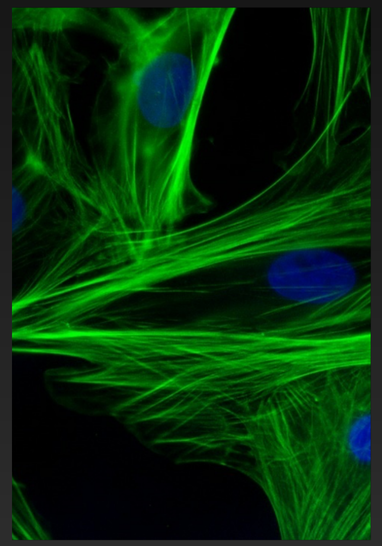
Dynamical phase transitions in complex fluids and non-equilibrium systems

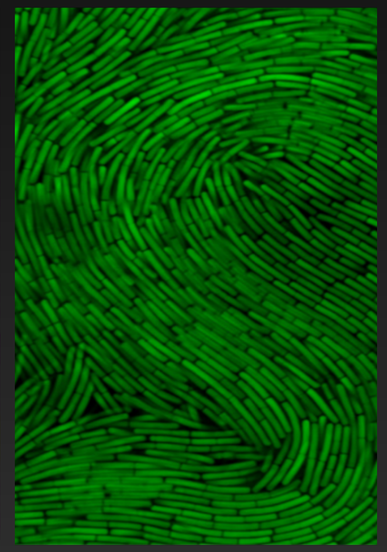
WP1 Spoke 2 b5 Physics of Complex Systems (UniBa)

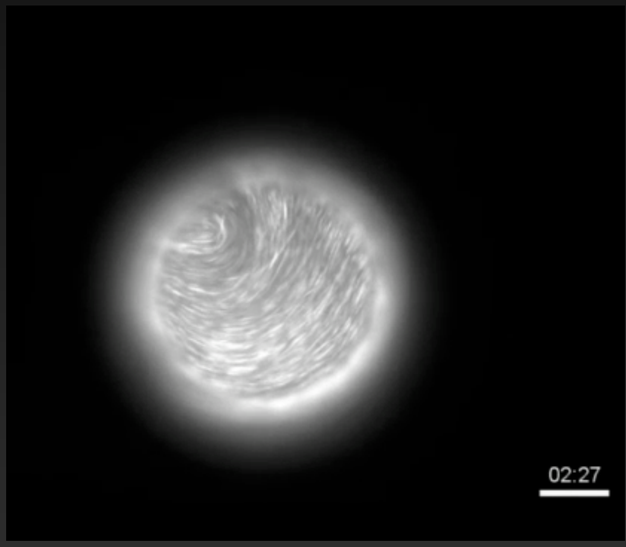
- Ordering properties in complex fluids and non-equilibrium systems
  Active fluids (dense suspensions of bacteria, cytoskeletal extracts, Microtubules bundles)

- Hydrodynamic and Statistical mechanics modelling

- High Performance Computing







- Prof. Giuseppe Gonnella
- Antonio Suma (RTB)
- Antonio Lamura

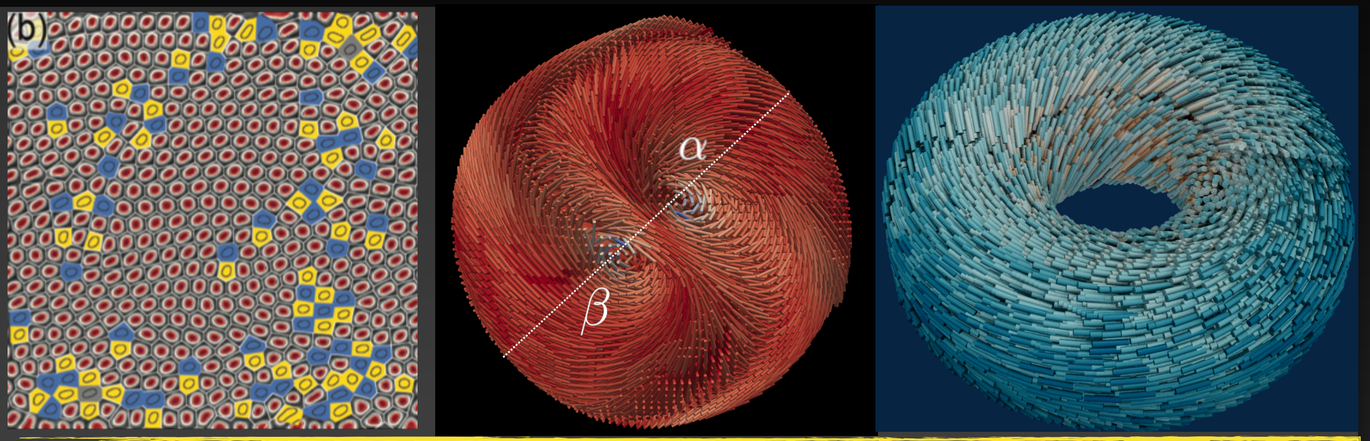
Dr. Giuseppe Negro

6/03/2023

gnegro2@ed.ac.uk

USE CASES

Phase Field Theories of complex and active fluids



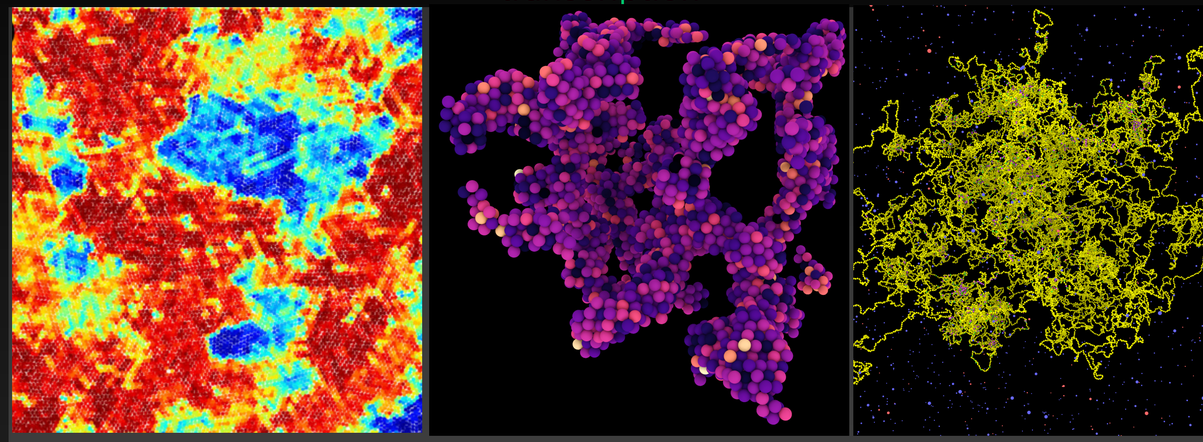
Topological Phase transitions of Choleric Shells Confined in Shells

Self-Propulsions of active droplets in 3D

Active Turbulence

Lattice Boltzmann Methods
MPI

Non-equilibrium statistical models for self propelled particles and DNA transcription



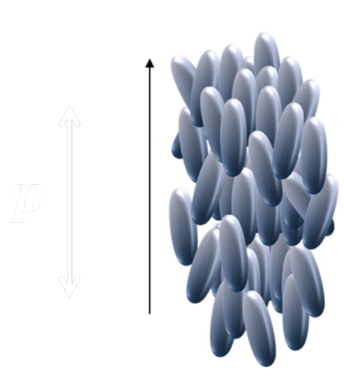
Non equilibrium Phase transitions in Active Brownian Particles

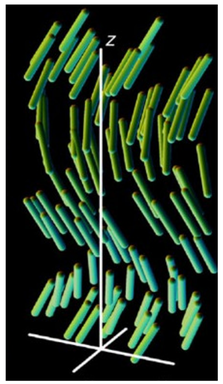
Polymer models to study transcription and dynamics in Human Chromosomes

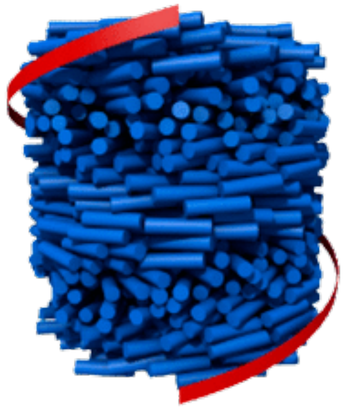
Molecular dynamics simulations with implicit and explicit solvents (LAMMPS+ CustomMulti Particle collision Dyanamics Package)

