



Cholesteric Liquid Crystals & Active Emulsions

DOTTORANDO: LIVIO NICOLA CARENZA

SUPERVISOR: PROF. GONNELLA

Summary

- ▶ General Framework
- ▶ Lattice Boltzmann Method for Liquid Crystals in three-dimensional geometries
- ▶ Cholesteric Liquid Crystals
- ▶ Active Emulsions
- ▶ Active Turbulence

General Framework

- ▶ Model & Methods of numerical fluid dynamics: coarse grained approach

General Framework

- ▶ Model & Methods of numerical fluid dynamics: coarse grained approach
- ▶ Generalized Navier-Stokes equation

$$\begin{aligned} \partial_t(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \otimes \vec{v}) \\ = -\nabla p + \nabla \cdot \left(\underline{\underline{\sigma}}^{viscous} + \underline{\underline{\sigma}}^{complex} \right) \end{aligned}$$

General Framework

- ▶ Model & Methods of numerical fluid dynamics: coarse grained approach
- ▶ Generalized Navier-Stokes equation
- ▶ Binary mixtures \longrightarrow Concentration scalar field φ

$$\begin{aligned} \partial_t(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \otimes \vec{v}) \\ = -\nabla p + \nabla \cdot \left(\underline{\underline{\sigma}}^{viscous} + \underline{\underline{\sigma}}^{complex} \right) \end{aligned}$$

$$\partial_t \varphi + \nabla \cdot (\varphi \vec{v}) = M \nabla^2 \mu \quad , \quad \mu = \frac{\delta F^{bm}}{\delta \varphi}$$

General Framework

- ▶ Model & Methods of numerical fluid dynamics: coarse grained approach
- ▶ Generalized Navier-Stokes equation
- ▶ Binary mixtures \longrightarrow Concentration scalar field φ
- ▶ Anisotropic contributions: vector/tensor order parameters Ψ

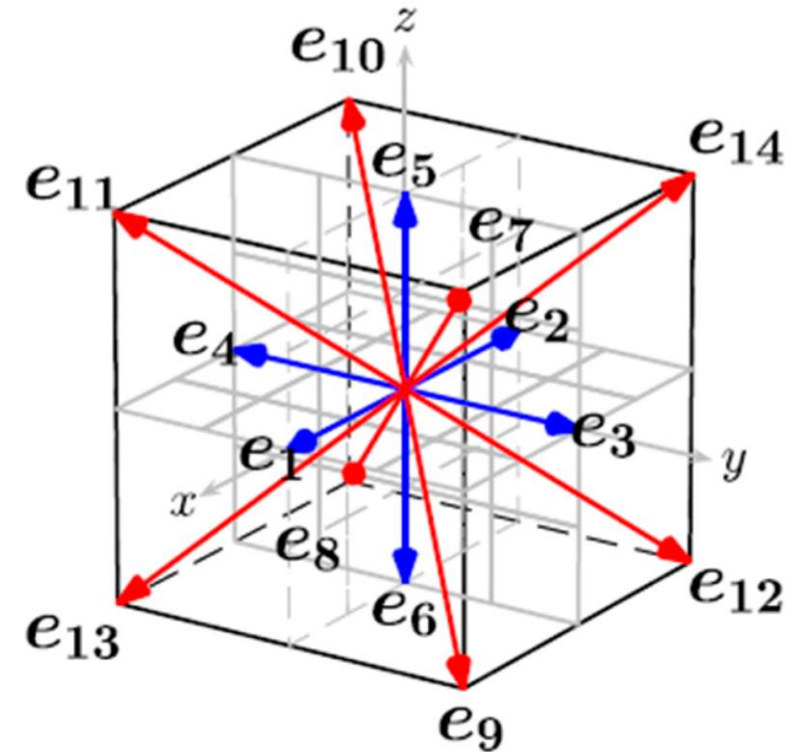
$$\partial_t(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \otimes \vec{v}) = -\nabla p + \nabla \cdot (\underline{\underline{\sigma}}^{viscous} + \underline{\underline{\sigma}}^{complex})$$

$$\partial_t \varphi + \nabla \cdot (\varphi \vec{v}) = M \nabla^2 \mu, \quad \mu = \frac{\delta F^{bm}}{\delta \varphi}$$

$$\partial_t \Psi + \vec{v} \cdot \nabla \Psi + S = \Gamma \frac{\delta F}{\delta \Psi}$$

3d Lattice Boltzmann Method

- ▶ Boltzmann Equation \longrightarrow Discretized time, space and velocity
- ▶ Distribution functions $f_i(\vec{x}_\alpha, t)$
- ▶ Physical observables $\rho(\vec{x}_\alpha, t) = \sum_i f_i(\vec{x}_\alpha, t)$ $\rho \vec{v} = \sum_i \vec{e}_i f_i(\vec{x}_\alpha, t)$
- ▶ DF dynamics
 - ▶ Collision (BGK approximation)
$$f_i^{coll}(\vec{x}_\alpha, t) = f_i(\vec{x}_\alpha, t) - \frac{1}{\tau} [f_i(\vec{x}_\alpha, t) - f_i^{eq}(\vec{x}_\alpha, t)]$$
 - ▶ Streaming $f_i(\vec{x}_\alpha + \vec{e}_i \Delta t, t + \Delta t) = f_i^{coll}(\vec{x}_\alpha, t)$
- ▶ Equilibrium DF \longrightarrow Expansion at II order in $\vec{v} \longrightarrow$ Recover continuum equations



