Cornered!
anisotropic fluids in confined geometries

Prof. Nigel Mottram
Department of Mathematics and Statistics
University of Strathclyde, Glasgow

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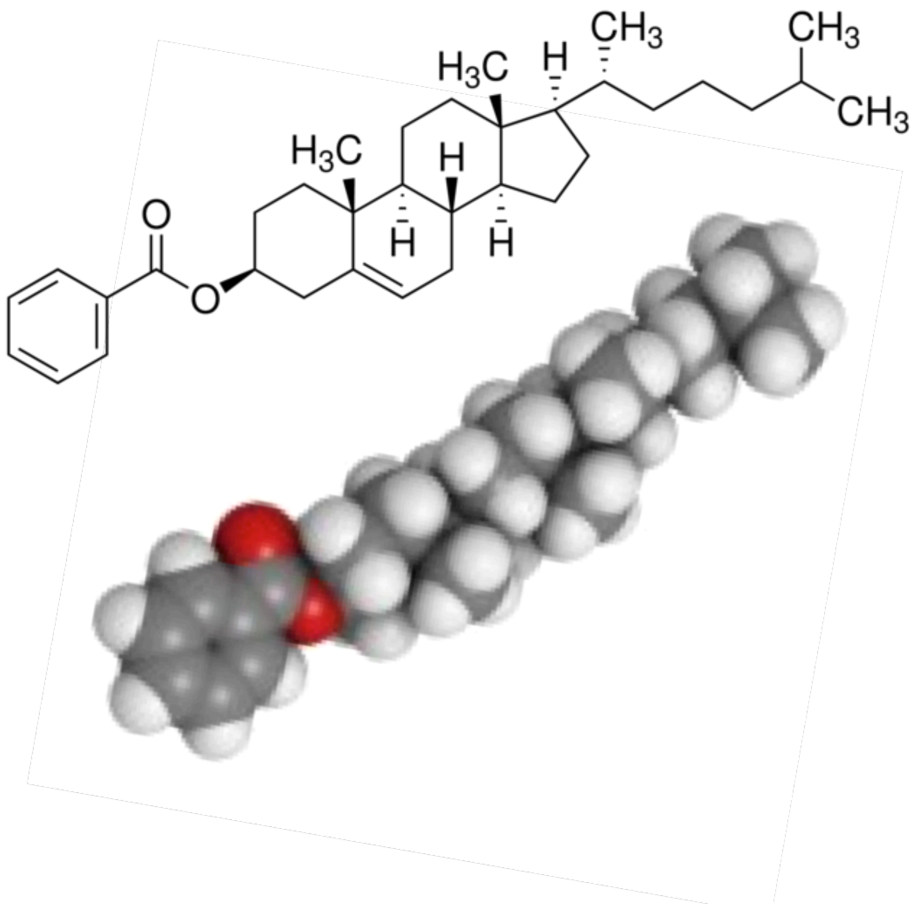
Dr Geoff McKay, Dr Andrew Davidson, Josh Walton (Strathclyde)

Prof Carl Brown, Dr Costas Tsakonas, Dr Sam Ladak, Dr Gary Wells (Nottingham Trent)

Liquid Crystals

Elongated molecules can have **orientational** order **without** having **positional** order.



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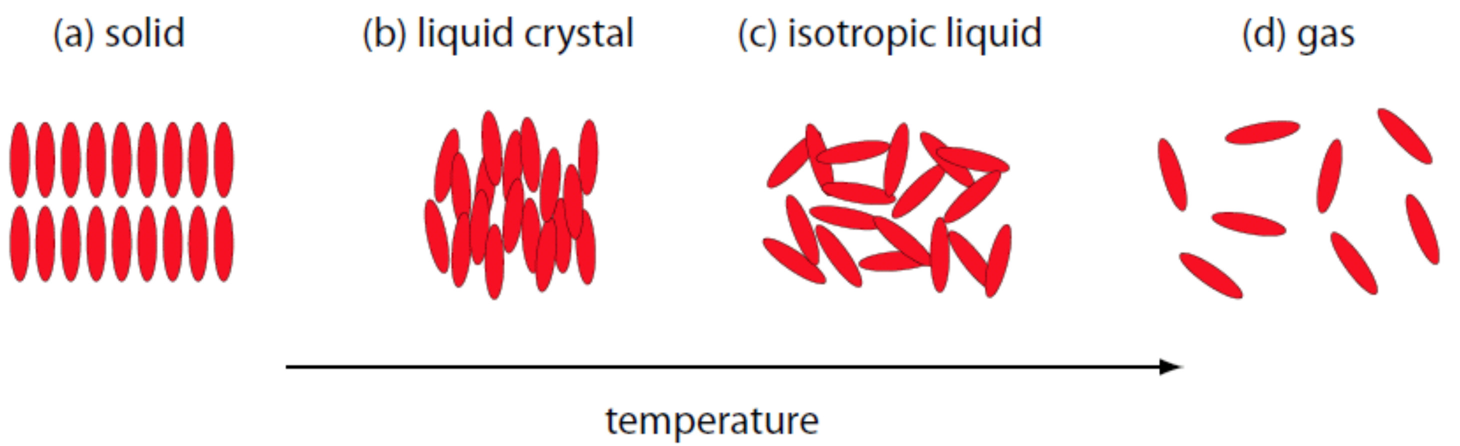

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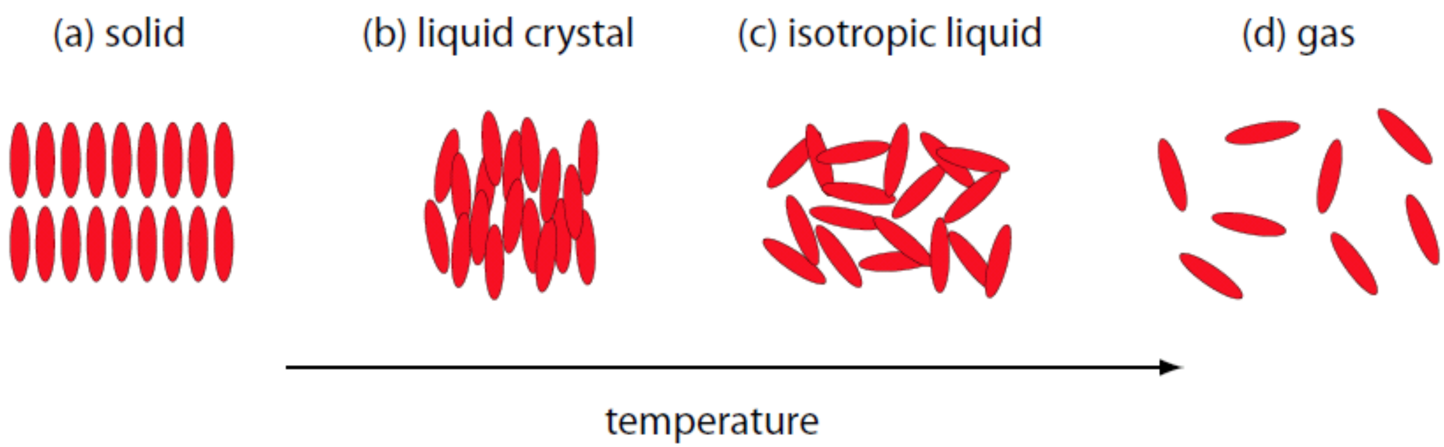
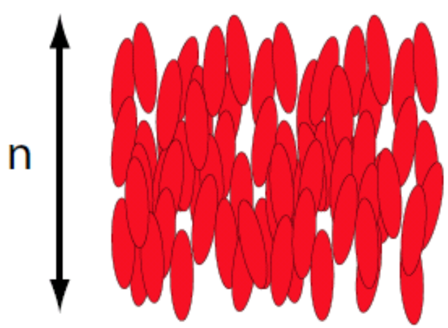


A group of molecules can then have an **average direction (the director n)**



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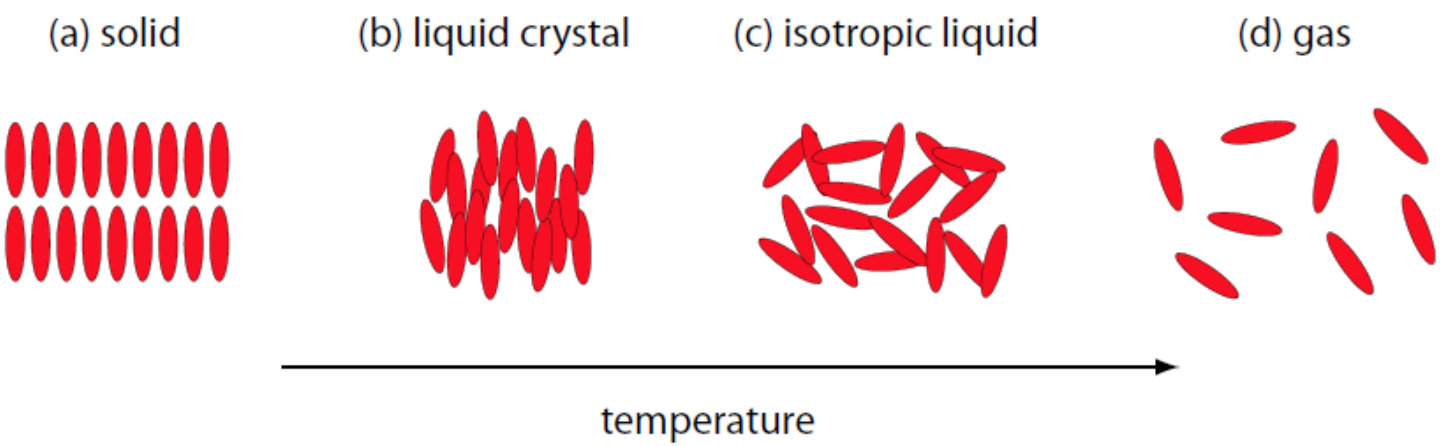
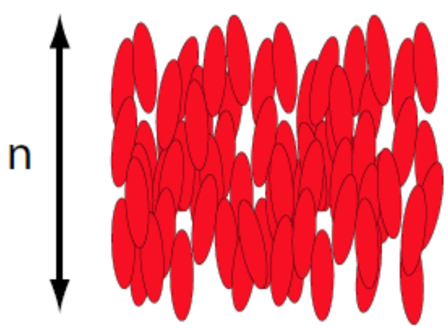
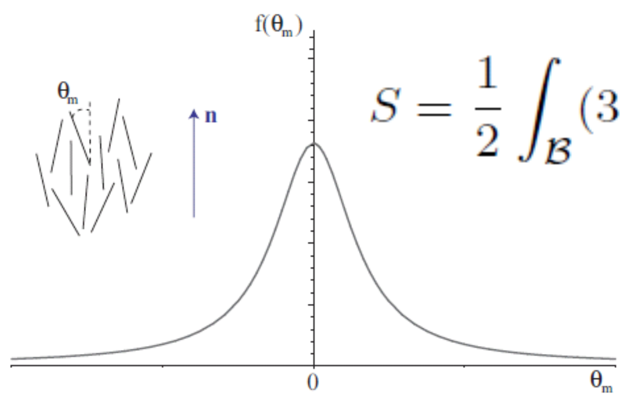


A group of molecules can then have an average direction (the director **n**) and a measure of the distribution **spread around this director (scalar order parameter S)**.

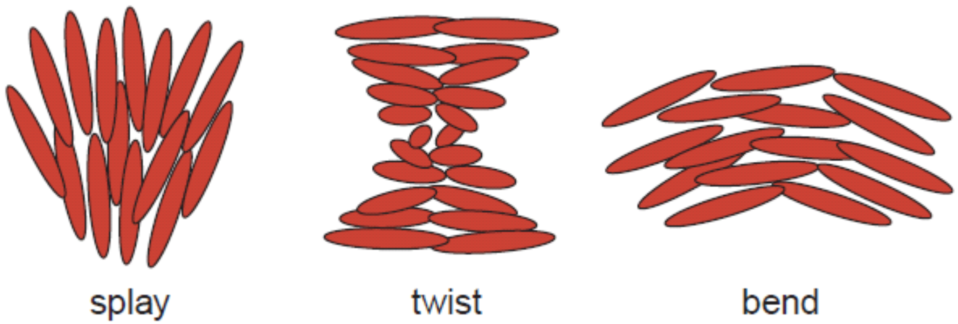




$$S = \frac{1}{2}\int_{\mathcal{B}} (3\cos^2\theta_m - 1)\, f(\theta_m)\, dV.$$

Liquid Crystals – elastic energy

- **Frank-Oseen-Zöcher elastic energy**



$$\boxed{\begin{aligned}\mathcal{F}_d \quad = \quad & \frac{K_1}{2}(\nabla.\mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n}.\nabla\times\mathbf{n} - q_0)^2 + \frac{K_3}{2}(\mathbf{n}\times\nabla\times\mathbf{n})^2 \\ & + \frac{1}{2}(K_2+K_4)\,\nabla.\left((\mathbf{n}.\nabla)\,\mathbf{n} - (\nabla.\mathbf{n})\,\mathbf{n}\right)\end{aligned}}$$

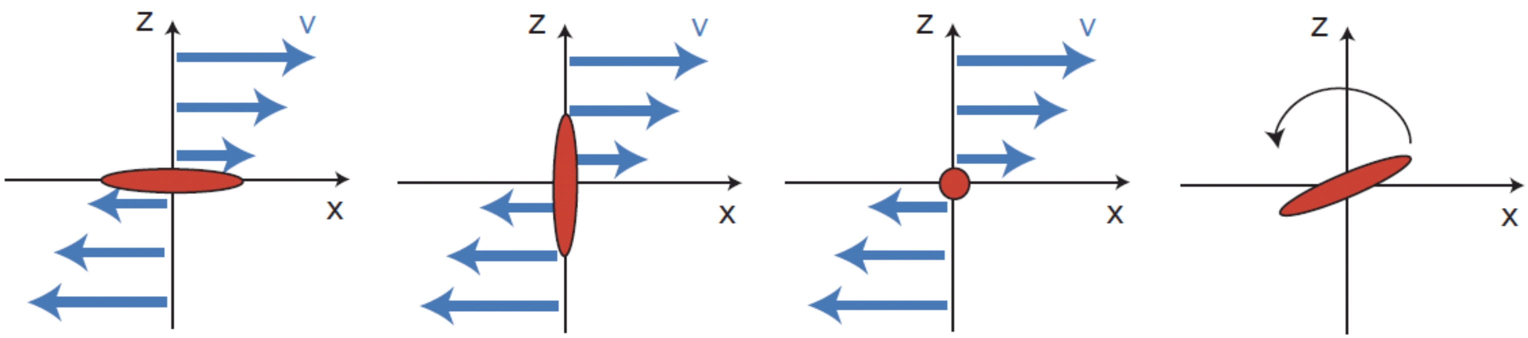
In 5CB (at 26° C):

$$K_1 = 6.2\times 10^{-12}\,\mathrm{N},\ K_2 = 3.9\times 10^{-12}\,\mathrm{N},\ K_3 = 8.2\times 10^{-12}\,\mathrm{N}.$$

Liquid Crystals – stress tensor

- **The stress tensor in a liquid crystal depends of the molecular orientation**

$$\tilde{t}_{ij} = \alpha_1 n_k n_p D_{kp} n_i n_j + \alpha_2 N_i n_j + \alpha_3 N_j n_i + \alpha_4 D_{ij} + \alpha_5 D_{ik} n_k n_j + \alpha_6 D_{jk} n_k n_i$$



(a) $\eta_1 = \frac{1}{2}(\alpha_3 + \alpha_4 + \alpha_6)$, (b) $\eta_2 = \frac{1}{2}(-\alpha_2 + \alpha_4 + \alpha_5)$, (c) $\eta_3 = \frac{1}{2}\alpha_4$, (d) $\gamma_1 = \alpha_3 - \alpha_2$

- this means that rotating the molecules induces a flow

Liquid Crystals as Soft Solids…

- Nematics are almost exclusively used as reconfigurable elastic media

Optical birefringence device (light switching/guiding etc.)

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	switchable	optical contrast
1: isotropic liquid	YES (i.e. EM-phoresis)	POOR (unless dye added)
2: nematic	YES	GOOD
3: elastomer	YES (but slow)	BETTER
4: solid	NO	BEST

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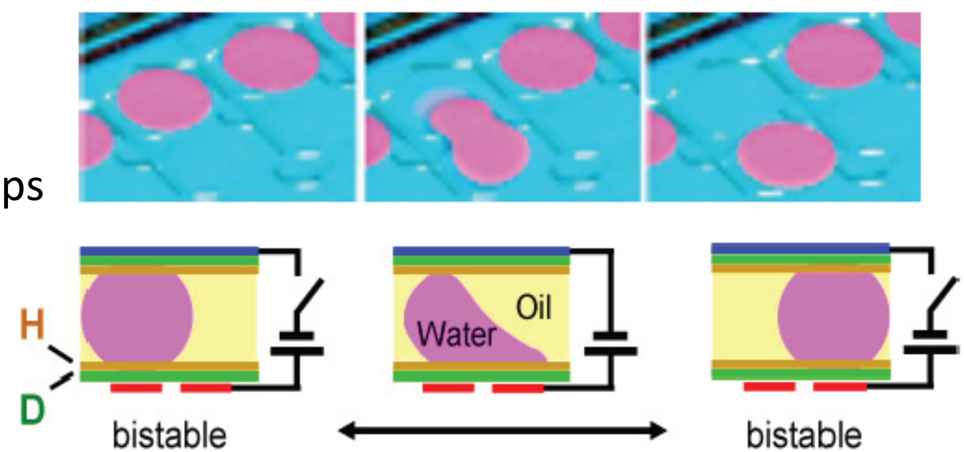
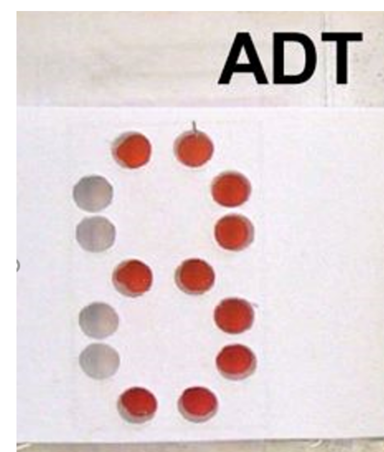
1: isotropic liquid

coloured liquid drops
moved by E-field





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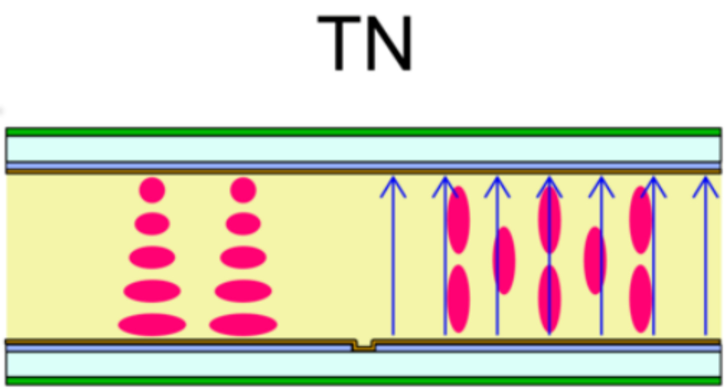
molecular orientation switched by E-field but order parameter is not perfect



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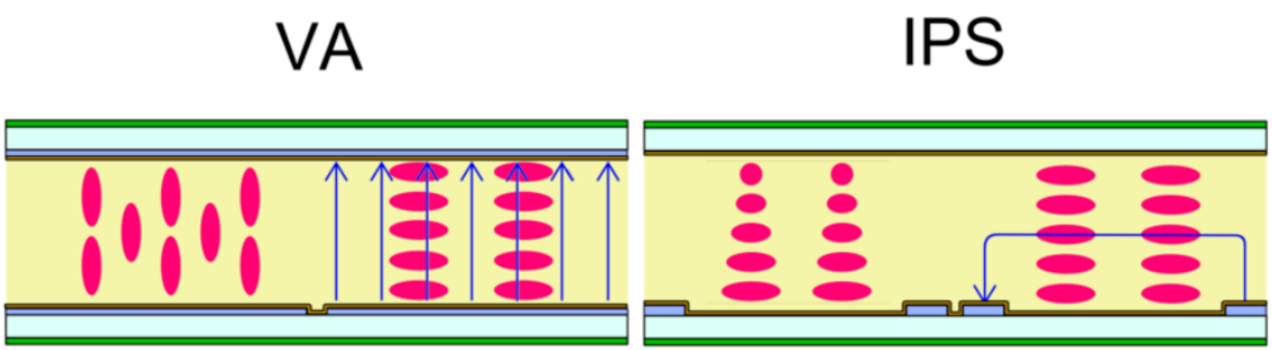

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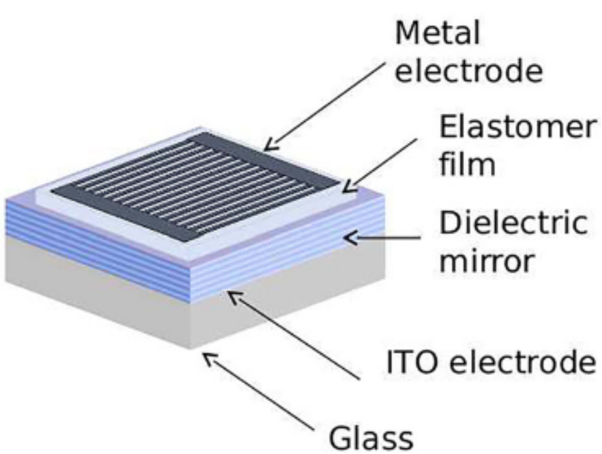
3: elastomer

solid material but optic axis can be switched by E-field or deformation



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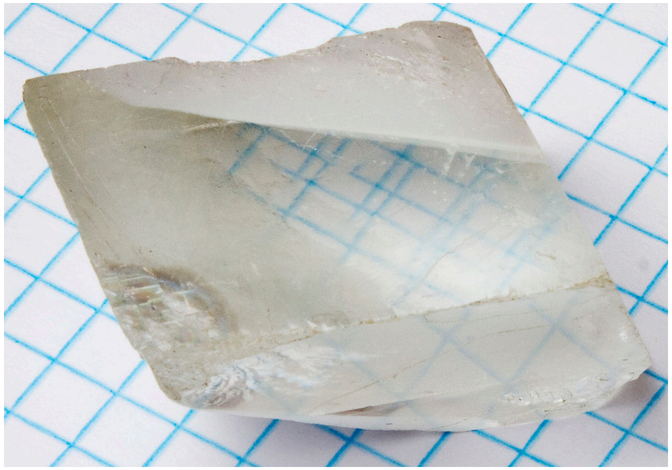
4: solid

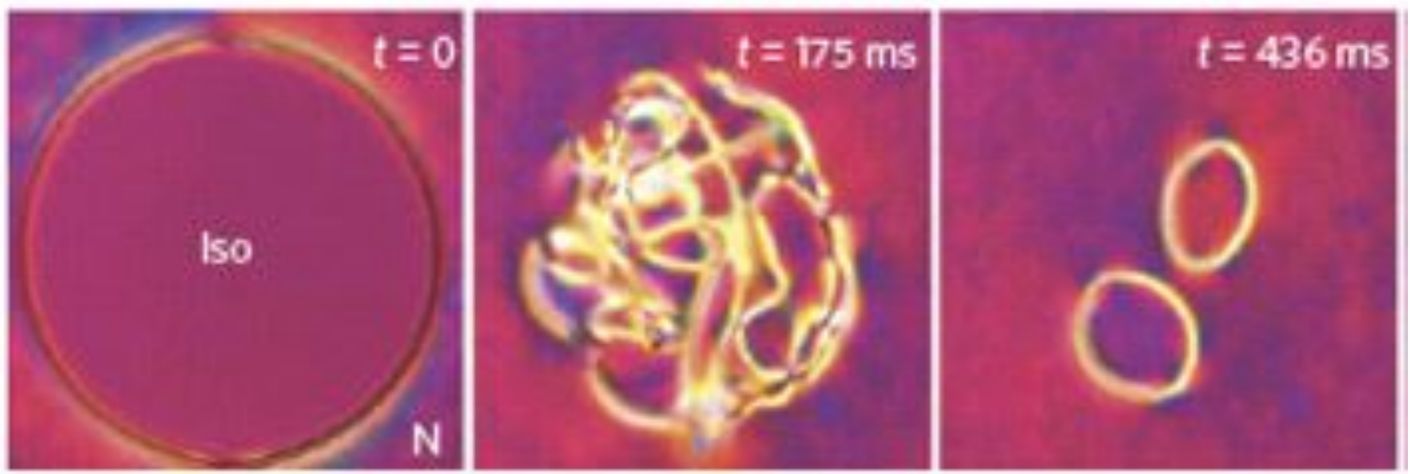
high order parameter means better optical performance



