Liquid Crystals and Continuum Mechanics – Research and Applications

University of Strathclyde Science

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UNIVERSITY OF STRATHCLYDE

LMS Prospects in Mathematics
10th September 2020

A bit about myself…

- 2006 – Ph.D. in applied mathematics, University of Bristol

CASE (Competitive Awards in Science and Engineering) student with Hewlett Packard
Thesis title: Liquid crystals and tangent unit-vector fields in polyhedral geometries

- University of Oxford:

❖ Royal Commission for the Exhibition of 1851 Research Fellow, Oxford Centre for Nonlinear Partial Differential Equations

❖ Oxford Centre for Collaborative Applied Mathematics Research Fellow

- University of Bath: EPSRC Career Acceleration Fellowship

- University of Strathclyde, United Kingdom.

Research overview

- Mathematics of Materials Science motivated by Applications in Science and Industry
  - Primary research programme : mathematical theories and modelling for **liquid crystals** and **liquid crystal devices**
  - Related areas

- Partially ordered materials : colloids, bent-core mesophases, composites
- Collaborations with University of Luxembourg, Indian Institute of Technology Delhi, Illinois Institute of Technology

- Complex Fluids and Microfluidics

Collaborations with University of Oxford (OCIAM Visiting Fellowship)

- Solid Mechanics and Nonlinear Elasticity

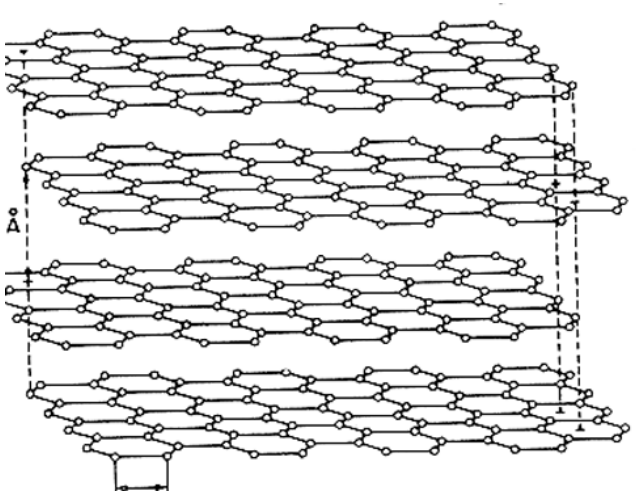
- Industrial Mathematics

Collaborations with Hewlett Packard and Merck.

The 4th phase of matter….

Liquid crystals are soft ordered phases – an intermediate phase of matter between the solid and liquid states.

SOLID



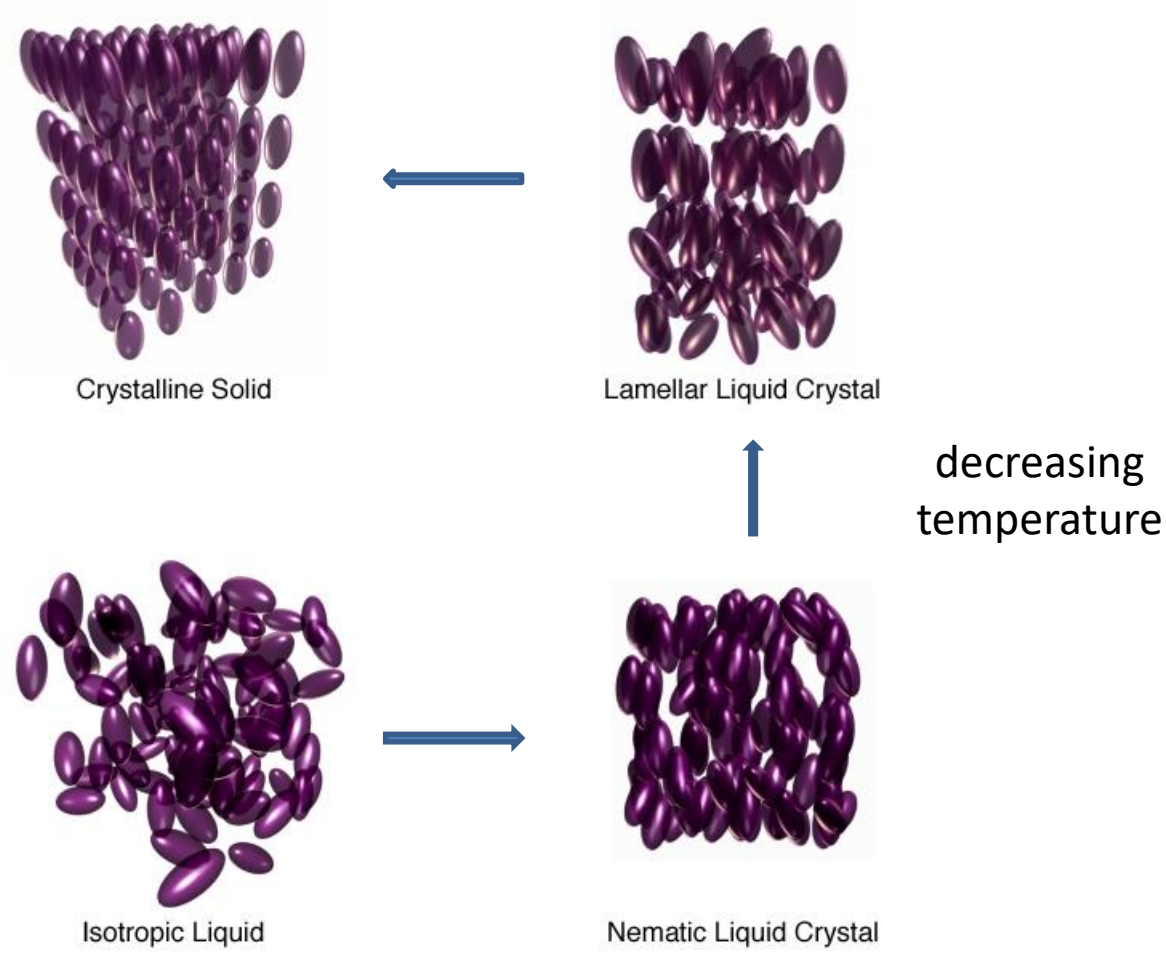
- 3D lattice structure
- molecules have fixed positions and orientations

LIQUID

- no lattice structure
- isotropic medium – molecules are free to point in any direction

Liquid Crystals – what are they?