PHASE FIELD THEORIES

liquid crystals



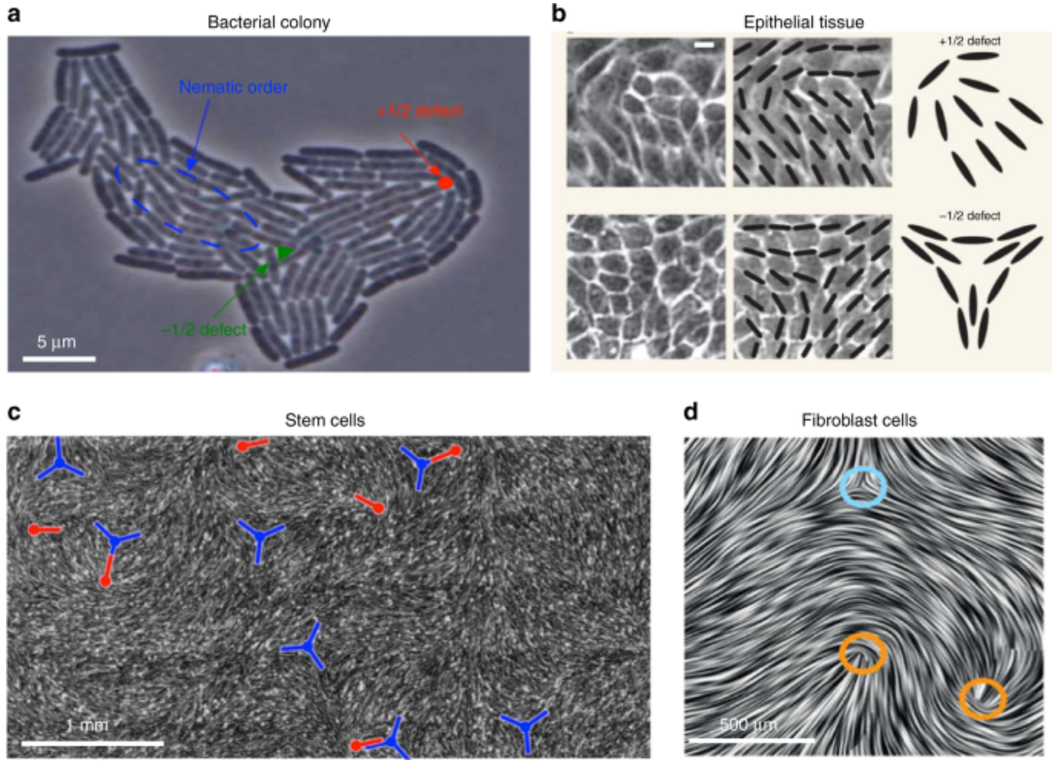




Oriental Order ⟶ Smooth Deformations

Described by a second rank traceless symmetric Tensor Order Parameter

$$Q_{\alpha\beta} = S\,\langle \mathbf{n}_\alpha \mathbf{n}_\beta - \frac{1}{d}\delta_{\alpha\beta} \rangle$$



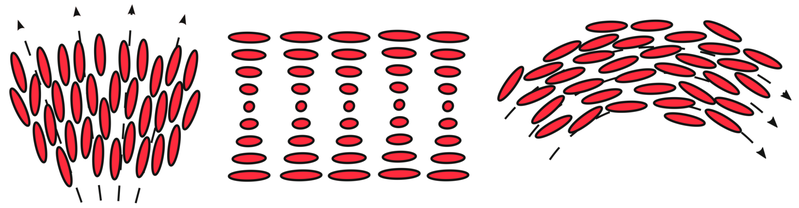
Landau-De Gennes Theory

Tensor order parameter
First order transition for orientational order

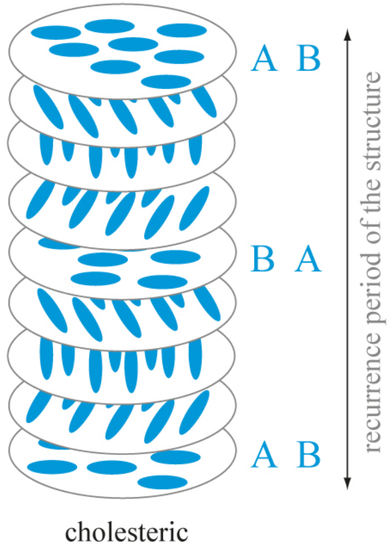
$$\mathcal{F}\left[\phi, Q_{\alpha\beta}\right] = \int dV \left[A_0\left[\frac{1}{2}\left(1-\frac{\chi(\phi)}{3}\right)\mathbf{Q}^2 - \frac{\chi(\phi)}{3}\mathbf{Q}^3 + \frac{\chi(\phi)}{4}\mathbf{Q}^4\right] + \frac{L}{2}\left[(\nabla\cdot\mathbf{Q})^2 + (\nabla\times\mathbf{Q} + 2q_0\mathbf{Q})^2\right]\right]$$

First order I-N phase transition

$$\chi(\phi) = \chi_0 + \chi_s(\nabla\phi)^2 > 2.7$$



Splay Twist Bend
Elastic Contributions



$$q_0 = 2\pi/p_0$$

Number of windings
In a droplet of radius

$$N = 2R/p_0$$

3 Control Parameters

Radius of Confinement

Chirality

Elastic energy

Activity

DYNAMICAL EQUATIONS

Dynamical fields

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

Advection relaxation for the tensor order parameter

$$(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{Q} - \mathbf{S}(\mathbf{W},\mathbf{Q}) = -\frac{1}{\Gamma}\mathbf{H}$$

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

Navier Stokes equation for the velocity field

$$(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{v} = \nabla\cdot\sigma$$

Advection diffusion for concentration field

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

$$\sigma^{el}_{\alpha\beta} = -\xi H_{\alpha\gamma}\left(Q_{\gamma\beta} + \frac{1}{3}\delta_{\gamma\beta}\right) - \xi\left(Q_{\alpha\gamma} + \frac{1}{3}\delta_{\alpha\gamma}\right)H_{\gamma\beta} + 2\xi\left(Q_{\alpha\beta} - \frac{1}{3}\delta_{\alpha\beta}\right)Q_{\gamma\mu}H_{\gamma\mu} + Q_{\alpha\gamma}H_{\gamma\beta} - H_{\alpha\gamma}Q_{\gamma\beta}$$

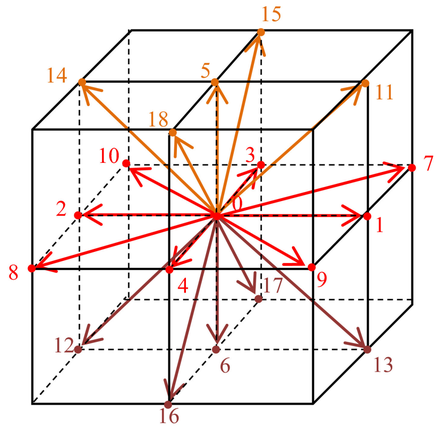
$$\sigma^{bm} = \left(f - \frac{\delta\mathcal{F}}{\delta\phi}\right)\delta_{\alpha\beta} - \frac{\delta\mathcal{F}}{\delta(\partial_\beta\phi)}\partial_\alpha\phi$$

Numerically solved via a hybrid Lattice Boltzmann Scheme

LATTICE BOLTZMANN MODELS

Based on phase-space discretisation form of the Boltzmann equation

$$\partial_t f + \xi_\alpha \partial_\alpha f + \frac{F_\alpha}{\rho} \partial_{\xi_\alpha} f = \Omega(f)$$



Discretised both in real and velocity space

$$f_i(\vec{r} + \vec{\xi}_i \Delta t, t + \Delta t) - f_i(\vec{r}, t) = \mathscr{C}(f_i, t)$$

$$\mathscr{C}(f_i, t) = -\frac{1}{\tau}(f_i - f_i^{eq})$$

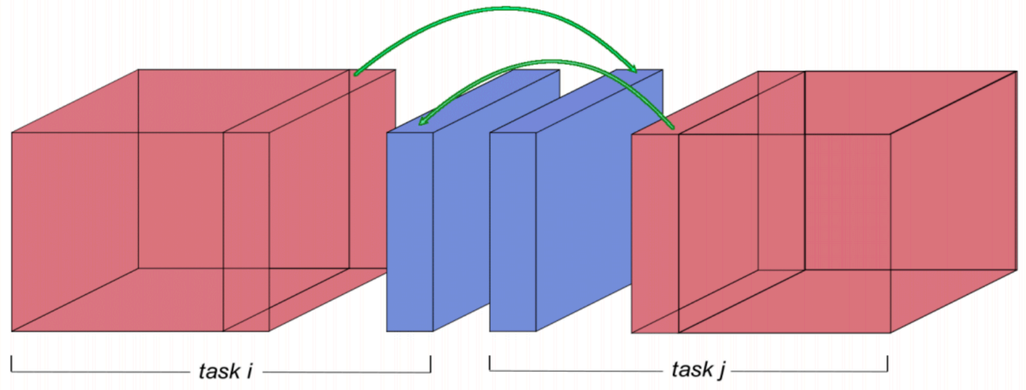
Mass and momentum density are defined as

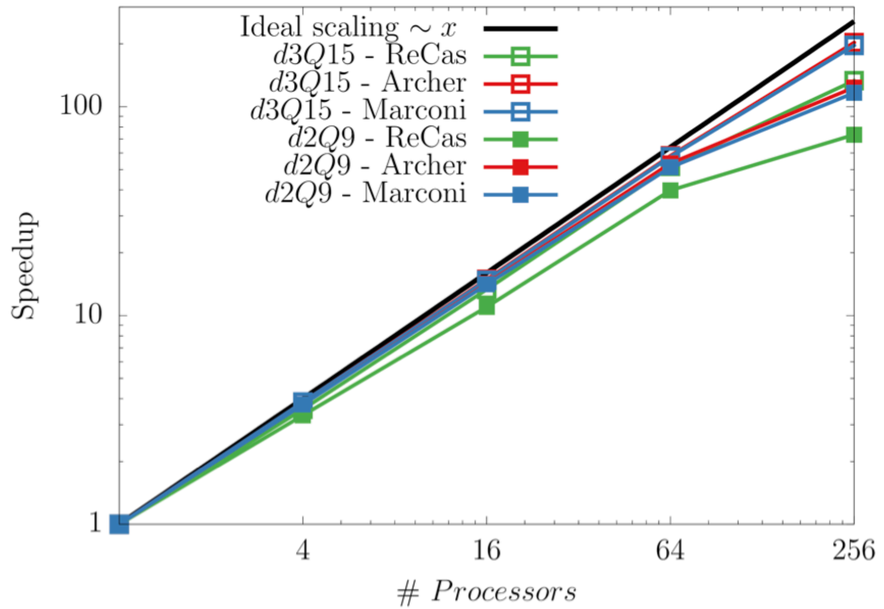
$$\sum_i f_i^{eq} \xi_{i\alpha} = \rho u_\alpha \qquad \sum_i f_i^{eq} = \rho$$

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

- The Equilibrium distribution functions are expanded up to a given order in the fluid velocity
- The Navier Stokes equations can be formally derived from the Lattice Boltzmann equation in the long wave length limit through Chapman-Enskog expansion

