Active Turbulence & Complex Fluids

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Project Plan

- Active Turbulence
- Complex Fluids
  - Active Nematics
  - Analysis of defects in 3D systems
  - Cholesteric droplet gauged to electric fields
- Development of high performance computing skills

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Active Fluids

- What is **active matter**?
  - Living organisms, Janus particles, biological compounds *etc.* $\Rightarrow$ Internal Energy Consumption;
  - Far-from-equilibrium dynamics $\Rightarrow$ NESS (Non Equilibrium Steady States);
  - Collective effects (*i.e.* Assembling)
- **Active Fluids**: why are they important?
  - Significant contribution to the understanding of peculiar fluid machanisms;
  - Medical and technological applications.
- Both theoretical and experimental interest

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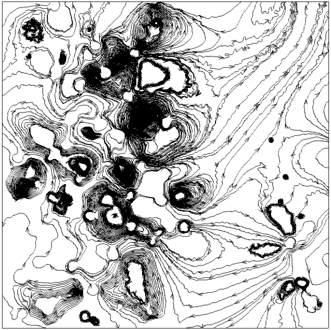
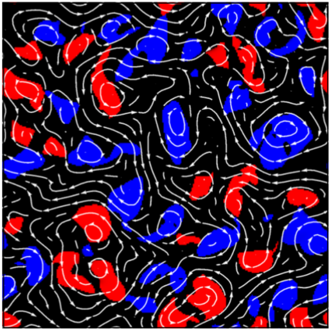
Tipical flow structure in active fluids



(a) Bonelli, Carenza, Gonnella, Marenduzzo, Orlandini, Tiribocchi



(b) Giomi

Is This Turbulence? Not yet any definitive answer in literature!

The state of art

- Until now in literature:
  - Single-component fluids;
  - 2D computer simulations;
- Our project
  - **Multi-component fluid** ⇒ **Confining Turbulence**
    - Active Polar Component
    - Passive Isotropic Component
    - Surfactant (favours emulsification)
  - 3D computer simulations ⇒ **HPC skills required**
  - Matching experimental research

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Our model (Bonelli, Carenza, Gonnella, Marenduzzo, Orlandini, Tiribocchi)

We have studied a model for **polar active binary mixture** based on a **field theory** approach.

$$\mathcal{F}[\phi, \boldsymbol{P}] = \int \mathrm{d}\boldsymbol{r} \left[\frac{a}{4\phi_{cr}^2}\phi^2(\phi-\phi_0)^2 + \frac{k}{2}(\nabla\phi)^2 + \frac{c}{2}(\nabla^2\phi)^2 - \frac{\alpha}{2}\frac{(\phi-\phi_{cr})}{\phi_{cr}}\boldsymbol{P}^2 + \frac{\alpha}{2}\boldsymbol{P}^4 + \frac{\kappa}{2}(\nabla\boldsymbol{P})^2 + \beta\boldsymbol{P}\cdot\nabla\phi \right]$$

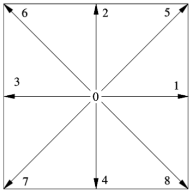
$$\rho\left(\partial_t + \boldsymbol{v}\cdot\nabla\right)\boldsymbol{v} = -\nabla P + \nabla\cdot\boldsymbol{\sigma}$$

$$\sigma_{\alpha\beta}^{act} = -\zeta\phi\left(P_\alpha P_\beta - \frac{\boldsymbol{P}^2}{3}\right)$$

Lattice Boltzmann Method

Discretized version of the Boltzmann Transport Equation

- Space discretization;
- Velocity dicretization.



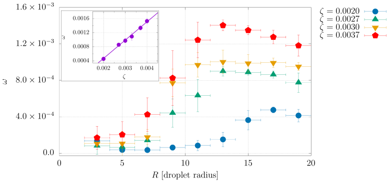
$$f_k(\boldsymbol{x}_k+\boldsymbol{e}_k\Delta t, t+\Delta t)-f_k(\boldsymbol{x}_k, t) = -\frac{1}{\tau}(f_k - f_k^{eq})$$

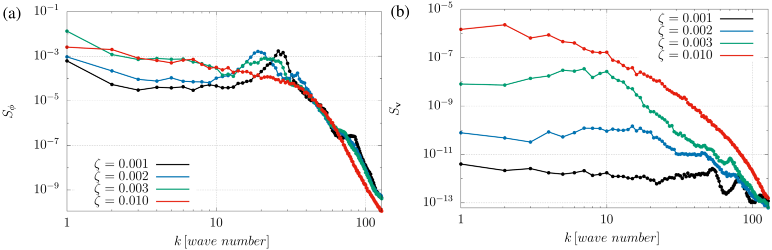
Riproducing N-S equation if constraints are satisfied:

$$\rho(\boldsymbol{x}, t) = \sum_k f_k(\boldsymbol{x}, t) \qquad \rho\boldsymbol{v} = \sum_k f_k(\boldsymbol{x}, t)\boldsymbol{e}_k$$

