A Mesoscopic Particle-based Method for Active-Nematics

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Physics and Biology of Active Systems
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Motivation

EMBO Fellow

Microscopic Models

- Active colloids
- Simulations of motile microbes

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Continuum Models

- Active-nematic hydrodynamics

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Mescoscale Models

- Coarse-grain many microscopic entities without calculating molecular interactions

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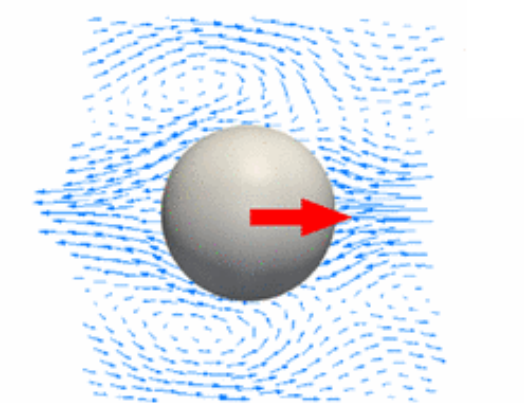
Conclusion:

- Coarse-graining solvents successful in passive soft matter
  - We would like a "toolbox" of similar simulation techniques for active fluids



Colloids in Active Fluids: Anomalous Microrheology and Negative Drag by Foffano, *et. al.*

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Active-Nematic Hydrodynamic Equations to be Simulated

- Continuity equation $D_t \rho + \rho \partial_i u_i = 0$

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- Review: recreate Navier-Stokes Equations by mesoscopic MPCD

Technique: Multi-Particle Collision Dynamics

EMBO Fellow

Traditional MPCD

- Particle-based algorithm for moderate Péclet numbers.

Each point-like particle i has

1. position $\underline{x}_i$
2. velocity $\underline{v}_i$
3. mass m_i

Each cell has

1. population N_c
2. centre of mass velocity $\underline{v}_{\mathrm{cm}}$
3. (moment of inertia $\underline{\underline{I}}_c$)

Advantages

- Finite temperature
- No explicit pair-wise interactions
  - Point-like particles
- Highly parallelizable

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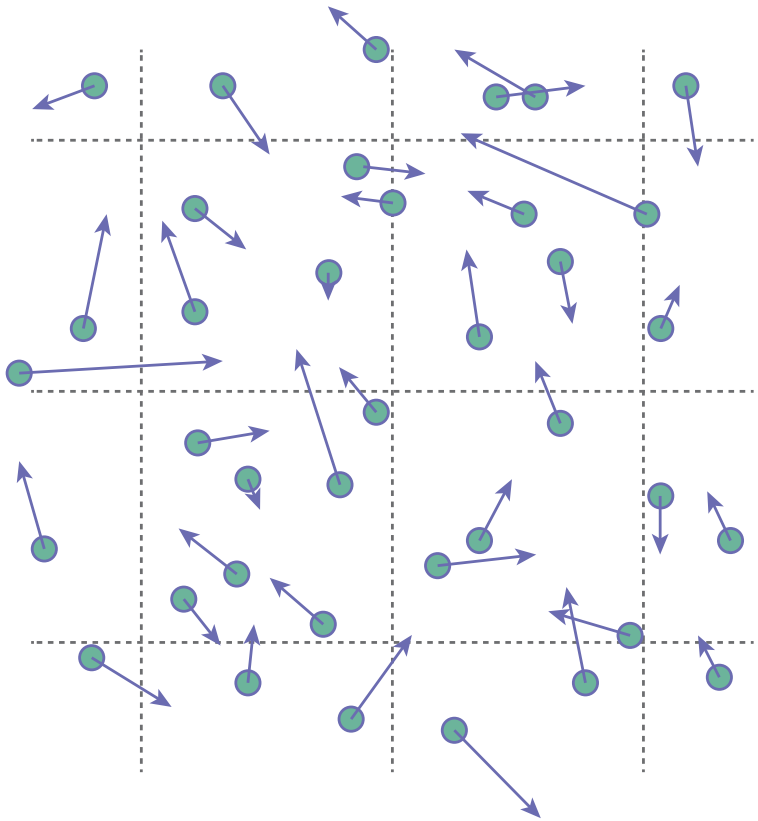
Technique: Multi-Particle Collision Dynamics



Streaming

$$\underline{x}_i\left(t+\delta t\right)=\underline{x}_i\left(t\right)+\underline{v}_i\left(t\right)\delta t$$

† Modelling the separation of macromolecules: A review of current computer simulation methods, Slater *et. al.* , Electrophoresis, 30, 2009.

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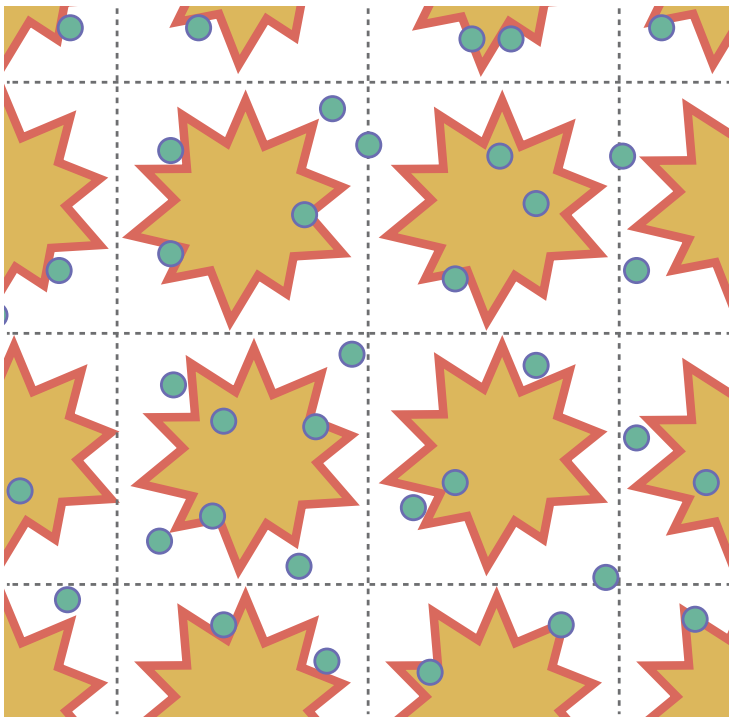

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Collision (Andersen MPCD)

$$\underline{v}_i\left(t+\delta t\right)=\underline{v}_{\mathrm{CM}}\left(t\right)+\Xi$$

where Ξ is a collision operation

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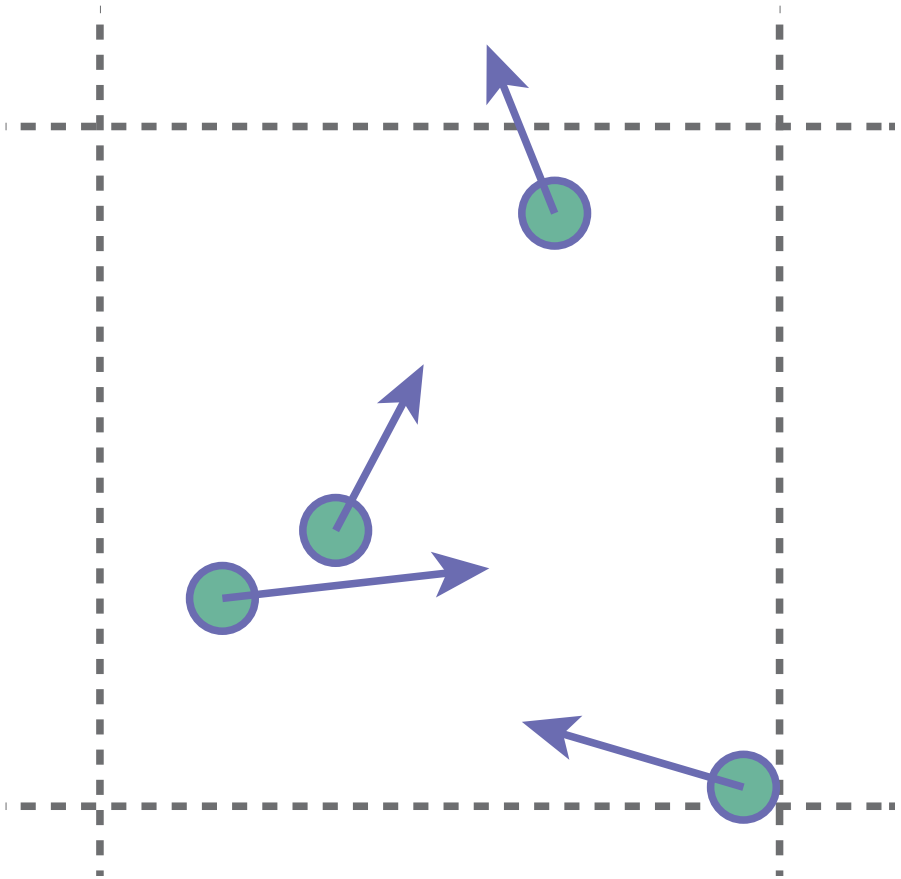

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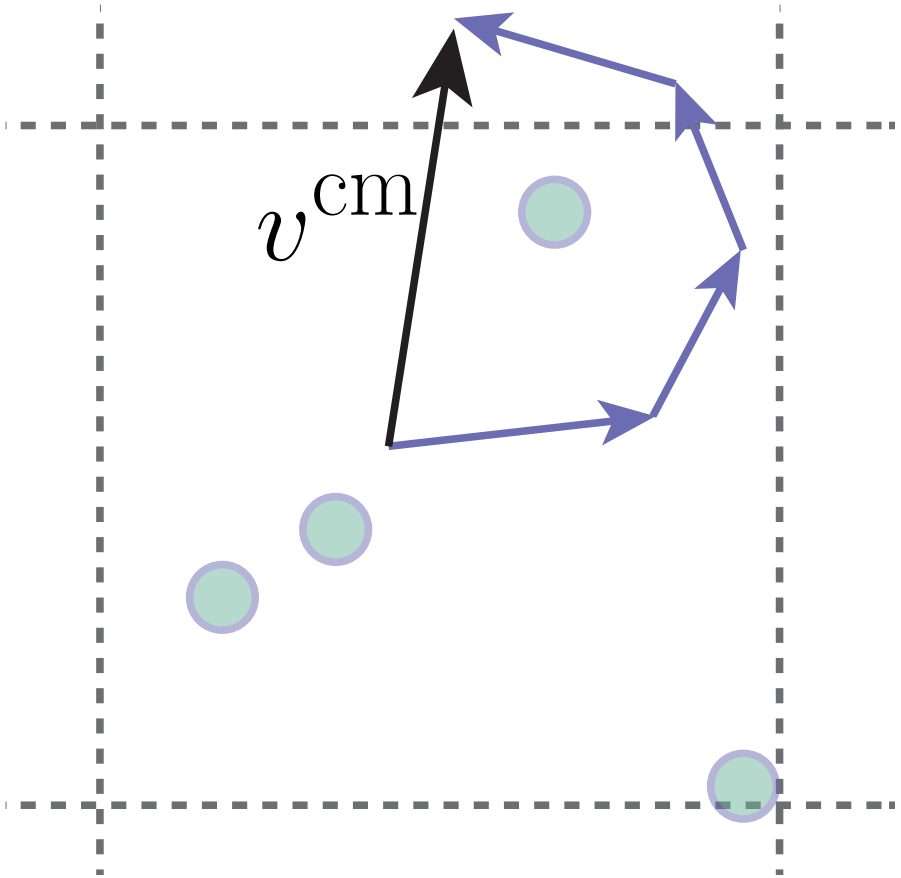

