Theoretical models and simulations for complex and active fluids

DOTTORATO IN FISICA TEORICA
XXXII CICLO

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SUMMARY

- Theoretical models for Complex and active fluids
- Numerical methods
- Active Fluids
- Cholesteric LC
- Active cholesteric droplet

COMPLEX AND ACTIVE FLUIDS

- Fluids with internal structure and active components (bacteria suspended in passive fluids)**‘’soft matter systems”**
- Intermediate scales of organization **continuous description with coarse grained fields**

Continuity equation

$$\partial_t \rho = -\partial_\alpha (\rho u_\alpha)$$

Navier-Stokes

$$\partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha \; u_\beta) = -\partial_\alpha p + \partial_\alpha \sigma_{\alpha\beta}$$

Stress Tensor

$$\sigma_{\alpha\beta} = \sigma_{\alpha\beta}^{\text{passive}} + \sigma_{\alpha\beta}^{\text{active}}$$

Convection-diffusion

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \nabla \cdot (M \nabla \frac{\delta F}{\delta \phi})$$

Advection relaxation

$$(\partial_t + \mathbf{u} \cdot \nabla)\mathbf{Q} - \mathbf{S}(\mathbf{W}, \mathbf{Q}) = \Gamma \nabla \cdot (\frac{\delta F}{\delta \mathbf{Q}})$$

LB METHODS

Based on phase-space discretize form of the Boltzmann equation

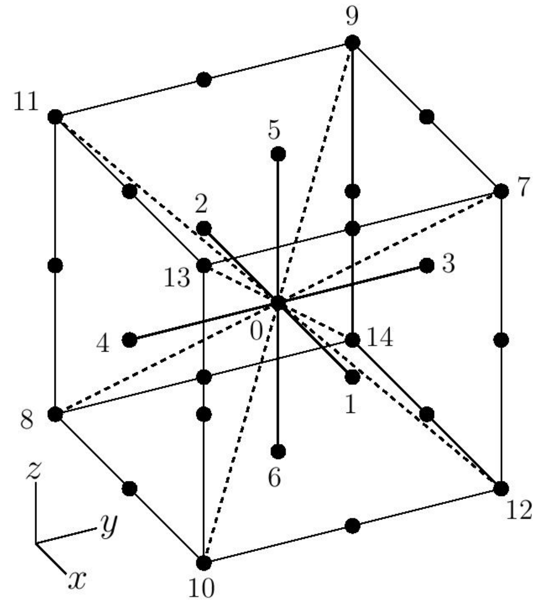
Discretization both in real and velocity space: algorithm expressed in terms of a set of discretized distribution functions $\{f_i(\mathbf{x}_\alpha, t)\}$

$$f_i(\mathbf{x} + c\mathbf{e_i}\Delta t, t + \Delta t) - f(\mathbf{x}, t) = -\Delta t \frac{f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t)}{\tau} + \Delta t F_i$$

Mass and momentum density are defined as

$$\sum_i f_i^{\mathrm{eq}} e_{i\alpha} = \rho u_\alpha \qquad \sum_i f_i^{\mathrm{eq}} = \rho$$

$$\sum_i f_i^{\mathrm{eq}} e_{i\alpha} e_{i\beta} = -\sigma_{\alpha\beta} + \rho u_\alpha u_\beta$$

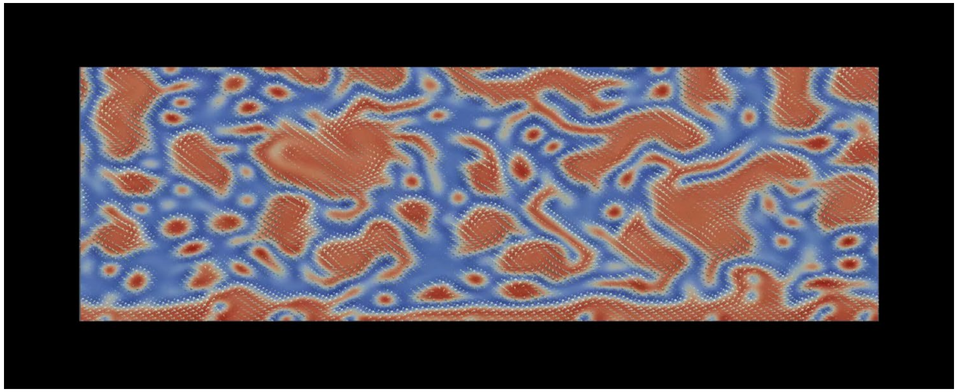


D3Q15 geometry

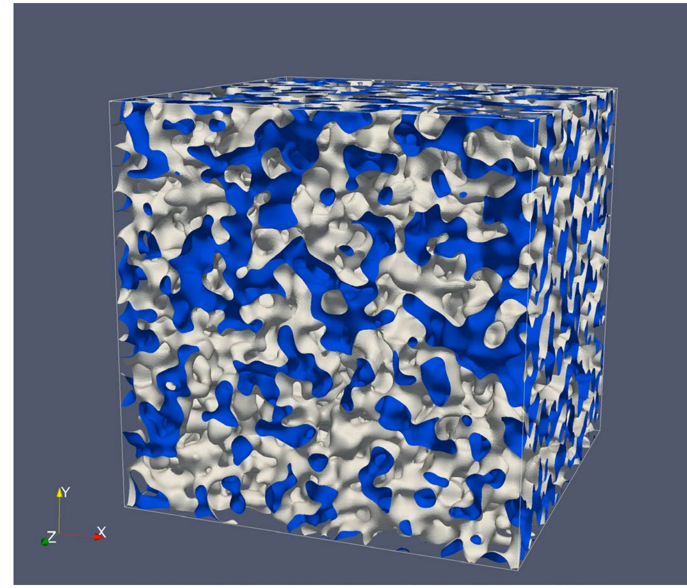
The equilibrium distribution functions are expanded up to a given order in the fluid velocity **u.** The expansion coefficients are determined imposing the above constraints

- Development and Implementation of a 3D LB scheme
- Parallelization

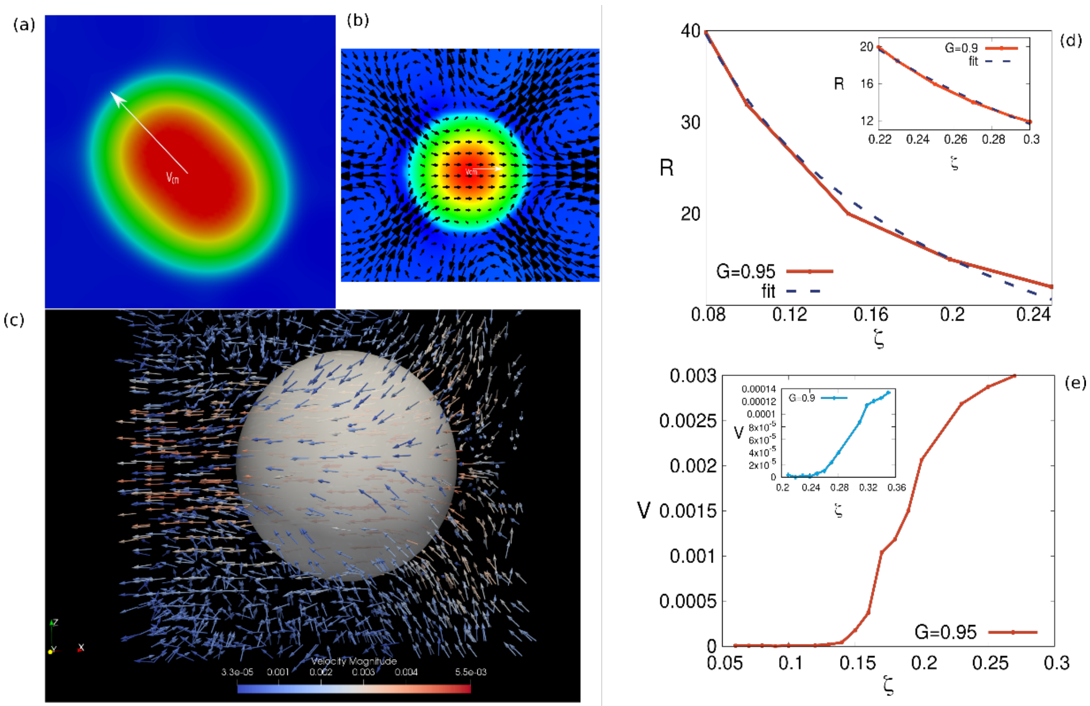
Int. Journal modern physics C (2019) **& The European Physical Journal E** 42 (6), 81, (2019)