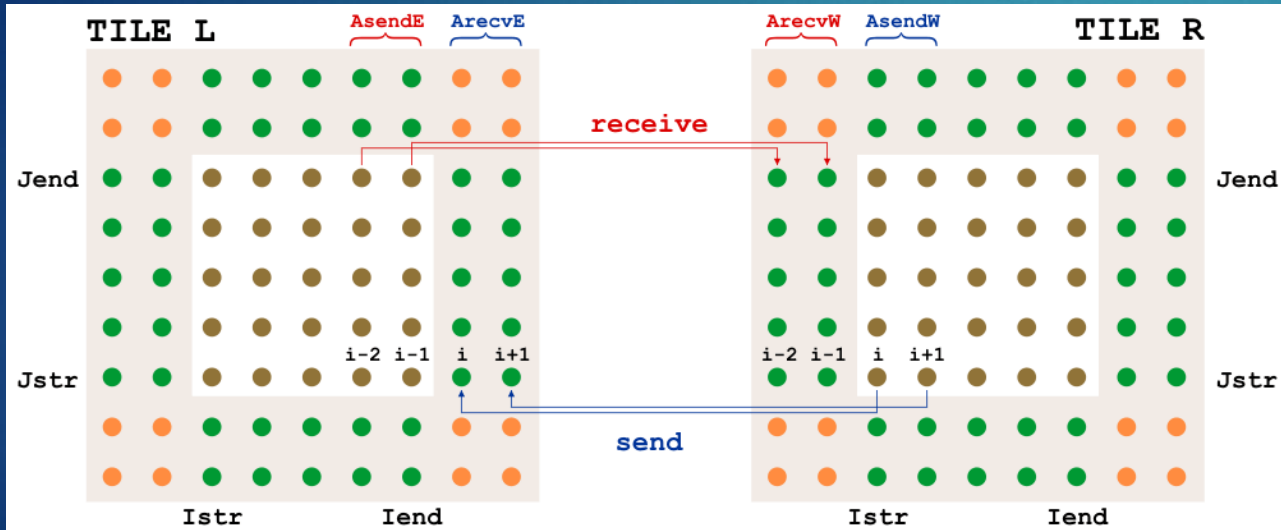
Parallelization

- ▶ Long simulation times
- ▶ Huge amount of memory

Parallelization

- ▶ Long simulation times
- ▶ Huge amount of memory

Be Wise... Parallelize!!!



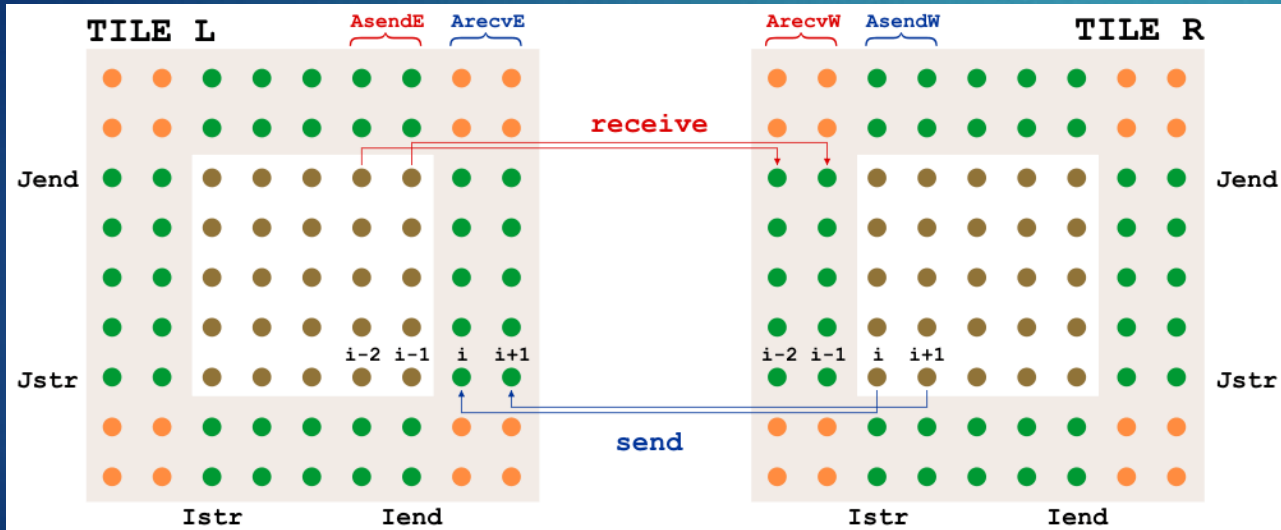
- ▶ Summer school on Parallel Computing – Cineca (BO)
- ▶ Advanced School on Parallel Computing – Cineca (BO)