Liquid Crystals as Soft Solids…

- **An additional advantage is that liquid crystals are self-annealing**

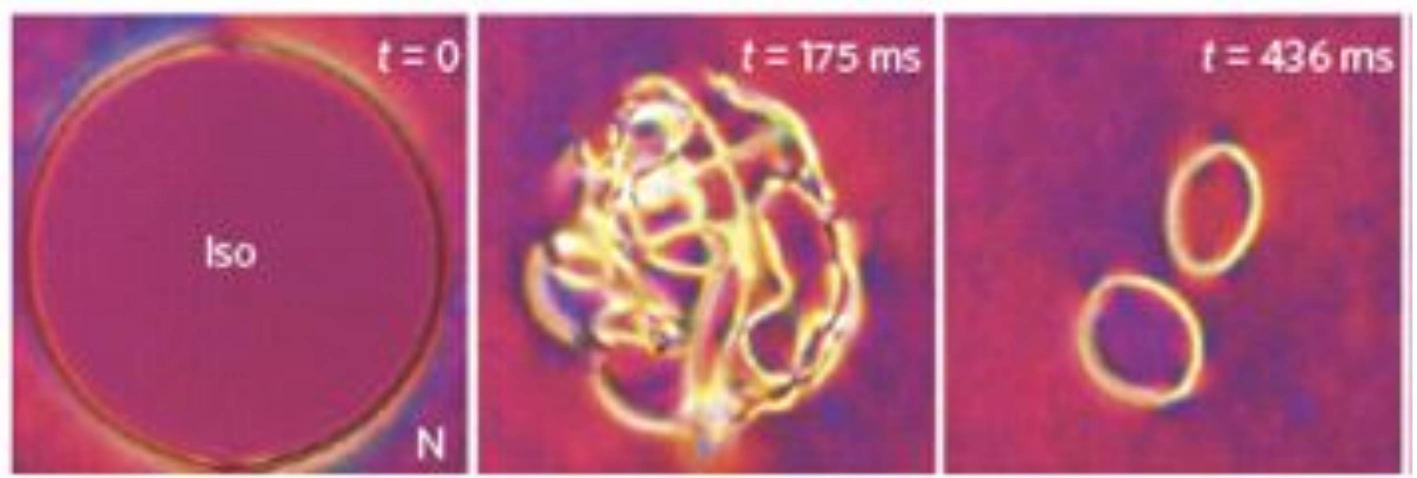
defects that occur in the manufacturing process will anneal out



Liquid Crystals as Soft Solids…

- **An additional advantage is that liquid crystals are self-annealing**

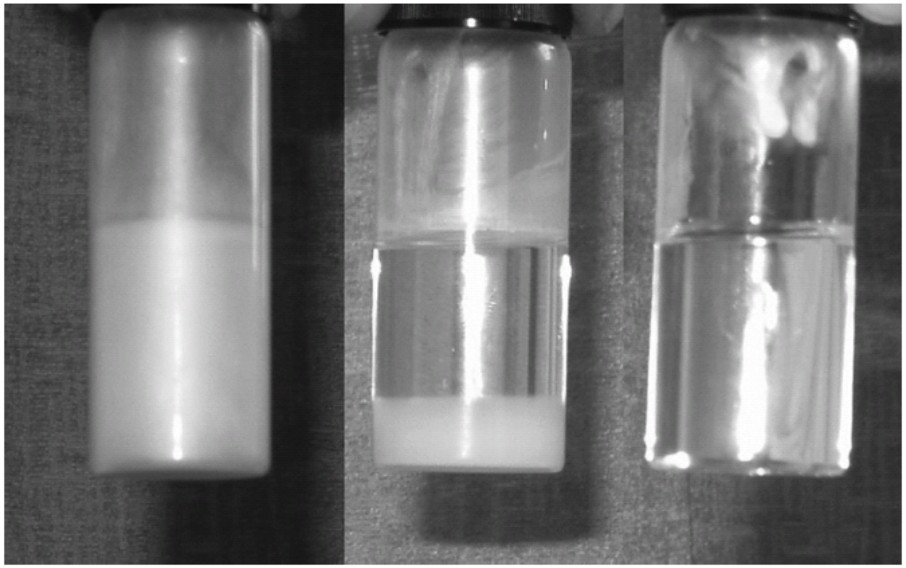
defects that occur in the manufacturing process will anneal out (usually)



In the beginning…there were defects

Reinitzer's original experiments demonstrated a second "melting" point from a scattering liquid to a clear liquid

- **random arrangements of the director lead to scattering**
- **defects can lead to these random alignments**

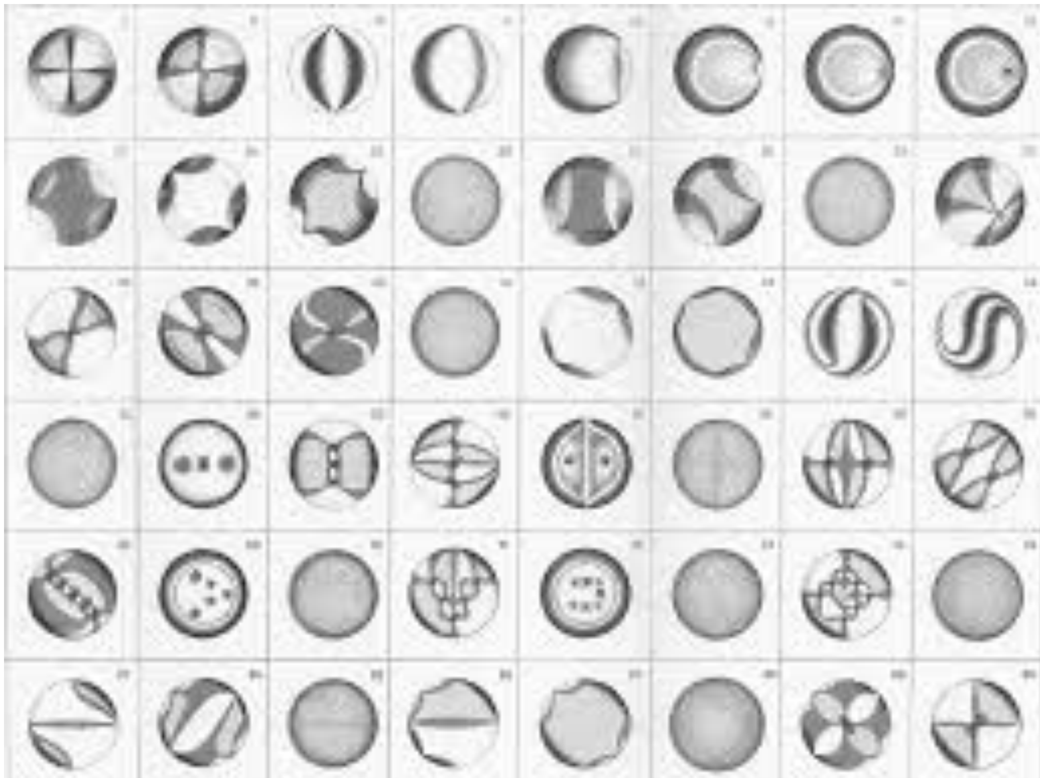


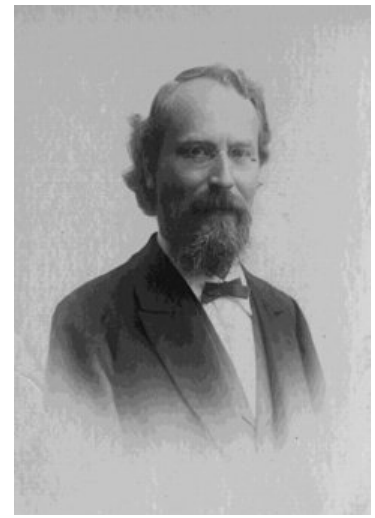
temperature

Freidrich Reinitzer

Identification

- **Reinitzer then sent samples to Otto Lehmann…**





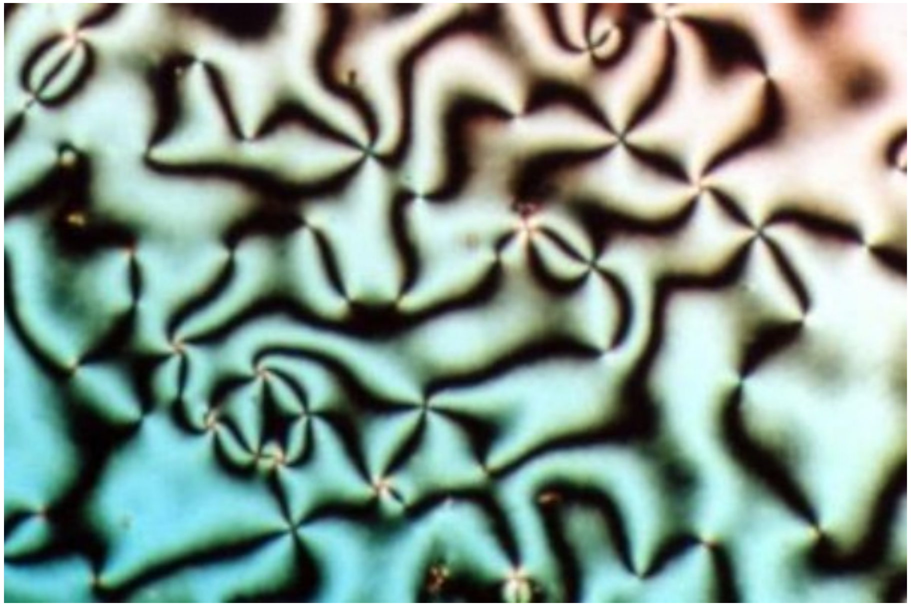
Lehmann's "copulating droplets"

Resembled oil drops except for the 'stains' found as drops merged

The stains or *schliere* led to the term schlieren texture

Identification

- Defects played a significant role in the development of liquid crystal science
- **these materials were classified through their defects**



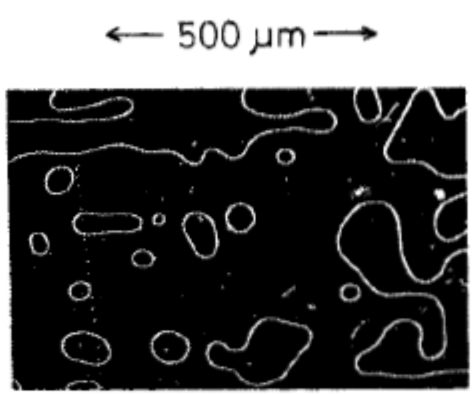
Banishment

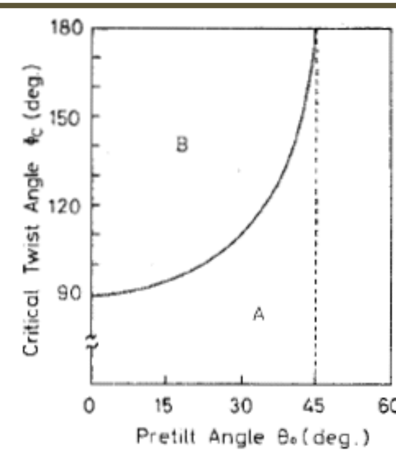
- After intense interest in textures and defects in the early years, the invention of the liquid crystal displays meant that defects were suddenly unwanted.

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. ED-24, NO. 7, JULY, 1977 811

Control and Elimination of Disclinations in Twisted Nematic Liquid-Crystal Displays

AKIRA MIYAJI, MORIE YAMAGUCHI, AKIRA TODA, HITOSHI MADA, AND SHUNSUKE KOBAYASHI, MEMBER, IEEE





Enlightenment

- **The development of a continuum theory of liquid crystals that could also model disclinations was crucial**

Research article

Short Range Order Effects in the Isotropic Phase of Nematics and Cholesterics

P. G. De Gennes

Page 193-214 | Received 22 Sep 1970, Published online: 21 Mar 2007

Photo: L. Falk

The Q tensor is based on the second moment of molecular orientations

$$\mathbf{Q} = S_1\,(\mathbf{n}\otimes\mathbf{n}) + S_2\,(\mathbf{m}\otimes\mathbf{m}) - \frac{1}{3}(S_1+S_2)\mathbf{I}$$

- **People looked again at defects…**

Enlightenment

University of Strathclyde Glasgow

- **For the first time, the core of defects could be investigated…**

VOLUME 59, NUMBER 22 PHYSICAL REVIEW LETTERS 30 NOVEMBER 1987

Defect Core Structure in Nematic Liquid Crystals

N. Schopohl and T. J. Sluckin[a]

Institut Laue-Langevin, 38042 Grenoble Cédex, France

(Received 6 July 1987)

The core structure of half-integer wedge disclinations in nematic liquid crystals has been investigated within the Landau–de Gennes theory, by solution of the appropriate Euler-Lagrange equations. Close to the nematic-isotropic transition the energy density exhibits a domain-wall-like structure around the core which disappears at low temperatures. The inner core does not consist of isotropic fluid, and the core is heavily biaxial at all temperatures.

$$F_{\text{bulk}} = A\,\mathrm{tr}\mathbf{Q}^2 + \tfrac{2}{3}B\,\mathrm{Tr}\mathbf{Q}^3 + \tfrac{1}{2}C\,\mathrm{Tr}\mathbf{Q}^4,$$

$$F_{\text{kin}} = L_1 \frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ij}}{\partial x_k} + L_2 \frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k} + L_3 \frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ik}}{\partial x_j},$$

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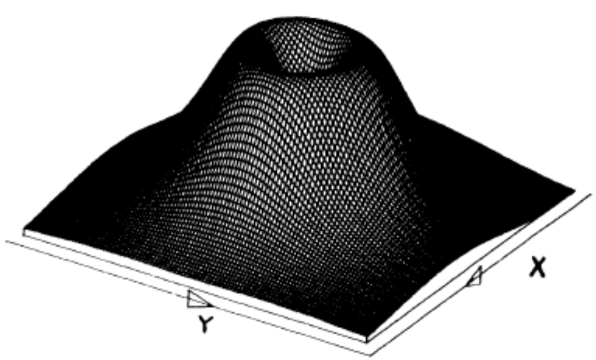
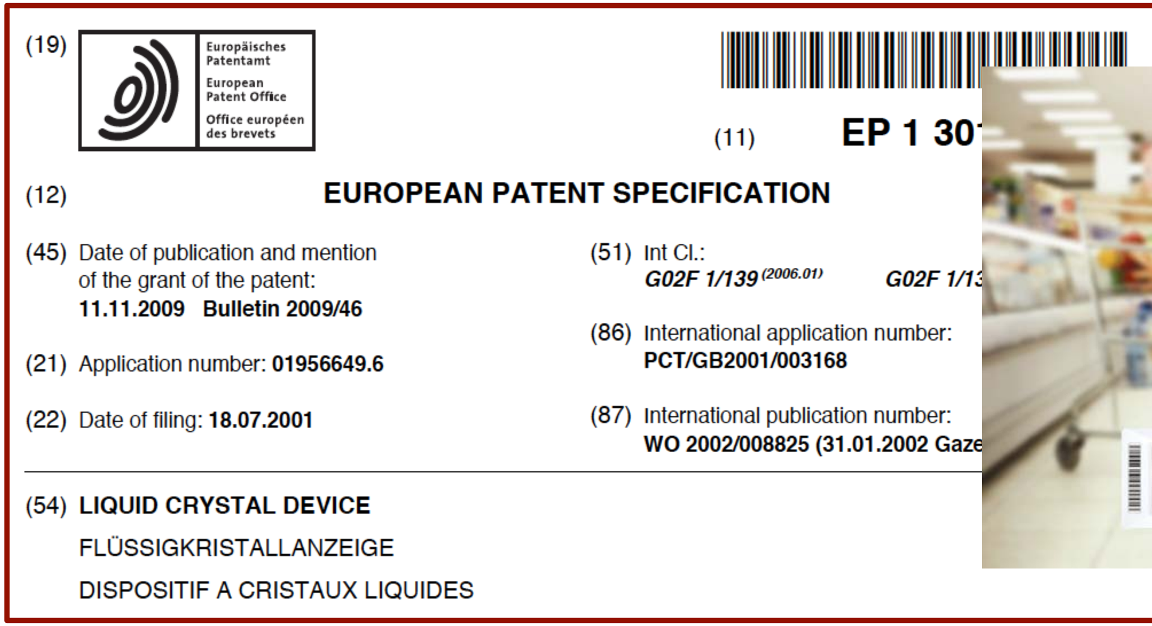


FIG. 2. Energy surface $\xi(x,y)$ in the region $-12 < x,y < 12$ for the same defect as in Fig. 1, showing the crater structure.

In conclusion we have used the Landau–de Gennes formalism to make an exact calculation of the structure of a wedge disclination in a nematic liquid crystal. The core is always biaxial, sometimes contains structures which resemble an isotropic-nematic interface, but never contains a core of isotropic fluid.

Renaissance

- Zenithal Bistable Display (DERA: WO 2002/008825)



(19) Europäisches Patentamt
European Patent Office
Office européen des brevets

(11) EP 1 30

(12) EUROPEAN PATENT SPECIFICATION

(45) Date of publication and mention of the grant of the patent:
11.11.2009 Bulletin 2009/46

(21) Application number: **01956649.6**

(22) Date of filing: **18.07.2001**

(51) Int Cl.:
G02F 1/139 (2006.01) *G02F 1/13*

(86) International application number:
PCT/GB2001/003168

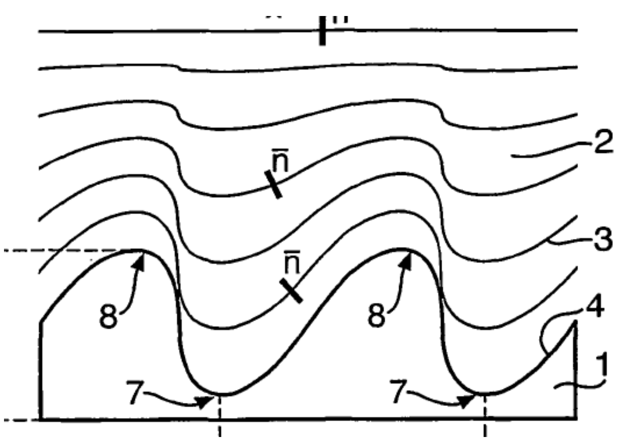
(87) International publication number:
WO 2002/008825 (31.01.2002 Gaze

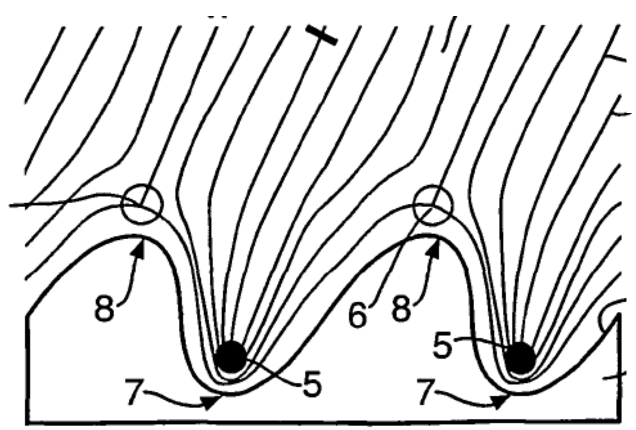
(54) **LIQUID CRYSTAL DEVICE**

FLÜSSIGKRISTALLANZEIGE

DISPOSITIF A CRISTAUX LIQUIDES

University of Strathclyde Glasgow

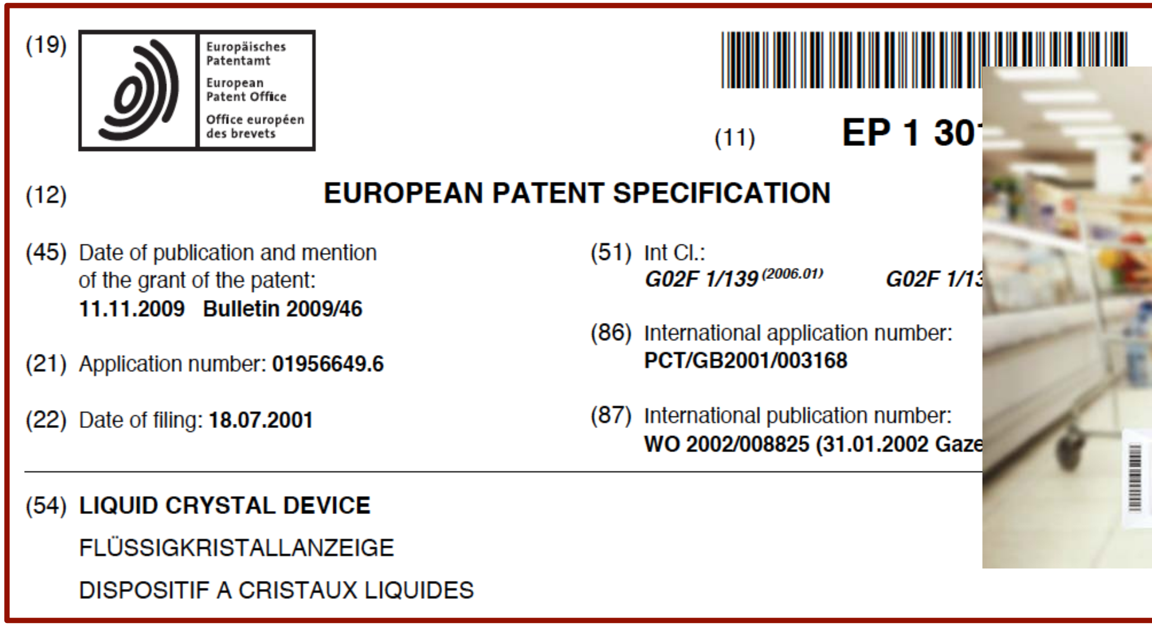




Displaydata
DYNAMIC. DIGITAL. DELIVERS.

Renaissance

- **Zenithal Bistable Display (DERA: WO 2002/008825)**



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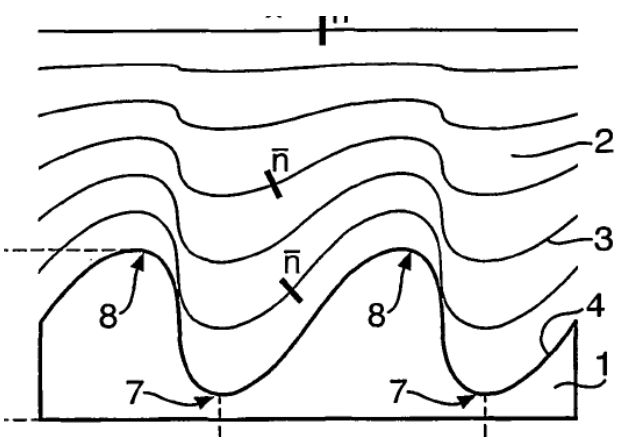
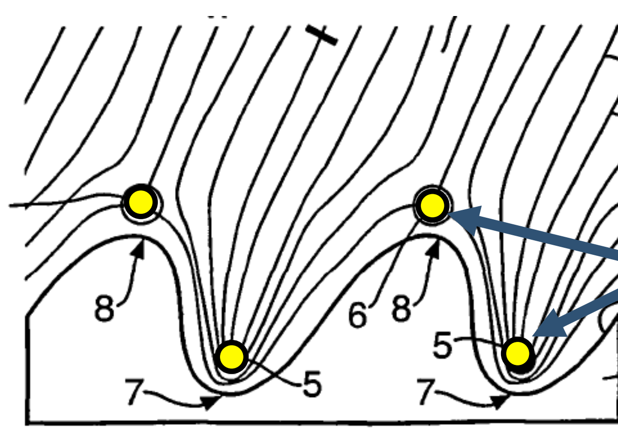




stabilised defects

DYNAMIC. DIGITAL. DELIVERS.

