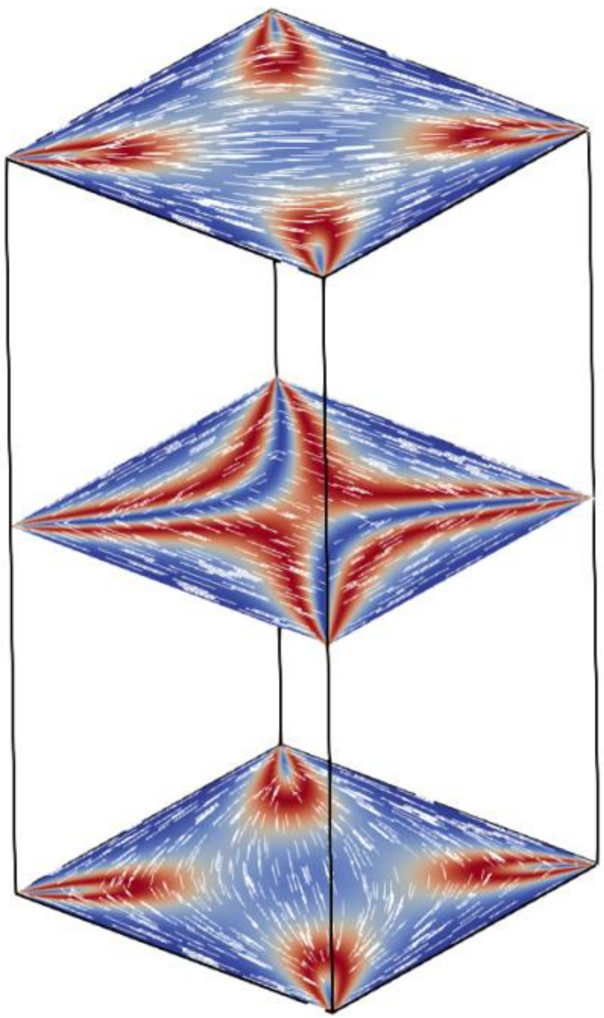


THE WELL ORDER RECONSTRUCTION SOLUTION FOR THREE-DIMENSIONAL WELLS

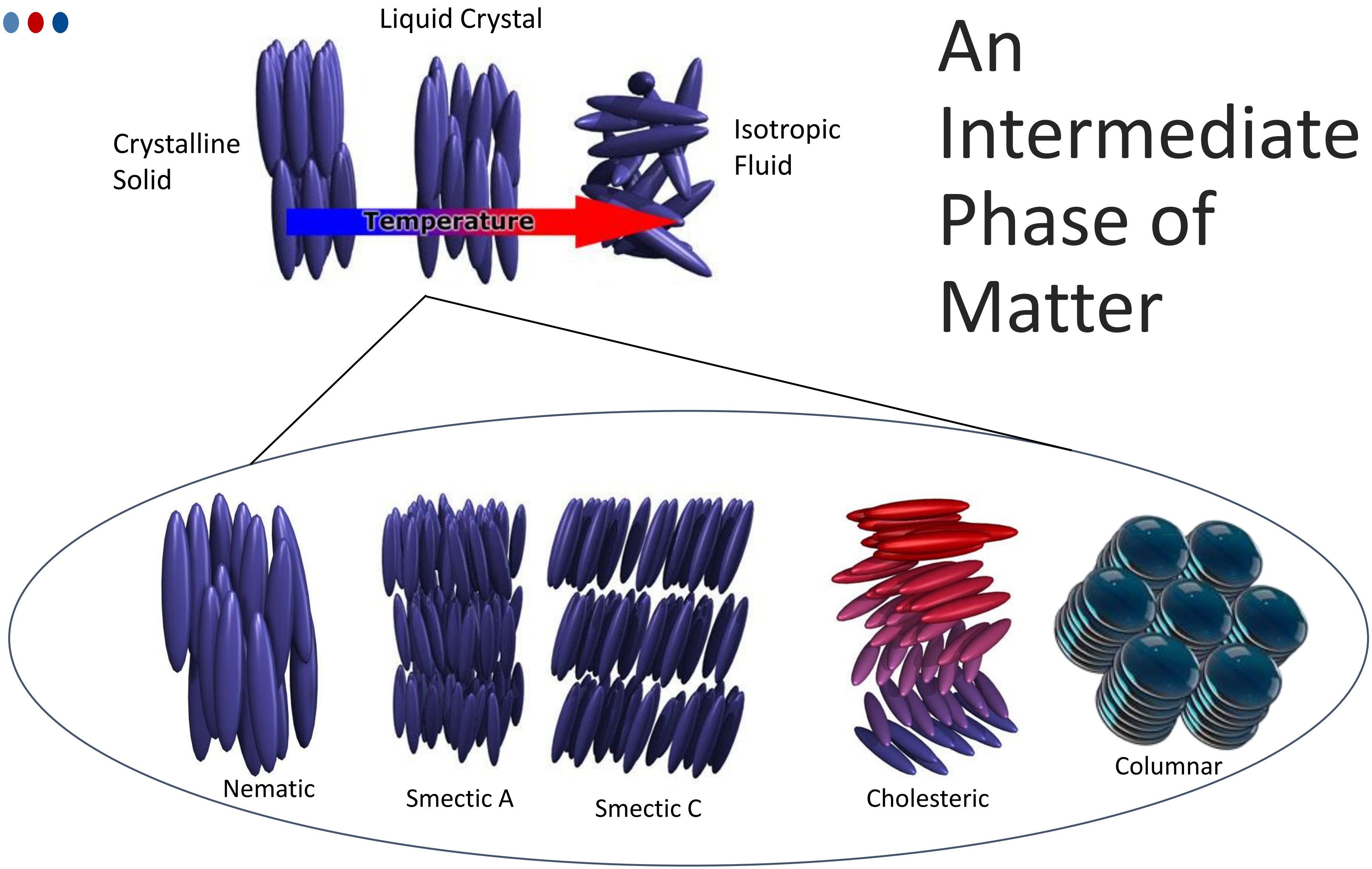
Joseph Harris

Joint work with Apala Majumdar (PhD Supervisor), Giacomo Canevari and Yiwei Wang

Department of Mathematical Sciences

University of Bath, UK

An Intermediate Phase of Matter



THE LANDAU-DE GENNES MODEL

We describe the nematic state by the macroscopic order parameter $\boldsymbol{Q}$ (traceless, symmetric 3x3 matrix).

In the absence of surface energies, we minimize the LdG energy given by

