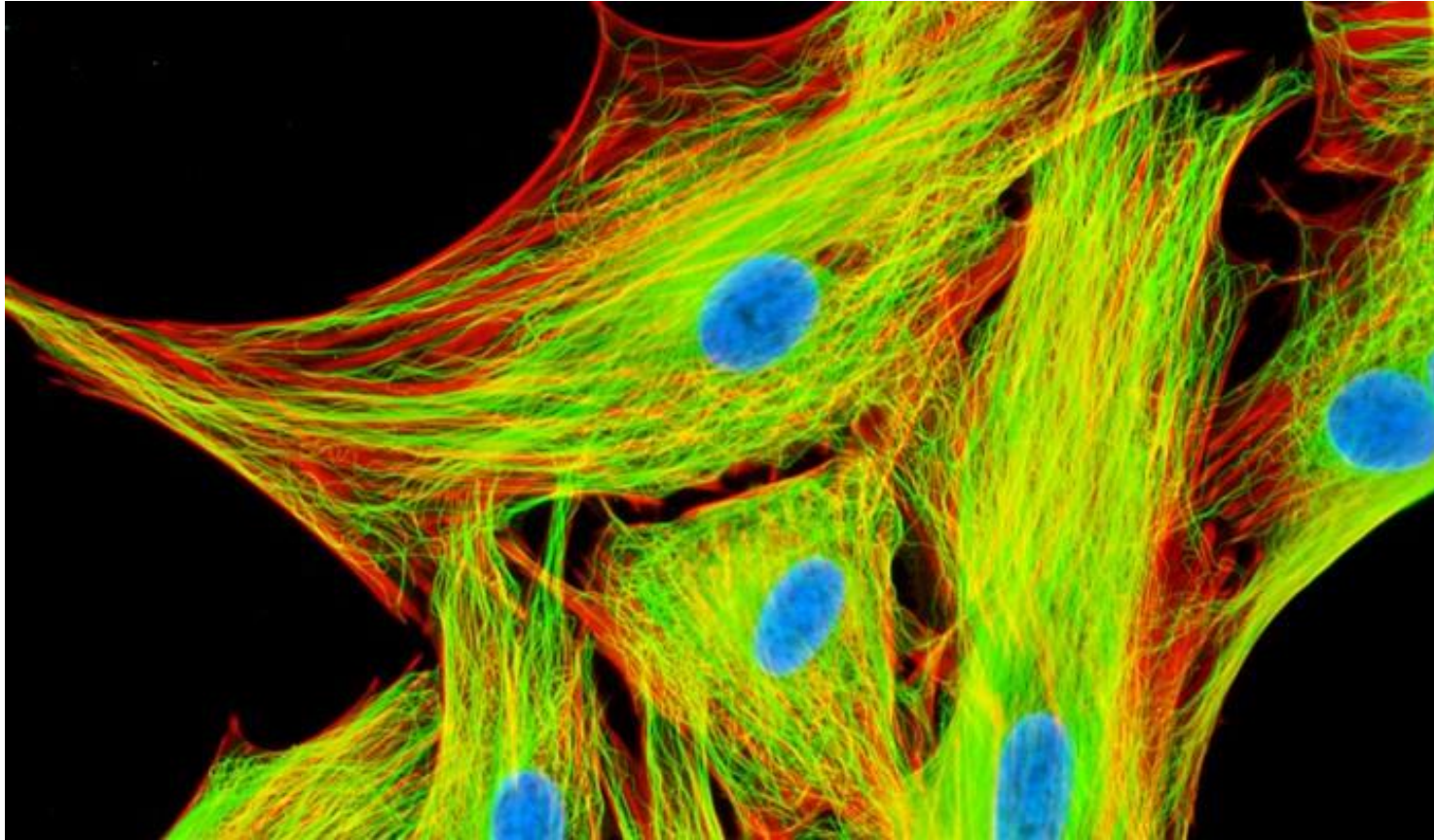
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Dry or Wet?

Active constituents interact with each other leading to interesting and unexpected properties.

In some cases, the interaction with the surrounding environment becomes important.

A basic classification of active systems can be done as follows:

- Dry systems: the interaction between constituents does not conserve momentum. *"No action-reaction principle holds for a lion chasing a gazel"*
- Wet system: active constituents exchange momentum among themselves and with the environment. We will refer to this kind of systems with the name *active fluids*

Bacterial, algae, cytoskeletal suspensions fall in this latter class.

Spontaneous Flow

Energy injection due to consumption of internal/chemical energy is capable to set up self-sustained flows.

Superfluidity and Negative Viscosity

Experimental and numerical studies on rheological properties of active fluids revealed the emergency of a superfluidity phase under suitable environmental and boundary conditions. Astonishingly, negative viscosities have been observed in bacterial suspensions.

Active Turbulence

Active flows have been found to develop vortical structures, resembling those typical of hydrodynamic Kolmogorov turbulence.

WHY ACTIVE MATTER?