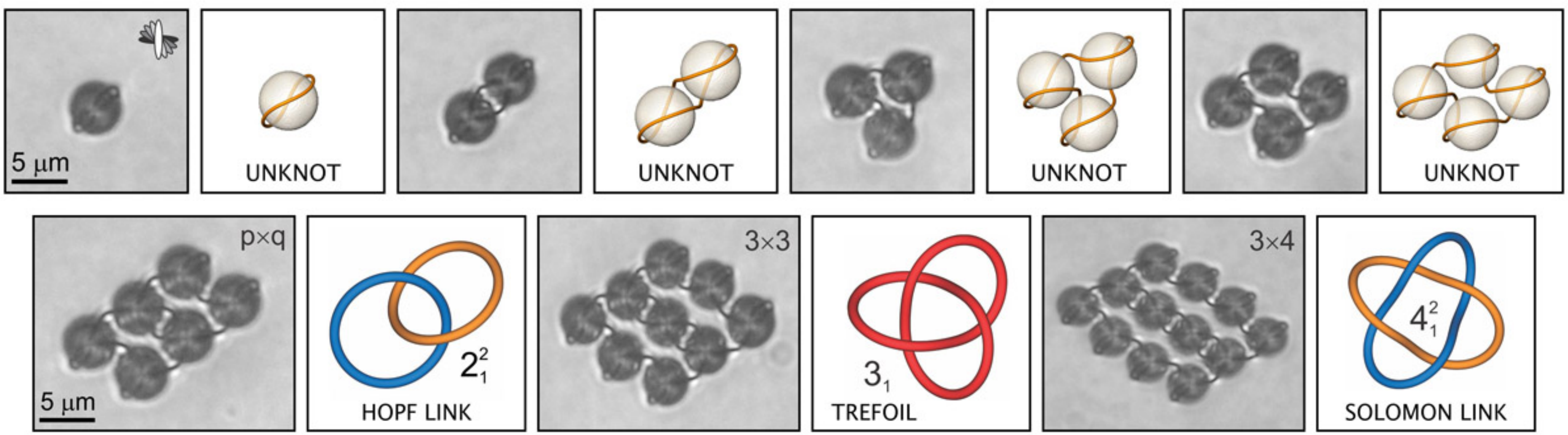
Renaissance

- **Manipulation of defect entanglements**

Reconfigurable Knots and Links in Chiral Nematic Colloids

Uroš Tkalec,[1]*† Miha Ravnik,[2,3] Simon Čopar,[3] Slobodan Žumer,[1,3] Igor Muševič[1,3]*

Tying knots and linking microscopic loops of polymers, macromolecules, or defect lines in complex materials is a challenging task for material scientists. We demonstrate the knotting of microscopic topological defect lines in chiral nematic liquid-crystal colloids into knots and links of arbitrary complexity by using laser tweezers as a micromanipulation tool. All knots and links with up to six crossings, including the Hopf link, the Star of David, and the Borromean rings, are demonstrated, stabilizing colloidal particles into an unusual soft matter. The knots in chiral nematic colloids are classified by the quantized self-linking number, a direct measure of the geometric, or Berry's, phase. Forming arbitrary microscopic knots and links in chiral nematic colloids is a demonstration of how relevant the topology can be for the material engineering of soft matter.



Renaissance

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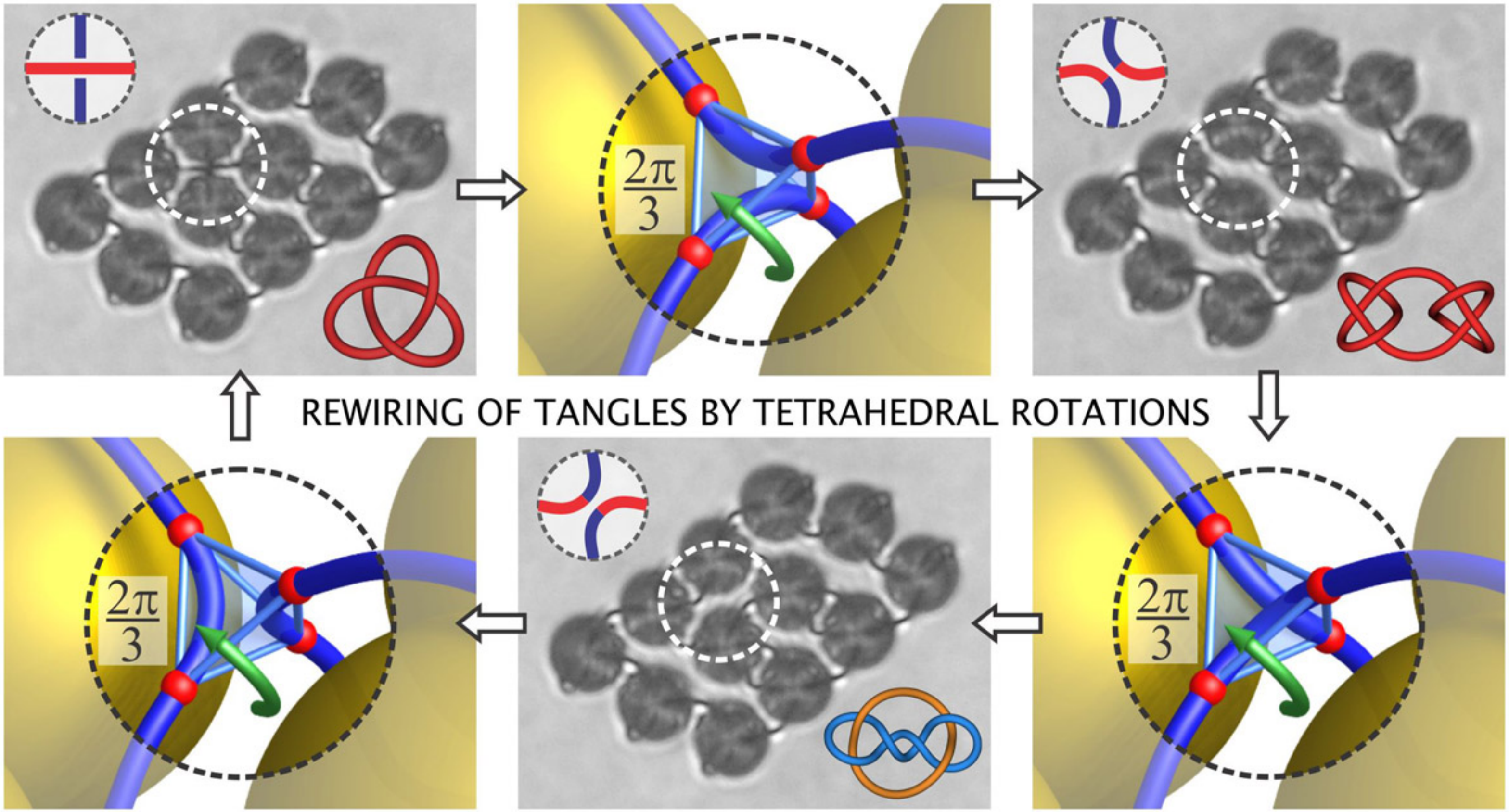

Renaissance

- **Manipulation of defect entanglements**

nature physics

LETTERS

PUBLISHED ONLINE: 22 DECEMBER 2014 | DOI: 10.1038/NPHYS3194

Light-controlled topological charge in a nematic liquid crystal

Maryam Nikkhou[1], Miha Škarabot[1], Simon Čopar[1,2], Miha Ravnik[2], Slobodan Žumer[1,2] and Igor Muševič[1,2]*

Renaissance

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nature physics

LETTERS

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liquid crystal

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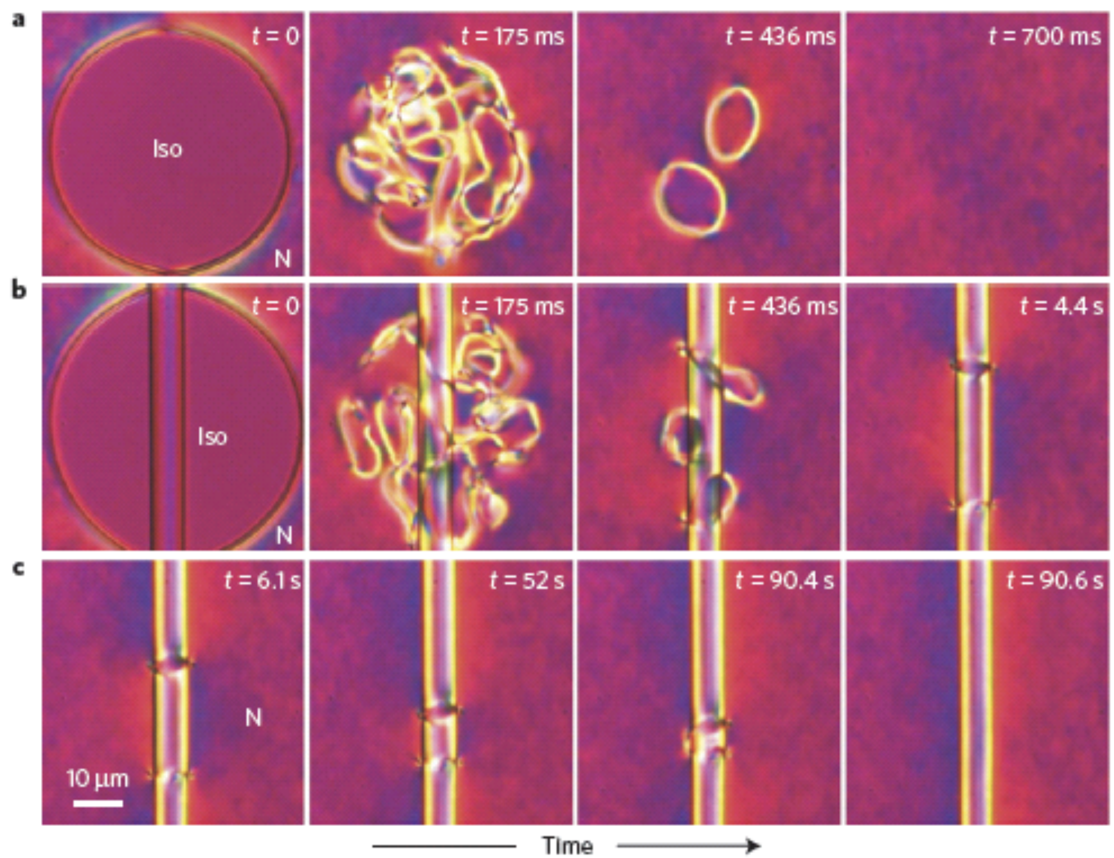


The future

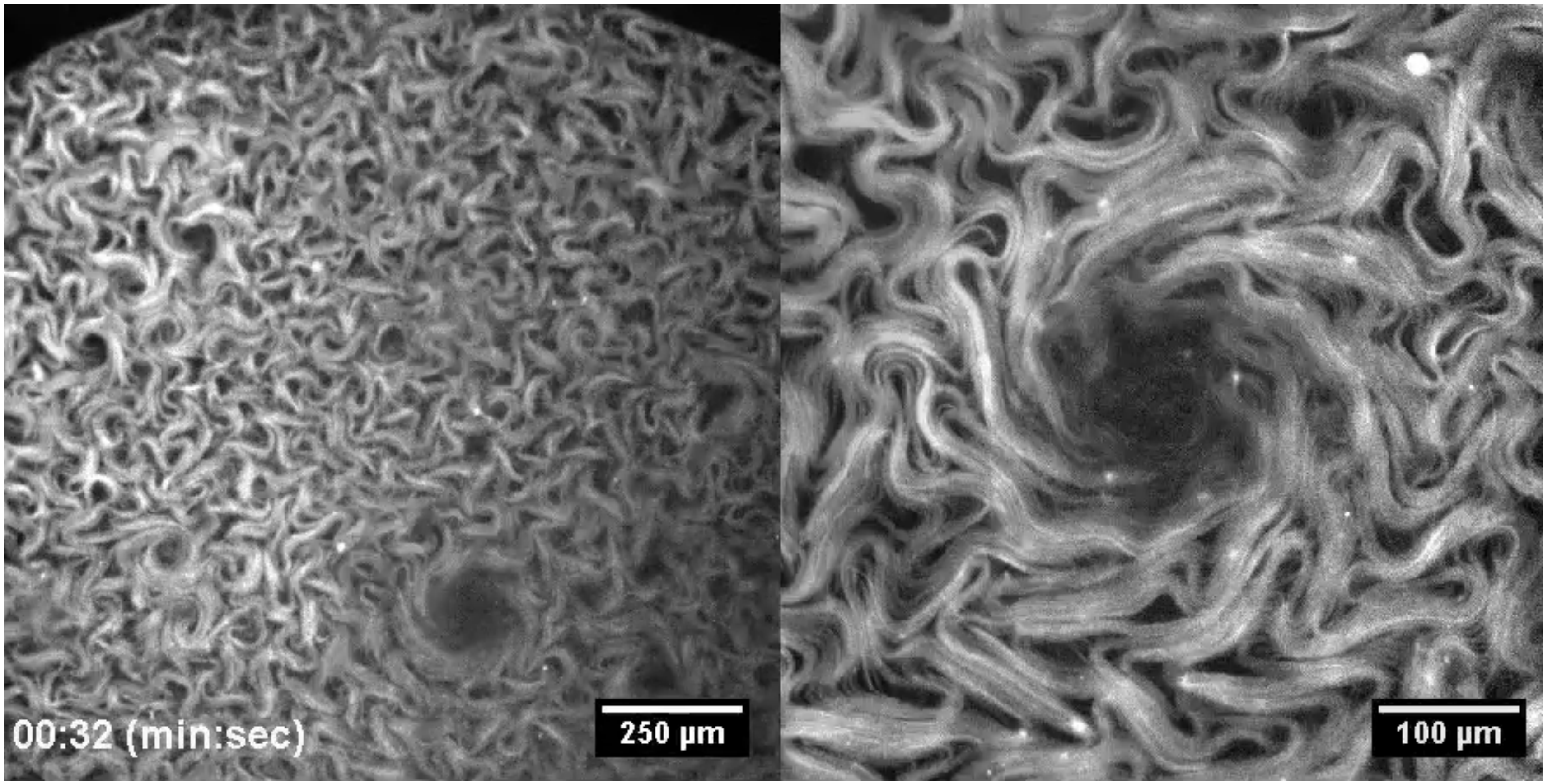
PNAS | May 17, 2016 | vol. 113 | no. 20

Control of active liquid crystals with a magnetic field

Pau Guillamat[a,b], Jordi Ignés-Mullol[a,b], and Francesc Sagués[a,b,1]

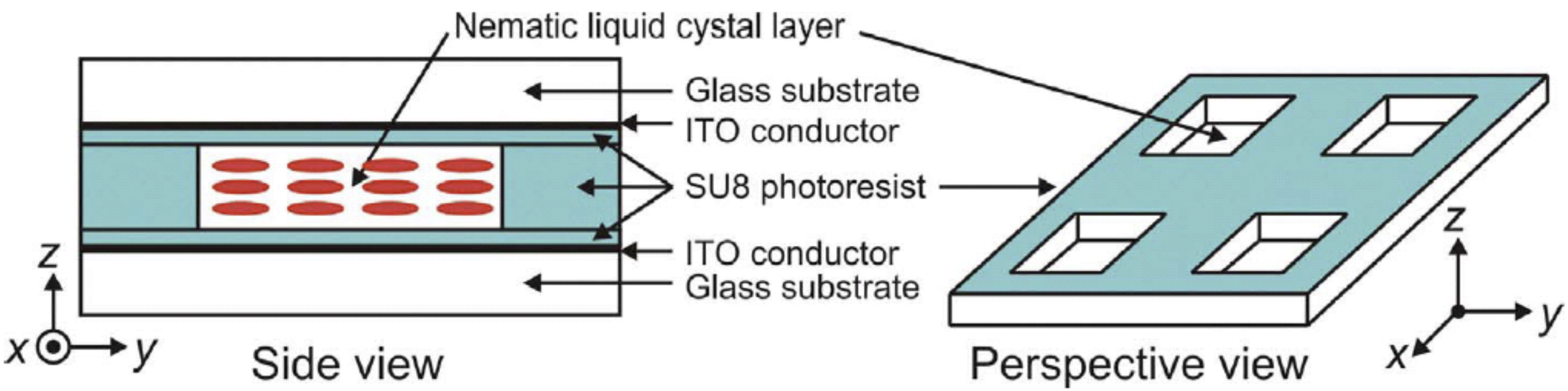
[a]Departament de Química Física, Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain; and [b]Institute of Nanoscience and Nanotechnology, Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain

Edited by Nicholas L. Abbott, University of Wisconsin, Madison, WI, and accepted by the Editorial Board April 4, 2016 (received for review January 8, 2016)



Confined nematics: shallow cavities

- **Nematic within a shallow square well:**

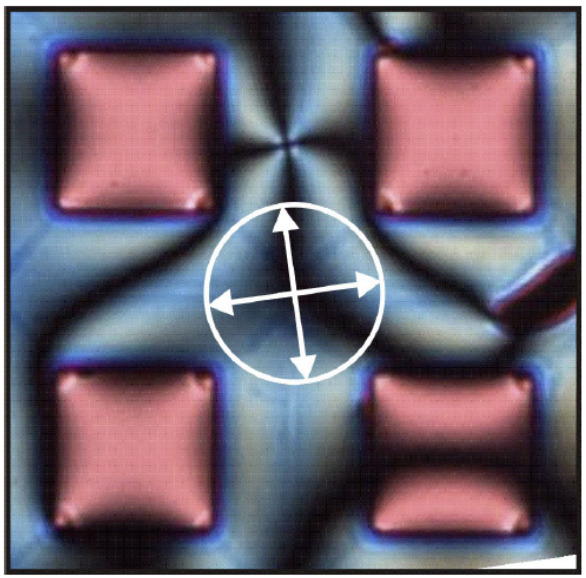


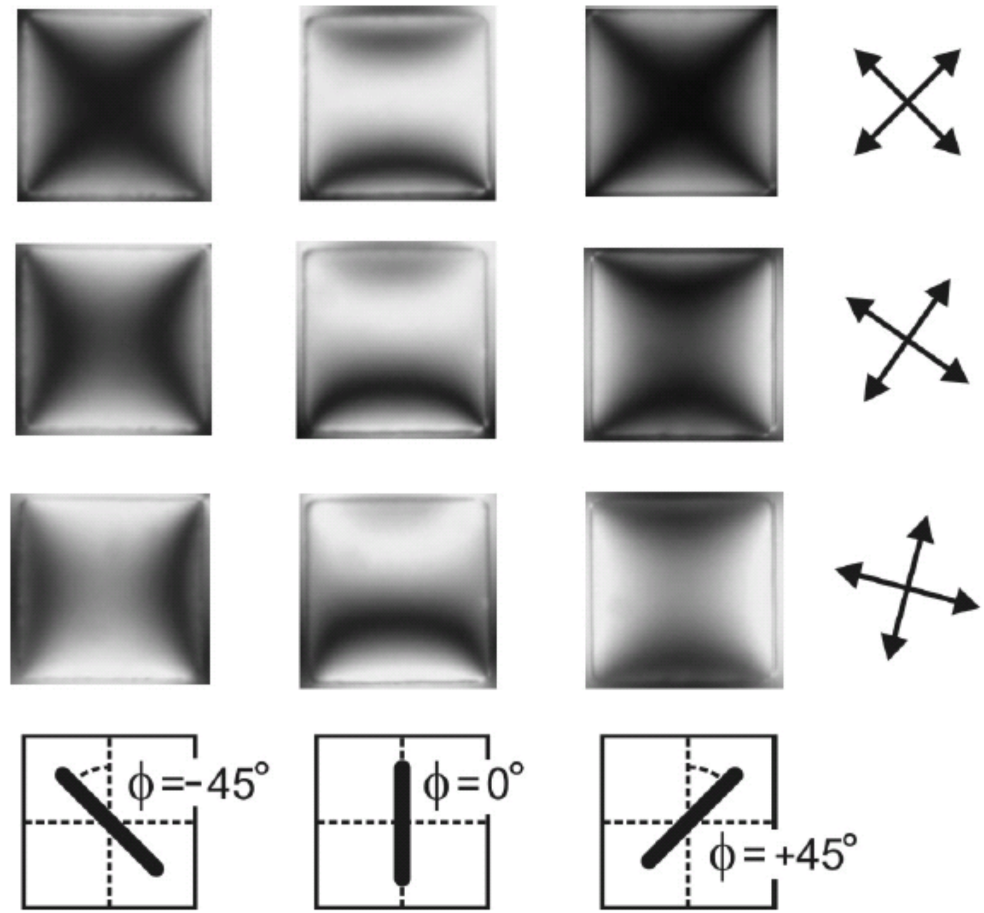
- square wells formed by photolithography
- well depth 15 μm, wells of side 20 - 100 μm
- filled with nematic material E7 whilst upper SU8 layer is "wet"

C. Tsakonas, A. Davidson, C.V. Brown, N. J. Mottram, *Appl. Phys. Lett.* **90**, 111913 (2007)

Confined nematics: shallow cavities

- **Nematic within a square cavity: experiments**





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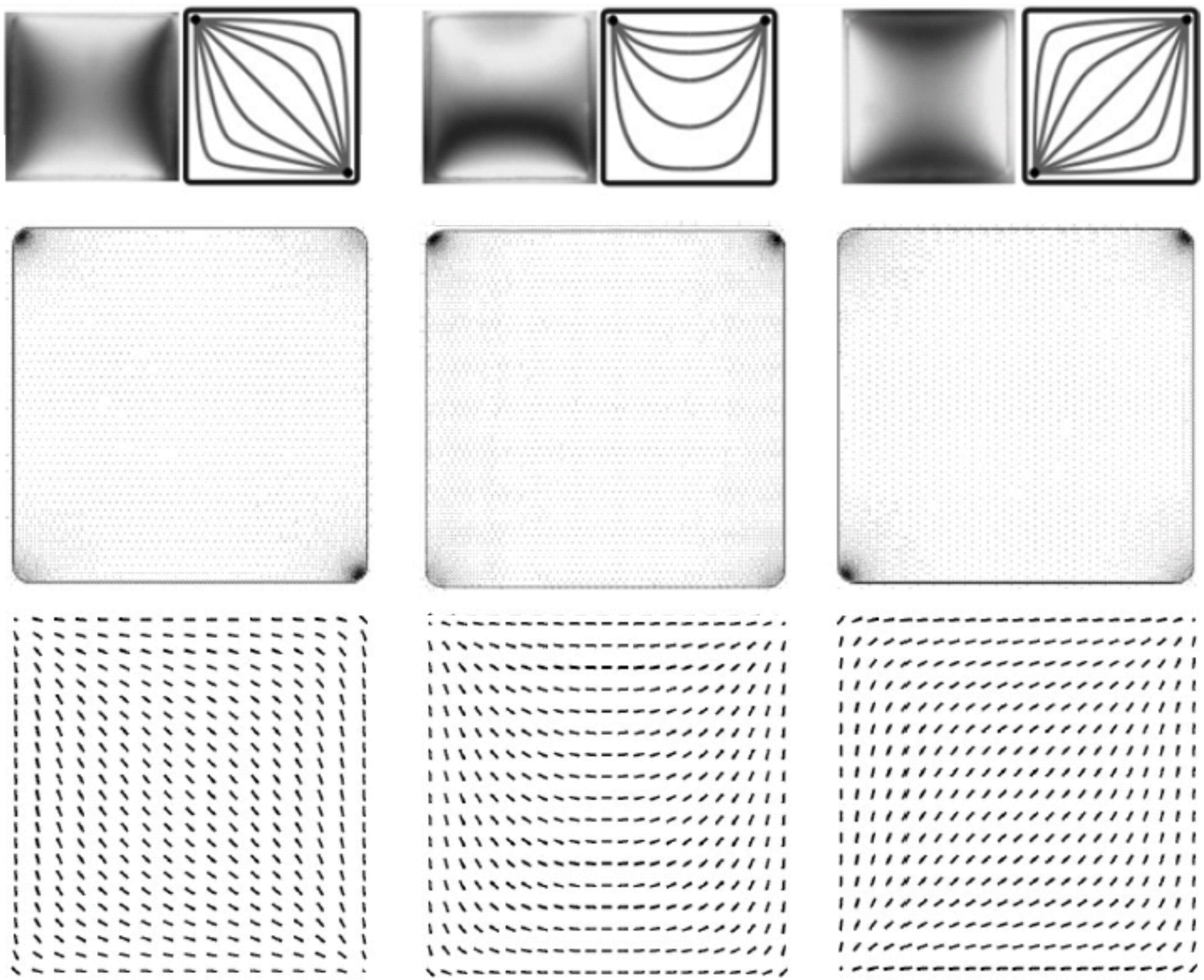
G.G. Wells and C.V. Brown, *Appl. Phys. Lett.* **91**, 223506 (2007)