$$\mathcal{F}_\lambda[\boldsymbol{Q}] = \iiint \frac{1}{2}|\nabla \boldsymbol{Q}|^2 + \frac{\lambda^2}{L} f_b(\boldsymbol{Q})\, dV$$

where λ is a characteristic length scale, $L > 0$ a material-dependent elastic constant.

The thermotropic bulk potential is given by

$$f_b(\boldsymbol{Q}) = \frac{A}{2} tr\boldsymbol{Q}^2 - \frac{B}{3} tr\boldsymbol{Q}^3 + \frac{C}{4}(tr\boldsymbol{Q}^2)^2$$

For a given $A < 0$, minimizers of f_b have the form:

$$\boldsymbol{Q} = s_+\left(\boldsymbol{n}\otimes\boldsymbol{n} - \frac{\boldsymbol{I}}{3}\right), \quad \boldsymbol{n} \in S^2$$

where

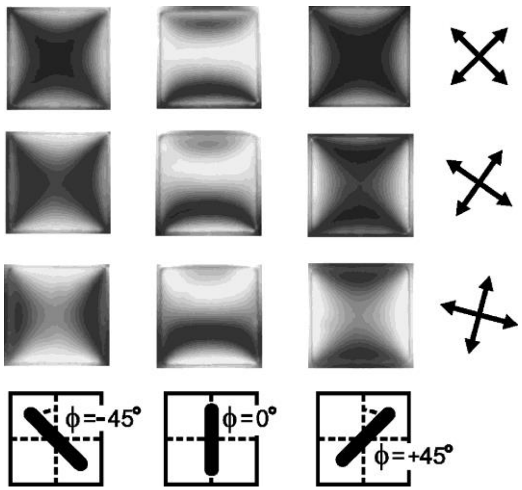
$$s_+ = \frac{B + \sqrt{B^2 + 24|A|C}}{4C}$$