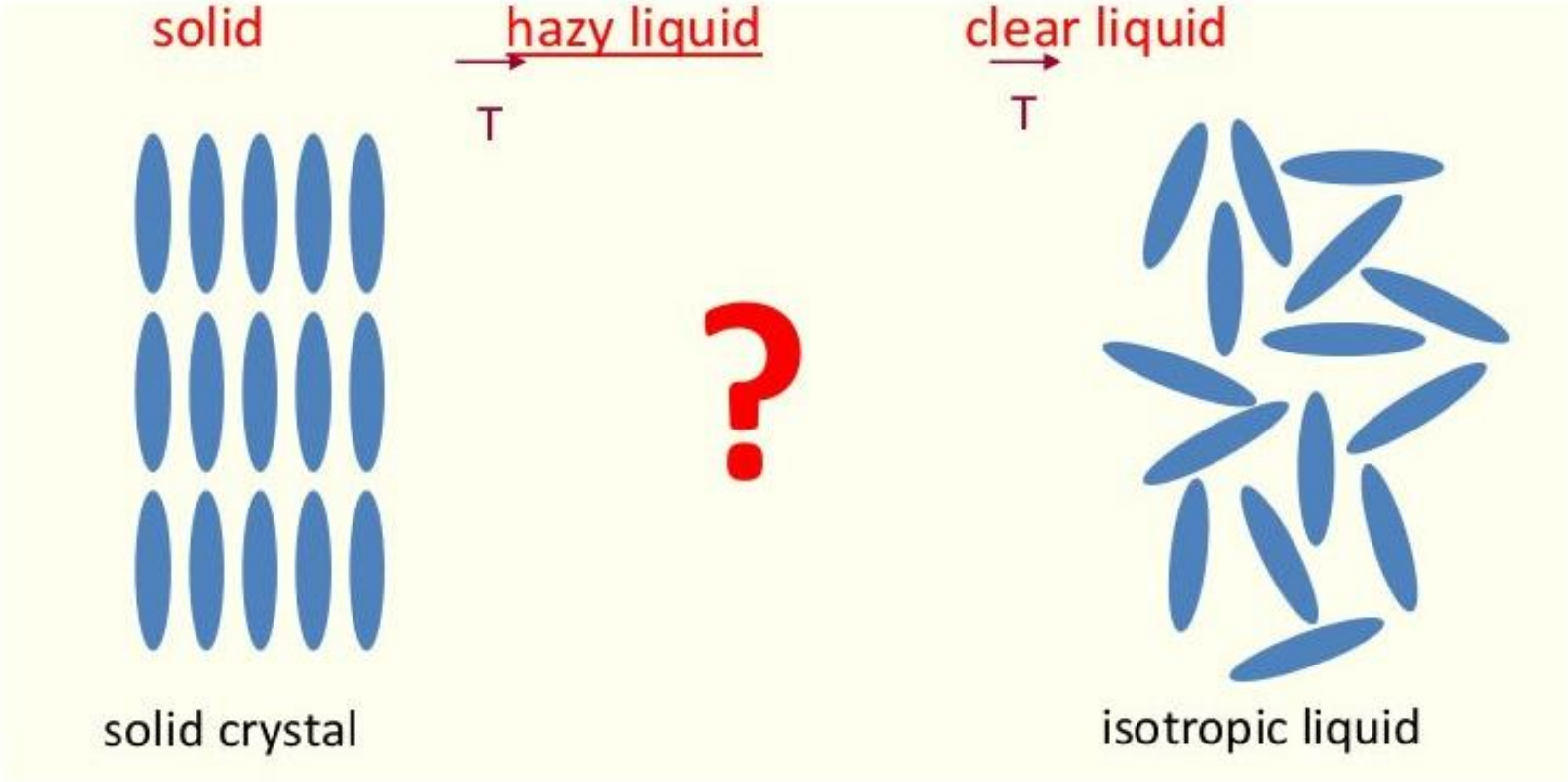
- Mesogenic phases of matter



- Intermediate between solids and liquids

History

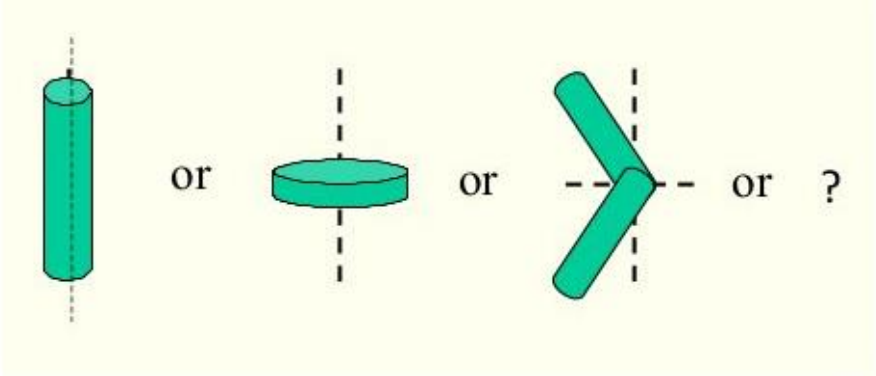
- Discovered by Reinitzer in 1888 : two melting points for cholesterol! !



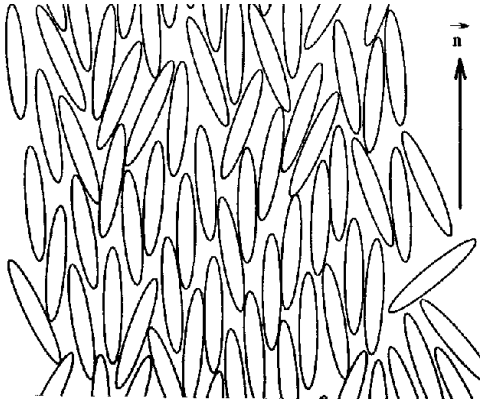
Courtesy: Peter Palffy-Muhoray Lectures at Colorado - Boulder