- Design of new smart material
- Medical applications (drug delivery)
- Testing ground for theoretical topics regarding non-equilibrium systems

Dynamic modelling for active matter

- Molecular dynamics vs. Coarse Grained Hydrodynamics

Numerical and computational methods

- Lattice Boltzmann Method
- MPI

Active Cholesteric Droplet

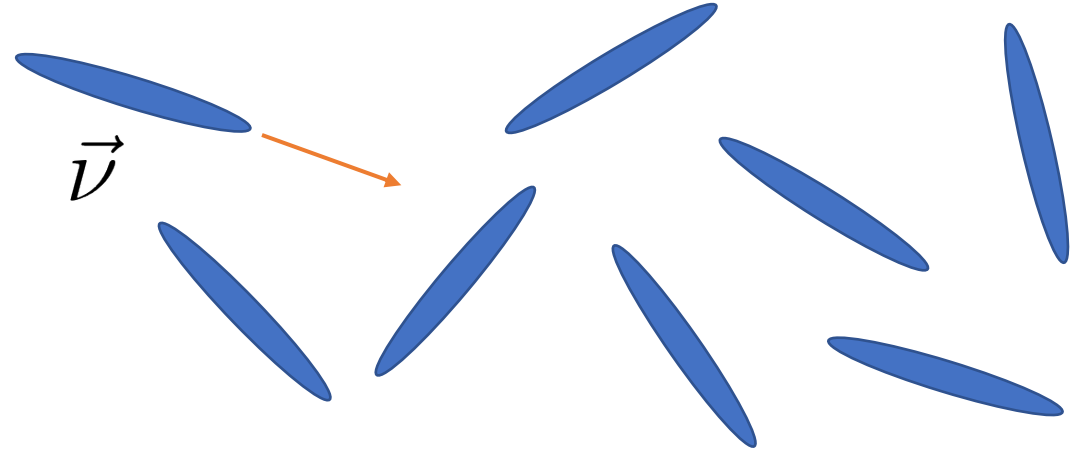
- Cholesteric Liquid Crystals
- Some preliminary results

Summary

Modelling active matter

Many theories have been developed so far to describe active matter, ranging from agent-based models to continuum (coarse-grained) theories.

Most active constituents are capable to move in the direction of their axes of symmetry, that we denote with a vector \vec{v} .



It is reasonable to assume that the swimming speed of such active constituents is proportional to a certain active force \vec{F}_{act} directed in the same direction of \vec{v} .

$$\gamma \dot{\vec{r}} = F_{act} \vec{v}$$

The effect of the environment can be included in this description introducing some Gaussian noise, both in the velocity evolution equation and in the orientation of the swimmer.

$$\dot{\theta} = \eta \quad \gamma \dot{\vec{r}} = F_{act} \vec{v} + \vec{\xi} - \nabla \sum_j U(|\vec{r} - \vec{r}_j|)$$

What if the swimmer is not alone?

In this case we need to consider a suitable interaction term too!

Towards a continuum theory of active matter

The Active Brownian Model presented succeeds in catching the swarming dynamics of a few individual constituents, but unfortunately suffers of some issues:

- Limited number of constituents can be considered
- Environment only appears as a background noise

Particle-based theories cannot be used to model active fluids, where the density of active constituents can be very high and the hydrodynamic feedback due to the gauge between the swimmers and the flow is fundamental to catch the essential features of active fluids.

Polar or Nematic Active Liquid Crystals

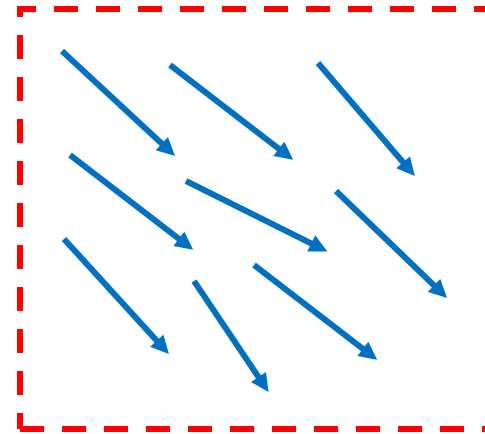
We now consider a volume containing many (rod-like) active particles. We denote by \vec{v}_i the orientation of each particle.

We can thus define a mean local orientation:

$$\vec{P}(\vec{r}) = \langle \sum_i \vec{v}_i \delta(\vec{r} - \vec{r}_i) \rangle_{cg}$$

We describe the concentration of active constituents by introducing a scalar field defined as:

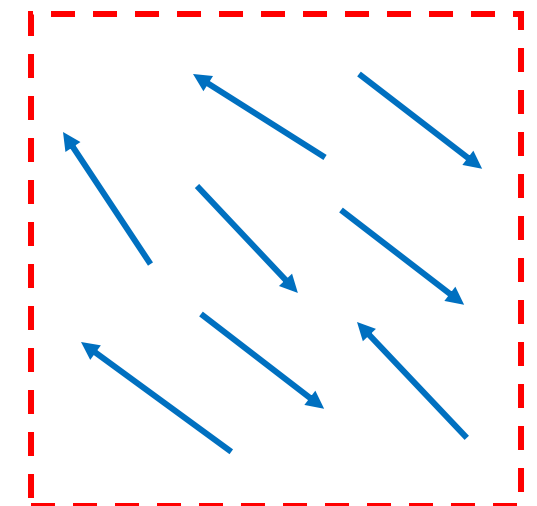
$$\phi(\vec{r}) = \langle \sum_i \delta(\vec{r} - \vec{r}_i) \rangle_{cg}$$



In many situations the mean polarization can be null even if some orientational order is preserved. This can occur in systems whose constituent exhibit head-tail symmetry, or if particles pointing in opposite directions are equally represented.

