Interacting Defects and their Dynamics in 2D Active Nematics

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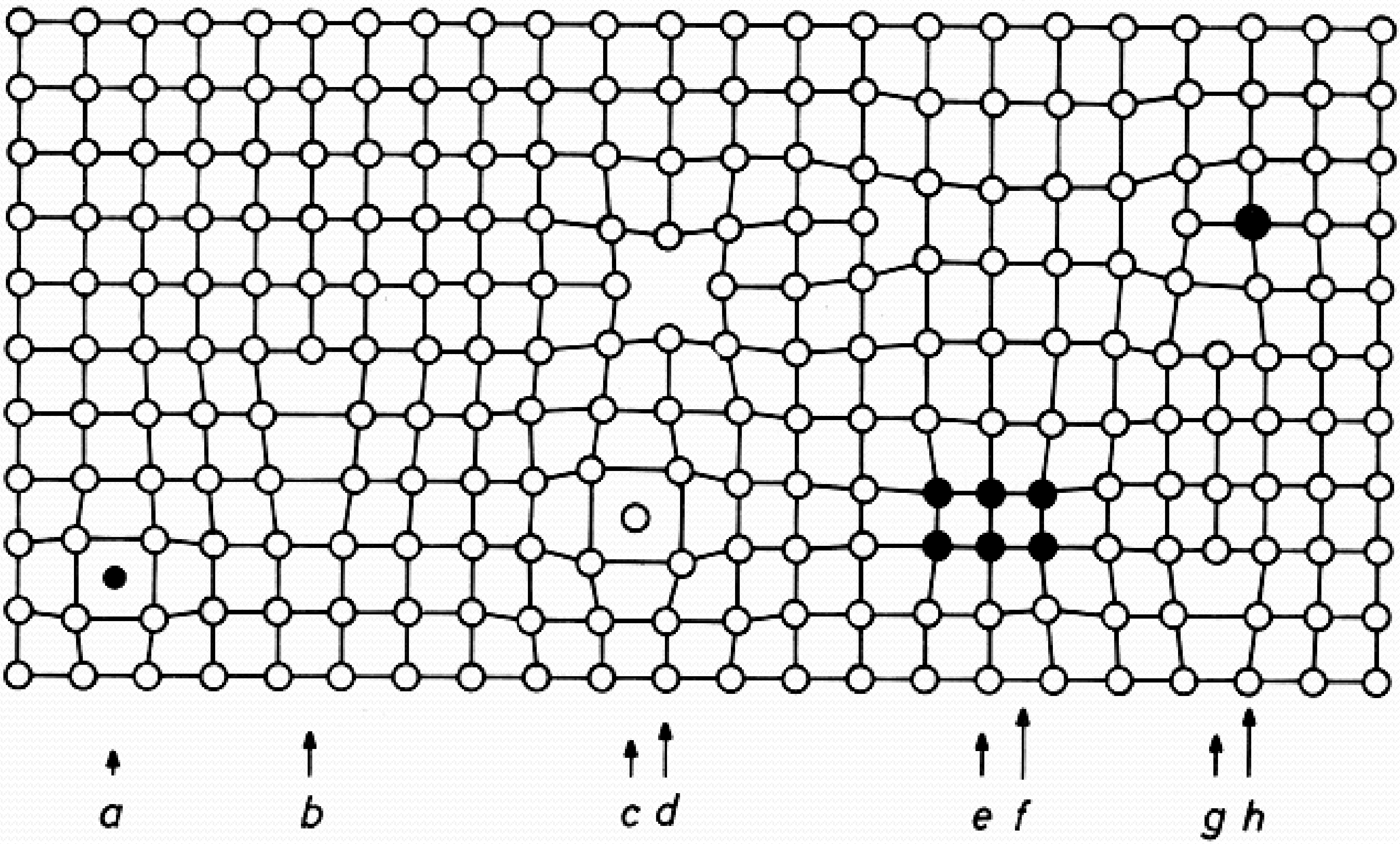
6th Dynamics Days Central Asia, Nazarbayev University, May 2020, (virtual)

The city Tehran

Soft Condensed matter @ Sharif University of Technology

The Soft and Biological Matter

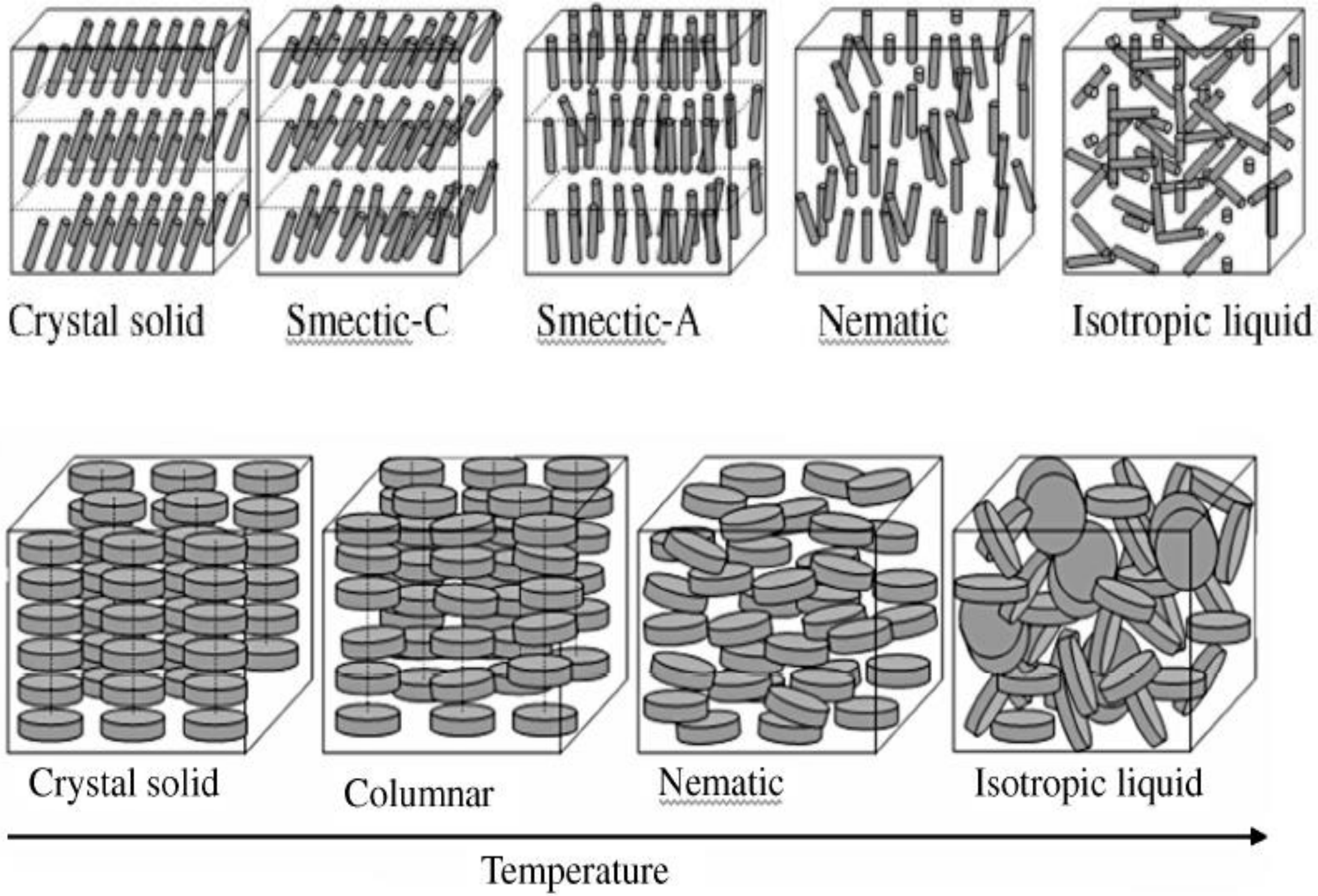
Defects in Crystals



Defects in nature and their effects

- Color
- Resistivity
- Mechanical properties
- Magnetic properties
- Hysteresis

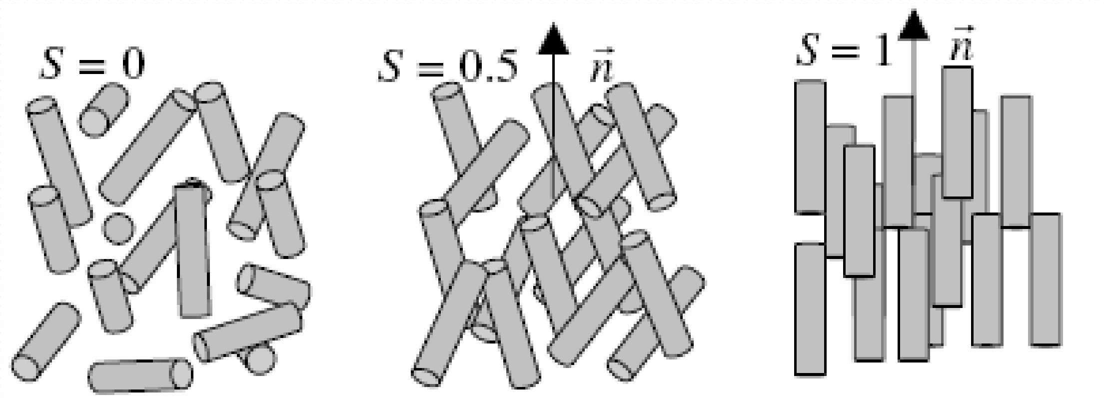
Liquid Crystals phases



Order Parameter

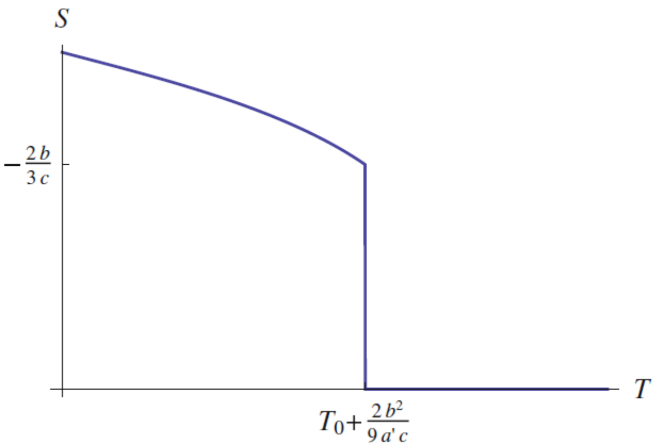
- The average directions of the molecular axes are along a common direction: namely, the liquid crystal ***director*** , n

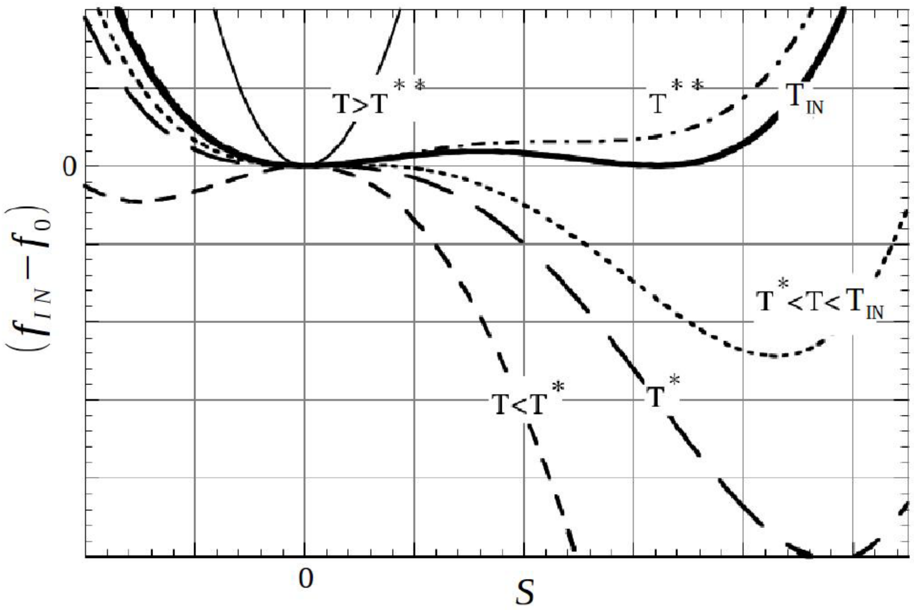
- Order parameter tensor is defined as $$Q_{ij} = \left\langle \frac{3n_i n_j - \delta_{ij}}{2} \right\rangle$$
  The largest eigenvalue of ***Q*** gives schaler order parameter, ***S,***
  and the corresponding eigenvector determines the director.



