Particle-based Mesoscale Algorithm for Active Matter

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Rudolf Peierls Centre for
Theoretical Physics
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17 December, 2014

Motivation

Active Solvents Suspensions:

- Colloids
  - PRL, 109, 028103 (2012)
- Passive Droplets
  - Soft Matter, 10, 7826-78307 (2014)
- Casmir-like Interactions
  - PRE, 90, 013019 (2014)
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- Living Liquid Crystals
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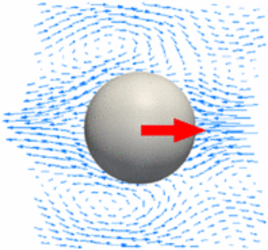

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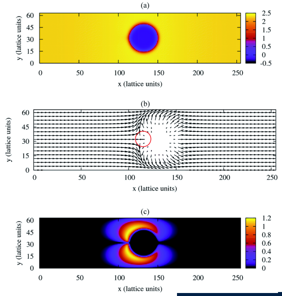

Spontaneous motility of passive emulsion droplets in polar active gels
by De Magistris, *et. al.*

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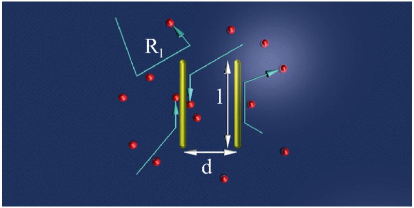

Casimir effect in active matter systems
by Ray, *et. al.*

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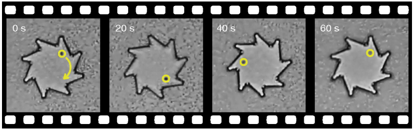

Bacterial ratchet motors by Di Leonardo, *et. al.*

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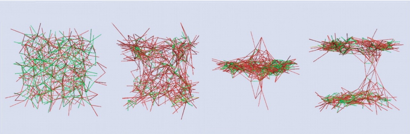

On the spontaneous collective motion of active matter by Wang & Wolynes

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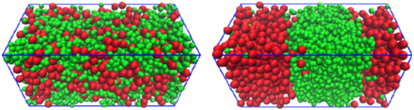

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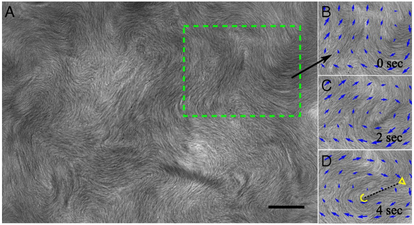

Living liquid crystals by Zhou, *et. al.*

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Conclusion:

- Coarse-graining solvents successful in passive soft matter
  - "Toy-models" have been enlightening, re: Vicsek model
  - Active-nematic LB has been quite successful

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Technique: Multi-Particle Collision Dynamics

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Traditional MPCD

- Particle-based algorithm for moderate Péclet numbers.

Each point-like particle i has

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

Each cell has

1. population N_c
2. centre of mass velocity $\vec{v}_{\mathrm{cm}}$
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

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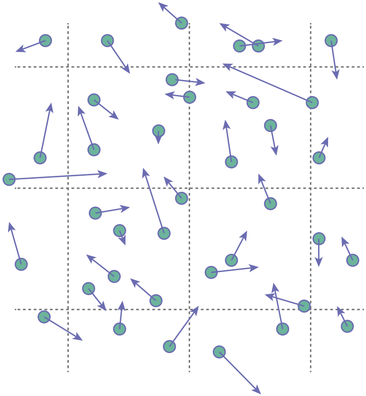

Streaming

$$\vec{x}_i\,(t+\delta t) = \vec{x}_i\,(t) + \vec{v}_i\,(t)\,\delta t$$

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

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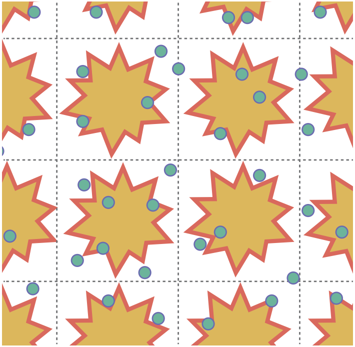

Streaming

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

Collision (Andersen MPCD)

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

where Ξ is a collision operation

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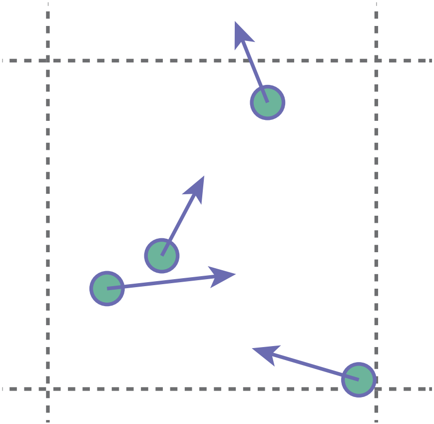

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$$\Xi = \underbrace{\vec{\xi}_i}_{\text{noise}} - \underbrace{\frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i}}_{\text{av. cell noise}}$$

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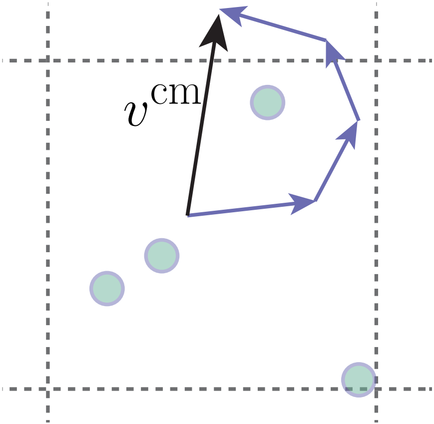

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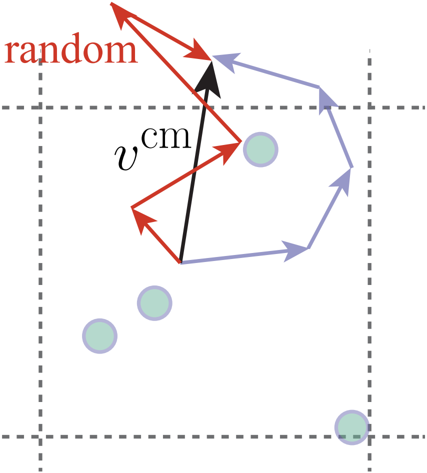