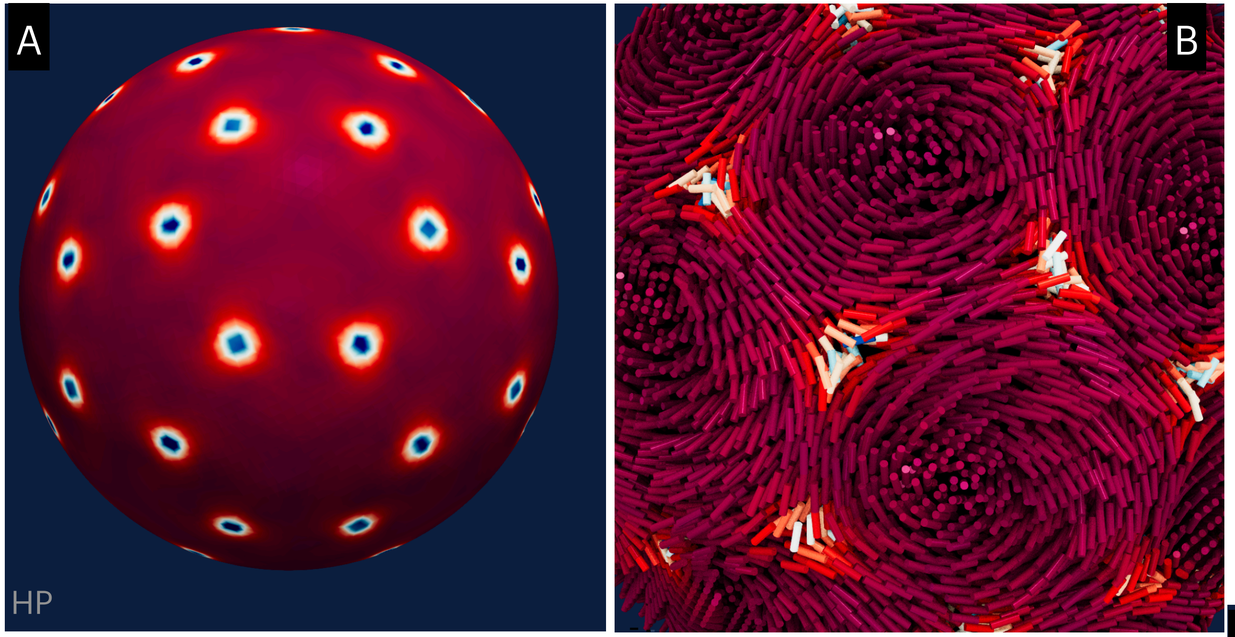
MPI Parallelization



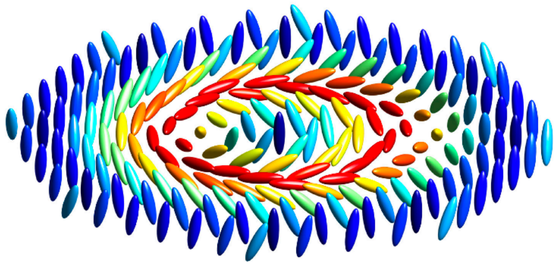


HPC facilities Cineca (Bologna), Recas (Bari), Archer2 (Edinburgh), Snellius (Amsterdam)

Chiral liquid crystals confined in shells

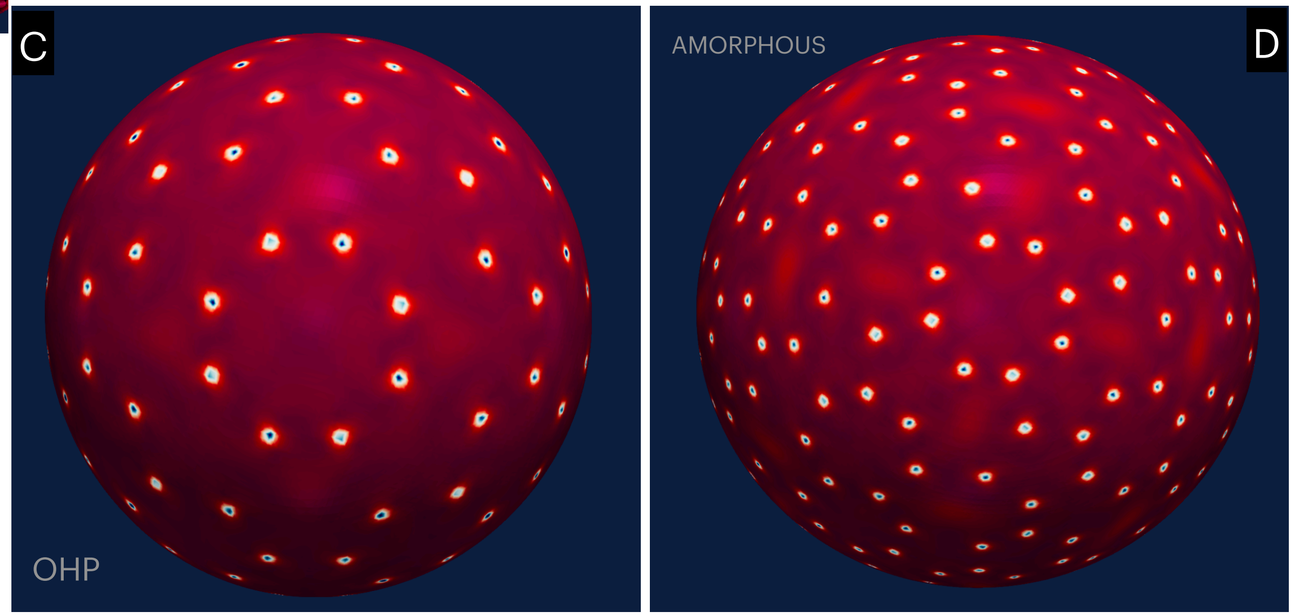


Football configuration



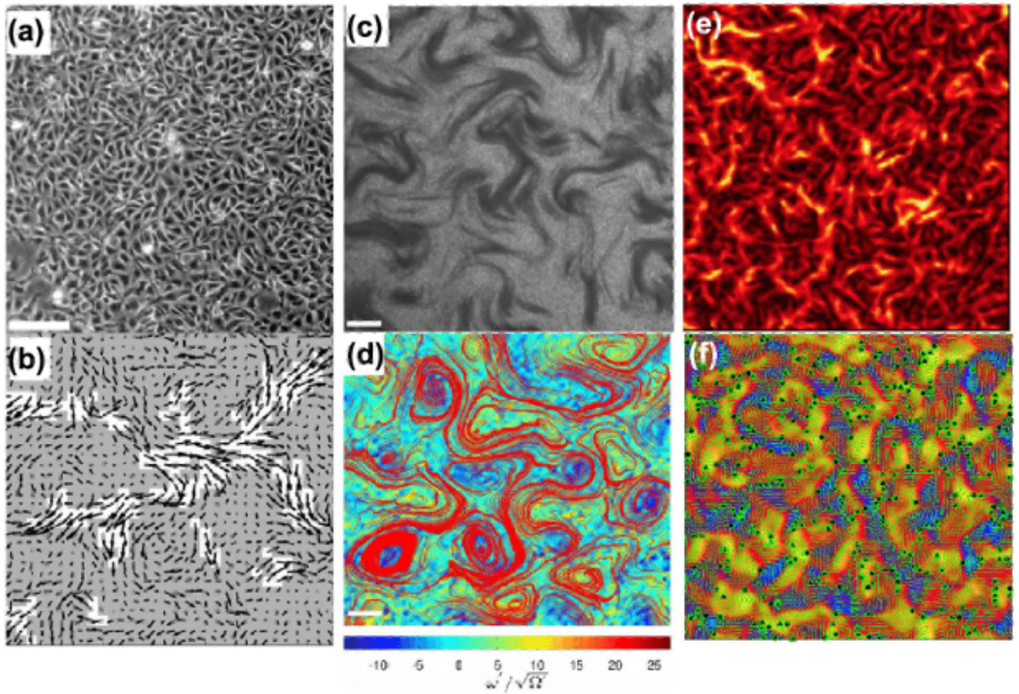
BABY SKYRMION

Increasing chirality or increasing R

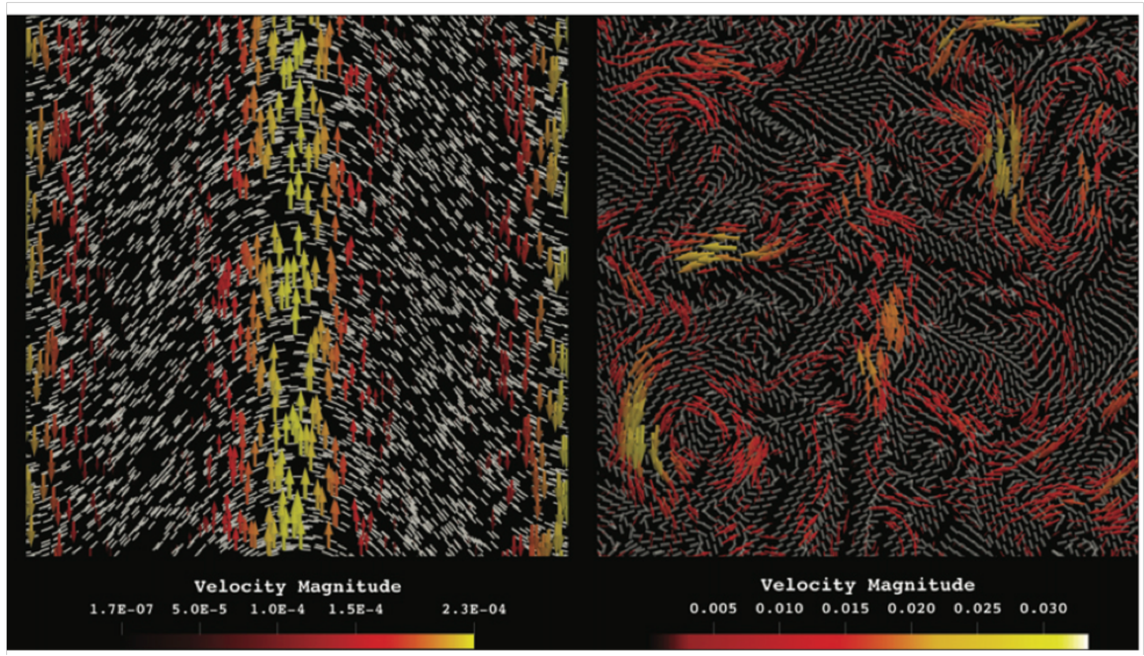


G. Negro* et al. “Cholesteric Shells: two-dimensional blue fog and finite quasycrystals” In: **Physical Review Letters,** 128 (2022)

