Microhydrodynamics of Liquid Crystals

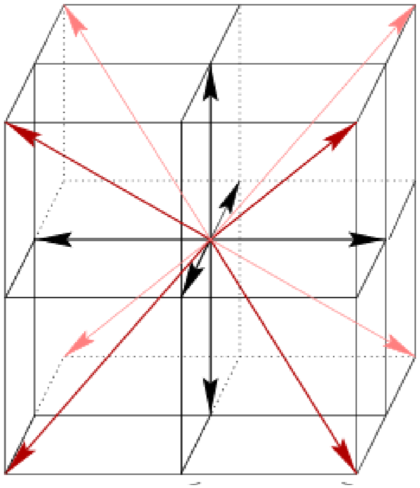
- Hybrid LB approach
- Gallery of examples
- Nematic/cholesteric hydrodynamics
    - Phase diagram: the elusive BPIII
    - Particles in cholesterics: microrheology
    - Dimers in cholesterics: self-assembled rotors
    - Particles in active nematics: negative drag coefficient

With: *O. Henrich, J. Lintuvuori, K. Stratford,*
G. Foffano, D. Marenduzzo

Antecedents: *J. Yeomans Group, Oxford*

Lattice Boltzmann for Simple Fluids

= fast fluid mechanics on a lattice



- each site $\mathbf{x}$ has velocity set $\{\mathbf{c}_i\}$: $\mathbf{c}_i \Delta t$ = lattice vector
- $f_i(\mathbf{x},t)$: population of fluid "particles" at $\mathbf{x}$ with velocity $\mathbf{c}_i$

$\rho(\mathbf{x},t) = \sum_i f_i$ fluid density

$\rho\mathbf{v}(\mathbf{x},t) = \sum_i f_i\, \mathbf{c}_i + O(\Delta t)$ fluid velocity

- local streaming, and relaxation:

$$f_i(\mathbf{x}+\mathbf{c}_i,t+1) - f_i(\mathbf{x},t) = \sum_j L_{ij}\ (f_j(\mathbf{x},t) - f_j^0(\mathbf{x},t)) - \mathbf{F}.\nabla_c f_i + O(\Delta t)$$

- continuum limit: Navier Stokes equation

$$\rho(\partial \mathbf{v}/\partial t + \mathbf{v}.\nabla\mathbf{v}) = -\nabla P + \eta\nabla^2\mathbf{v} + \mathbf{F}_{\text{ext}}$$

Lattice Boltzmann for Liquid Crystals

$$\mathbf{F}_{\mathsf{ext}} = \nabla . \Pi[\mathbf{Q}]$$

Stress tensor Π derives from a mesoscopic free energy functional $\mathcal{F}[\mathbf{Q}]$

Couple LB to finite difference code that updates **Q**

$$\rho(\partial \mathbf{v}/\partial t + \mathbf{v}.\nabla \mathbf{v}) = -\nabla P + \eta \nabla^2 \mathbf{v} + \nabla . \Pi[\mathbf{Q}]$$

$$\mathcal{D}\mathbf{Q}/\mathcal{D}t = \Gamma \mathbf{H} + \zeta$$

Total derivative knows about advection by **v** and flow alignment by vorticity

ζ = thermal noise

Molecular field: $\mathbf{H} = -\delta\mathcal{F}/\delta\mathbf{Q} + \frac{\mathbf{I}}{3}\mathsf{Tr}\,(\delta\mathcal{F}/\delta\mathbf{Q})$

A. N. Beris and B. J. Edwards, Thermodynamics of Flowing Systems, OUP (1994)

*D. Marenduzzo, E. Orlandini, MEC, J. Yeomans, PRE **76**, 031921 (2007)*

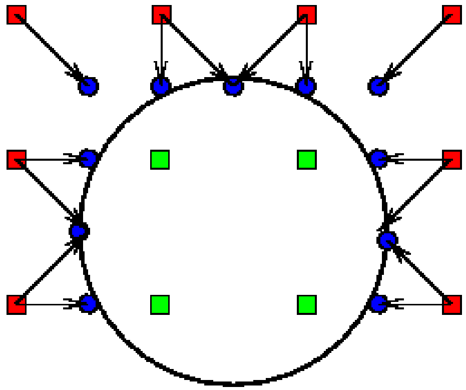
Lattice Boltzmann

Discretizes momentum space

$\Rightarrow$ fast momentum transfer across lattice

Fully local dynamics

$\Rightarrow$ excellent for parallel supercomputers



Adding colloids (bounce-back of momentum):

K. Stratford et al., J Stat Phys ***121****, 163 (2005)*

Adding thermal noise:

R. Adhikari et al., EPL ***71****, 473 (2005)*

Adding subgrid stokeslet/stresslet particles:

R. Nash et al., PRL ***104****, 258101 (2010)*

Compressible flows e.g. liquid-vapour systems:

No hybrid route; noise etc now in place

M. Gross et al., PRE ***82****, 056714 (2010), JSTAT P03030 (2011), Phil Trans* ***369****, 2274 (2011)*

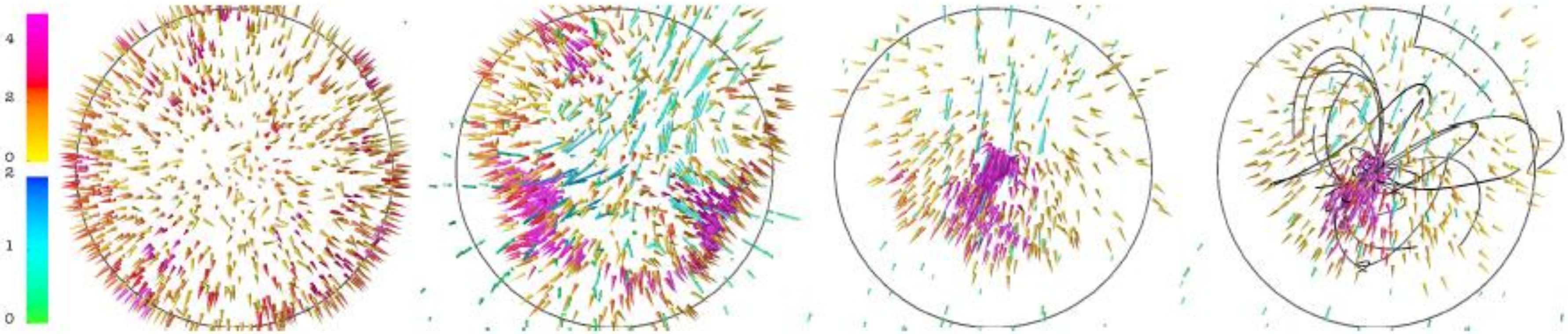
[Compare Dunweg Talk]

Lattice Boltzmann

Sub-grid swimming
stresslets (active
colloids/bacteria)
in harmonic trap

R. Nash et al, PRL ***104,*** *258101 (2010)*

MOVIE AVAILABLE AT PRL



Lattice Boltzmann

Binary fluid mixture
+ interfacial particles
+ gravity
*E. Kim et al PRE **85**, 020403 (2012)*

MOVIE AVAILABLE AT PRE

Nematic Liquid Crystals

s = molecular axis

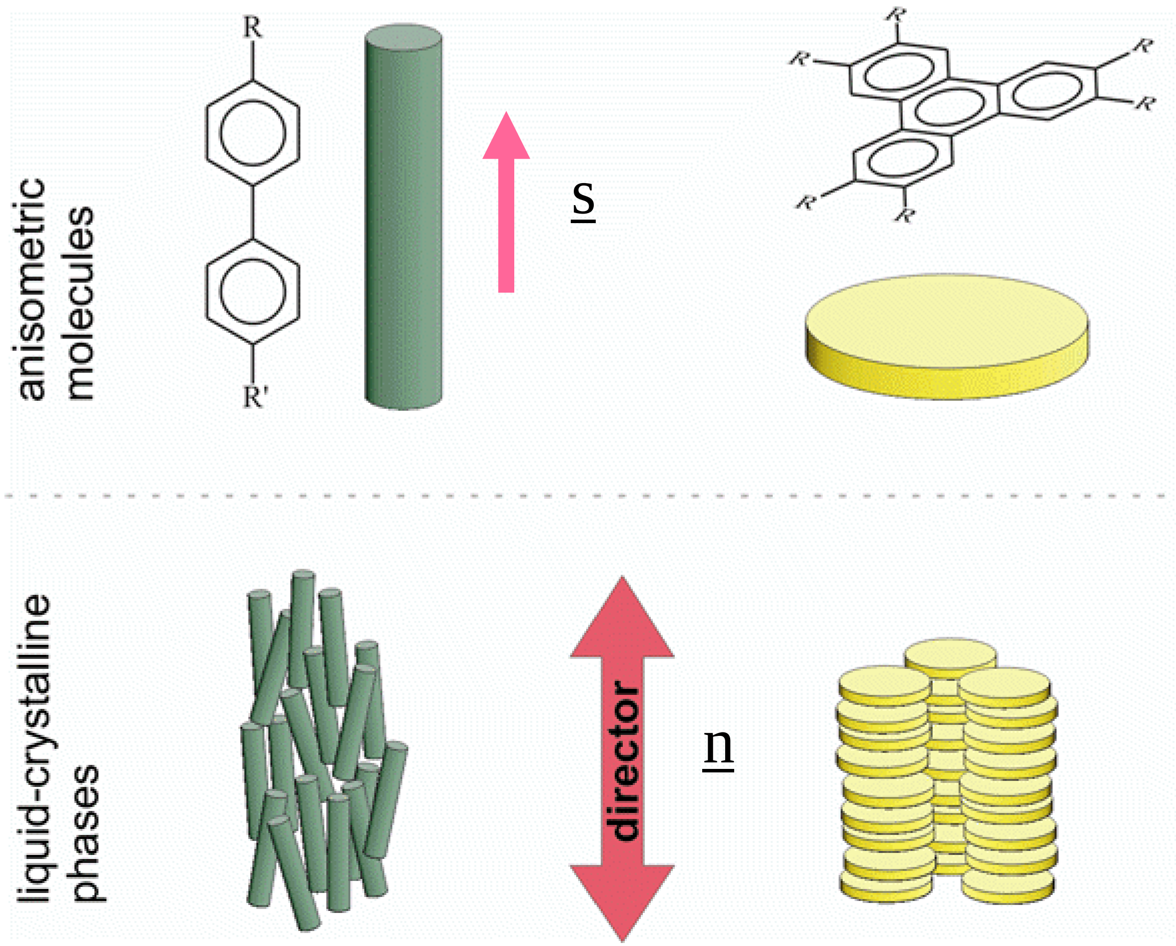
$\langle s_\alpha \rangle = 0$ (apolar)

