Nematic Liquid Crystals in Lipschitz domains

Anupam Pal Choudhury Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria

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In this talk, we shall discuss the simplified Ericksen–Leslie model for nematic liquid crystals in three dimensional bounded Lipschitz domains. Applying a semilinear approach, we shall discuss the proof of local and global well-posedness (assuming a smallness condition on the initial data) in critical spaces for initial data in L^3_σ for the fluid and $W^{1,3}$ for the director field. The analysis of such models, so far, has been restricted to domains with smooth boundaries.

Based on a joint work with Amru Hussein and Patrick Tolksdorf

Reference:

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Outline of the talk

- Introduction
- The case of Neumann boundary data
- ▶ The case of Dirichlet boundary data
- Concluding remarks and Future directions

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At the molecular level:

Crystals- Groups of molecules are regularly stacked. Molecular order is present, that is, certain pattern repeats.

Isotropic liquids- Properties independent of directions in which they are measured. Molecular patterns are not present.

Liquid crystals- Order exists at least in one-direction in space combined with anisotropy.

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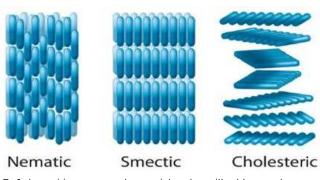
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Three phases of liquid crystals:

- Nematic phase: No positional order present but a long-range translational order. Thus, it differs from isotropic liquids in which molecules are arbitrarily oriented. Preferred direction varies throughout the medium.
- Smectic phase: Set of two-dimensional liquid layers on top of each other. Preferred direction within each layer but the preference varies over layers.
- ▶ Cholesteric phase: Two-dimensionally ordered systems in three dimensions following a helical structure. As in the smectic phase, no positional ordering within layers but a preferred direction in each layer.

In this talk, we shall focus on a simplified model for nematic liquid crystals.



 $Ref:\ http://www.qsstudy.com/chemistry/liquid-crystals$

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Definition (Lipschitz boundary)

The boundary $\partial\Omega$ of a bounded domain $\Omega\subset\mathbb{R}^n$ is said to be $\mbox{\it Lipschitz}$ if for each point $x\in\partial\Omega$, there exist r>0 and a $\mbox{\it Lipschitz}$ continuous mapping $\gamma:\mathbb{R}^{n-1}\to\mathbb{R}$ such that, upon rotating and relabeling the coordinate axes if necessary, we have

$$\Omega \cap Q(x,r) := \{y | \gamma(y_1, \cdots, y_{n-1}) < y_n\} \cap Q(x,r),$$

where

$$Q(x,r) := \{y | |y_i - x_i| < r, i = 1, \dots, n\}.$$

In other words, near each point $x \in \partial \Omega$, the boundary is the graph of a Lipschitz continuous function.

The isothermal simplified Ericksen-Leslie model

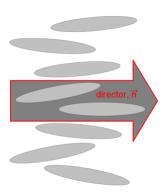
Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary $\partial \Omega$. The isothermal simplified Ericksen-Leslie model is given by

$$\begin{aligned} \partial_t u + (u \cdot \nabla) u - \nu \Delta u + \nabla \pi &= -\lambda \text{div}([\nabla d]^\top \nabla d) \text{ in } (0, T) \times \Omega, \\ \partial_t d + (u \cdot \nabla) d &= \gamma (\Delta d + |\nabla d|^2 d) \text{ in } (0, T) \times \Omega, \\ \text{div } u &= 0 \text{ in } (0, T) \times \Omega, \\ (u, d) \Big|_{t=0} &= (a, b) \text{ in } \Omega. \end{aligned}$$

- ▶ $u:(0,\infty)\times\Omega\to\mathbb{R}^n$ denotes the velocity field, $\pi:(0,\infty)\times\Omega\to\mathbb{R}$ denotes the pressure.
- ▶ $d:(0,\infty)\times\Omega\to\mathbb{R}^n$ denotes the molecular orientation of the liquid crystal at the macroscopic level (we shall also refer to this as the director field). This physical interpretation of d further imposes the condition

$$|d|=1$$
 in $(0,T)\times\Omega$.

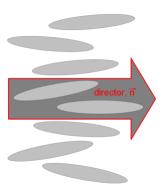
• Without loss of generality, we shall also assume that $\nu = \gamma = \lambda = 1$.



Ref: Wikipedia

- ▶ The notation *n* corresponds to *d* in the pde.
- ► Ericksen-Leslie theory for nematic liquid crystals was developed in 1960's.