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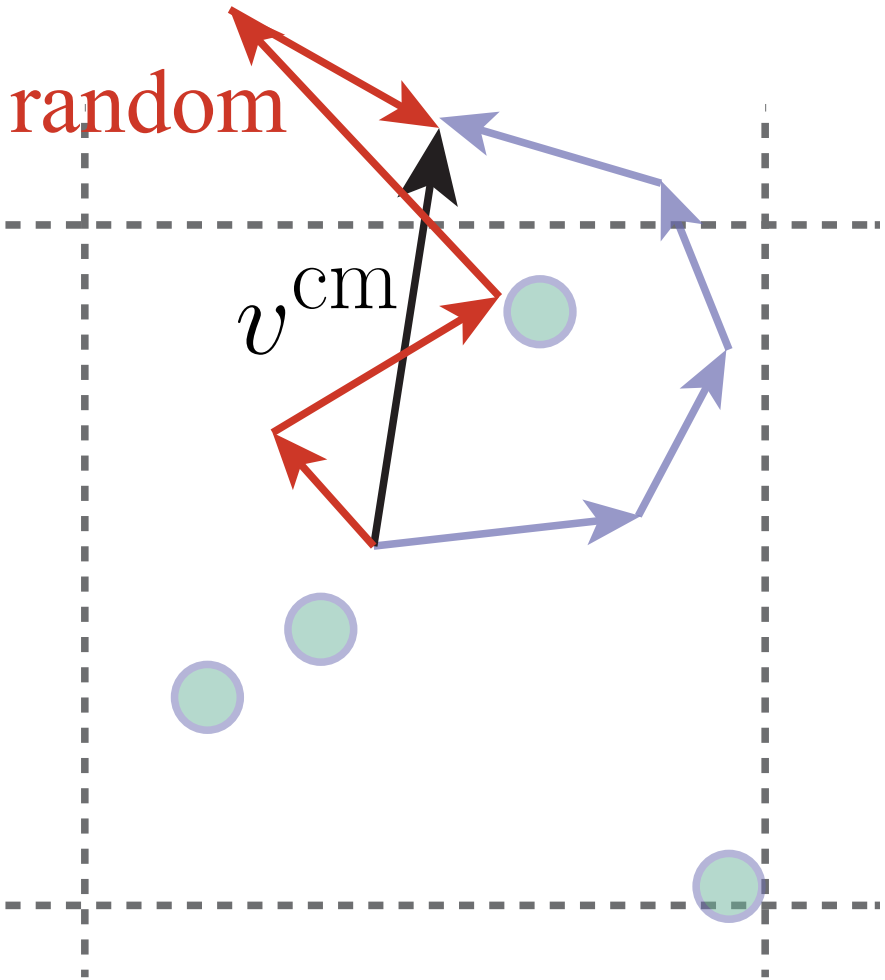

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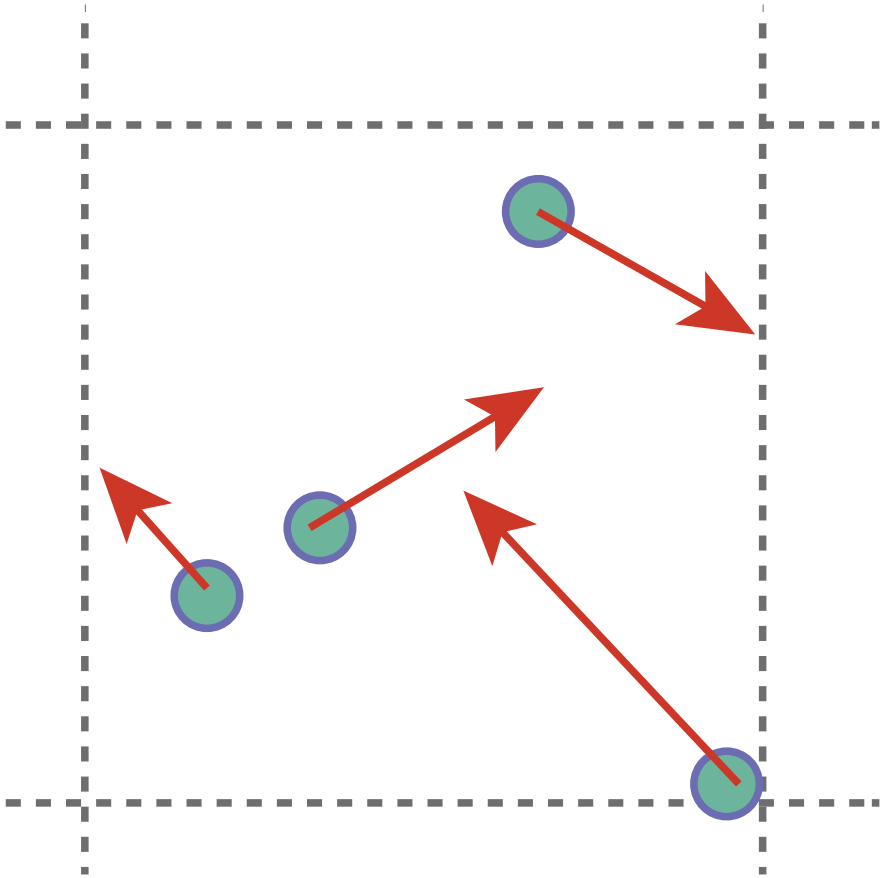

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Equations to Simulate

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- Orientation equation $D_t Q_{ij} - S_{ij} = \Gamma H_{ij}$

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- *i.e.* Navier-Stokes Equations on long time and length scales

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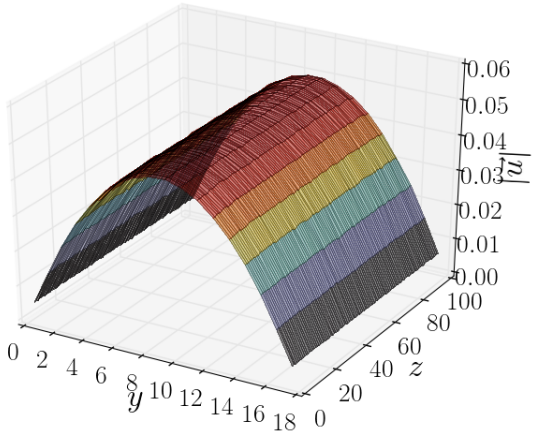
Example: MPCD Flow Profiles



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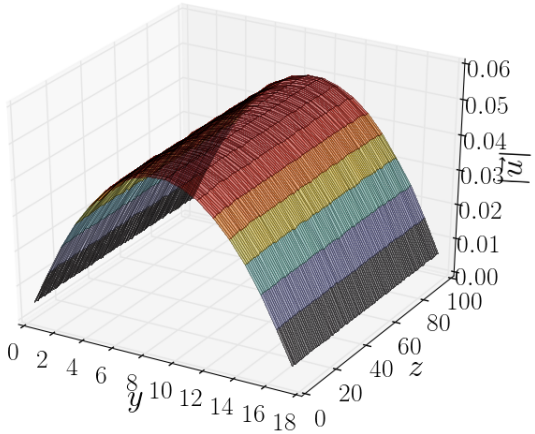

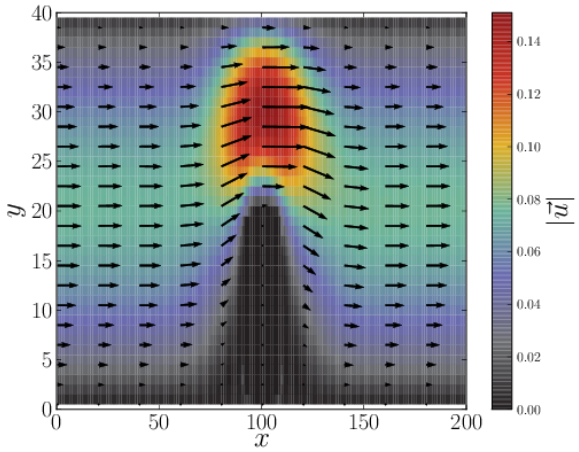

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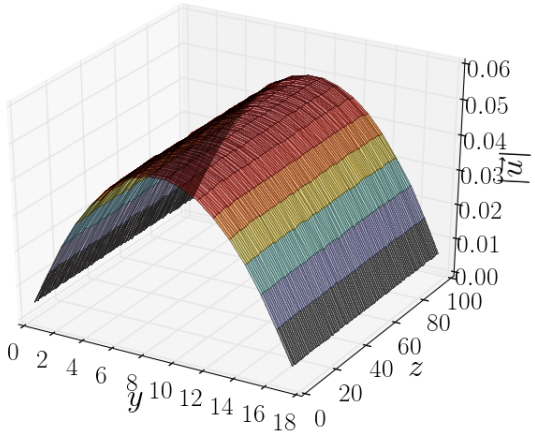