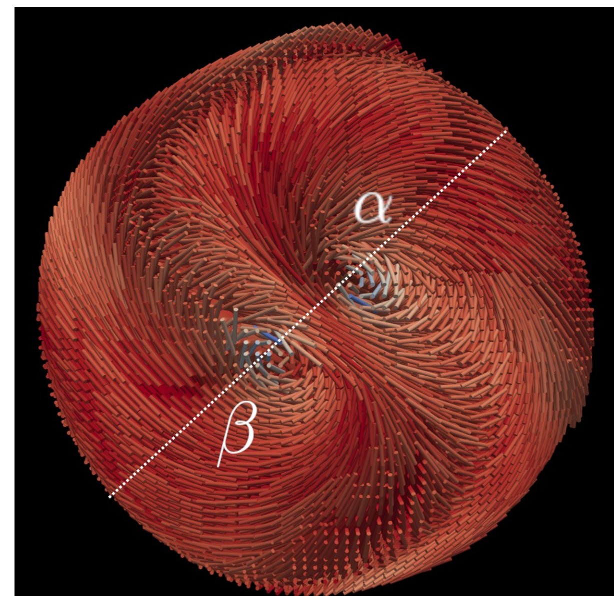
Entropy production in out of equilibrium active-fluids
Soft Matter (2018)



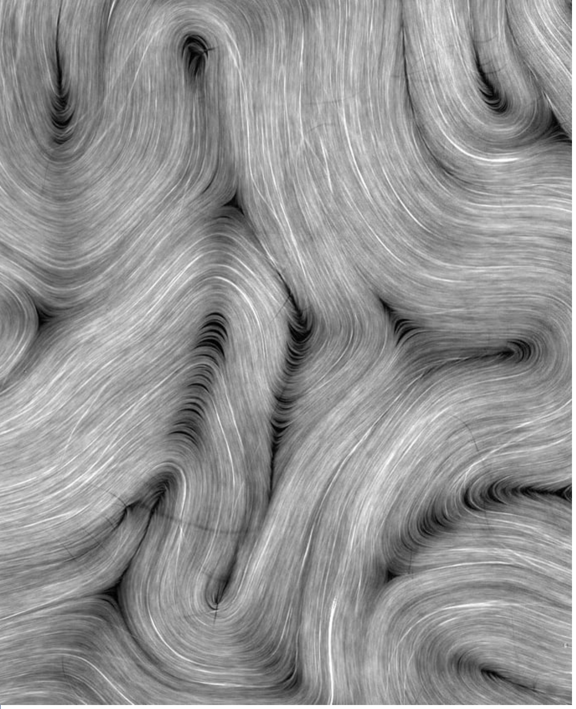
Kinetics of Liquid-Vapor phase separation (In preparation) & **Int. Journal modern physics C (2019)**

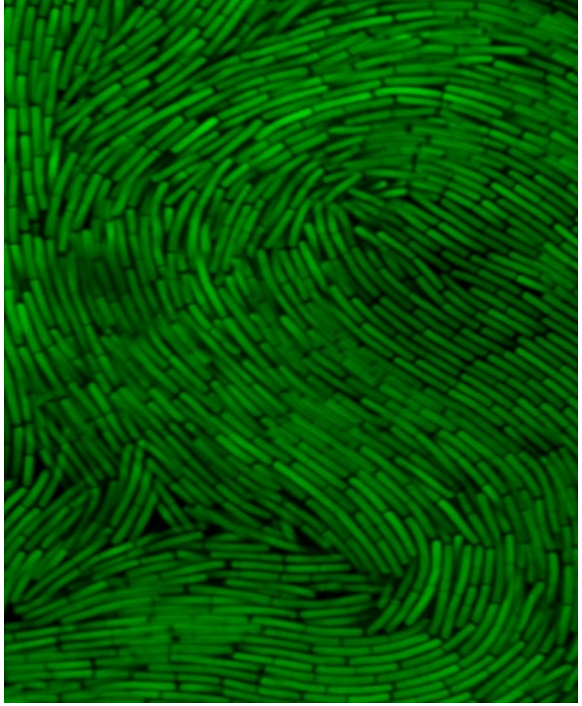


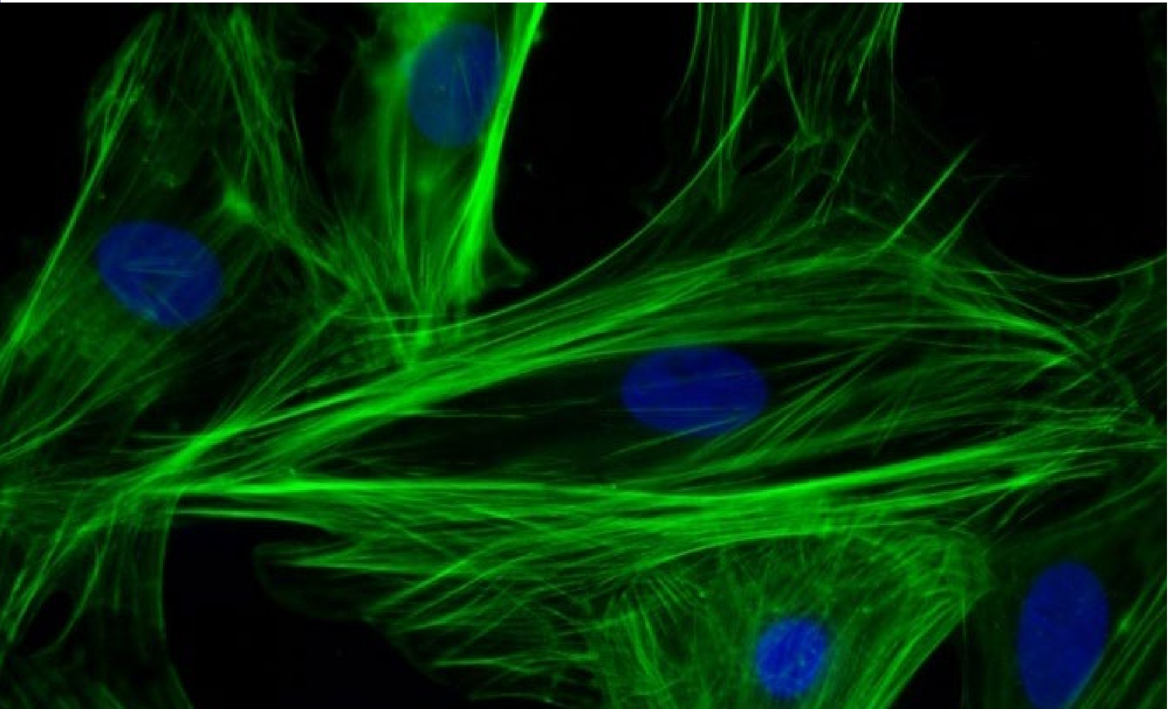
Role of compressibility in contraction based droplets motility
EPL (2019) 127 (5), 58001



Rotation and propulsion in 3D active chiral droplets
PNAS (2019) doi_10.1073/pnas.1910909116