Nematic Liquid Crystals

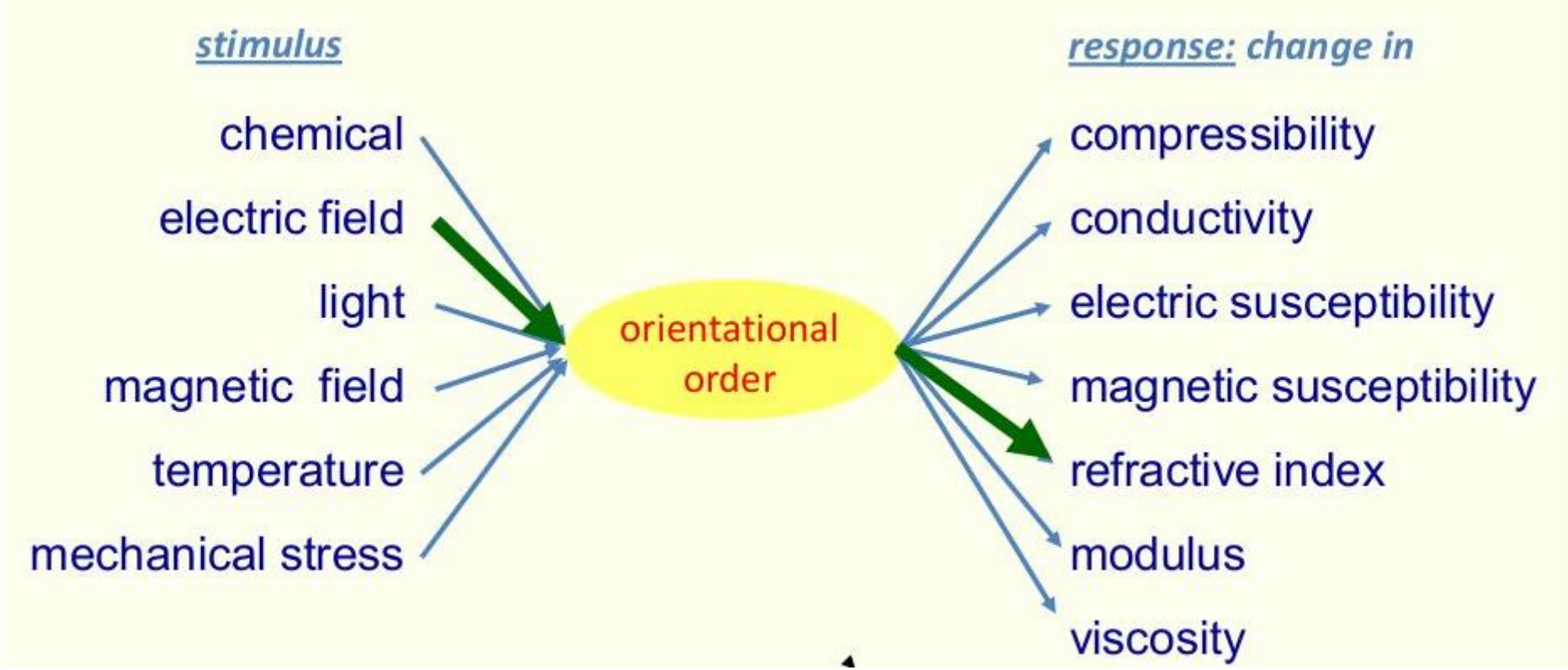
- Anisotropic rod-like molecules with directional properties



- Long-range orientational ordering: molecules line up with one another



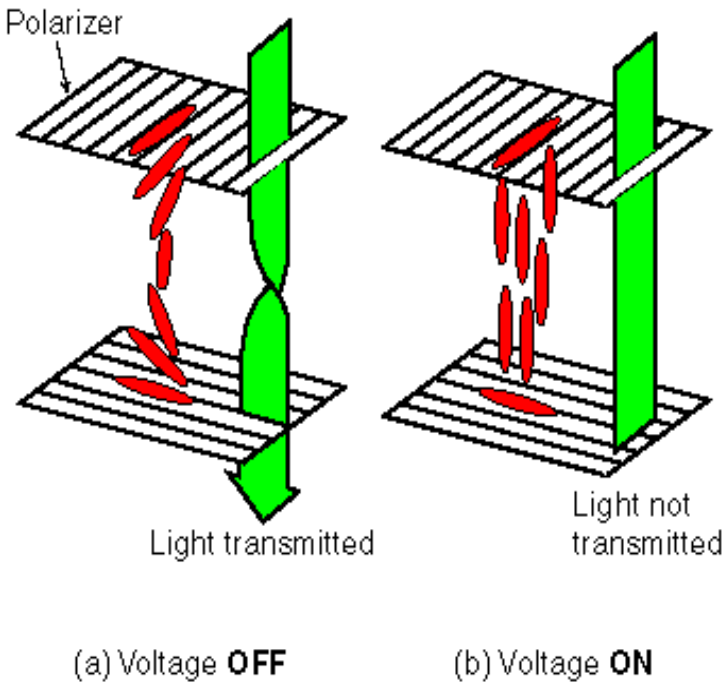
Key word: anisotropy!!!



Courtesy: Images from Peter Palffy-Muhoray's lectures at Colorado – Boulder (*Physics Today 60 (9), 54 (2007)*)

Nematic Anisotropy to Applications …

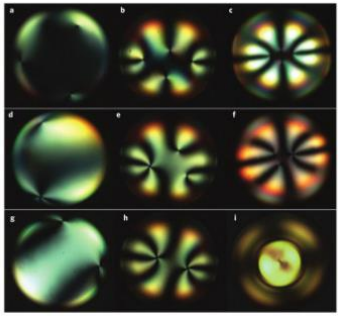
- Best known as the working material of the multi-billion dollar liquid crystal display (LCD) industry.



- Biology, Meta-materials, Photonics, Security Applications and many more…

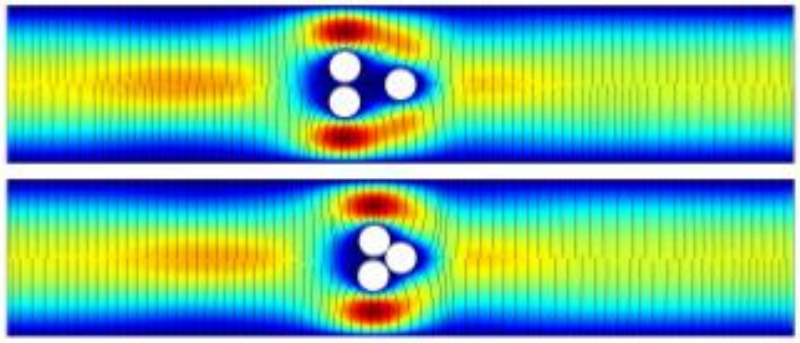
New Applications and New Research

- New Materials and Colloid Science



Liquid crystals in micron-scale droplets, shells, and fibers , *J. Phys.: Condens. Matter,*,(2017)

- Soft Robotics, Materials with Memory, Security Applications
- Microfluidics and Biomimetic Systems



S. Mondal, A. Majumdar and I.M. Griffiths 2017 Nematohydrodynamics for Colloidal Self-Assembly and Transport Phenomena. Journal of Colloid and Interface Science. 528, p. 431-442.