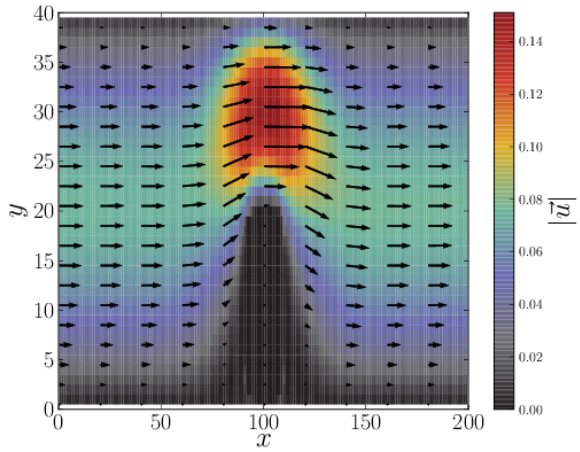

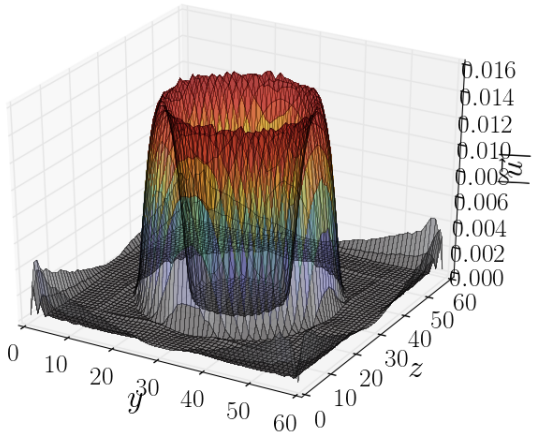

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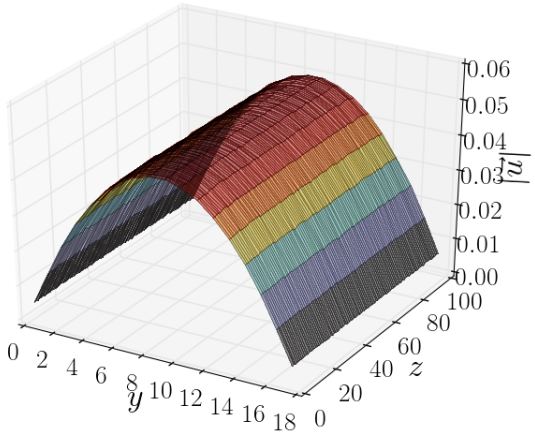

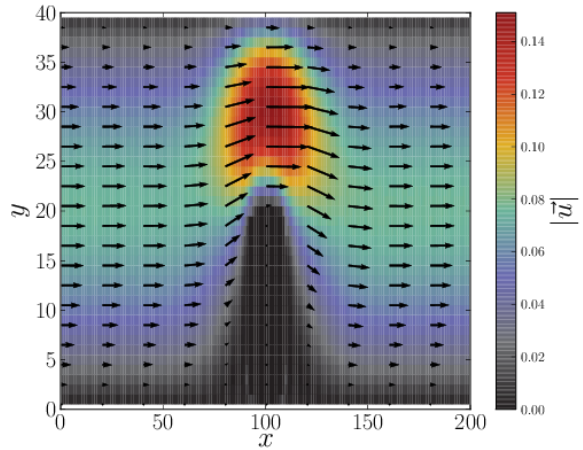

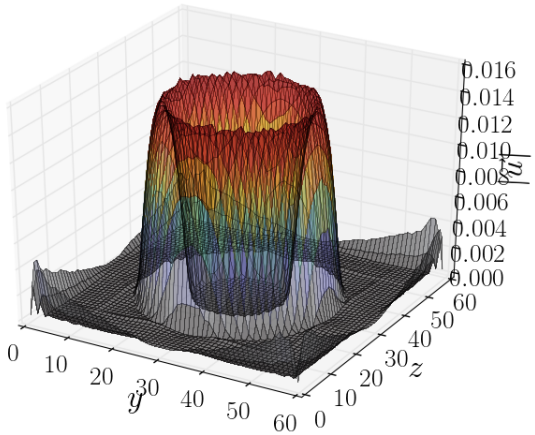

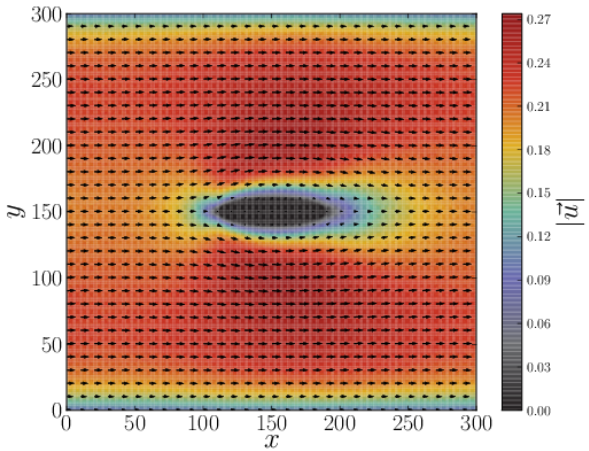

Intermission I

Questions on the operation of the traditional MPCD algorithm?

EMBO Fellow

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1. position $\underline{x}_i$
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3. mass m_i

Each cell has

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Nematic Multi-Particle Collision Dynamics

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Nematic MPCD

Each must additionally have

1. orientation $\underline{u}_i$
2. molecular potential U
3. rotational coefficient γ_R
4. tumbling parameter λ

Each cell must have

1. order parameter $\underline{\underline{Q}}_c$
   - **1.1** scalar order parameter S_c
   - **1.2** director $\underline{n}_c$

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Nematic Multi-Particle Collision Dynamics

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Momentum Collision Operation

$$\underline{v}_i\left(t+\delta t\right)=\underline{v}_{\mathrm{CM}}\left(t\right)+\Xi$$

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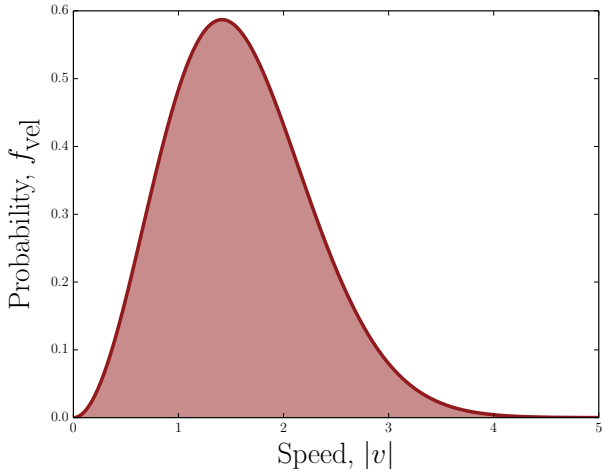

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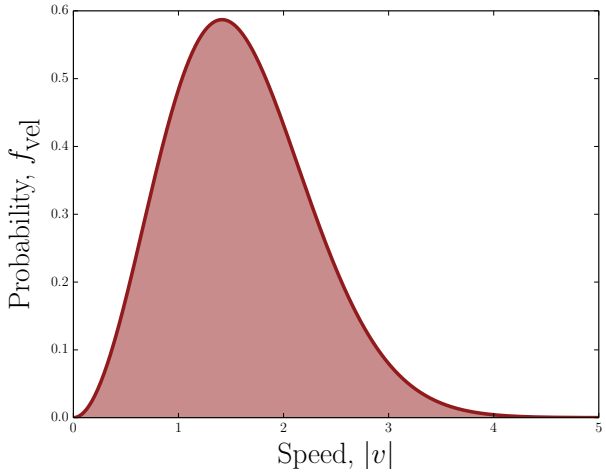

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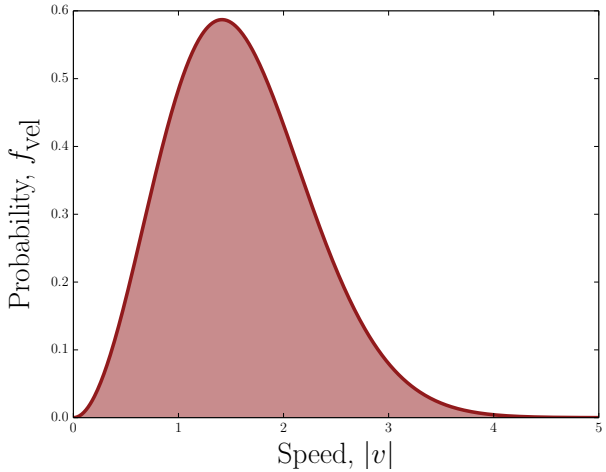

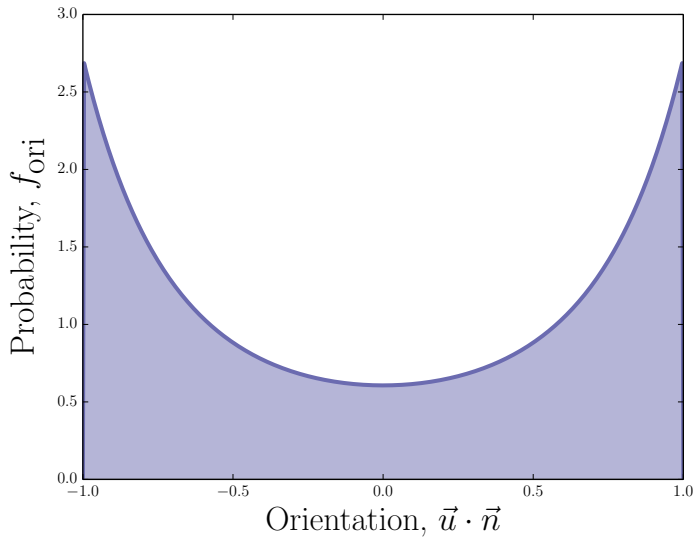

Orientation Collision Operation

$$\underline{u}_i\left(t+\delta t\right)=\underline{\eta}_i\left(\beta U,S,\underline{n}\right),$$

where $\underline{\eta}_i$ is a random orientation drawn from the equilibrium Maier-Saupe probability distribution

$$f_{\mathrm{ori}}=\exp\left(\frac{\beta US}{d-1}\left[d\left(\underline{\eta}\cdot\underline{n}\right)^2-1\right]\right)\propto\exp\left(\frac{d\beta US}{d-1}\eta_n^2\right)$$

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Nematic Multi-Particle Collision Dynamics