Parallelization

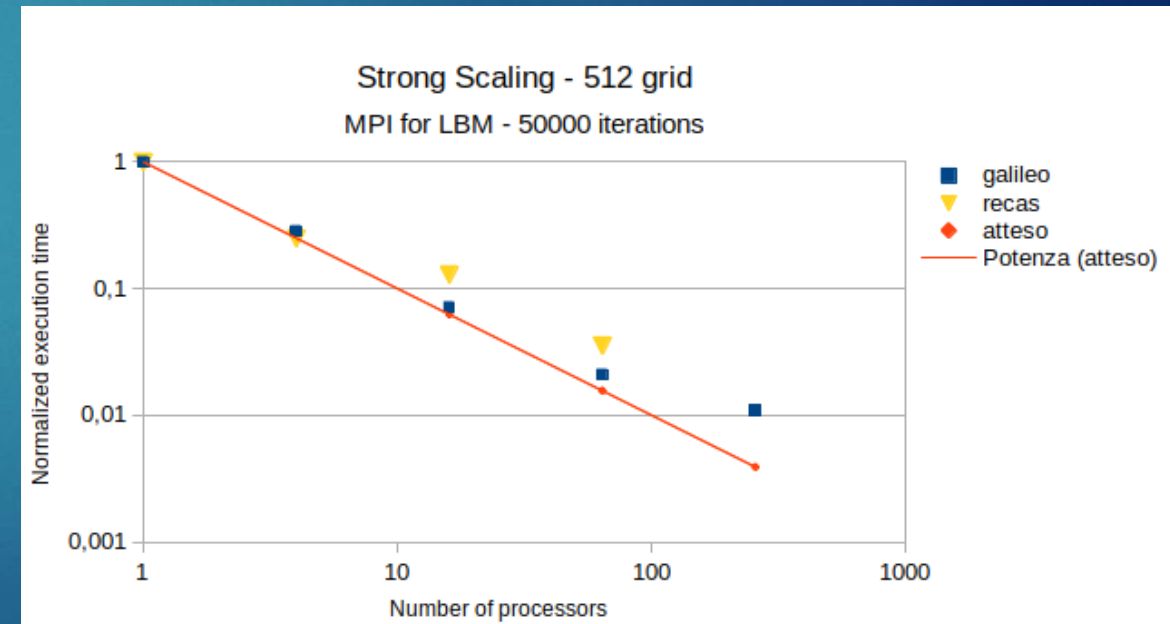
- ▶ Long simulation times
- ▶ Huge amount of memory

Be Wise... Parallelize!!!

- ▶ Message Passing Interface
- ▶ ~ 40Gb of Memory
- ▶ ~ 3y of CPU

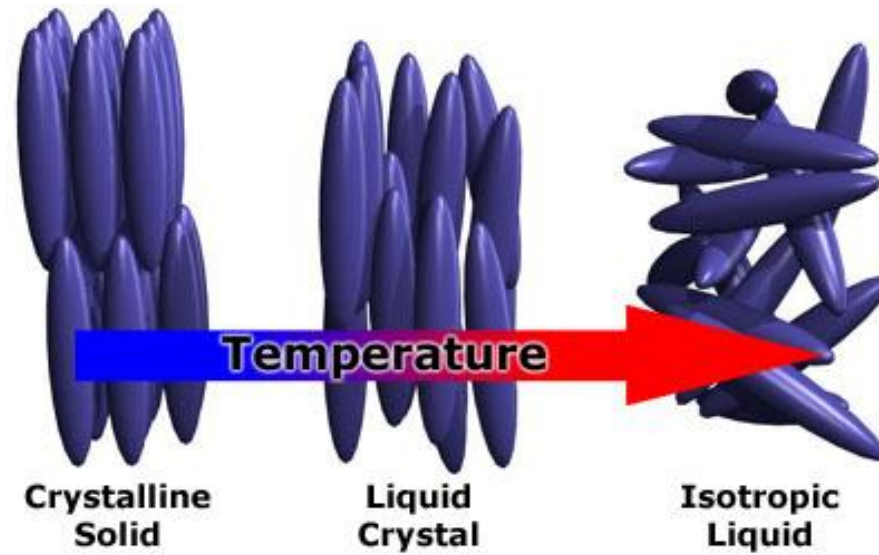


- ▶ Summer school on Parallel Computing – Cineca (BO)
- ▶ Advanced School on Parallel Computing – Cineca (BO)