Landau - de Gennes Theory

$$f = \frac{F}{V} = f_0 + \frac{1}{2} A Q_{\alpha\beta} Q_{\alpha\beta} + \frac{1}{3} B Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} + \frac{1}{3} C_1 (Q_{\alpha\beta} Q_{\alpha\beta})^2$$
$$+ \frac{1}{3} C_2 Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\delta} Q_{\delta\alpha} + \cdots ,$$

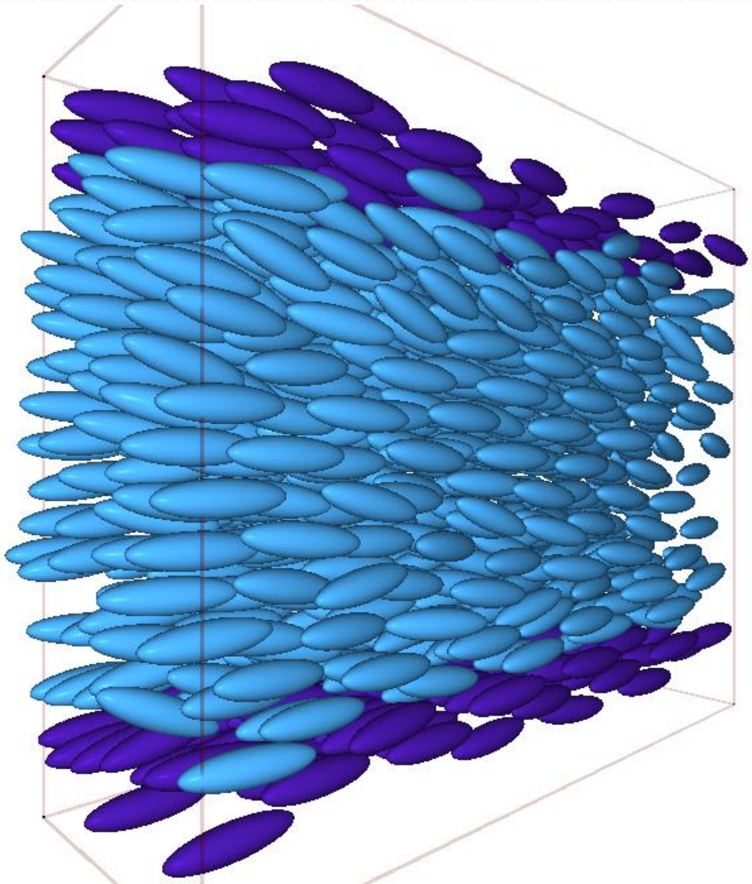




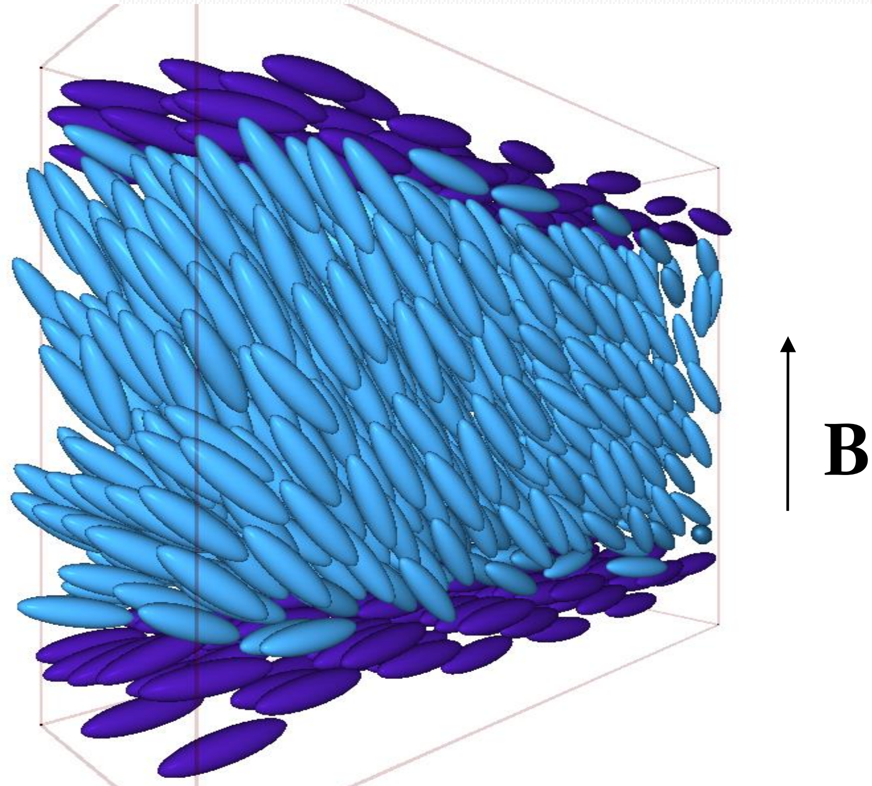
$$f = f_0 + \frac{1}{2} a S^2 + \frac{1}{3} b S^3 + \frac{1}{4} c S^4$$

$a = \frac{3}{2} A$, $b = \frac{3}{4} B$, and $c = \frac{9}{4} C_1 + \frac{9}{8} C_2$.

Liquid Crystal Elasticity

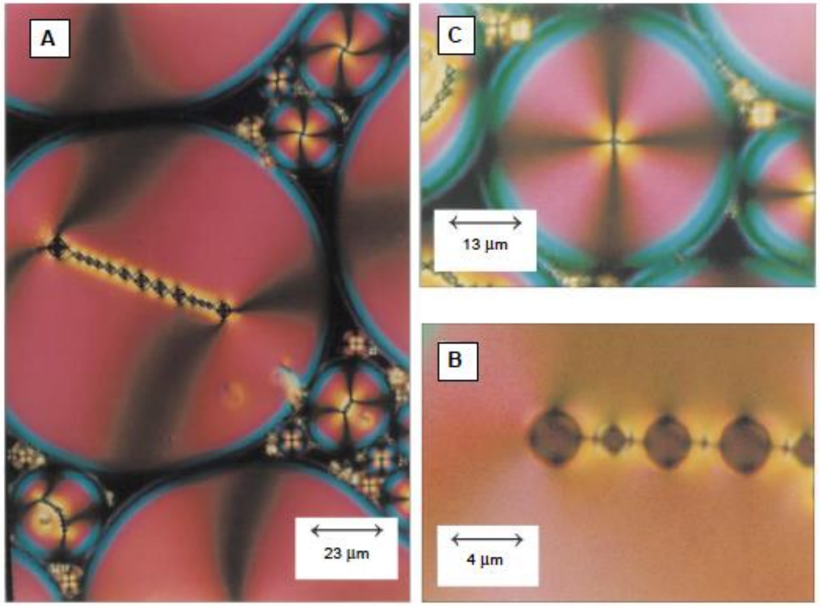


B = 0



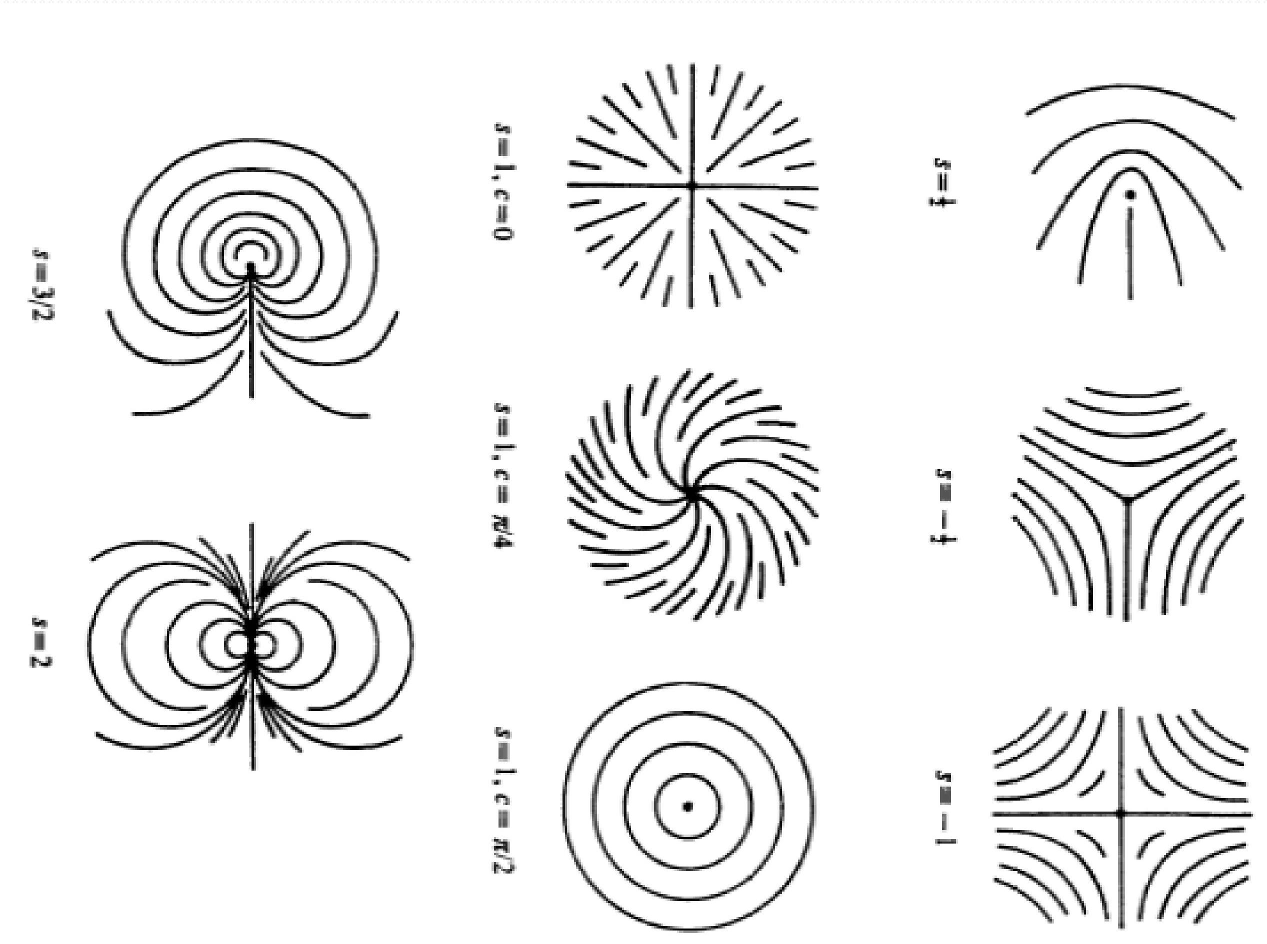
Defects on nematic fluids

- Although in an ideal Nematic the liquid prefers to save its director and order parameter globally constant, in reality boundary interactions and surface anchoring induce defects on the system.

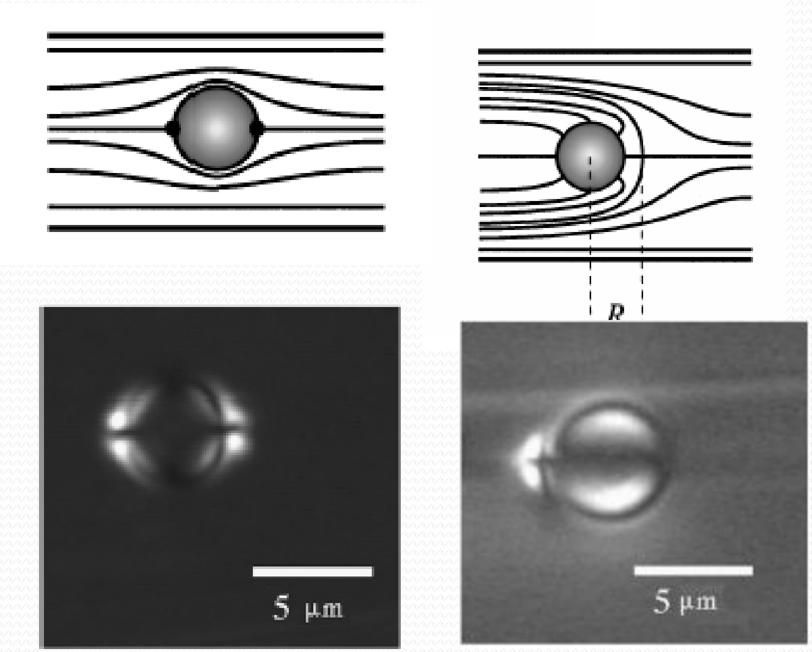


Poulin, Stark, Lubensky & Weitz, Science (1997)

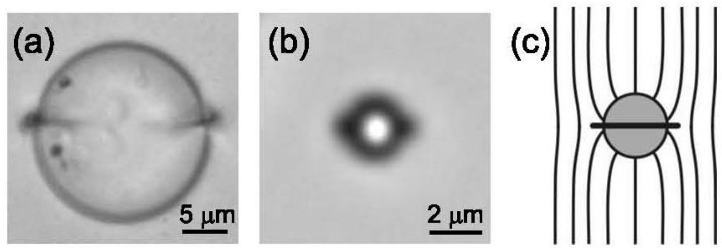
Boundary conditions induced defects



Induced defects by colloids in Nematic



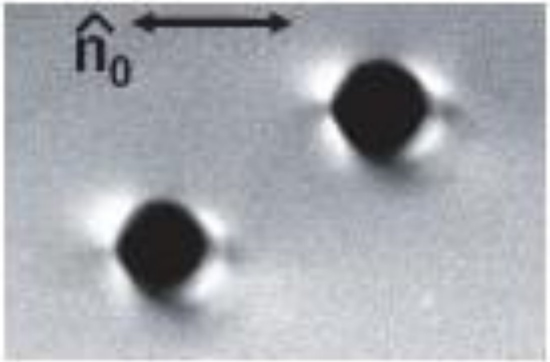
[P. Poulin, and D. A. Weitz, Phys. Rev. E , 1998]

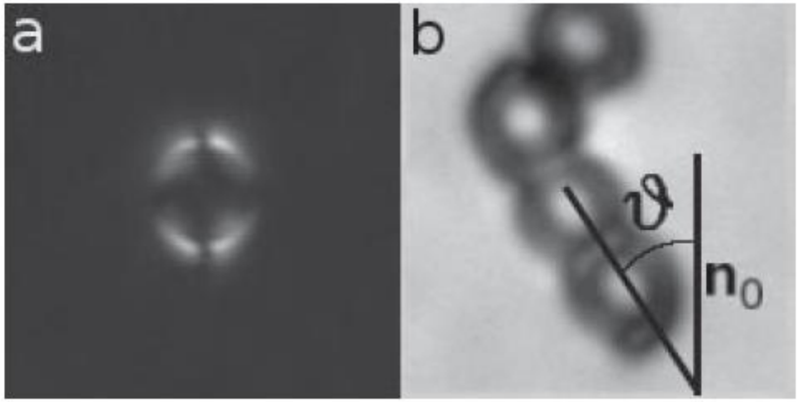


Skarabot et al, Phys. Rev. E (2008)

The control of the anchoring is achieved experimentally by using various amphiphilic compounds which are adsorbed at the water–liquid-crystal interface.