order parameter

$Q_{\alpha\beta} = \langle s_\alpha s_\beta \rangle - \delta_{\alpha\beta}/3$

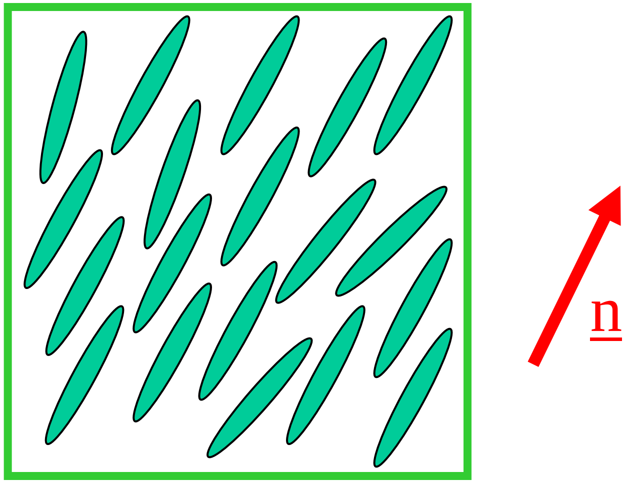
largest eigenvector = **n**

eigenvalue q



Cholesterics: Nematics with a twist

Chiral nematic molecules

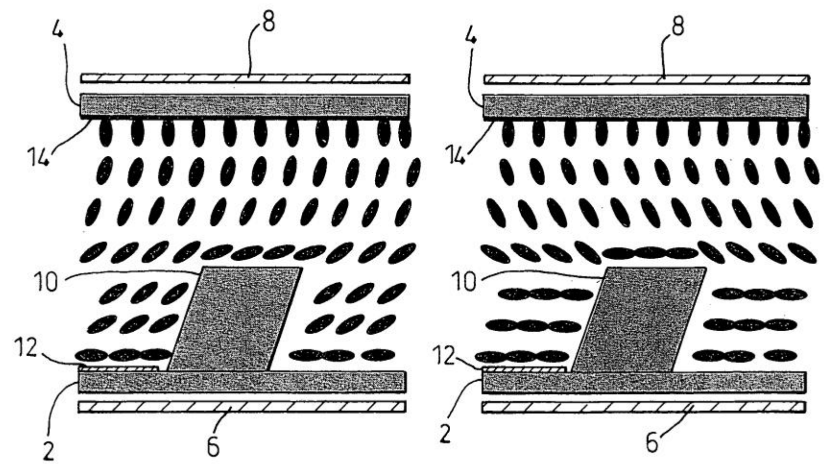


cholesteric: $\underline{n}$ has helical pitch (~ 1μm)

nematic: $\underline{n}$ uniform

$Q_{\alpha\beta} = q(n_\alpha n_\beta - \delta_{\alpha\beta}/3)$

in uniaxial case

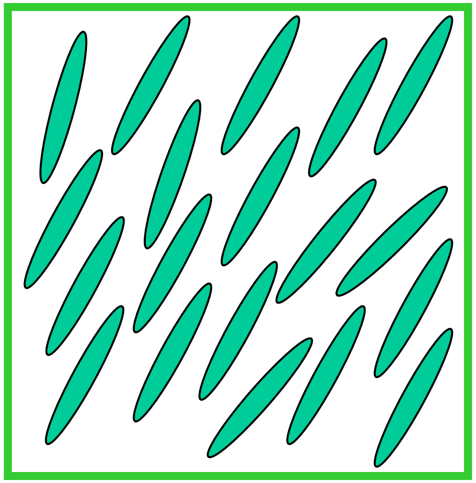


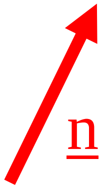
bistable (powerless) displays: e-paper

Cholesterics: Bistable (powerless) LCDs

Cholesterics: Nematics with a twist

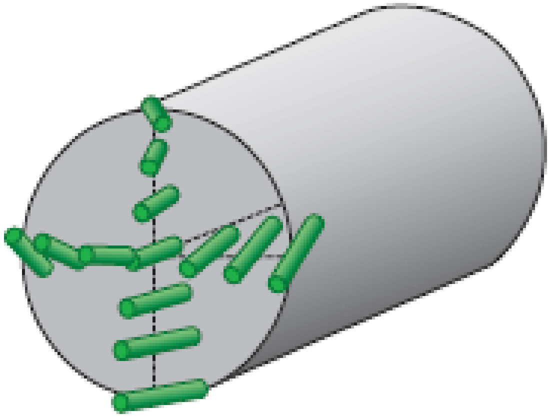
Chiral nematic molecules

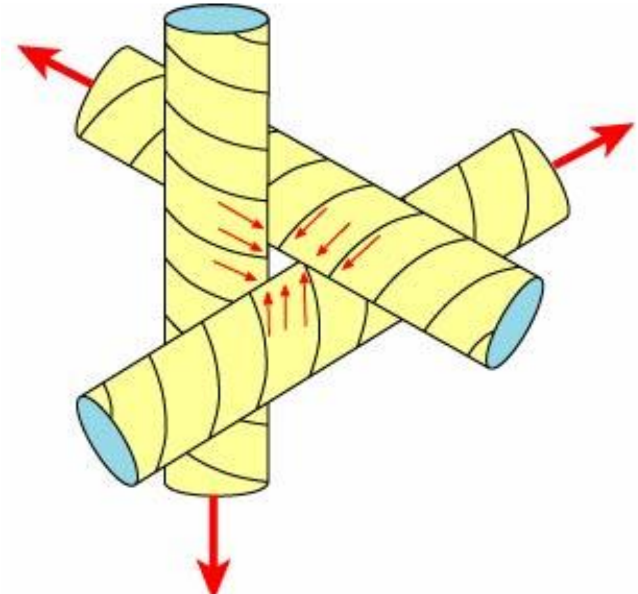


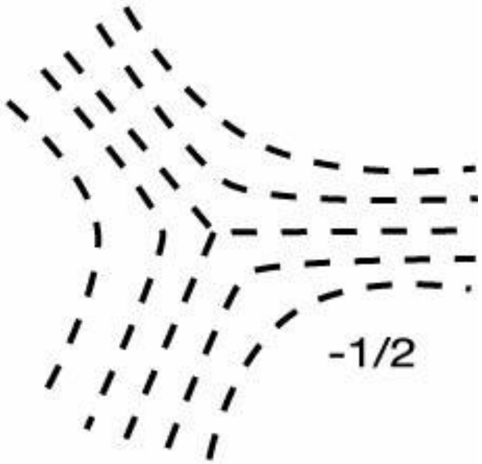


Topological defects (disclination lines)

forced into system by too much chirality
and/or boundary conditions







Landau – de Gennes Free Energy Functional

$$\mathcal{F}[\mathbf{Q}] = \int (f_1 + f_2 + f_3)\, dV$$

f_1 = bulk nematic free energy density

$$f_1 = A_0 \left[\frac{1}{2}\left(1 - \frac{\gamma}{3}\right) Q_{\alpha\beta}^2 - \frac{\gamma}{3} Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} + \frac{\gamma}{4} Q_{\alpha\beta}^4\right]$$

$A_0 \sim 10^6$ Pa ~ kT/nm^3
I-N transition at $\gamma = 2.7$, spinodal at $\gamma = 3$

reduced temperature
$\tau = 27/\gamma - 9$

$$f_2 = \frac{K}{2}\left[(\partial_\beta Q_{\alpha\beta})^2 + (\epsilon_{\alpha\gamma\delta}\partial_\gamma Q_{\delta\beta} + 2q_0 Q_{\alpha\beta})^2\right]$$

K = elastic constant
p = $2\pi/q_0$ = pitch of cholesteric helix

κ: reduced chirality
$\kappa^2 = 108Kq_0^2/A_0\gamma$

LC dynamics: Beris-Edwards equations

Navier Stokes (η = viscosity)

$$\rho(\partial \mathbf{v}/\partial t + \mathbf{v}.\nabla \mathbf{v}) = -\nabla P + \eta \nabla^2 \mathbf{v} + \nabla.\Pi$$

Stress tensor (ξ = flow alignment parameter)

$$\Pi_{\alpha\beta} = -P_0\delta_{\alpha\beta}+2\xi(Q_{\alpha\beta}+\frac{1}{3}\delta_{\alpha\beta})Q_{\gamma\epsilon}H_{\gamma\epsilon}-\xi H_{\alpha\gamma}(Q_{\gamma\beta}+\frac{1}{3}\delta_{\gamma\beta})$$

$$-\xi(Q_{\alpha\gamma}+\frac{1}{3}\delta_{\alpha\gamma})H_{\gamma\beta}-\partial_\beta Q_{\gamma\nu}\frac{\delta F}{\delta\partial_\alpha Q_{\gamma\nu}}+Q_{\alpha\gamma}H_{\gamma\beta}-H_{\alpha\gamma}Q_{\gamma\beta}$$