$A = \frac{B^2}{24C}$

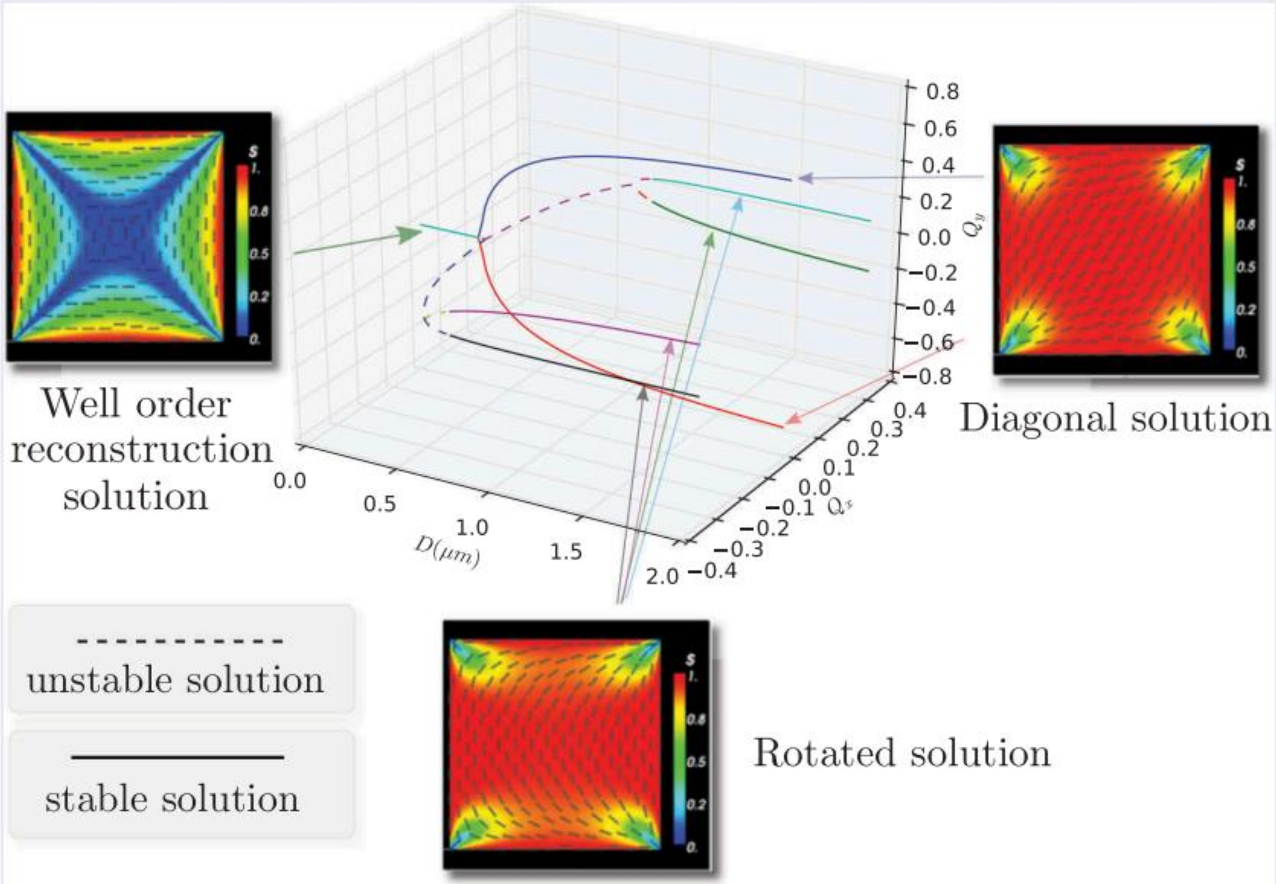
$A = \frac{B^2}{27C}$

$A = 0$

$A = -\frac{B^2}{3C}$



Tsakonas et.al. (2007). Multistable alignment states in Nematic liquid crystal filled wells. *Appl. Phys. Lett*, 1-18. https://doi.org/10.1063/1.2713140



Robinson et.al. (2017). From molecular to continuum modelling of bistable liquid crystal devices. *Liquid Crystals*, 1-18. https://doi.org/10.1080/02678292.2017.1290284

THE WELL ORDER RECONSTRUCTION SOLUTION (WORS)

The WORS is an interesting nematic liquid crystal equilibria for two reasons:

- It partitions the square into four quadrants and the nematic director is approximately constant in each quadrant according to the tangent condition on the corresponding edge
- The WORS has a defect line along each square diagonal and the two intersect at the centre, yielding the quadrant structure

The WORS has a constant eigenframe and is uniaxial along the square diagonals with negative order parameter and can therefore be described by solutions of the form –

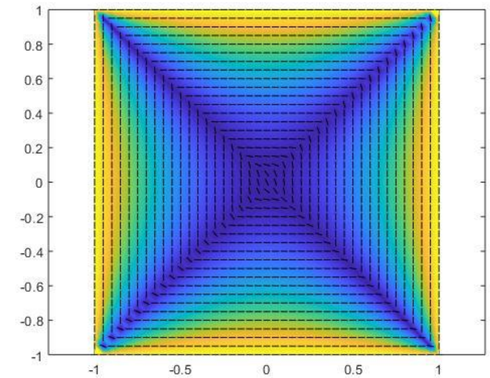
$$\boldsymbol{Q} = q_1(\boldsymbol{n}_1 \otimes \boldsymbol{n}_1 - \boldsymbol{n}_2 \otimes \boldsymbol{n}_2) + q_3(\hat{\mathbf{z}} \otimes \hat{\mathbf{z}} - \boldsymbol{I}/3)$$