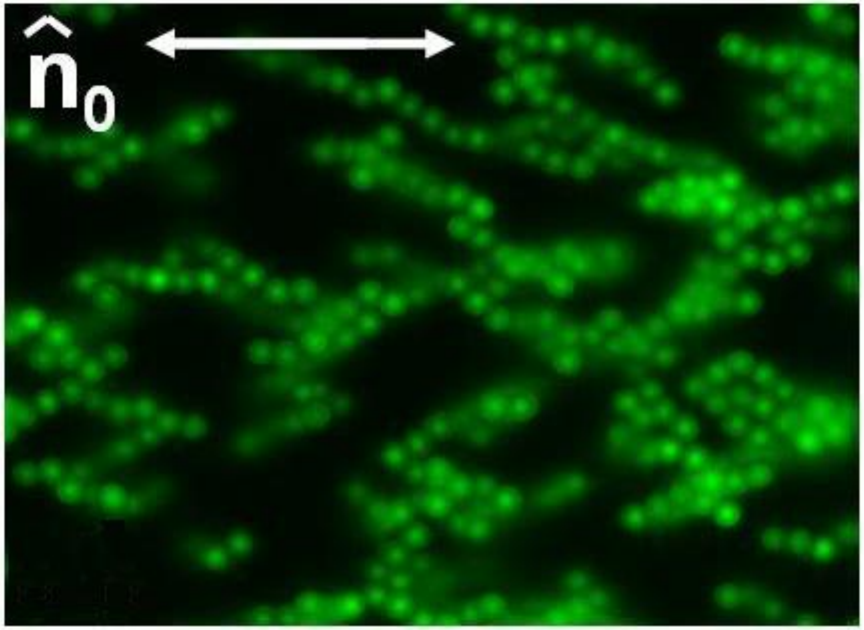
Interacting colloids in Nematics





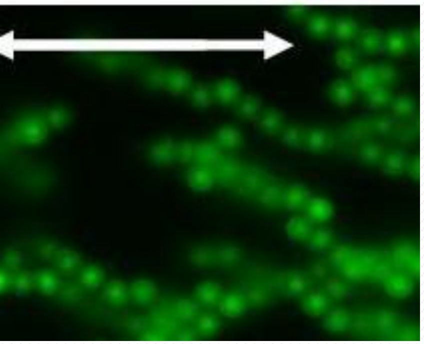
$$\vartheta = 25^\circ - 35^\circ$$

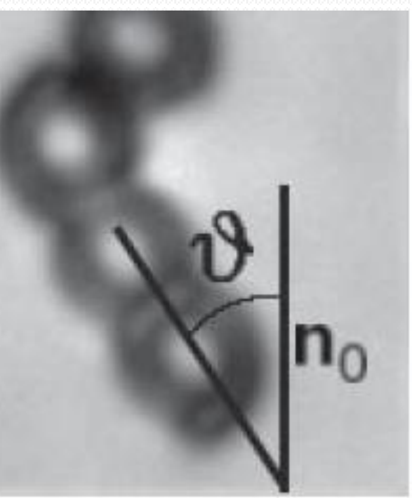
[Kotar , et al., Phys Rev Lett, 2006]

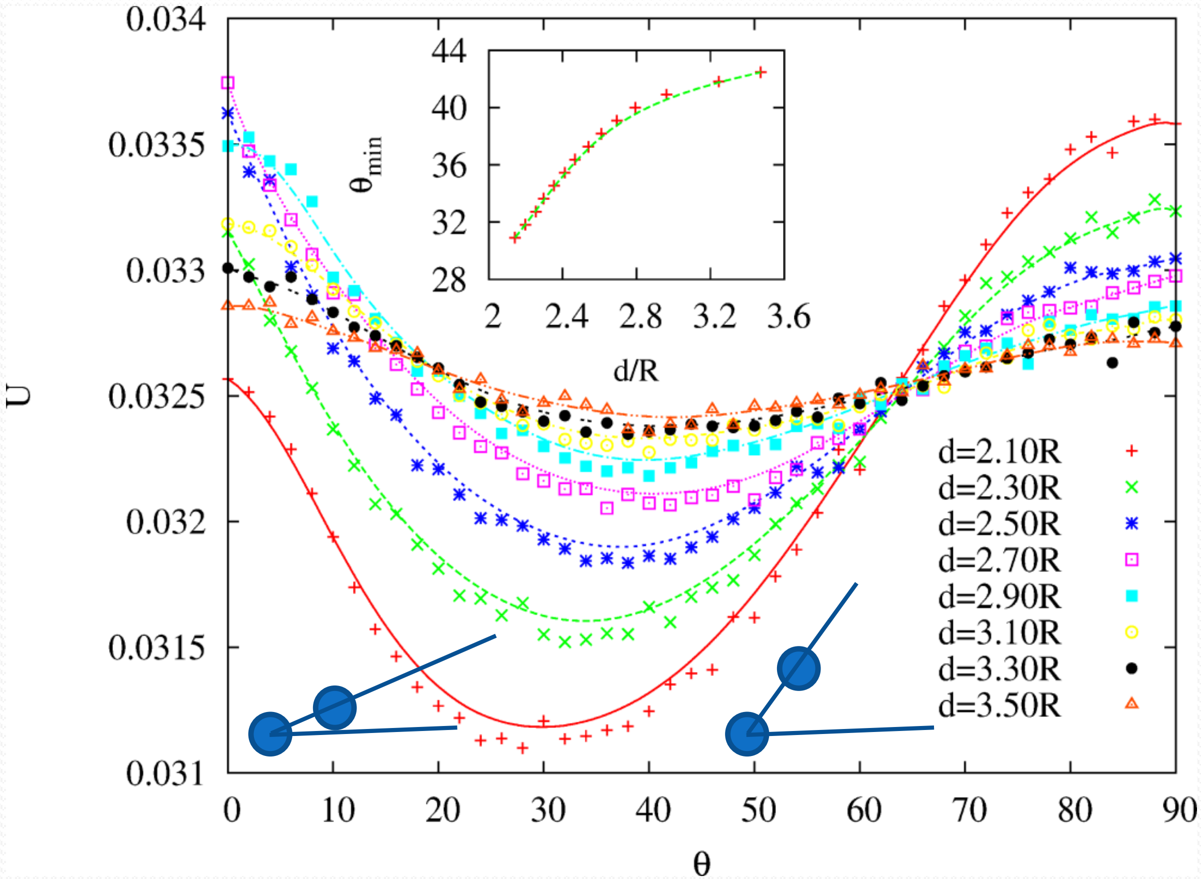


[I. Smalyukh, et al., Phys Rev Lett, 2005]

Free Energy minimization







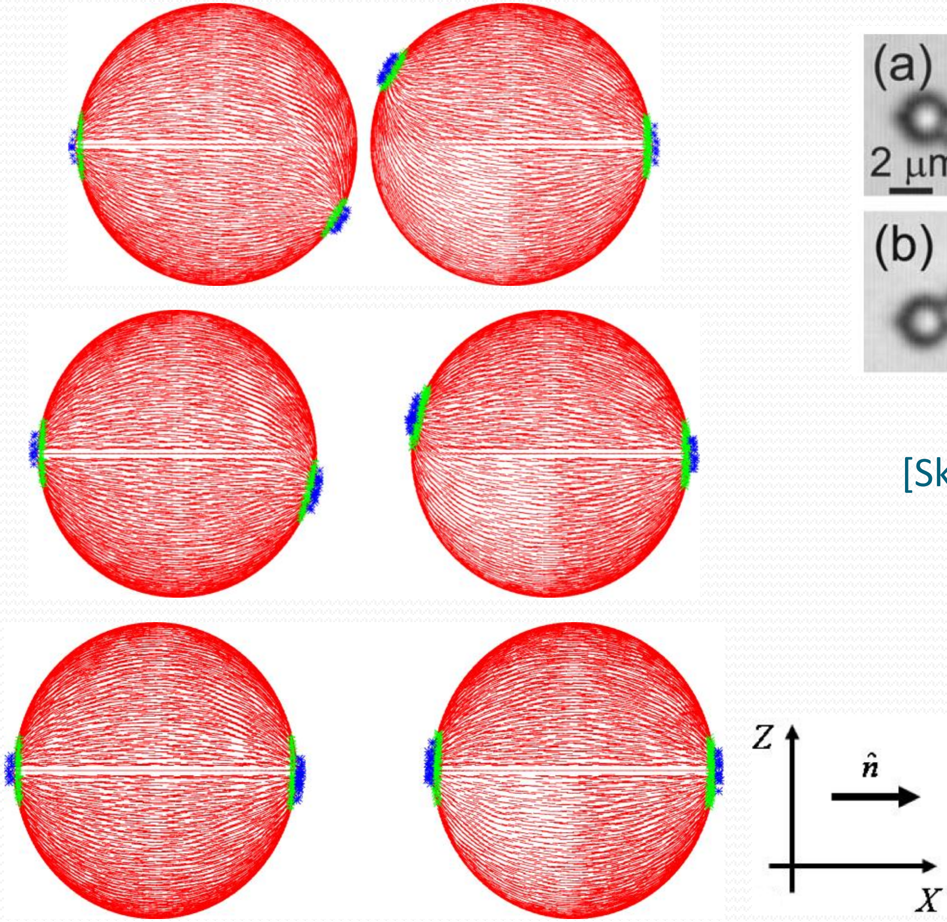
[Mozaffari, Babadi, Fukuda and Ejtehadi, Soft Matter, 2011]

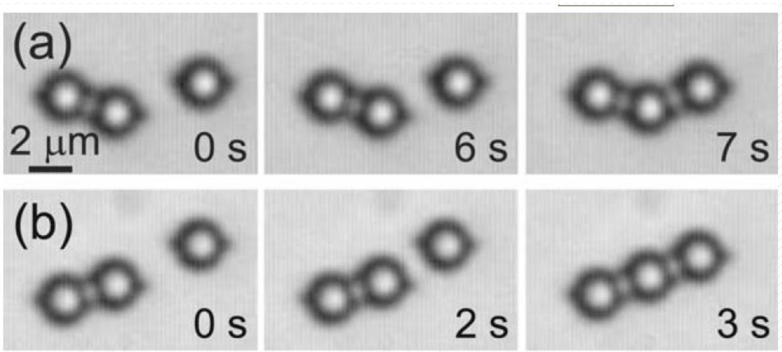
Defect reconfiguration causes attraction

$\frac{d}{R} = 2.1$
$\theta = 0^\circ$

$\frac{d}{R} = 2.7$
$\theta = 0^\circ$

$\frac{d}{R} = 3.0$
$\theta = 0^\circ$

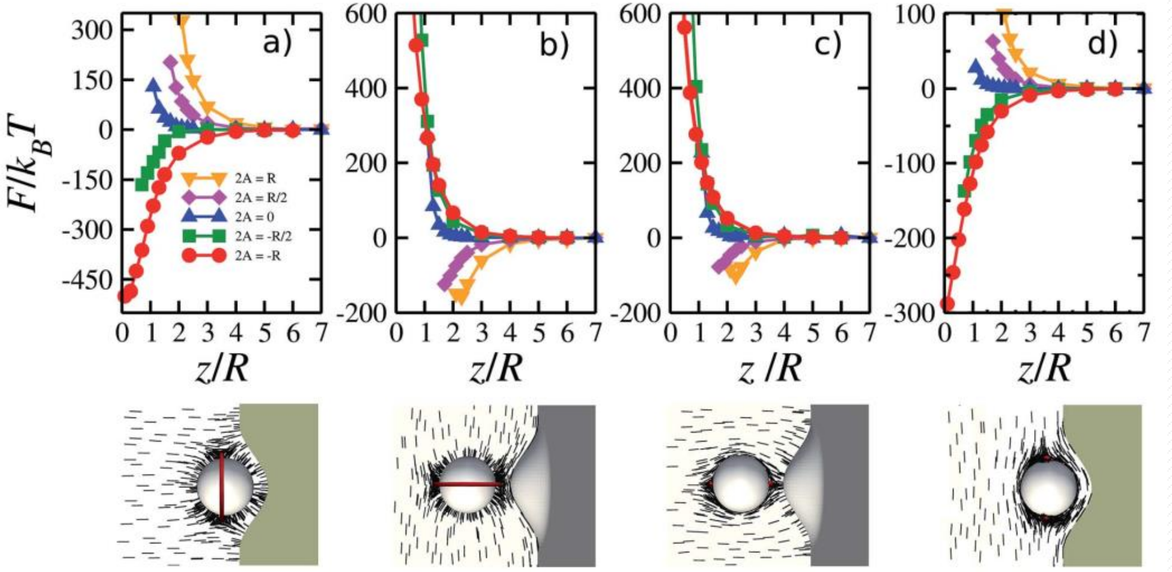


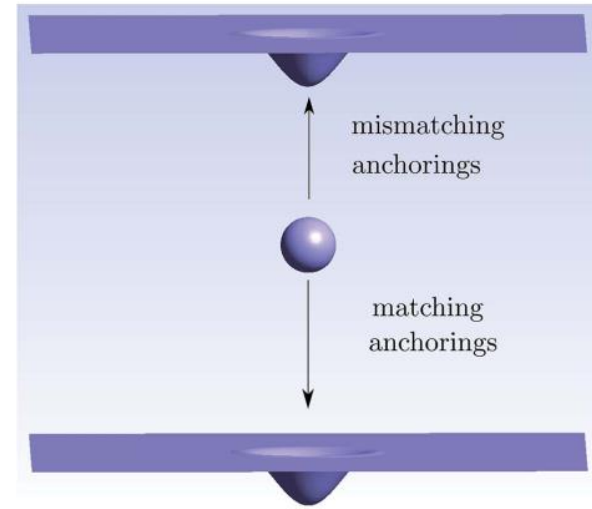


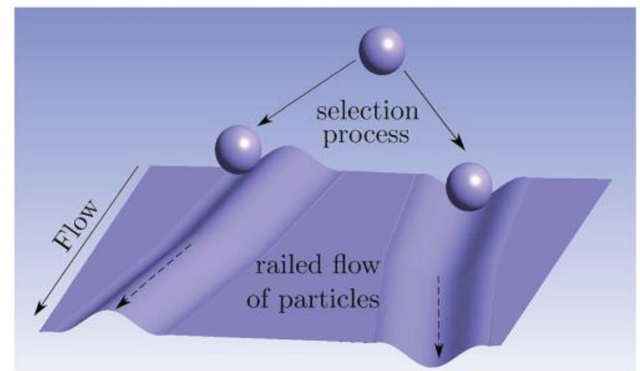
[Skarabot et al, Phys. Rev. E , 2008]