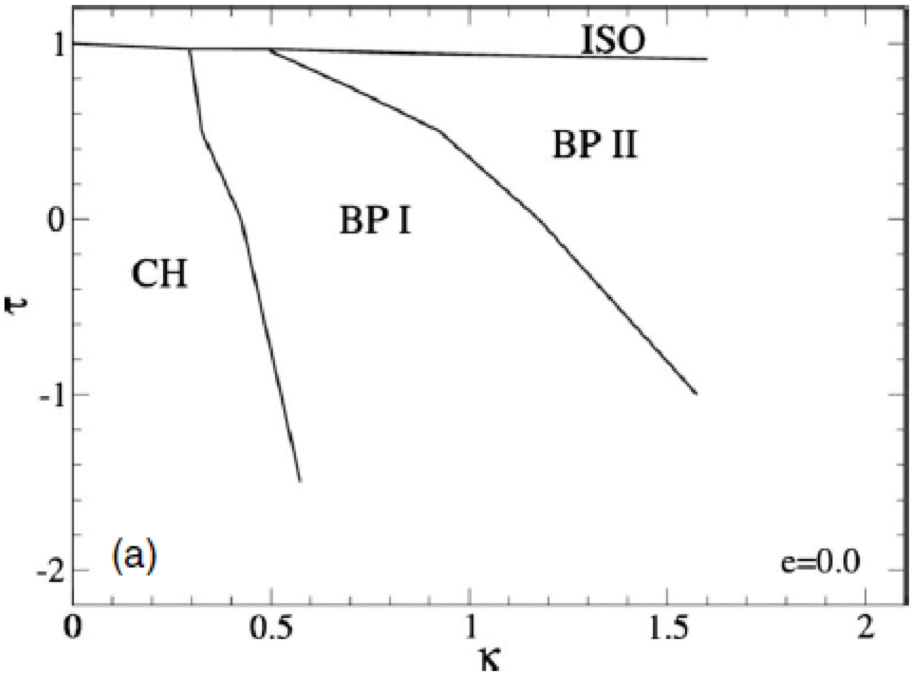
Order parameter relaxation (Γ = rotational mobility, S = rotational advector)

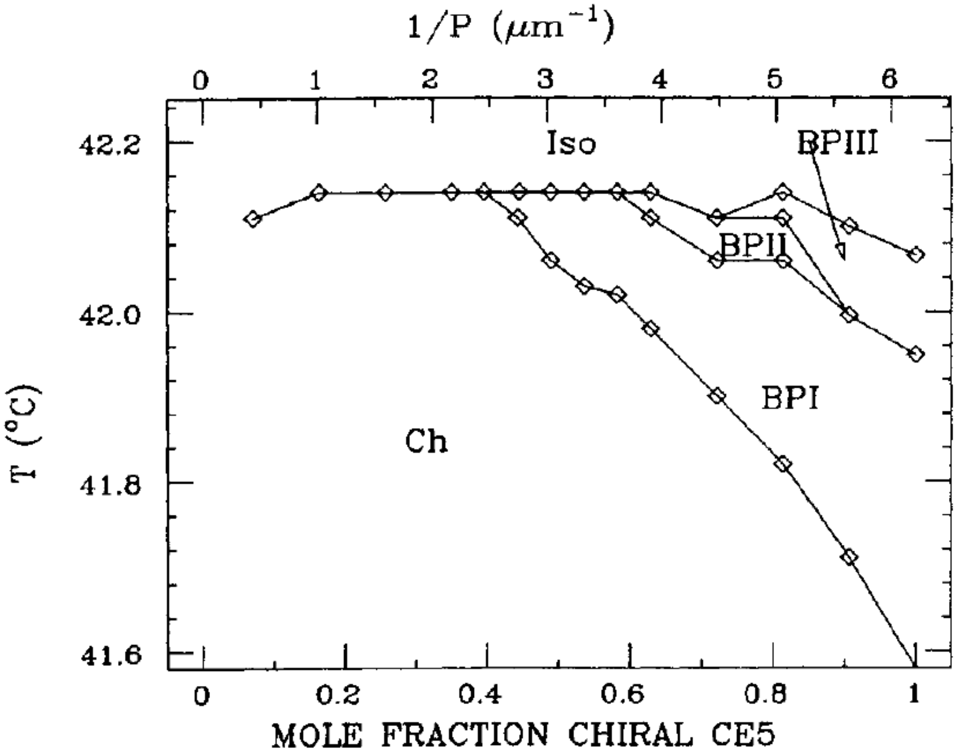
$$(\partial_t + \mathbf{v}.\nabla)Q_{\alpha\beta} + S_{\alpha\beta}(\xi, \nabla\mathbf{v}, \mathbf{Q}) = \Gamma H_{\alpha\beta}$$

Molecular field (F = ∫fdV)

$$\mathbf{H} = -\frac{\delta F}{\delta \mathbf{Q}} + (\mathbf{I}/3)\mathrm{Tr}\frac{\delta F}{\delta \mathbf{Q}}$$

Phase diagram of Landau–de Gennes model





[Periodic phases only]

[+Aperiodic BPIII]

Numerical phase diagram

G. Alexander+ J. Yeomans, PRE ***74,*** *061706 (2006)*

Classic experiments

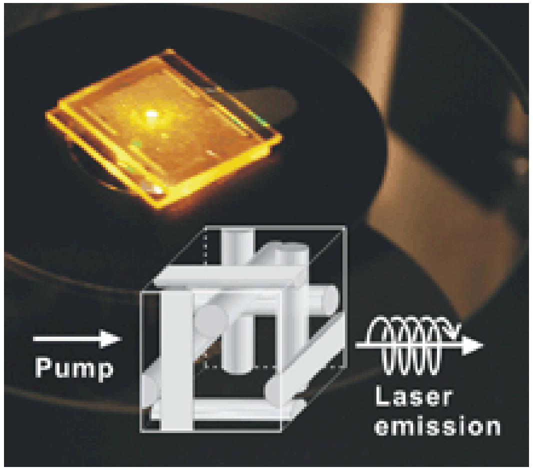
Yang + Crooker, PRA ***35,*** *4419 (1987)*