In this case the order parameter for the nematic phase must satisfy the head-tail symmetry.

$$\underline{\underline{Q}} = \vec{P} \otimes \vec{P} - \frac{P^2}{3} \underline{\underline{I}}$$



Dynamical Equations

We need evolution equations for the two order parameters, namely the concentration of active material and their orientation. Moreover we need a further equation to describe momentum transfer within the fluid.

$$d_t \phi = \nabla \cdot \left(M \nabla \frac{\delta \mathcal{F}}{\delta \phi} \right)$$

Advection-Diffusion equation for the (conserved) concentration field

$$d_t \vec{P} + \underline{\underline{\Omega}} \cdot \vec{P} = \xi \underline{\underline{D}} \cdot \vec{P} - \frac{1}{\Gamma} \frac{\delta \mathcal{F}}{\delta \vec{P}}$$

Adapted Ericksen-Leslie equation for the treatment of a vector field

$$\rho(\partial_t \vec{v} + \vec{v} \cdot \nabla \vec{v}) = \nabla \cdot \underline{\underline{\sigma}}^{pass} + \underline{\underline{\sigma}}^{act}$$

Incompressible Navier-Stokes equation

$$\underline{\underline{\sigma}}^{pass} = \underline{\underline{\sigma}}^{hydro} + \underline{\underline{\sigma}}^{viscous} + \underline{\underline{\sigma}}^{elastic} + \underline{\underline{\sigma}}^{binary}$$

$$\underline{\underline{\sigma}}^{hydro} = -p \underline{\underline{I}}$$

$$\underline{\underline{\sigma}}^{viscous} = 2\eta \underline{\underline{D}}$$

Material derivative

$$d_t = (\partial_t + \vec{v} \cdot \nabla)$$

Vorticity tensor

$$\Omega_{\alpha\beta} = \frac{1}{2} (\partial_\beta v_\alpha - \partial_\alpha v_\beta)$$

Strain-rate tensor

$$D_{\alpha\beta} = \frac{1}{2} (\partial_\beta v_\alpha + \partial_\alpha v_\beta)$$

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:

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

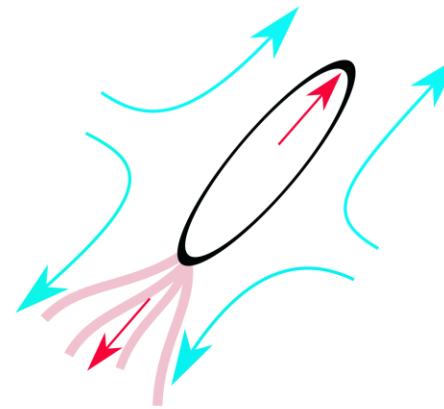
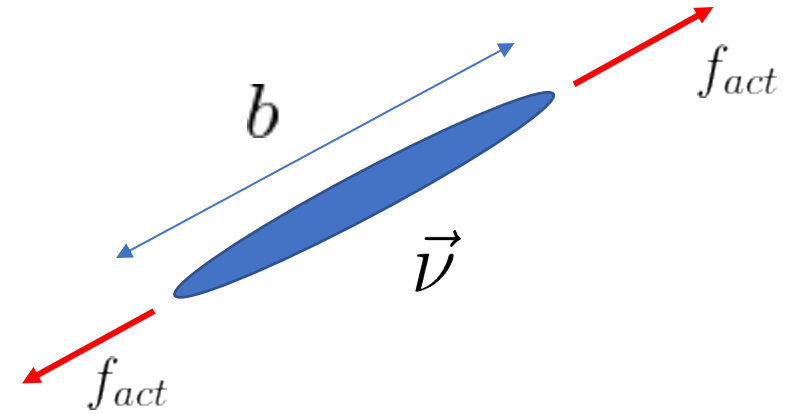
Expanding we can derive an expression for the active force exerted by a collection of swimmers as the divergence of a stress tensor:

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

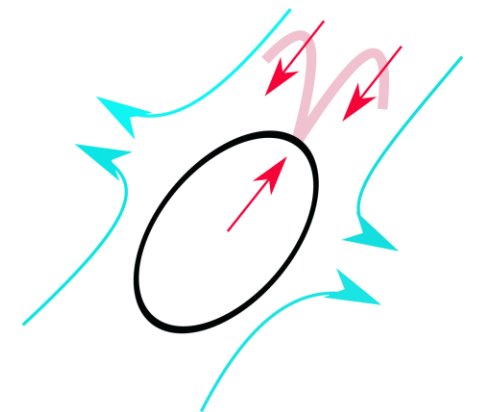
In general we can write:

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

Where we introduced ζ the activity parameter.



Pusher/Extensile



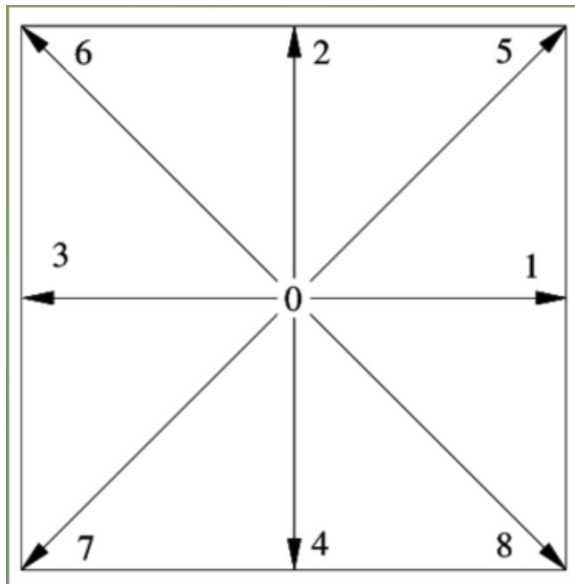
Puller/Contractile

Lattice Boltzmann Method

LBM 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 discrete lattice on grid points and along lattice velocities.