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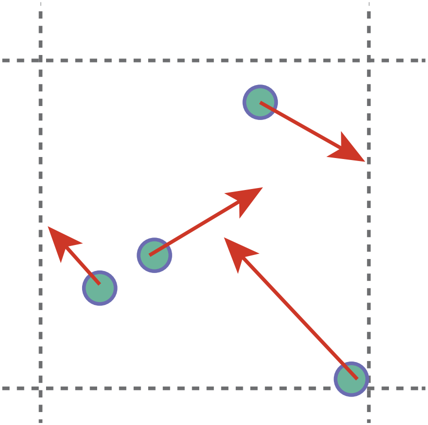

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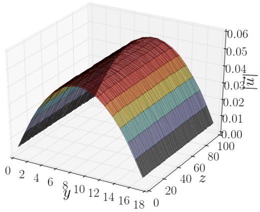
Example: MPCD Flow Profiles



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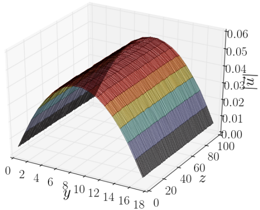

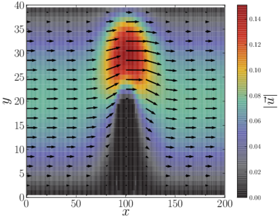

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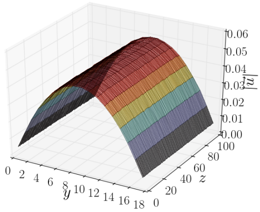

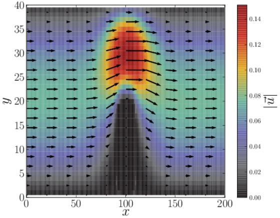

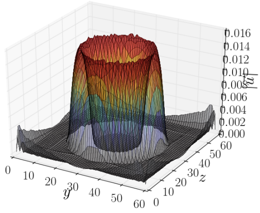

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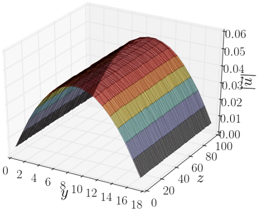

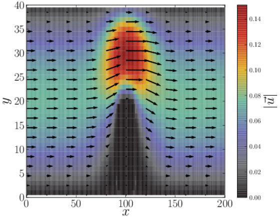

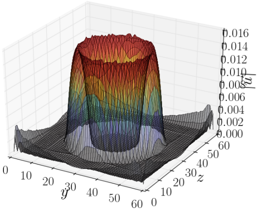

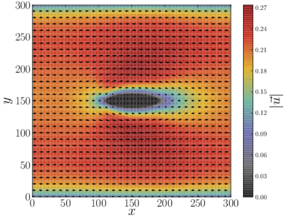

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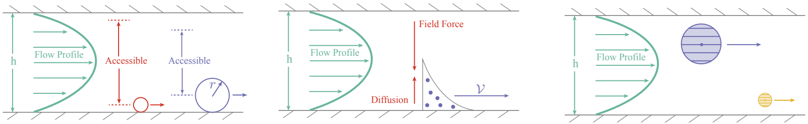
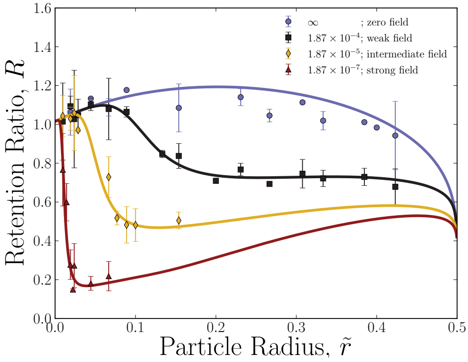
Example: Microfluidic Field-Flow Fractionation





$$\lambda = \frac{k_B T}{fh} \equiv \Lambda \tilde{r}^{-\alpha}$$

$$R = \frac{\langle \mathcal{V} \rangle}{\langle u \rangle}$$

$$\tilde{r} = \frac{r}{h}$$

† TNS & Slater, J. Chromato. A, 1233, 2012.
⋆ TNS, Tahvildari, *et. al.* , Anal. Chem, 85 (12), 2013.

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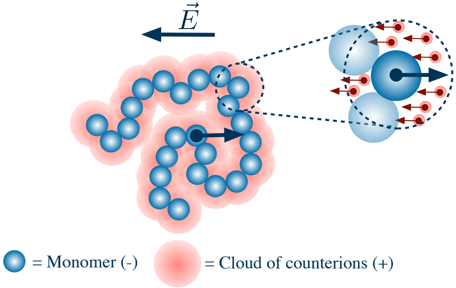
Example: Mean-Field MPCD-MD Debye-Hückel



Free-Draining Mobility

- $\mu_0 = v/E = Q^{\text{eff}}/\zeta^{\text{eff}}$ is **independent** of **length** and **conformation**
- Counterion clouds (λ_D) screen **both**
  - electrostatics
  - hydrodynamics

† Electrophoresis: When hydrodynamics matter, TNS, Hickey, Slater & Harden, Colloid Interface Sci, 17(2), 2012.

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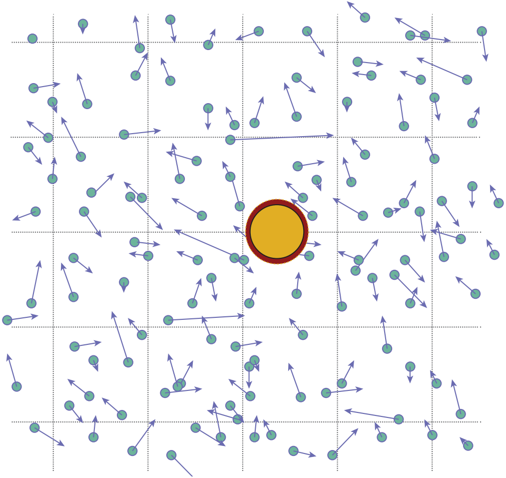

Implicit Counterions

† Simulations of the free-solution electrophoresis of polyelectrolytes with a finite Debye length using the Debye-Hückel approximation, Hickey, TNS, Harden & Slater, PRL, 109(9), 2012.