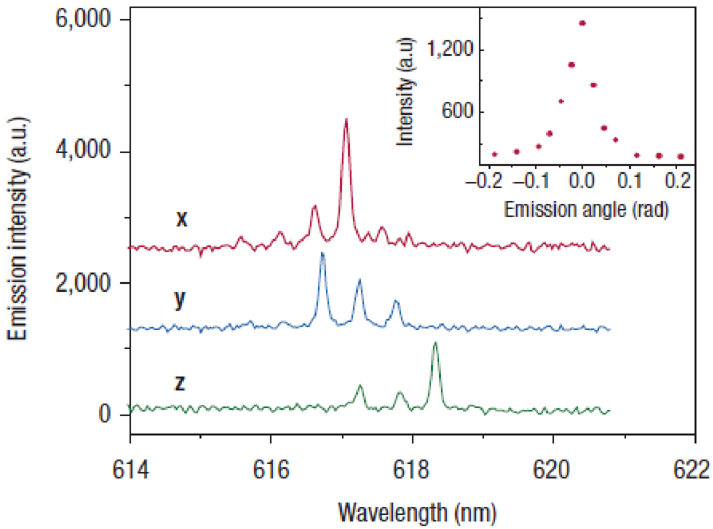
BP Devices

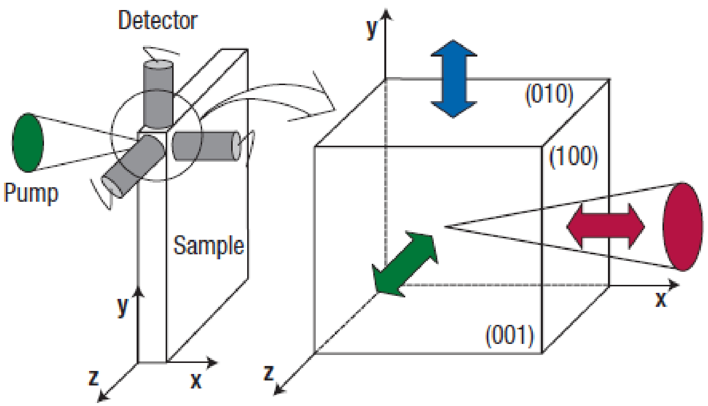
Tri-directional pumped laser

Mirrorless operation

Tunable colour

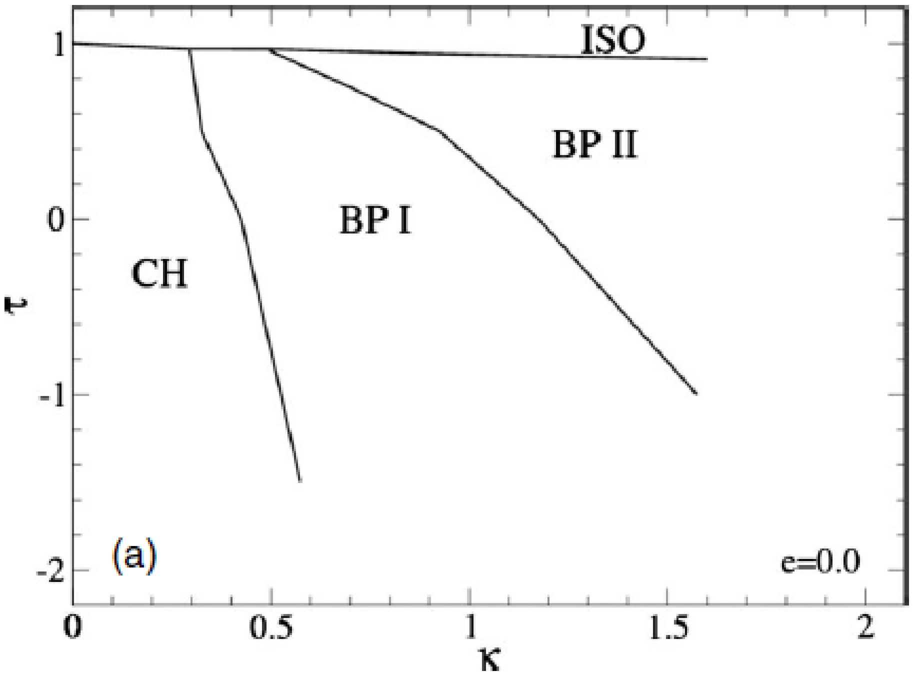


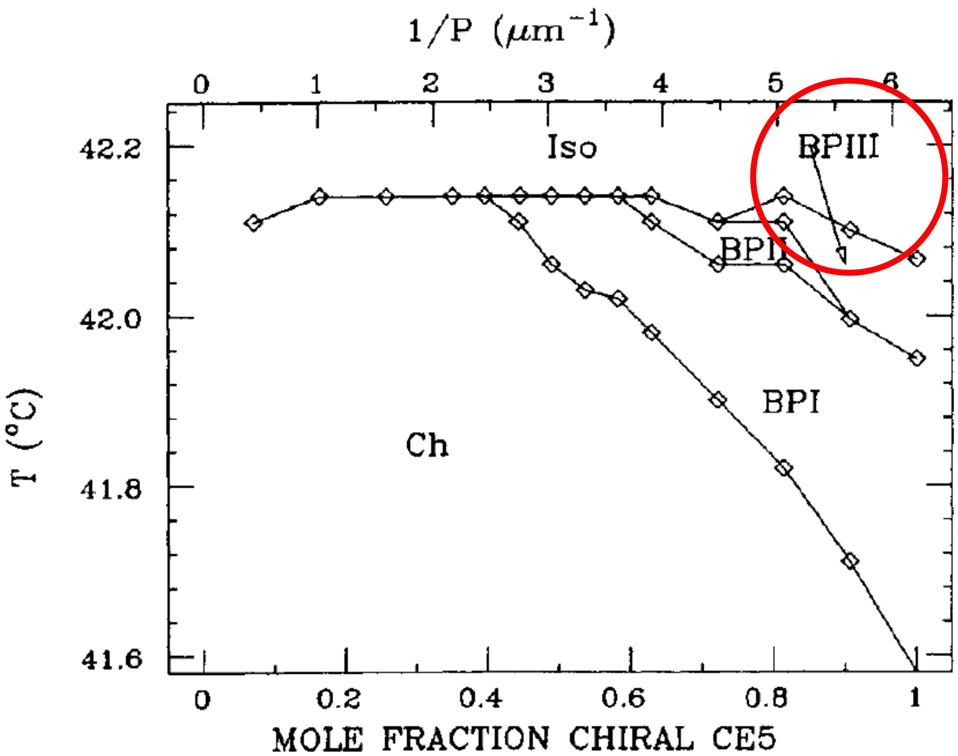




*W. Cao et al, Nat Mat **1**, 111 (2002)*

Phase diagram of Landau–de Gennes model





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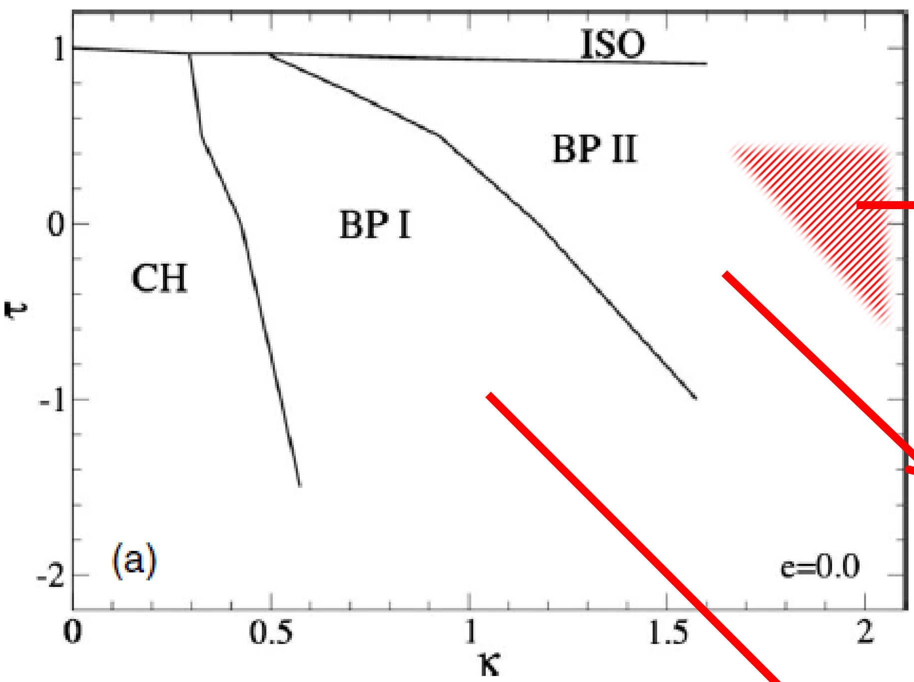
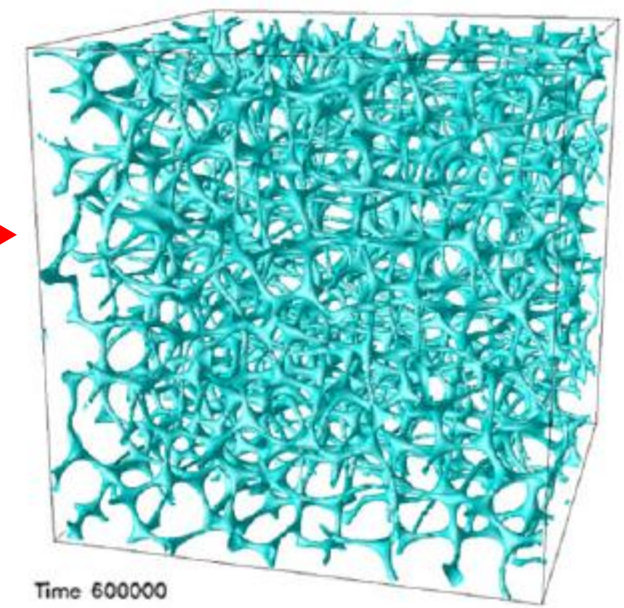
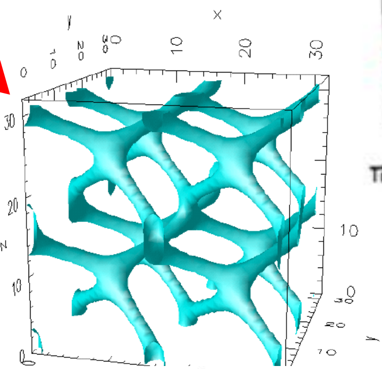
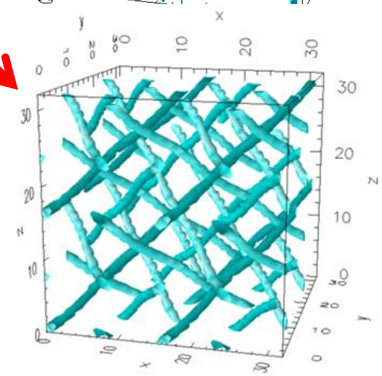








BPIII
BPII-like amorph
O. Henrich et al
*PRL **106**, 107801 (2011)*

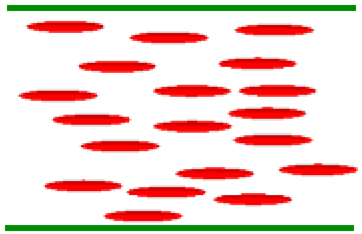
BPI,II
Ordered lattices of disclinations

Colloids in Cholesterics

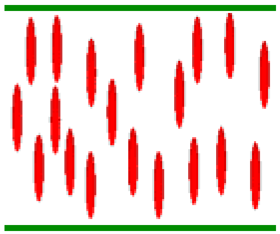
Statics

Equilibrium defect structure for planar or homeotropic anchoring

Dependence on colloid/pitch size ratio



Planar Texture



Homeotropic Texture

Microrheology

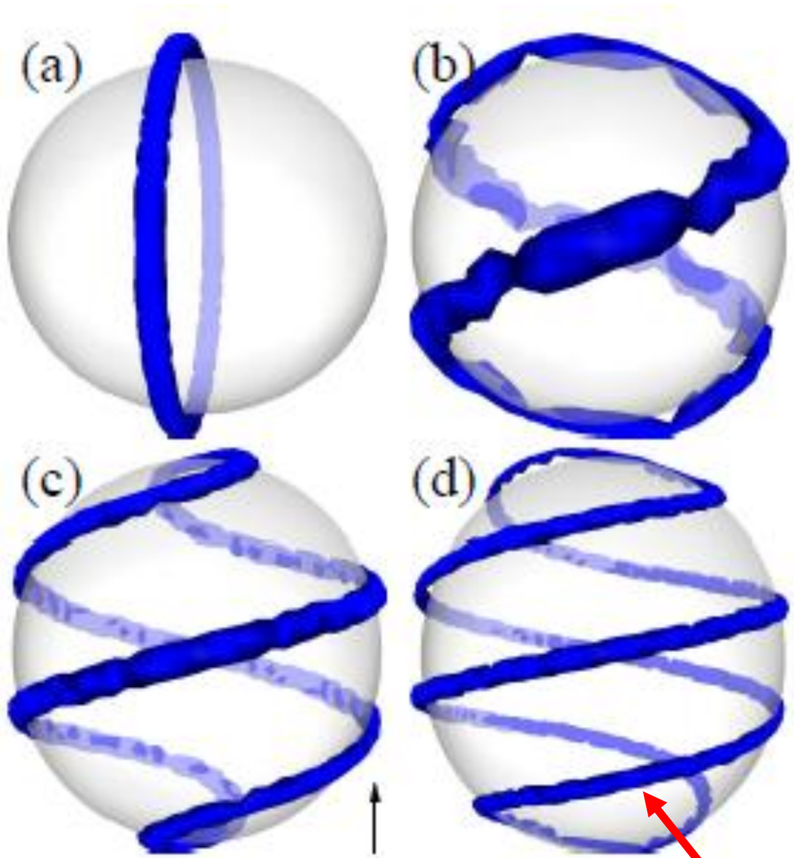
What is force **f** to drag a colloid through the system at speed **v**

(a) in the plane of cholesteric layers?