[Mozaffari, Babadi, Fukuda and Ejtehadi, Soft Matter, 2011]

Surface topography

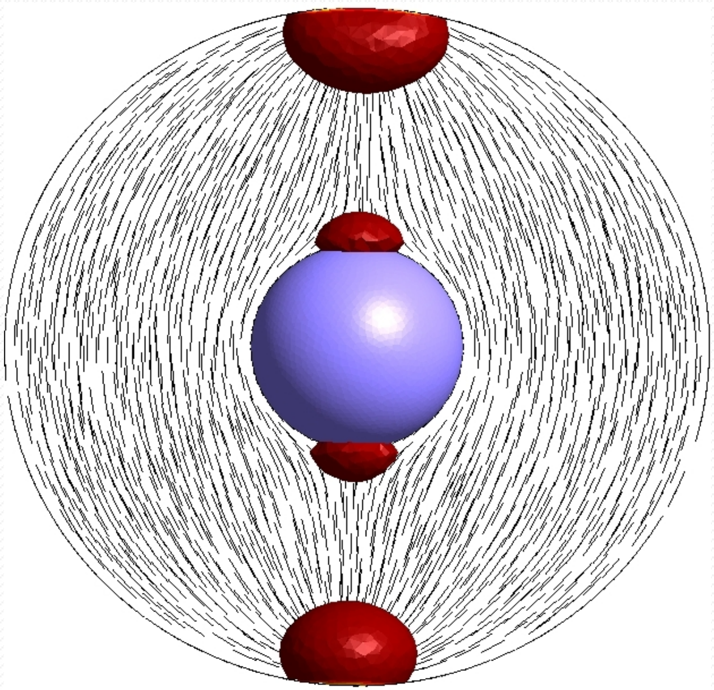


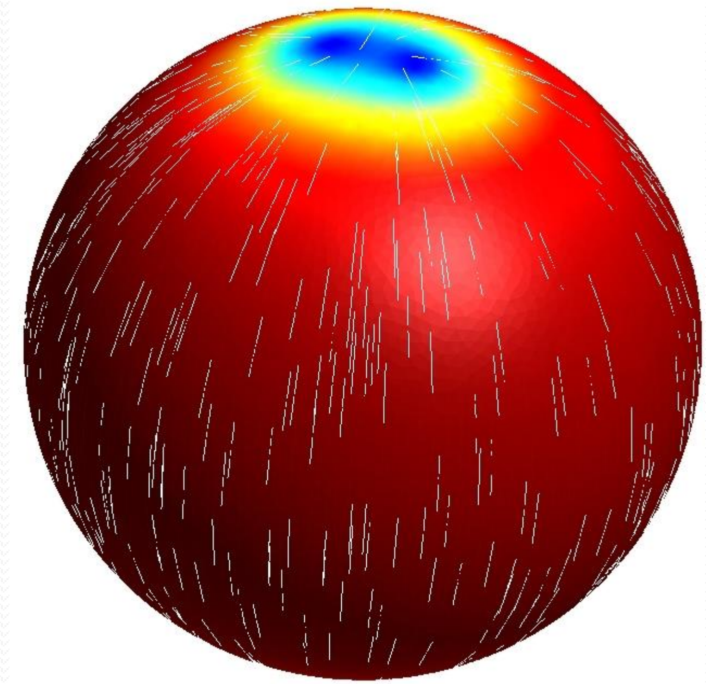




[Eskandari, Silvestre, Telo da Gamaa and Ejtehadi, Soft Matter (2014)]

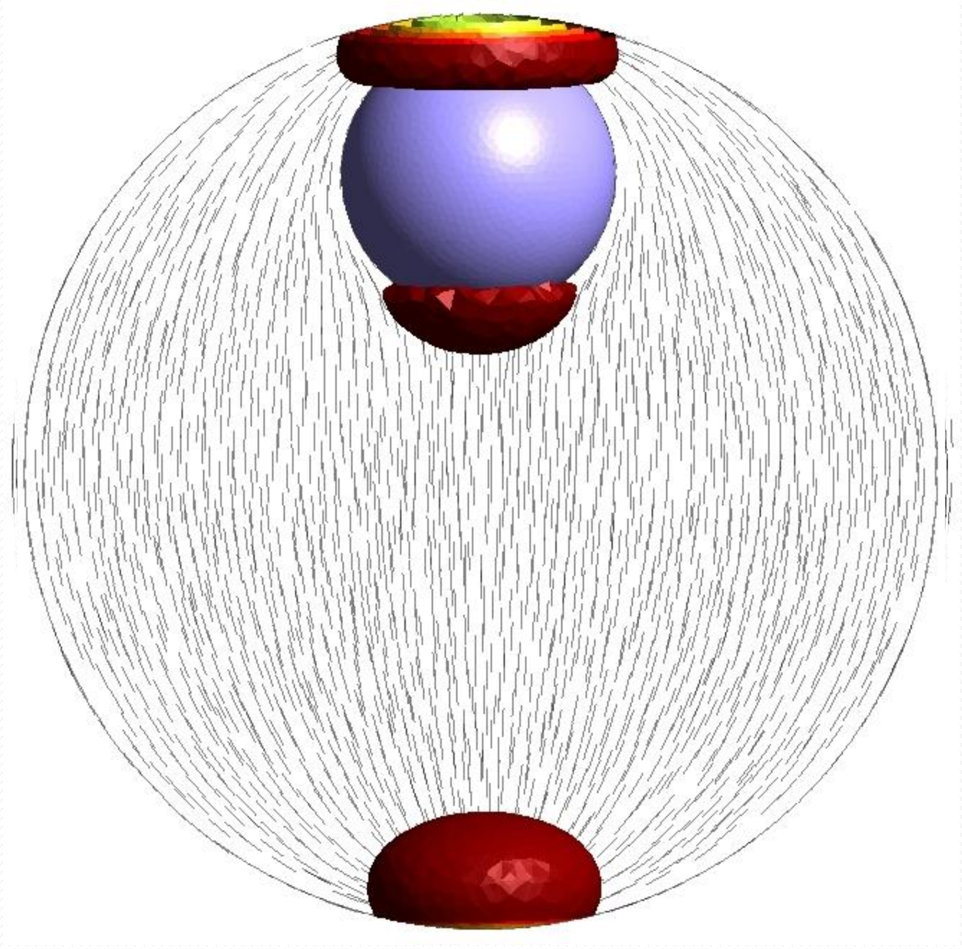
Defect structure in the nematic shells



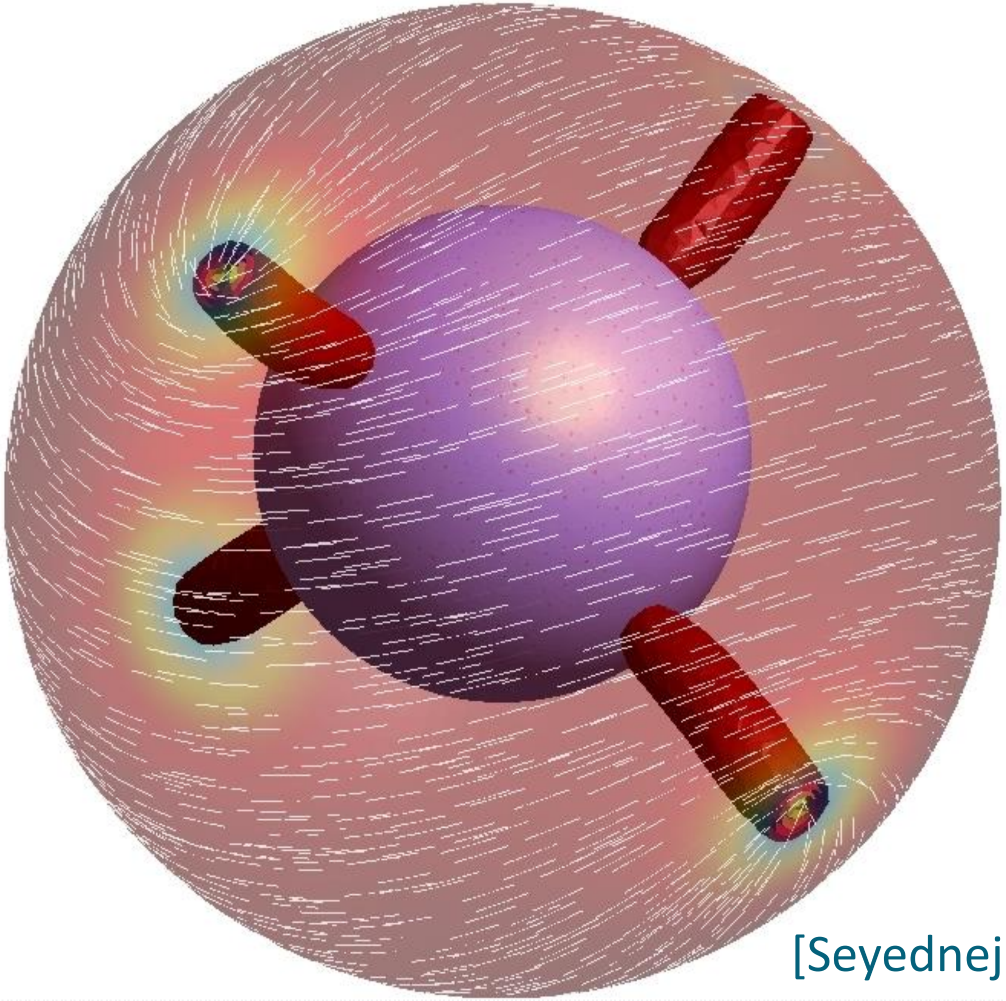


[Seyednejad, Mozaffari, and Ejtehadi, PRE 2013]

Off-center droplets (thick shells)

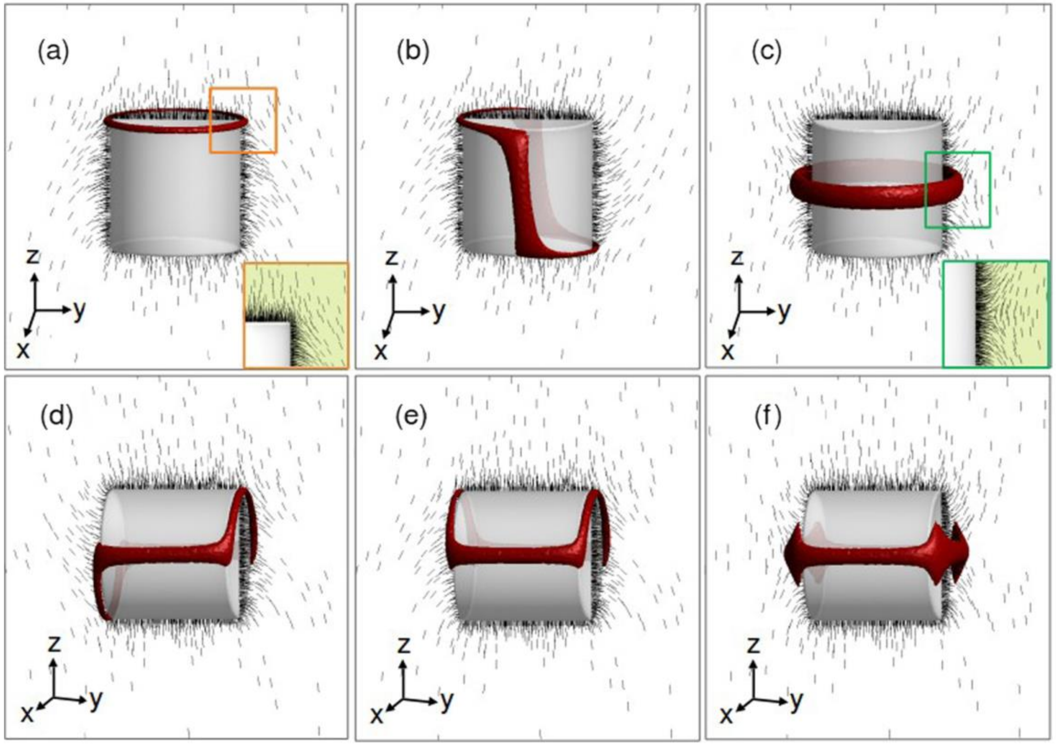


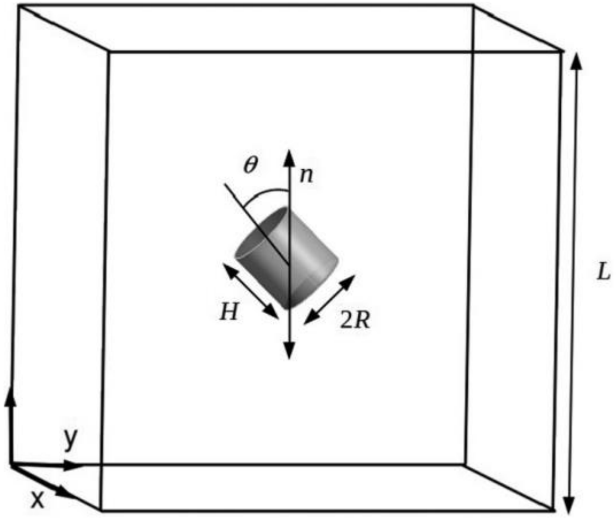
PRE Kaleidoscope



[Seyednejad, Mozaffari, and Ejtehadi, PRE 2013]