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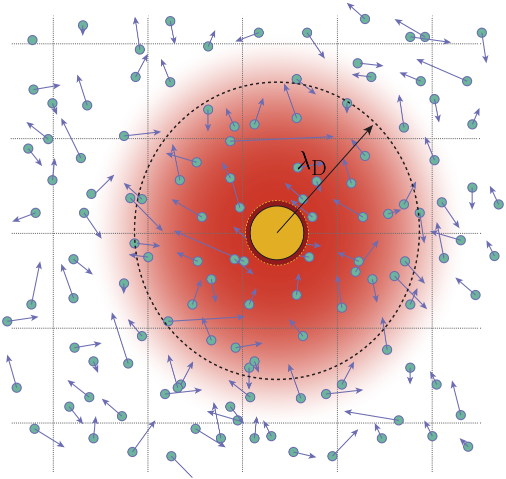

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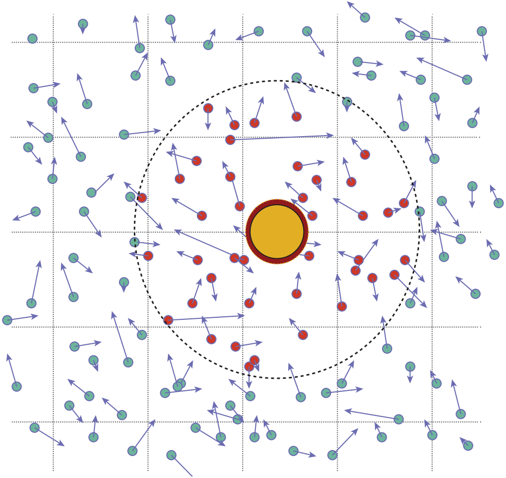

Implicit Counterions

- Finite λ_D
- Debye-Hückel approx. gives charge
  - Implicit counterions
  - Zero-salt limit

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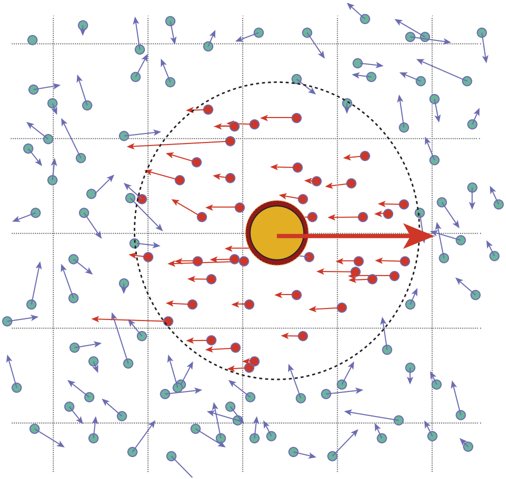

Implicit Counterions

- Finite λ_D
- Debye-Hückel approx. gives charge
  - Implicit counterions
  - Zero-salt limit
- Electric force $\propto$ charge

† Simulations of the free-solution electrophoresis of polyelectrolytes with a finite Debye length using the Debye-Hückel approximation, Hickey, TNS, Harden & Slater, PRL, 109(9), 2012.

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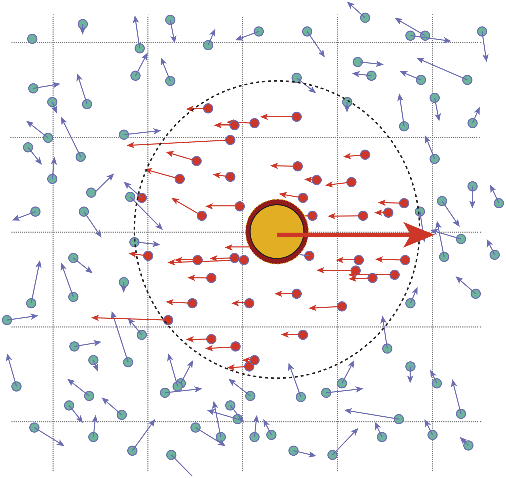

Implicit Counterions

- Finite λ_D
- Debye-Hückel approx. gives charge
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- Electric force $\propto$ charge
- Charge cutoff for counterion condensation

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Proposal: Active MPCD

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

Dry Active Polar MPCD

Vicsek-like Andersen Collision

- Particle interactions align velocities
- In the Vicsek model this is a rotation with noise and a constant speed α_{act}
- In active polar MPCD this is a relaxation to a prescribed speed:

$$\Xi = \underbrace{\vec{\xi}_i}_{\text{noise}} - \underbrace{\frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i}}_{\text{av. cell noise}} + \underbrace{\tau \left[\alpha_{\text{act}} \frac{\vec{v}_{\text{CM}}(t)}{|v_{\text{CM}}(t)|} - \vec{v}_i(t) \right]}_{\text{activity}}$$

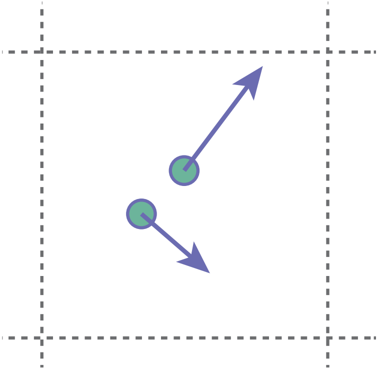

Figure: Polar flocking transition

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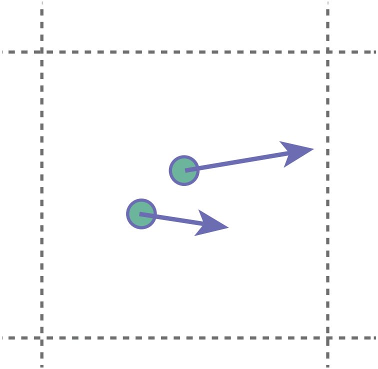

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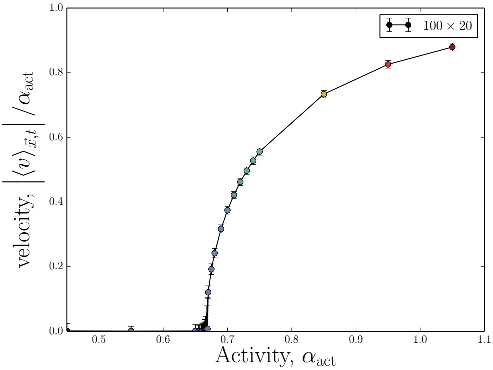