(b) along the helical axis?

Homeotropic (normal) anchoring

R/p = 0
(nematic)

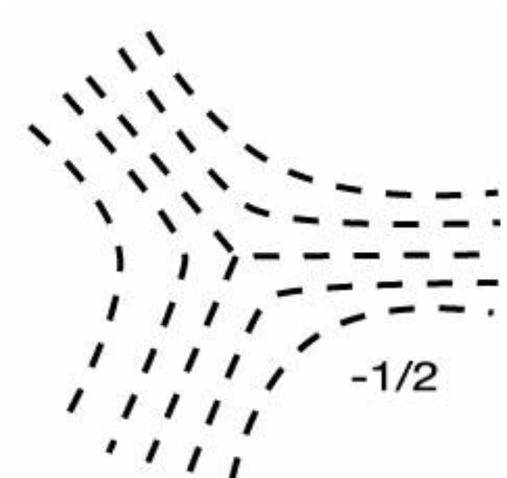


R/p = 0.25

R/p = 0.5

R/p = 0.75

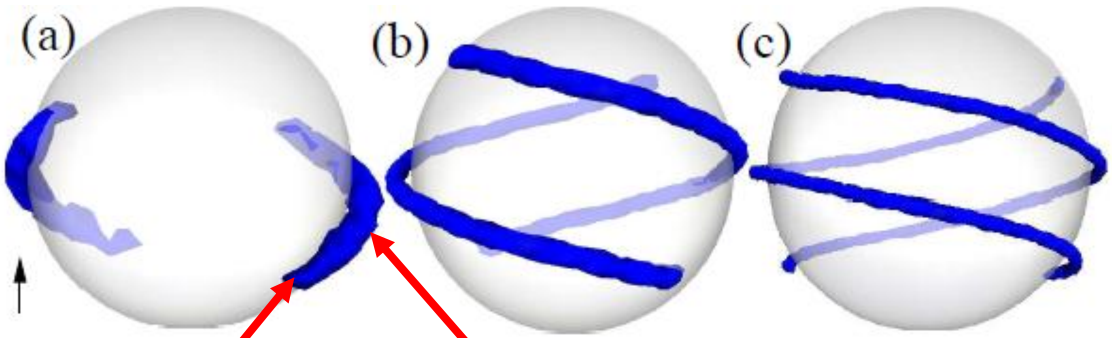
closed disclination line



J. Lintuvuori et al, J. Mat. Chem. ***20,*** *10547 (2010)*

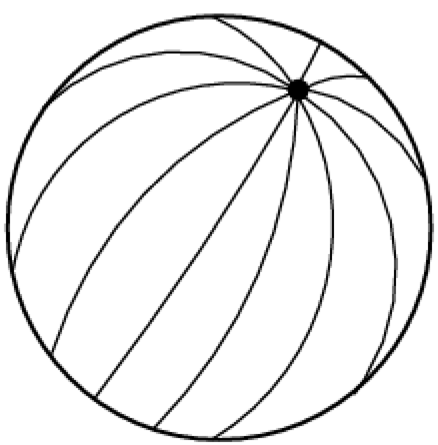
Planar anchoring

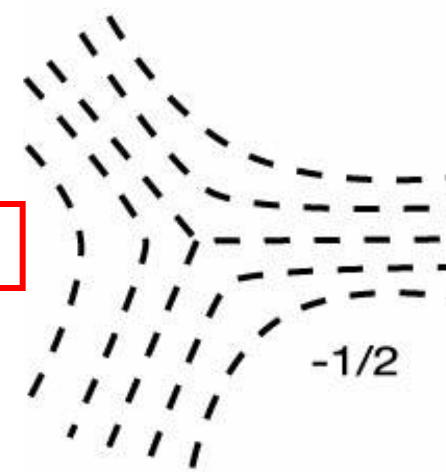
R/p: 0.25 0.50 0.75



2D boojum

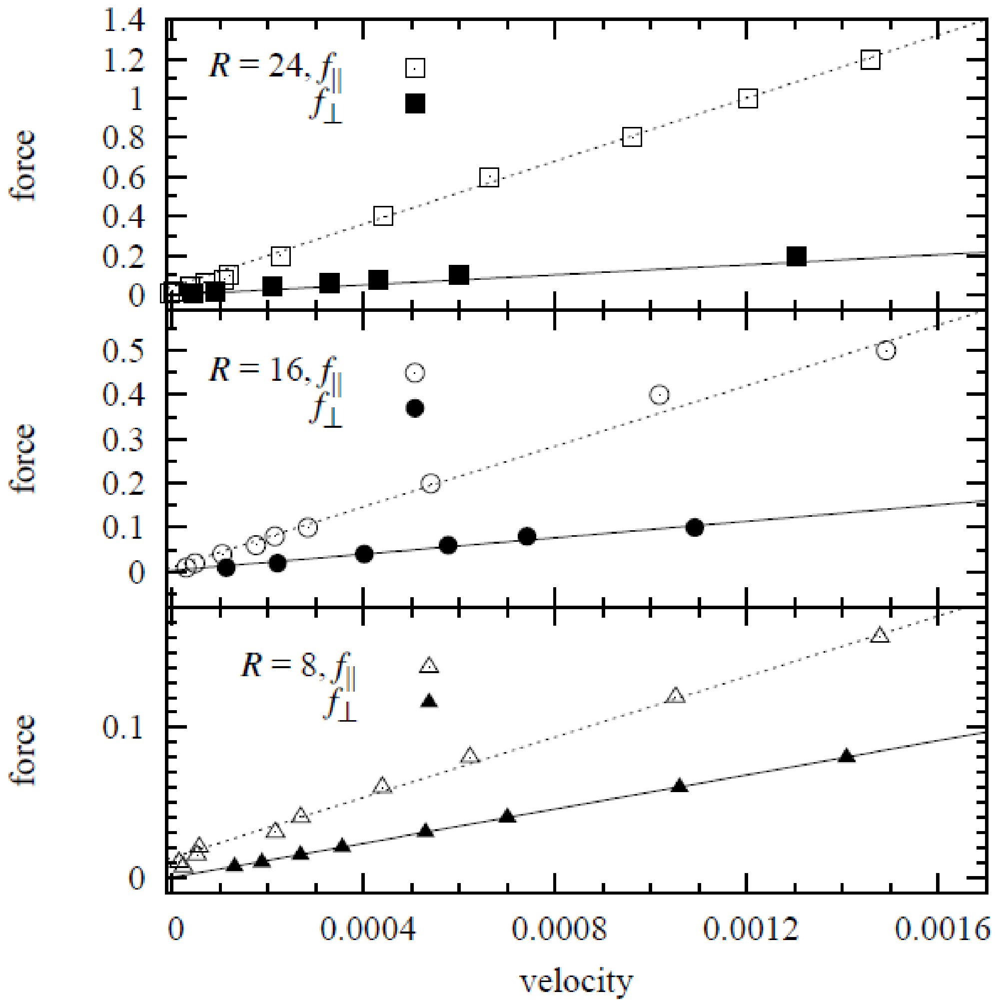
open disclination line





*J. Lintuvuori et al, PRL, **105**, 178302 (2010)*

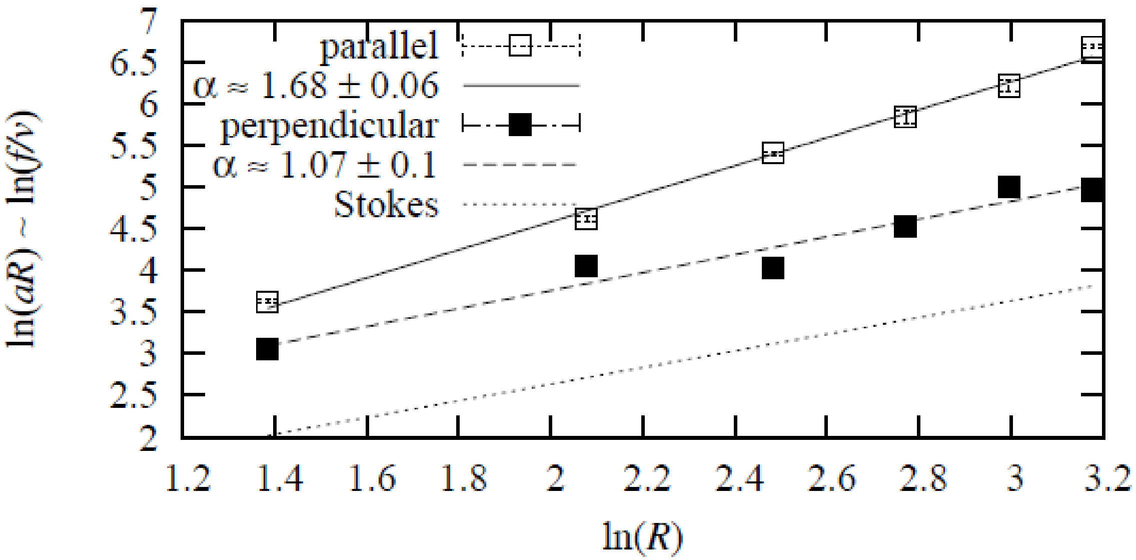
Microrheology: small speeds



force is linear in velocity
for both || and ⊥ motion...