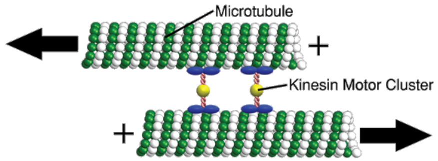


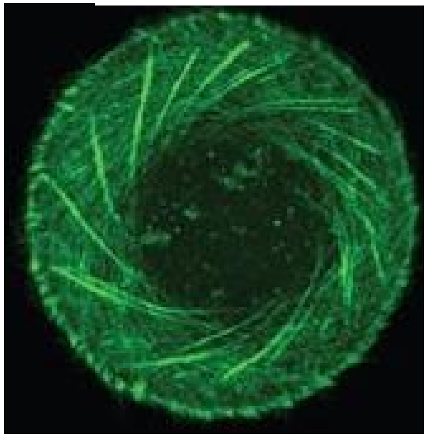


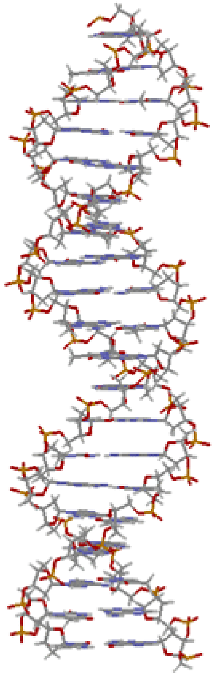
ACTIVE FLUIDS

CHIRALITY IN BIOLOGICAL SYSTEMS

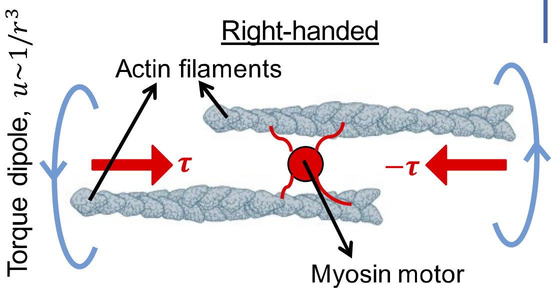
Spiral arrangement in confined cytoskeletal extracts

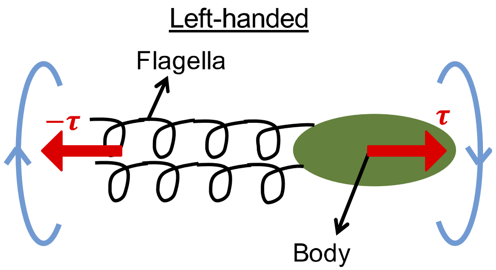






DNA





Actomyosin

Bacteria

DYNAMICAL MODEL

Dynamical fields:

- Concentration field ϕ
- Nematic field $Q_{\alpha\beta}$
- Velocity field $\mathbf{v}$

$$\partial_t \varphi + \nabla \cdot (\varphi \mathbf{v}) = \nabla \cdot \left(M \nabla \frac{\delta \mathcal{F}}{\delta \varphi} \right)$$

$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{Q} - \mathbf{S}(\mathbf{W}, \mathbf{Q}) = \Gamma \mathbf{H}$$

Numerical method:

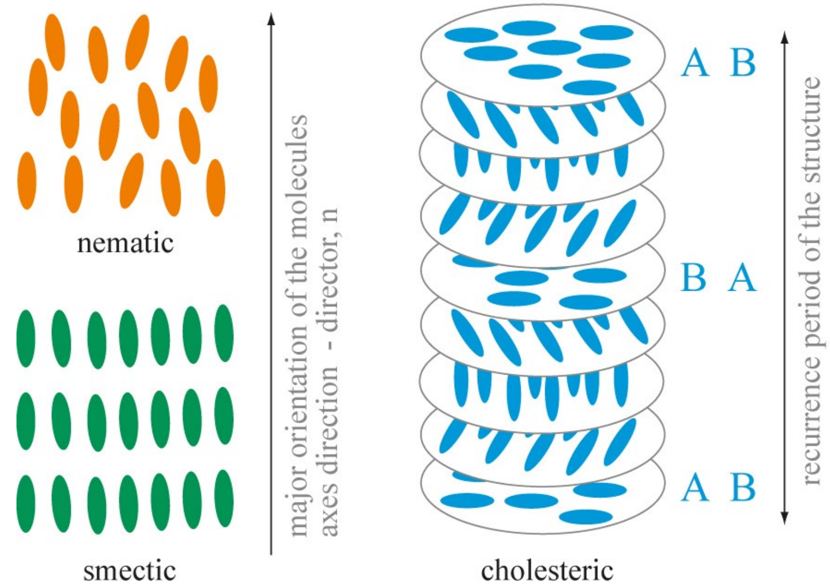
- Lattice Boltzmann
- Finite difference
- MPI implementation

$$\mathbf{H} = -\frac{\delta \mathcal{F}}{\delta \mathbf{Q}} + \frac{\mathbf{I}}{3} Tr \left(\frac{\delta \mathcal{F}}{\delta \mathbf{Q}} \right)$$

$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{v} = \nabla \cdot \left[\sigma^{pass} + \sigma^{act} \right]$$

Lattice Boltzmann methods and active fluids, The European Physical Journal E 42 (6), 81, (2019)

LANDAU-DE GENNES THEORY



$$\mathcal{F}[\phi, Q_{\alpha\beta}] = \int dV \Big[\frac{a}{4}\phi^2(\phi-\phi_0)^2 + \frac{k_\phi}{2}(\nabla\phi)^2 + A_0\left[\frac{1}{2}\left(1-\frac{\chi(\phi)}{3}\right)\mathbf{Q}^2 - \frac{\chi(\phi)}{3}\mathbf{Q}^3 + \frac{\chi(\phi)}{4}\mathbf{Q}^4\right] + \frac{K}{2}\left[(\nabla\mathbf{Q})^2 + (\nabla\times\mathbf{Q} + 2q_0\mathbf{Q})^2\right] + W(\nabla\phi)\cdot\mathbf{Q}\cdot(\nabla\phi)\Big]$$