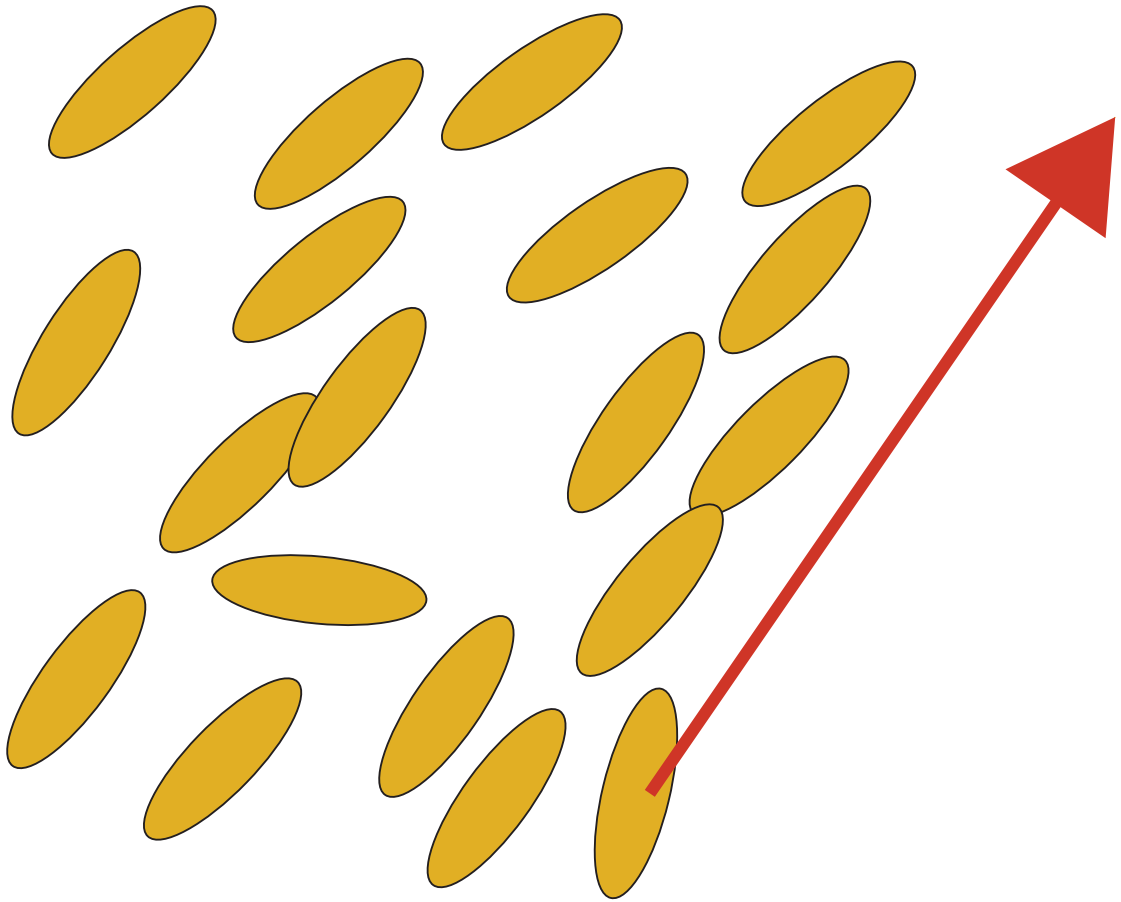
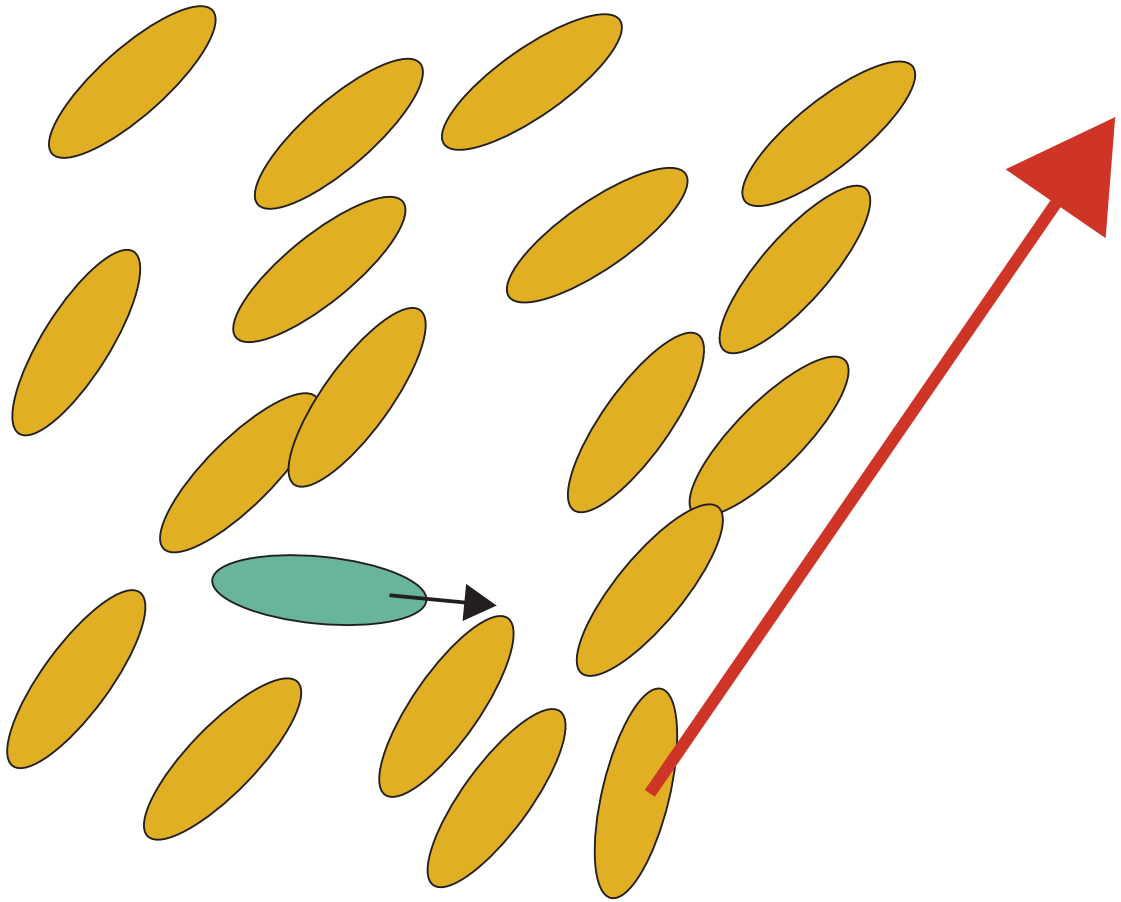


Figure: Nematic $S \approx 1$; $U \gg k_{\mathrm{B}}T$

Nematic Multi-Particle Collision Dynamics



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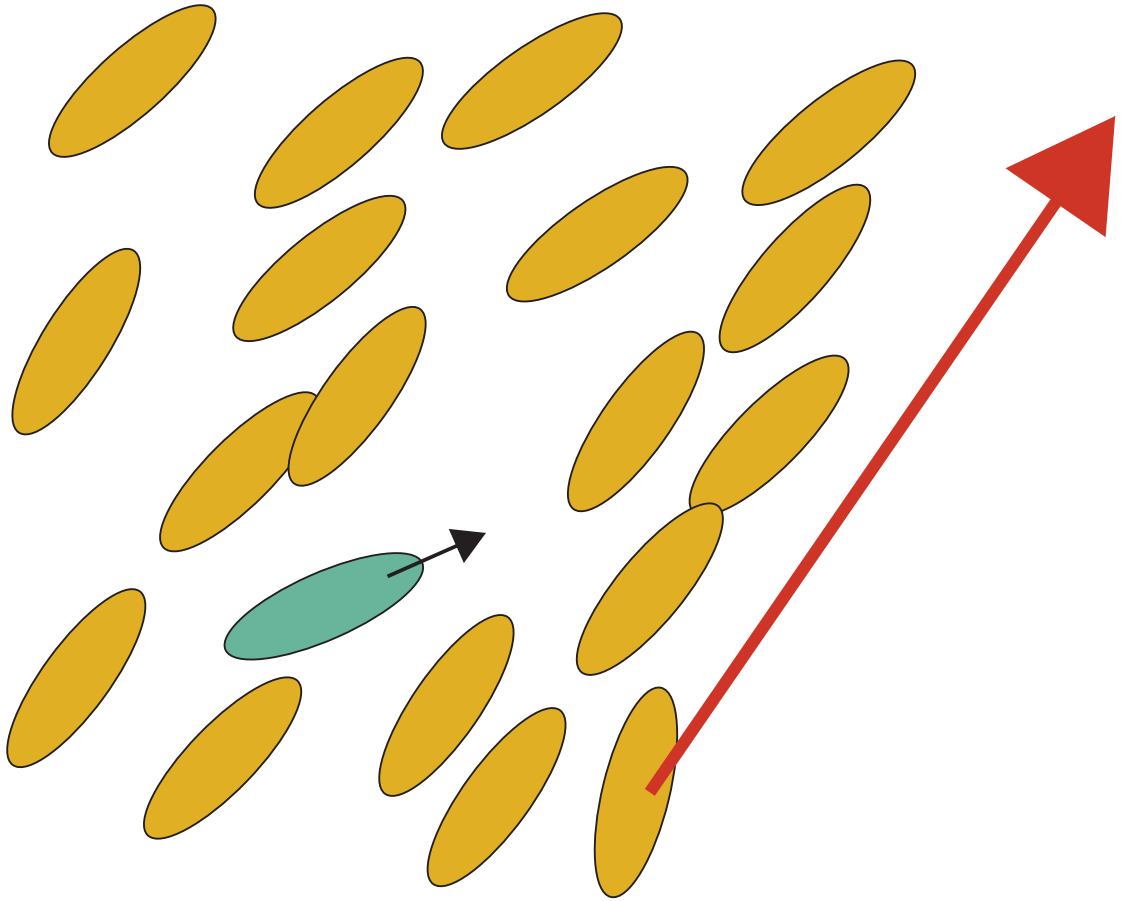

Figure: Nematic $S \approx 1$; $U \gg k_{\mathrm{B}}T$

Isotropic-Nematic Transition

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Figure: Isotropic phase ($U \ll k_{\mathrm{B}}T$)

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Isotropic-Nematic Transition

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Figure: Nematic phase (note: topological defects)

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Isotropic-Nematic Transition