ACTIVE TURBULENCE



Jörn Dunkel, Sebastian Heidenreich, Knut Drescher, Henricus H. Wensink, Markus Bär, and Raymond E. Goldstein
Phys. Rev. Lett. **110**, 228102 – Published 28 May 2013

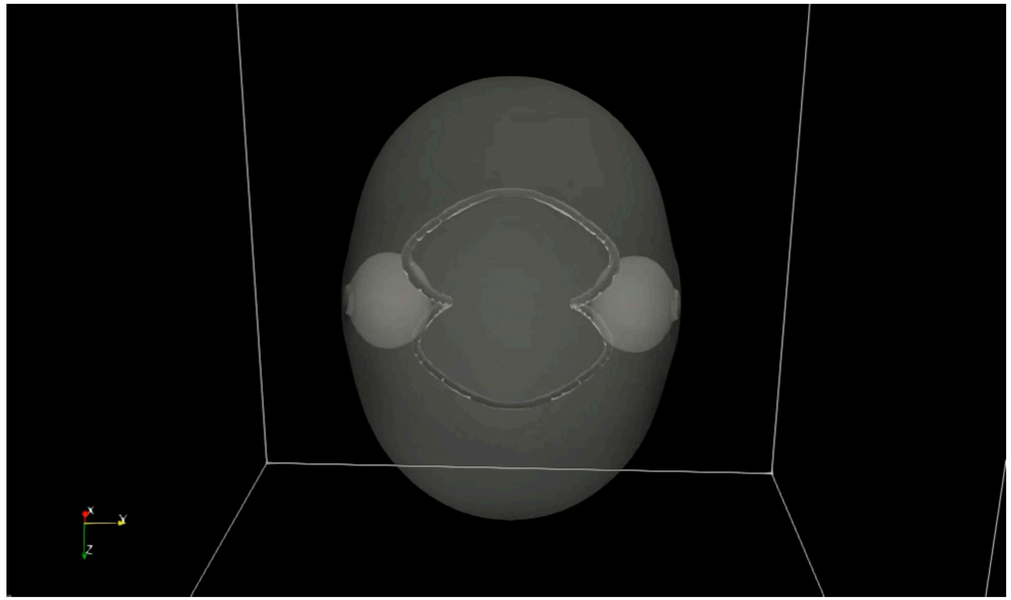


Cascade or not cascade? Energy transfer and elastic effects in active nematics
LN Carenza, L Biferale, G Gonnella
Europhysics Letters 132 (4), 44003 (2021)

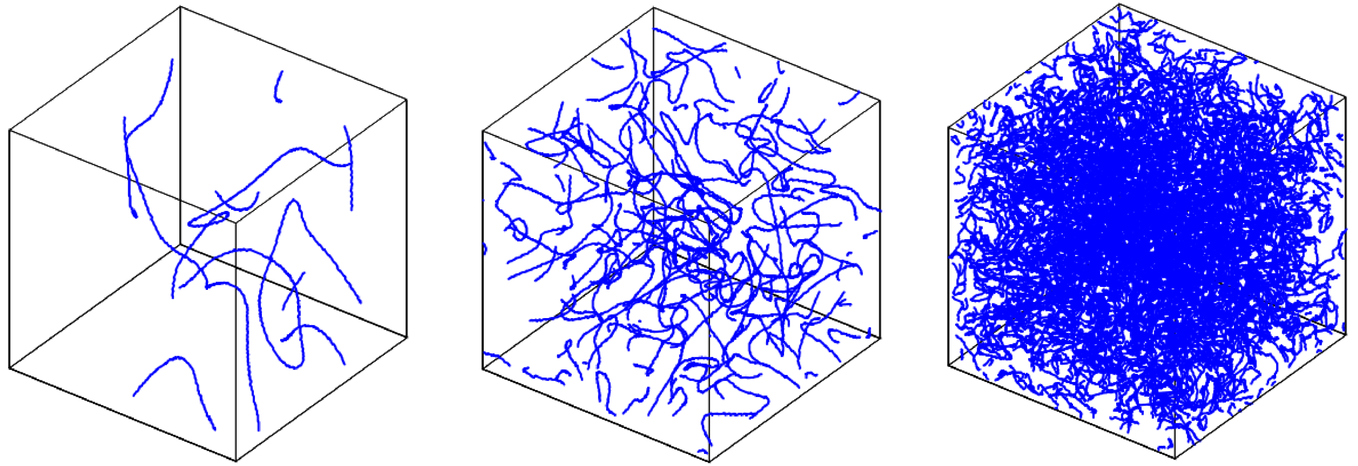
Multiscale control of active emulsion dynamics
LN Carenza, L Biferale, G Gonnella
Physical Review Fluids 5 (1), 011302 (2020)