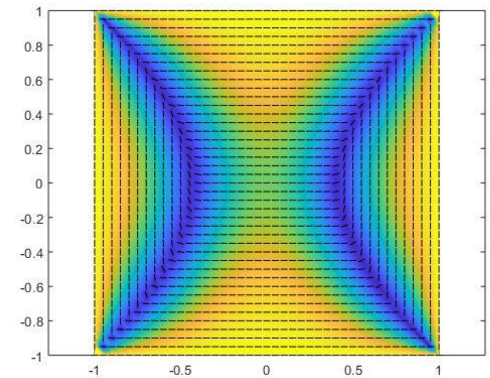
- The WORS was numerically reported by **Kralj, Majumdar (2014)** in 2D

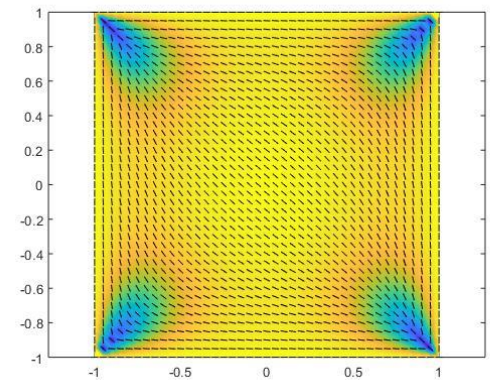
- This was analysed further in **Majumdar et.al. (2016)**, **Canevari et.al. (2017)** and **Wang et.al. (2018)** at a fixed temperature

- As proven in **Wang et.al. (2018)**, the WORS survives in the *thin film limit*

- It is our aim to observe the WORS for square wells with a finite height, exemplifying the 3D relevance of WORS-type solutions for all temperatures below the nematic supercooling temperature (i.e. the deep nematic regime $A < 0$)