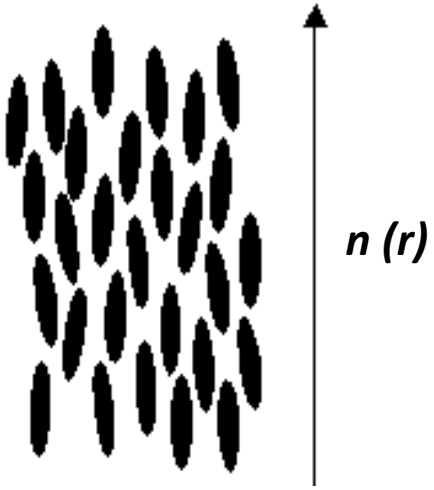
How do we mathematically model nematic liquid crystals?

Three popular "continuum" approaches - model "directions of preferred local molecular alignment/orientational order" and the "degree of orientational order".

- Oseen-Frank theory: restricted to "uniaxial phases" with a single direction of locally preferred alignment and "constant degree of orientational order".

- Ericksen theory: restricted to "uniaxial phases" with "variable degree of orientational order".

- Landau-de Gennes theory: account for primary and secondary directions of alignment and "variable degrees of orientational order".



Research themes

Theme I: Foundational aspects of continuum liquid crystal theories

- mathematics of defects: asymptotic analysis, structure and size of defect cores, approximate descriptions etc.

- analogies with other variational theories in materials science e.g. Ginzburg-Landau theory of superconductivity, nonlinear elasticity, micromagnetics.

- qualitative properties of solutions, stability?

D.Henao, A.Majumdar and A.Pisante 2017 Uniaxial versus Biaxial Character of Nematic Equilibria in Three Dimensions. Calculus of Variations and PDEs 56: 55.

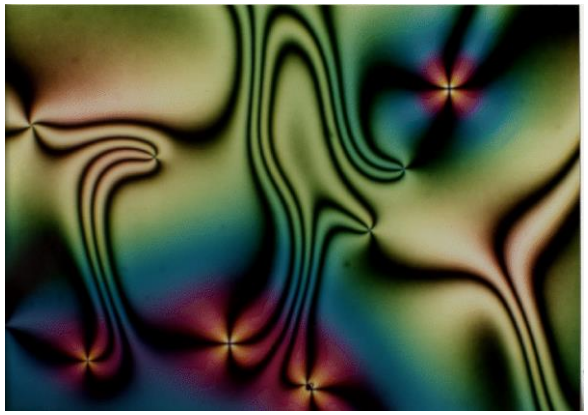
Canevari, G., Majumdar, A. and Spicer, A., 2017. Order reconstruction for nematics on squares and hexagons:a Landau-de Gennes study. *SIAM Journal on Applied Mathematics*, 77 (1), pp. 267-293.

Canevari, G., Ramaswamy, M. and Majumdar, A., 2016. Radial symmetry on three-dimensional shells in the Landau-de Gennes theory. *Physica D: Nonlinear Phenomena*, 314, pp. 18-34.

D. Henao & A.Majumdar 2012 Symmetry of uniaxial global Landau-de Gennes minimizers in the theory of nematic liquid crystals. SIAM Journal on Mathematical Analysis 44-5, 3217-3241.

A.Majumdar & A.Zarnescu, 2010 The Landau-de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. Archive of Rational Mechanics and Analysis, 196, 1, 227--280.

A.Majumdar, 2010 Equilibrium order parameters of liquid crystals in the Landau-de Gennes theory.European Journal of Applied Mathematics,21 , 181-203.



Point defects in liquid crystals.

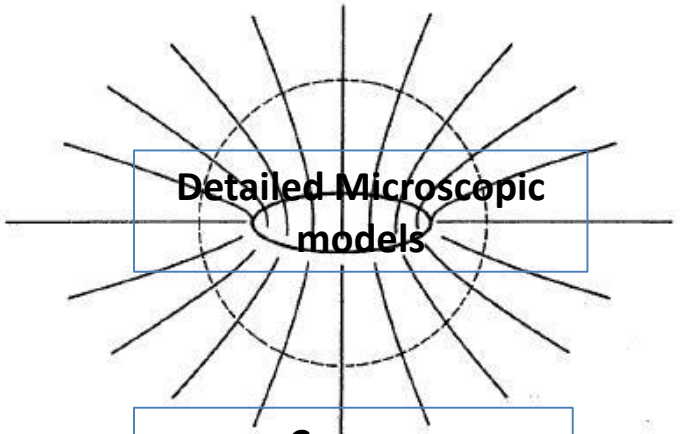
(**www.lci.kent.edu/defect.html**)

- **Theme II : Non-classical approaches**

- continuum theories can break down in critical scenari

- new continuum approaches

- new multiscale approaches that couple mean-field and macroscopic theories.



- G.Canevari, A.Majumdar and B.Stroffolini 2019 Minimizers of a Landau-de Gennes Energy with a Subquadratic Elastic Energy. Archive for Rational Mechanics and Analysis.

- M.Robinson, C.Luo, P.Farrell, R.Erban, and A.Majumdar 2017 From molecular to continuum modelling of bistable liquid crystal devices. Liquid Crystals, Volume 44, Issue 14-15, 2267-2284.

- J. Ball and A. Majumdar, 2010 Nematic liquid crystals : from Maier-Saupe to a continuum theory. Molecular Crystals and Liquid Crystals, 525, 111.