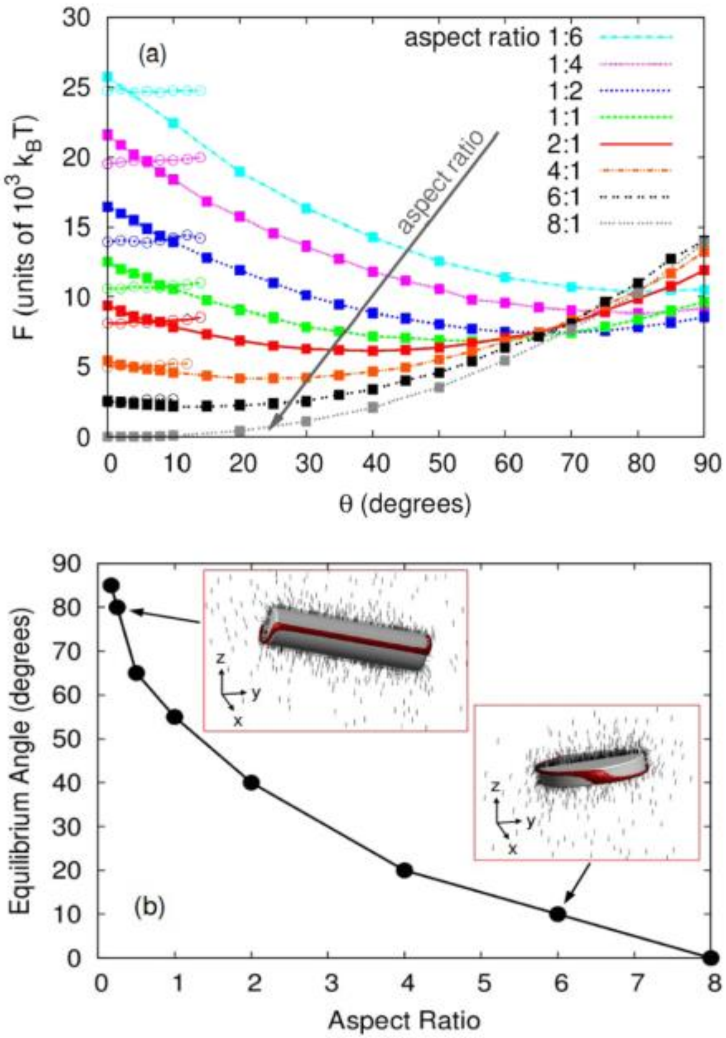
Cylindrical particles

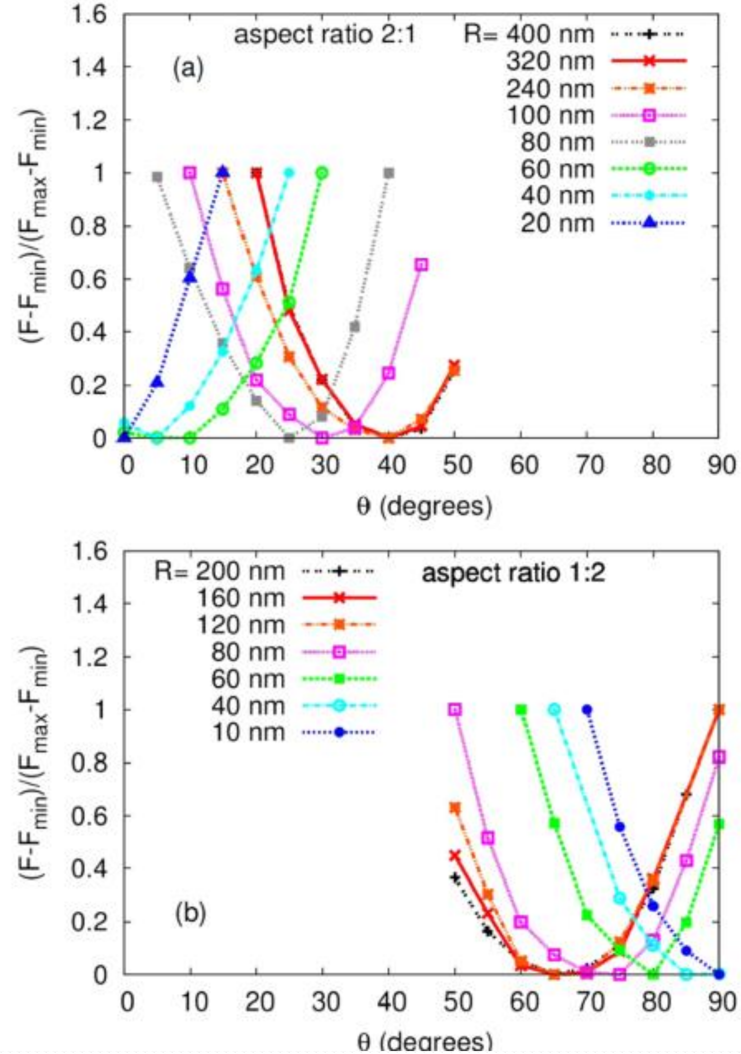




[Hashemi and Ejtehadi, PRE 2015]

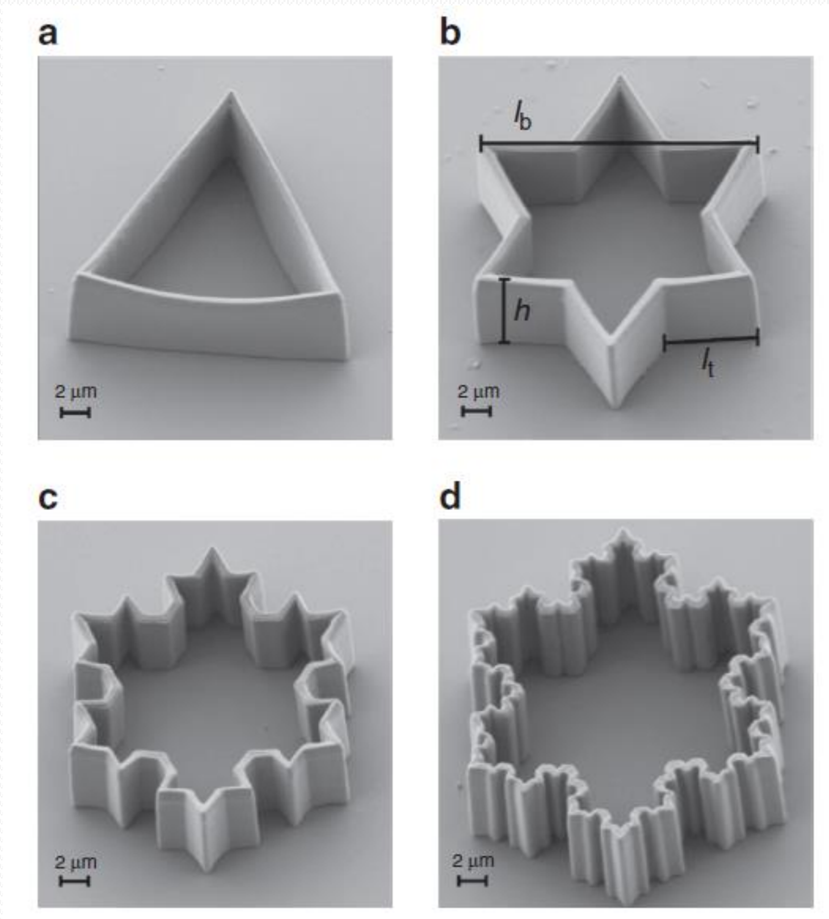
Cylinder orientation

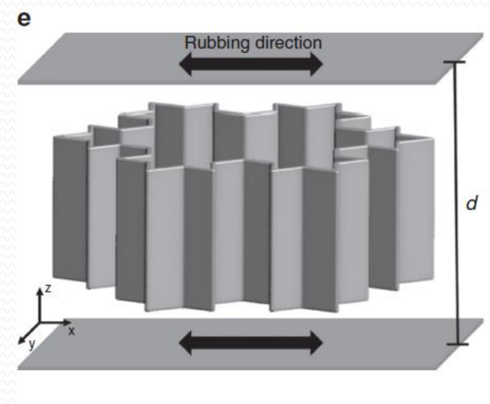




[Hashemi and Ejtehadi, PRE 2015]

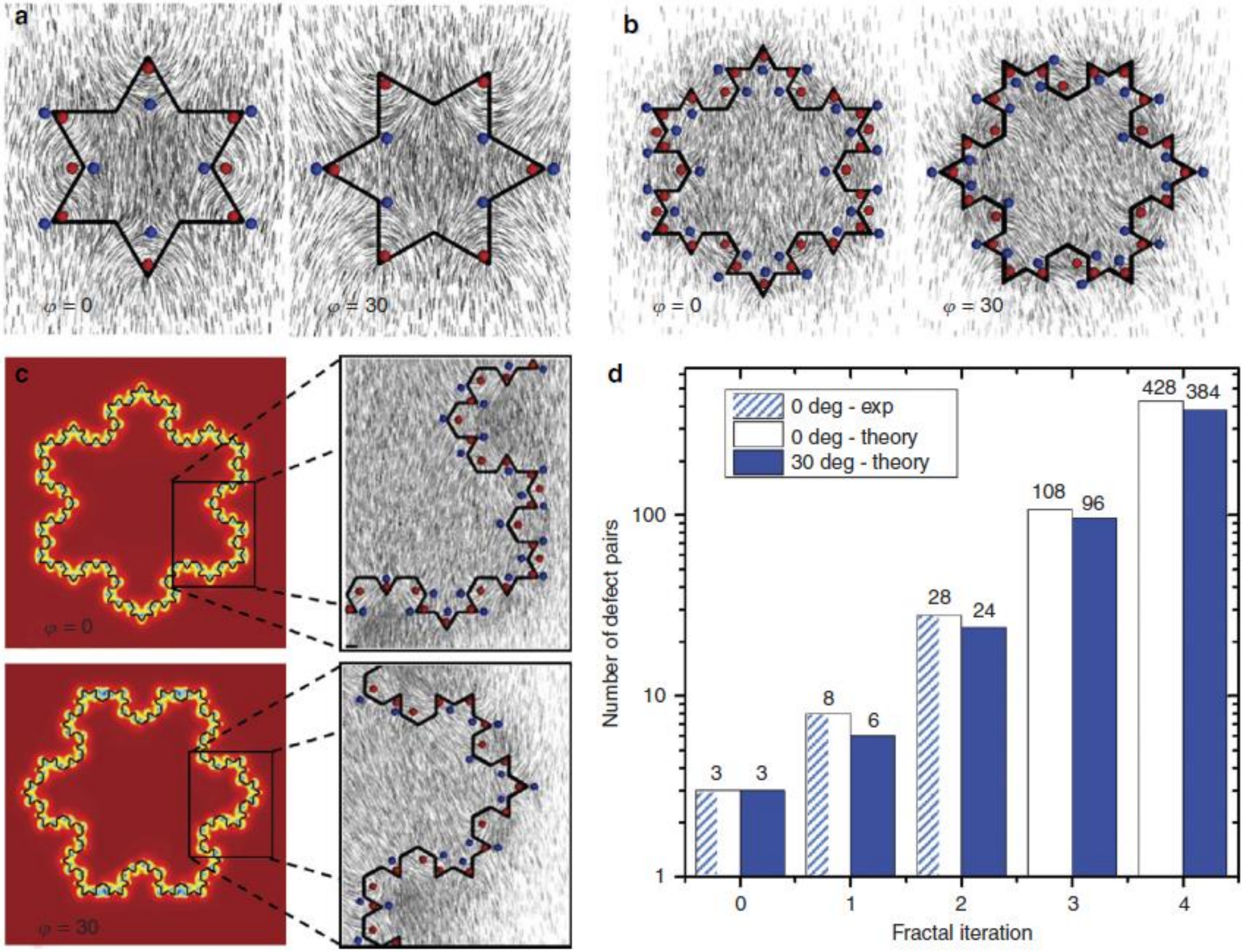
Real Fractal particles





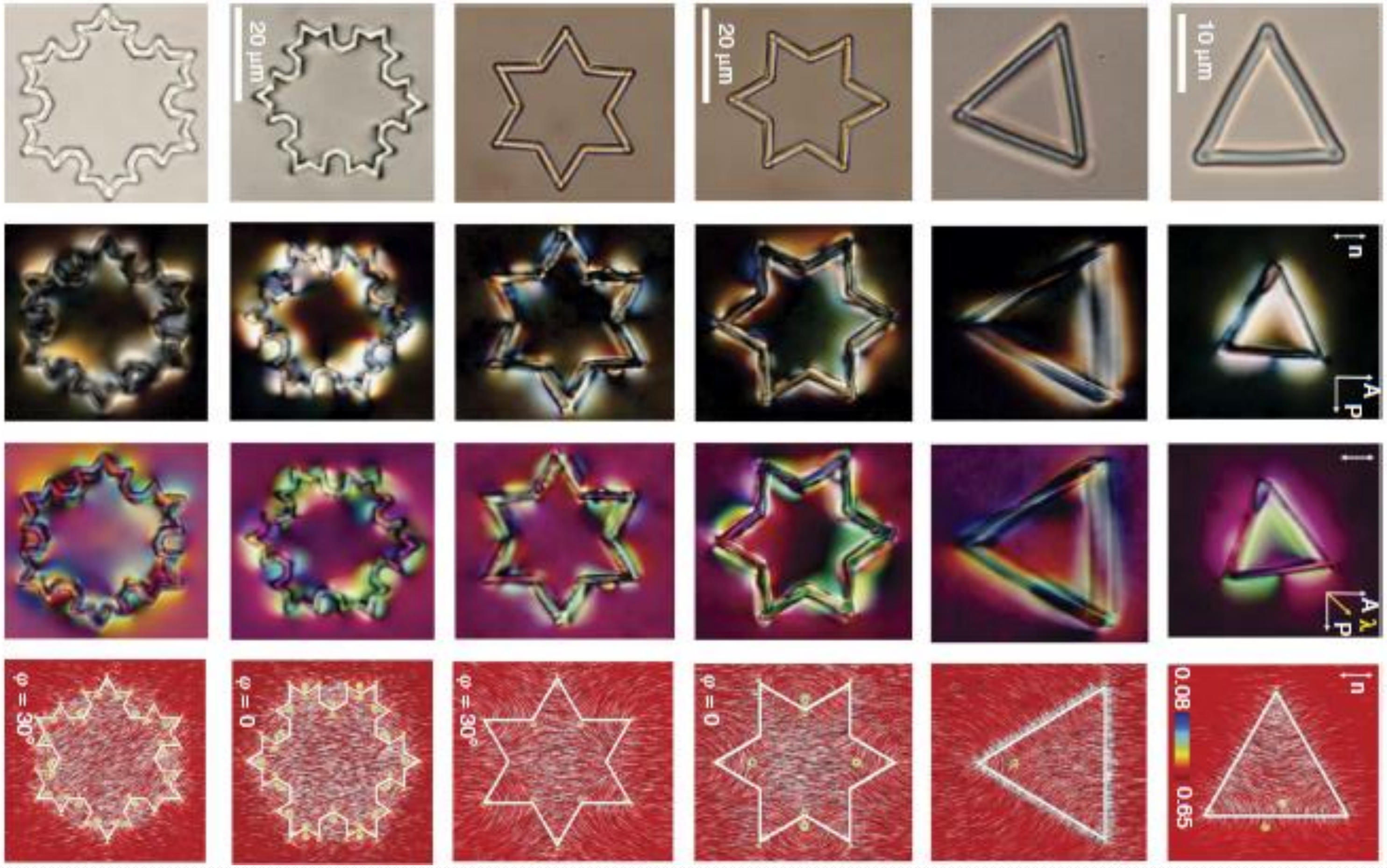
[Hashemi, Jagodic, Mozaffari, Ejtehadi, Musevic and Ravnik, Nature Communications 2017]