Assuming the system close to equilibrium the collision operator can be expanded 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

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

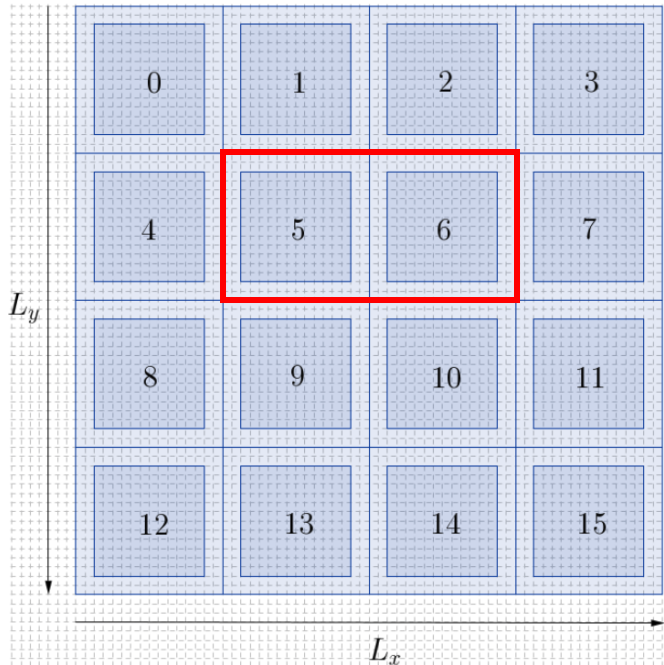
In this scope viscosity arises directly from discretization effects

$$\nu = c^2 \Delta t \frac{2\tau - 1}{6}$$

High Performance Computing for LBM

Numerical implementation of LBM must face some computational issues:

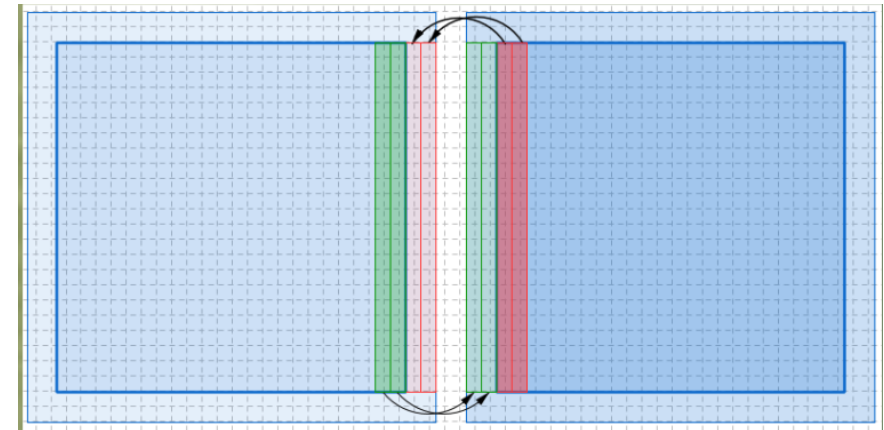
- Memory resources
- Long processing times (the typical amount of time required to perform $10E7$ LB iterations on a squared 256 grid with a C code $\sim 200h$ of CPU time using proc. Intel® Core™ i7)



"Be wise... parallelize!"

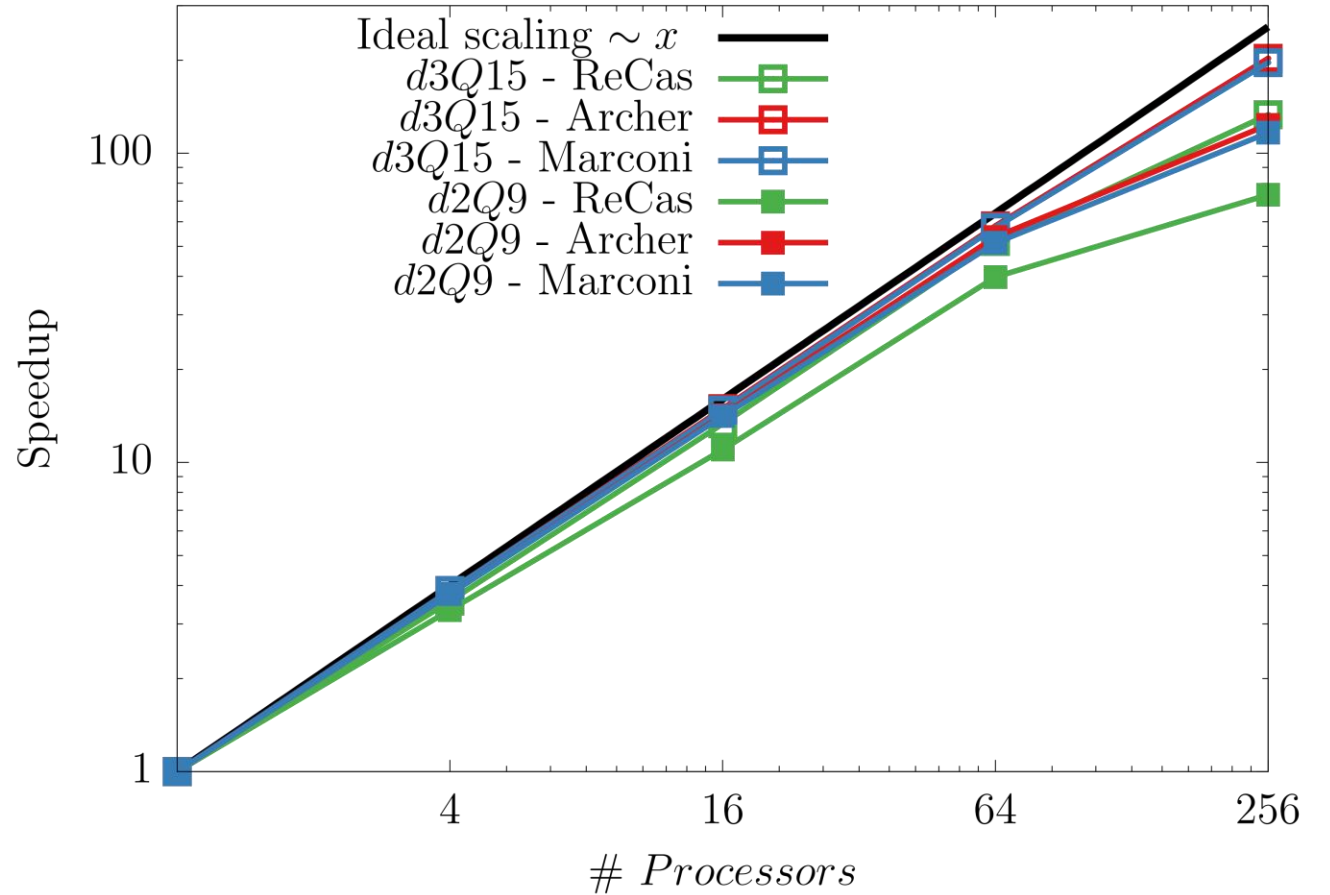
- MPI protocol
- Distributed memory systems