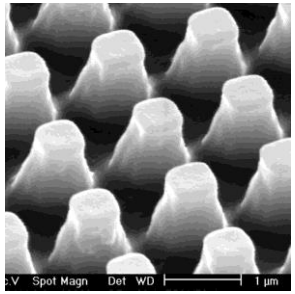
Theme III: Multistable Systems and Applications

- Directly motivated by industrial applications

- **Bistable liquid crystal displays**

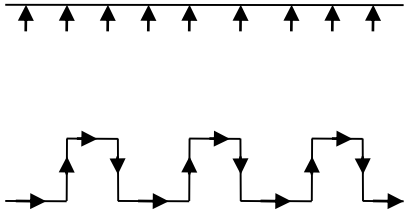
e.g. Planar Bistable Nematic Device; Post Aligned Bistable Nematic Device (Hewlett Packard) : **stable equilibria and switching**

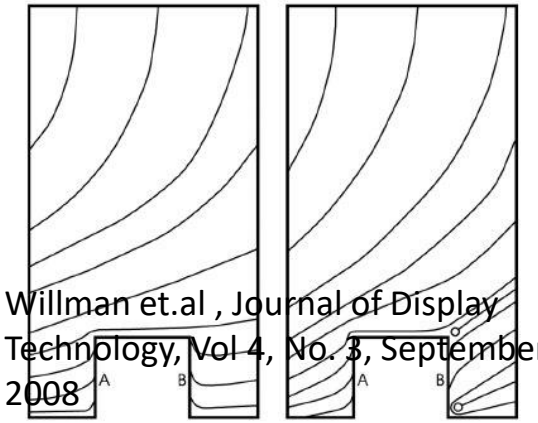
- modelling, optimisation and performance



Kitson and Geisow, Applied Physics Letters, 80,2002.

The Post Aligned Bistable Nematic Device, HP



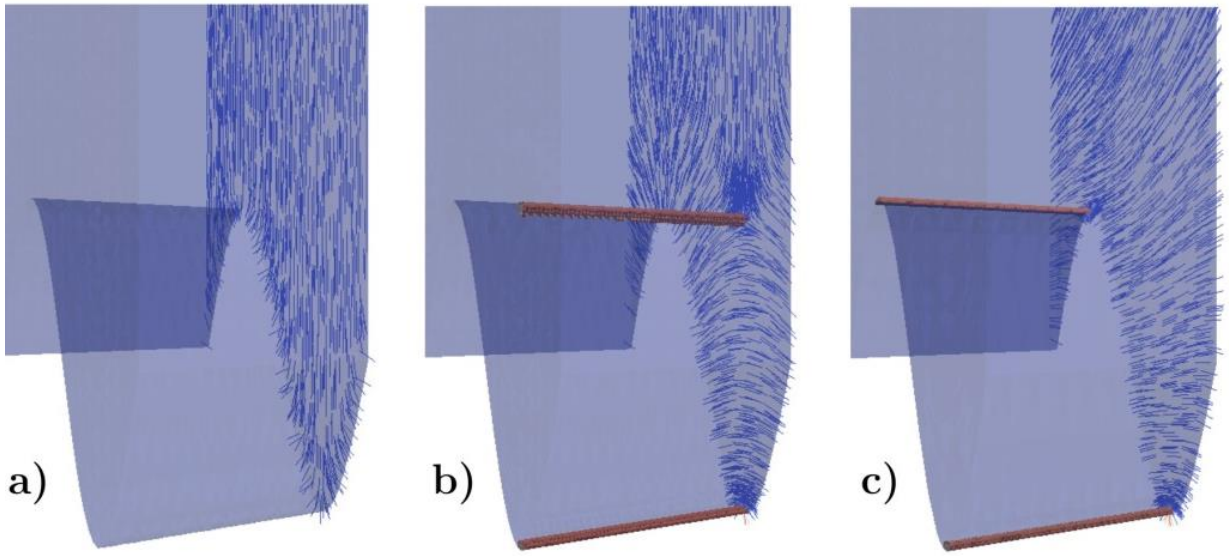


Willman et.al , Journal of Display Technology, Vol 4, No. 3, September 2008

A.Majumdar. C.J.P.Newton, J.M.Robbins and M.Zyskin 2007 Topology and bistability in liquid crystal devices. Physical Review E, 75, 051703 051714.

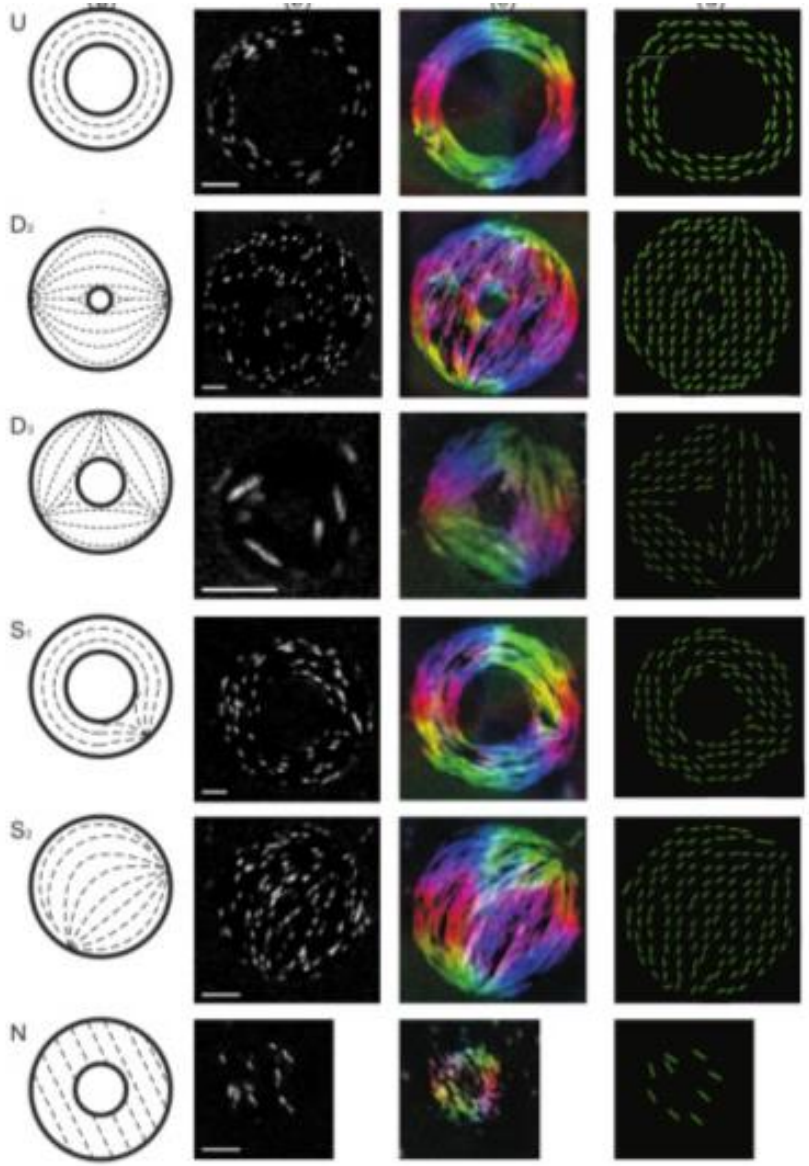
Theme III: Multistable Systems and Applications continued…

- The Zenithally Bistable Nematic Device



Raisch, A. and Majumdar, A., 2014. Order reconstruction phenomena and temperature-driven dynamics in a 3D zenithally bistable device. *EPL (Europhysics Letters)*, 107 (1), 16002.