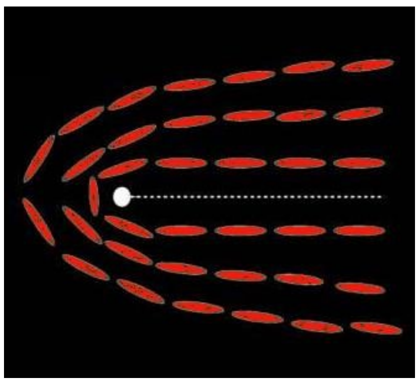
$$p_0 = \frac{2\pi}{q_0}$$

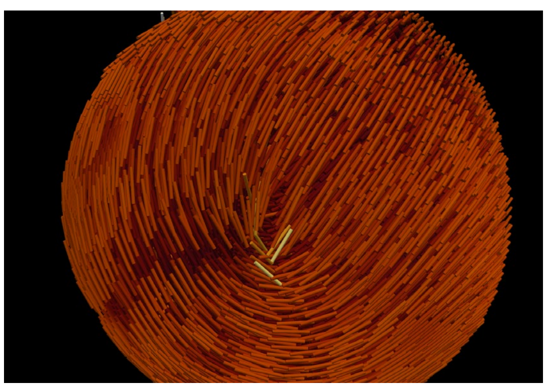
First order phase transition
I-N

$$\chi(\phi) = \chi_0 + \chi_s\phi > 2.7$$

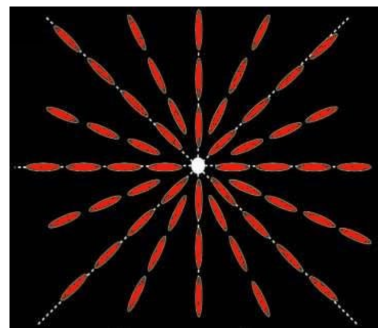
TOPOLOGICAL DEFECTS ON A HAIRY BALL: THE GAUSS-BONNET THEOREM

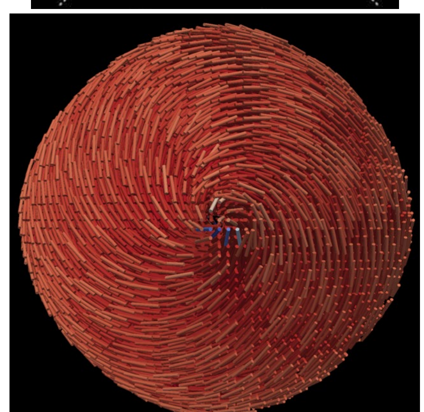
+1/2





+1





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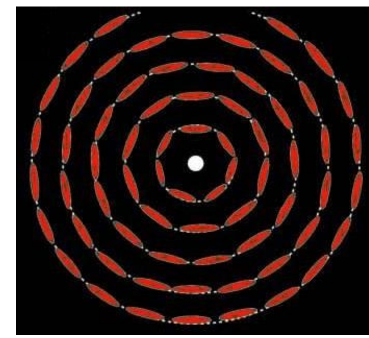
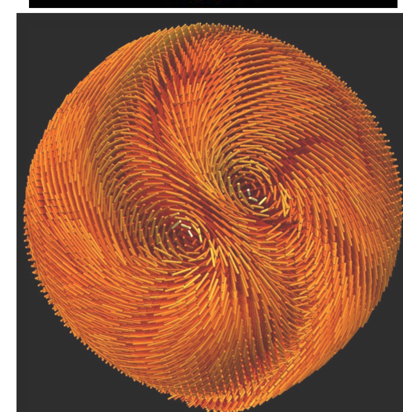




THE ACTIVE STRESS TENSOR

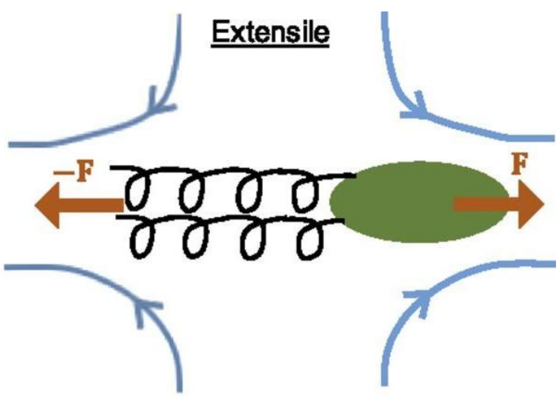
$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{v} = \nabla \cdot \left[\sigma^{pass} + \sigma^{act}\right]$$

Dissipative/Reactive terms

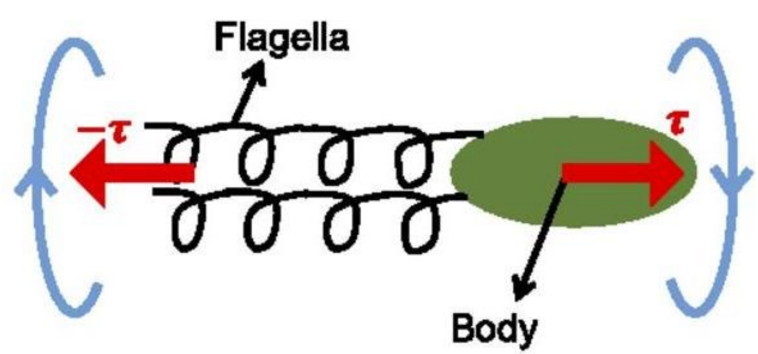
Non-Equilibrium terms

$$\sigma^{act}_{\alpha\beta} = -\zeta \phi Q_{\alpha\beta} - \bar{\zeta} \epsilon_{\alpha\mu\nu} \partial_\mu (\phi Q_{\nu\beta})$$