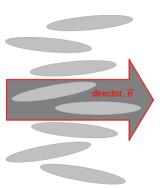
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Boundary conditions:

$$\begin{split} u &= 0 \text{ on } (0,T) \times \partial \Omega, \\ \partial_{\nu} d &= 0 \text{ on } (0,T) \times \partial \Omega \text{ (Neumann boundary condition) or } \\ d &= \tilde{d} \text{ on } (0,T) \times \partial \Omega \text{ (Dirichlet boundary condition)}. \end{split}$$

In case of Dirichlet boundary conditions, we shall also assume that $|\tilde{d}(t,x)|=1 \text{ on } (0,T)\times\partial\Omega.$

Two types of approach: Fluid-type approach (couple equation for *d* with Navier-stokes), Geometric approach (fluid equation coupled with theory of harmonic maps on spheres).

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- ▶ A semilinear approach to study the system with Neumann boundary data was followed in Li-Wang (2012) but their
- ▶ It was observed in Choudhury-Hieber-Hussein (unpublished note) that the quasilinear approach, as in the Neumann boundary data case, can be adapted when the Dirichlet boundary data for the director field is a constant vector e.

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$$u=0$$
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The case of Neumann boundary data

$$X = L^q_{\sigma}(\Omega) \times L^q(\Omega)^3,$$

and obtains the equivalent equation without pressure.

Then omitting the condition |d| = 1 one obtains

$$\begin{cases}
\partial_t u + Au &= -\mathbb{P}u \cdot \nabla u - \mathbb{P} \text{div } \left[(\nabla d)^T (\nabla d) \right], & \text{in } \Omega \times (0, T), \\
\partial_t d + Bd &= -u \cdot \nabla d - |\nabla d|^2 d, & \text{in } \Omega \times (0, T),
\end{cases}$$
(1)

with initial conditions u(0) = a and d(0) = b.

The operators A, B are defined as

$$A:=-\mathbb{P}\Delta,\ B:=-\Delta_{N,q}.$$

Nematic Liquid Crystals in Lipschitz domains

▶ Define for any $b \in L^1(\Omega)$ the average and the complementary mean-value free part

$$\overline{b} := \frac{1}{|\Omega|} \int_{\Omega} b d\omega$$
 and $b_s := b - \overline{b},$ (2)

where the subscript in b_s refers to stable, since for the Cauchy problem defined by the Neumann Laplacian it corresponds to the exponentially stable part.

Note that (2) define bounded projections in all L^p spaces, $p \in [1, \infty]$,

$$P_c d = \overline{d}$$
 and $P_s d = d_s$.

Now, using (2) one defines the variables

$$x = \overline{d} - \overline{b}$$
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We, therefore, obtain the following reformulation of (1)

$$\begin{cases} \partial_{t}u + Au &= -\mathbb{P}u \cdot \nabla u - \mathbb{P}\mathrm{div}\left[\left(\nabla y\right)^{T}\left(\nabla y\right)\right], & \text{in } \Omega \times (0, T), \\ \partial_{t}y + By &= -u \cdot \nabla y - P_{s}|\nabla y|^{2}(x + y + \overline{b}), & \text{in } \Omega \times (0, T), \\ \partial_{t}x &= -P_{c}|\nabla y|^{2}(x + y + \overline{b}), & \text{in } \Omega \times (0, T) \end{cases}$$

$$(3)$$

which defines a system in the space

$$L^q_\sigma(\Omega) \times L^q_0(\Omega)^3 \times \mathbb{R}^3$$
.

$$F_{u}(u, \nabla y) = -\mathbb{P} \operatorname{div} \left(u \otimes u + (\nabla y)^{T} (\nabla y) \right),$$

$$F_{y}(u, \nabla y, y, x, \overline{b}) = -u \cdot \nabla y - P_{s} |\nabla y|^{2} (x + y + \overline{b}),$$

$$F_{x}(\nabla y, y, x, \overline{b}) = -P_{c} |\nabla y|^{2} (x + y + \overline{b}).$$

Starting with the mild formulation of the problem one can define now the iteration scheme as follows.

$$u_{0} := e^{-tA}a, \ u_{j+1} := u_{0} + \int_{0}^{t} e^{-(t-s)A}F_{u}(u_{j}(s), \nabla y_{j}(s))ds,$$

$$y_{0} := e^{-tB}b_{s},$$

$$y_{j+1} := y_{0} + \int_{0}^{t} e^{-(t-s)B}F_{y}(u_{j}(s), \nabla y_{j}(s), y_{j}(s), x_{j}(s), \overline{b})ds,$$

$$x_{0} = 0, \ x_{j+1} := \int_{0}^{t} F_{x}(\nabla y_{j}(s), y_{j}(s), x_{j}(s), \overline{b})ds.$$