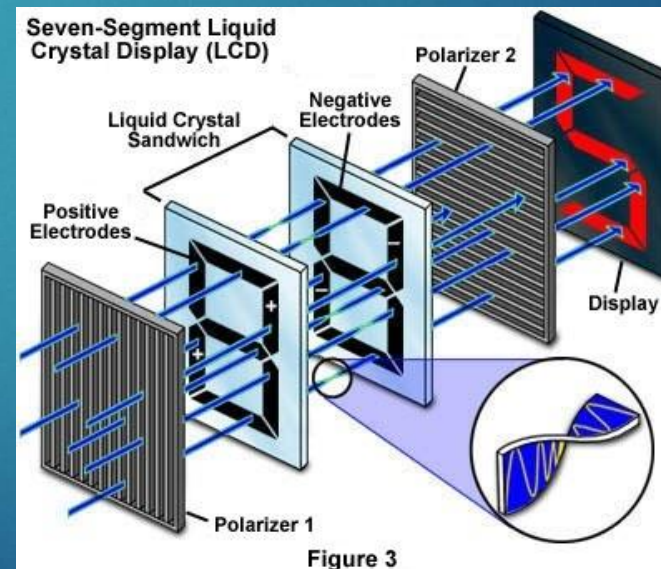
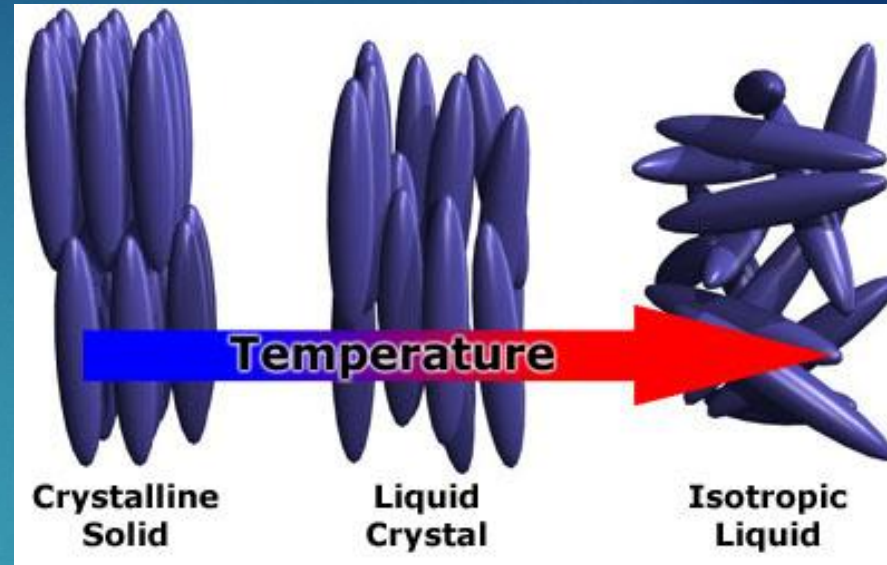
Cholesteric Liquid Crystals

- ▶ Long chained molecules in solution
- ▶ Lost translational order, preserved directional order



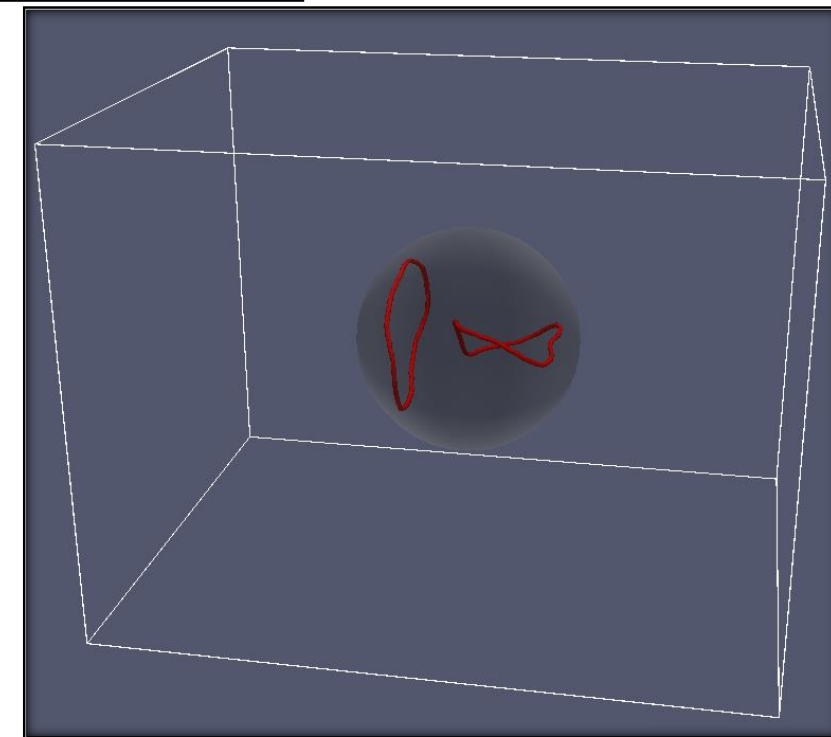
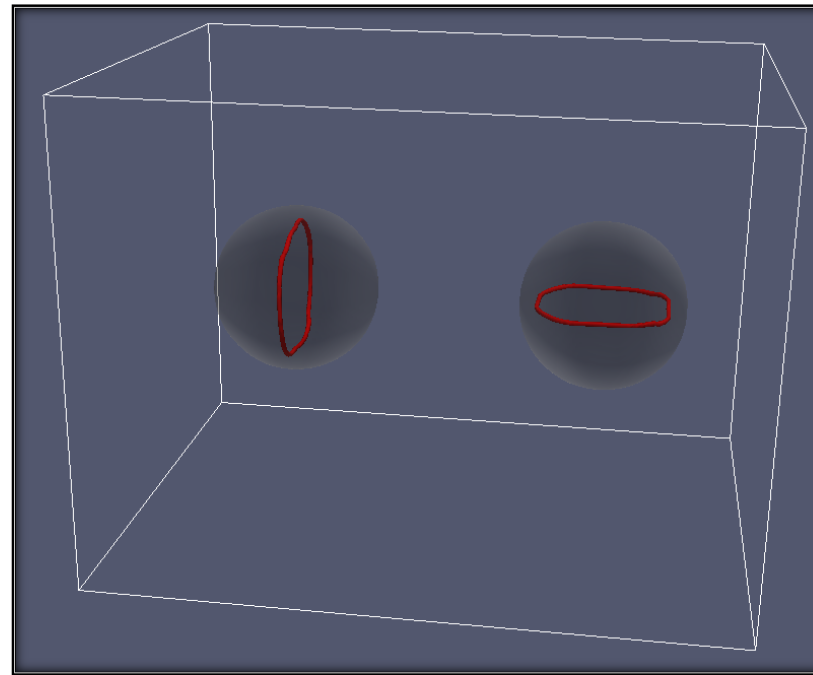
Cholesteric Liquid Crystals