Force dipole

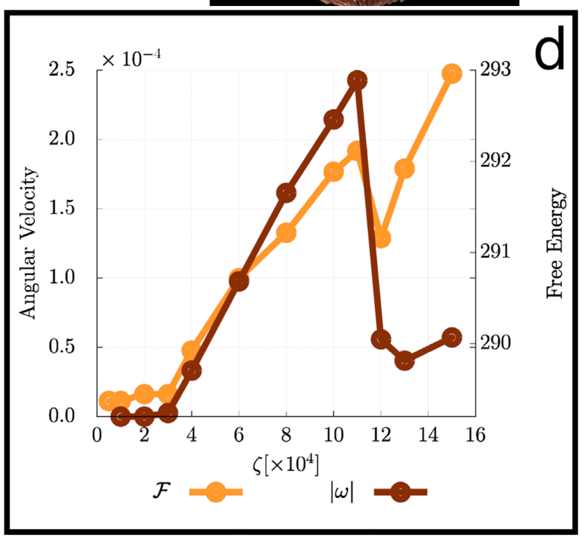


Torque dipole

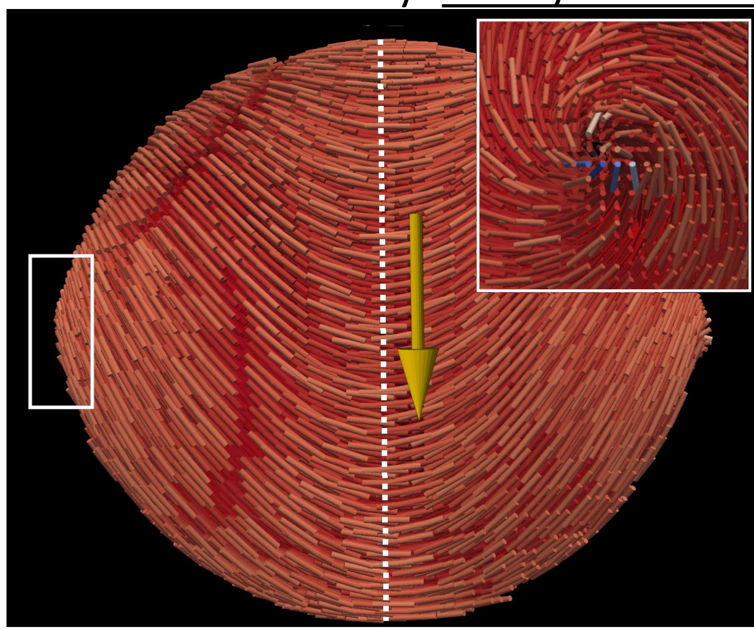


NEMATIC DROPLET

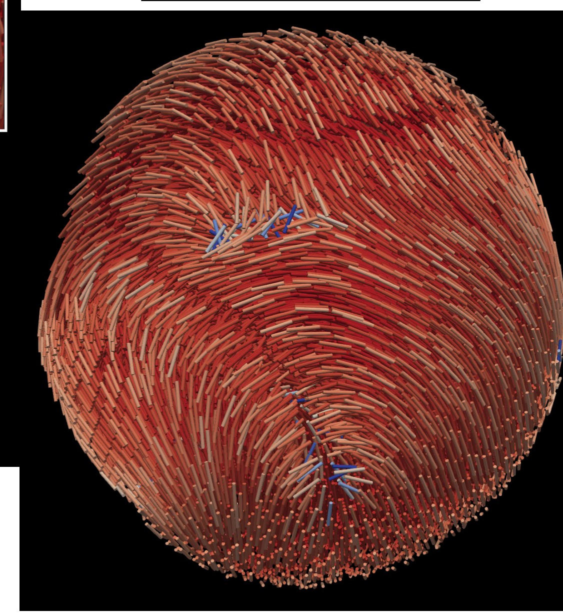
Small activity: quiescent state



Intermediate activity: steady rotational state

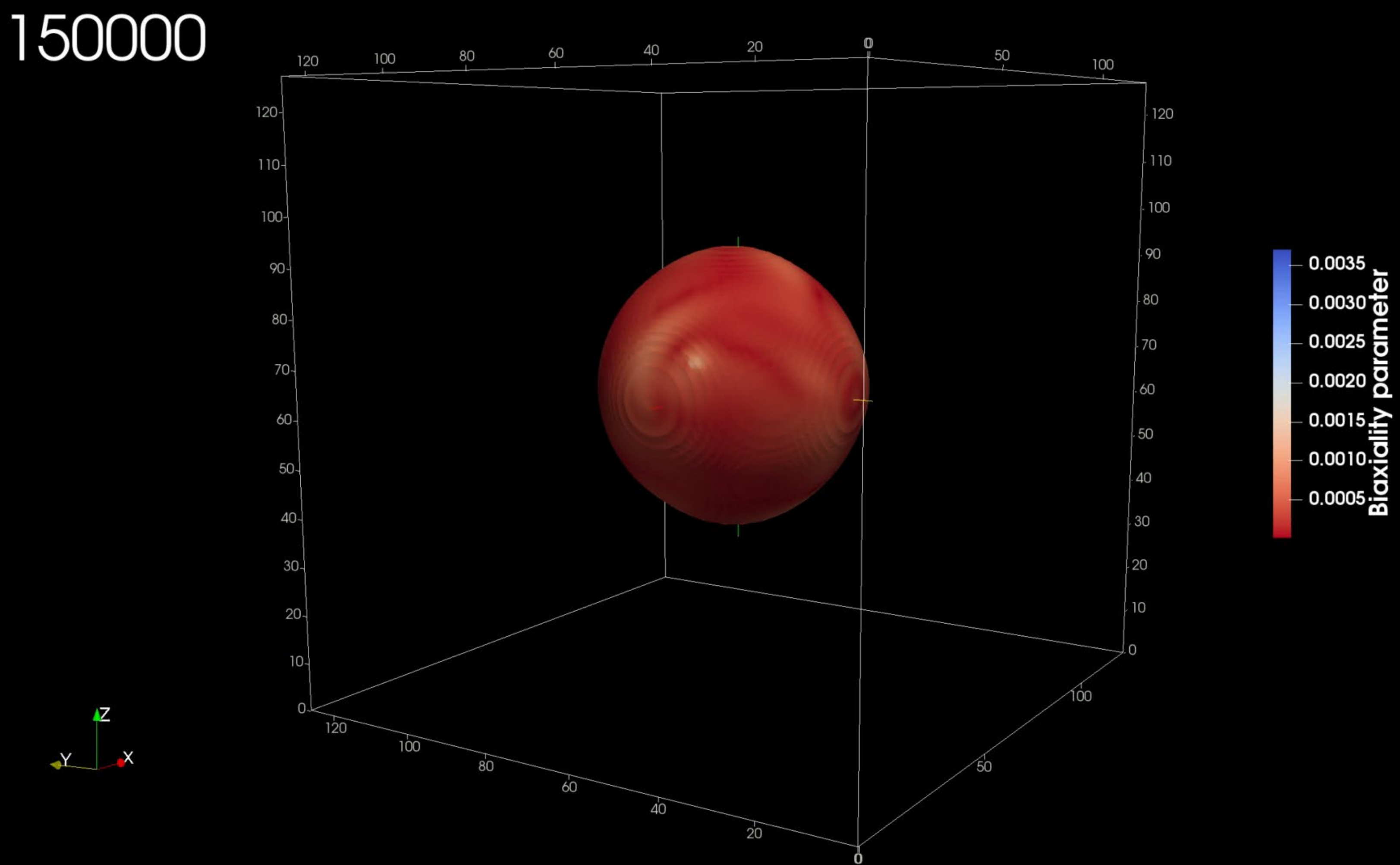


High activity:
active turbulence

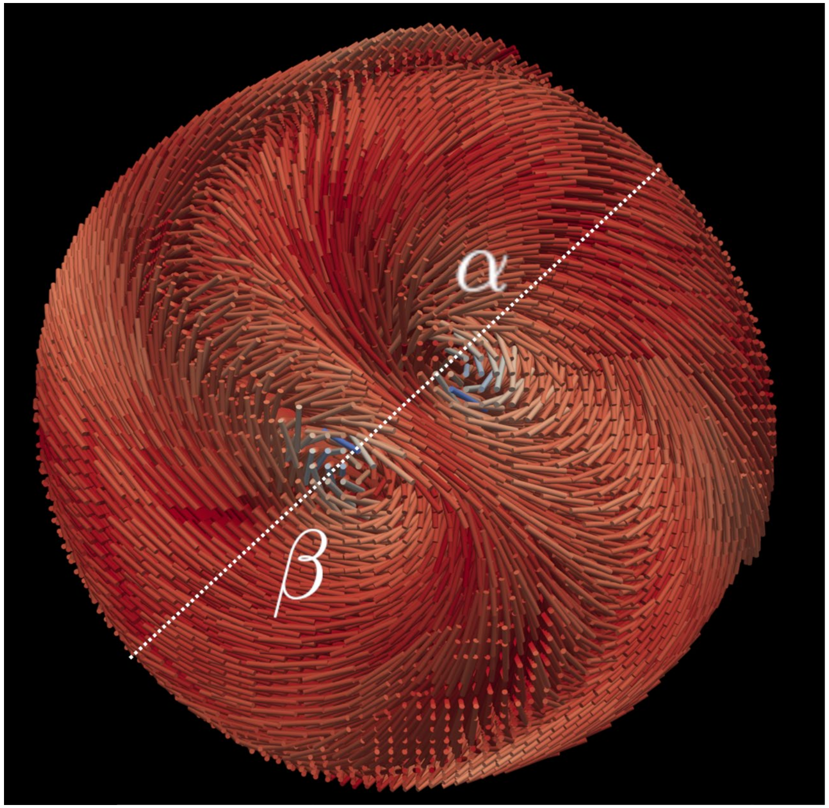


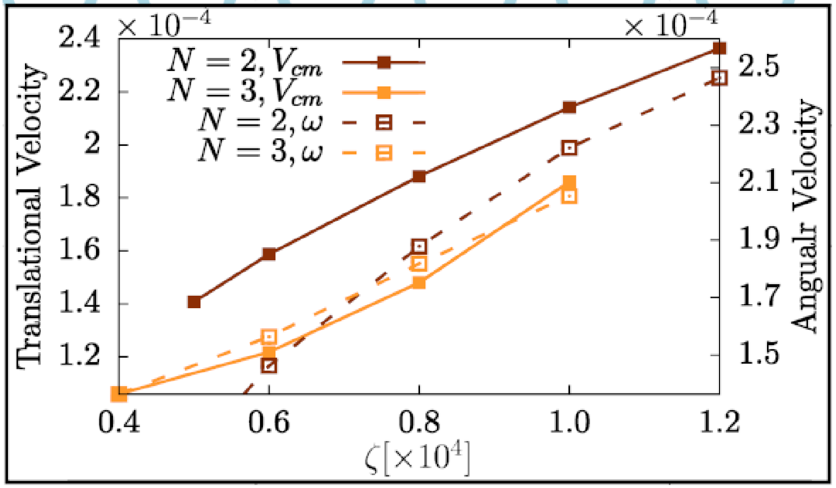
Rotation and propulsion in 3D active chiral droplets. **PNAS (2019).**
doi_10.1073/pnas.1910909116