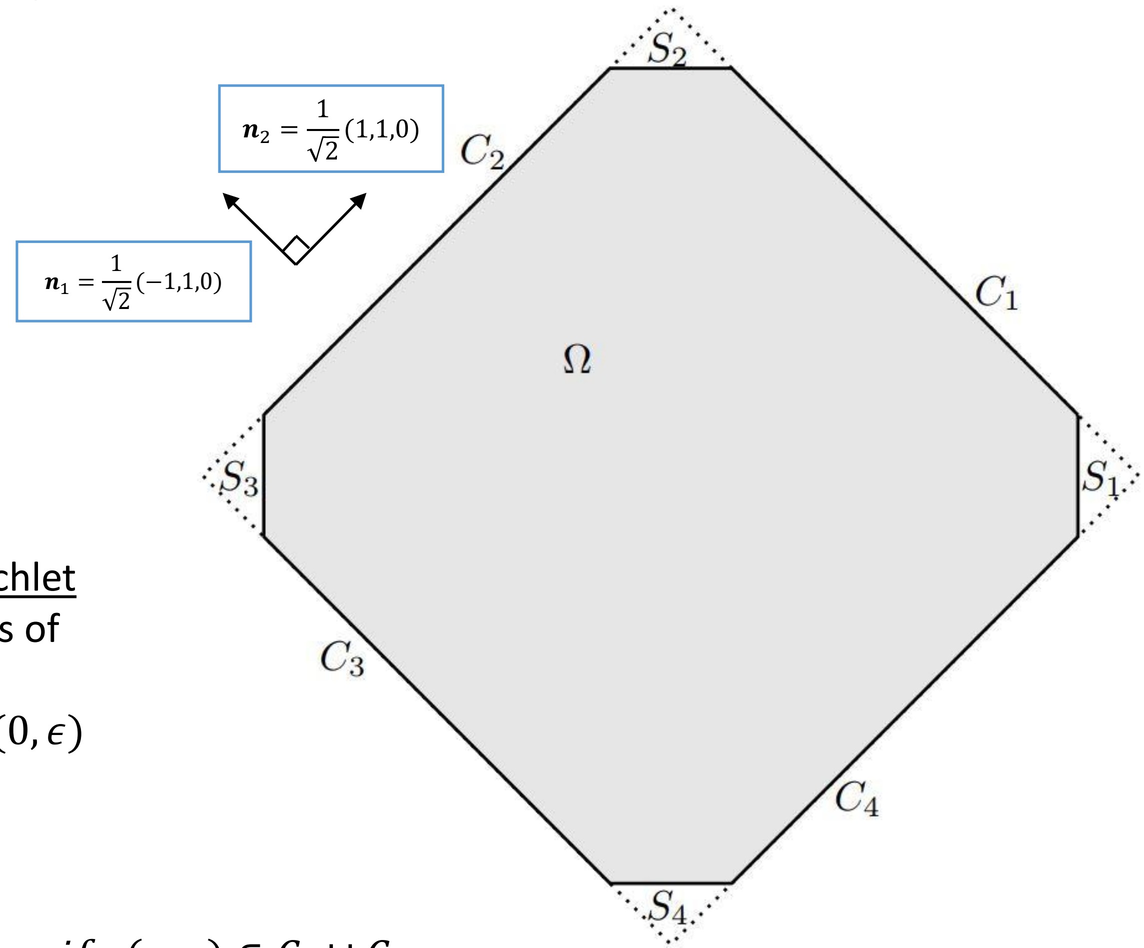






BOUNDARY CONDITIONS ON THE LATERAL SURFACES

Define $V = \Omega \times (0, \epsilon)$, for ϵ finite.



We impose tangent uniaxial Dirichlet conditions on the lateral surfaces of the well:

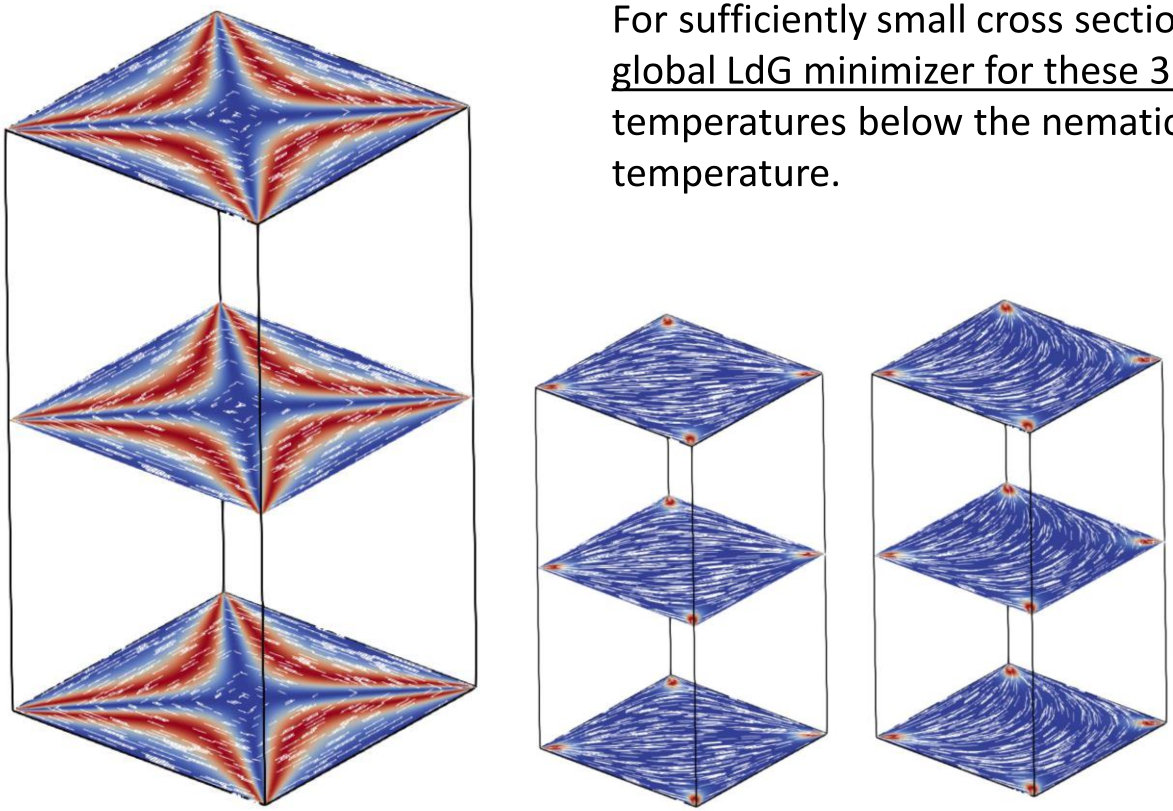
$$\boldsymbol{Q} = \boldsymbol{Q}_b \quad \text{on} \quad \partial\Omega \times (0, \epsilon)$$

$$\boldsymbol{Q}_b(x, y, z) := \begin{cases} s_+\left(\boldsymbol{n}_1 \otimes \boldsymbol{n}_1 - \frac{\boldsymbol{I}}{3}\right) & if \quad (x, y) \in C_1 \cup C_3 \\ s_+\left(\boldsymbol{n}_2 \otimes \boldsymbol{n}_2 - \frac{\boldsymbol{I}}{3}\right) & if \quad (x, y) \in C_2 \cup C_4 \end{cases}$$