- ▶ Long chained molecules in solution
- ▶ Lost translational order, preserved directional order
- ▶ Chirality → Cholesteric LC
- ▶ Optical properties



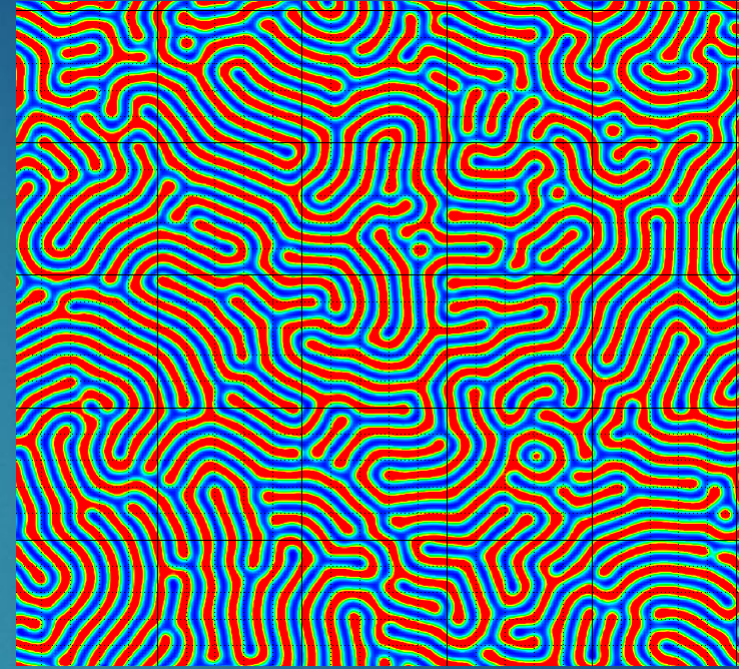
Defects in CLC droplets

- ▶ Fundamental for optical properties
- ▶ Strong dependence on geometry and boundary condition
- ▶ Relaxing dynamics*
- ▶ Merging droplets*
- ▶ Droplets under shear
- ▶ Switching dynamics under electric field



Active Emulsions

- ▶ Active matter: energy injection on small scales
 - ▶ Bacteria Suspensions
 - ▶ Cytoskeleton extracts
- ▶ Polar order
- ▶ Confinement of active behavior