ACTIVE CHOLESTERIC DROPLET: A NOVEL MOTILITY MODE



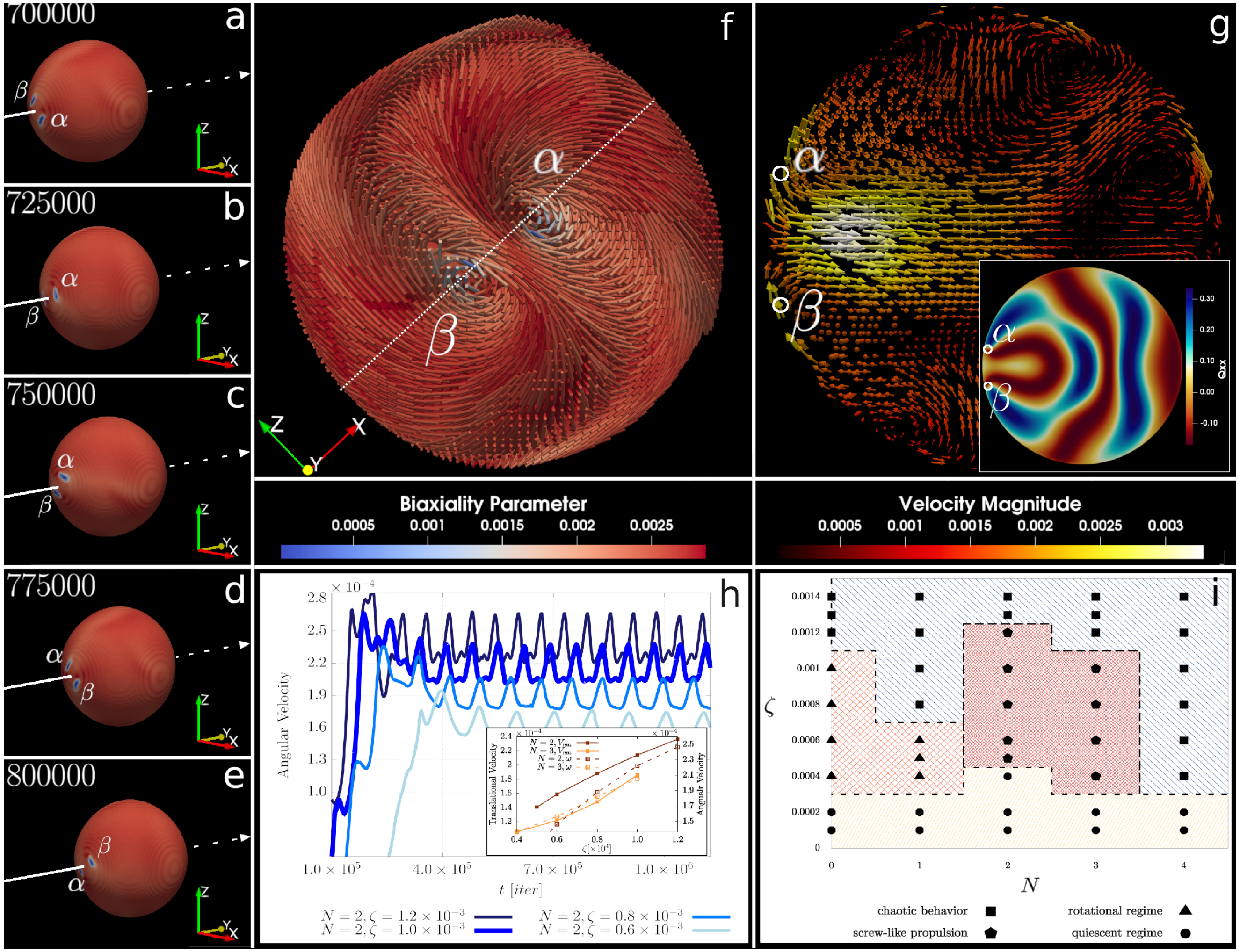
ACTIVE CHOLESTERIC DROPLET: A NOVEL MOTILITY MODE



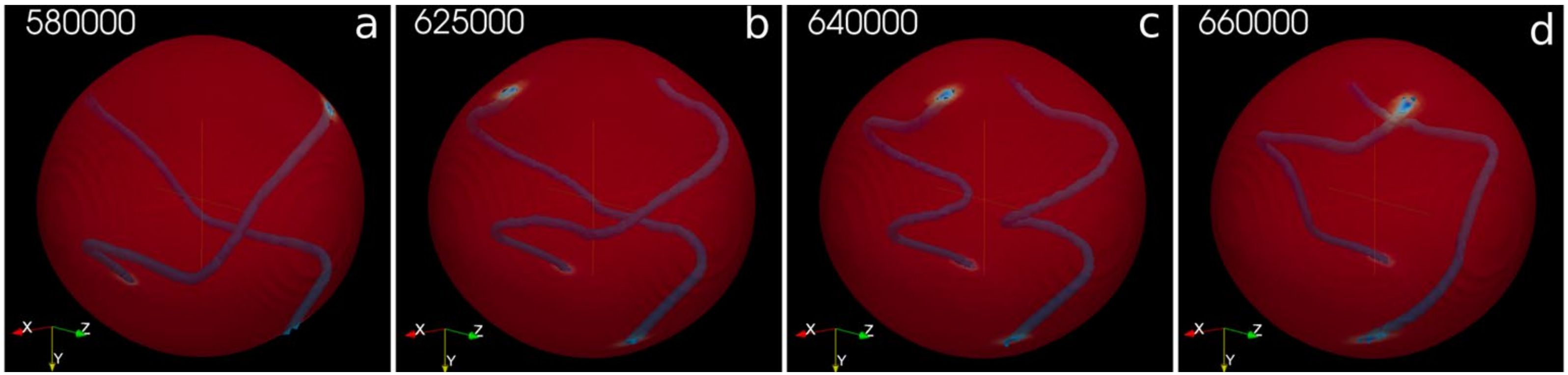


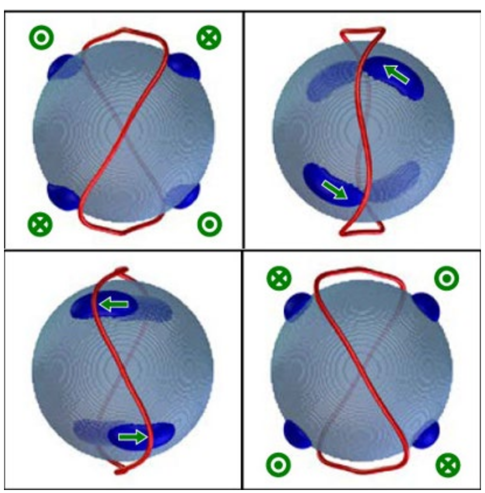
- Defects recombine in a configuration reminiscent of Frank-Pryce structure
- Activity sustains rotational motion
- Asymmetric defect configuration & rotational motion result in the propulsion of the droplet
- Velocity of the c.o.m. is tuned by activity

ACTIVE CHOLESTERIC DROPLET: A NOVEL MOTILITY MODE



ACTIVE TORQUE IN CHIRAL DROPLETS





Guillamat *et al,* Science Advances. 2018;4

$$\sigma_{\alpha\beta}^{act} = -\bar{\zeta}\epsilon_{\alpha\mu\nu}\partial_{\mu}(\phi Q_{\nu\beta})$$

- 4 defects of charge +½ are formed on droplet surface connected by two disclination lines
- Activity power mirror rotation of defects
- Defects dynamics observed in experiments of nematic active shells