Theme III: Multistable Systems and Applications continued



- A.Lewis et.al , 2014 Colloidal liquid crystals in rectangular confinement : Theory and experiment. Soft Matter, 39, pp. 7865-7873.
- A.H.Lewis, P.D.Howell, D.G.A.L.Aarts and A.Majumdar 2017 Nematic equilibria on a two-dimensional annulus: defects and energies. Studies in Applied Mathematics, 138, 438466.
- A.Lewis, P.Howell, D.Aarts and A.Majumdar 2017 Revisiting the two-dimensional defect-free azimuthal nematic equilibrium on an annulus. SIAM J. Appl. Math., 77(6), 18511875.

Why Liquid Crystals - Rich Mathematical Landscape

Partial Differential Equations

Calculus of Variations

Scientific Computation

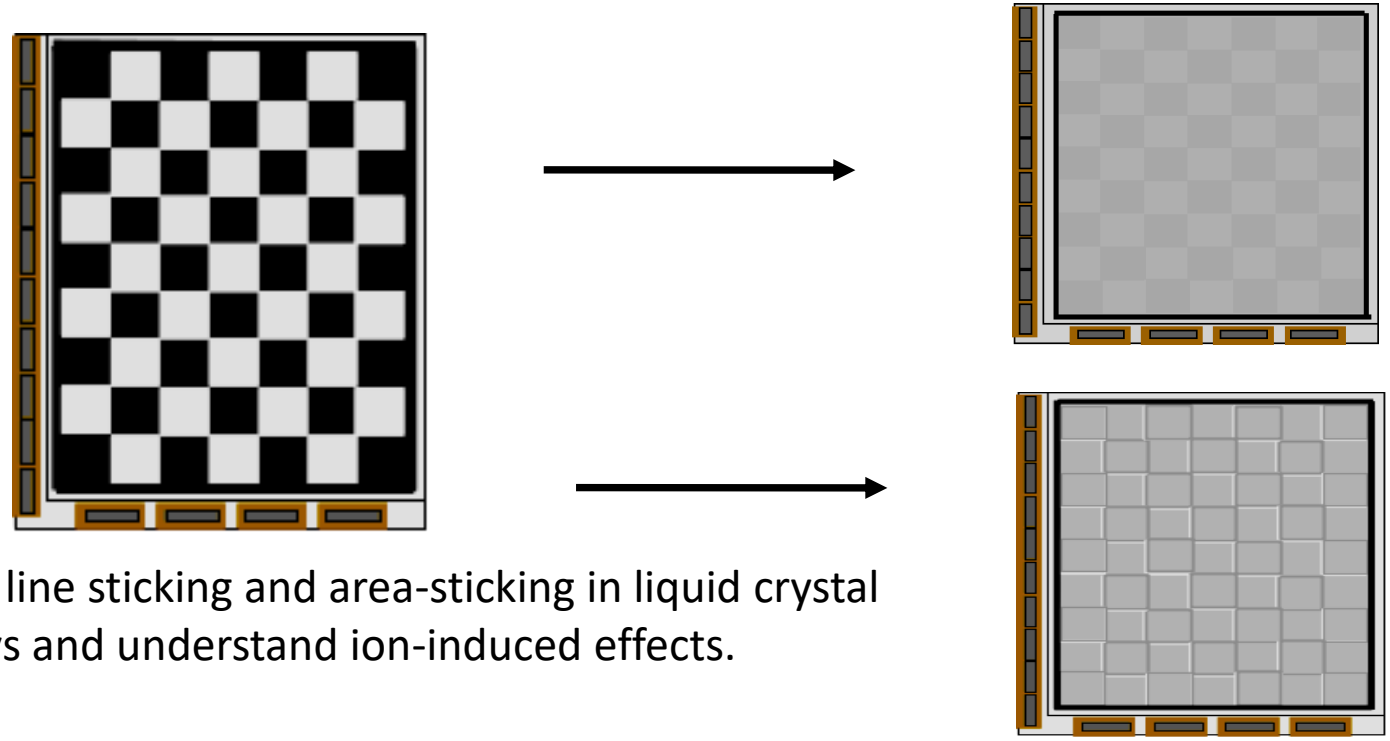
Algebra and Topology, Functional Analysis

Dynamical Systems

Postgraduate Students

- 2011- 2015: Alexander Lewis, University of Oxford
- 2012 – 2016: Amy Spicer, University of Bath
- 2017 – : Joseph Harris, University of Bath; University of Strathclyde
- 2019 - : James Dalby, University of Strathclyde
- 2018 - : Oliver Whitehead, University of Oxford
- 2017 - : Ruma Maity, Indian Institute of Technology Bombay.
- University of Bath – Aaron Pim, Tina Zhou
- International junior researchers – India, China, Luxembourg

The MERCK Problem



- Model line sticking and area-sticking in liquid crystal displays and understand ion-induced effects.