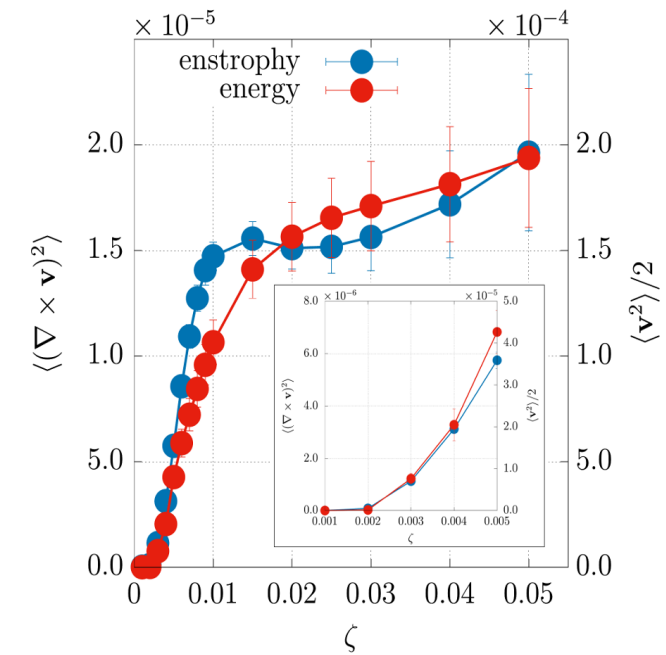
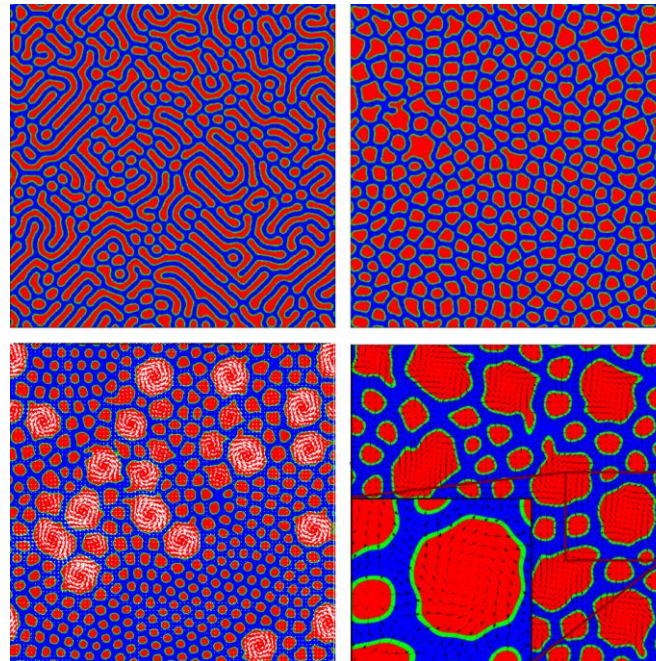
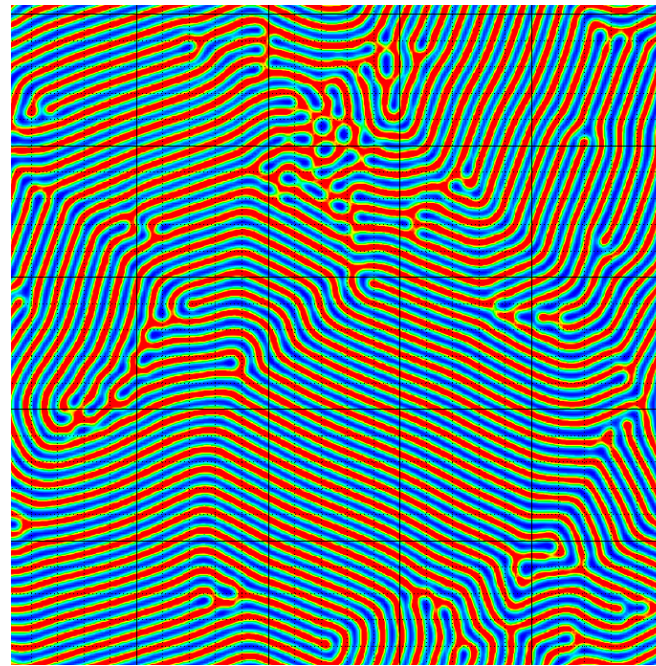
$$F = \int dV \left[\frac{a}{4 \varphi_{cr}} \varphi^2 (\varphi - \varphi_0)^2 + \frac{k_\varphi}{2} (\nabla \varphi)^2 + \frac{c}{2} (\nabla^2 \varphi)^2 + \frac{\alpha}{2} \varphi \vec{P}^2 + \frac{\alpha}{4} \vec{P}^4 + \frac{k_P}{2} (\nabla \vec{P})^2 + \beta \vec{P} \cdot \nabla \varphi \right]$$

- ▶ Lamellar phase if $a < \frac{k_\varphi^2}{4c} + \frac{\beta^2}{k_P}$ $k_\varphi < 0, c > 0$
- ▶ Active stress tensor $\sigma^{active} = -\zeta \varphi \vec{P} \otimes \vec{P}$