*J. Lintuvuori et al, PRL, **105**, 178302 (2010)*

Microrheology: small speeds



but force not linear in R when v || to helix

violation of Stokes law: $f/v = 6\pi\eta R$

force law probes mesoscopic state, not local material properties

effective viscosity $\eta_{||}(R) \sim R^{\alpha}$, $\alpha \sim 0.7$

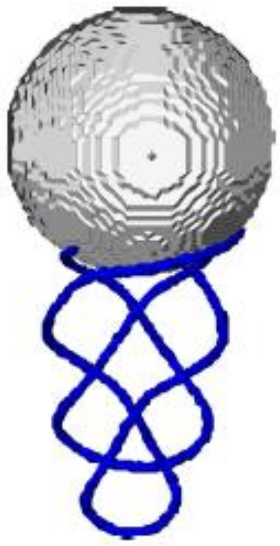
theory suggests $\alpha \sim 1$

*J. Lintuvuori et al, PRL, **105**, 178302 (2010)*

Microrheology: larger speeds

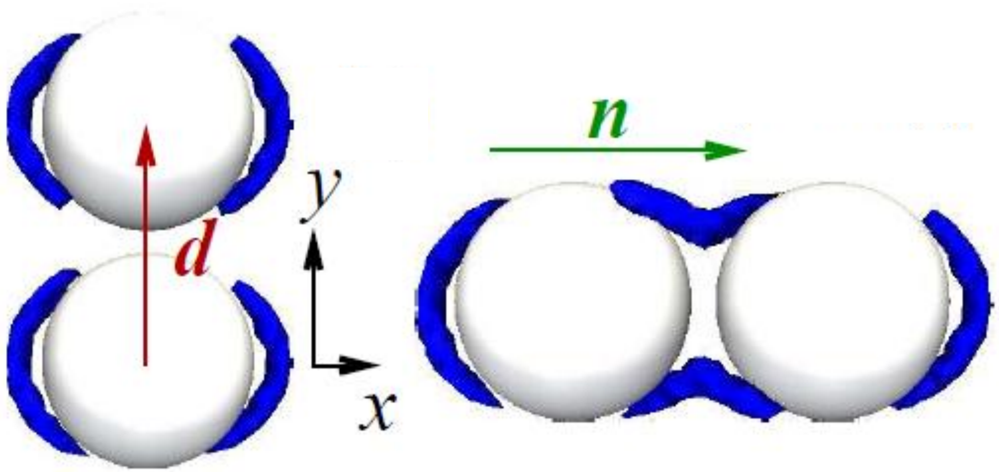
High Ericksen number: $Er = 2q^2vR/\Gamma K = 0.7$

$R/p \sim 0.75$



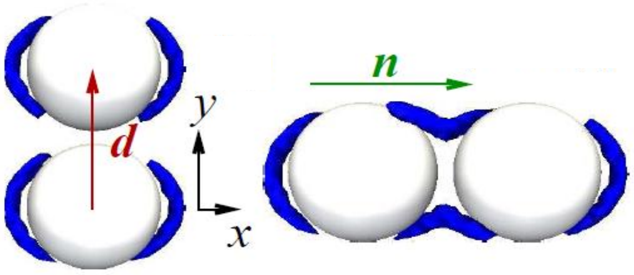
Dimers in cholesterics

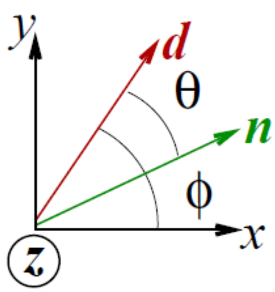
- planar anchoring creates anisotropic short range attraction
- bonding by boojum exchange
- strong dependence on orientation of dimer axis to director

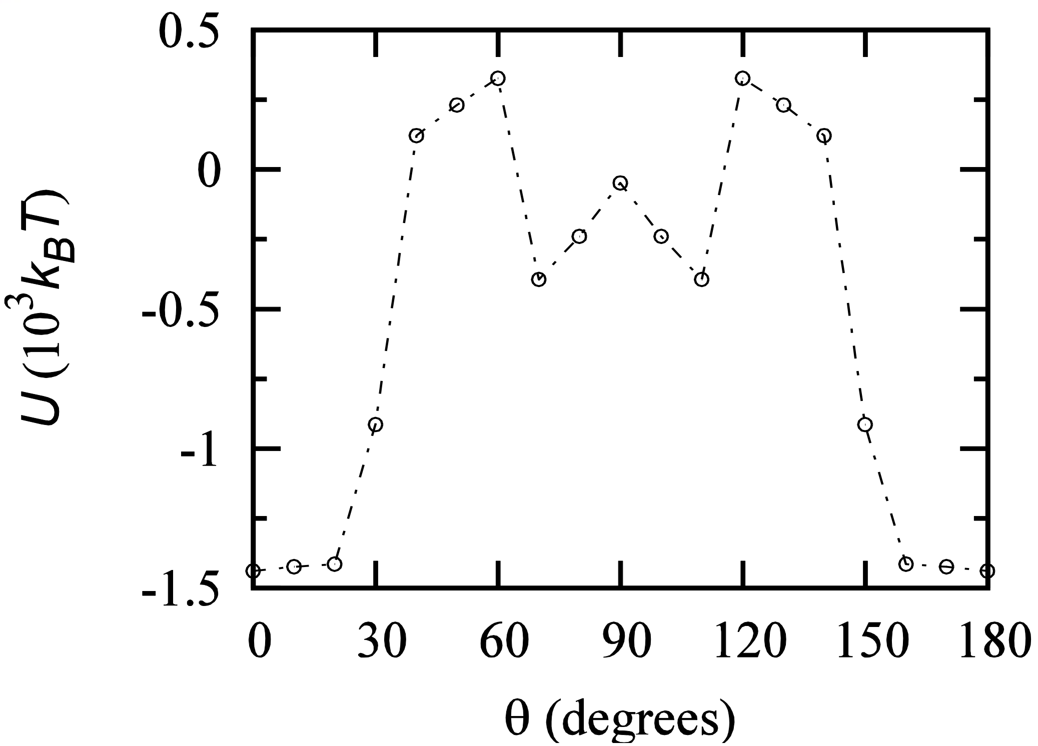


F. E. Mackay and C. Denniston, EPL, ***94****, 66003 (2011)*

Dimers in x-y plane



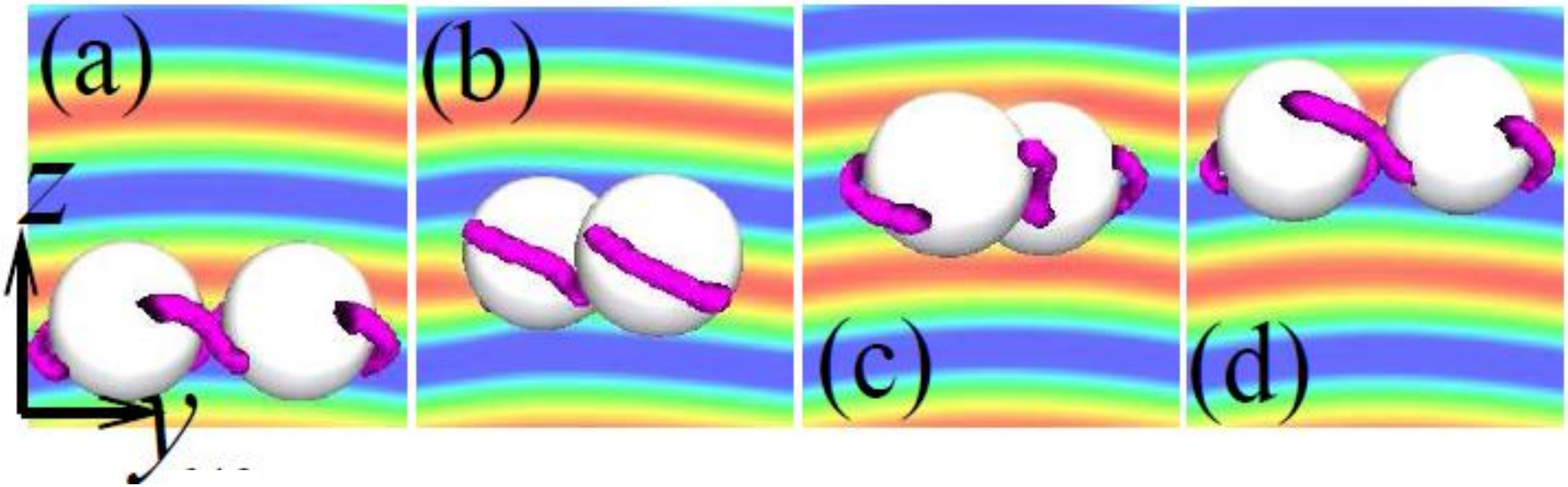




*F. E. Mackay and C. Denniston, EPL, **94**, 66003 (2011)*
*J. Lintuvuori et al, PRL **107**, 268102 (2011)*

Pulling dimers through a cholesteric

- rotation of **d** axis resulting from z translation
- small **f**: rotor phase, lock-in (with wobbles) between **d** and **n**
- larger **f**: phase slip