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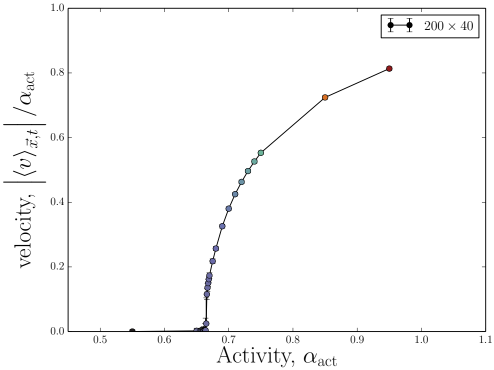

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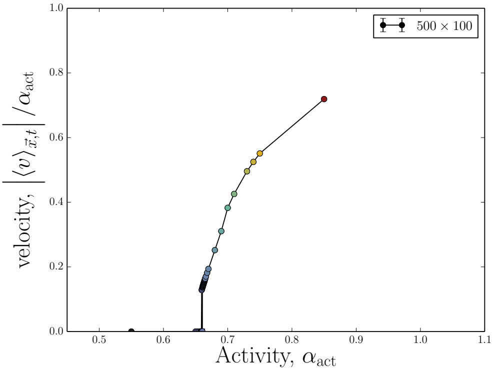

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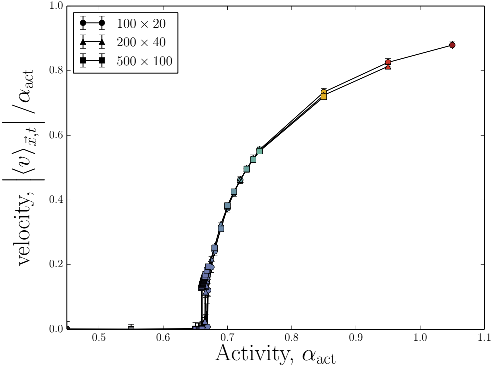

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Figure: Flocking coexistence

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Dry Active Apolar MPCD

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Chaté-like Andersen Collision

- Particles align along orientation, rather than vector

$$\Xi = \underbrace{\vec{\xi}_i}_{\text{noise}} - \underbrace{\frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i}}_{\text{av. cell noise}} \pm \underbrace{\tau \left[\alpha_{\text{act}} - |v_i(t)|\right] \hat{n}}_{\text{activity}}$$

where $\hat{n}$ of each cell is the primary eigenvector of

$$\underline{\underline{Q}} = \frac{1}{d-1} \left\langle d\hat{v}_i \hat{v}_i - \underline{\underline{\delta}} \right\rangle_{N_c}$$

and S is the eigenvalue (flocking scalar order parameter)

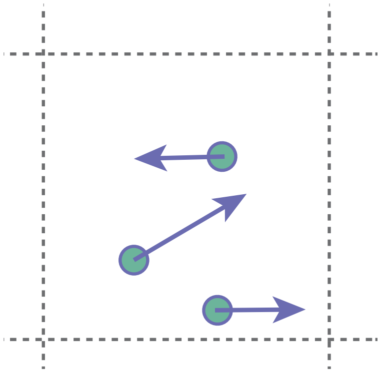

Figure: Nematic ordering transition

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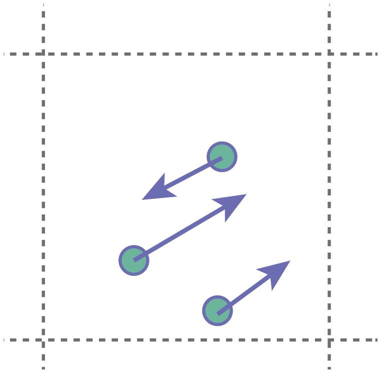

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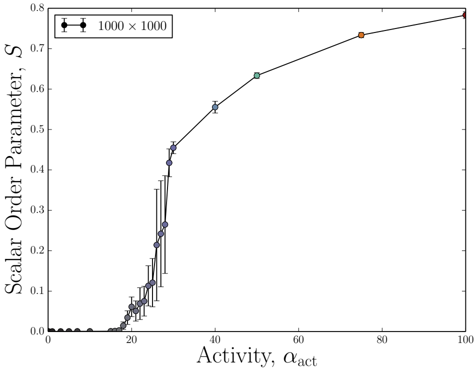

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Figure: Coexistence

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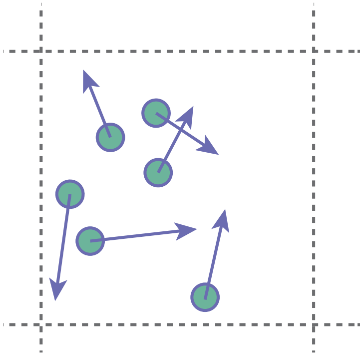
Dry Active Dipolar MPCD

Dipole-Force Andersen Collision

- MPCD cells are subject to dipolar force

$$\Xi = \underbrace{\vec{\xi}_i}_{\text{noise}} - \underbrace{\frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i}}_{\text{av. cell noise}} + \kappa\left(\vec{x}_i, \vec{x}_{\text{cm}}\right) \underbrace{\frac{\alpha_{\text{act}} m_i}{N_c}\hat{n}}_{\text{activity}}$$

where $\kappa = \pm 1$ and the fluid is thermostated by velocity rescaling



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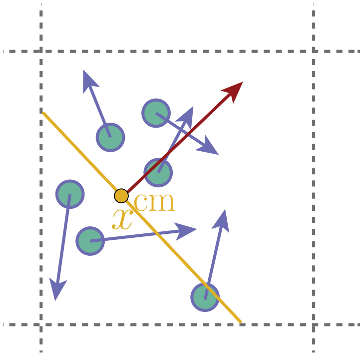

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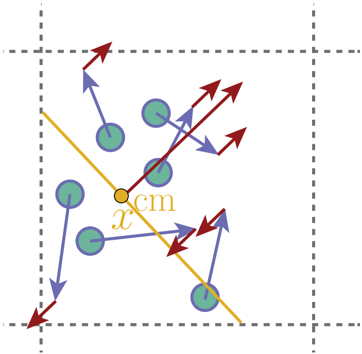

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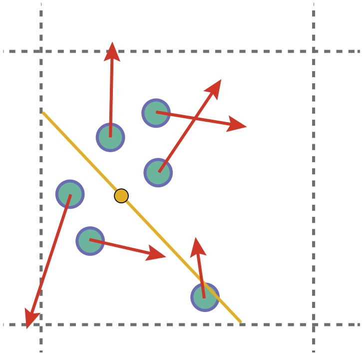