Planned Activity

Multi-Phase models



Active Turbulence in 3D

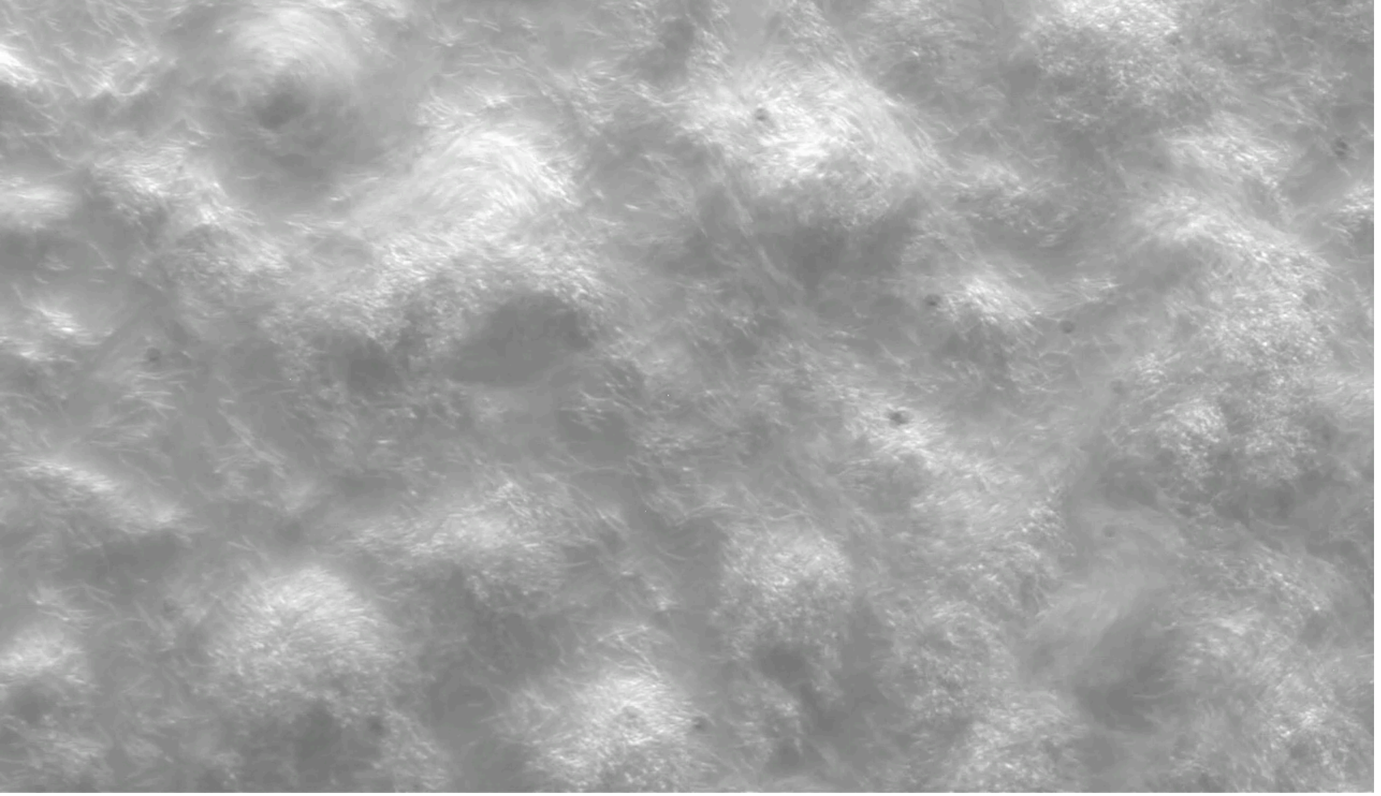


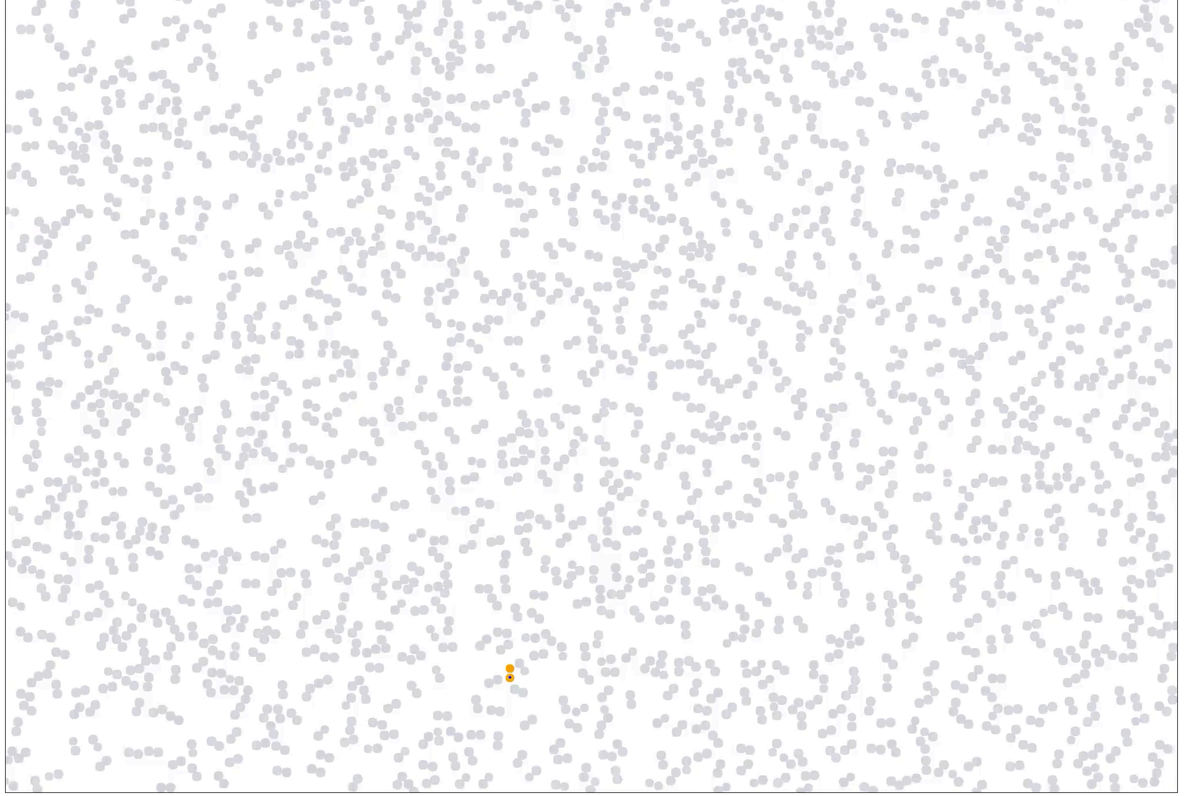
α=0.0001 0.001 0.01

Defects tracking in 3D Active turbulence

Typical Runs: 128/256 cores for 48 hours
50 exploratory runs
307200 core hours

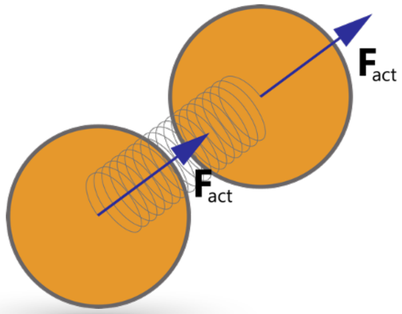
Non-equilibrium statistical models for self propelled particles and DNA transcription





- $U(r) = \begin{cases} U_{\text{Mie}}(r) - U_{\text{Mie}}(r_{min}) & \text{if } r < r_{min} \\ 0 \quad \text{if } r \geqslant r_{min} \end{cases}$

- $\mathbf{F}_{FENE} = -\dfrac{k(\mathbf{r}_i - \mathbf{r}_j)}{1 - r_{ij}^2/r_0^2}$

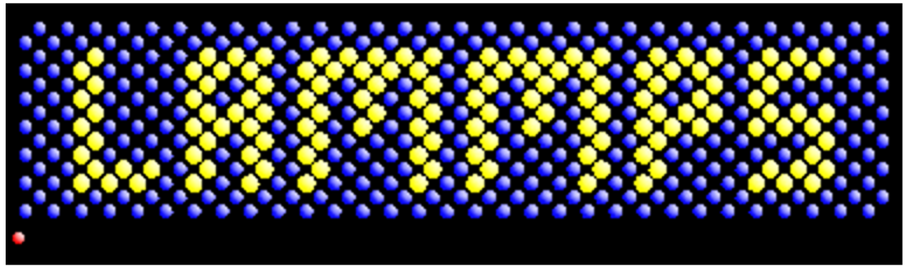


ACTIVE PARTICLES

$$m\ddot{\mathbf{r}}_i = -\gamma\dot{\mathbf{r}}_i - \frac{\partial U_{FENE}}{\partial r_{i,i+1}}\,\hat{\mathbf{r}}_{i,i+1} - \sum_{j\neq i}^{2N}\frac{\partial U}{\partial r_{ij}}\,\hat{\mathbf{r}}_{ij} + F_{\text{act}}\hat{\mathbf{n}}_i + \sqrt{2D_0}\,\eta_i\ ,$$

$$m\ddot{\mathbf{r}}_{i+1} = -\gamma\dot{\mathbf{r}}_{i+1} + \frac{\partial U_{FENE}}{\partial r_{i,i+1}}\,\hat{\mathbf{r}}_{i,i+1} - \sum_{j\neq i+1}^{2N}\frac{\partial U}{\partial r_{i+1,j}}\,\hat{\mathbf{r}}_{i+1,j} + F_{\text{act}}\hat{\mathbf{n}}_{i+1} + \sqrt{2D_0}\,\eta_{i+1}$$

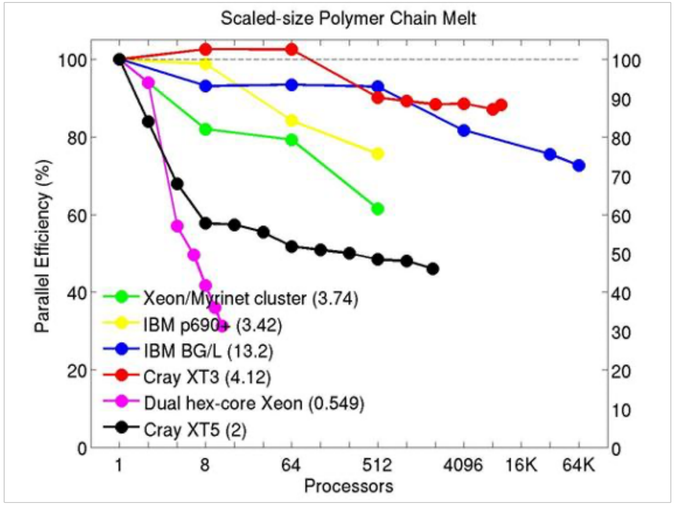
Molecular Dynamics Methods



LAMMPS is a classical molecular dynamics code with a focus on materials modeling.

It's an acronym for **Large-scale Atomic/Molecular Massively Parallel Simulator**.

It can be used with multiple CPUs and with a GPU



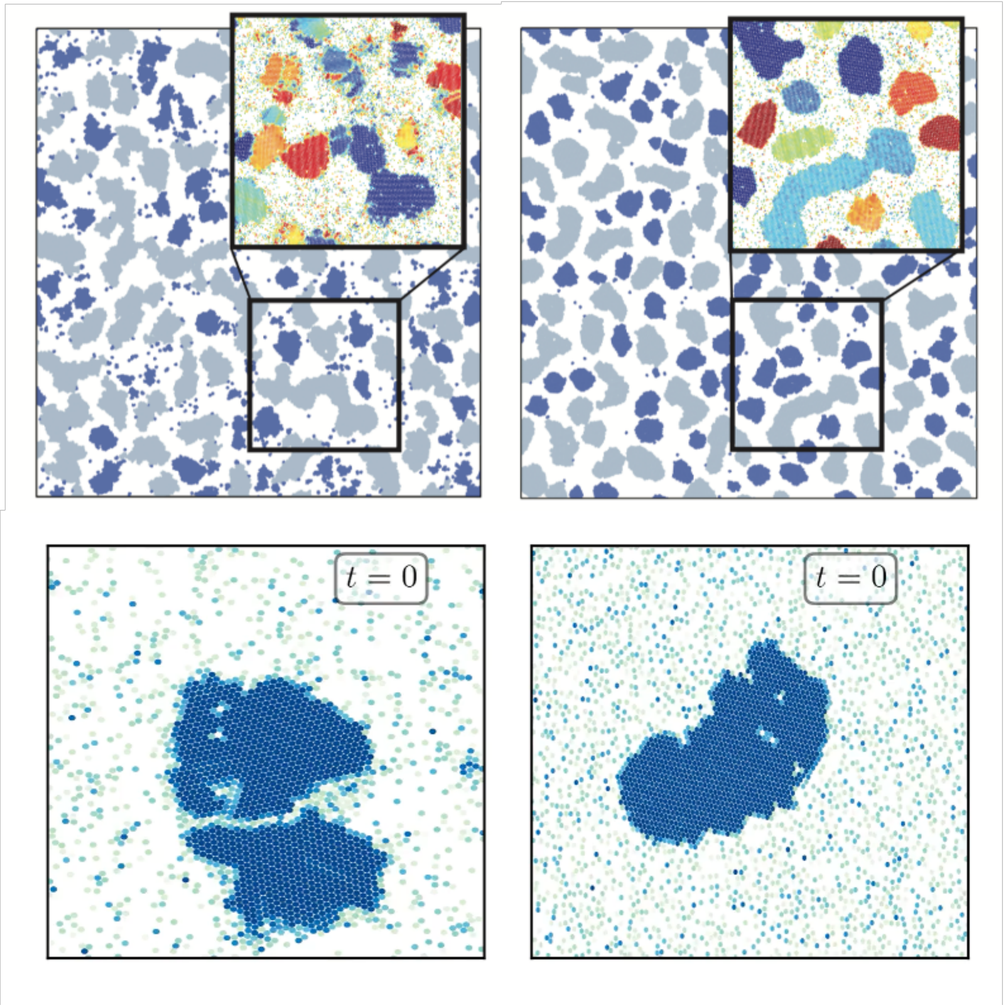
Bead-spring polymer melt with 100-mer chains and FENE bonds:

- 32,000 atoms for 100 timesteps
- reduced density 0.8442 (liquid)
- force cutoff of 2^(1/6) sigma
- neighbor skin = 0.4 sigma
- neighbors/atom = 5 (within force cutoff)
- NVE time integration

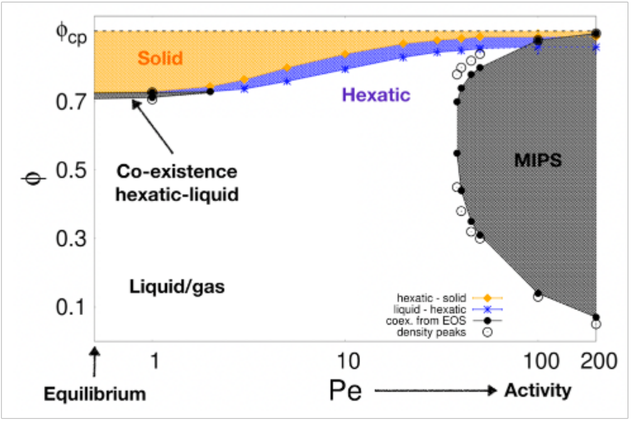
Molecular Dynamics Methods

Active self-propelled particles

Active (with repulsion) Passive (with attraction)



- Micro and macro phase separation of active systems
- Self-organization and dynamics of active clusters
- Phase diagram



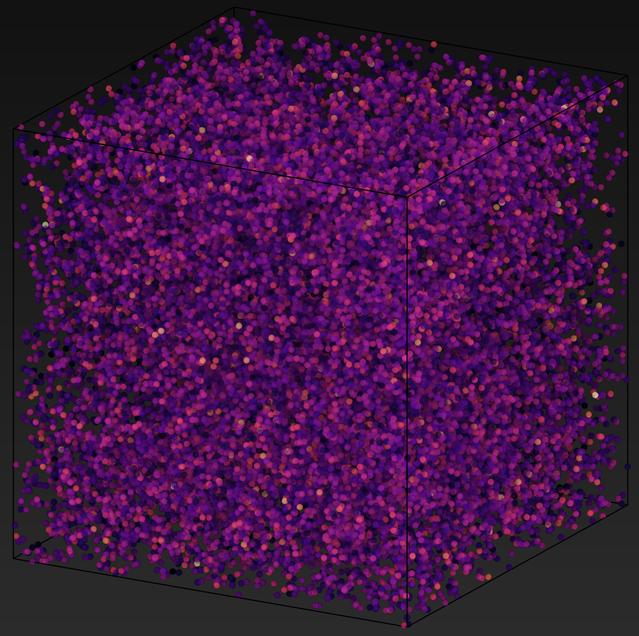
Cugliandolo et al. PRL 119 (26), 268002 2017

Digregorio et al. PRL 121, 098003 2018

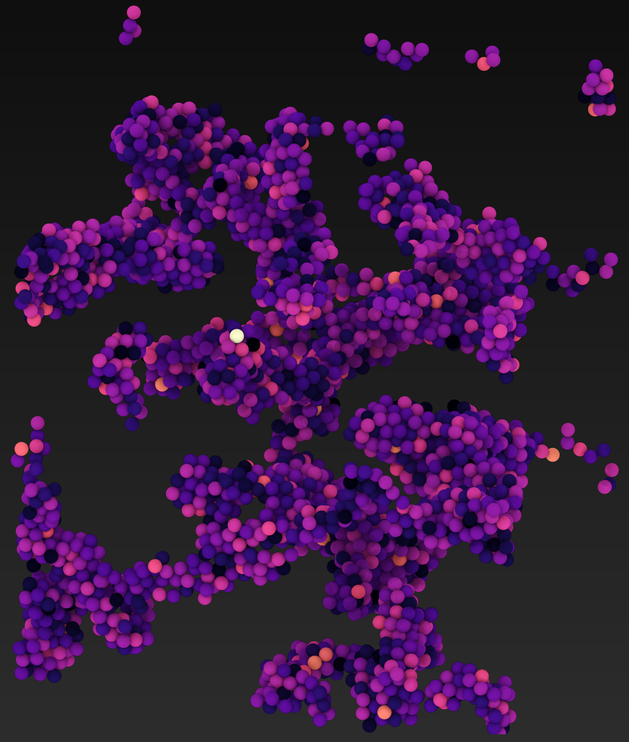
Caporusso et al. PRL 125 (17), 178004 2020

Planned Activity

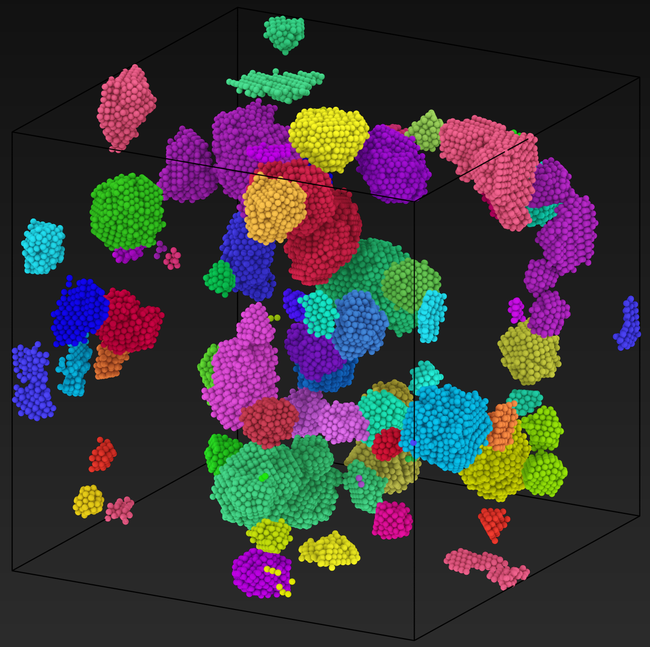
Three control parameters Attraction Activity Density



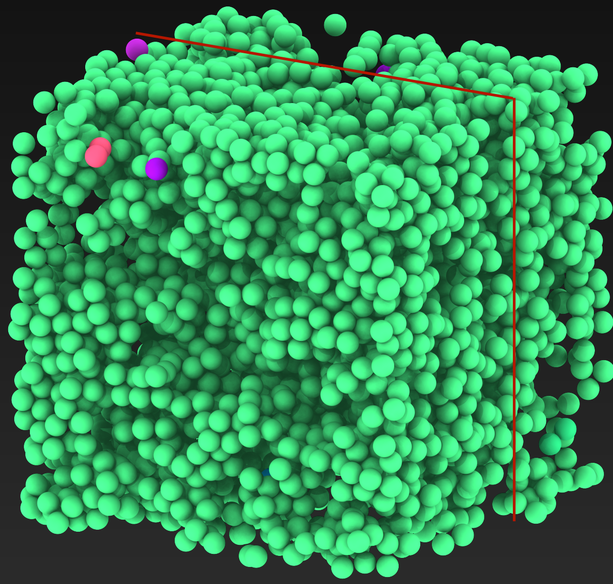
No Attraction, Any value of density and activity



Attraction, low activity, low density: Gel Phase



Attraction, higher activity, low density: Arrested Phase Separation



Attraction, high activity, high density: Percolating Network

Typical Runs: 256 cores for 48 hours
30 exploratory runs
368640 core hours

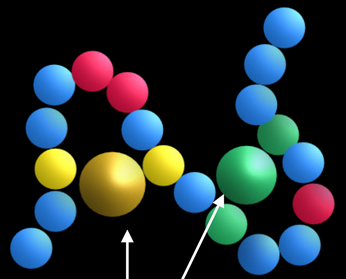
THANK YOU

POLYMER MODEL FOR GENE ORGANIZATION AND TRANSCRIPTION

Neutral

Binding sites (TU)

3Mbp-> 1000 beads (each 30nm in diameter->3Kbp)



Binders (TF) Weakly with all others

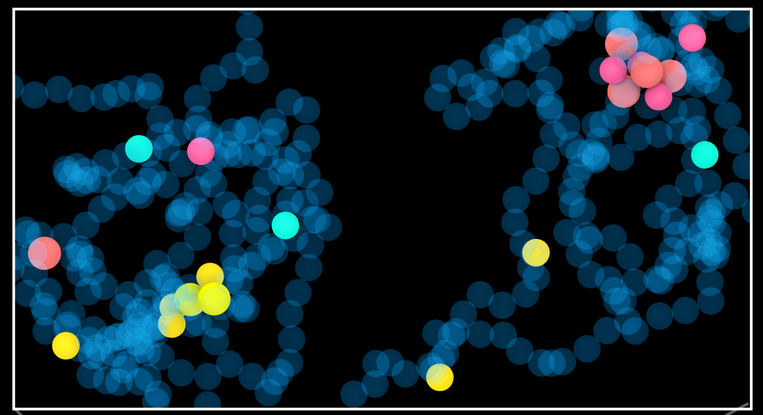
TFs SWITCH BETWEEN ACTIVE AND INACTIVE STATES

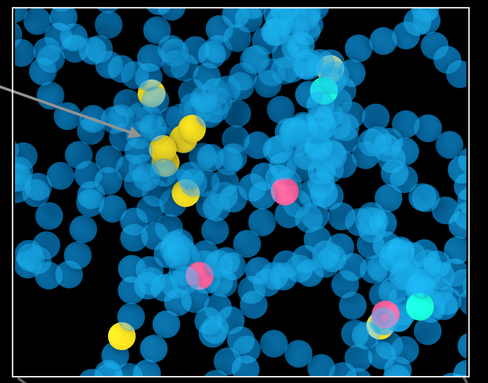
Rapid exchange of factors and polymerases between bound and free states seen in photobleaching experiments