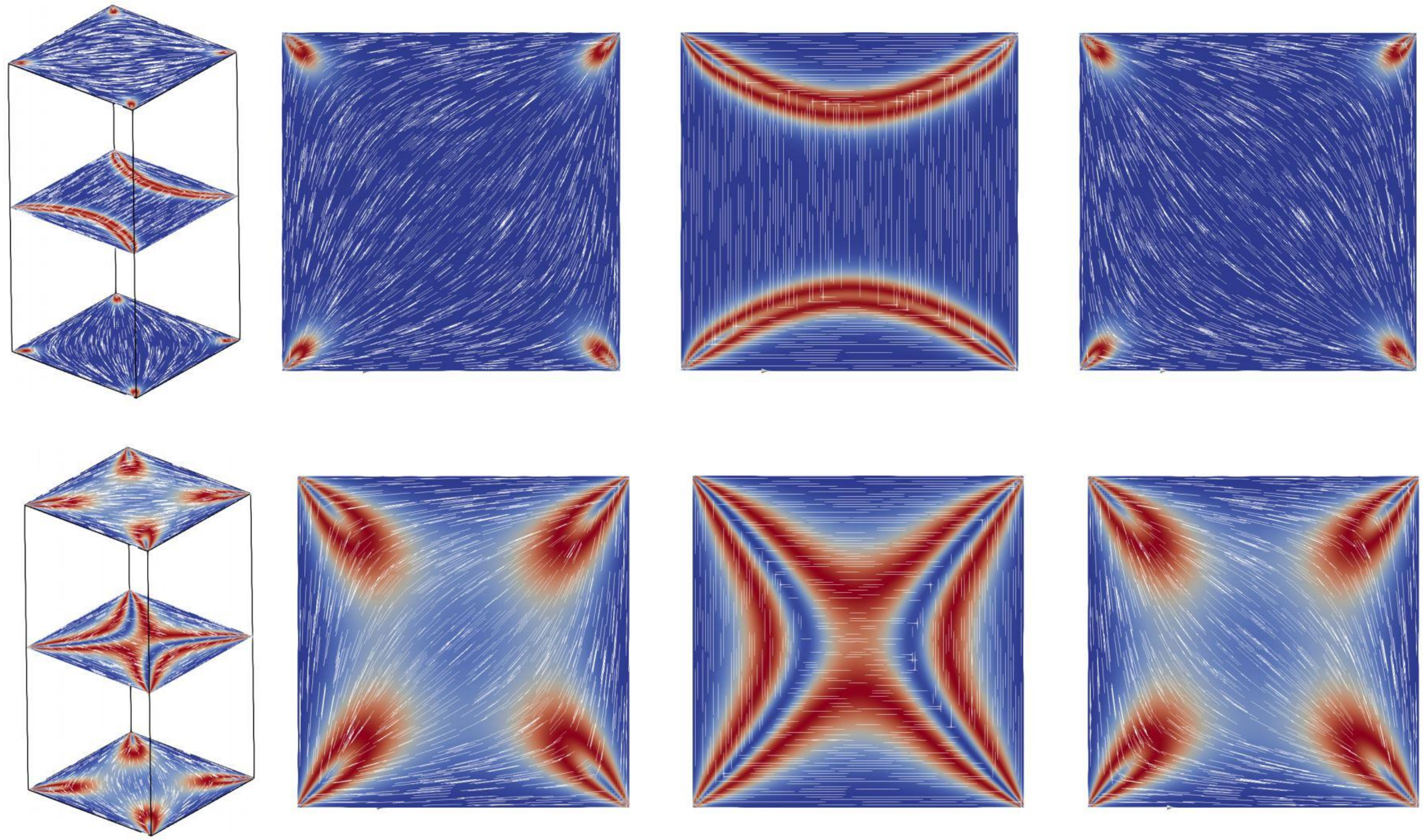
NATURAL BOUNDARY CONDITIONS ON THE TOP AND BOTTOM PLATES

$$\partial_z \boldsymbol{Q} = 0 \quad on \quad \Omega \times \{0, \epsilon\}$$

For sufficiently small cross section size, λ, the WORS is the global LdG minimizer for these 3D problems for all temperatures below the nematic supercooling temperature.