Fractal-like particles



[Hashemi, Jagodic, Mozaffari, Ejtehadi, Musevic and Ravnik, Nature Communications 2017]

Experiment + Theory

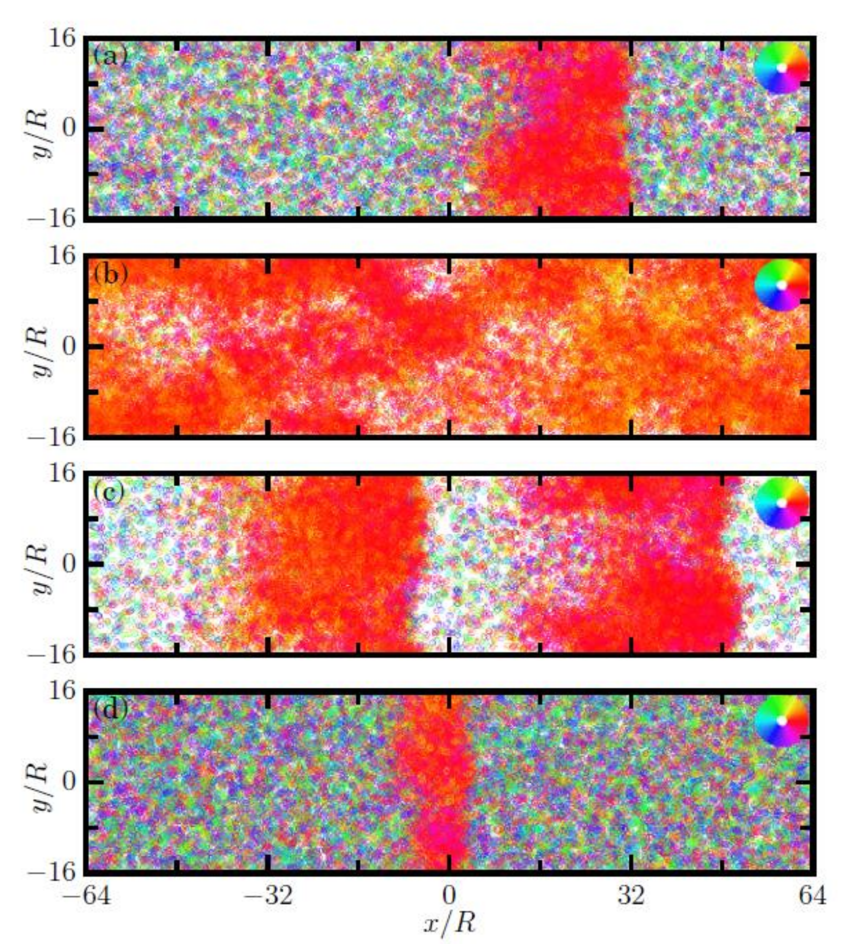


[Hashemi, Jagodic, Mozaffari, Ejtehadi, Musevic and Ravnik, Nature Communications 2017]

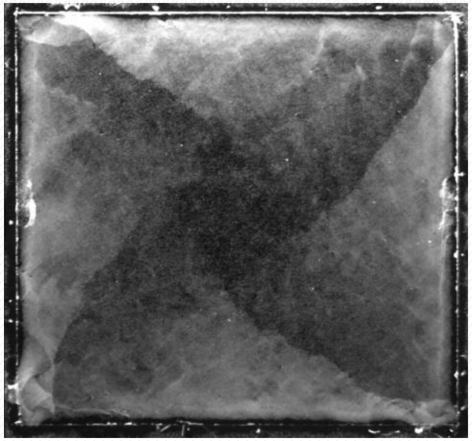
Analogy between

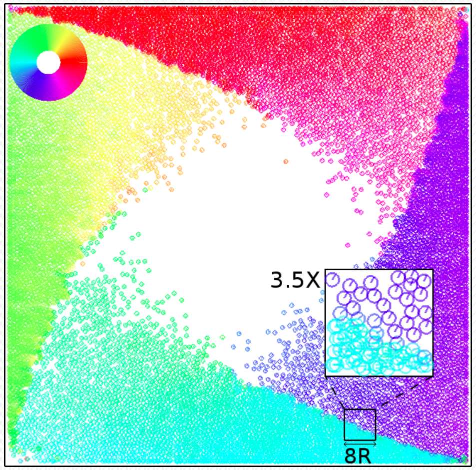
Active matter
And
Liquid Crystals

Defect in polar active matter



[Seyed-Allaei, Schimansky-Geier, and Ejtehadi, PRE 2016]





[Seyed-Allaee and Ejtehadi, PRE (2015)]

Polar Order

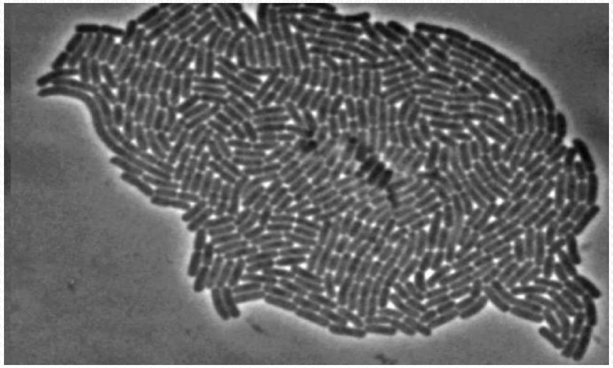
- **Defects in Active particles with directed movements have integer topological charge.**

School of sardine fish

Sheep

Active nonpolar particles in nematic phase

- As like as liquid crystals half-integer defects are possible.



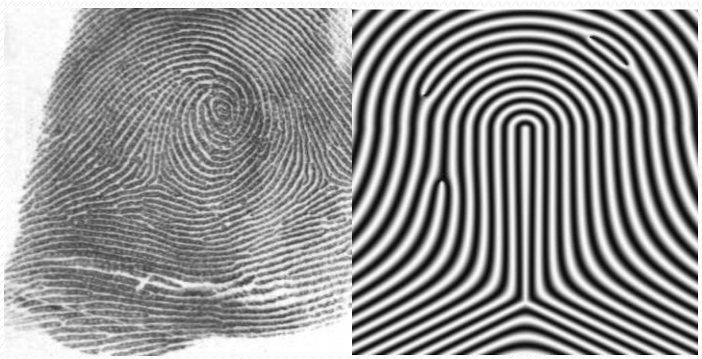
[2] E.Coli

[1] Myxococcus xanthus

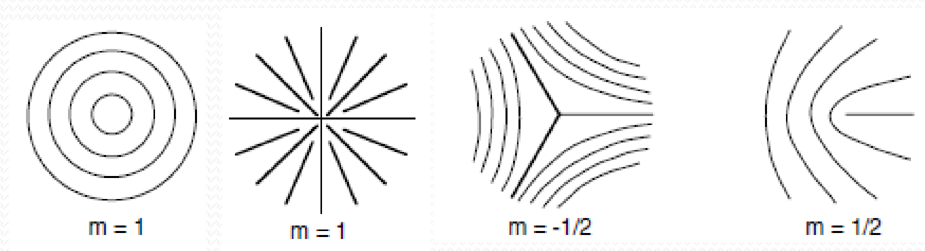
[1] Rüegg, Peter. "The Winner Doesn't Always Take All." Phys.org. June 11, 2015. Accessed May 28, 2019. https://phys.org/news/2015-06-winner-doesnt.html.
[2] Dell'Arciprete, D., M. L. Blow, A. T. Brown, F. D. C. Farrell, J. S. Lintuvuori, A. F. McVey, D. Marenduzzo, and W. C. K. Poon. "A Growing Bacterial Colony in Two Dimensions as an Active Nematic." Nature News. October 10, 2018. Accessed May 28, 2019. https://www.nature.com/articles/s41467-018-06370-3.

Topological Defects:

These are singular configurations of director field which can be changed to a homogenous state through a process called pair annihilation.



[2] Finger print, an example of defects in body

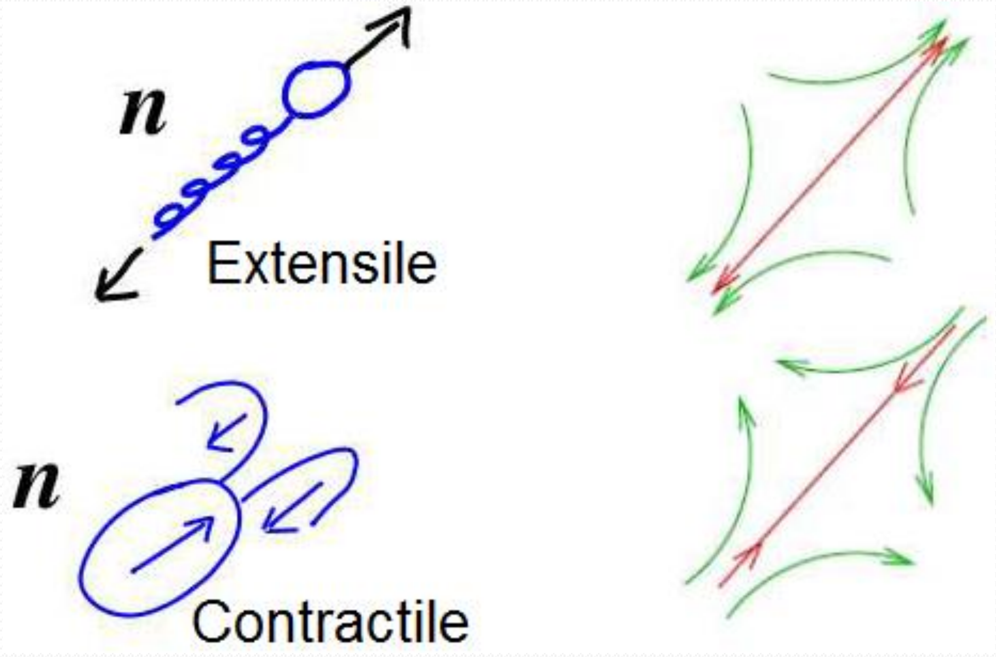


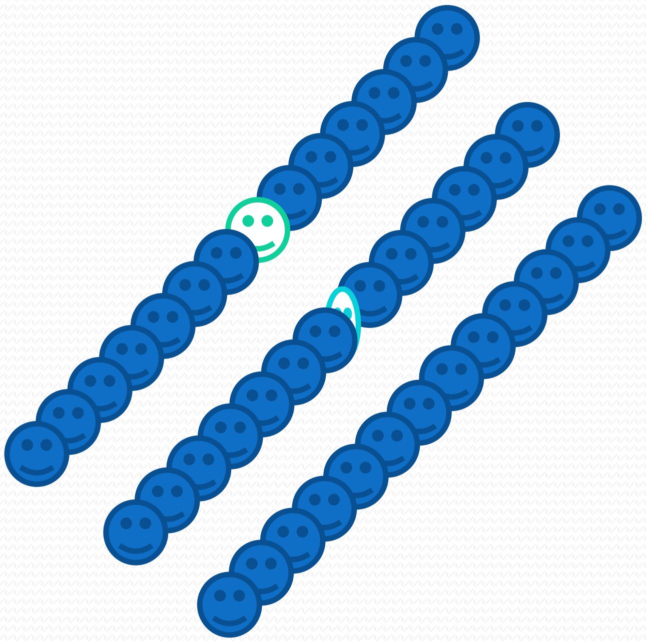
[1] Director orientation in some topological defects.

[1] Oswald, Patrick, and Pawel Pieranski. *Nematic and Cholesteric Liquid Crystals: Concepts and Physical Properties Illustrated by Experiments*. Boca Raton: Taylor & Francis, 2005.

[2] Larkin, Kieran G., and Peter A. Fletcher. "A Coherent Framework for Fingerprint Analysis: Are Fingerprints Holograms?" *Optics Express*15, no. 14 (2007): 8667. doi:10.1364/oe.15.008667.

How an active swimmer affects surrounding flow field.





Ramaswamy, Sriram. The mechanics and statistics of active matter. *Annual Review of Condensed Matter Physics*, 1(1):323–345, 2010.