C. A. Brackley et al. Nat. Comm. (2021)

TU in a cluster

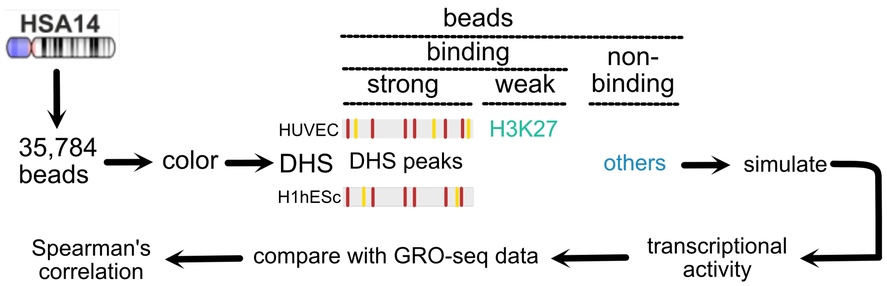
TU+TF

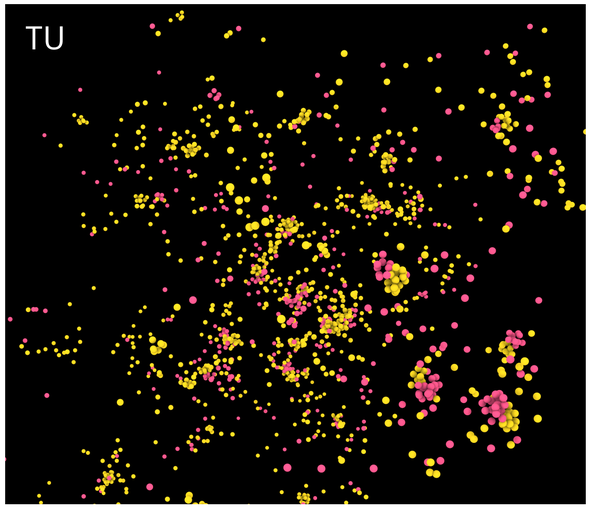


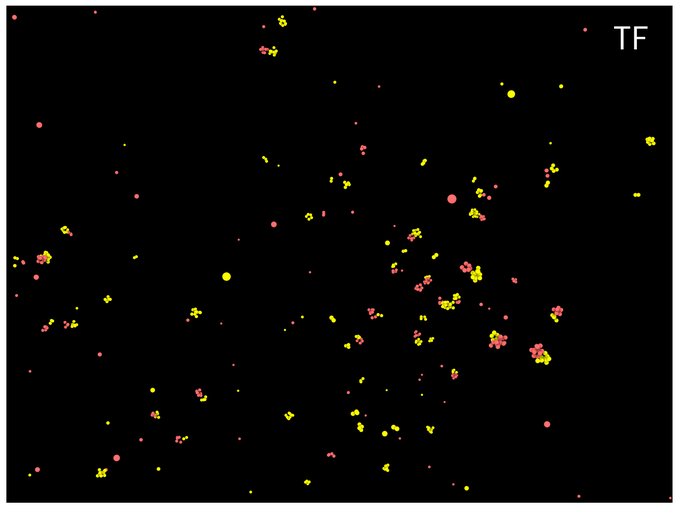


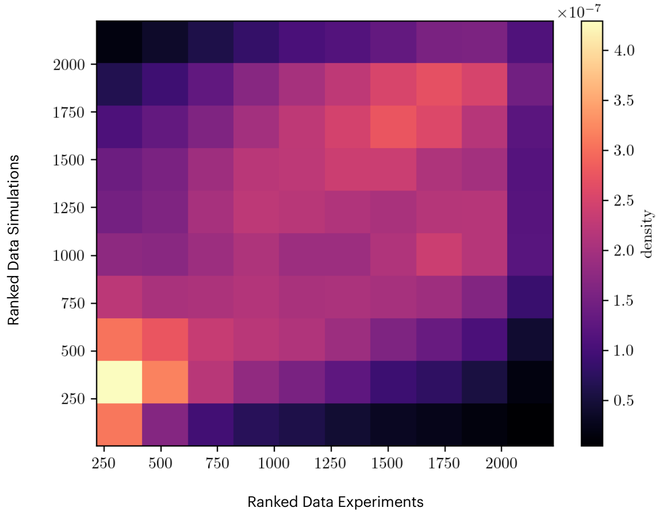
MD SIMULATION

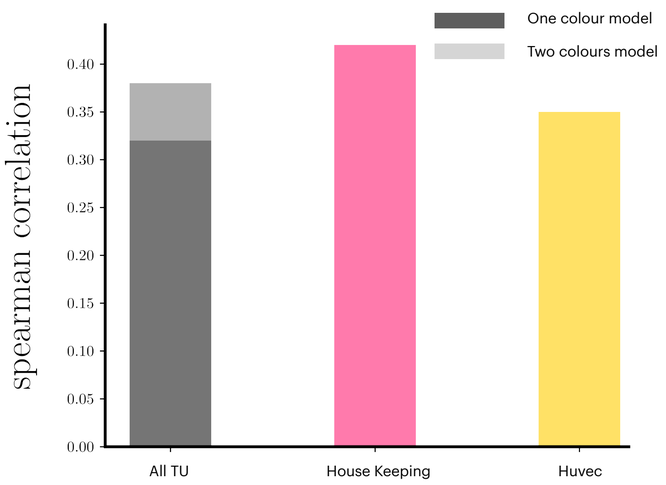
CHR 14

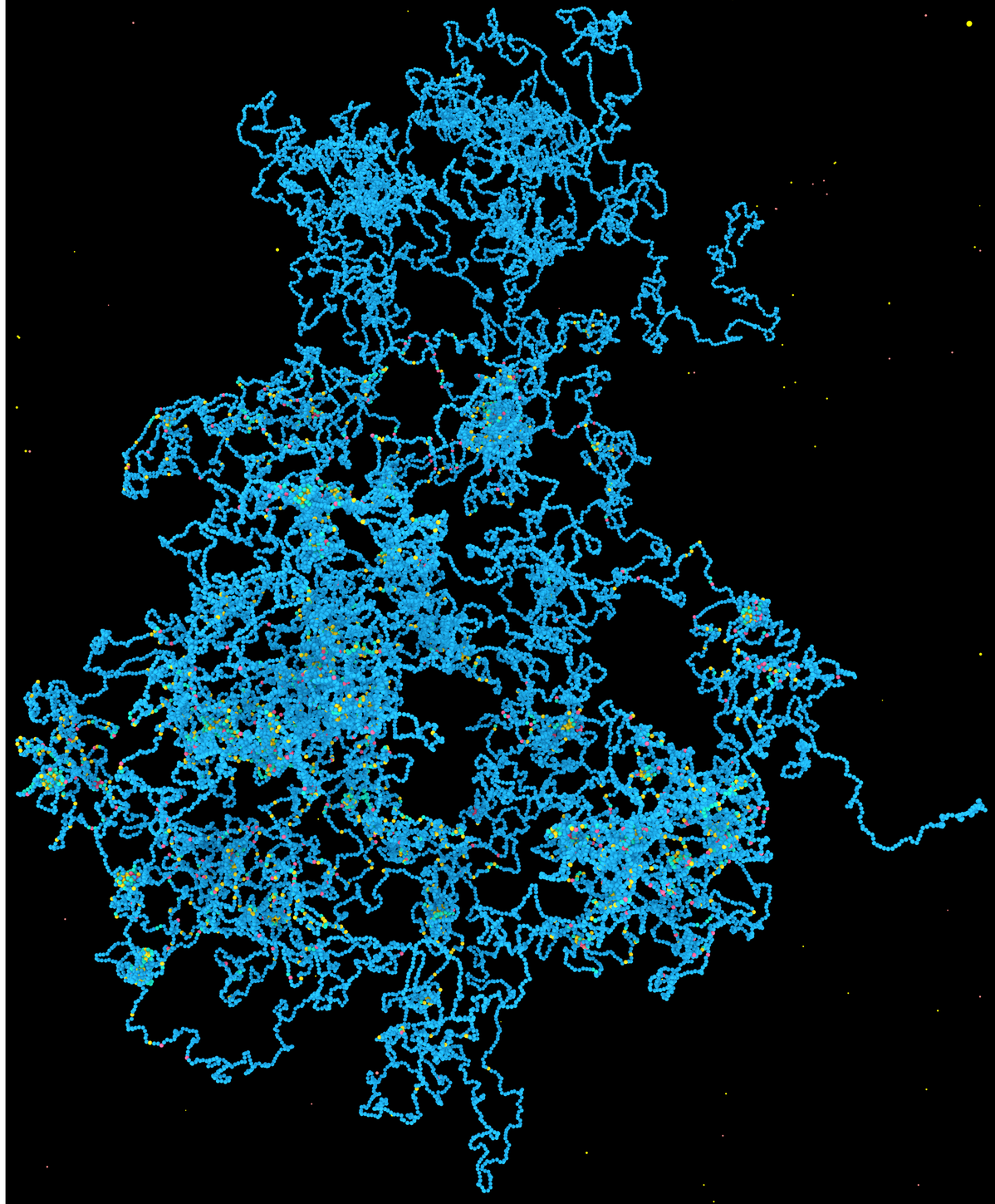

HSA14
35,784 beads
color
DHS
DHS peaks
HUVEC
H1hESc
H3K27
beads
binding
strong
weak
non-binding
others
simulate
transcriptional activity
compare with GRO-seq data
Spearman's correlation


TU


TF


Ranked Data Simulations
Ranked Data Experiments
density
×10⁻⁷


One colour model
Two colours model
spearman correlation
All TU
House Keeping
Huvec