PUBBLICAZIONI

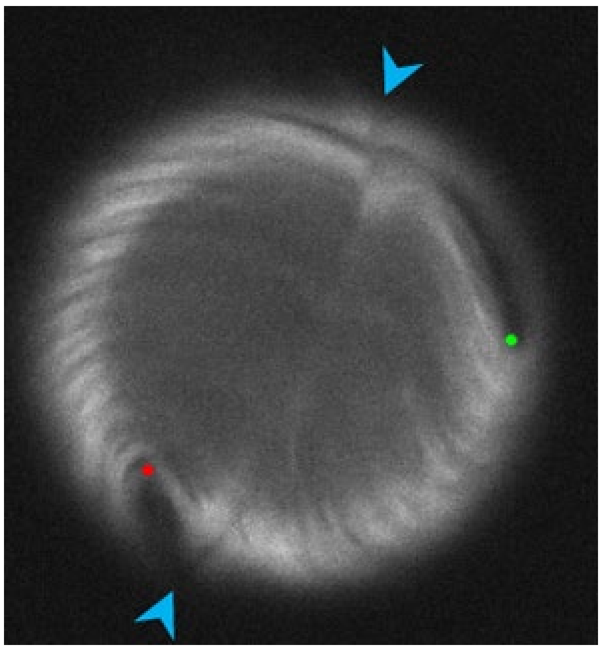
- Morphology and flow patterns in highly asymmetric active emulsions, Physica A: Statistical Mechanics and its Applications 503, 464-475
- Lattice Boltzmann methods and active fluids, The European Physical Journal E 42 (6), 81
- Hydrodynamics of contraction-based motility in a compressible active fluid, EPL (Europhysics Letters) 127 (5), 58001
- Comparison between isothermal collision-streaming and finite-difference lattice Boltzmann models, International Journal of Modern Physics C
- Rheology of active polar emulsions: from linear to unidirectional and inviscid flow, and intermittent viscosity, Soft matter
- Dynamically asymmetric and bicontinuous morphologies in active emulsions, International Journal of Modern Physics C, 1941002
- Rotation and propulsion in 3d active chiral droplets, PNAS (2019)

Proceedings

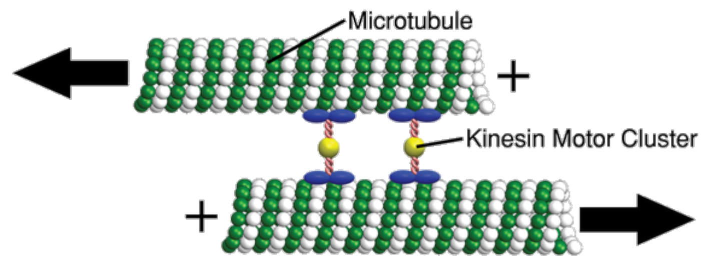
- In silico characterization of asymmetric active polar emulsions, G. Negro, L.N. Carenza, P. Digregorio, G. Gonnella, A. Lamura, AIP Conference Proceedings 2071 (1), 020012

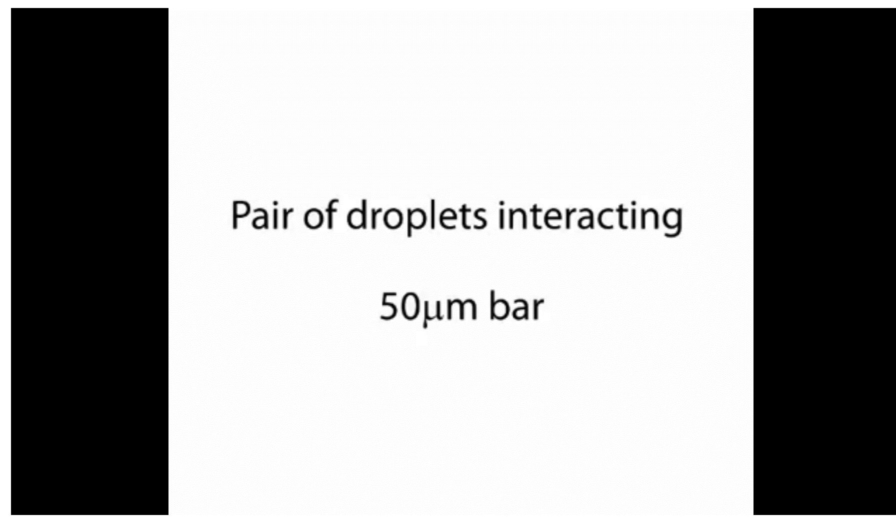
Thank you for your attention

EXPERIMENTS ON ACTIVE DROPLETS



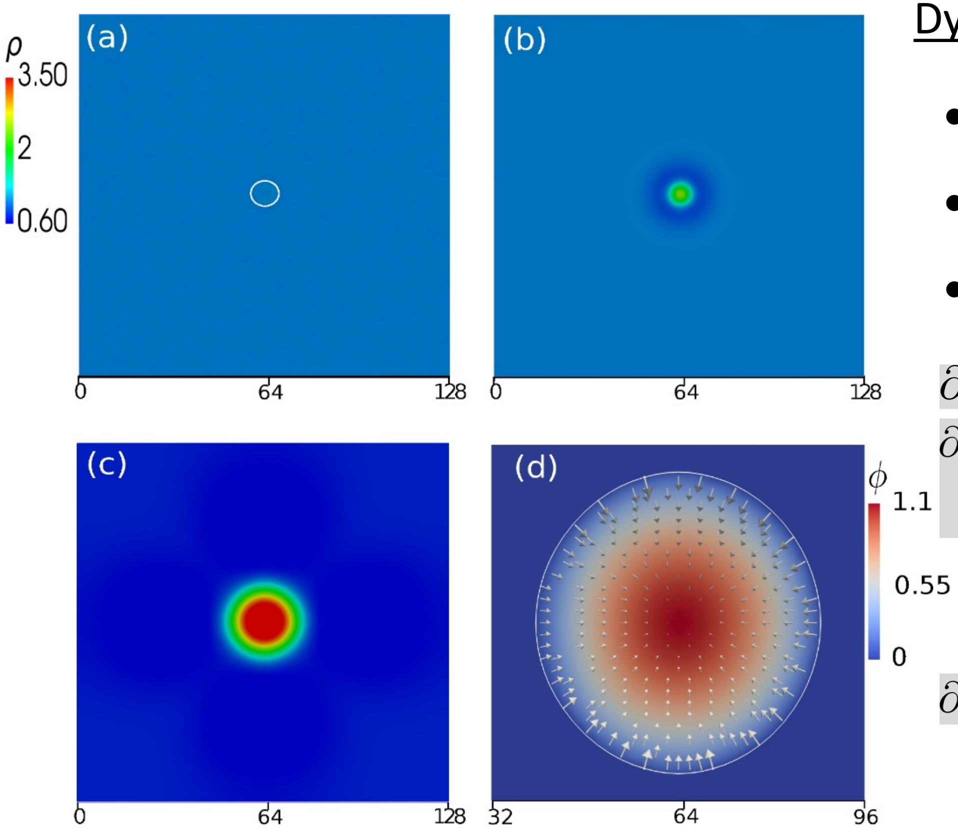
Guillmat et al. Active nematic emulsions
Science Advances Apr. 2018;





Keber *et al.* Topology and dynamics of active nematic vesicles, Science, Sept 2014; 345(6201), 1135-1139.