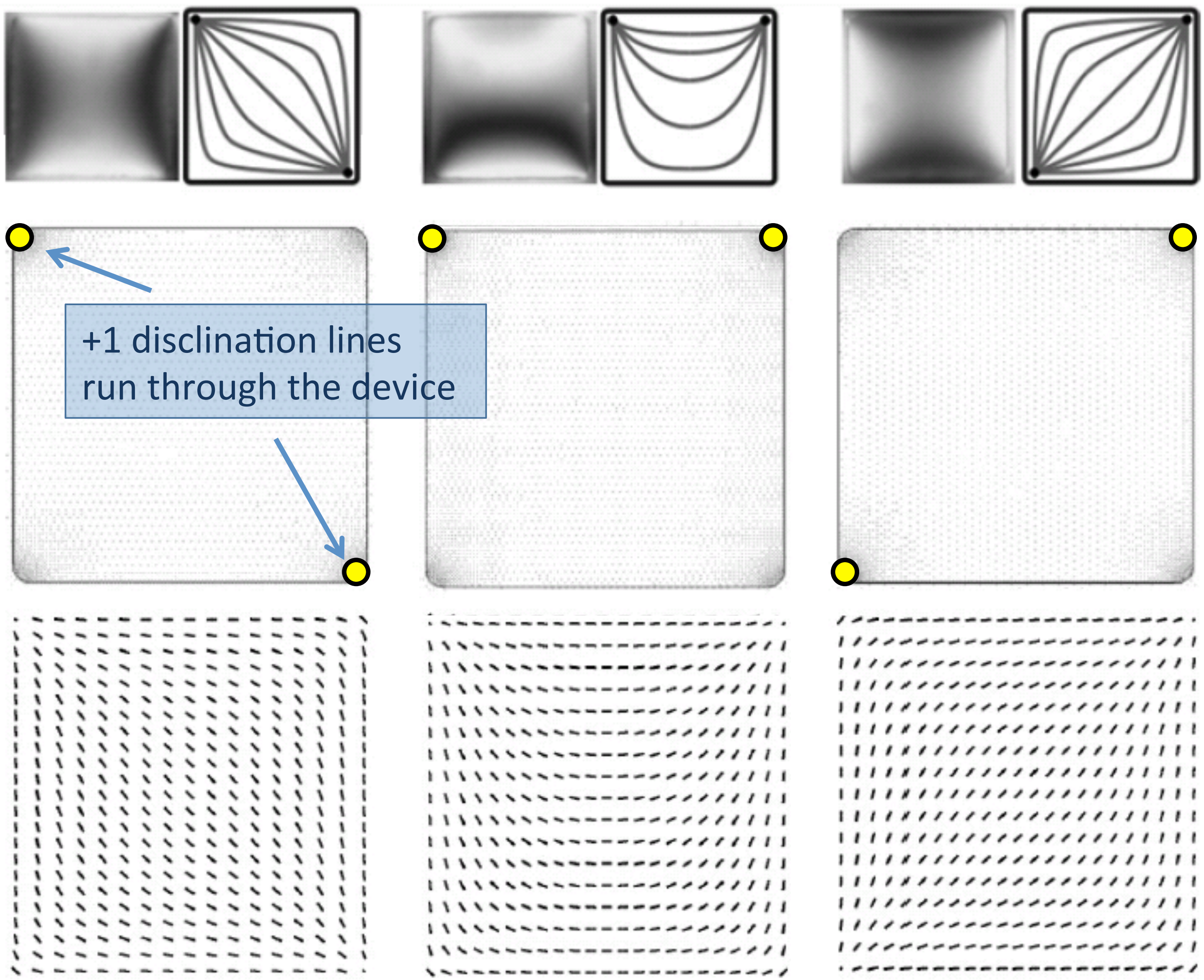
Confined nematics: shallow cavities



order parameter model (largest eigenvalue)

director model (eigenvector of largest eigenvalue)

Confined nematics: shallow cavities

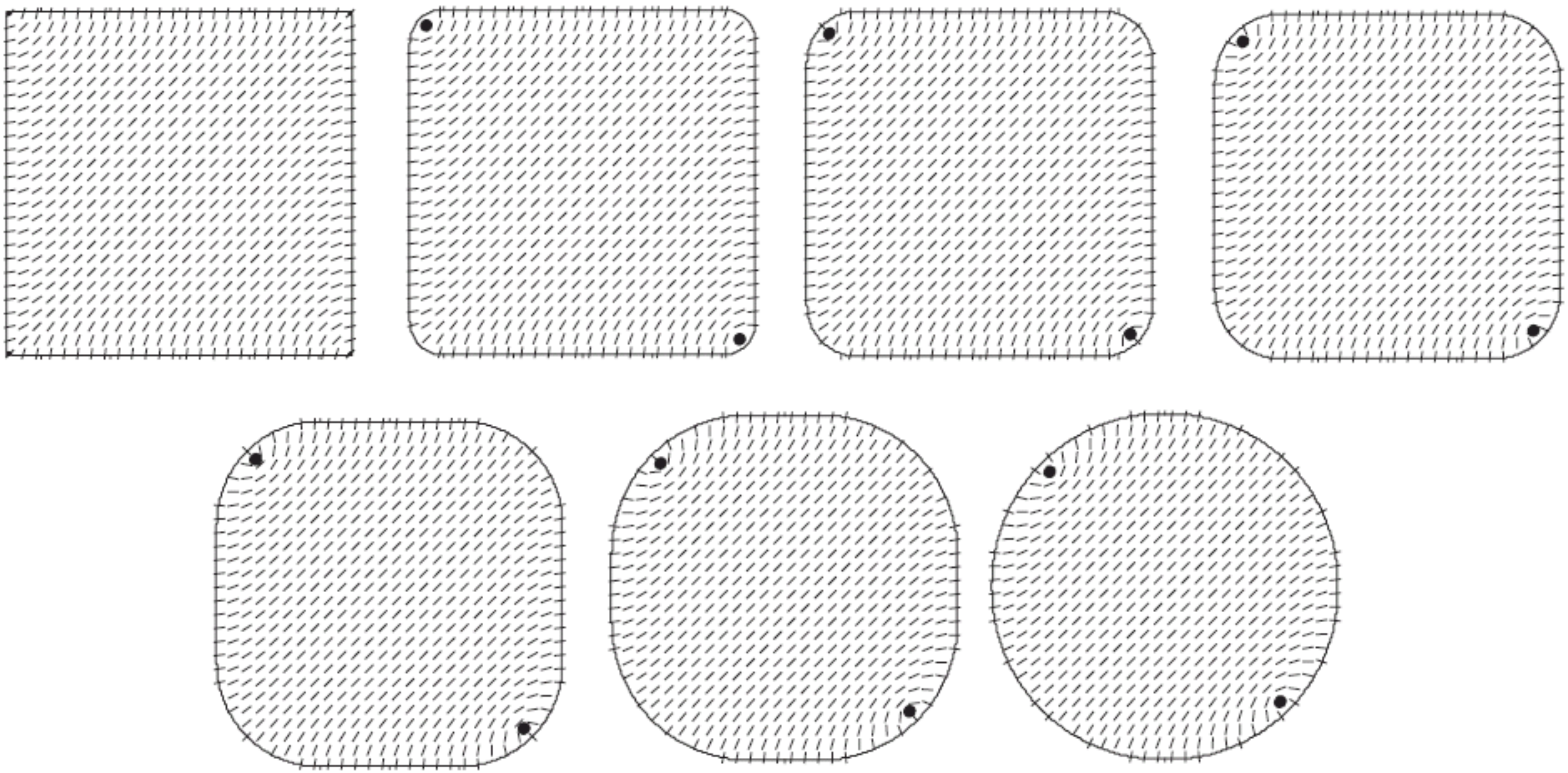


order parameter model (largest eigenvalue)

director model (eigenvector of largest eigenvalue)

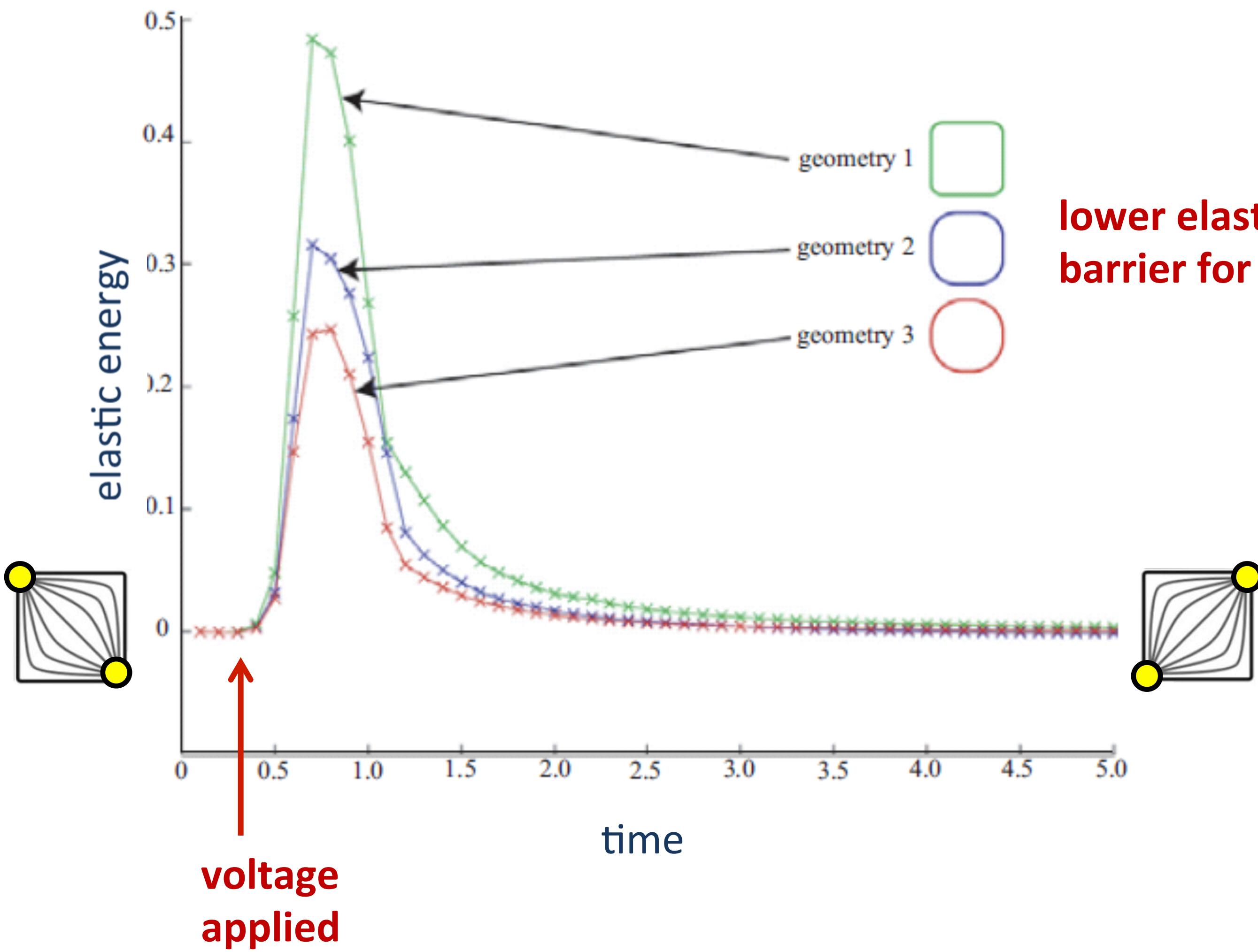
Confined nematics: shallow cavities

- **Nematic within a square(ish) cavity:**
- rounding the corners brings two disclinations into the bulk
- …and two disclinations move out of the region



Confined nematics: corners stabilise defects

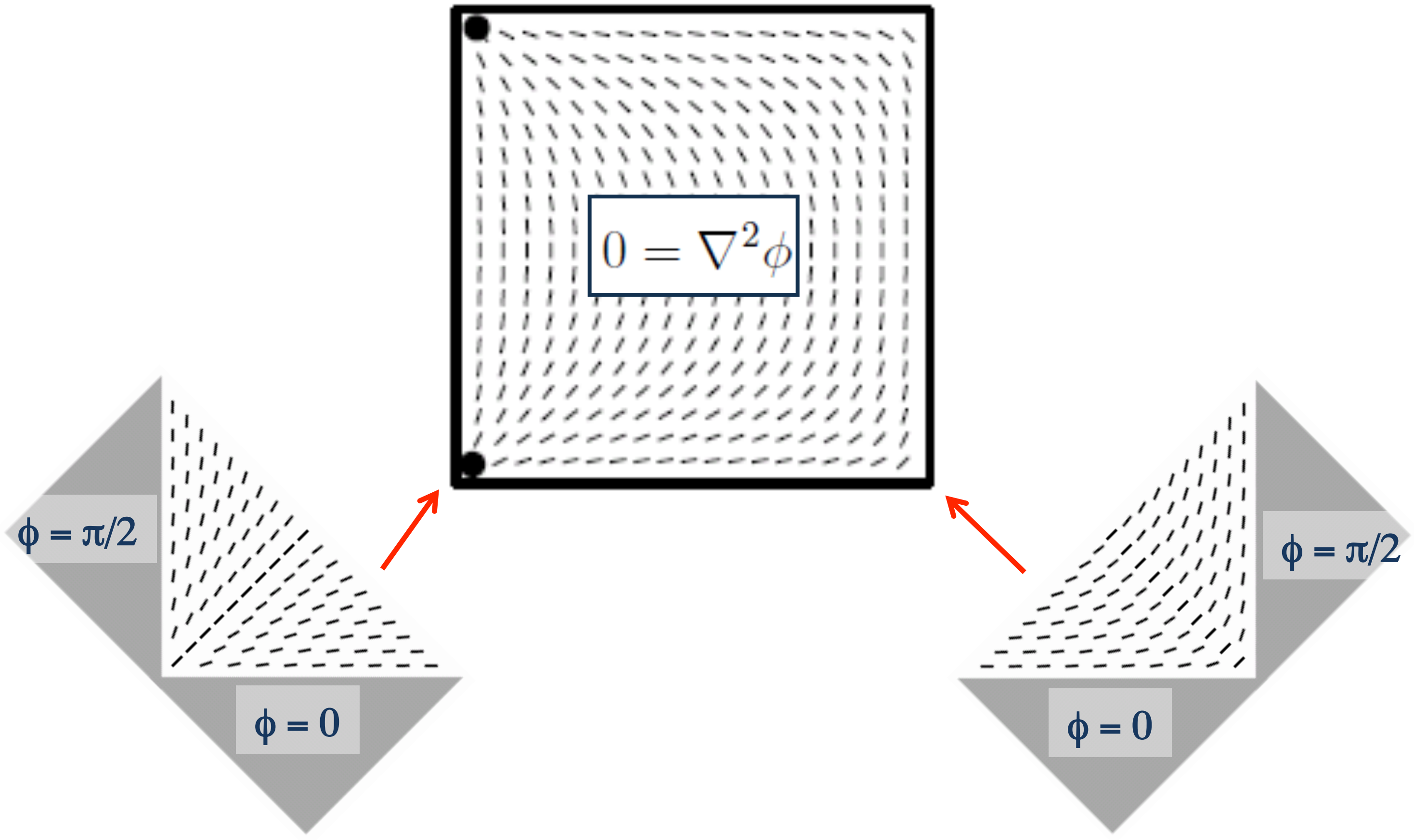
- **Nematic within a square(ish) cavity: switching between states**
- the curvature of the corner determines the stability of the states



lower elastic energy barrier for round corners

Director profile in corners

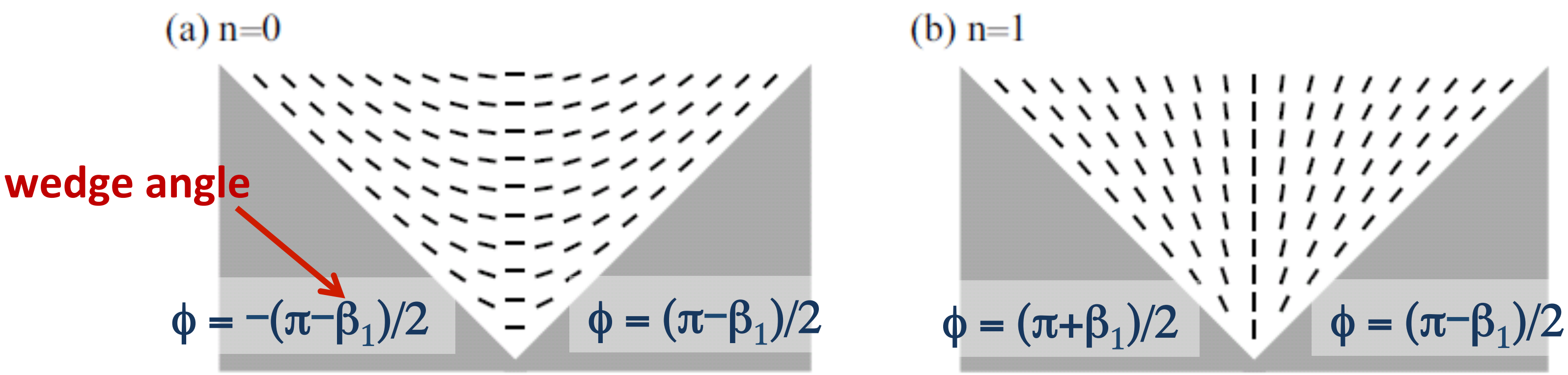
- Nematic within a **square cavity**:



Director profile in corners

- **Nematic within a triangular cavity:**

- for infinite planar anchoring we get solutions like…



- where **n measures the rotation of the director from one wall to the other**.
- the elastic energy is then

$$F_e = \frac{KL((1-n)\pi - \beta_1)^2}{2\beta_1} \ln\left(\frac{R}{\epsilon}\right)$$

Director profile in corners

- **Nematic within a triangular cavity:**

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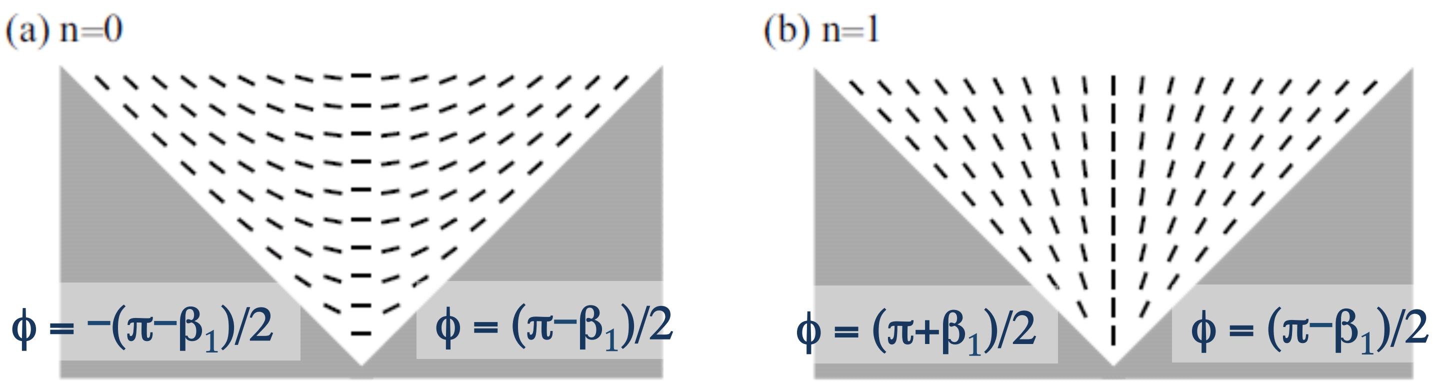


- where **n measures the rotation of the director from one wall to the other**.
- the elastic energy is then

$$F_e = \frac{KL((1-n)\pi - \beta_1)^2}{2\beta_1}\ln\left(\frac{R}{\epsilon}\right)$$

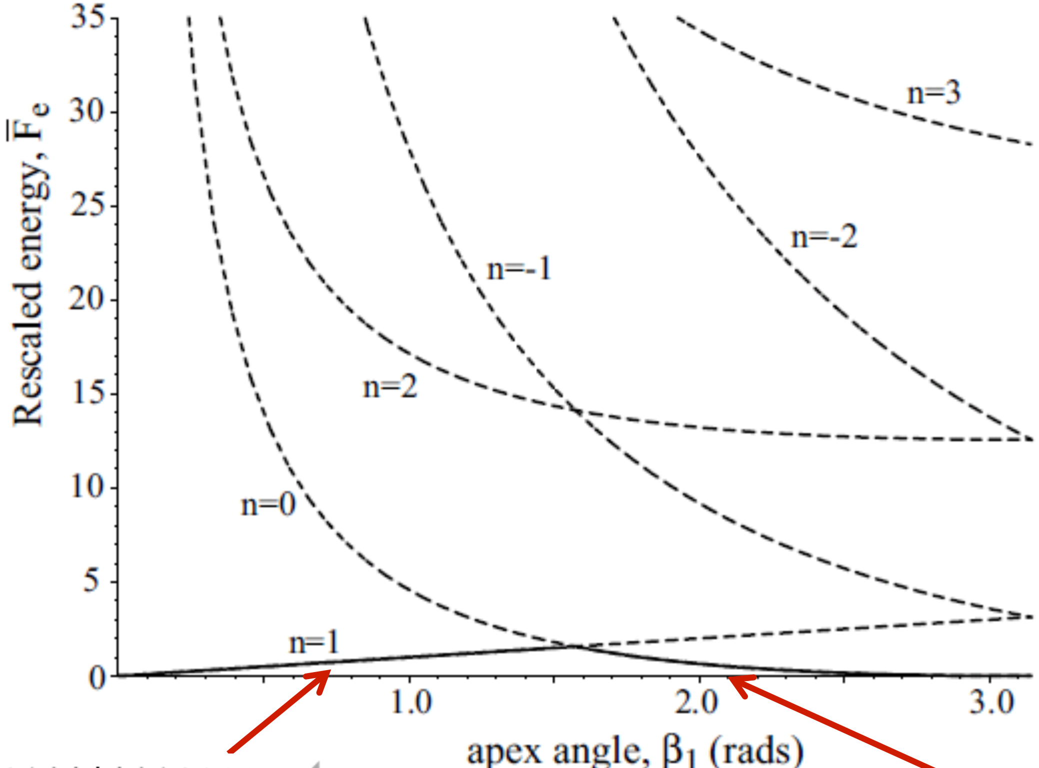
region size

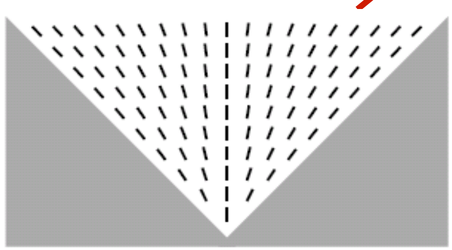
"defect core" size

wedge angle

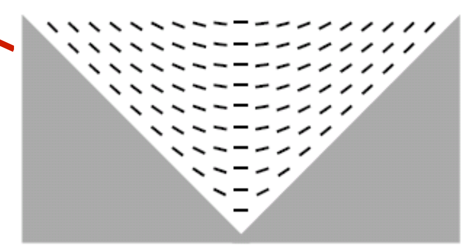
Director profile in corners: energy

- **Nematic within a triangular cavity:**



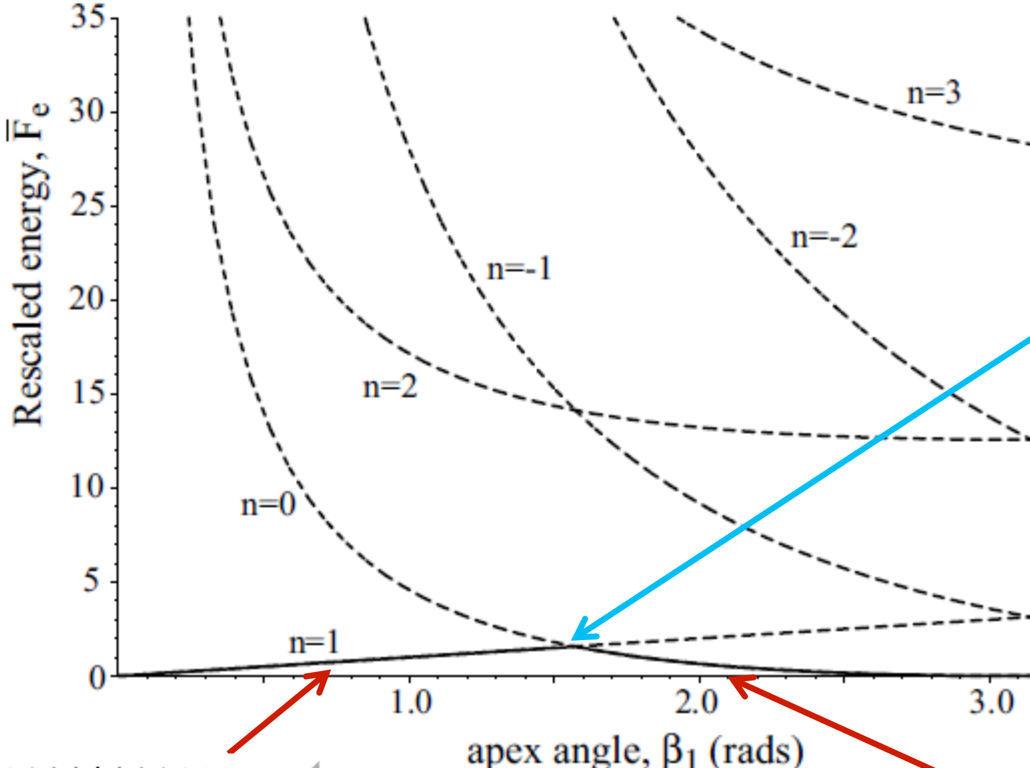


lowest energy solutions

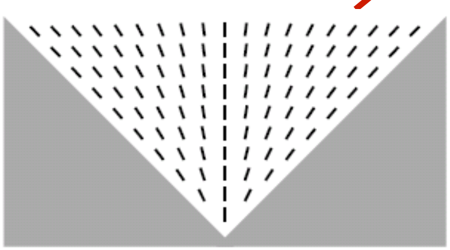


Director profile in corners: energy

- Nematic within a **triangular cavity**:



energy barrier



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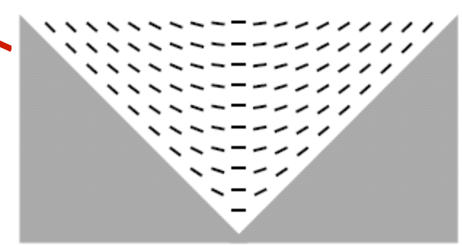
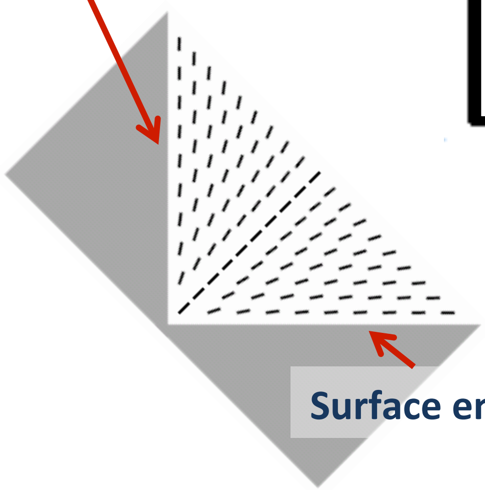