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The non-linear terms are comprised using the representation $u\cdot \nabla u=\operatorname{div} u\otimes u$ for $\operatorname{div} u=0$ by the notation

$$F_{u}(u, \nabla y) = -\mathbb{P} \text{div} \left(u \otimes u + (\nabla y)^{T} (\nabla y) \right),$$

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$$x_0 = 0, \ x_{j+1} := \int_0^t F_x(\nabla y_j(s), y_j(s), x_j(s), \overline{b})ds.$$

Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Then there exists $\varepsilon > 0$ such that,

(a) there exists $\omega>0$ and a constant C>0 such that for $\frac{3}{2}-\varepsilon< p\leq q<3+\varepsilon$ and t>0,

$$\begin{split} \|e^{-tA}f\|_{L^{q}_{\sigma}(\Omega)} &\leq Ce^{-\omega t}t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|f\|_{L^{p}_{\sigma}(\Omega)}, \ f \in L^{p}_{\sigma}(\Omega), \\ \|e^{-tA}\mathbb{P}\mathrm{div}\,F\|_{L^{q}_{\sigma}(\Omega)} &\leq Ce^{-\omega t}t^{-\frac{1}{2}-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|F\|_{L^{p}(\Omega)^{3\times 3}}, \ F \in L^{p}(\Omega)^{3\times 3}, \end{split}$$

(b) there exists $\omega>0$ and a constant C>0 such that for all $1< p\leq q\leq \infty$ with $p<\infty$ and t>0,

$$\|e^{-tB}f\|_{L^q(\Omega)^3} \le Ce^{-\omega t}t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|f\|_{L^p(\Omega)^3}, \quad f \in L^p_0(\Omega)^3.$$

Moreover, for all $\frac{3}{2} - \varepsilon and for <math>t > 0$,

$$\|\nabla e^{-tB}f\|_{L^{q}(\Omega)^{3\times 3}} \leq Ce^{-\omega t}t^{-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|\nabla f\|_{L^{p}(\Omega)^{3\times 3}}, \ f\in L_{0}^{p}\cap W^{1,p},$$

$$\|\nabla e^{-tB}f\|_{L^{q}(\Omega)^{3\times 3}} \leq Ce^{-\omega t}t^{-\frac{1}{2}-\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|f\|_{L^{p}(\Omega)^{3}}, \ f\in L_{0}^{p}(\Omega)^{3}.$$

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For
$$0 < T \le \infty$$
 and $3 \le p < q$, the class of solutions considered is defined using

$$S_q^u(\mathit{T}) := \Big\{ u \in \mathit{C}((0,\mathit{T});\mathit{L}_\sigma^q(\Omega)) \mid \sup_{0 < s < \mathit{T}} e^{\frac{\omega s}{2}} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|\mathit{u}(s)\|_{\mathit{L}_\sigma^q(\Omega)} < \infty \Big\},$$

$$S_q^d(\mathit{T}) := \Big\{ d \in \mathit{C}((0,\mathit{T}); \mathit{W}^{1,q}(\Omega)^3) \mid \sup_{0 < s < \mathit{T}} e^{\frac{\omega_\mathit{S}}{2}} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|\nabla d(s)\|_{\mathit{L}^q(\Omega)^{3 \times 3}}$$

where $\omega > 0$ is the minimum of the corresponding constants appearing earlier.

Theorem

Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, then there exists $\varepsilon > 0$ such that given initial conditions $a \in L^p_{\sigma}(\Omega)$ and $b \in W^{1,p}(\Omega)^3 \cap L^{\infty}(\Omega)^3$ where $3 \leq p < 3 + \varepsilon$, the following hold true for $q \in (p, 3 + \varepsilon)$.

(a) There exists T > 0 depending on the initial data such that equation (1) has a local mild solution (u, d) satisfying

$$u \in S_q^u(T) \cap BC([0,T); L_\sigma^p(\Omega)), \ \overline{d} \in BC([0,T); \mathbb{R}^3),$$

 $d_s \in S_q^d(T) \cap BC([0,T); W^{1,p}(\Omega)^3) \cap BC([0,T); L^\infty(\Omega)^3),$

where in the limit $s \to 0+$, one has

$$\|u(s)-a\|_{L^p(\Omega)}\to 0, \|d(s)-b\|_{L^\infty(\Omega)^3}\to 0, \|\nabla[d(s)-b]\|_{L^p(\Omega)^{3\times 3}}\to 0.$$