MINIMAL MODEL TO STUDY THE ROLE OF COMPRESSIBILITY IN CELL MOTION



Dynamical fields:

- Myosin Concentration field ϕ
- Actin density ρ
- Velocity field $\mathbf{v}$

$$\partial_t \rho + \partial_\alpha \rho v_\alpha = 0$$

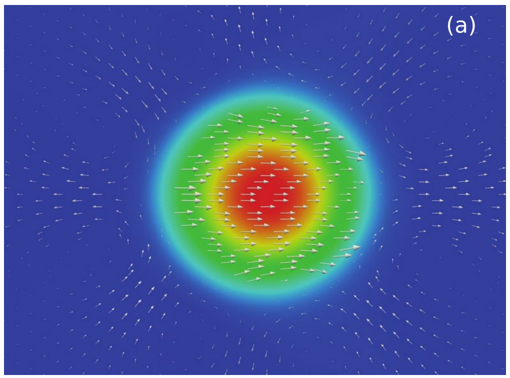
$$\partial_t v_\alpha + \partial_\beta(\rho v_\alpha v_\beta) = F_\alpha^{\text{int}} + F_\alpha^{\text{active}} + F_\alpha^{\text{interface}} + F_\alpha^{\text{viscous}}$$

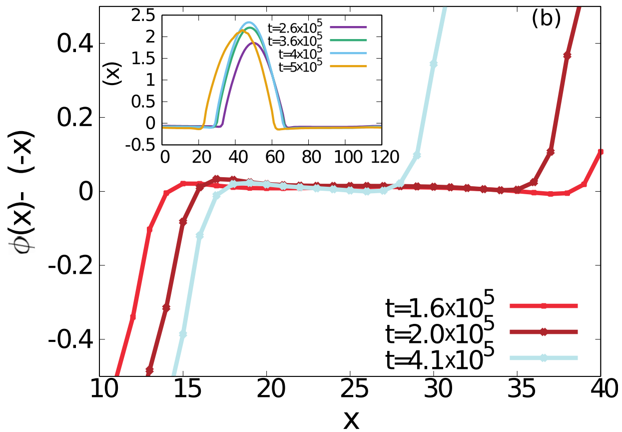
$$F_\alpha^{active} = \zeta \partial_\alpha \phi \qquad F_\alpha^{int} = -\partial_\alpha P^i + \partial_\alpha G\rho$$

$$\partial_t \phi + \partial_\beta(\phi v_\beta) = +D\nabla^2\phi - b\nabla^2\rho - K(\nabla^2)^2\phi$$

Contraction induced clustering

DROPLET MOTION AND STABILITY

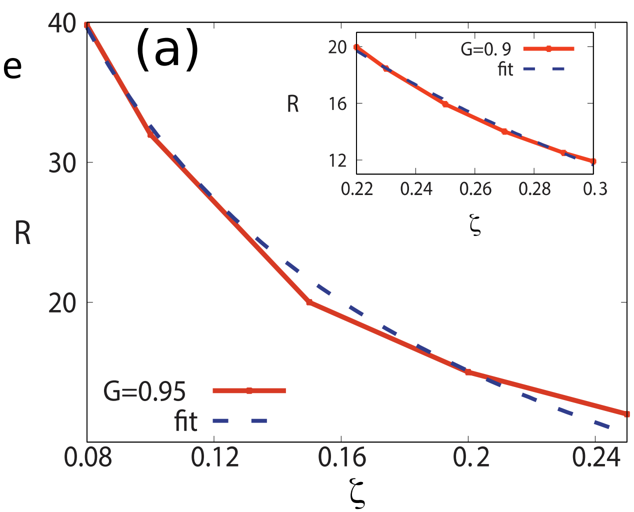


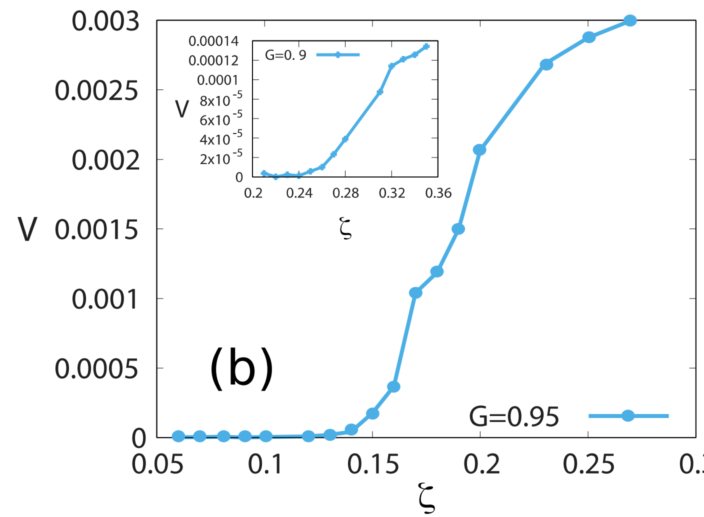


- Droplet first polarize
- Simple directed flow

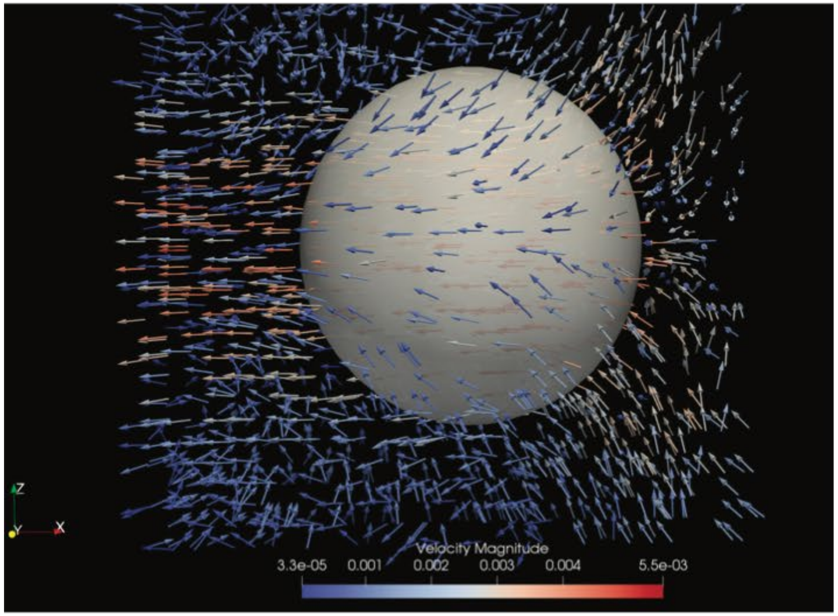
- Transition to a motile droplet

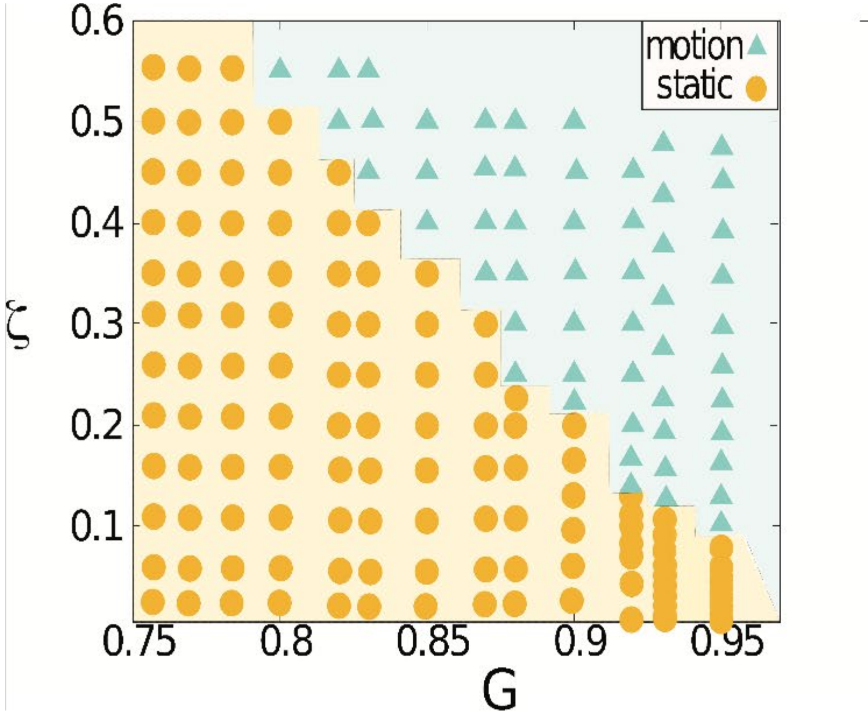
$$R_c \sim \sqrt{\frac{1}{\zeta}}$$





PHASE DIAGRAM: ONSET OF DROPLET MOTILITY





<u>Flow of a droplet in 3D strongly resemble that of a cell swimming in a matrigel</u>