WORS, diagonal and rotated solutions with $|\partial_z \boldsymbol{Q}|^2 \approx 10^{-12}$. With square cross section $\lambda^2 = 5$ (left), and $\lambda^2 = 100$ (right).



For large enough well height, ϵ, and relatively large λ, we demonstrate the existence of stable mixed 3D solutions with two different diagonal profiles on the top and bottom plates.

Mixed 3D solutions for $\lambda^2 = 100$ (top), and $\lambda^2 = 10$ (bottom), with cross sections at $z = 0, 2, 4$.

SURFACE ANCHORING ON THE TOP AND BOTTOM PLATES

$$\mathcal{F}_\lambda[\boldsymbol{Q}] = \iiint \frac{1}{2}|\nabla \boldsymbol{Q}|^2 + \frac{\lambda^2}{L} f_b(\boldsymbol{Q})\, dV + \frac{\lambda}{L}\int f_s(\boldsymbol{Q})\ dS$$

$$f_s(\boldsymbol{Q}) = \alpha_z\left(\boldsymbol{Q}\hat{\boldsymbol{z}}\cdot\hat{\boldsymbol{z}} + \frac{s_+}{3}\right)^2 + \gamma_z|(\boldsymbol{I} - \hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{z}})\boldsymbol{Q}\hat{\boldsymbol{z}}|^2, \qquad \alpha_z, \gamma_z > 0$$

f_s favours $\boldsymbol{Q}$-tensors that have $\hat{\boldsymbol{z}}$ as an eigenvector with constant eigenvalue $-\frac{s_+}{3}$ on the top and bottom plates.

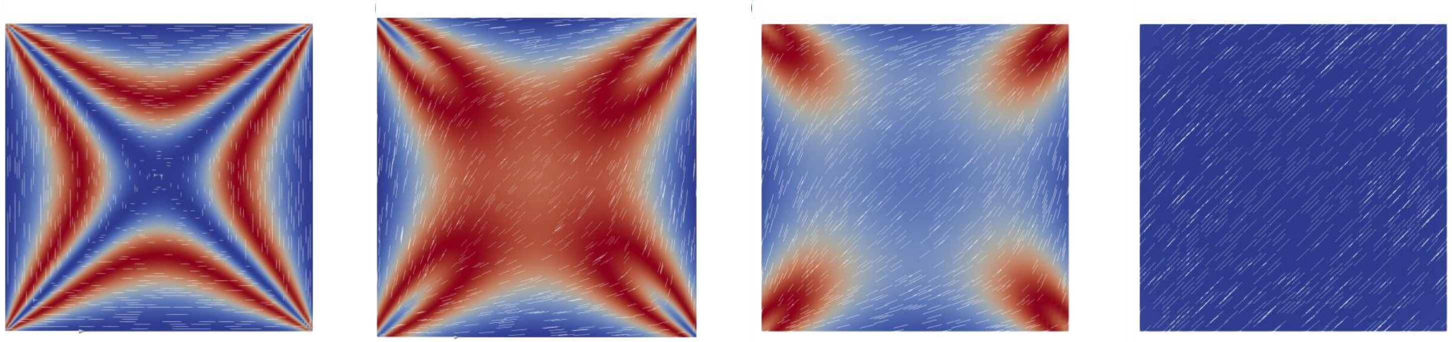
For sufficiently small λ, there is a unique WORS-type solution to this 3D problem.