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



Strong scaling test

- The size of the physical domain is kept fixed and divided among an increasing number of processors.
- The speedup is computed as the time needed to accomplish the calculation with # processors normalized with respect the time needed to perform the same calculation in a serial way.
- Scaling in 3d geometries (slice division) is close to the ideal behavior in the range explored.
- In 2d (strip division) scaling departs from ideal behavior for more than 64 processors, that is when the size of ghost strips gets close to that of the computational domain.



Active Droplets



Davide Marenduzzo



Giuseppe Gonnella



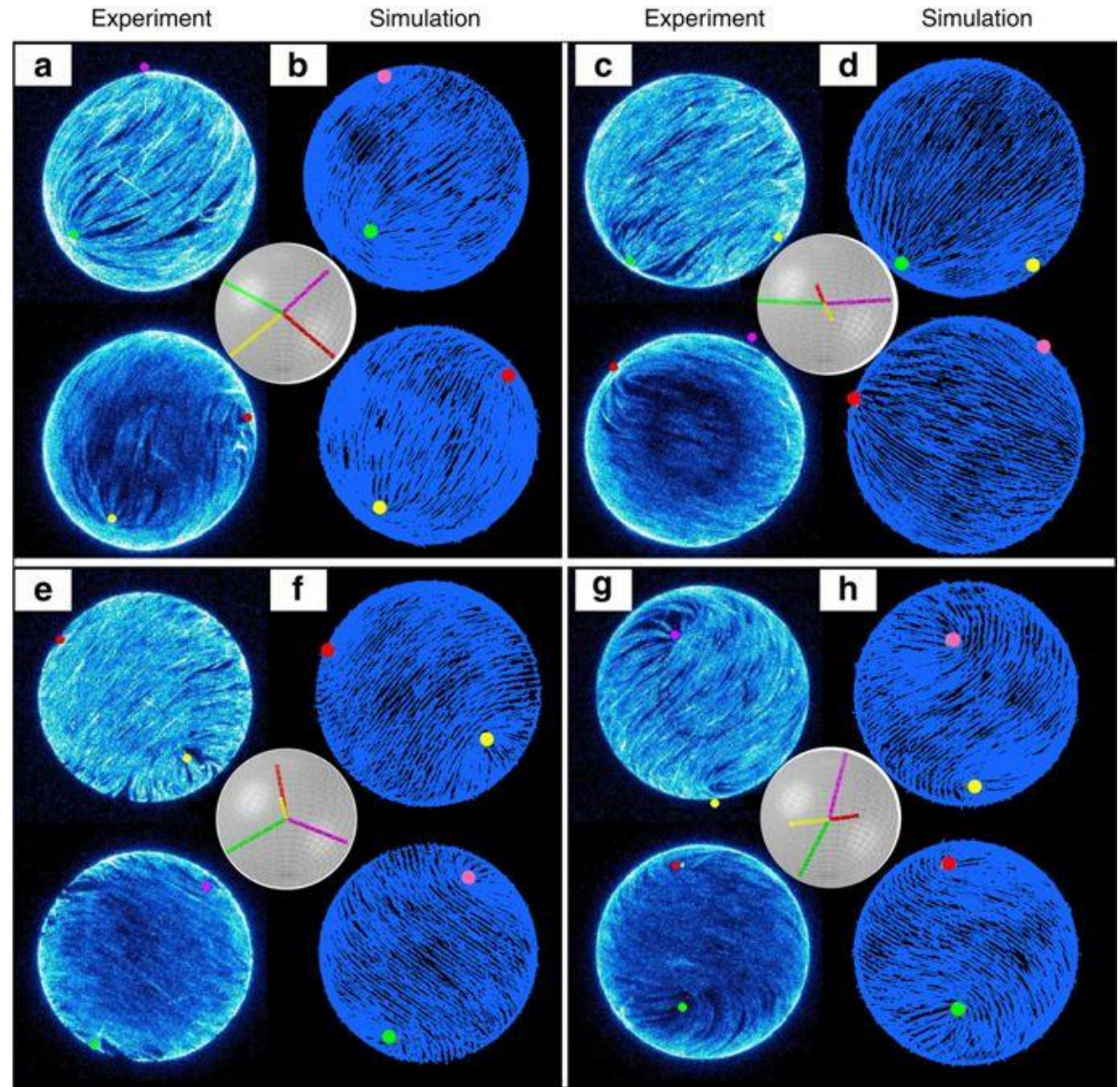
Giuseppe Negro



Livio Carenza

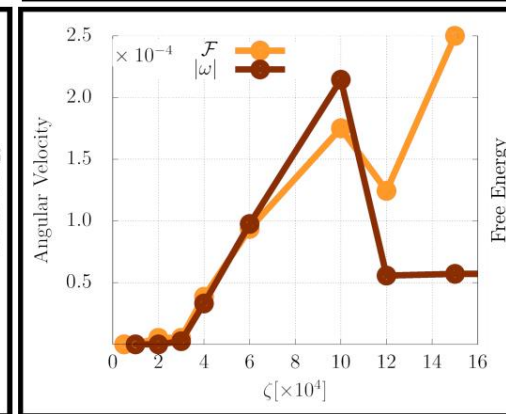
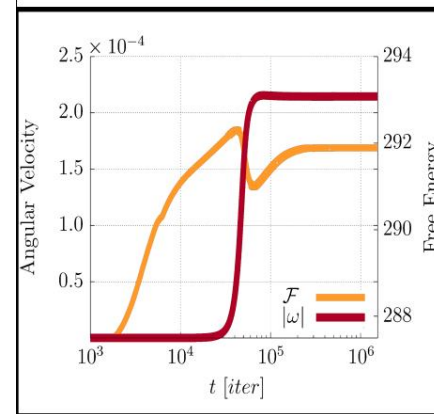
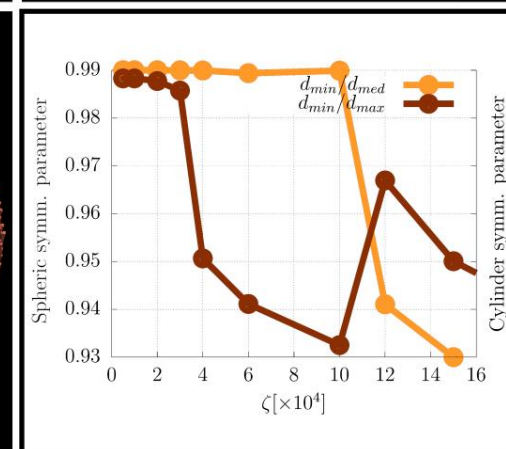
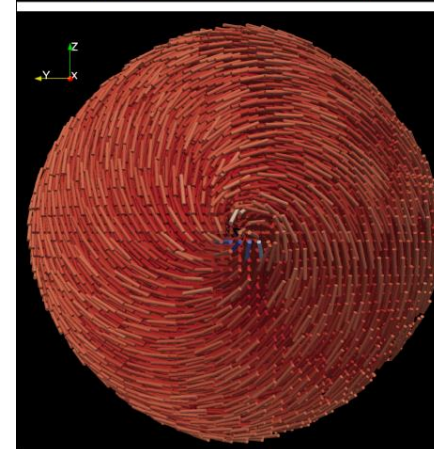
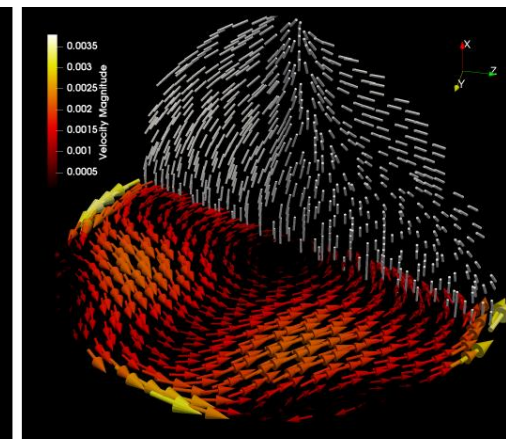
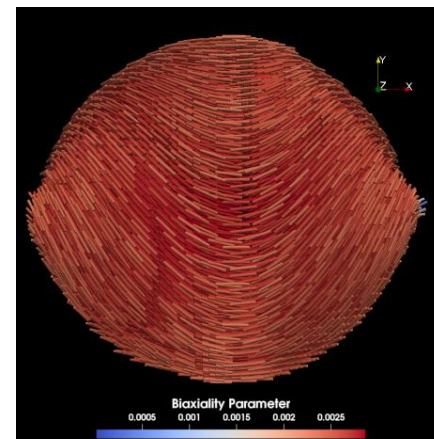
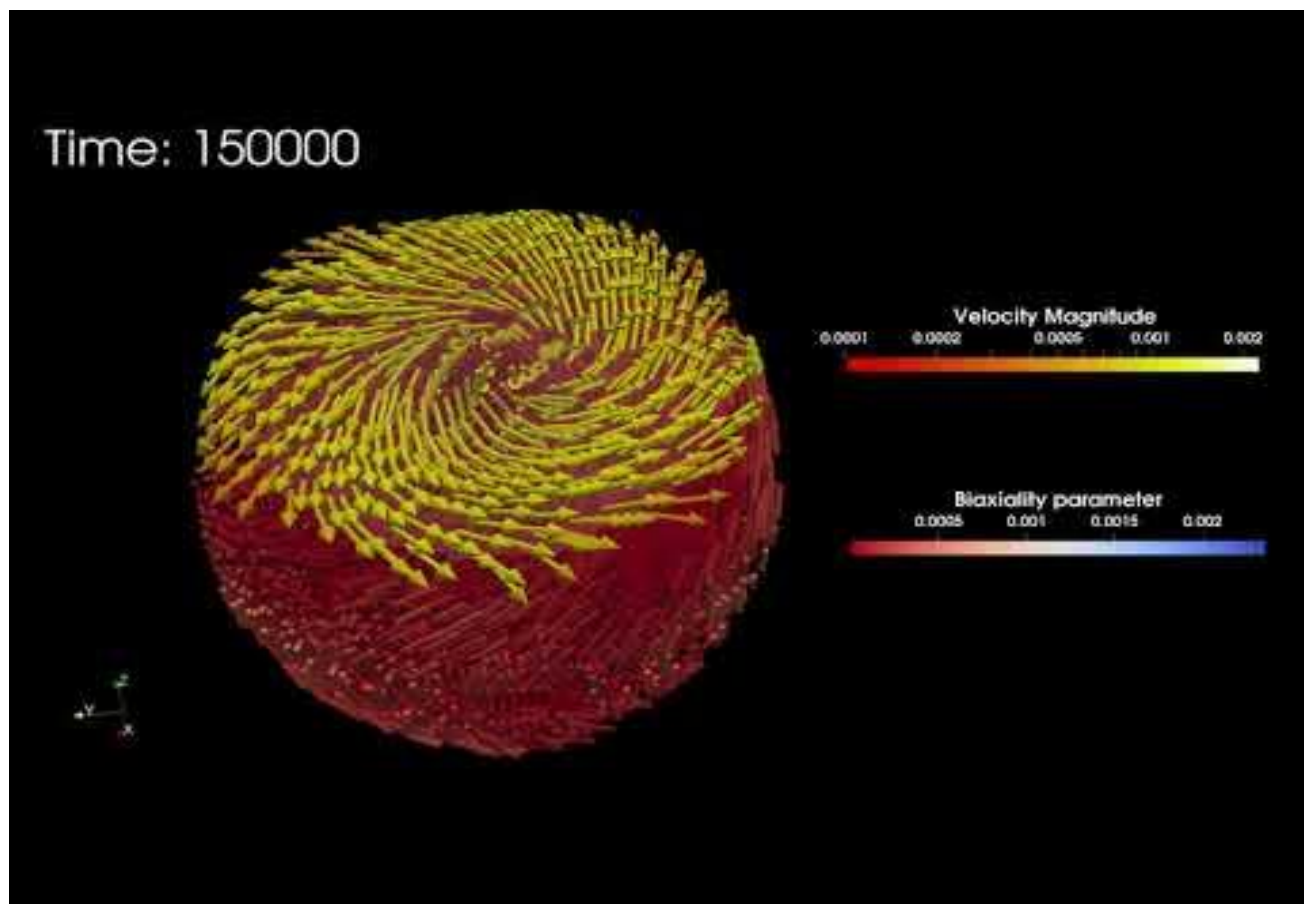
Active Droplets