J. Lintuvuori et al, PRL ***107****, 268102 (2011)*

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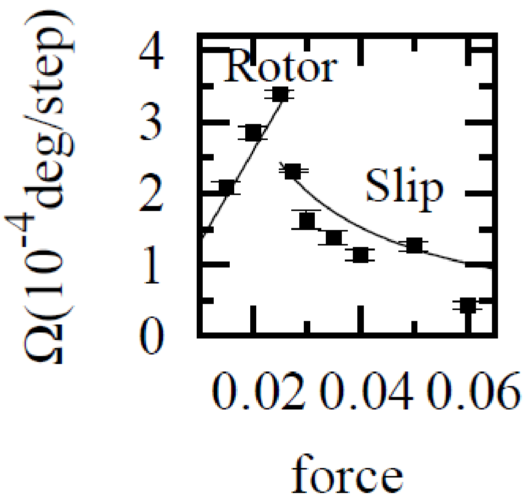

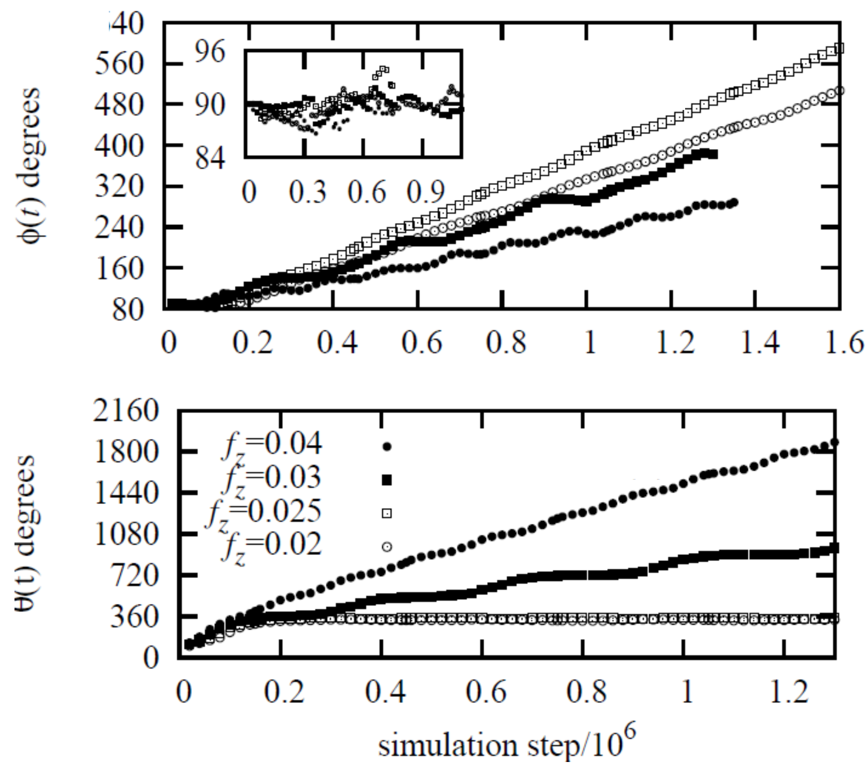

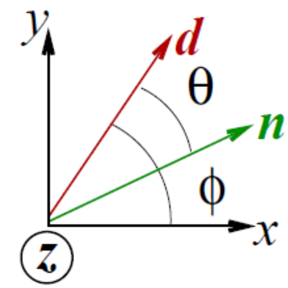

*J. Lintuvuori et al, PRL **107**, 268102 (2011)*

And finally…

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- Hybrid LB approach
- Gallery of examples
- Nematic/cholesteric hydrodynamics
  - Phase diagram: the elusive BPIII
  - Particles in cholesterics: microrheology
  - Dimers in cholesterics: self-assembled rotors
  - Particles in active nematics: negative drag coefficient

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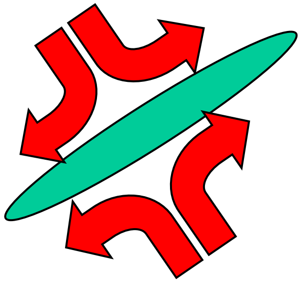
G. Foffano, D. Marenduzzo

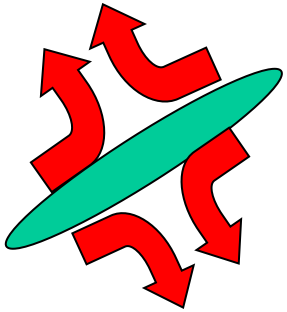
Antecedents: *J. Yeomans Group, Oxford*

Microrheology of active nematics

Active nematics:



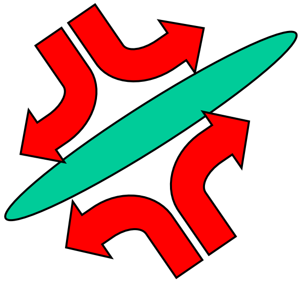
dense bacterial suspensions
(extensile, $\zeta > 0$)



cytoskeletal actomyosin
(contractile, $\zeta < 0$)

Microrheology of active nematics

Active nematics:



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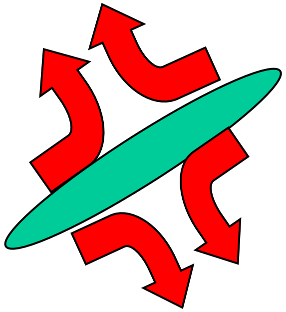


cytoskeletal actomyosin
(contractile, $\zeta < 0$)

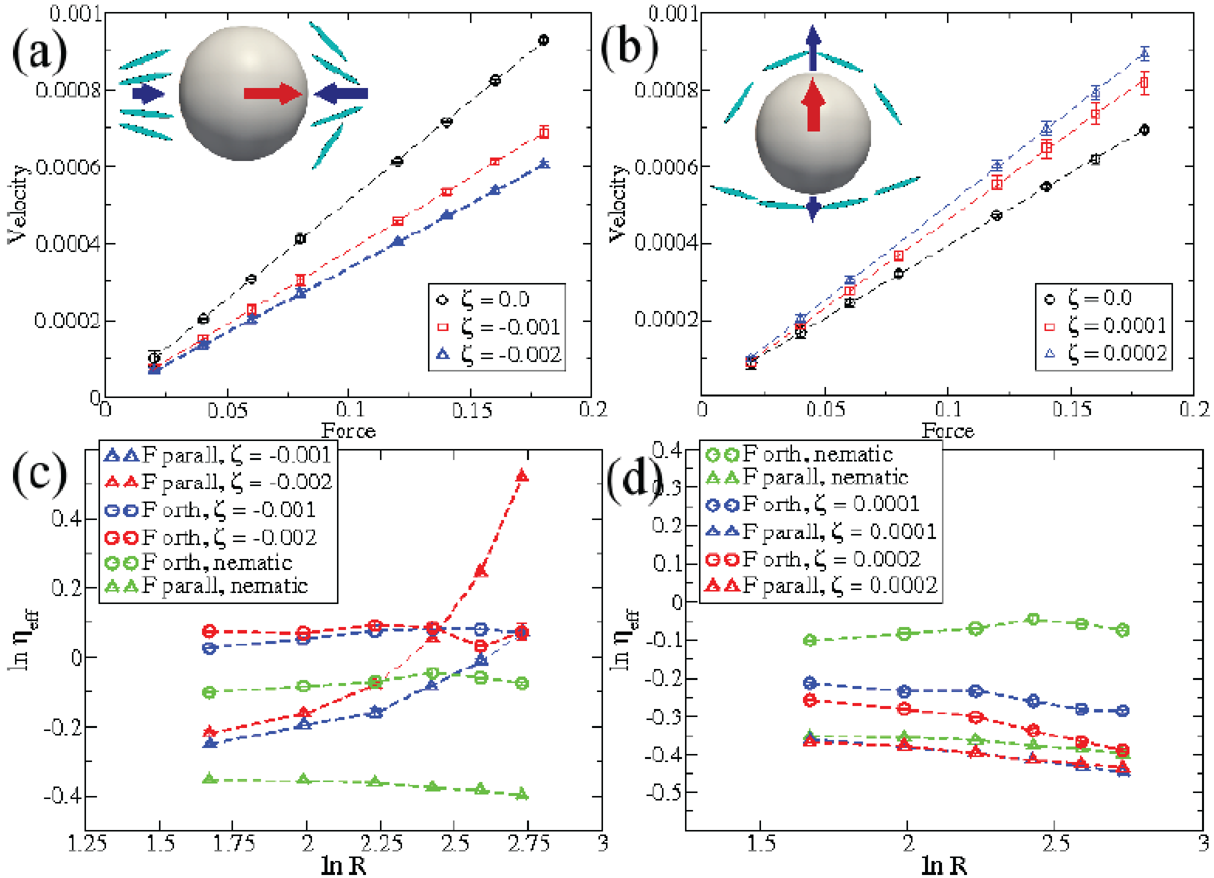
Equations of motion as previous ($p \to \infty$) with additional stress

$$\Delta\Pi = -\zeta[\mathbf{Q} + \mathbf{I}/3]$$

Flow instabilities in bulk samples (avoided here via PBCs)

R. Simha and S. Ramaswamy, PRL ***89****, 058101 (2002) , Y. Hatwalne et al PRL* ***92****, 118101 (2004), K. Kruse et al PRL* ***92****, 078101 (2004)*