Nemato-dynamics for active

With a little algebra and changing the parameter from director to Nematic order parameters, starting from Eriksen-Leslie theory of Nemato-Dynamics, one can arrive at these equation for describing the dynamics of the system [1]. Also we include an active contribution.

$$\omega_{ij} = (\partial_i v_j - \partial_j v_i)/2 \quad , \quad u_{ij} = (\partial_i v_j + \partial_j v_i)/2$$

$$\frac{Dc}{Dt} = \partial_i \left[D_{ij}\, \partial_j c + \alpha_1 c^2 \partial_j Q_{ij} \right] \quad , \qquad D_{ij} = D_0 \delta_{ij} + D_1 Q_{ij}$$

$$\rho \frac{Dv_i}{Dt} = \eta \nabla^2 v_i - \partial_i p + \partial_j\, \sigma_{ij} \quad , \qquad \sigma_{ij} = -\lambda S H_{ij} + Q_{ik} H_{kj} - H_{ik} Q_{kj} + \alpha_2 c^2 Q_{ij}$$

$$\frac{DQ_{ij}}{Dt} = \lambda S u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik} Q_{kj} + \frac{1}{\gamma} H_{ij}$$

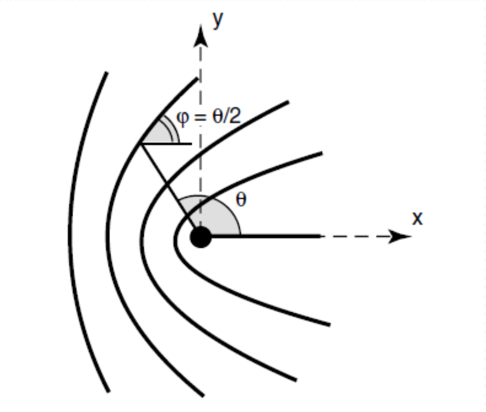
[1] Giomi, L., M. J. Bowick, P. Mishra, R. Sknepnek, and M. Cristina Marchetti. "Defect Dynamics in Active Nematics." *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*372, no. 2029 (2014): 20130365. doi:10.1098/rsta.2013.0365.

Isolated Defect

$$\oint d\varphi = 2k\pi \implies \varphi_d = k\theta$$

$$f = \frac{1}{2}A(c)tr(Q^2) + \frac{1}{4}C(tr(Q^2))^2 + \frac{1}{2}K|\nabla Q|^2$$

$$U_d = \frac{K}{2}\int (\nabla \varphi_d)^2 dxdy = \pi K k^2 ln(\frac{R}{a}) + \epsilon_c$$



[1] Details of +1/2 defect

Pair Defect +- 1/2

$$U_{pair} = 2\pi K k^2 ln(\frac{\Delta}{a}) \quad , \quad \Delta = x_+ - x_-$$

$$\frac{d\Delta}{dt} = -\frac{2\kappa}{\Delta} \quad , \quad \kappa = 2\pi K k^2/\zeta \sim 1/\gamma$$

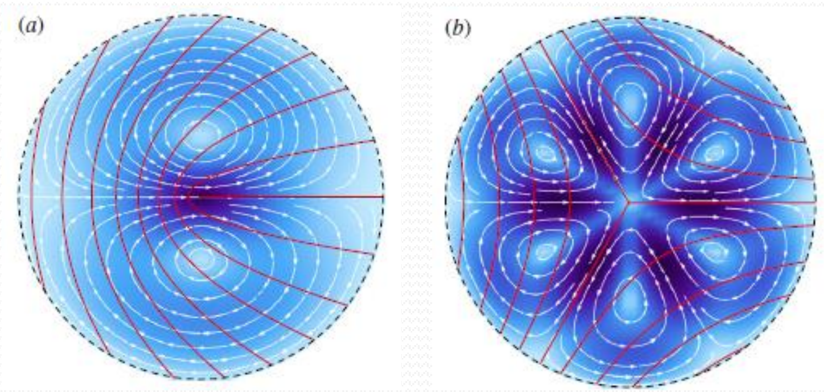
$$\frac{DQ_{ij}}{Dt} = \lambda S u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} + \frac{1}{\gamma}H_{ij}$$

[1] Oswald, Patrick, and Pawel Pieranski. *Nematic and Cholesteric Liquid Crystals: Concepts and Physical Properties Illustrated by Experiments*. Boca Raton: Taylor & Francis, 2005.

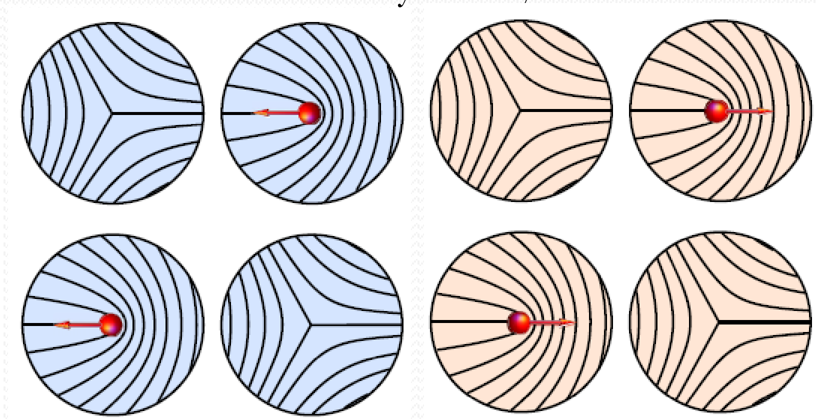
Back Flow:

$$\sigma_{ij} = -\lambda S H_{ij} + Q_{ik} H_{kj} - H_{ik} Q_{kj} + \alpha_2 c^2 Q_{ij}$$

The active term in stress tensor results a velocity field around the defect core which is called Back-flow. It is obvious from the symmetry of the defects that -1/2 has no backflow and the +1/2 has a constant backflow velocity resulting from constant force in a viscous fluid in the direction of its symmetry axis.



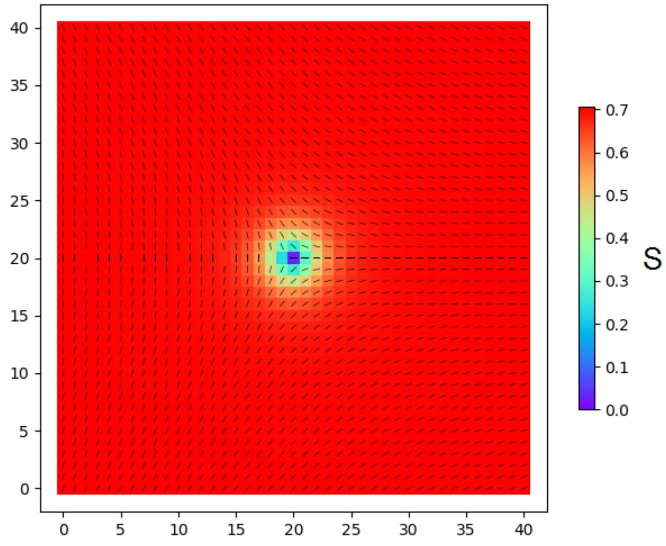
[1] Fluid velocity(white stream lines) and director field (red lines). (a) +1/2 , (b) -1/2.

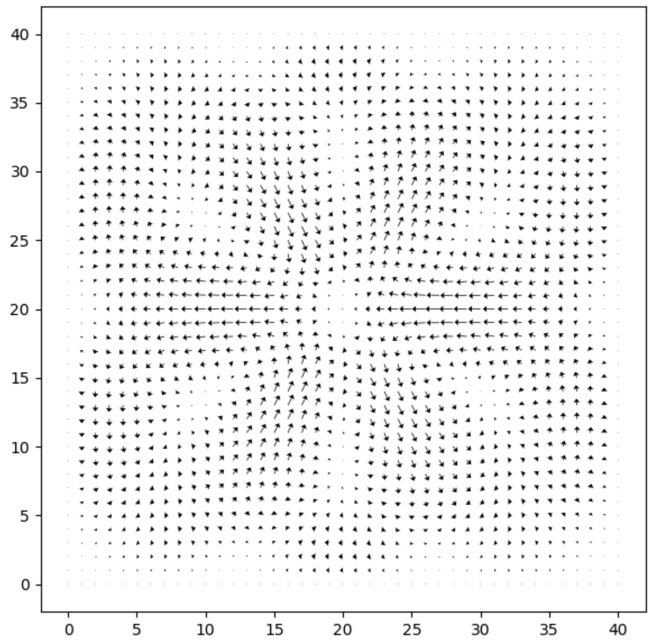


[2] Regarding the relative geometry of the position and orientation of pairs, backflow can facilitate or delay the pairs to annihilate.`

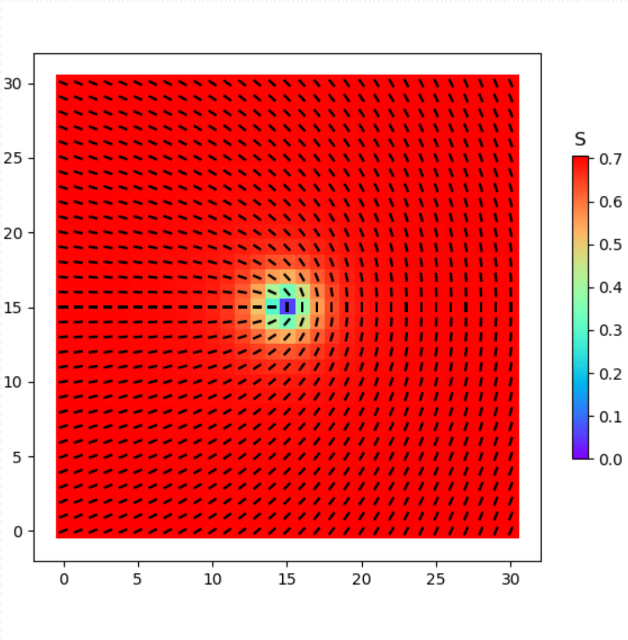
[1] , [2] Giomi, L., M. J. Bowick, P. Mishra, R. Sknepnek, and M. Cristina Marchetti. "Defect Dynamics in Active Nematics." *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*372, no. 2029 (2014): 20130365. doi:10.1098/rsta.2013.0365.

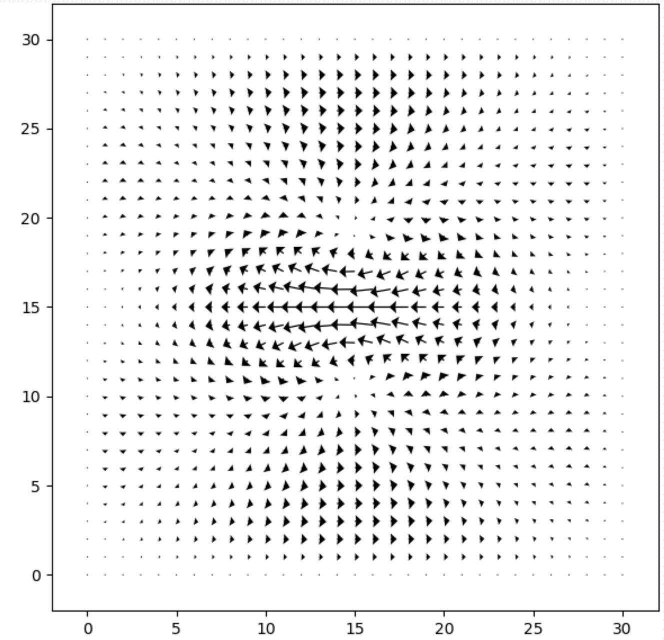
Backflow of -1/2





Backflow of +1/2



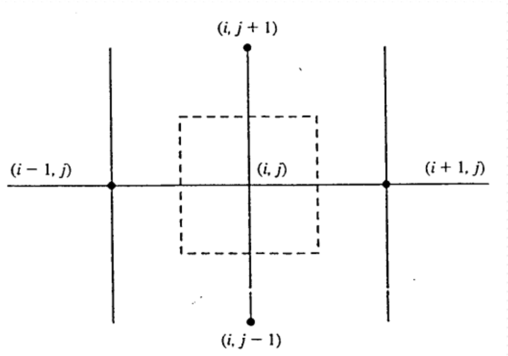


Finite Difference

Calculations have been preformed in a 80 by 80 domain.

Spatial derivatives have been calculated via Finite difference.

Dynamics of quantities have been evaluated via Runge-Kutta 4th orde



[1] Five point Star

$$\nabla^2 f\Big|_{(i,j)} = \frac{f(i+1,j) + f(i-1,j) + f(i,j+1) + f(i,j-1) - 4f(i,j)}{h^2}$$

$$k_1 = \Delta t f(t_n, y_n)$$

$$k_2 = \Delta t f(t_n + \frac{\Delta t}{2}, y_n + \frac{k_1}{2})$$

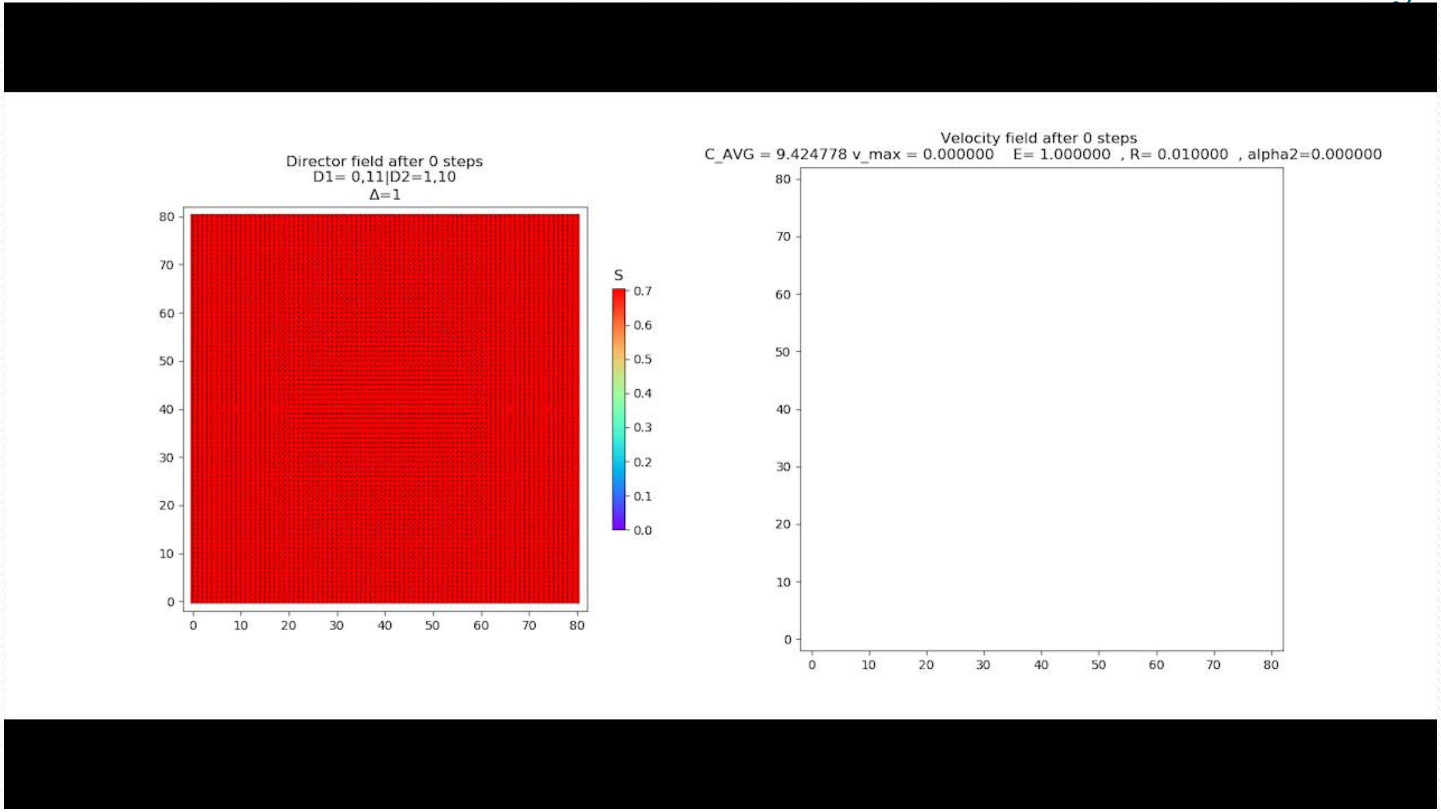
$$k_3 = \Delta t f(t_n + \frac{\Delta t}{2}, y_n + \frac{k_2}{2})$$