Director profile in corners: weak anchoring

- Consider the director profile in a corner with Rapini-Papoular anchoring

$$0 = \nabla^2 \phi$$

Surface energy = $\cos^2(\phi)$

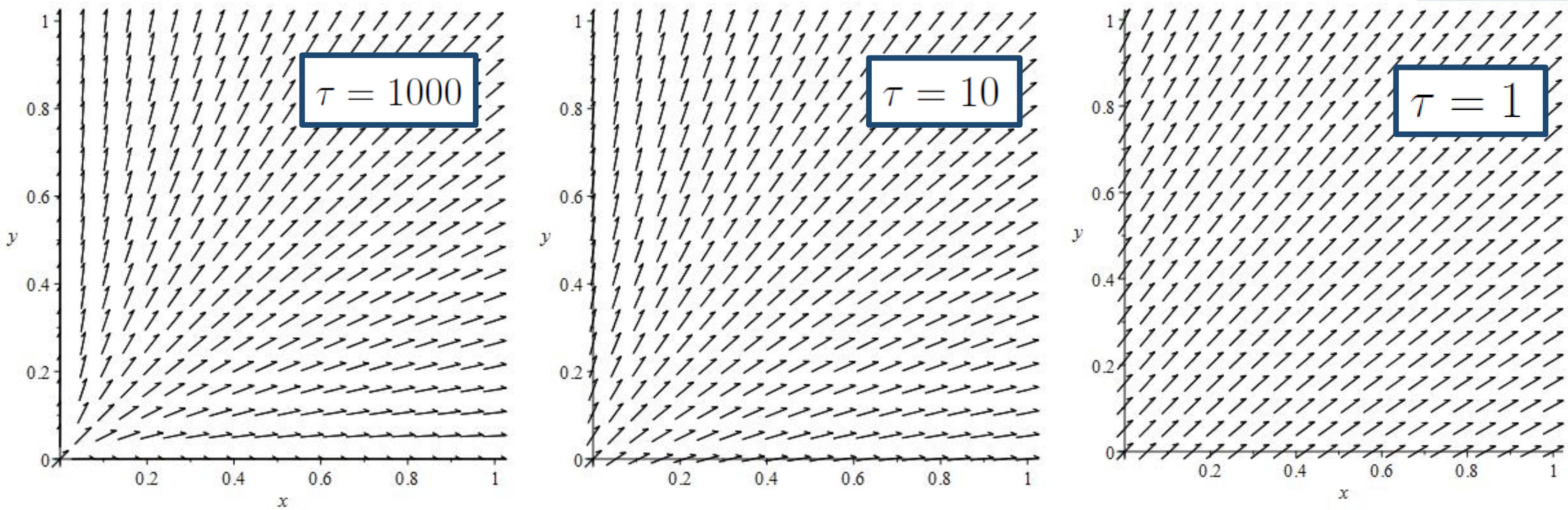


Surface energy = $\sin^2(\phi)$

In each corner our director angle is governed by a balance of elastic and surface energies

Director profile in corners: weak anchoring

- **Director structure near to a corner**

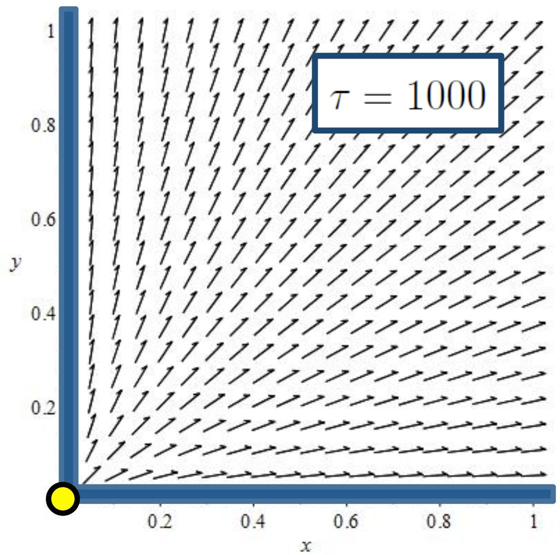


$$\phi = \tan^{-1}\left(\frac{y + 1/\tau}{x + 1/\tau}\right)$$

where $\tau = Wd/K$ is a nondimensionalised anchoring strength

This director angle solution solves Laplace's equation and the nonlinear Rapini-Papoular anchoring minimisation. (see *Points, Lines and Walls* – M. Kleman)

Director profile in corners: weak anchoring



a "virtual defect" outside the region

$$(x, y) = (-1/\tau,\ -1/\tau)$$

$$\phi = \tan^{-1}\left(\frac{y + 1/\tau}{x + 1/\tau}\right)$$

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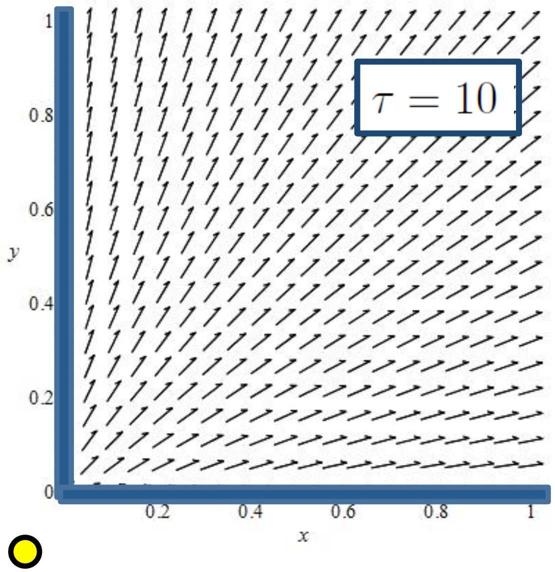
Director profile in corners: weak anchoring



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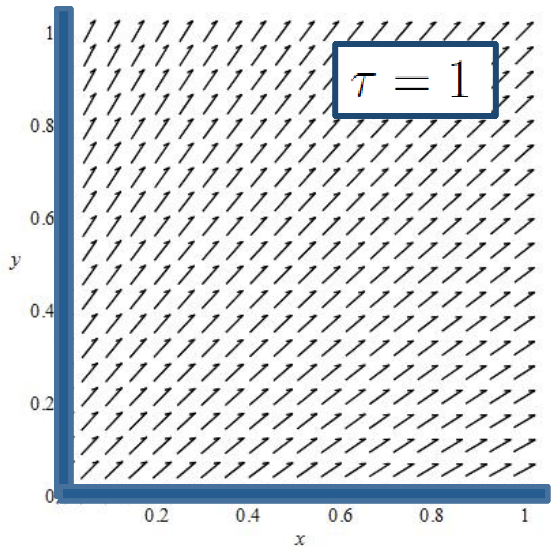

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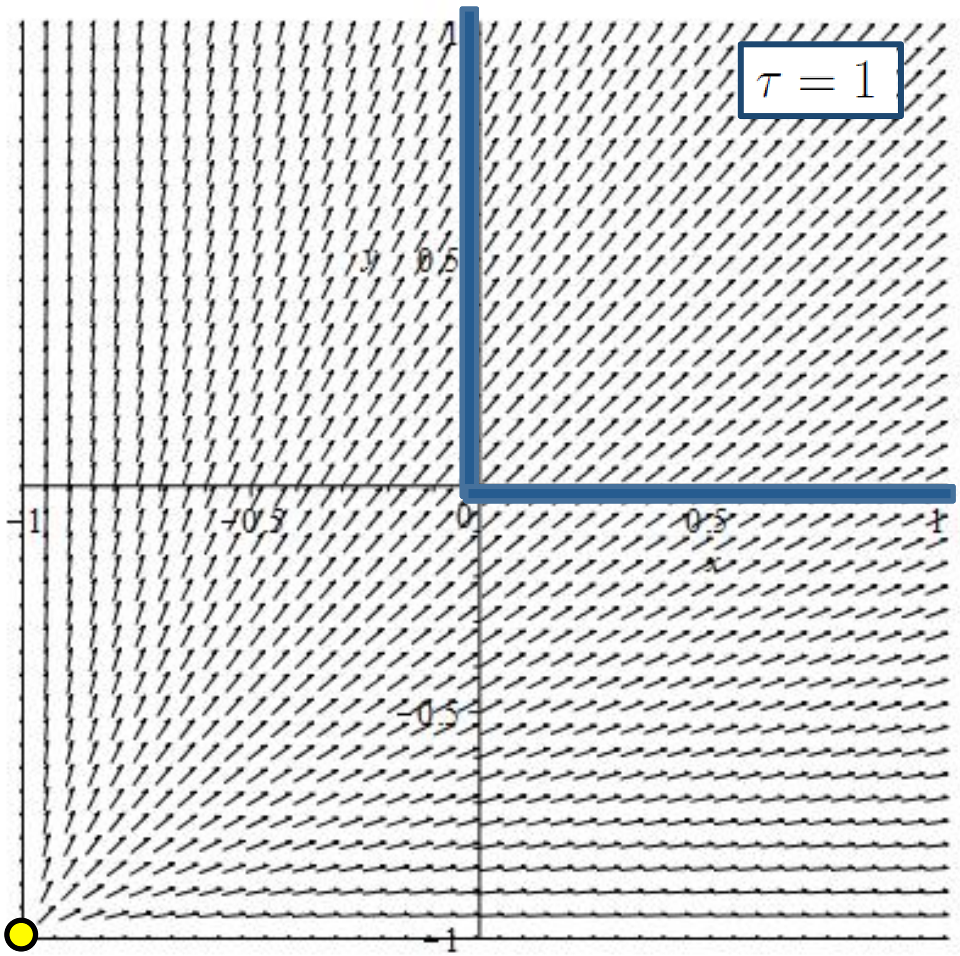

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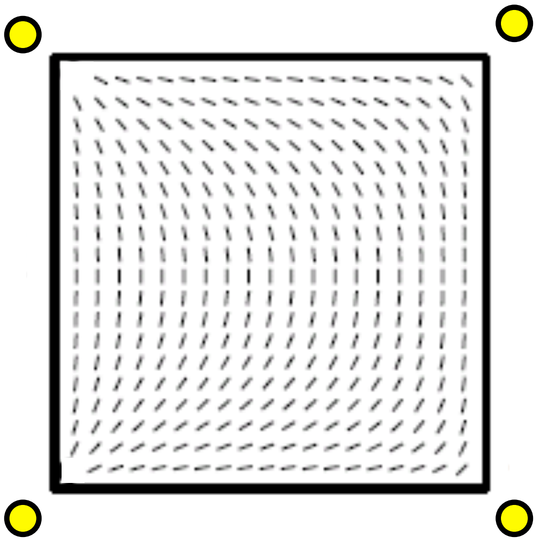
Confined nematics: director structure

- We can construct a director structure using the method of images



Confined nematics: director structure

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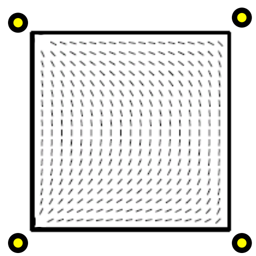

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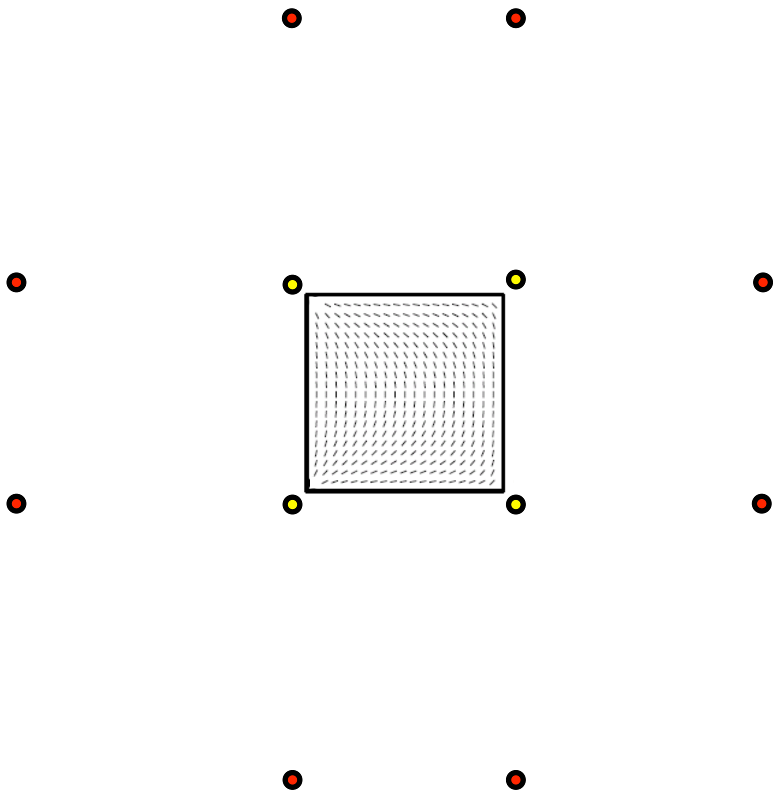
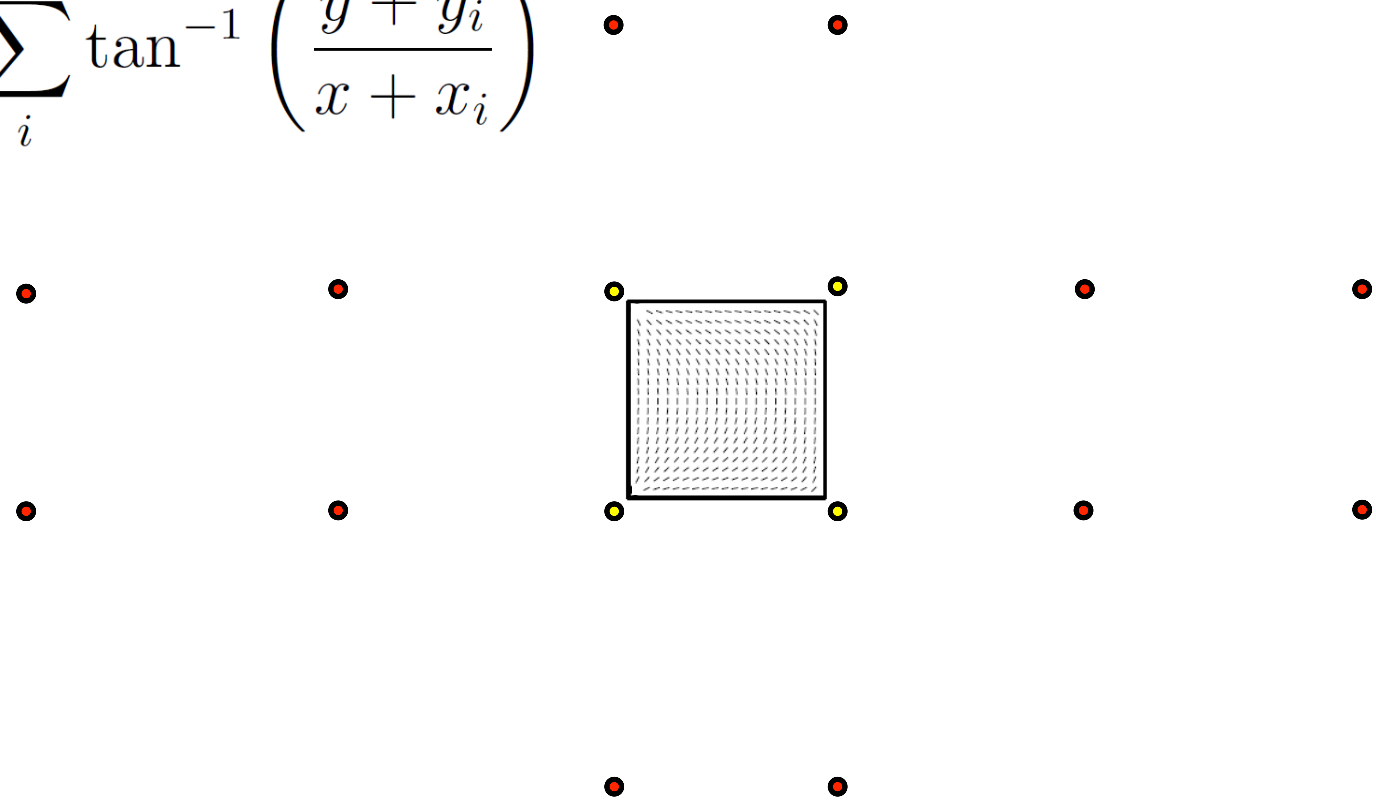


Confined nematics: director structure

- **We can construct a director structure using the method of images**

$$\phi = \sum_i \tan^{-1}\left(\frac{y + y_i}{x + x_i}\right)$$



Confined nematics: director structure

University of Strathclyde Glasgow

- **With weak anchoring, analytic forms of the director field are found**

PHYSICAL REVIEW E

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Nematic liquid crystal director structures in rectangular regions

J. Walton, N. J. Mottram, and G. McKay

Phys. Rev. E **97**, 022702 – Published 16 February 2018

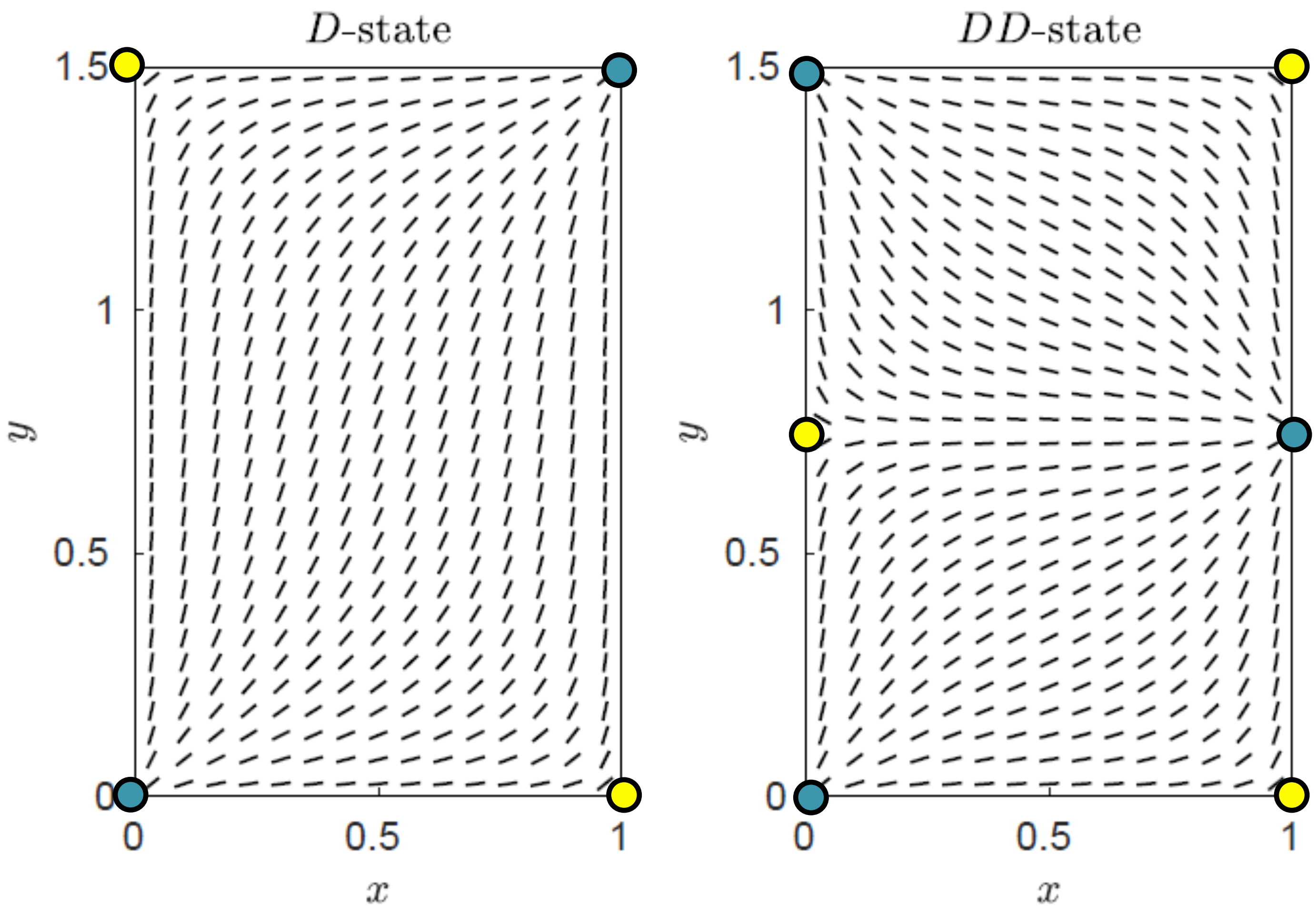
$$\theta(x,y)=\sum_{\substack{j=1\\ j\ \mathrm{odd}}}^{\infty}\left[\Theta_1\Phi_j\left(\frac{y}{\lambda},\frac{1-x}{\lambda},\frac{1}{\lambda},\lambda\tau\right)+\Theta_2\Phi_j\left(\frac{y}{\lambda},\frac{x}{\lambda},\frac{1}{\lambda},\lambda\tau\right)+\Theta_3\Phi_j(x,\lambda-y,\lambda,\tau)+\Theta_4\Phi_j(x,y,\lambda,\tau)\right],$$

where

$$\Phi_j(U,V,\Lambda,T)=\frac{-2[\cos(P_j)-1]\cos[P_j(U-1/2)][\cosh(P_jV)\cos(P_j/2)+\sinh(P_jV)\sin(P_j/2)]}{[\sin(P_j)+P_j][\cosh(P_j\Lambda)\sin(P_j)+\sinh(P_j\Lambda)]},$$