Results

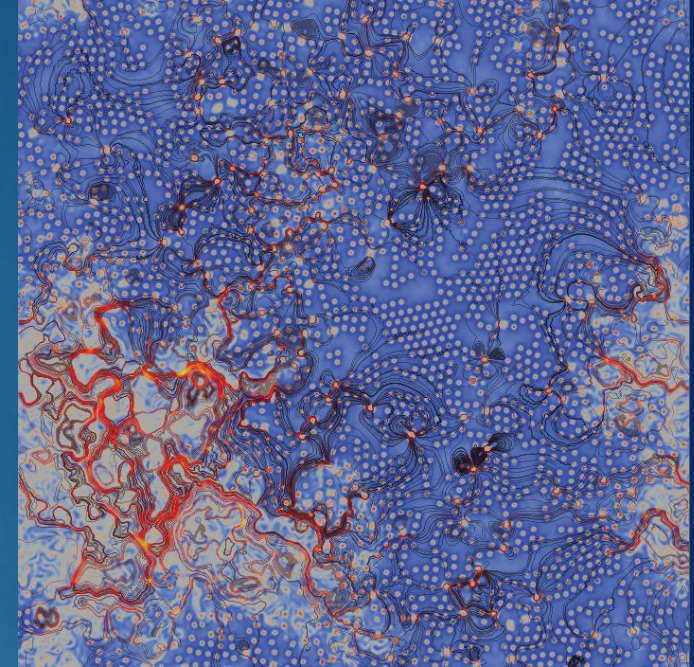
- ▶ Activity favours ordering
- ▶ Transition towards mesoscale turbulence
- ▶ Wealth of different morphologies

- ▶ [G.Negro, L.N.Carenza, P.Digregorio, G.Gonnella, A.Lamura](#) Morphology and flow patterns in highly asymmetric active emulsion, *Physica A*, Vol. 503, 2018, 464-475
- ▶ [F.Bonelli, L.N.Carenza, G.Gonnella, D.Marenduzzo, E.Orlandini, A.Tiribocchi](#) Lamellar ordering, droplet formation and phase inversion in exotic active emulsions, **Accepted with minor revisions Scientific Reports (Nature)**
- ▶ [L.N.Carenza, G.Gonnella, A.Lamura, G.Negro, A.Tiribocchi](#) Lattice Boltzmann Methods and Active Fluids, **Submitted to EPJ**



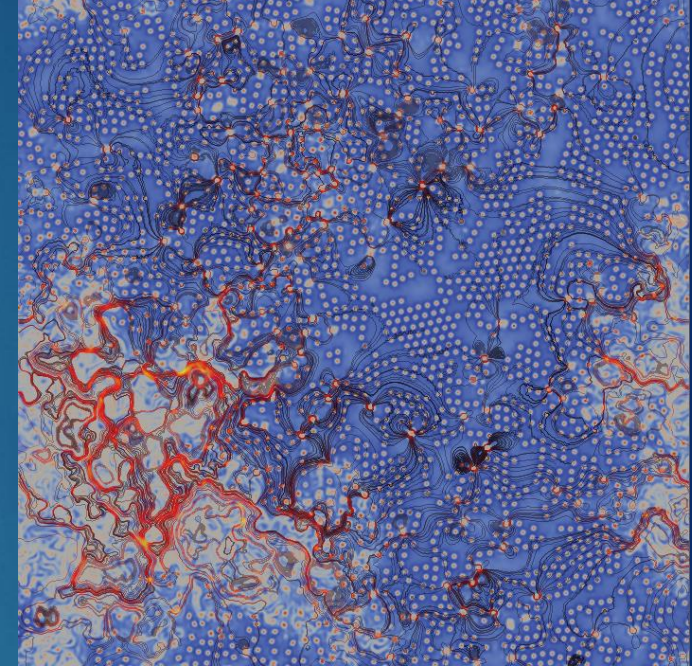
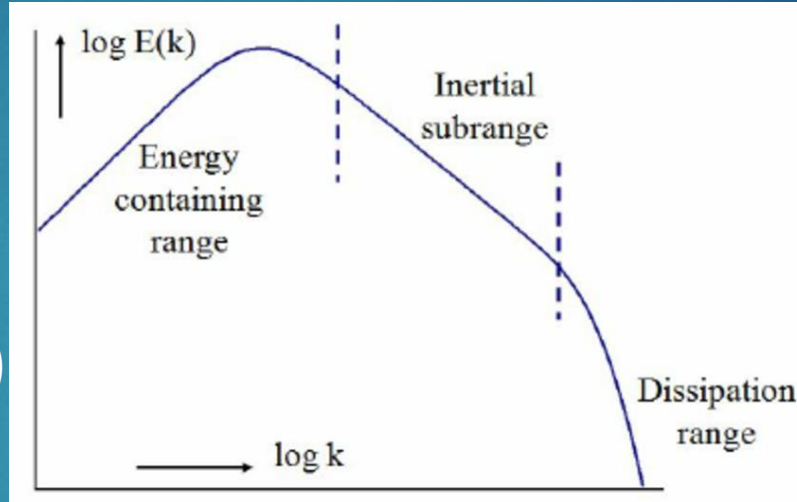
Active Turbulence

- ▶ Energy injection on small scales → Mesoscale turbulence
- ▶ What is new?