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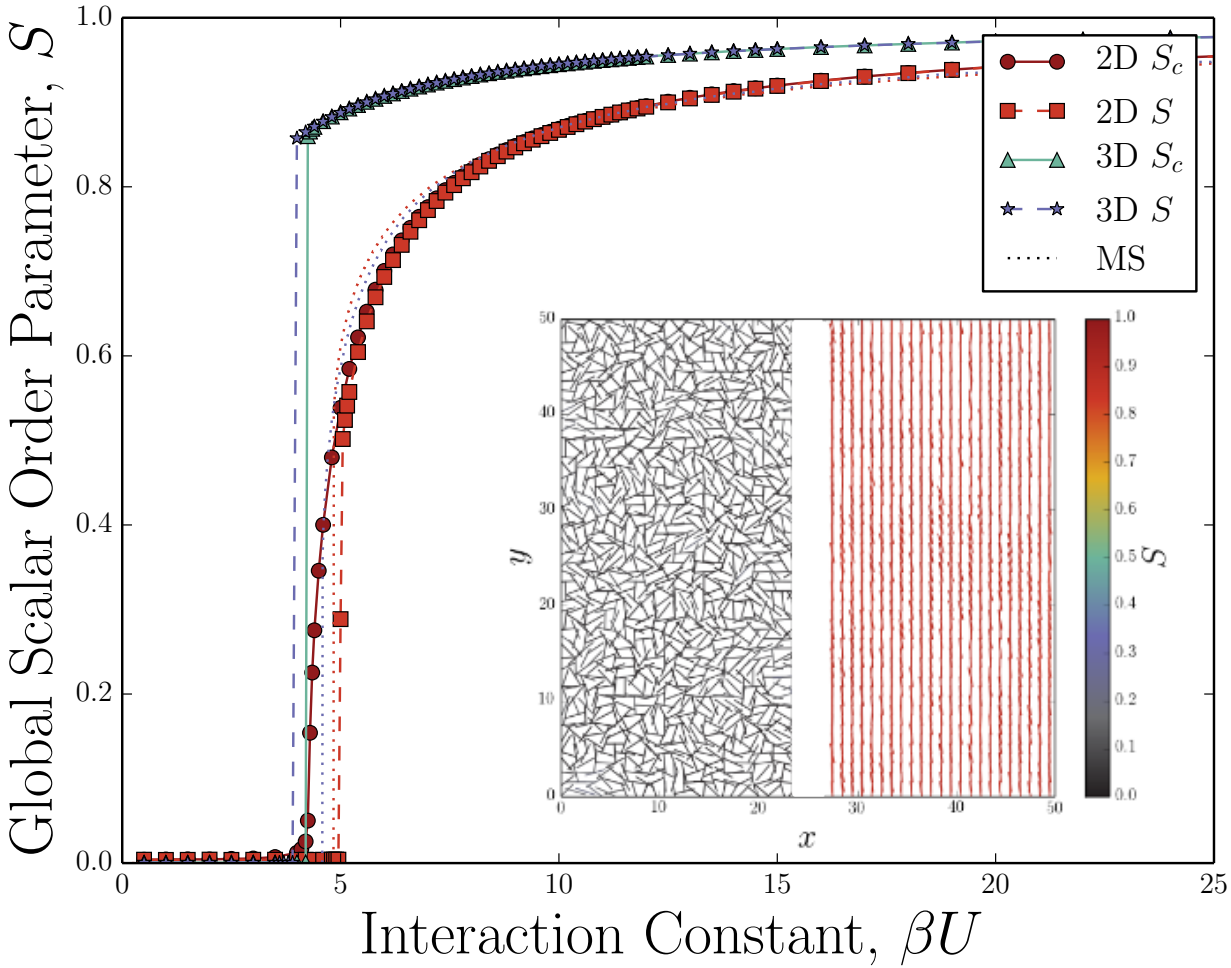

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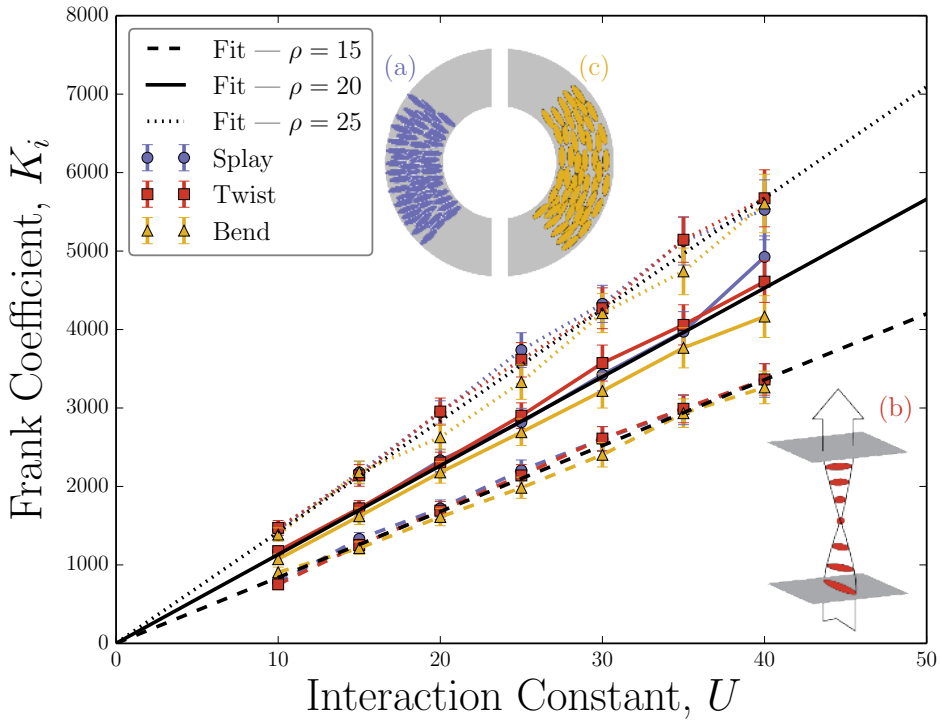
Frank Elastic Coefficient



Isotropic Elasticity

$K_i = \ell^2 \rho U S^2 \left[1 + C_i\right]/6 \sim U/a$

- $i = \{\text{splay}, \text{twist}, \text{bend}\}$
- $C_i \approx 0$ (rod length small compared to interaction length)
- $\ell \approx a$
- isotropic elasticity and one-constant approximation applies.

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Equations to Simulate

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- Nematohydrodynamics requires coupling momentum and orientation

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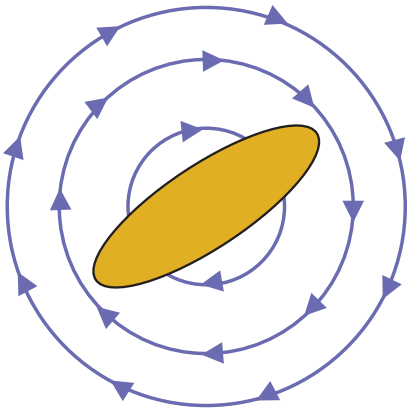
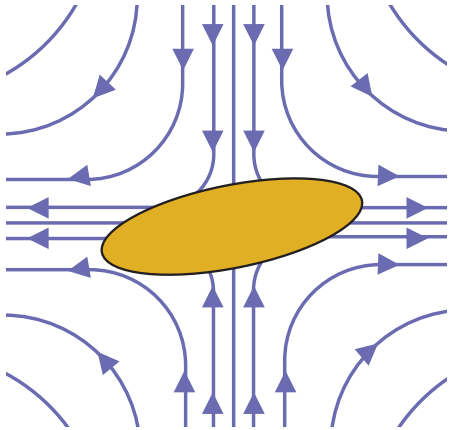
Shear Alignment: Velocity→Orientation Couplings

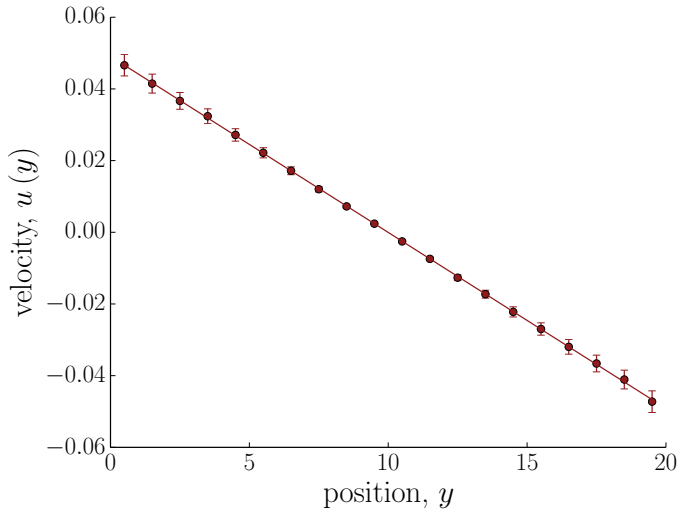




Flow-Induced Rotation

- Discretised Jeffery's equation for a slender rod
  $\frac{\delta \underline{u}_{\mathrm{HI},i}}{\delta t} = \chi_{\mathrm{HI}} \left[\underline{u}_i \cdot \underline{\underline{\omega}} + \lambda \left(\underline{u}_i \cdot \underline{\underline{D}} - \underline{u}_i \underline{u}_i \underline{u}_i : \underline{\underline{D}} \right) \right]$
- bare tumbling parameter λ
- heuristic shear coupling coefficient χ_{HI}

Tumbling & Shear Alignment



- Lees-Edwards BCs
- If $\lambda < 1$ then tumbling behaviour

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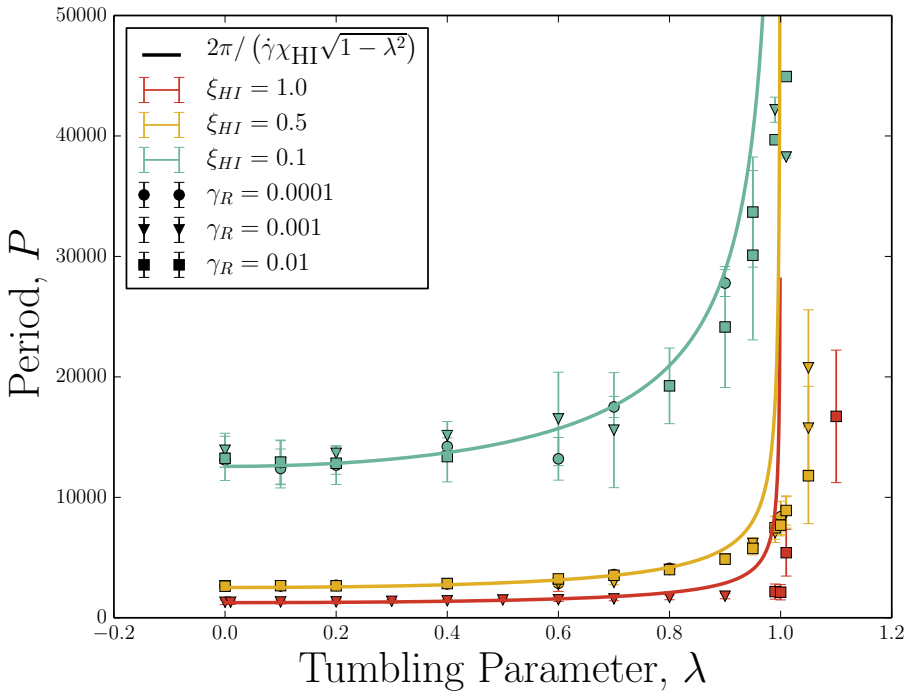