WEAK ANCHORING ON THE LATERAL SURFACES

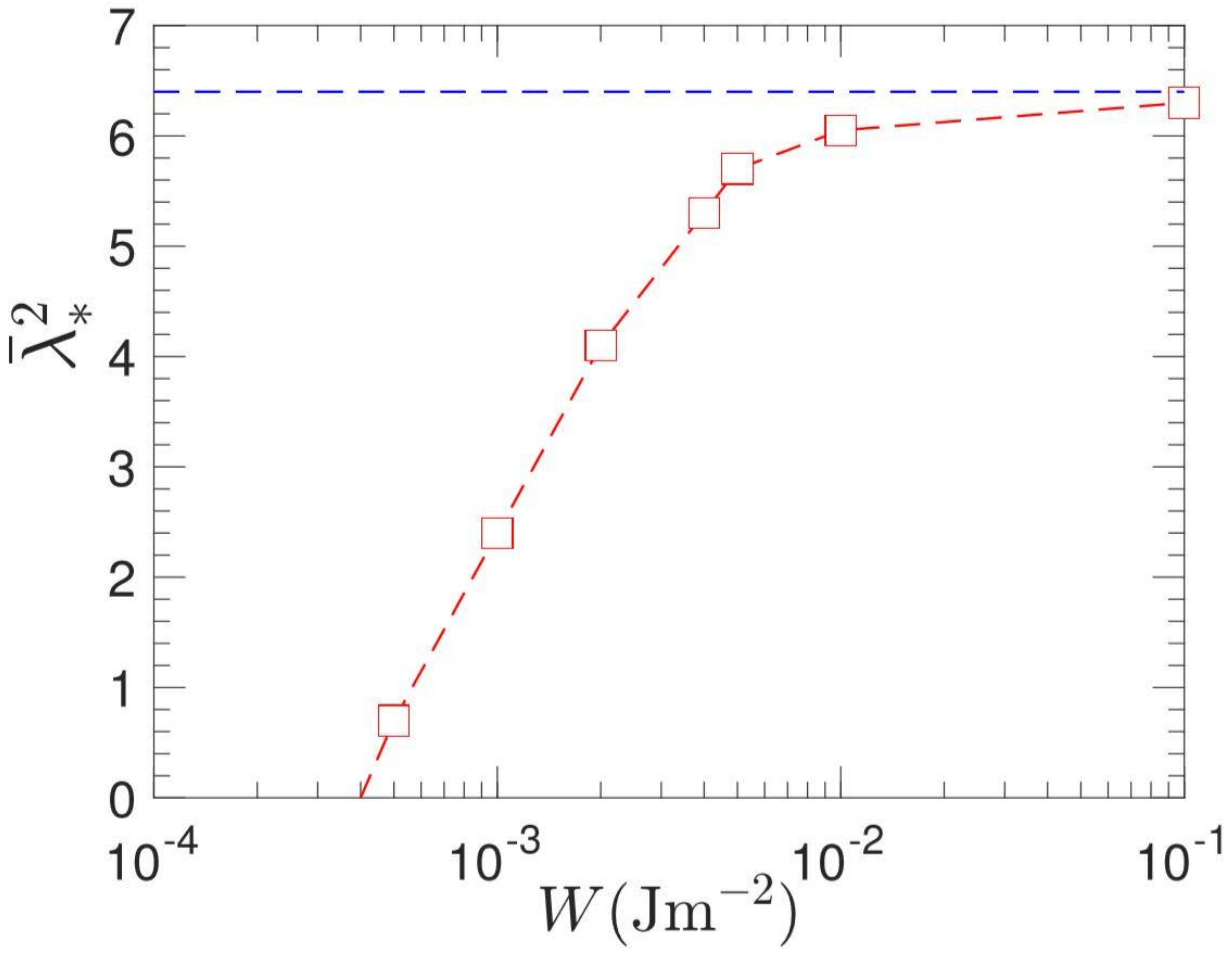
$$g(x) = s_+, \qquad \forall x \in [-1+\delta, 1-\delta]$$

$$f_s(\boldsymbol{Q}) = \begin{cases} \frac{W_1 \lambda}{L}\left(\boldsymbol{Q} - g(x)\left(\hat{\boldsymbol{x}} \otimes \hat{\boldsymbol{x}} - \frac{I}{3}\right)\right)^2, & y = 0,1 \\ \frac{W_2 \lambda}{L}\left(\boldsymbol{Q} - g(y)\left(\hat{\boldsymbol{y}} \otimes \hat{\boldsymbol{y}} - \frac{I}{3}\right)\right)^2, & x = 0,1 \end{cases}$$

Eliminates discontinuity at the corners.



Transition from the WORS to a diagonal solution by weakening the anchoring strength on the lateral surfaces for $W_i = 10^{-2} Jm^{-2}$ (left) to $W_i = 10^{-4} Jm^{-2}$ (right).



Bifurcation points, below which the WORS is the unique solution as a function of anchoring strength. The blue dashed line indicates the bifurcation point of the WORS for Dirichlet boundary condition in a 2D square well.

- This talk is based on joint work with collaborators **Giacomo Canevari**, **Apala Majumdar** and **Yiwei Wang**.

- Submitted paper: The Well Order Reconstruction Solution for Three-Dimensional Wells, in the Landau-de Gennes theory (2019).

- Preprint submitted to the **International Journal of Nonlinear Mechanics**.

THANK YOU

jh981@bath.ac.uk

arXiv:1903.03873