Active Turbulence

- ▶ Energy injection on small scales → Mesoscale turbulence
- ▶ What is new?
 - ▶ KOLMOGOROV TURBULENCE :
 - ▶ High Reynolds number
 - ▶ Hydrodynamics non-linearities
 - ▶ $-5/3$ spectrum (universal behavior)



Active Turbulence

► Energy injection on small scales → Mesoscale turbulence

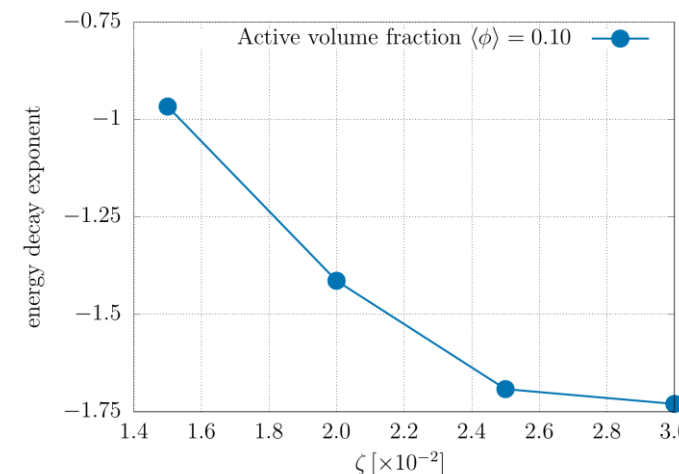
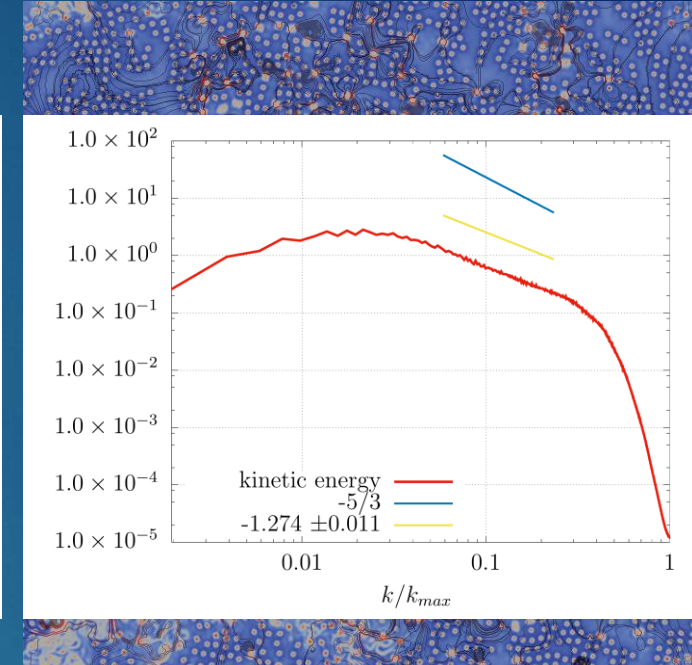
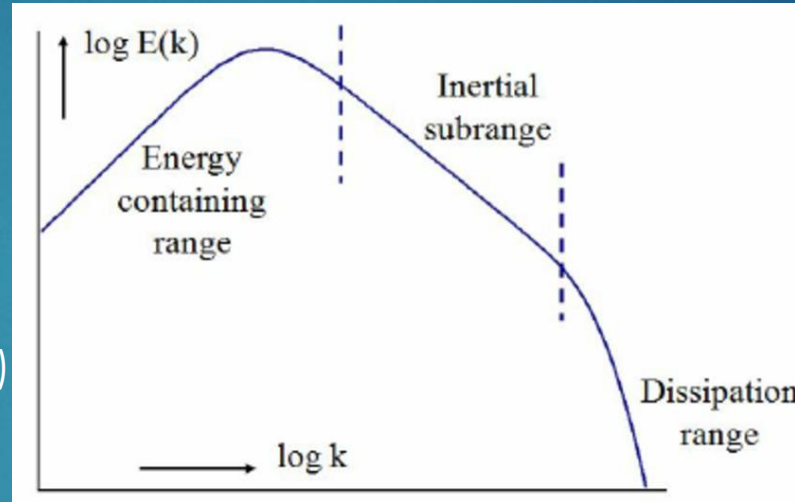
► What is new?

► KOLMOGOROV TURBULENCE :

- High Reynolds number
- Hydrodynamics non-linearities
- $-5/3$ spectrum (universal behavior)

► ACTIVE TURBULENCE

- Low Reynolds number
- Complex coupling source/sink power terms
- No universal behavior



Exams and Schools

PhD COURSES

- ▶ How to prepare a technical speech in English
- ▶ Management and knowledge of European research model and promotion of research results
- ▶ Introduction to parallel Computing and GPU Programming using CUDA
- ▶ C++
- ▶ Atom-photon interactions
- ▶ Standard model and beyond
- ▶ Linear stability analysis*
- ▶ Computational fluid dynamic*

PhD SCHOOLS

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

Courses labelled with * are being erogated.

Thank you for
your attention



Thank you for
your attention

questions?