Confined nematics: director structure

- **With weak anchoring, analytic forms of the director field are found**



Confined nematics: director structure

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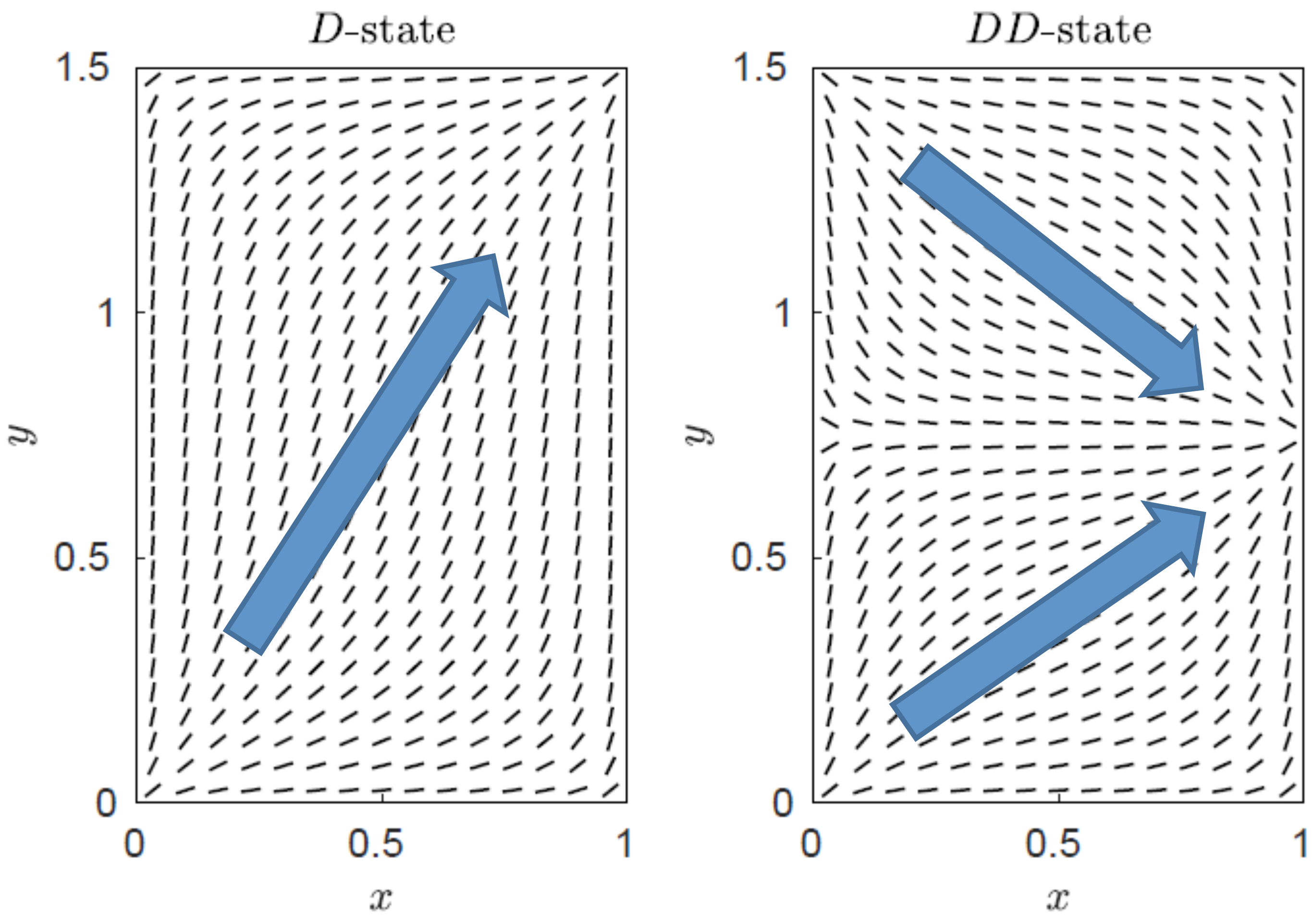

Confined nematics: director structure

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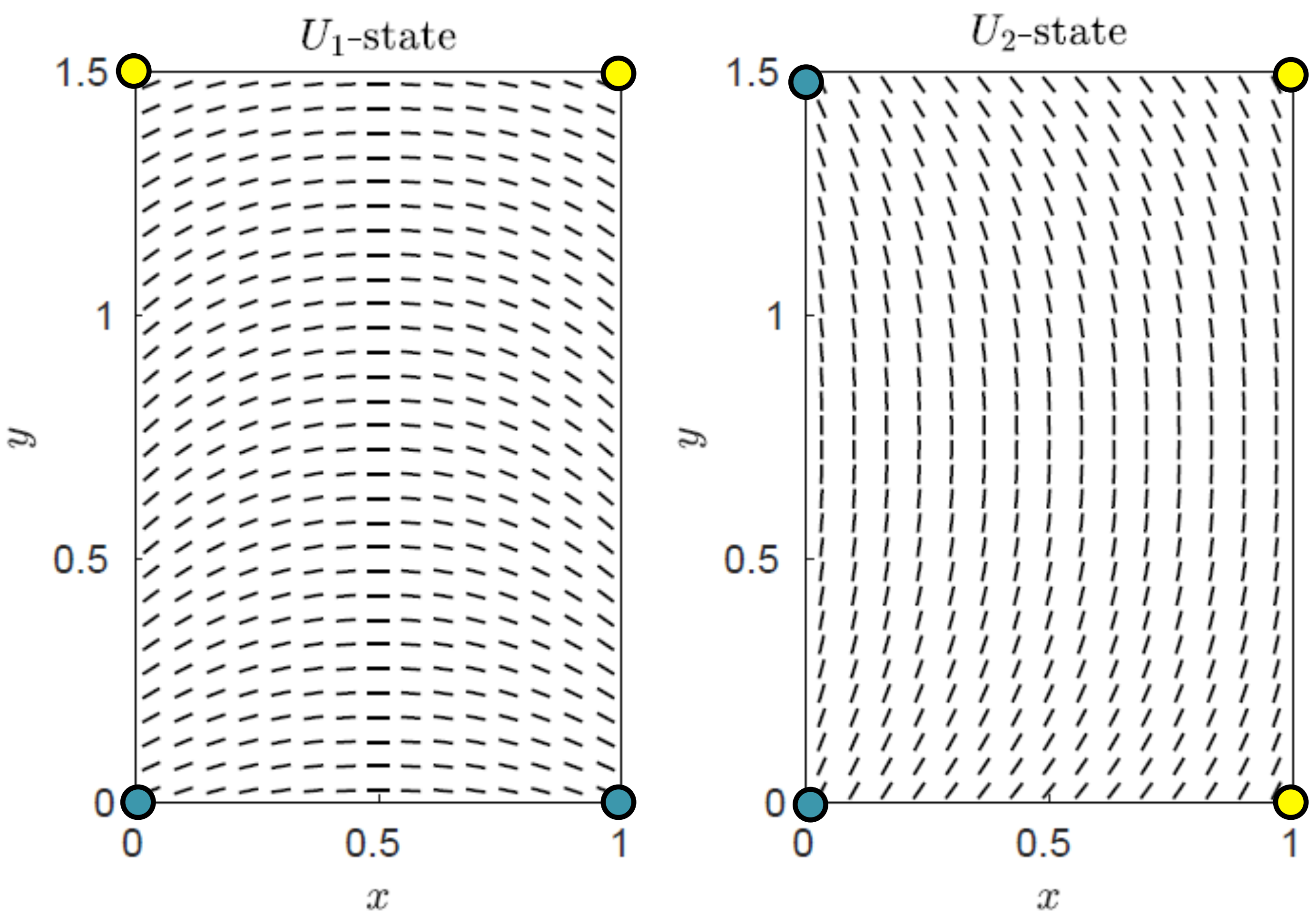

Confined nematics: director structure

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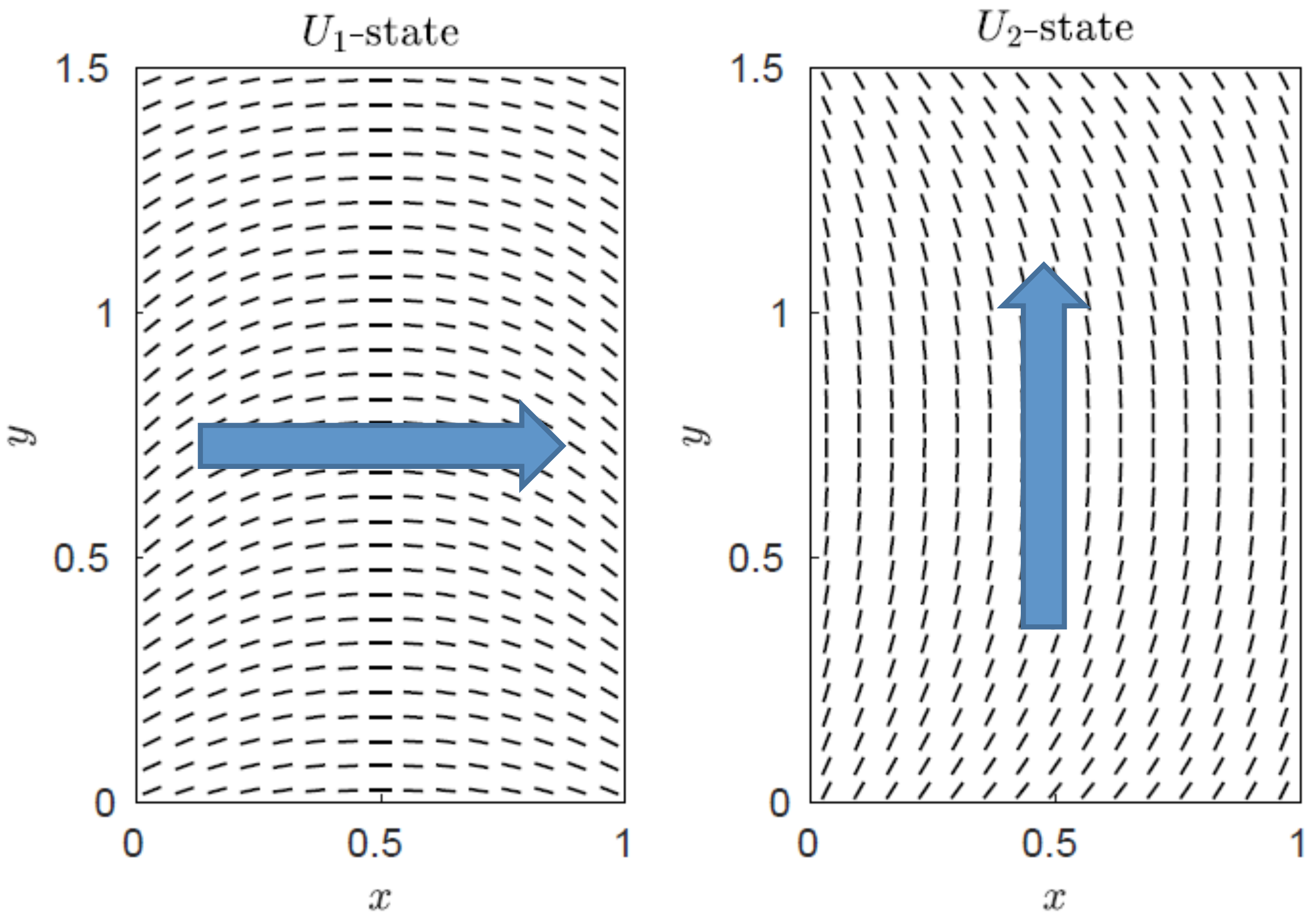

Confined nematics: director structure

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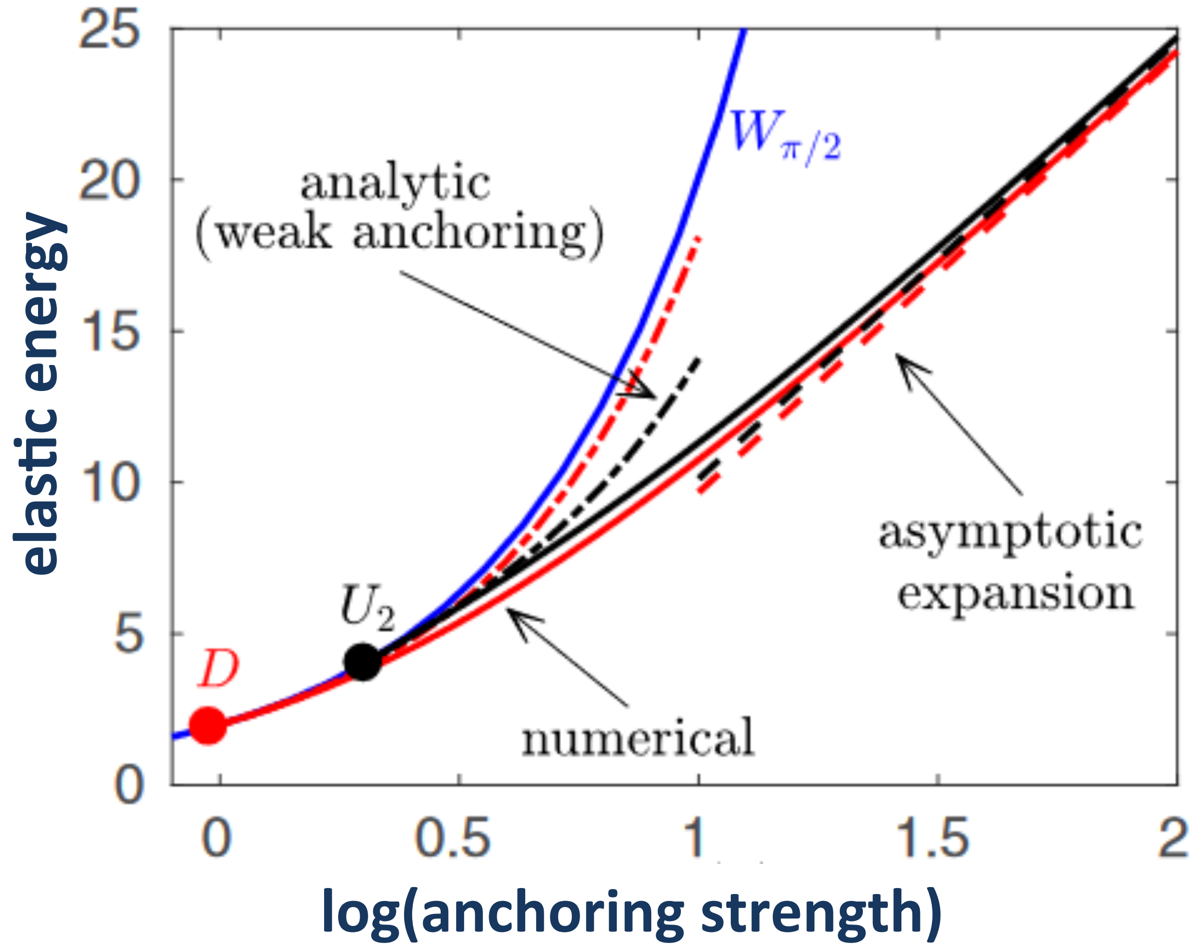
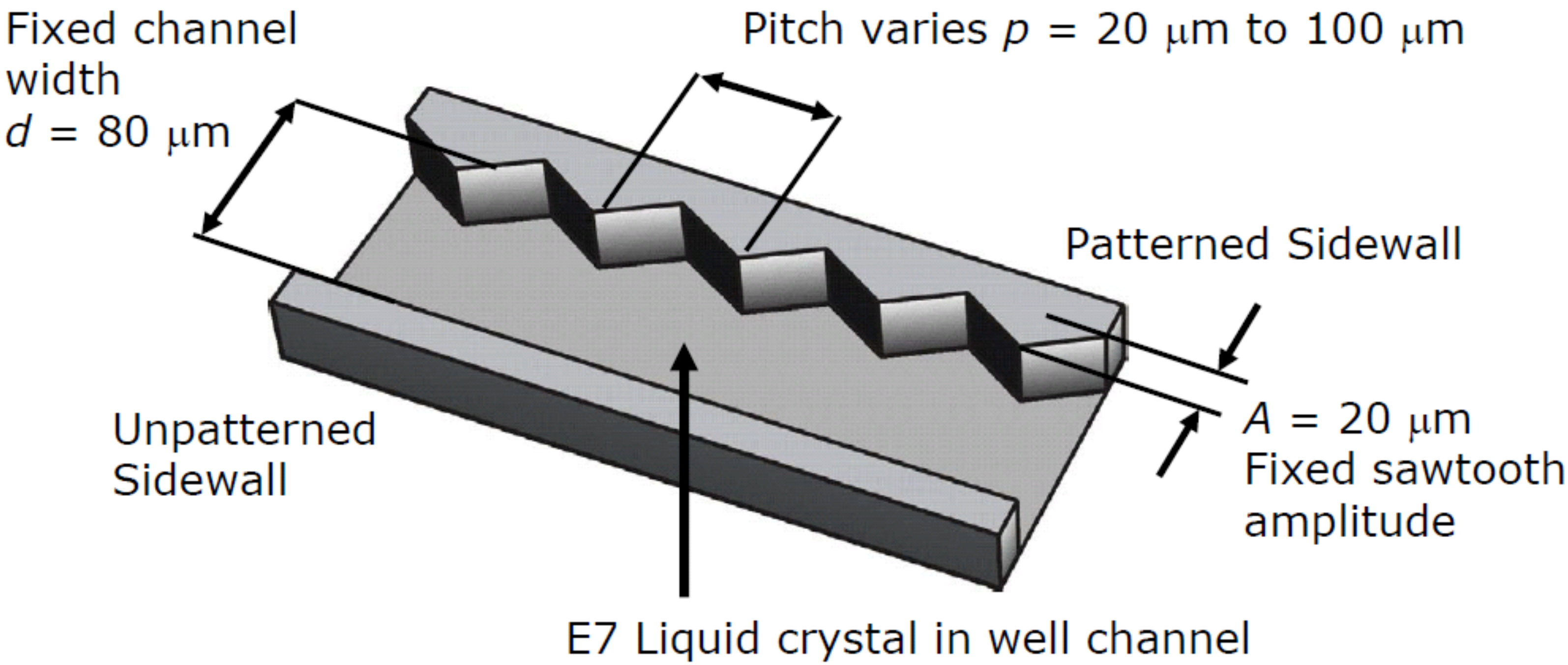


Confined nematics: channels

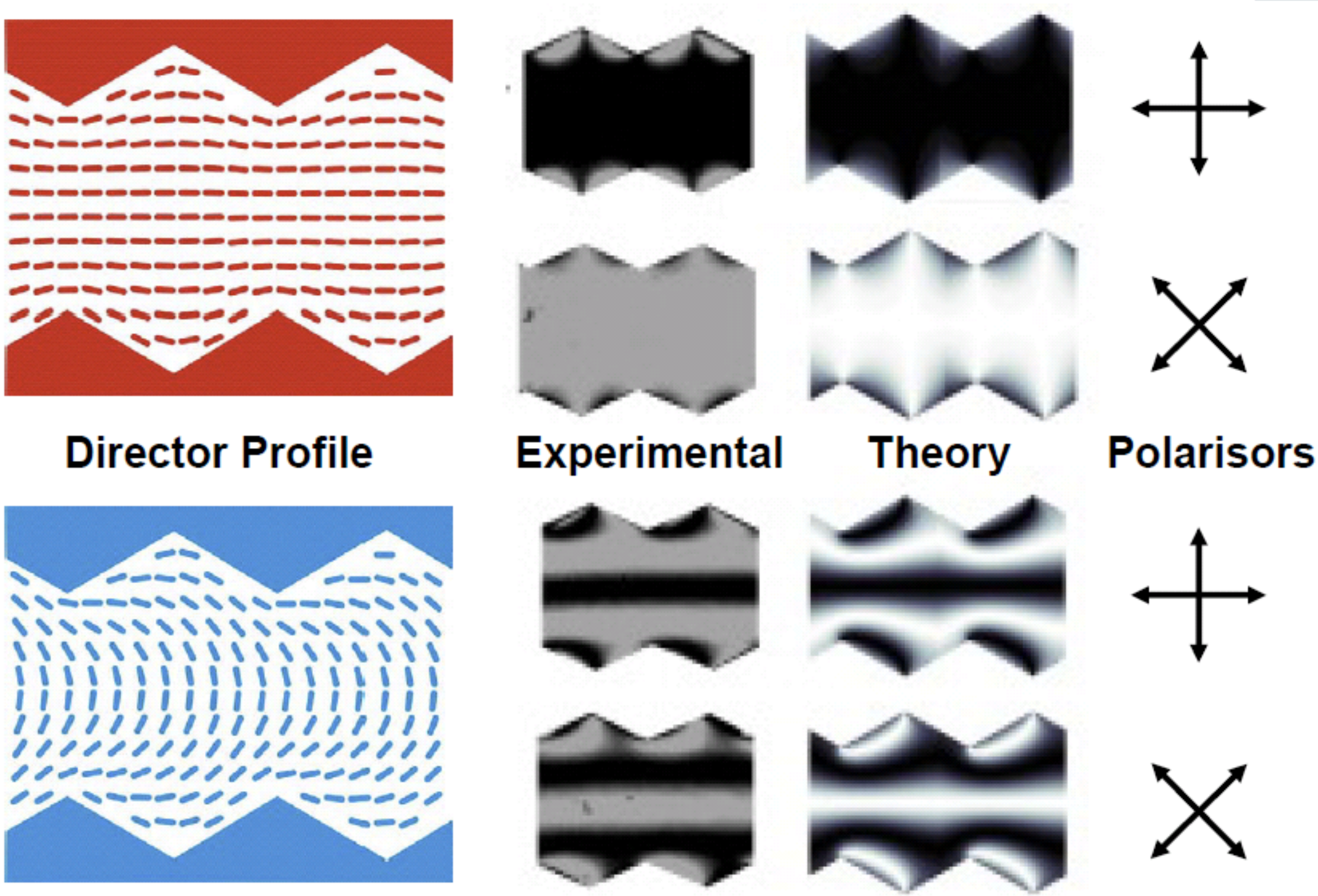
- **Liquid crystal sandwiched between a plane substrate and a sawtooth substrate**



S. Ladak, A. Davidson, C.V. Brown and N.J. Mottram, *J. Phys. D: Appl. Phys.* **42**, 85114 (2009)

Confined nematics: channels

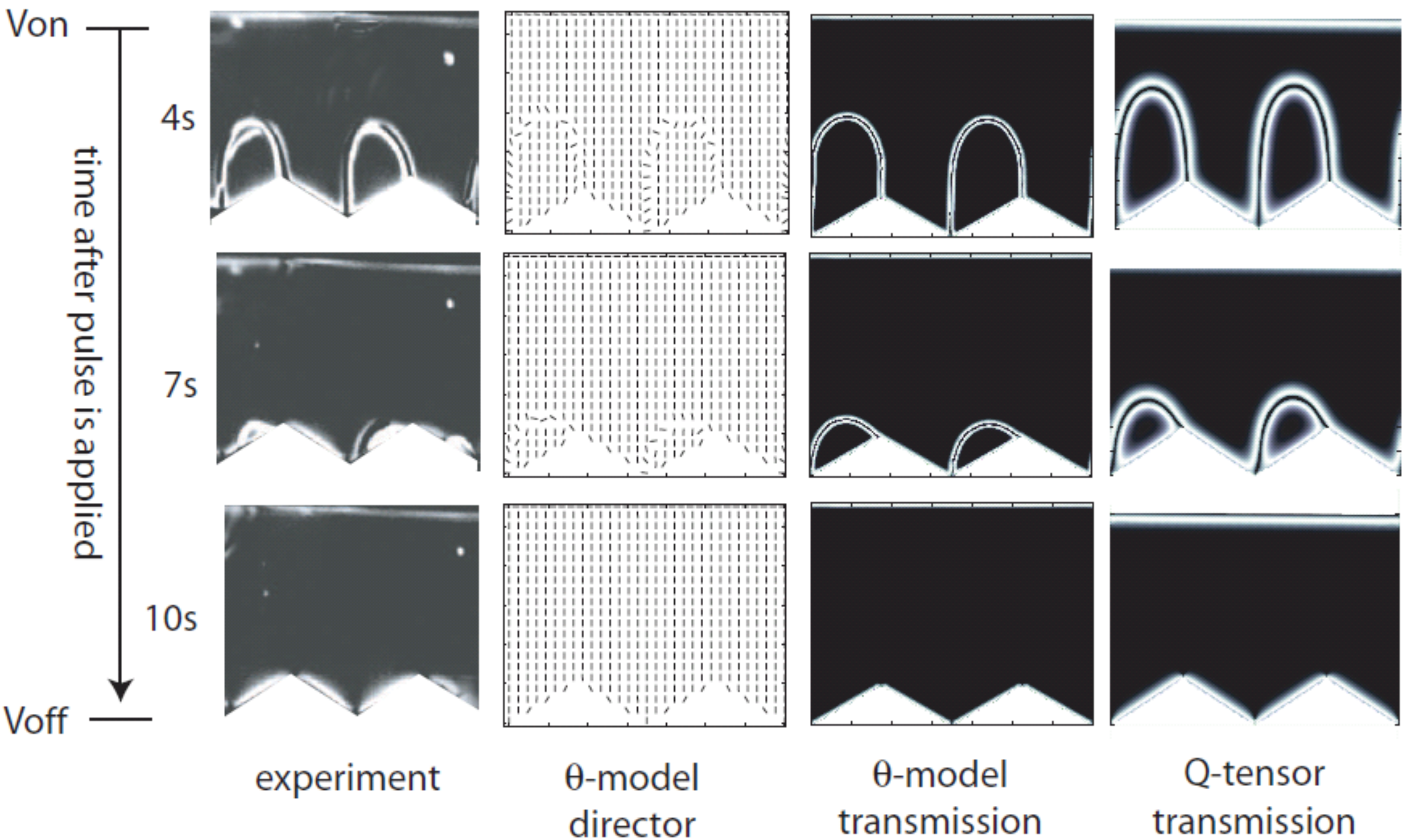
- Different wall geometries



S. Ladak, A. Davidson, C.V. Brown and N.J. Mottram, *J. Phys. D: Appl. Phys.* **42**, 85114 (2009)

Confined nematics: channels

- **Switching - switch voltage on**



Confined nematics: internal defects

University of Strathclyde Glasgow

- **Metastable states in rectangles**

LIQUID CRYSTALS, 2017
VOL. 44, NOS. 14–15, 2267–2284
http://dx.doi.org/10.1080/02678292.2017.1290284