Active Stress Tensor

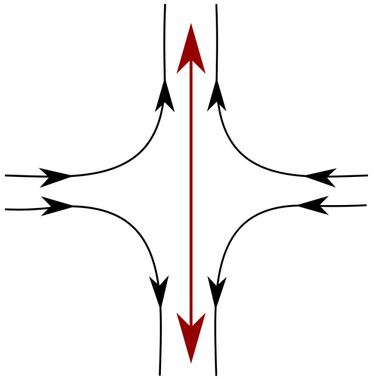
$$(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{v} = \nabla\cdot\left[\sigma^{pass} + \sigma^{act}\right]$$

Dissipative/reactive term

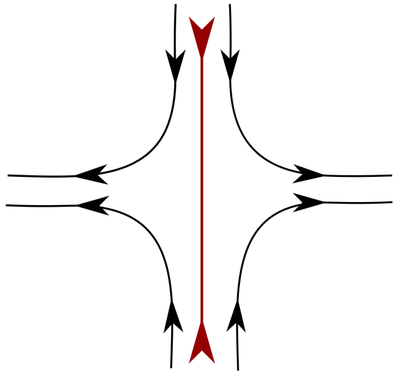
Non-Equilibrium terms

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

Force Dipoles

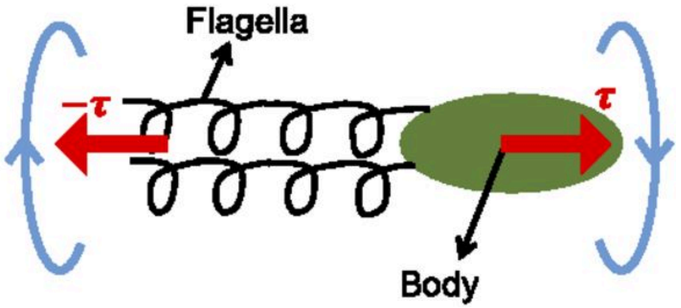


Extensile



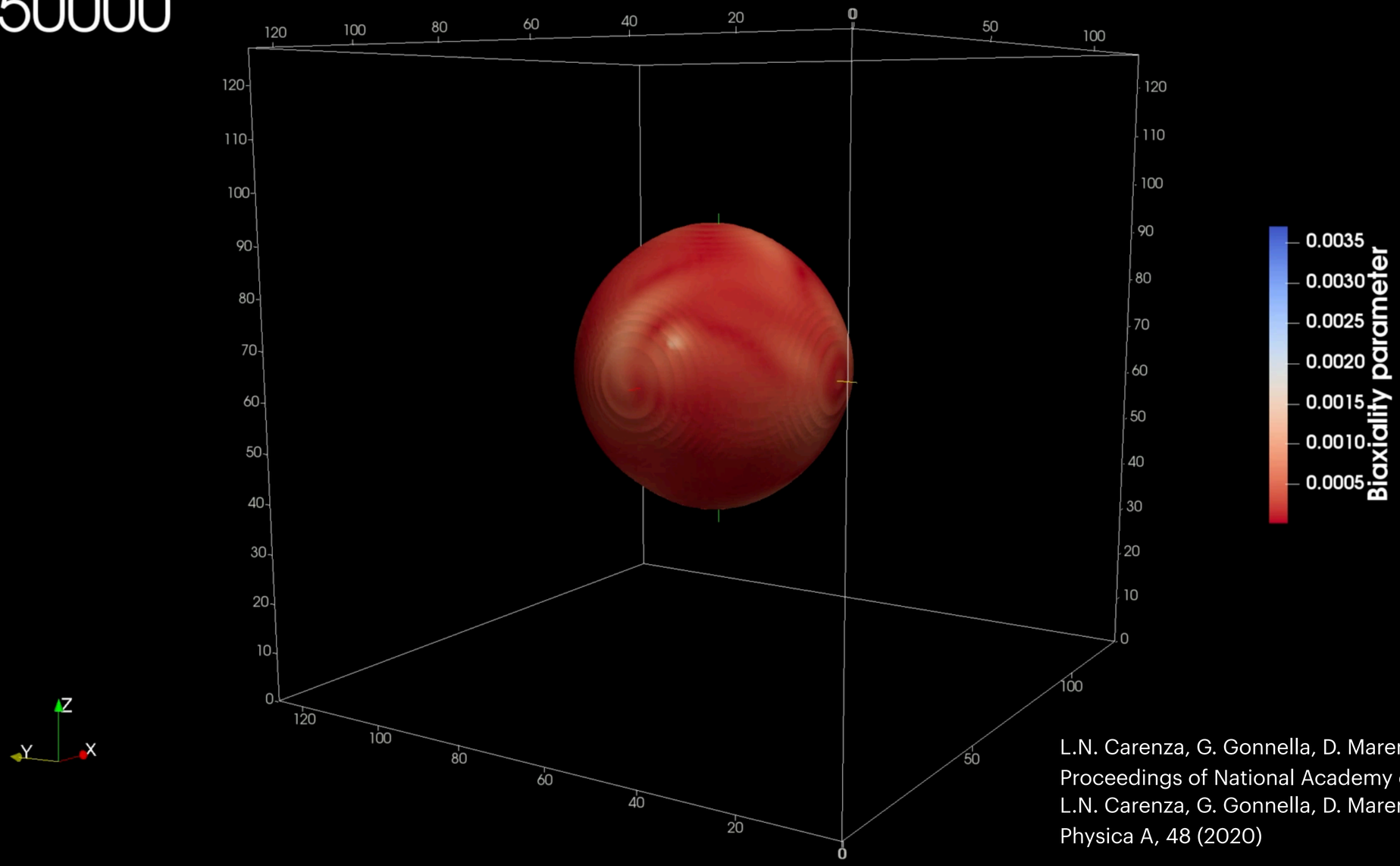
Contractile

Torque Dipoles



Active Cholesteric Droplet:
A novel Motility mode

150000



L.N. Carenza, G. Gonnella, D. Marenduzzo, and G. Negro*
Proceedings of National Academy of Science, 116 (2019)
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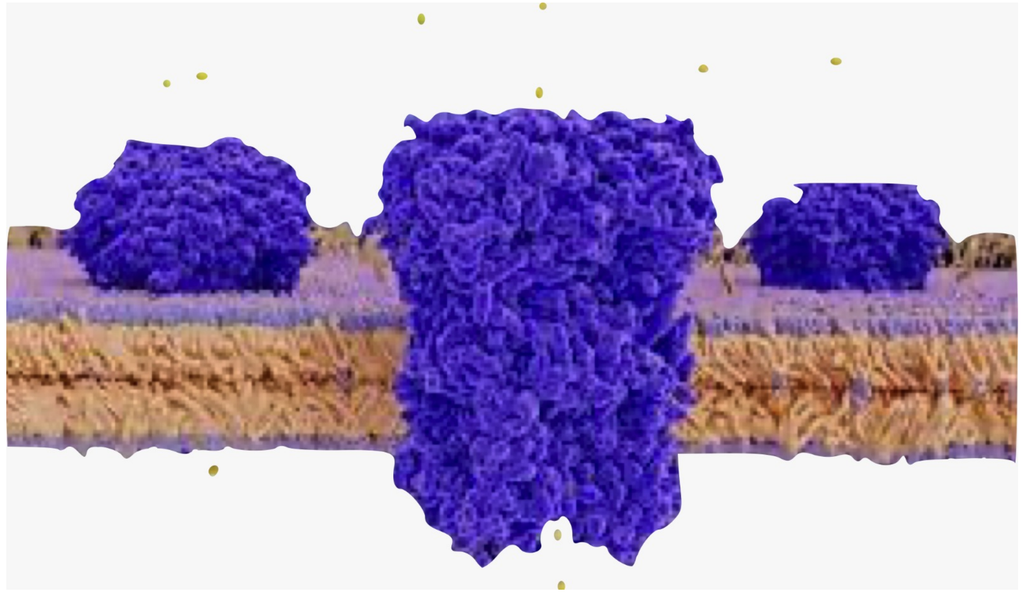
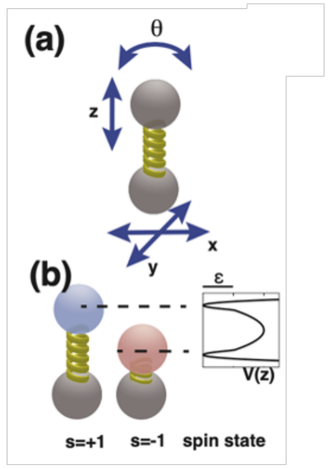
Physica A, 48 (2020)

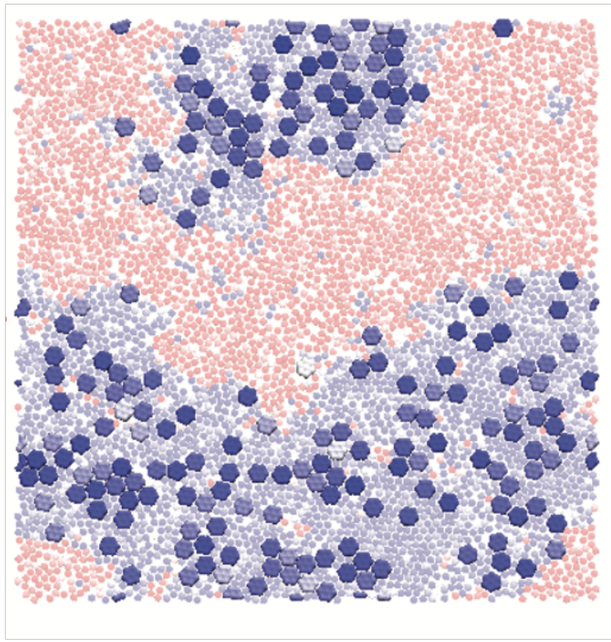
Molecular Dynamics Methods

Model for lipid bilayers and ion channels



Coarse-grained





Typical Runs: 128 cores for 48 hours
45 exploratory runs
276480 core hours