What has been done

- Morphology Characterization;
- Flow Characterization;
- Two articles submitted;





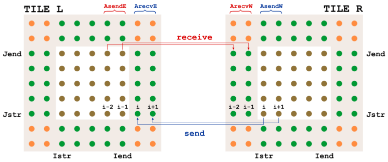
HPC for Grid Computation

Some common issues in computational fluid mechanics

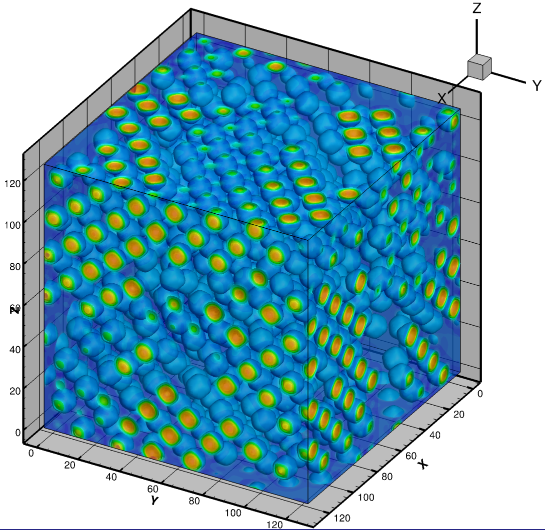
- Memory required (RAM $\sim 10^2 Gb$)
- Processing times ($\sim 3,5y$)

HPC approach required

- Pure MPI (grid division)
- Hybrid approach $\Rightarrow$ MPI+CUDA



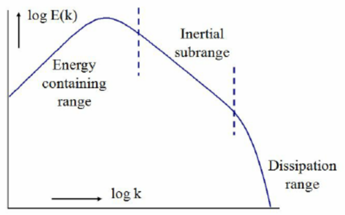
3d active emulsion



Kolmogorov Turbulence vs. Active Inverse Turbulence

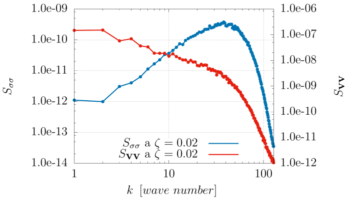
Kolmogorov Turbulence

- High Reynolds Number
- Energy flow from large to small scales

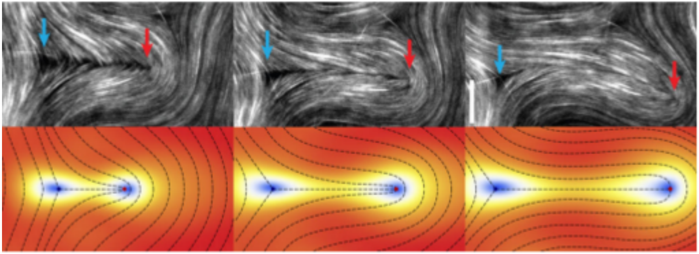


Active Inverse Turbulence

- Low Reynolds Number
- Inverse Energy Flow



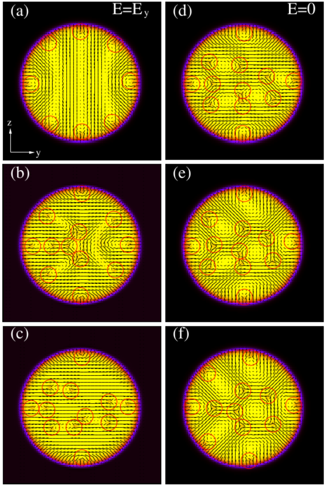
Defects Dynamics in 3D systems



Giomi, Bowick, Mishra, Sknepnek, Marchetti, *Defect dynamics in active nematics*, Phil.Trans.R. Soc.A 372

- Nematic Defects characterization in 3d geometries is still uncomplete ⇒ Advanced Mathematical Tools are required.
- Defects pair formation may play a crucial role in the onset of turbulence

Cholesteric Liquid Crystals



- Director field anchoring dramatically influences defect dynamics
- Coupling to electric field
- Expansion to the 3D systems: never treated before!

Fadda, Gonnella, Marenduzzo, Orlandini, Tiribocchi, *Switching dynamics in cholesteric liquid crystal emulsions*, The Journal of Chemical Physics 147, 064903 (2017)

Summary

- Active Turbulence Characterization;
- Devolepment of hybrid HPC tecniques for LBM (MPI+CUDA)
- 3D analysis of topological defects in polar and nematic systems
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