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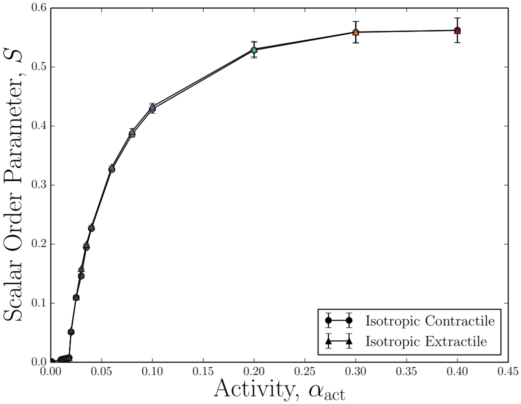

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EMBO Fellow

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Figure: Active Extensile Isotropic Fluid

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Nematic Multi-Particle Collision Dynamics

EMBO Fellow

Traditional MPCD

Each point-like particle i has

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

Each cell has

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

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Nematic MPCD

Each must additionally have

1. orientation $\vec{u}_i$

2. molecular potential U

3. rotational coefficient ξ_R

4. tumbling parameter λ

Each cell must have

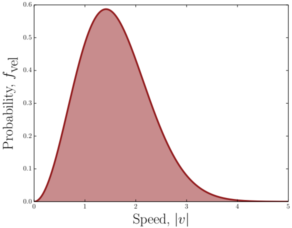
1. order parameter $\underline{\underline{Q}}$

- **1.1** scalar order parameter S
- **1.2** director $\vec{n}$

Momentum Collision Operation

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

$$\Xi = \underbrace{\vec{\xi}_i}_{\text{noise: MB-dist}} - \underbrace{\frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i}}_{\text{av. cell noise}} + \underbrace{\left(\underline{\underline{I}}_c^{-1} \cdot \delta \vec{L}_i\right) \times \vec{r}_i'}_{\text{correction to conserve ang mom}}$$



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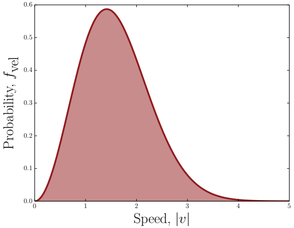

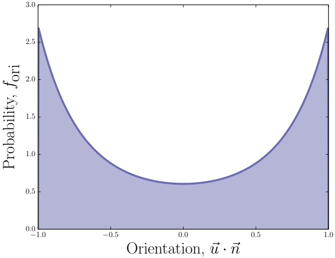

Orientation Collision Operation

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

where $\vec{\eta}_i$ is a random orientation drawn from the equilibrium probability distribution

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

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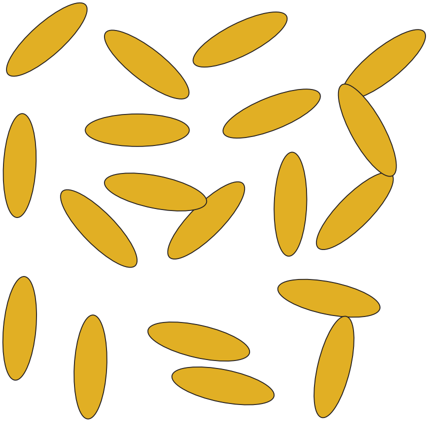


Figure: Isotropic $S \approx 0$; $U \ll k_{\mathrm{B}}T$

Nematic Multi-Particle Collision Dynamics

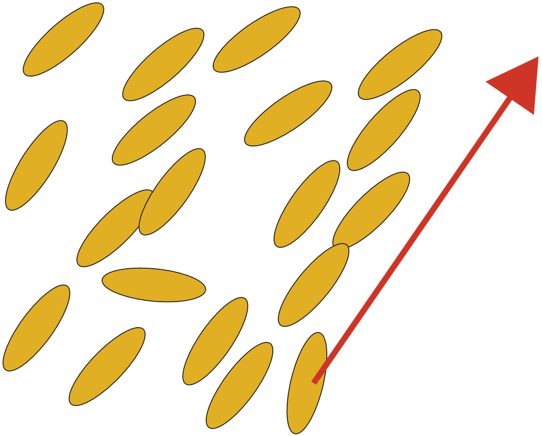
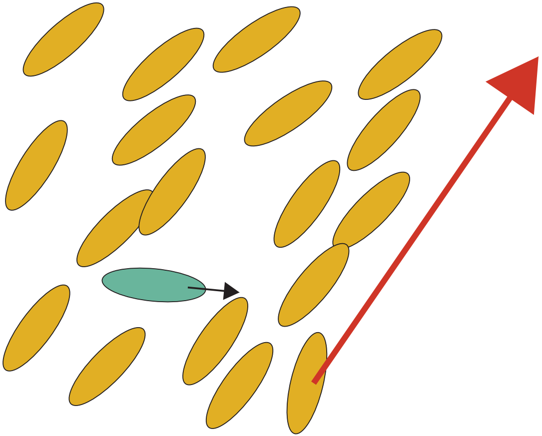


Figure: Nematic $S \approx 1$; $U \gg k_{\mathrm{B}}T$



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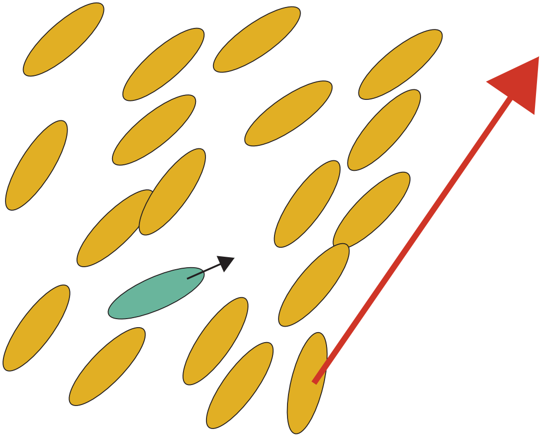