$$k_4 = \Delta t f(t_n + \Delta t, y_n + k_3)$$

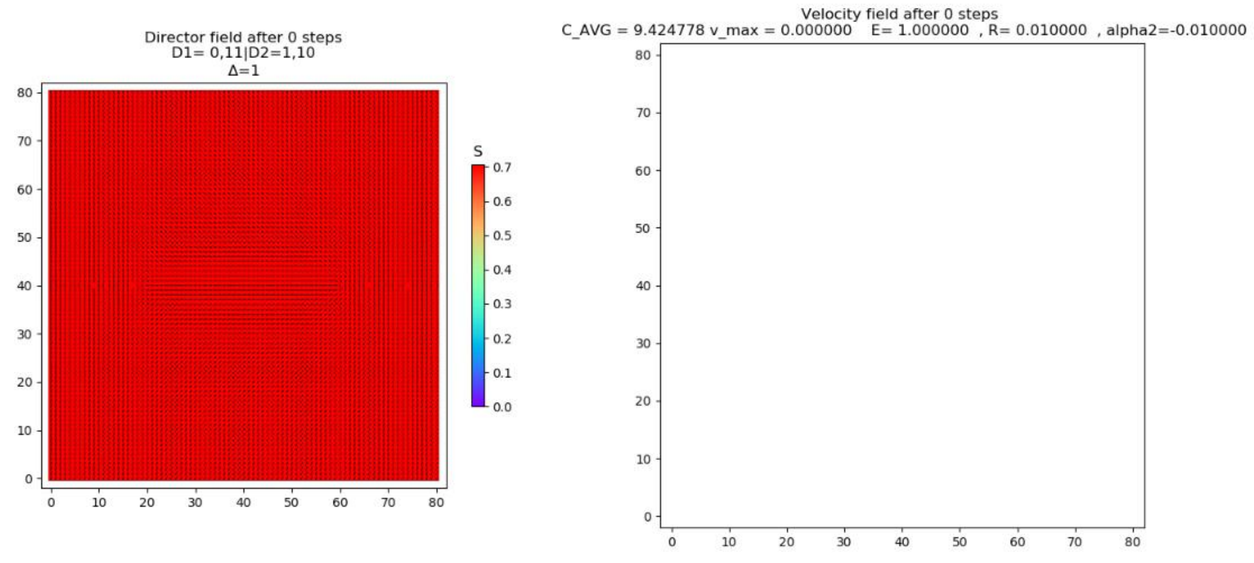
$$\Longrightarrow \quad y_{n+1} = y_n + \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}$$

[1] "Finite Difference Method for the Solution of Laplace Equation." Accessed May 31, 2019. https://www.andrew.cmu.edu/course/24-681/handouts/lectures/fdm_for_laplace_equation.pdf.

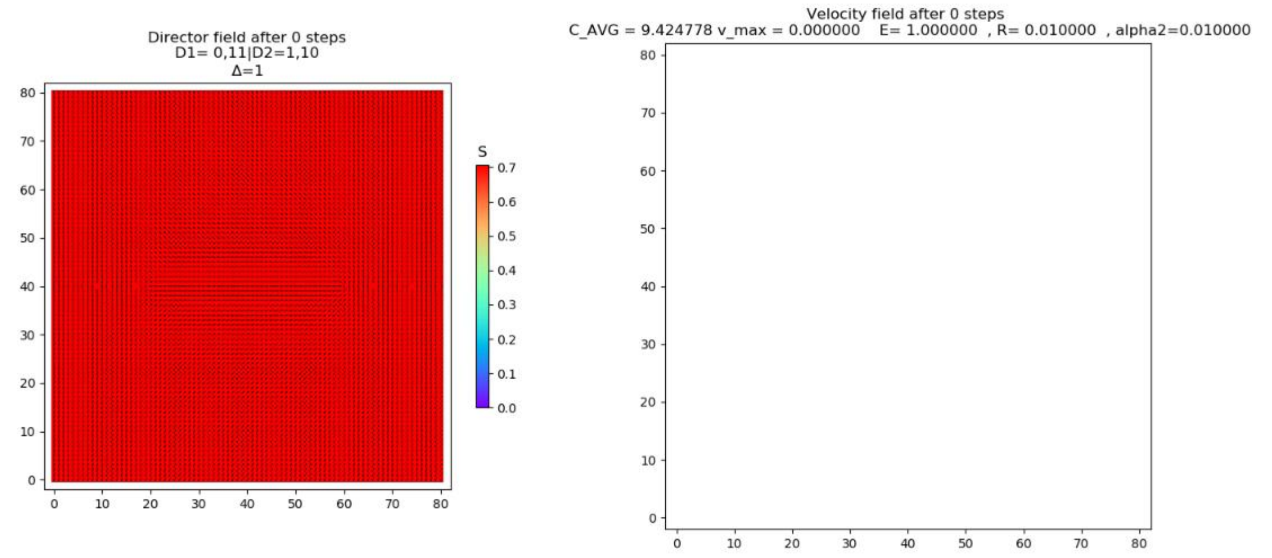
Annihilation with zero activity



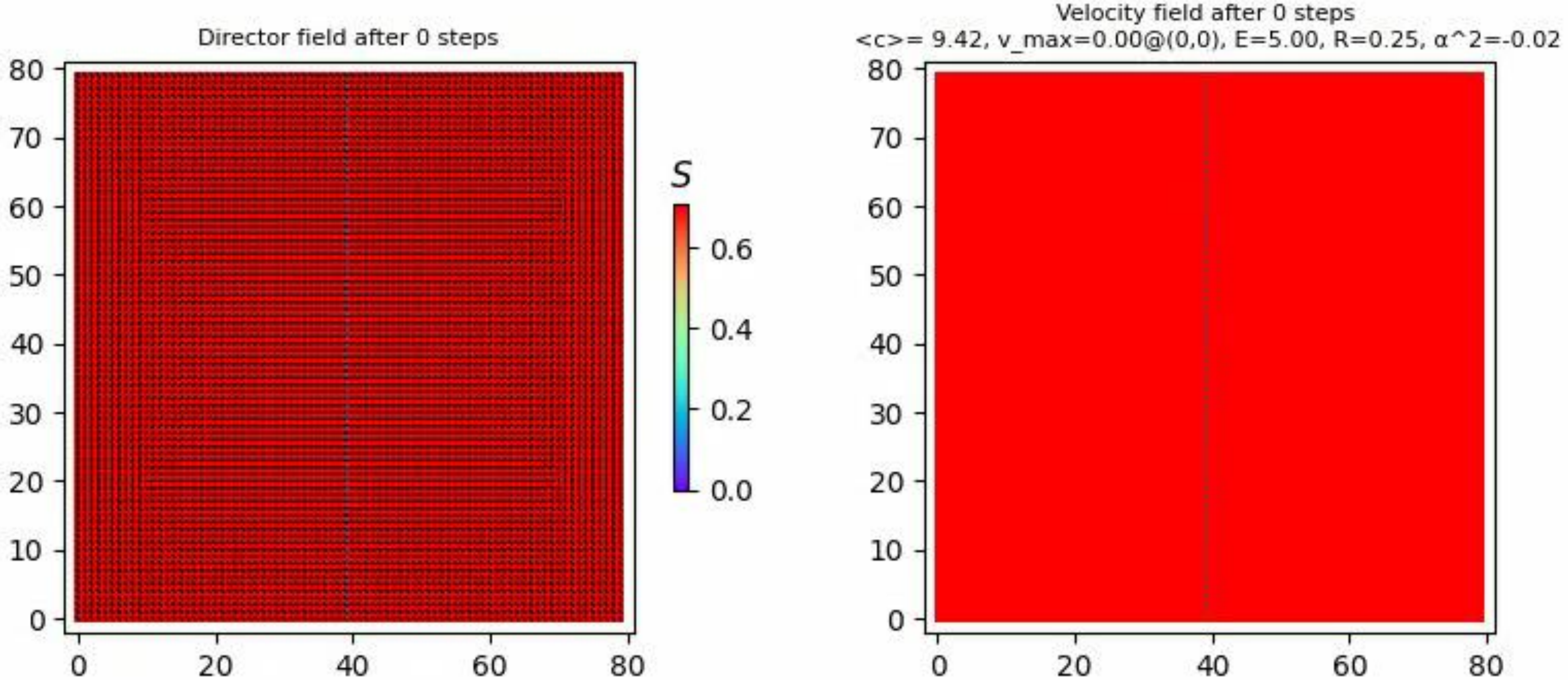
Annihilation with negative activity



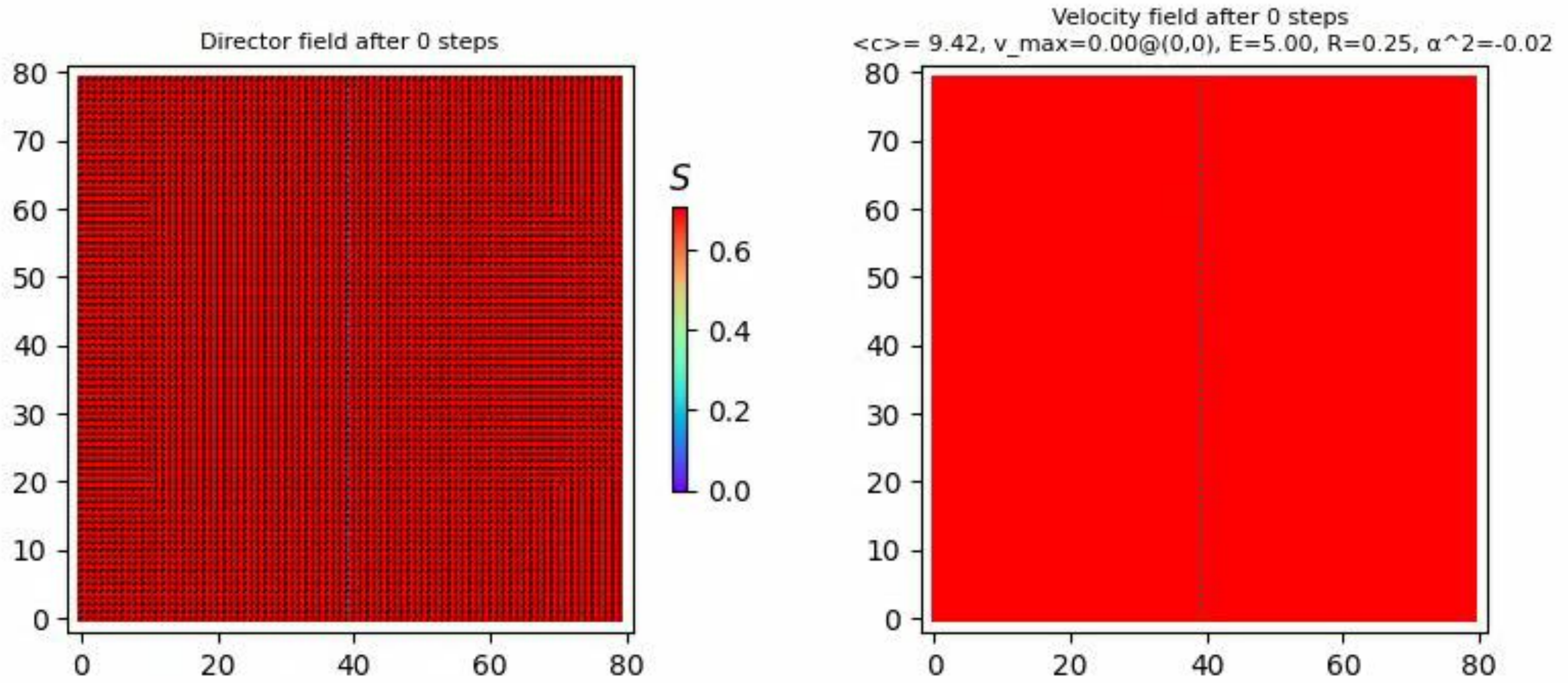
Annihilation with positive activity



Confined Annihilation with negative activity



Confined Annihilation with negative activity



Conclusion

- Topological defects interactions induced interesting dynamics to their configuration inside the nematic phase, both for passive and active nematics.
- In the case of active nematics in addition to the charge interaction potential between the defects, a back flow governs the defect dynamics due to active stress term.
- Numerical solution of the modified nemato-dynamics equations of the active nematic shows that the boundary conditions may affect the dynamics of the defects radically.
- The systems with the larger numbers of point defects behaves similar to self propelled charged particles.