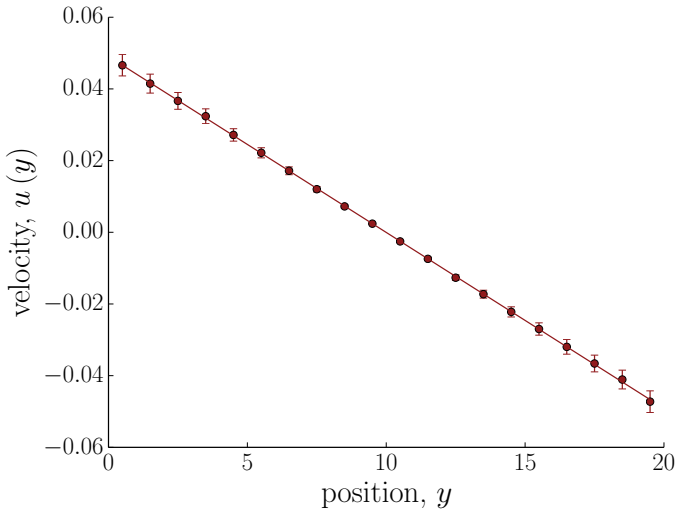

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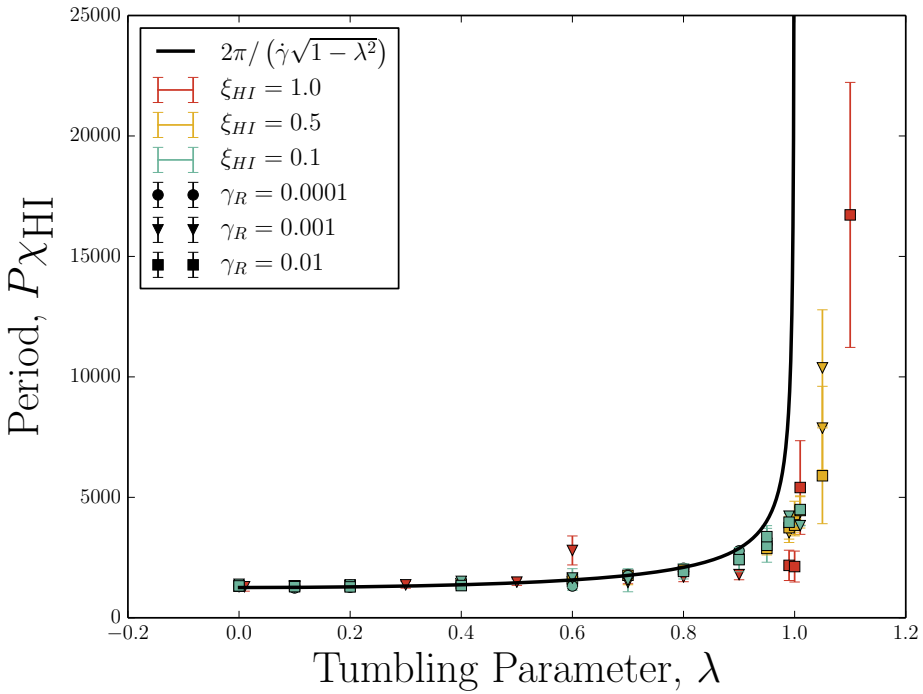

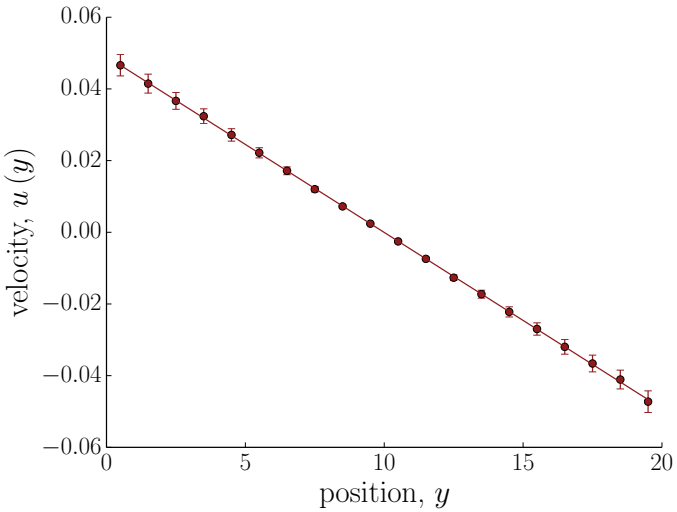

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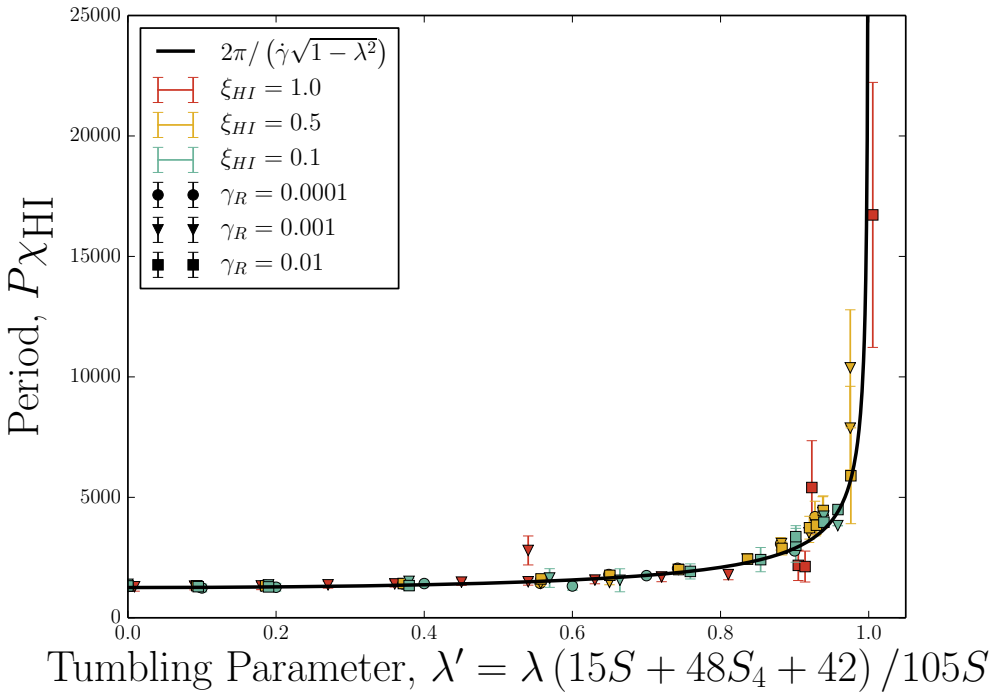

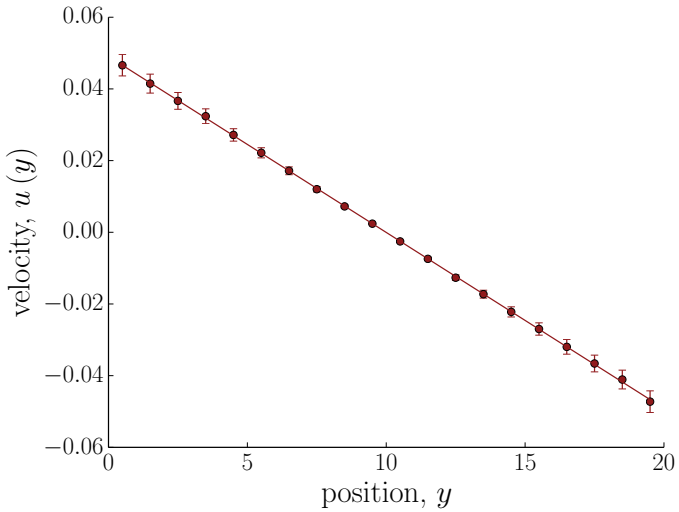

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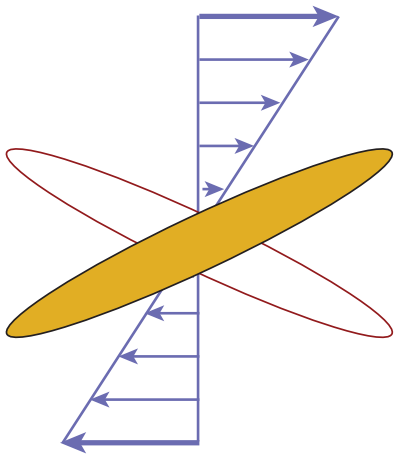
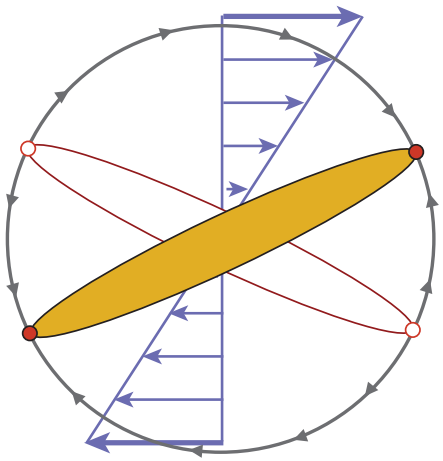


Expect:

- If $\lambda > 1$ then shear aligning

Tumbling & Shear Alignment



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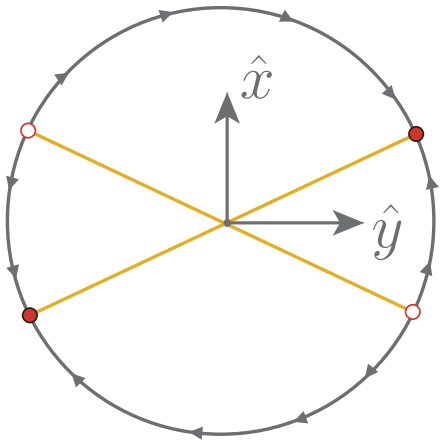

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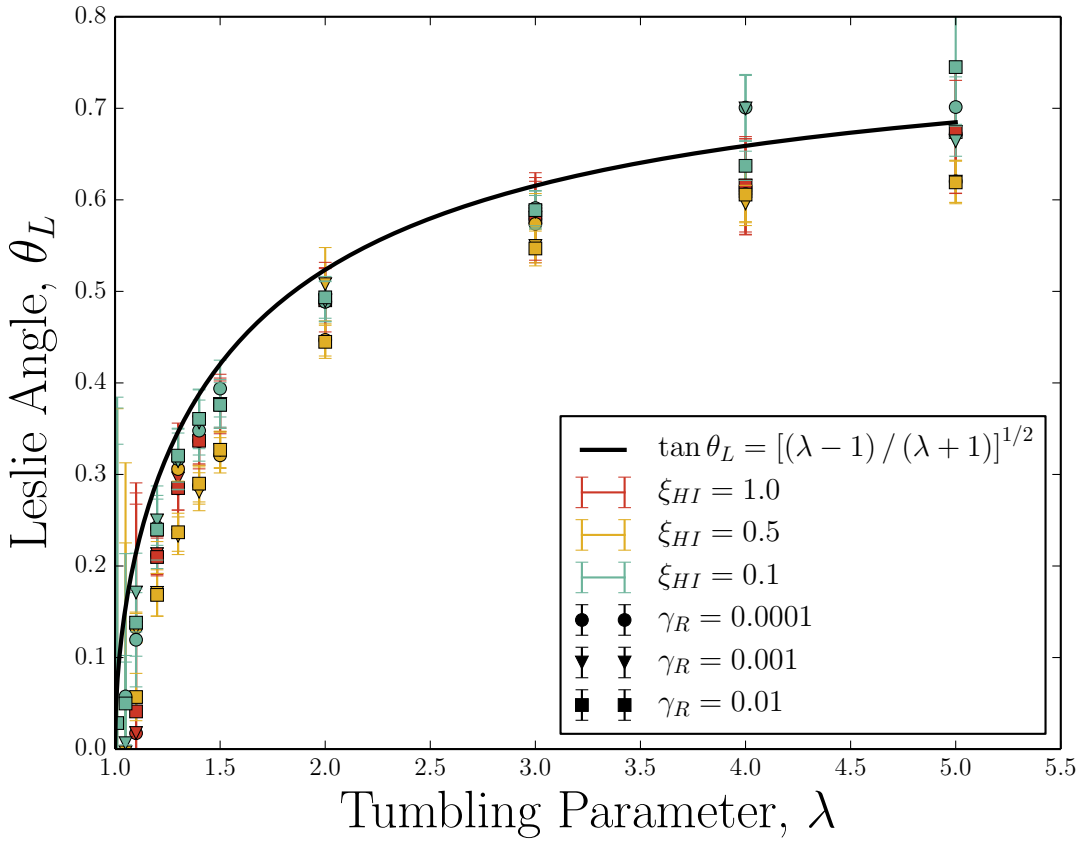