Figure: Nematic $S \approx 1$; $U \gg k_{\mathrm{B}}T$

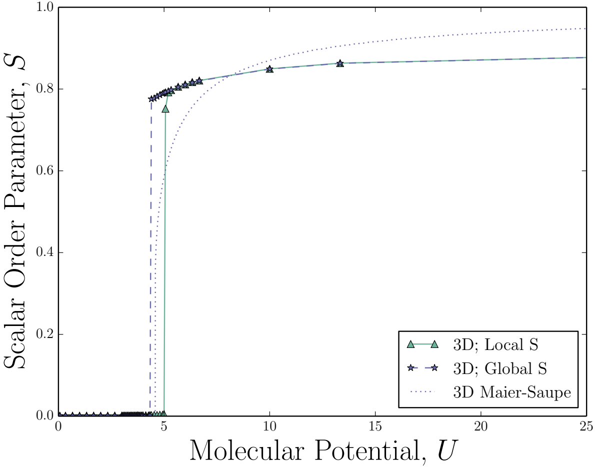
Isotropic-Nematic Transition

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

Isotropic-Nematic Transition

Figure: Nematic phase (note: topological defects)

Isotropic-Nematic Transition



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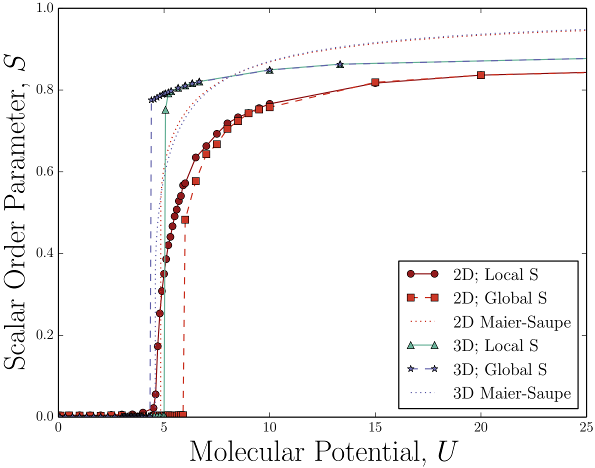

Coupling Velocity and Orientation Fields

Torque acting on nematogens:

1. from the collision operation
2. from an external magnetic field
3. from shear

Coupling Velocity and Orientation Fields

EMBO Fellow

Torque acting on nematogens:

1. from the collision operation
   $\vec{\tau}_{\text{col}} = \xi_R \vec{\Omega}_{\text{col}} = \xi_R \left[\vec{u} \times \frac{\Delta \vec{u}}{\delta t}\text{col}\right]$
2. from an external magnetic field
3. from shear

- torque $\vec{\tau} = \xi_R \vec{\Omega}$
- rotational friction coefficient $\xi_R \approx \frac{\pi \nu_0 L^3}{3 \ln(L/R)}$
- angular velocity $\vec{\Omega} = \vec{u} \times \dot{\vec{u}}$
- tumbling parameter $\lambda = \left(p^2 - 1\right) / \left(p^2 + 1\right)$
- ξ_{HI} phenomenological hydrodynamic susceptibility

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2. from an external magnetic field
   $\vec{\tau}_M = \vec{M} \times \vec{H} = \chi_a \left(\vec{H} \cdot \vec{u} \right) \vec{u} \times \vec{H}$
3. from shear

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- ξ_{HI} phenomenological hydrodynamic susceptibility

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Coupling Velocity and Orientation Fields

EMBO Fellow

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$\delta \vec{\mathcal{L}} = \vec{\tau} \delta t = \left[\vec{\tau}_{\text{col}} + \vec{\tau}_{\text{M}} + \vec{\tau}_{\text{E}} \right] \delta t$
reduces $\delta \vec{L}$ in the collision operation

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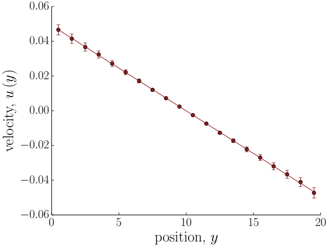
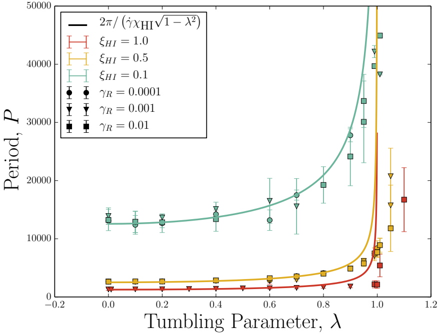
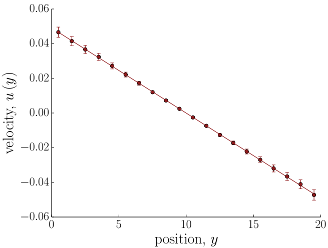
Tumbling & Shear Alignment



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

Tumbling & Shear Alignment





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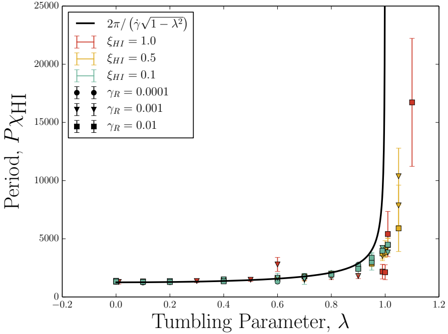

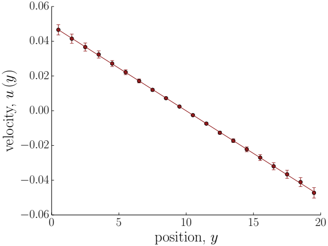

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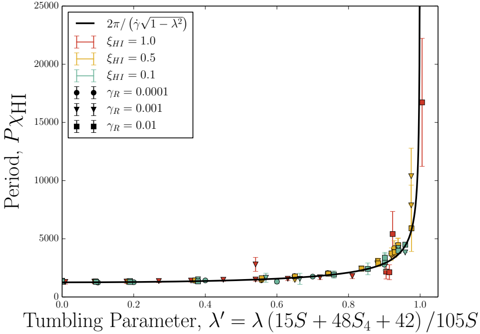

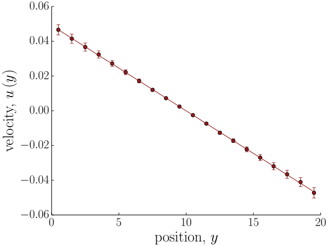

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Tumbling & Shear Alignment

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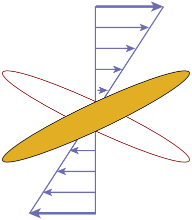

Expect:

- If $\lambda > 1$ then shear aligning

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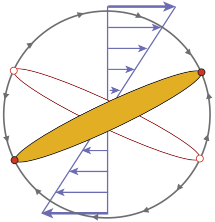
Tumbling & Shear Alignment



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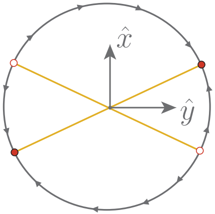

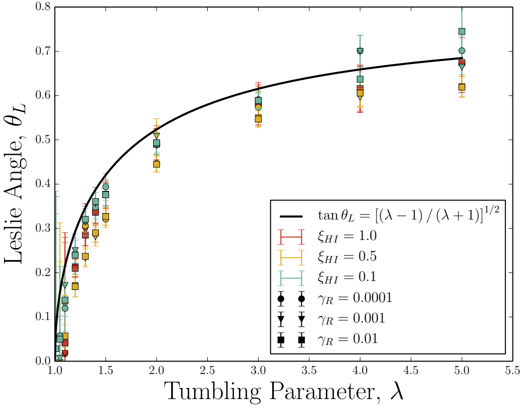

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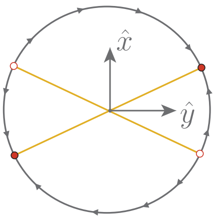

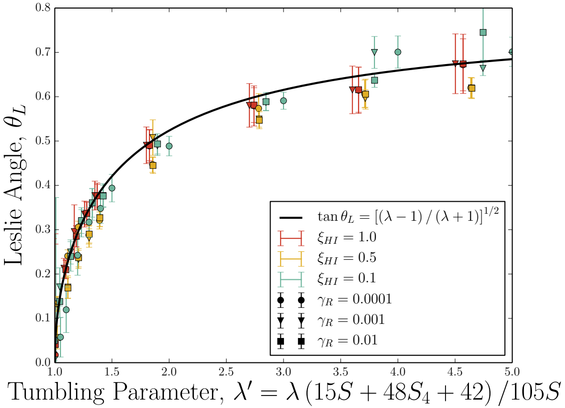

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Conclusion

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Recapitulation

- MPCD for active systems
  - Vicsek-like dry, active polar fluid
    - 1^{st} order flocking transition
    - Dense bands in dilute isotropic gas
  - Chaté-like dry, active apolar fluid
    - 1^{st} order nematic transition
    - Dense threads in dilute isotropic gas
  - Dipolar active fluid
    - Highly compressible
- MPCD for nematic liquid crystals
  - Isotropic-nematic transition
  - Topological defect dynamics
  - Frank elastic coefficients
  - Nematodynamics with backflow
  - Tumbling and aligning

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Conclusion

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Future work

- Precise determination of Frank coefficients and Leslie viscosities
- Embed solutes within LC
- Determine if homogeneous densities are possible in active dipolar MPCD
- Combine active dipolar and nematic MPCD algorithms
  - MPCD Active Gels

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Funding, Resources & Colleagues

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Example: Mean-Field MPCD-MD Debye-Hückel

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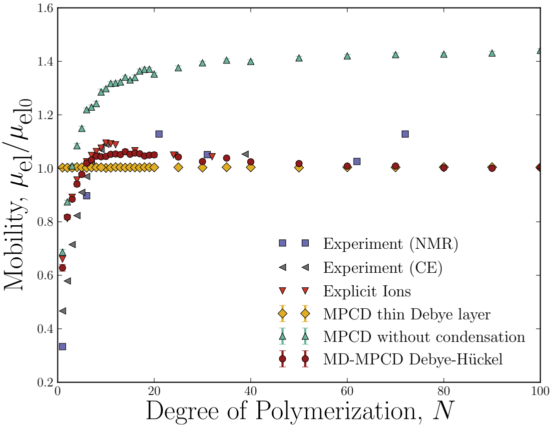

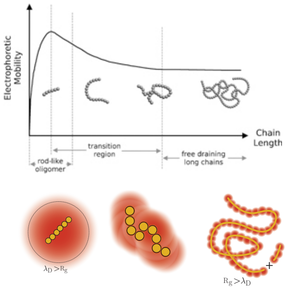

Full HI

Free-draining

† Importance of Hydrodynamic Shielding for the Dynamic Behavior of Short Polyelectrolyte Chains, Grass, Böhme, Scheler, Cottet & Holm, PRL, 100, 2008.

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Coupling Velocity and Orientation Fields

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   $\vec{\tau} = \xi_{\text{R}} \xi_{\text{HI}} \left(\vec{u} \times \dot{\vec{u}} \right)$

Orientation→Velocity Coupling

$$\delta \vec{\mathcal{L}} = \vec{\tau} \delta t = \left[\vec{\tau}_{\text{col}} + \vec{\tau}_{\text{M}} + \vec{\tau}_{\text{E}} \right] \delta t$$

$$\Xi = \vec{\xi}_i - \frac{\sum_j^{N_c} m_i \vec{\xi}_j}{\sum_j^{N_c} m_i} + \left(\underline{\underline{I}}_c^{-1} \cdot \left[\delta \vec{L}_i - \delta \vec{\mathcal{L}}_i \right] \right) \times \vec{r}_i'$$

- torque $\vec{\tau} = \xi_R \vec{\Omega}$
- rotational friction coefficient $\xi_R \approx \frac{\pi \nu_0 L^3}{3 \ln(L/R)}$
- angular velocity $\vec{\Omega} = \vec{u} \times \dot{\vec{u}}$
- magnetization $\vec{M}$
- magnetic susceptibility anisotropy $\chi_a = \chi_{\parallel} - \chi_{\perp}$
- rate of strain $2\underline{\underline{D}} = \underline{\underline{E}} + \underline{\underline{E}}^{\mathsf{T}}$
- vorticity $2\underline{\underline{\omega}} = \underline{\underline{E}} - \underline{\underline{E}}^{\mathsf{T}}$
- velocity gradient tensor $\underline{\underline{E}} = \vec{\nabla} \vec{v}$
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Tumbling & Shear Alignment