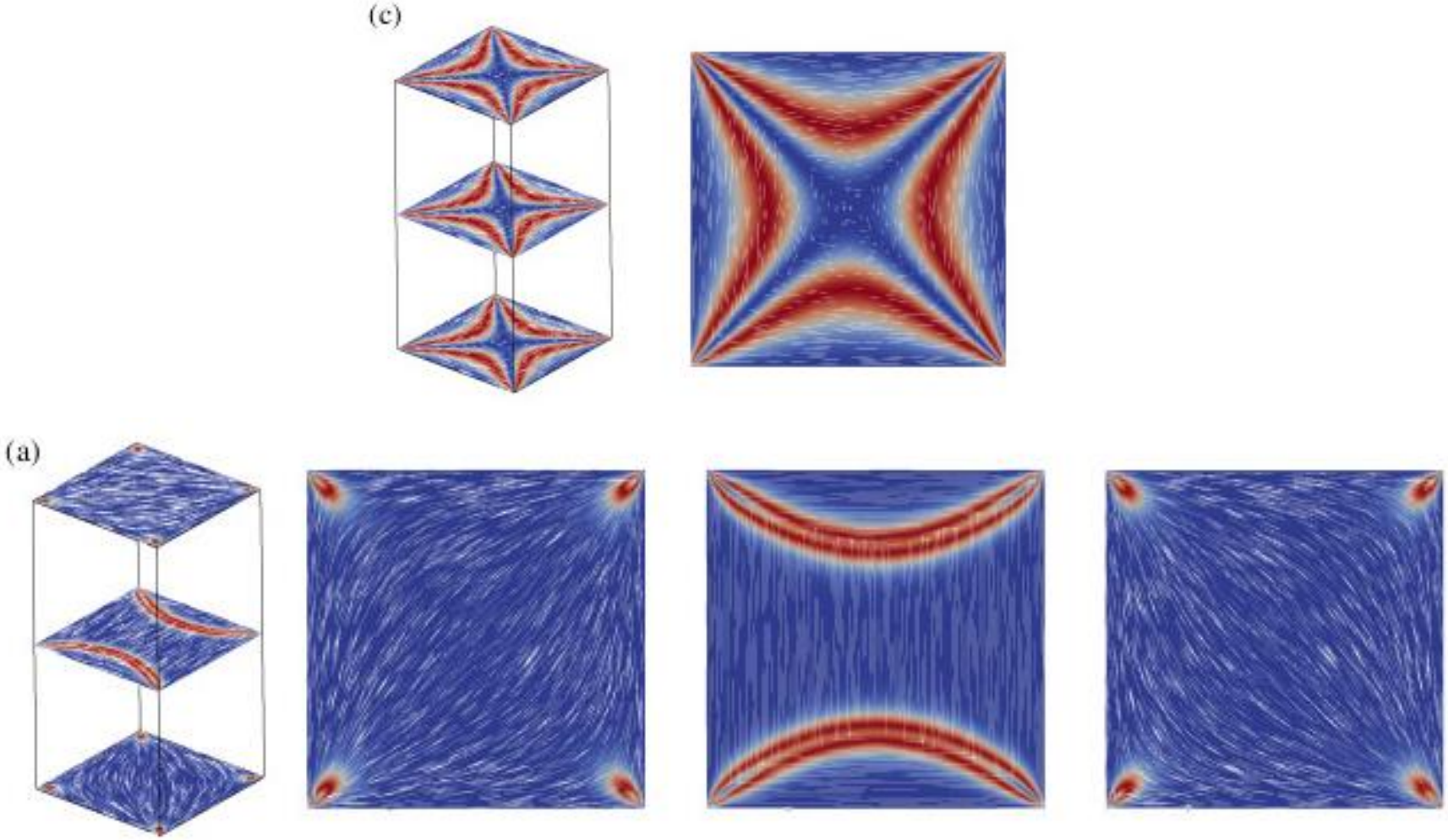
- The Team - Oliver Whitehead, Ian Griffiths, Colin Please, Apala Majumdar, Leo Weegels, David Wilkes, Rachel Tuffin

Multistability in Confined Nematics

- The Team: Joseph Harris (Strathclyde), Apala Majumdar (Strathclyde), Yucen Han (Peking University), Lei Zhang (Peking University)
-
- Analysis and Numerical Simulations of Nematics in Different Geometries – Square Wells, Hexagons, Pentagons.
-
- Complex solution landscapes – stability and multiplicity of stable profiles, their defect sets and control strategies for new systems.

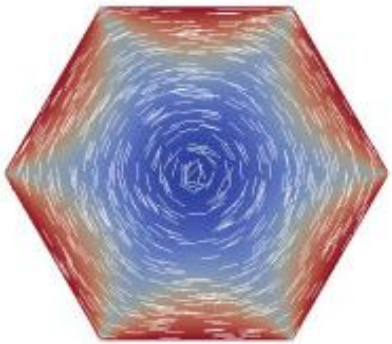
Joseph Harris

Some examples…



- See G.Canevari, J.Harris, Y.Wang and A.Majumdar 2020. The Well Order Reconstruction Solution for Three-Dimensional Wells, in the Landau-de Gennes theory. International Journal of Non-Linear Mechanics.

Some examples…



WORS

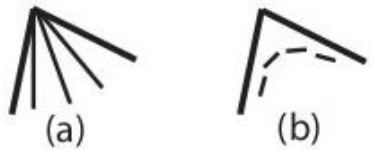
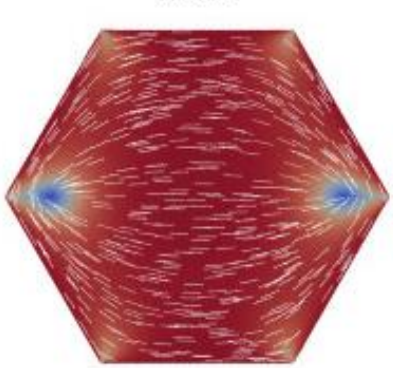
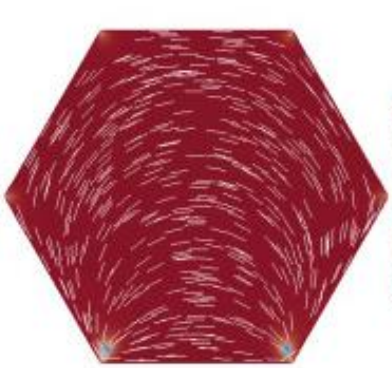


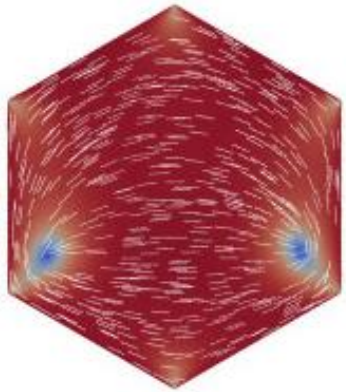
Figure 9: Two arrangements of nematics in the corner. (a) splay; (b) bend



Diagonal



Over Rotated



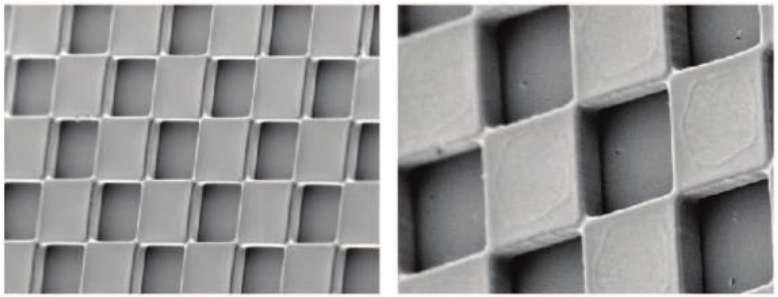
Rotated

- Joint work with Lei Zhang (Peking), Yucen Han (Peking)..