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From molecular to continuum modelling of bistable liquid crystal devices

Martin Robinson [a], Chong Luo [b], Patrick E. Farrell [c,d], Radek Erban [c] and Apala Majumdar [e]

[a] Department of Computer Science, University of Oxford, Oxford, UK; [b] Google Inc., Mountain View, CA, USA; [c] Mathematical Institute, Radcliffe Observatory Quarter, University of Oxford, Oxford, UK; [d] Center for Biomedical Computing, Simula Research Laboratory, Fornebu, Norway; [e] Department of Mathematical Sciences, University of Bath, Bath, UK

Confined nematics: internal defects

University of Strathclyde Glasgow

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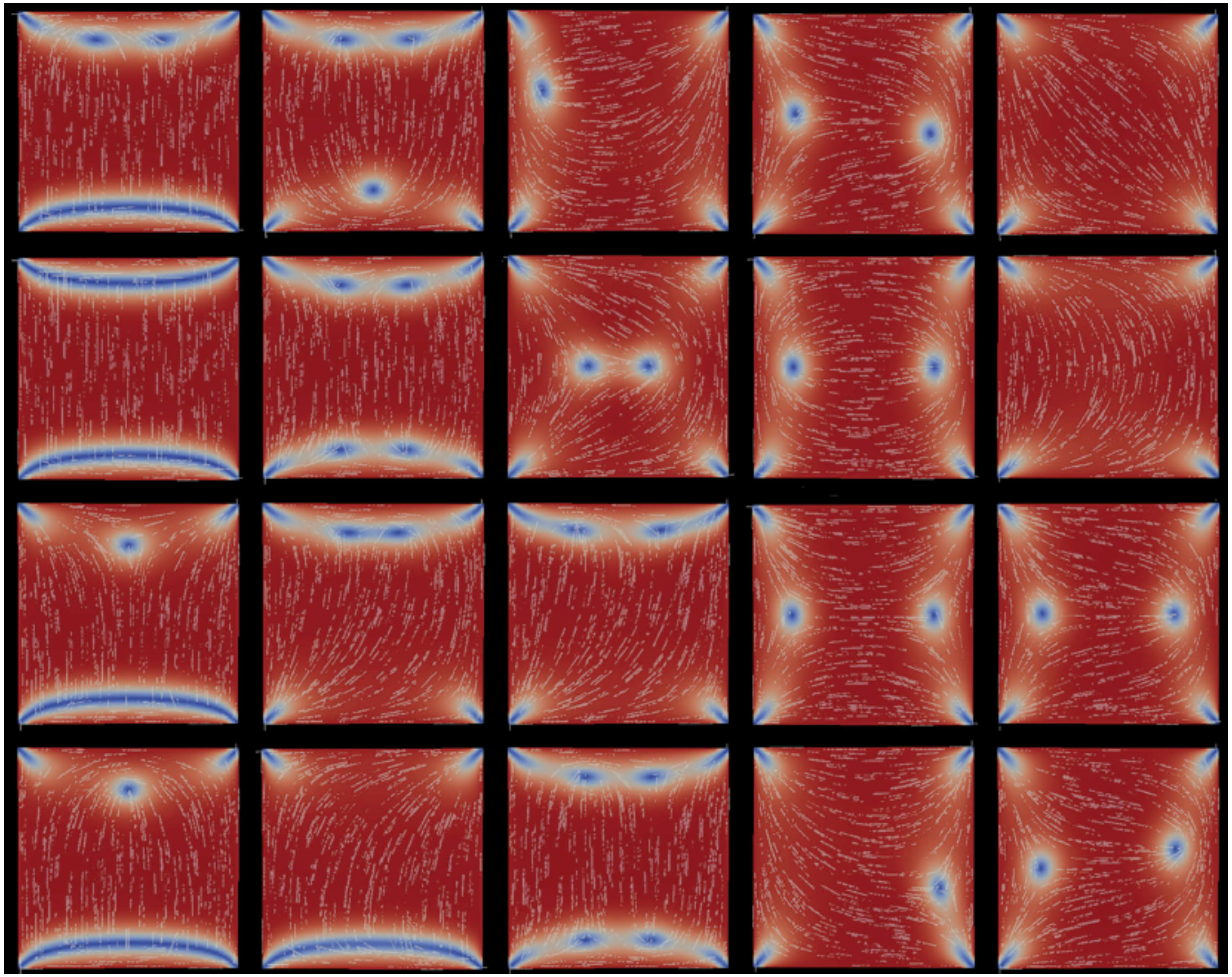
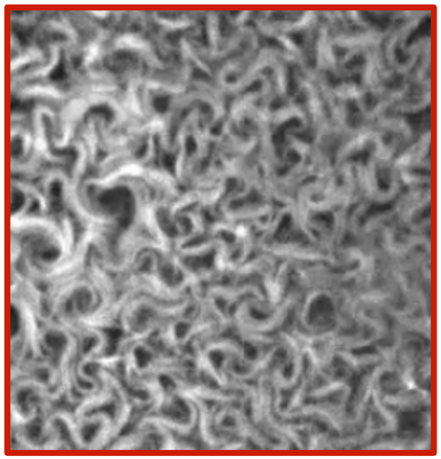
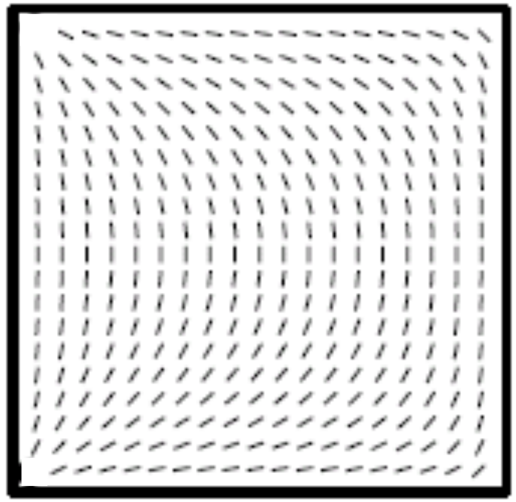


Confined active nematics

- We imagine an active nematics (i.e. suspension of bacteria) in a confined geometry





- …but assume low Reynolds number, low Ericksen number

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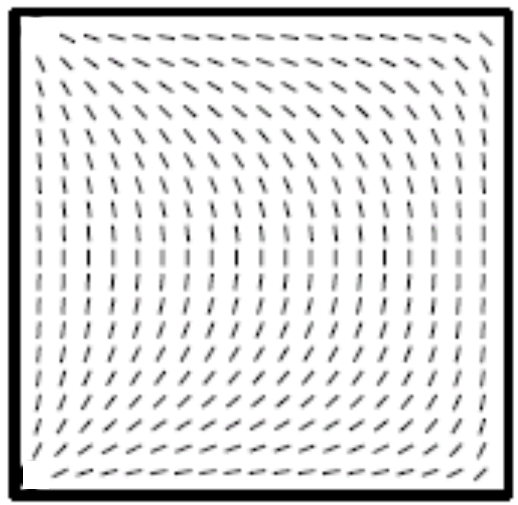

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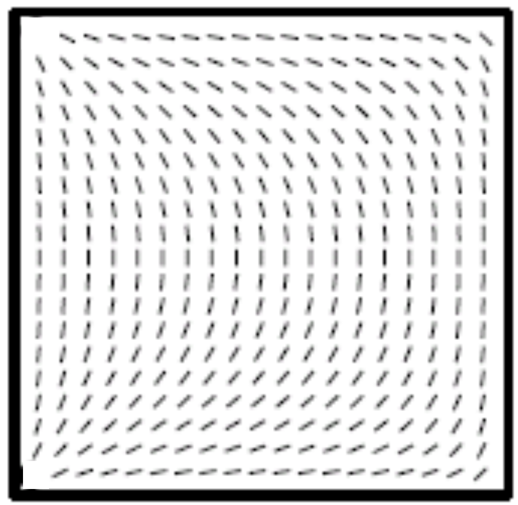

LIQUID CRYSTALS, 2016
VOL. 43, NOS. 13–15, 2332–2351
http://dx.doi.org/10.1080/02678292.2016.1239773

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INVITED ARTICLE

Multistable nematic wells: modelling perspectives, recent results and new directions

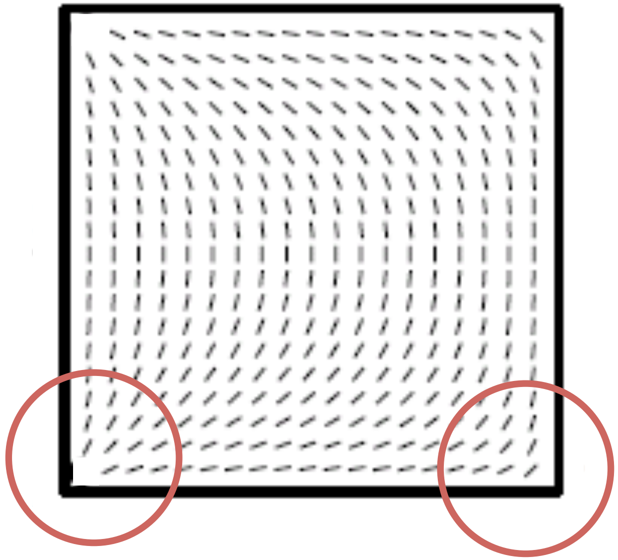
Apala Majumdar[a] and Alexander Lewis[b]

[a]Department of Mathematical Sciences, University of Bath, Bath, UK; [b]Mathematical Institute, University of Oxford, Oxford, UK

Confined active nematics

- We imagine an active nematics (i.e. suspension of bacteria) in a confined geometry

- Consider the corner regions



k=1

k=-1

Confined active nematics

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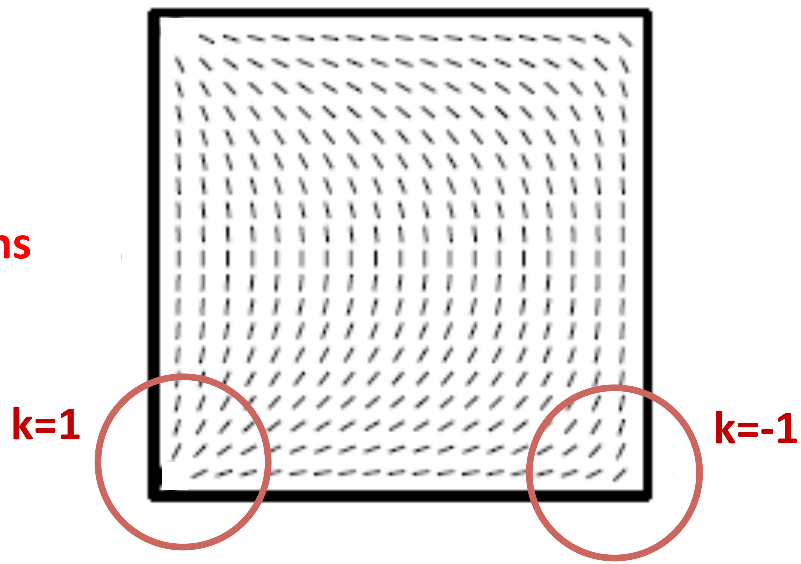
- Consider the corner regions



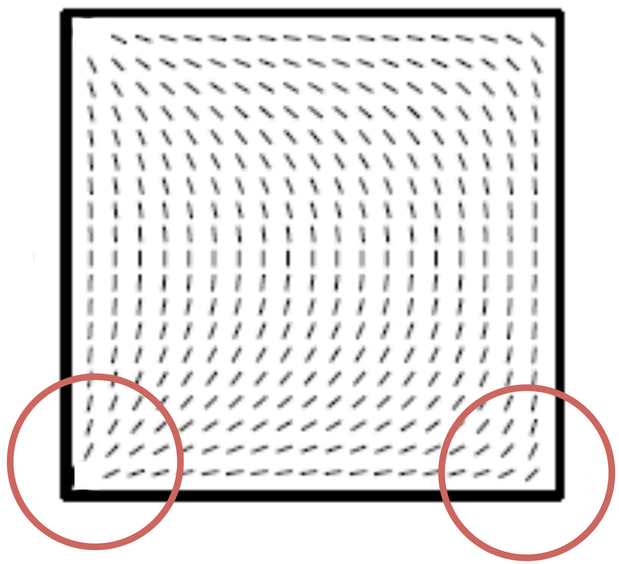
$$\nabla^4 \psi = \frac{2\mathcal{A}k(k-1)\sin(2(k-1)\phi)}{r^2}$$

streamfunction

director angle

Confined active nematics

- We imagine an active nematics (i.e. suspension of bacteria) in a confined geometry



strength of activity

strength of defect

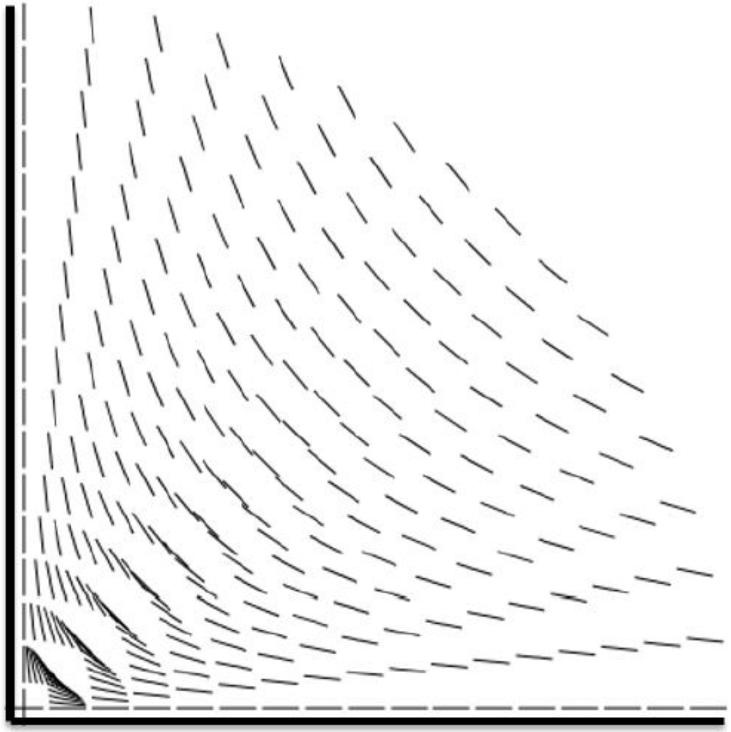
$$\nabla^4 \psi = \frac{2\mathcal{A}k(k-1)\sin(2(k-1)\phi)}{r^2}$$

streamfunction

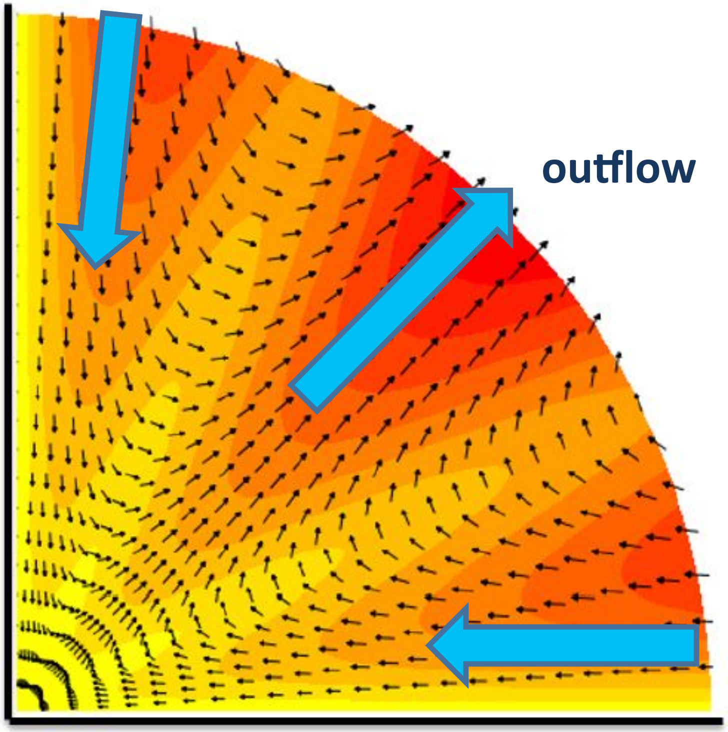
director angle

Confined active nematics

- Flow in a corner can be analytically calculated



director structure

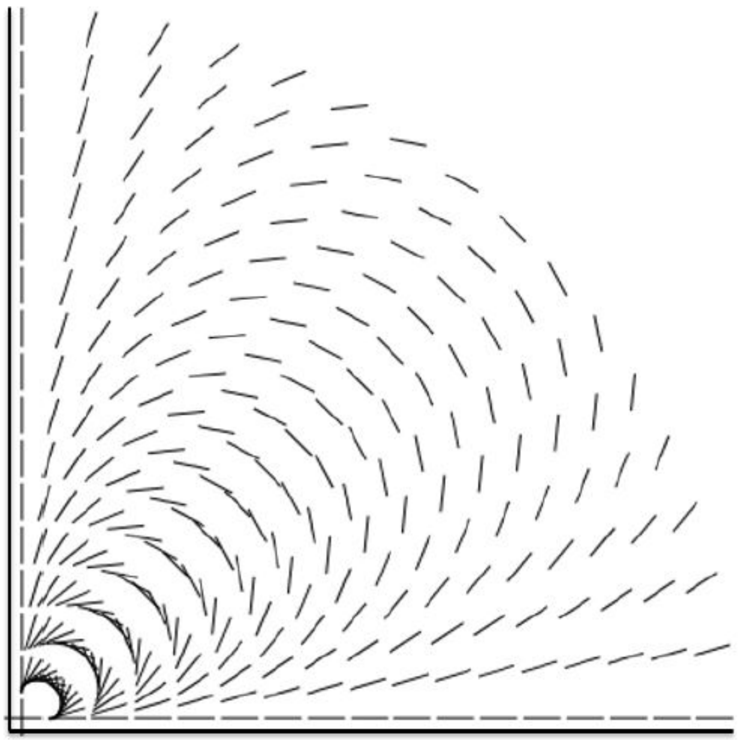


flow velocity
(yellow weak, red strong)

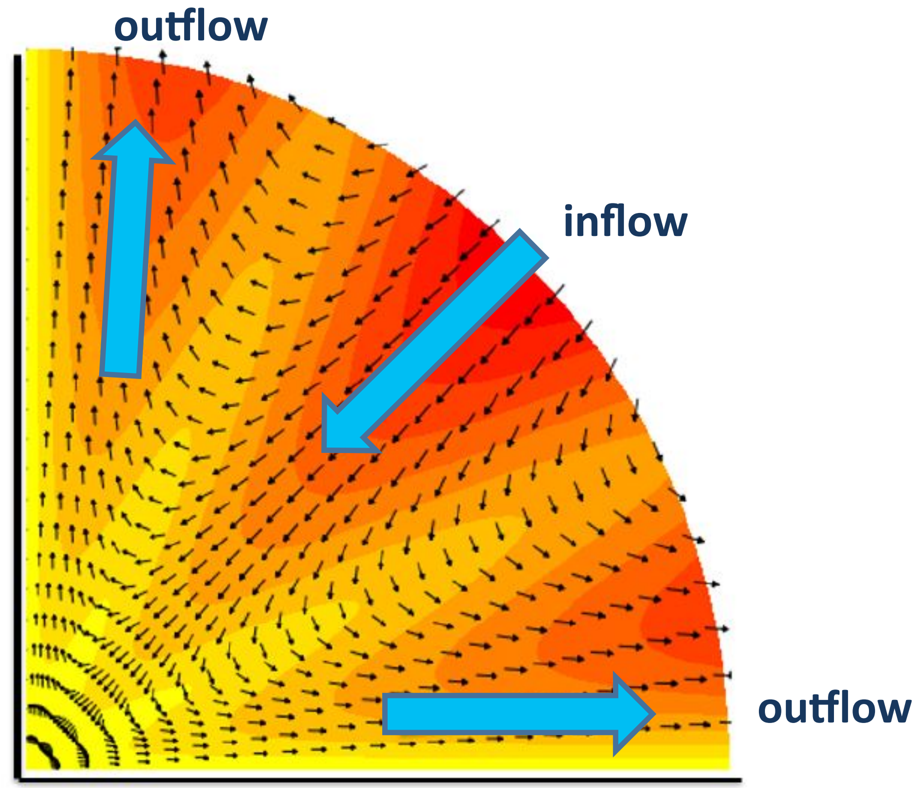
k=-1 defect

Confined active nematics

- **Flow in a corner can be analytically calculated**



director structure



flow velocity
(yellow weak, red strong)

k=3 defect

Confined active nematics

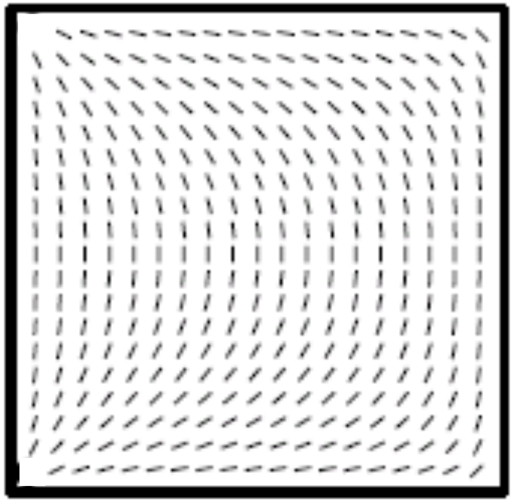
- **Flow in a corner can be analytically calculated**

for a k=1 defect there is NO FLOW

$$\nabla^4 \psi = \frac{2\mathcal{A}k(k-1)\sin(2(k-1)\phi)}{r^2}$$

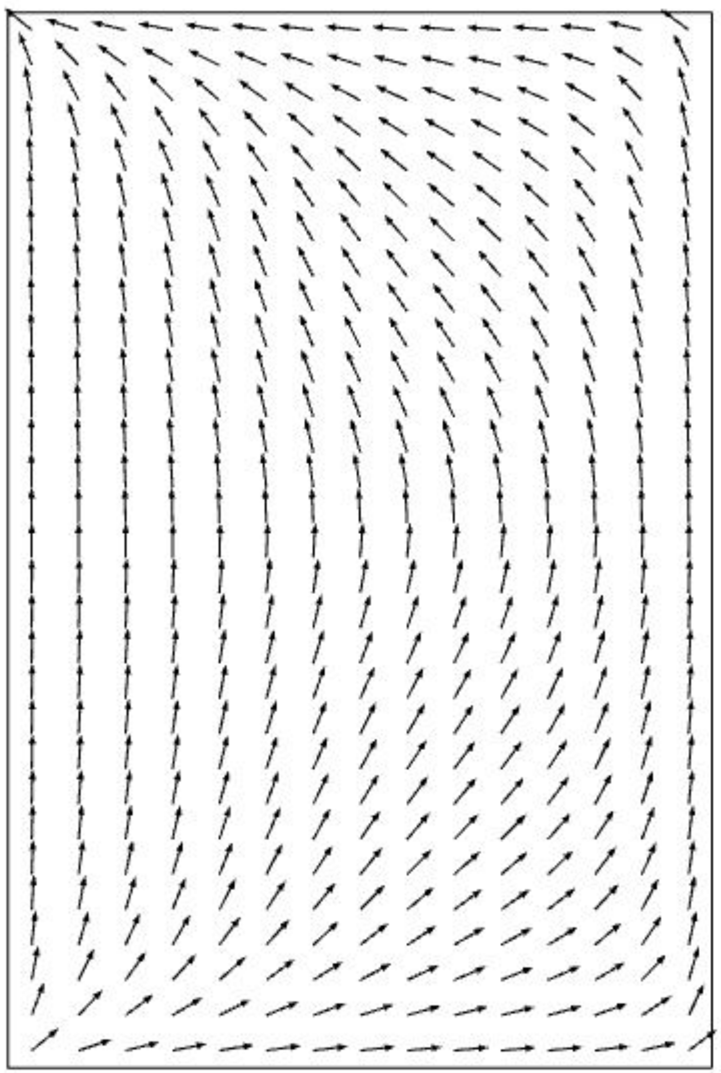
Confined active nematics

- Considering flow in the full rectangular region



We **solve the full coupled Ericksen-Leslie equations** for flow velocity and director angle with weak director anchoring (Rapini-Papoular) and no-slip velocity at boundaries.