- What happens if activity is confined?
- Recent experiments managed to confine active behavior in shells of liquid crystal
- Shells rotate under the effect of activity!
- Droplet propulsion may be exploited in applications aimed at drug delivery
- To simulate such system a three-dimensional approach is compulsory!



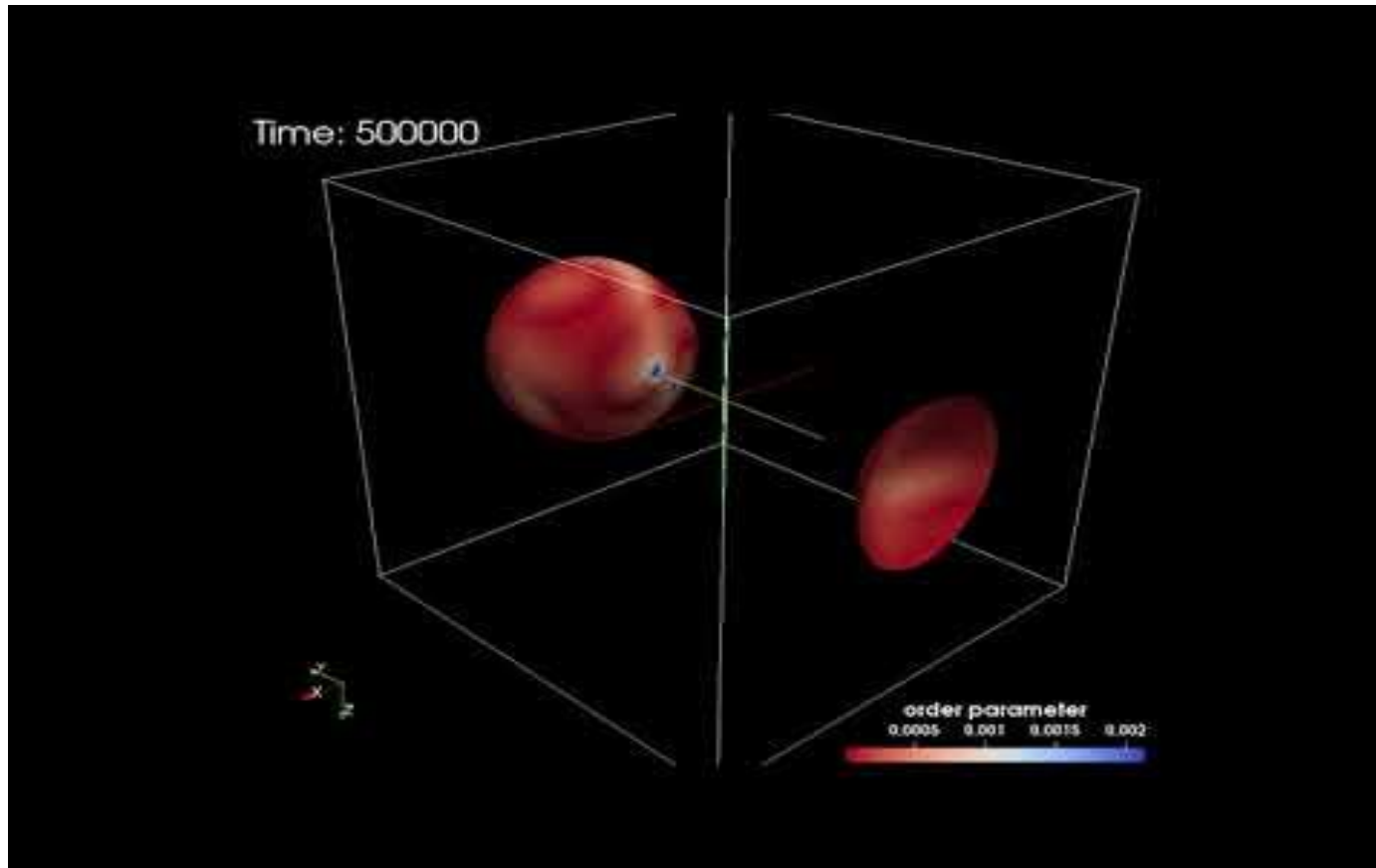
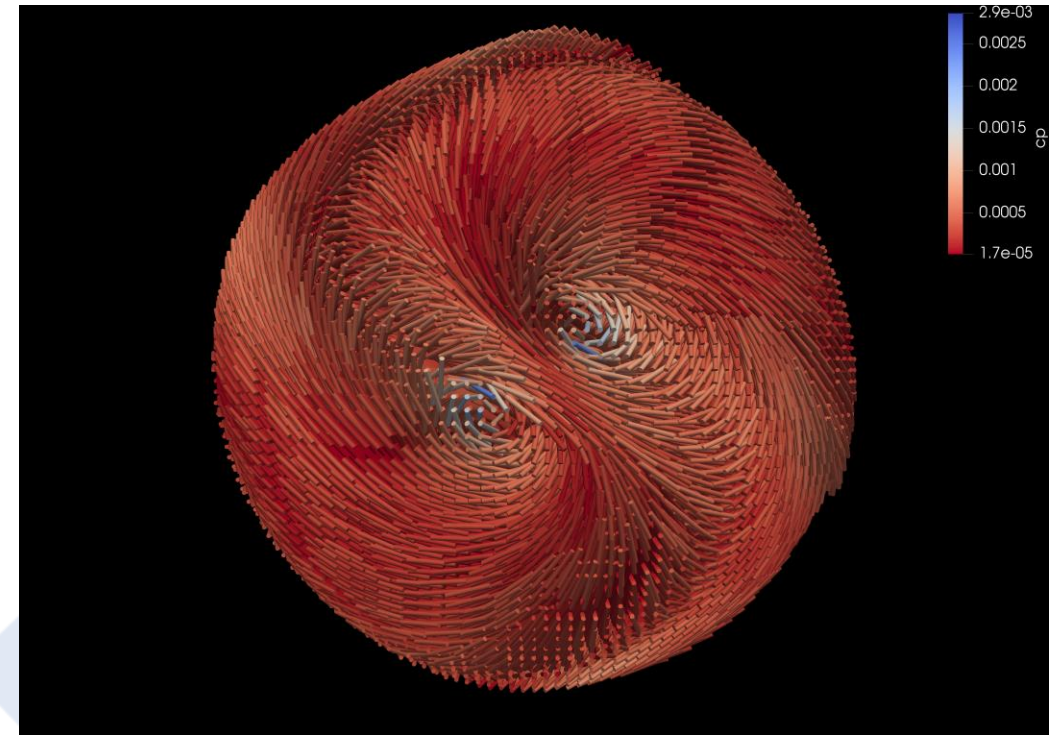
[R. Zhang, Y. Zhou, M. Rahimi, J.J. de Pablo](#), Dynamic structure of active nematic shells
Nat. Commun. [2016](#)

Active Nematic Droplet





Active Chiral Droplet



- Chirality is ubiquitous in biological matter (DNA, acto-myosin, microtubules, etc...)
- Chirality is at base of life and exploited in cell motility (motor proteins, flagella, etc...)
- Liquid Crystal can exhibit cholesteric features
- Active chiral droplets spontaneously sustain droplet propulsion

Thank you for your attention!