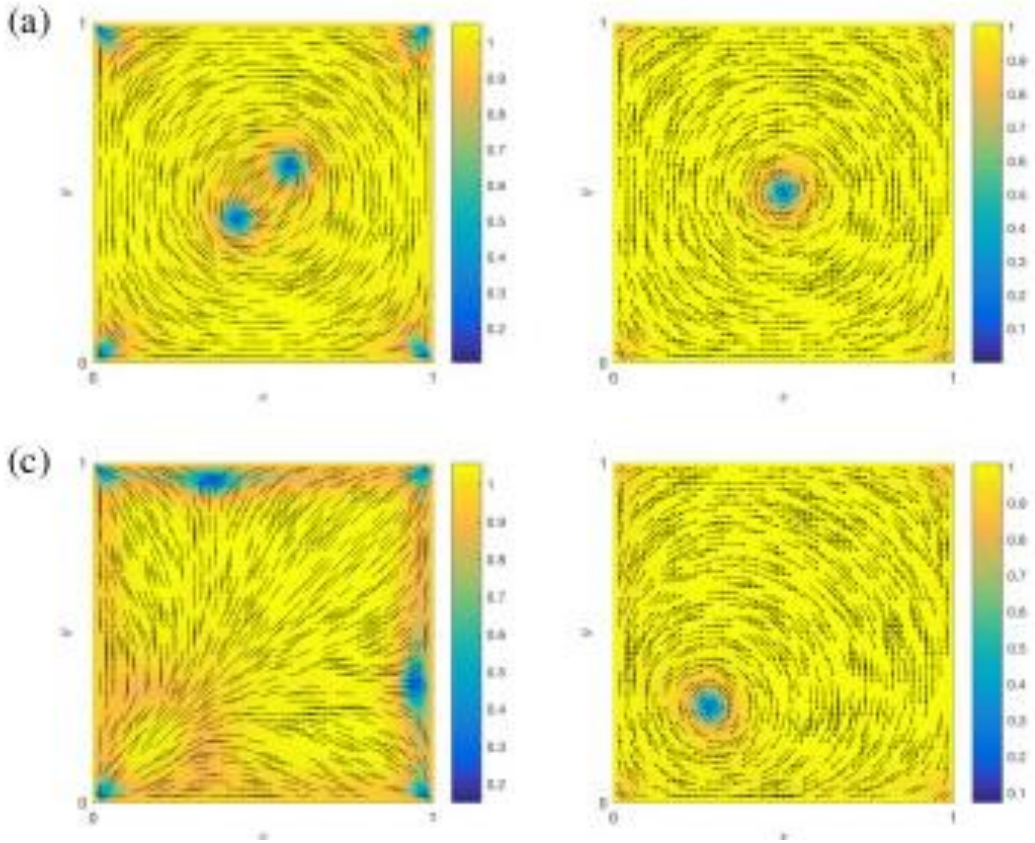
Ferronematics

- The Team: James Dalby (Strathclyde), Apala Majumdar (Strathclyde), Patrick Farrell (Oxford), Jingmin Xia (Oxford)
- Analysis and Numerical Simulations of ferronematics – examples of materials which have nematic and magnetic properties.
- Investigate the coupling between nematic and magnetic order and exotic defect profiles.
- Complex bifurcation diagrams.
- Continuum Mechanics, Nonlinear Partial Differential Equations, Topology and Numerical Methods.

James Dalby



Tsakonas, Davidson, Brown, Mottram , Appl. Phys. Lett. 90, 111913 (2007)



- https://journals.aps.org/pre/abstract/10.1103/PhysRevE.100.012703
- https://journals.aps.org/pre/abstract/10.1103/PhysRevE.101.022706https://arxiv.org/abs/1907.03833

Numerical Analysis of Confined Nematics

- The Team: Ruma Maity (IIT Bombay), Neela Nataraj (IIT Bombay), Apala Majumdar (Strathclyde)
- Analyse convergence and stability of numerical schemes for liquid crystals models.
- Discontinuous Galerkin Methods
- Conforming Finite Element Methods
- Nitsche Methods.

Ruma Maity

R.Maity, A.Majumdar and N.Nataraj 2020 Discontinuous Galerkin Finite Element Methods for the Landau-de Gennes Minimization Problem for Liquid Crystals. IMA Journal of Numerical Analysis.

Maity, Ruma Rani & Majumdar, Apala & Nataraj, Neela. (2020). A priori and a posteriori error analysis for the Nitsche's method of a reduced Landau-de Gennes problem.

Current UK Landscape

- **Strathclyde**

  - Continuum Mechanics and Industrial Mathematics
  - Numerical Analysis
  - Applied Analysis and Stochastic Analysis
  - Multiple postgraduate opportunities: Student Excellence Award, John Anderson Award, Project-Led Studentships, International Partners.
  - **Scottish University of the Year 2020**
  - **Times Higher Education University of the Year 2019**

Current UK Landscape (some examples)

- **University of Bath**

  - SAMBa (Statistical and Applied Mathematics at Bath)

  - Centre for Nonlinear Mechanics

- **University of Oxford**

  - InfoMM (Industrially Focused Mathematical Modelling)

- **University of Bristol; University of Manchester**

- **Many More!!**

  - Lots of postgraduate opportunities!!!

Liquid Crystals are a fascinating playground for mechanics, geometry, modelling and analysis to meet physics and real-life applications.

- Real opportunity for new mathematics-driven approaches to new materials, optimal design, optimal performance and efficient methodologies.

Acknowledgments:

- DST-UKIERI Project on “Theoretical and Experimental Studies of Magnetic Nanoparticles in Anisotropic Media”
- Royal Society Newton Advanced Fellowship
- Leverhulme Trust & Daiwa Foundation
- University of Strathclyde, New Professors Fund
- Visiting Professorship, University of Bath
- Visiting Fellowship, University of Oxford
- London Mathematical Society & the organizers!!

THANK YOU FOR YOUR ATTENTION !!