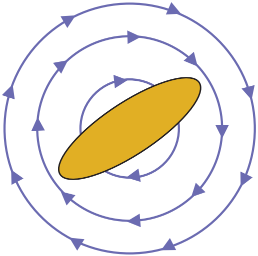


Figure: Rotational Component

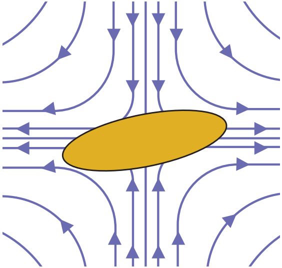


Figure: Strain Rate Component

$$\dot{\vec{u}} = \vec{u} \cdot \underline{\underline{\omega}} + \lambda \left(\vec{u} \cdot \underline{\underline{D}} - \vec{u}\vec{u}\vec{u} : \underline{\underline{D}} \right) \qquad ; \qquad \lambda = \frac{p^2 - 1}{p^2 + 1}$$

Frank Elastic Coefficients

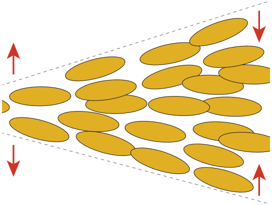


Figure: Splay

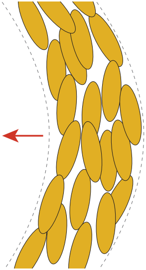


Figure: Bend

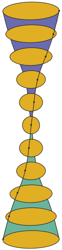


Figure: Twist

Free energy cost of deformation arises as difference in energy used in Maier-Saupe distribution

$$\beta\omega = \sum_i^N \frac{\beta U S}{d-1}\left[d\left(\vec{u}_i \cdot \vec{n}\right)^2 - 1\right]$$

†On going.

Confinement and Topological Defects

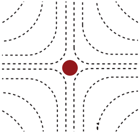


Figure: $m = -1$

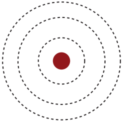
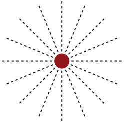


Figure: $m = +1$



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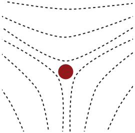

Figure: $m = -1/2$

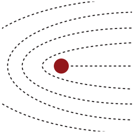

Figure: $m = +1/2$

Figure: Circular cavity with homeotropic BCs

Confinement and Topological Defects

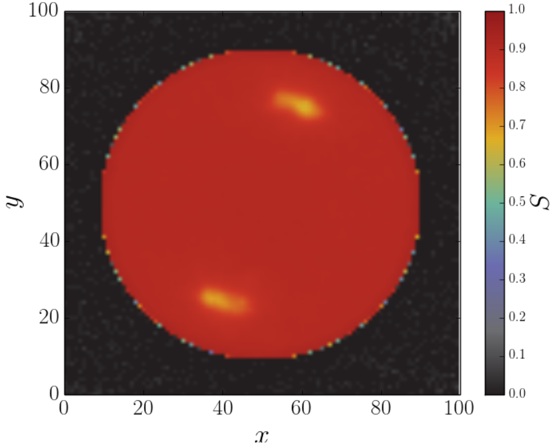

Figure: Circular cavity with homeotropic BCs

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Figure: Square cavity with homeotropic BCs

Confinement and Topological Defects

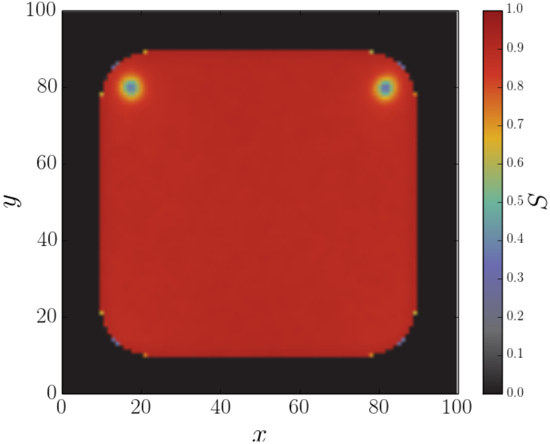


Figure: Square cavity with homeotropic BCs

Confinement and Topological Defects

Figure: Cavity with core

Confinement and Topological Defects

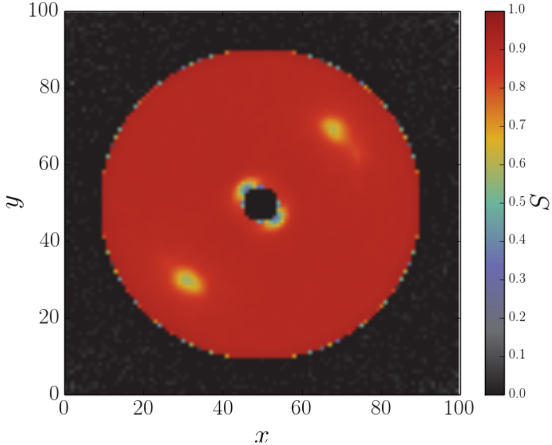


Figure: Cavity with core

Figure: Hemispherical barrier

Confinement and Topological Defects

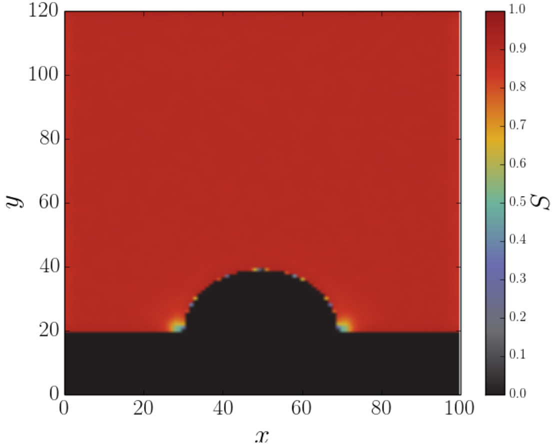
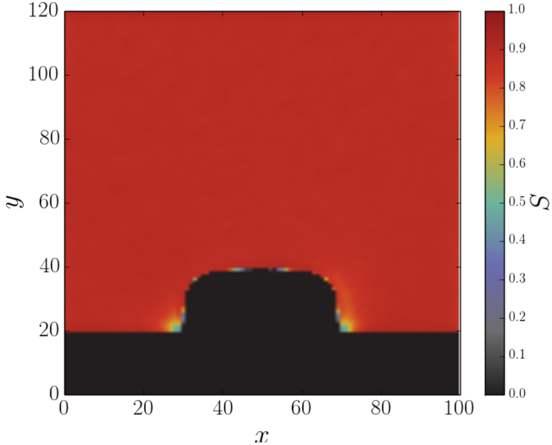


Figure: Hemispherical barrier

Figure: Craighead-like geometry

Confinement and Topological Defects



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