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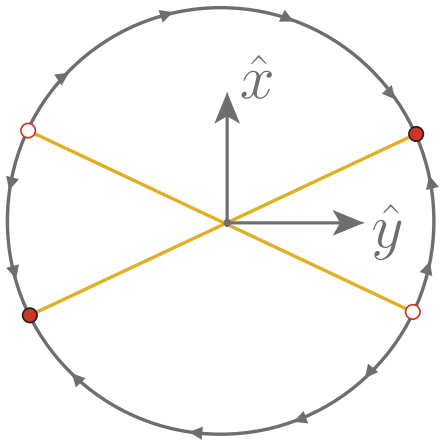

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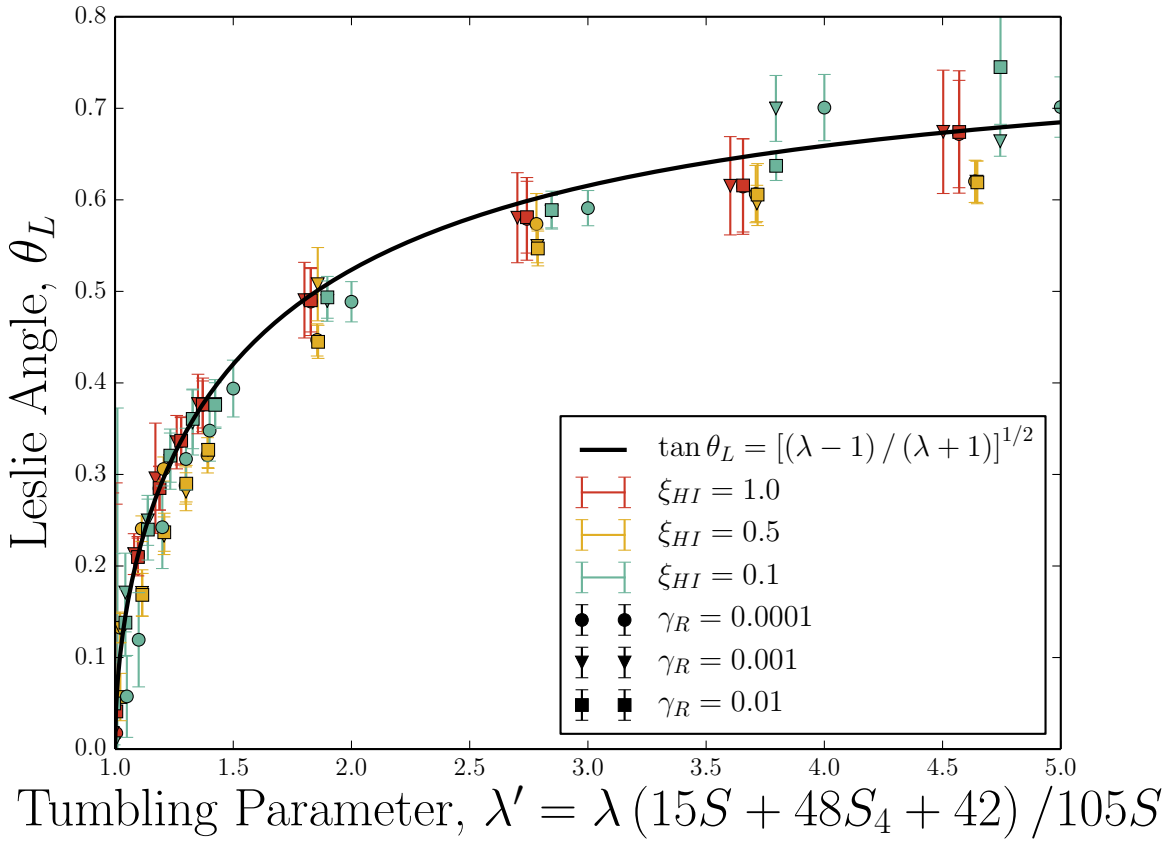

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- Backflow next

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Backflow: Orientation→Velocity Coupling

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Torque Balance

$$\underline{\Gamma}_{\text{net},i} = \underline{\Gamma}_{\text{HI},i} + \underline{\Gamma}_{\text{col},i} + \underline{\Gamma}_{\text{ext},i} = 0$$
$$\underline{\Gamma}_{\text{HI},i} = -\underline{\Gamma}_{\text{col},i} - \underline{\Gamma}_{\text{ext},i}$$

Hydrodynamic Drag Passes Angular Momentum To Fluid

The MPCD collision operator modified to

$$\Xi_{i,c} = \underline{\xi}_i - \left\langle \underline{\xi}_j \right\rangle_{N_c} + \left(\underline{\underline{I}}_c^{-1} \cdot [\delta \underline{L}_c + \delta \underline{\mathcal{L}}_c] \right) \times \underline{r}'_i$$

where $\delta \underline{\mathcal{L}}_c = \sum_i^{N_c} \delta \underline{\mathcal{L}}_i = -\sum_i^{N_c} \Gamma_{\text{HI},i} \delta t$

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- nematic-MPCD for fluctuating nematohydrodynamics
  - Shendruk and Yeomans, *Soft Matter*, 2015, 11, 5101.

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- nematic-MPCD for fluctuating nematohydrodynamics
  - Shendruk and Yeomans, *Soft Matter*, 2015, 11, 5101.
- Remaining: Activity

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Intermission II

Questions on the operation of the nematic-MPCD algorithm?

Proposal: Active MPCD

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Collision Operator

Passive Fluids

- MPCD collisions are artificial operations that stochastically exchange velocities while conserving energy and momentum

Active Fluids

- Active materials convert chemical potential energy to spontaneously drive dynamics
- MPCD collision operations can be conceived that lead to various classes of active matter

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Dipolar Active-Nematic MPCD

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Dipole-Force Andersen Collision

- MPCD cells are subject to dipolar force

$$\Xi_{i,c} = \underbrace{\underline{\xi}_i}_{\text{noise}} - \underbrace{\left\langle \underline{\xi}_j \right\rangle}_{\text{av. noise}} + \underbrace{\left(\underline{\underline{I}}_c^{-1} \cdot \left[\delta \underline{L}_c + \delta \underline{\mathcal{L}}_c \right] \right) \times \underline{r}_i'}_{\text{ang. mom.}}$$
$$+ \underbrace{\tau \left[\alpha_{\text{act}} - |v_i(t)| \right] \left(\kappa_i \underline{n}_c \right)}_{\text{activity}}$$
$$- \underbrace{\left\langle \tau \left[\alpha_{\text{act}} - |v_j(t)| \right] \left(\kappa_j \underline{n}_c \right) \right\rangle_{N_c}}_{\text{residuals}}$$

where

- τ relaxation coefficient
  - Extensile $0 < \tau \leq 1$
  - Contractile $-1 \leq \tau < 0$
- α_{act} out-of-equilibrium speed
- $\kappa_i = \pm 1$ based on plane:

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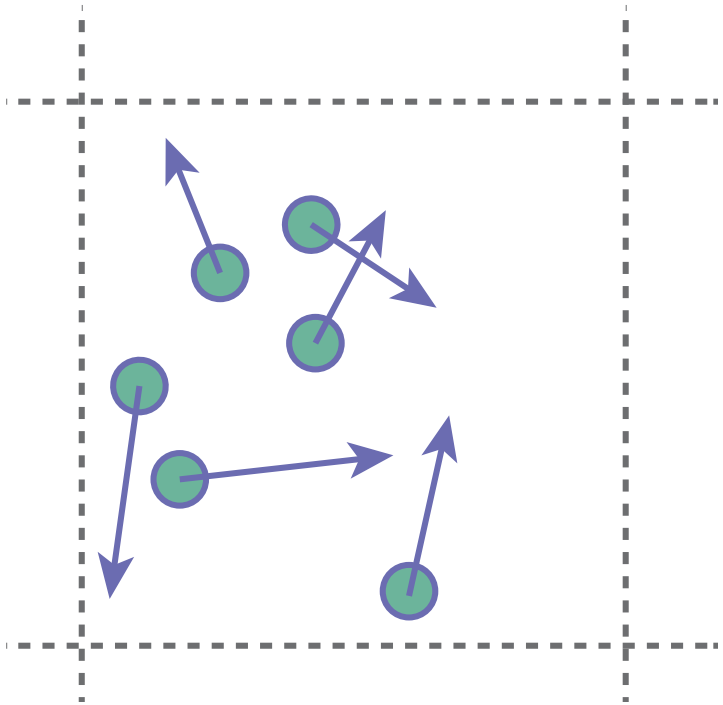

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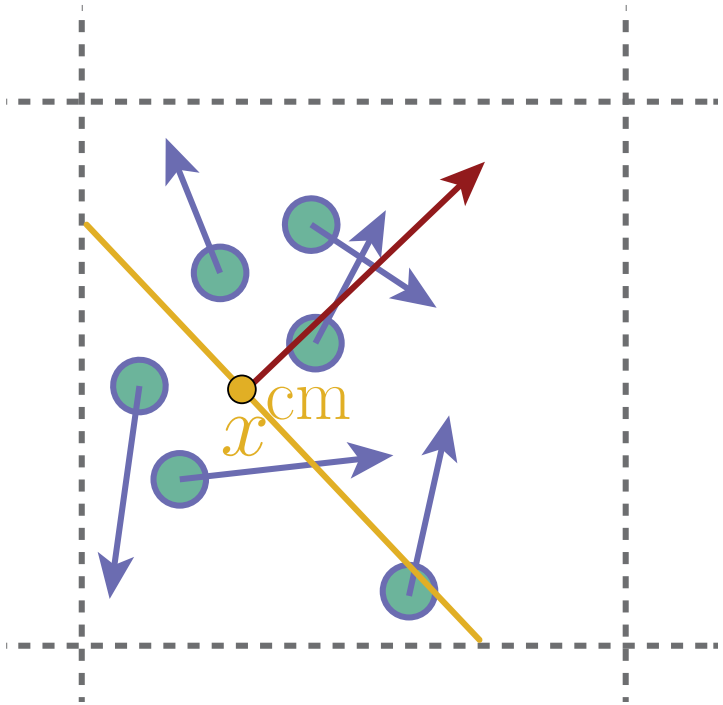