Confined active nematics



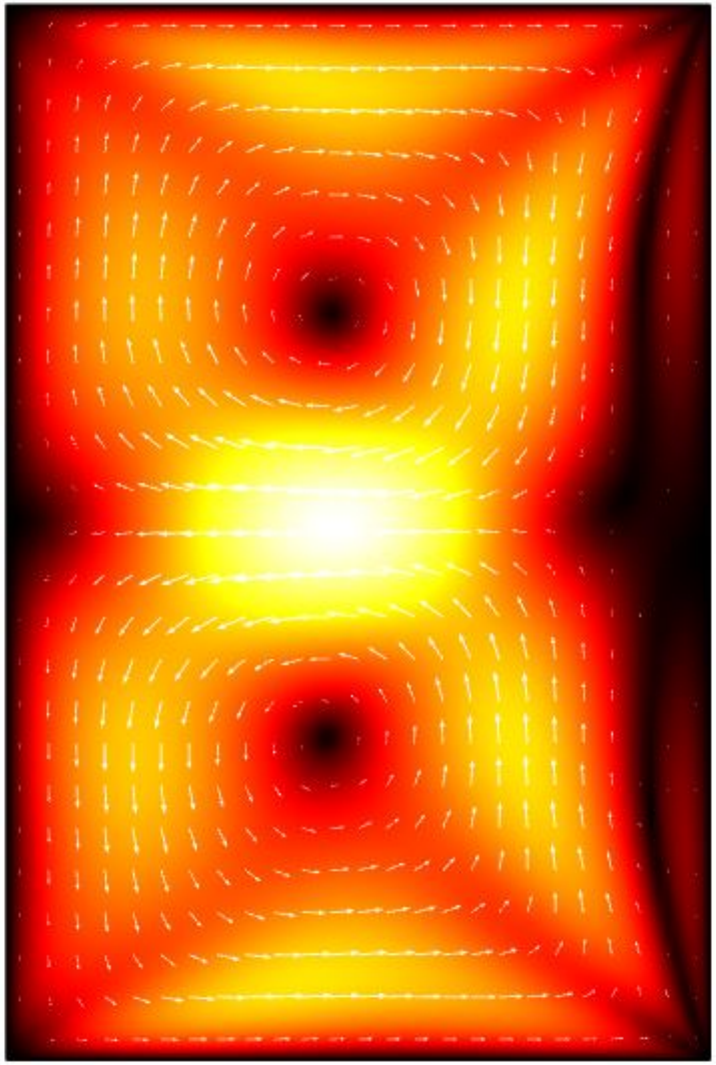
k=1 k=-1

director structure

For relatively small activity the **director is only slightly distorted from the inactive state**

Confined active nematics

This director structure leads to
double circulations in the flow

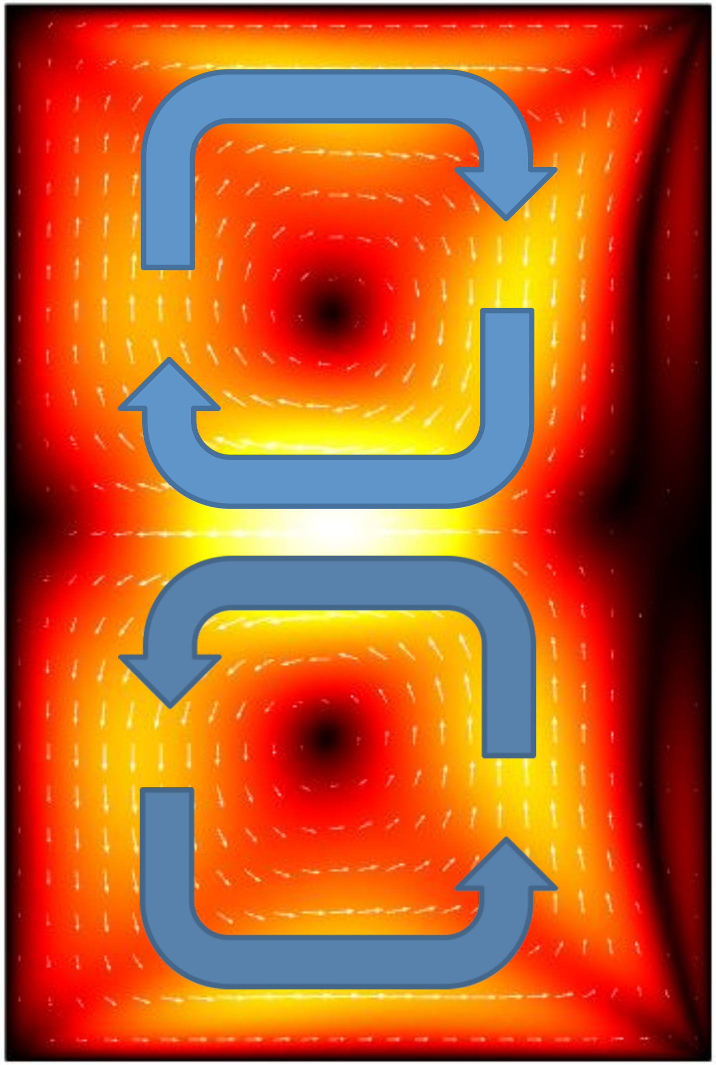


k=1 k=-1

flow velocity
(dark weak, light strong)

Confined active nematics

This director structure leads to
double circulations in the flow



k=1

k=-1

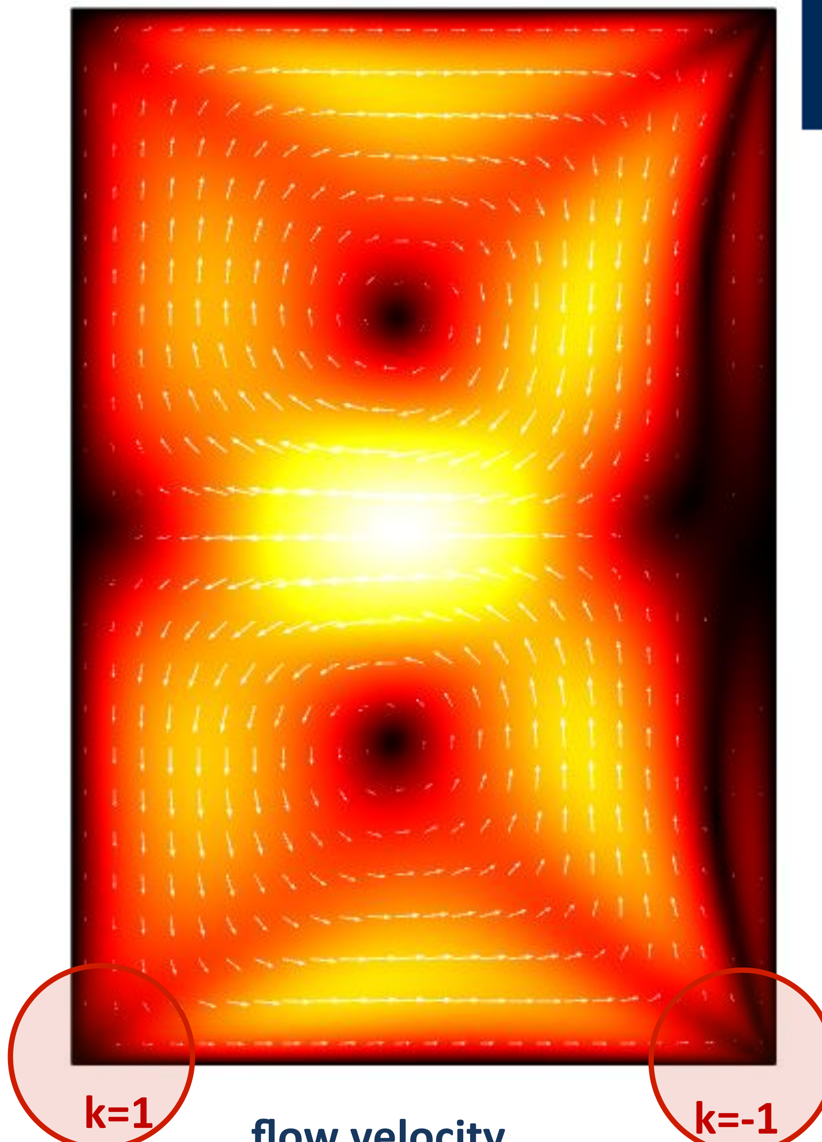
flow velocity

(dark weak, light strong)

Confined active nematics

This director structure leads to **double circulations in the flow**

Flow near to corners is similar to previous corner solutions



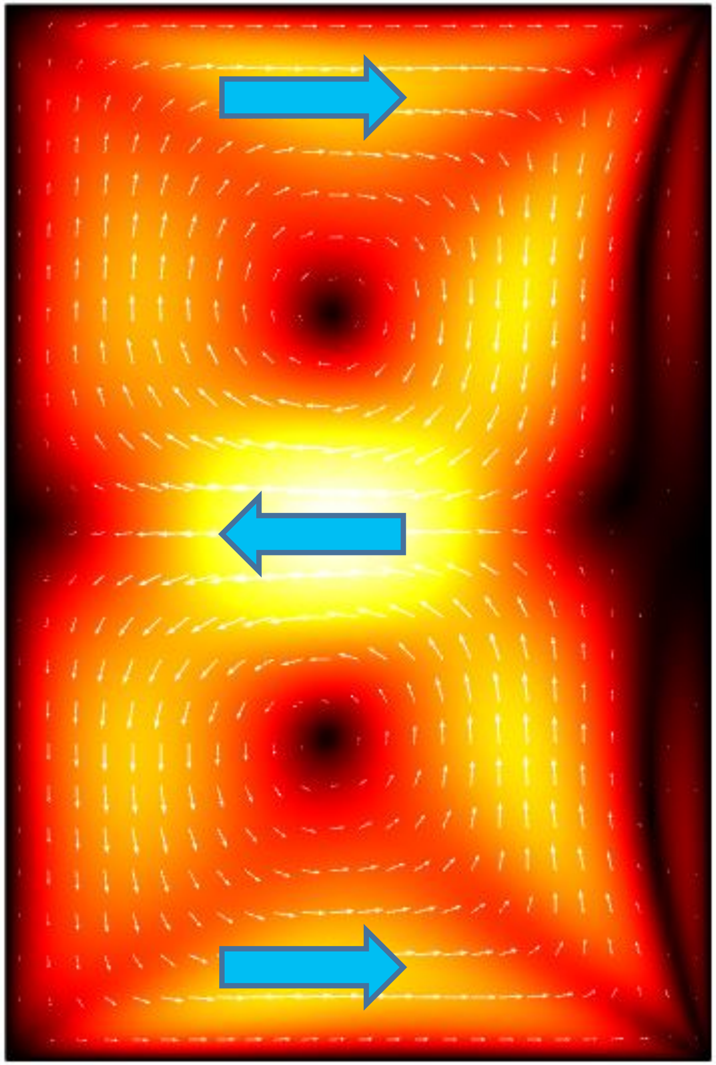
flow velocity

(dark weak, light strong)

Confined active nematics

This director structure leads to **double circulations in the flow**

We also see **jets of flow** in the bulk and near to boundaries

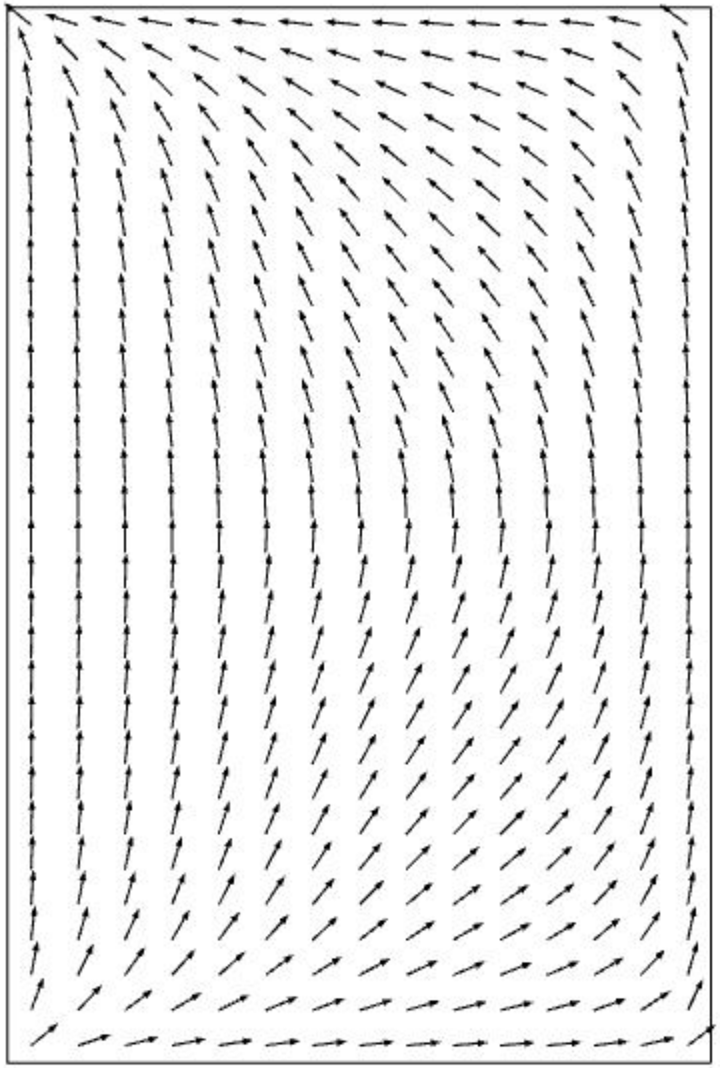


k=1 k=-1

flow velocity

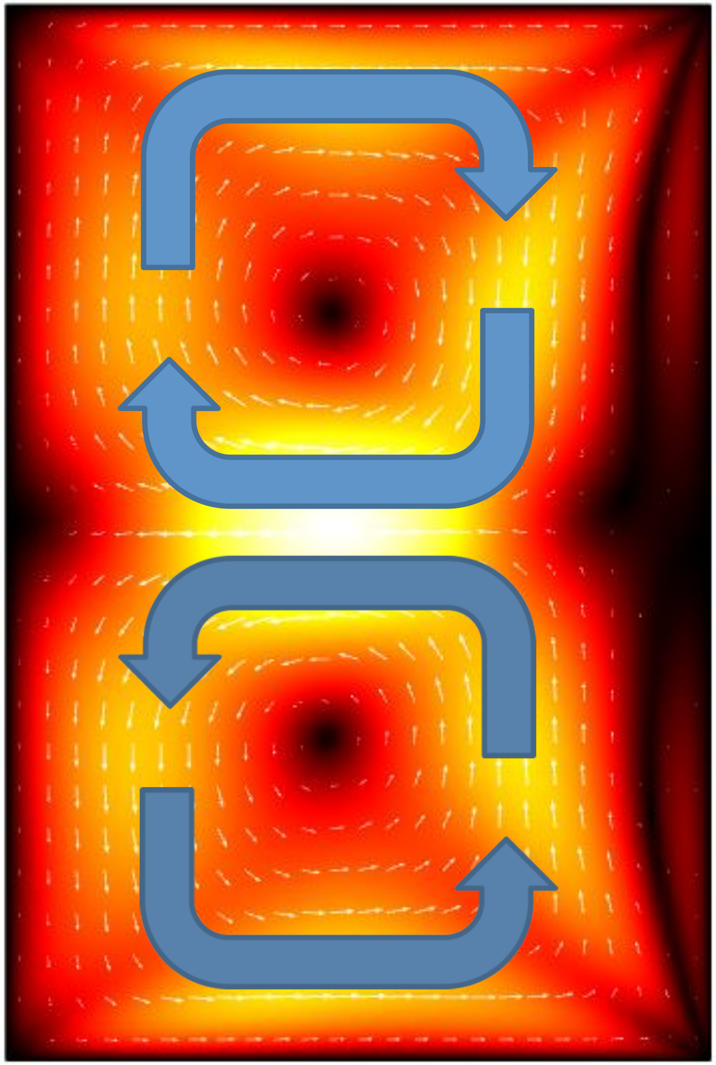
(dark weak, light strong)

Confined active nematics



k=1 k=-1

director structure



k=1 k=-1

flow velocity
(dark weak, light strong)

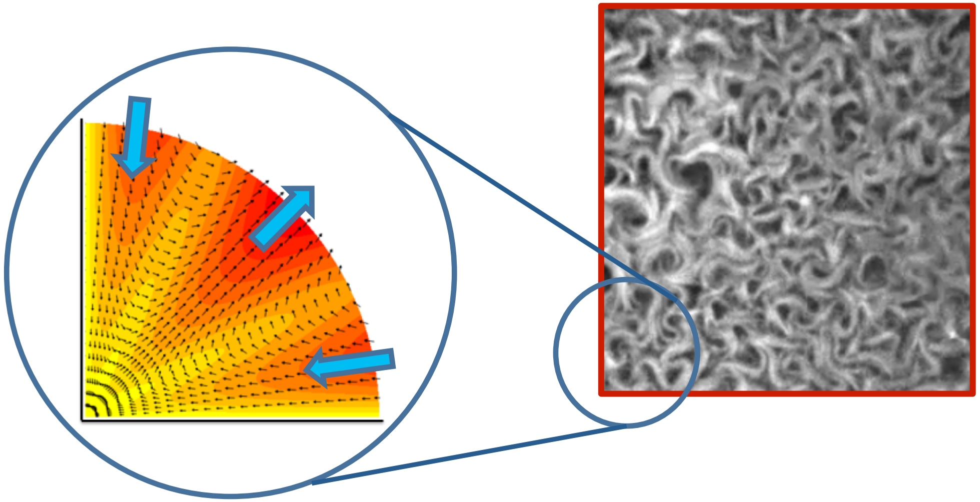
Cornered!

- **Corners induce distortion, multistability and stabilise defects and create virtual defects.**

Cornered!

- Corners induce distortion, multistability and stabilise defects and create virtual defects.

- Can they also generate flow?



Cornered!

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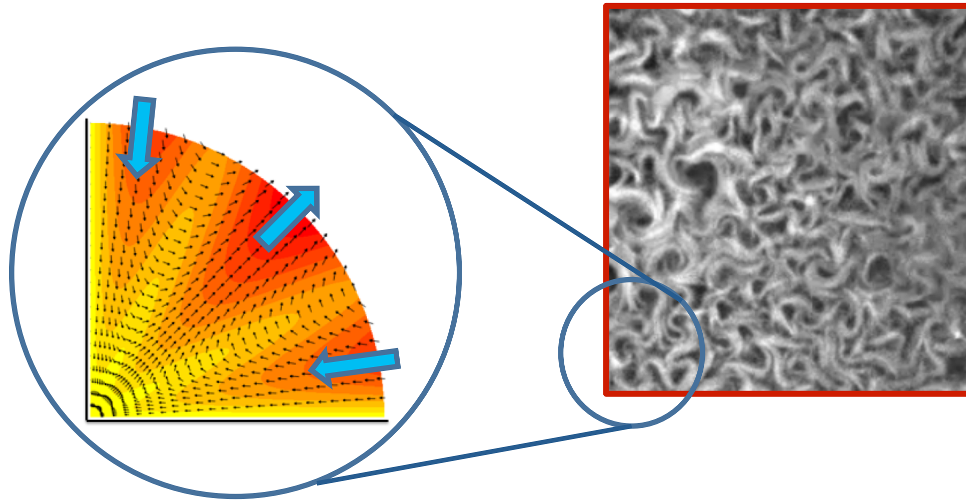
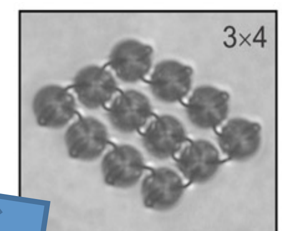
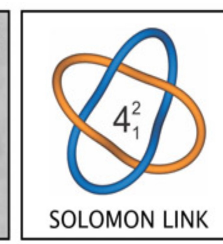


- Can they also generate flow?

- Can they help to stabilise defects externally?





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Replication of anisotropic dispersed particulates and com
templates

Olga Shchepelina, Veronika Kozlovskaya, Srikanth Singamaneni, Eugenia Kharlam
and Vladimir V. Tsukruk*

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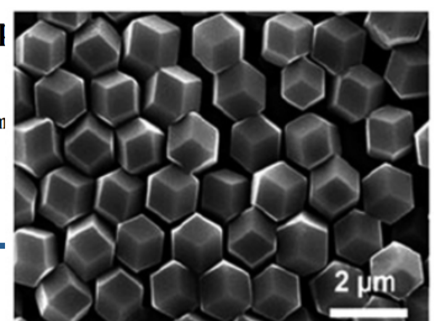
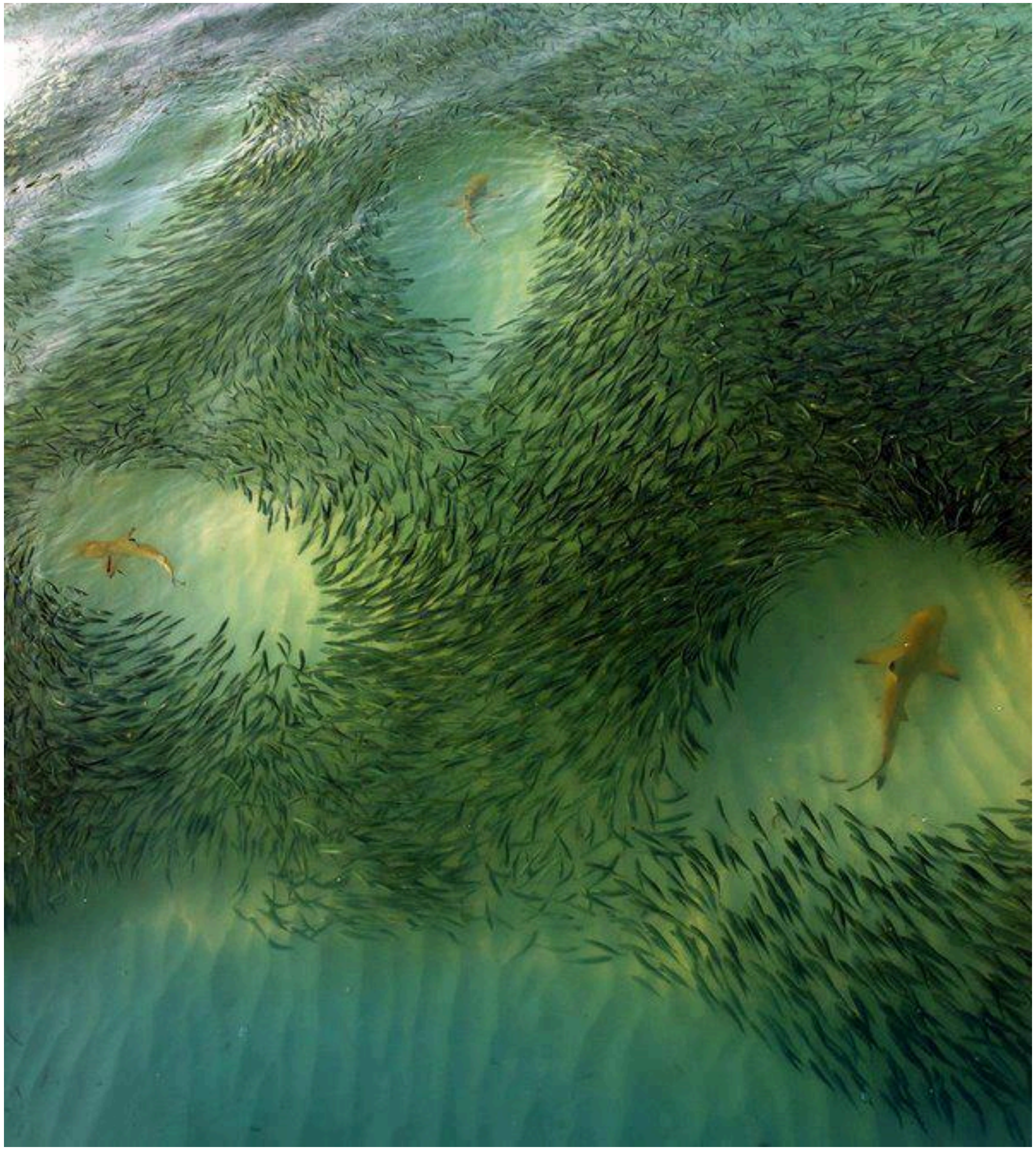


Cornered!



Colloid particles causing defects

Cornered!

Prof. Nigel Mottram
Department of Mathematics and Statistics
University of Strathclyde, Glasgow

Dr Geoff McKay, Dr Andrew Davidson, Josh Walton (Strathclyde)

Prof Carl Brown, Dr Costas Tsakonas, Dr Sam Ladak, Dr Gary Wells (Nottingham Trent)