Microrheology of active nematics



contractile

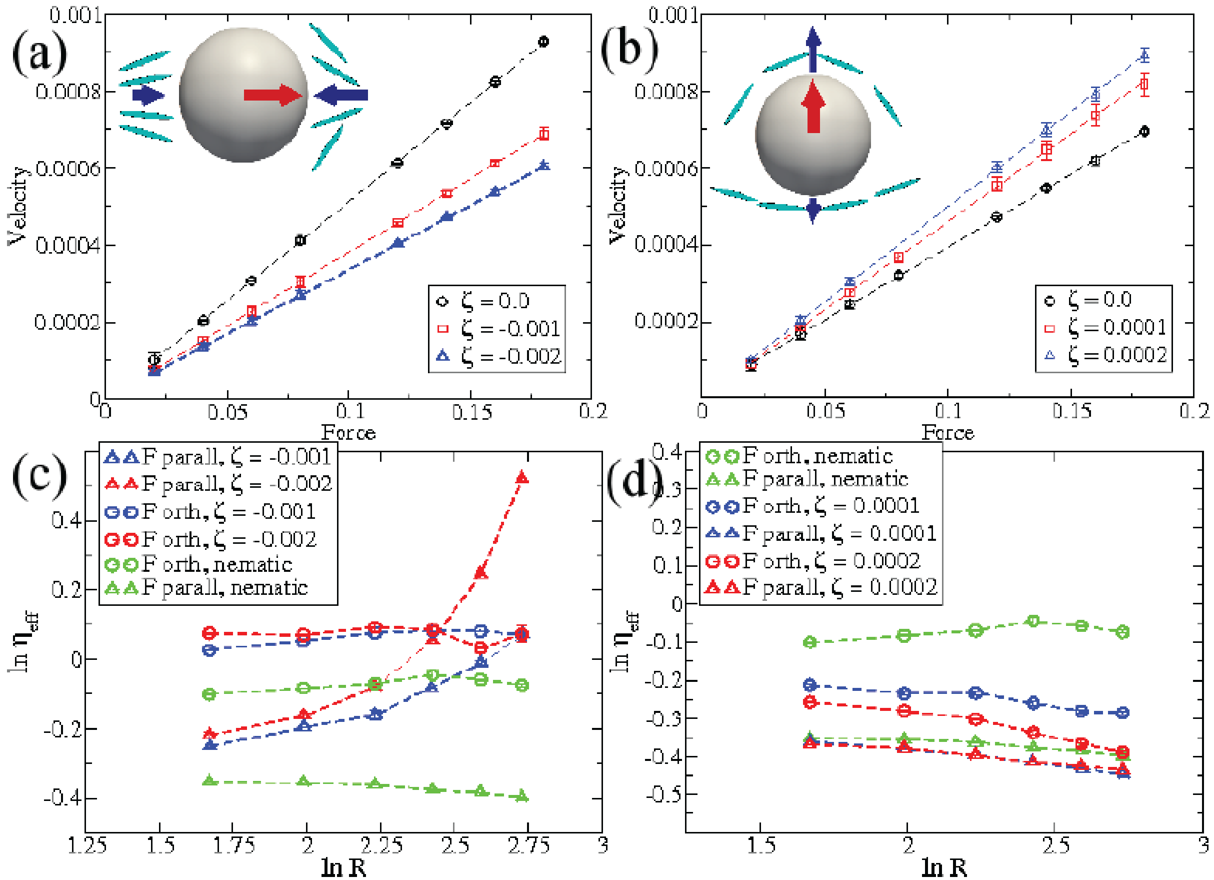
+ homeotropic

extensile

+ planar

G. Foffano et al, in review (2012)

Microrheology of active nematics



contractile

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+ planar

G. Foffano et al, in review (2012)

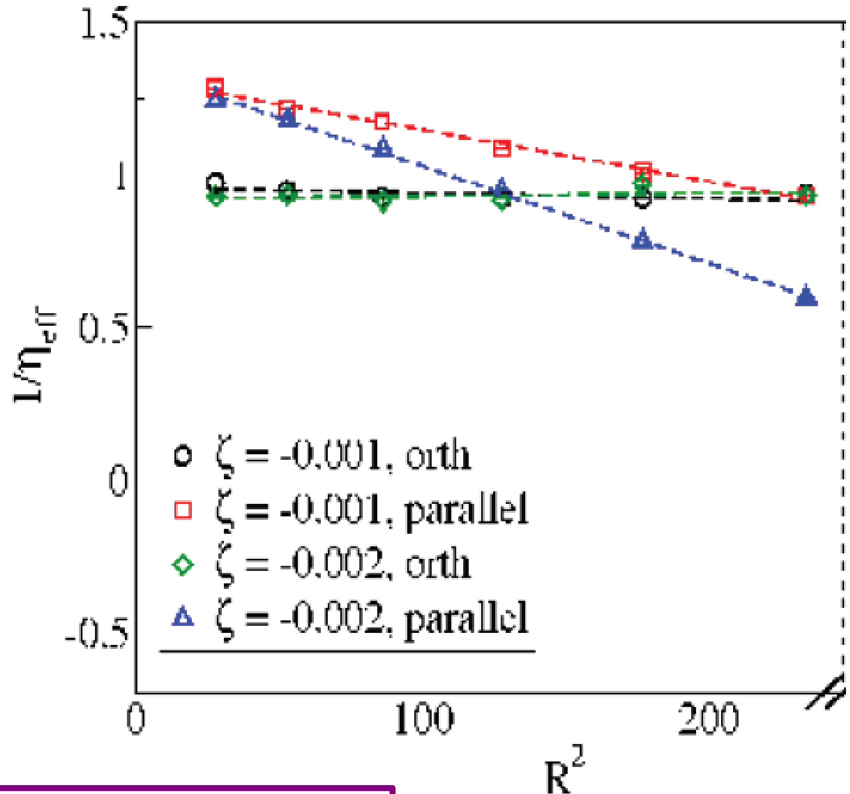
Microrheology of active nematics

Colloid in contractile fluid:

net active force $\propto \zeta F R^2/K$

$$\frac{1}{\eta_{\text{eff}}} = \frac{1}{\eta_{\text{passive}}}\left(1 - \frac{\alpha\zeta R^2}{K}\right)$$

Good fit to data at modest R

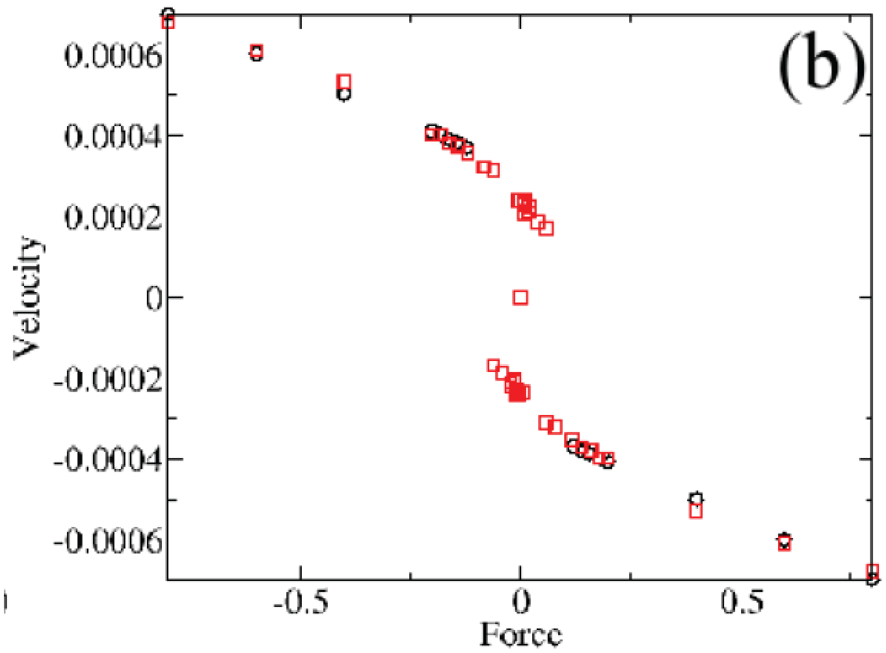


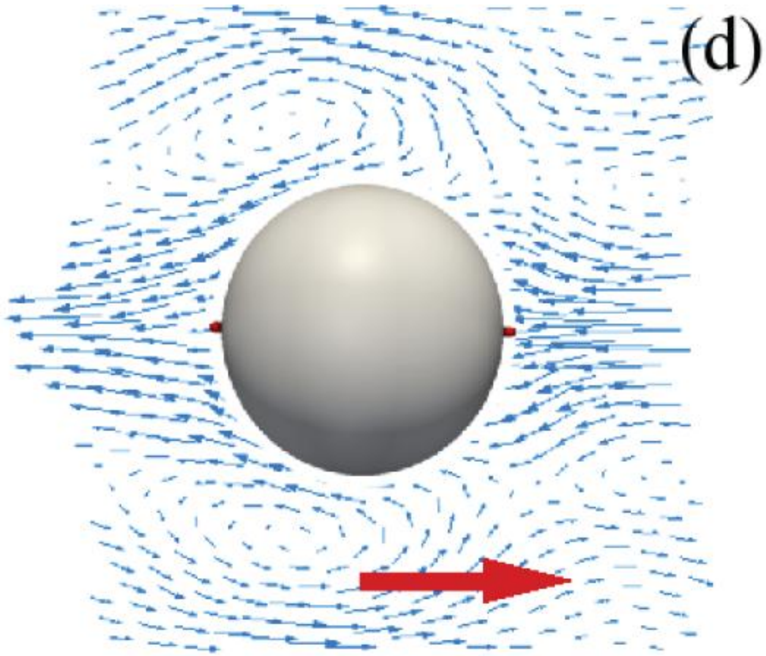
Negative drag coefficient at large R?

G. Foffano et al, in review (2012)

Microrheology of active nematics

$\alpha\zeta R^2/K = 3.4$





Negative drag coefficient at large R

Activity + anchoring creates a packet of fluid moving in opposite direction to **F**

G. Foffano et al, in review (2012)

Microhydrodynamics of Liquid Crystals

- Hybrid LB approach
- Gallery of examples
- Nematic/cholesteric hydrodynamics
  - Phase diagram: the elusive BPIII
  - Particles in cholesterics: microrheology
  - Dimers in cholesterics: self-assembled rotors
  - Particles in active nematics: negative drag coefficient

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