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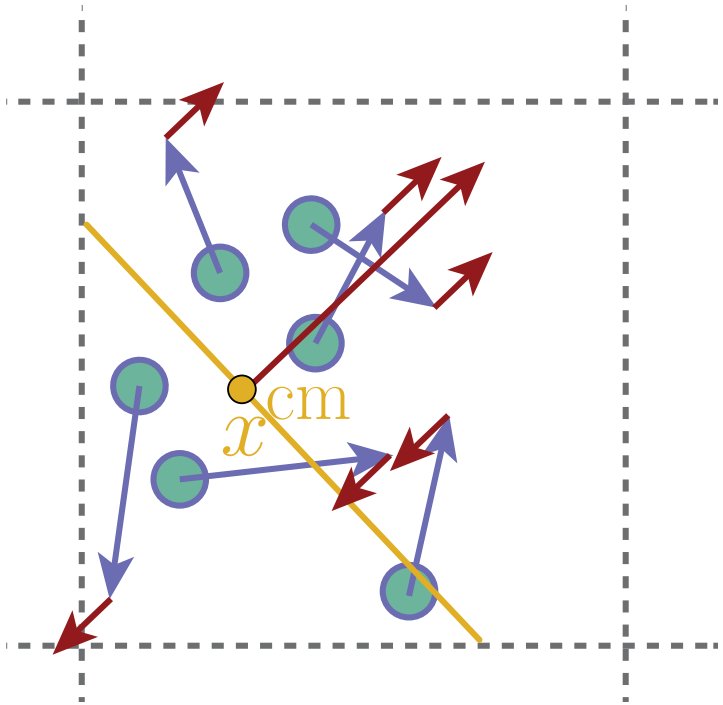

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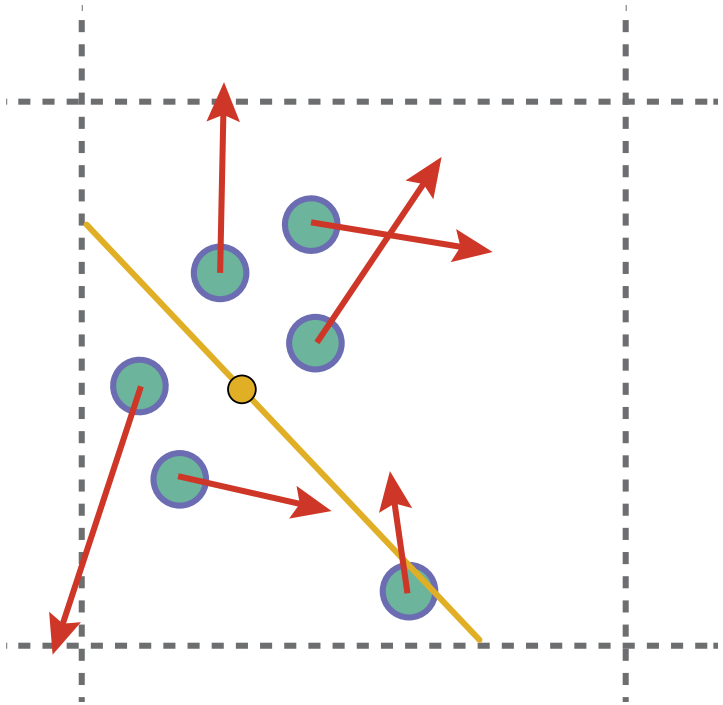

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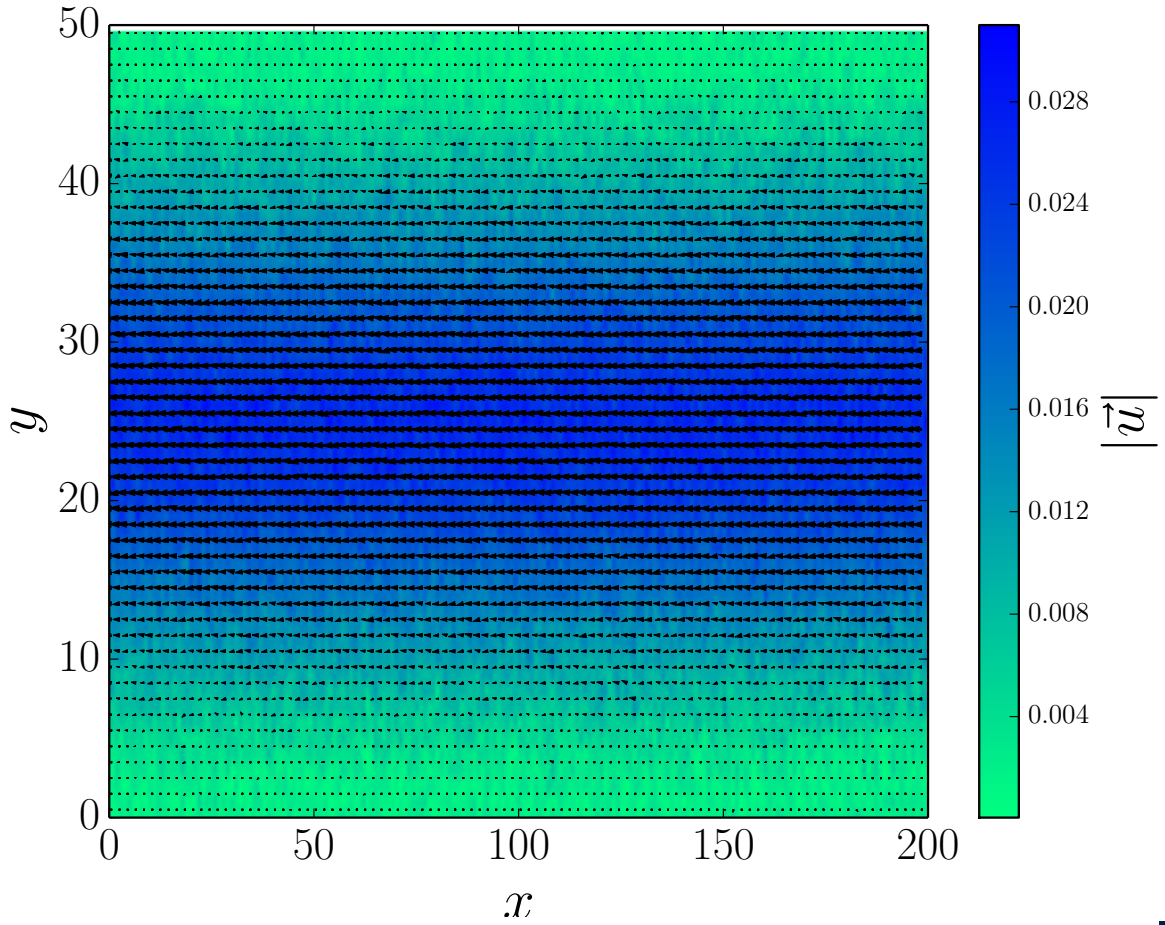
Wall and Defect Pairs Formation

Wall and Defect Pairs Formation

Spontaneous Flows



Active Colloidal Liquid Crystals

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Conclusion

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Recapitulation

- MPCD traditional mesoscale algorithm for isotropic solvent
- MPCD for nematic liquid crystals
  - Isotropic-nematic transition
  - Topological defect dynamics
  - Frank elastic coefficients
  - Nematodynamics with backflow
  - Tumbling and aligning
- MPCD for active nematic
  - Modified collision operator
  - Dipolar active fluid

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Defect Annihilation Dynamics

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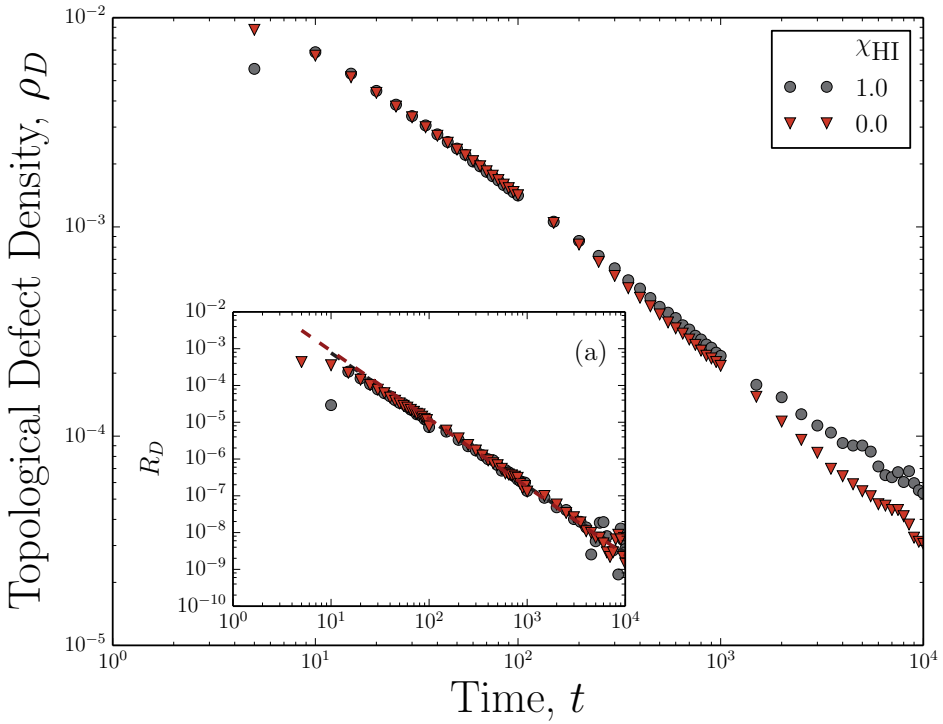
Defect Annihilation Dynamics



Annihilation Rate

- $R_D = -\dot{\rho}_D \sim t^{-(\nu+1)}$
- Liu and Muthukumar: $\nu = 6/7$
- Varies in time: $\nu = 0.74 \pm 0.02$ for $t \in [10, 10^3]$ but $\nu = 0.83 \pm 0.04$ over $t \in [10^2, 10^4]$