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$$s^{\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|u(s)\|_{L^{q}_{\sigma}(\Omega)}\to 0\quad \text{and}\quad s^{\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|\nabla d(s)\|_{L^{q}(\Omega)^{3\times 3}}\to 0.$$

(c) If a and ∇b are sufficiently small, then the solution exists globally in the class

$$u \in S_q^u(\infty) \cap BC([0,\infty); L_{\sigma}^p(\Omega)),$$

$$d_s \in S_q^d(\infty) \cap BC([0,\infty); W^{1,p}(\Omega)^3) \cap BC([0,\infty); L^{\infty}(\Omega)^3),$$

$$\overline{d} \in BC([0,\infty); \mathbb{R}^3).$$

- (d) The solution is unique in the class given in (a) provided p > 3, and in the case p = 3, it is unique in the subset of this class satisfying in addition the limit conditions (b).
- (e) Equation (1) subject to Neumann boundary conditions preserves the condition |d| = 1 if |d(0)| = |b| = 1.

The smallness condition in the previous theorem can be made precise in the sense that there exists a constant C>0 depending only on $p,\ q$, and Ω such that if

$$\max\{\kappa,\kappa^2\}(1+\|b\|_{L^\infty(\Omega)^3}) < C, \text{ where } \kappa:=\|a\|_{L^p_\sigma(\Omega)}+\|\nabla b\|_{L^p(\Omega)^{3\times 3}},$$

then the solution exists globally.

Theorem

For every $s \in (1,2)$, the solution has the following additional regularity properties

$$u \in W^{1,s}(0,T;W_{\sigma}^{-1,\frac{p}{2}}(\Omega)) \cap L^{s}(0,T;W_{0,\sigma}^{1,\frac{p}{2}}(\Omega)),$$

$$d',B_{\frac{p}{2}}d \in L^{s}(0,T;L^{\frac{p}{2}}(\Omega)^{3}).$$

$$k_{j}^{u}(T) := \sup_{0 < s < T} e^{\omega s / 2} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|u_{j}(s)\|_{L_{\sigma}^{q}(\Omega)},$$

$$k_{j}^{\nabla y}(T) := \sup_{0 < s < T} e^{\omega s / 2} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|\nabla y_{j}(s)\|_{L^{q}(\Omega)^{3}},$$

$$k_{j}^{y}(T) := \sup_{0 \le s < T} \|y_{j}(s)\|_{L^{\infty}(\Omega)^{3}}, k_{j}^{x}(T) := \sup_{0 \le s < T} \|x_{j}(s)\|_{\mathbb{R}^{3}}.$$

Let us introduce the notations

$$k_j^q := k_j^u + k_j^{\nabla y}, \ k_j^{\infty} := k_j^y + k_j^x.$$

Next, let us denote

$$W_j(t) := u_{j+1}(t) - u_j(t), \ Z_j(t) := \nabla y_{j+1}(t) - \nabla y_j(t),$$

 $Y_j(t) := y_{j+1}(t) - y_j(t), \ X_j(t) := x_{j+1}(t) - x_j(t),$

and the corresponding quantities

$$\begin{split} \delta_{j}^{u}(T) &:= \sup_{0 < s < T} e^{\omega s/2} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|W_{j}(s)\|_{L_{\sigma}^{q}(\Omega)}, \\ \delta_{j}^{\nabla y}(T) &:= \sup_{0 < s < T} e^{\omega s/2} s^{\frac{3}{2} \left(\frac{1}{p} - \frac{1}{q}\right)} \|Z_{j}(s)\|_{L^{q}(\Omega)^{3}}, \\ \delta_{j}^{y}(T) &:= \sup_{0 < s < T} \|Y_{j}(s)\|_{L^{\infty}(\Omega)^{3}}, \ \delta_{j}^{x}(T) &:= \sup_{0 < s < T} \|X_{j}(s)\|_{\mathbb{R}^{3}}. \end{split}$$

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Now, one estimates for $3 \le p < q < 3 + \epsilon$,

$$\begin{split} k_{j+1}^{u}(T) &\leq k_{0}^{u}(T) + CC_{1,T}[k_{j}^{u}(T)^{2} + k_{j}^{\nabla y}(T)^{2}], \\ k_{j+1}^{\nabla y}(T) &\leq k_{0}^{\nabla y}(T) \\ &\quad + CC_{1,T}\Big[k_{j}^{u}(T)k_{j}^{\nabla y}(T) + k_{j}^{\nabla y}(T)^{2}(k_{j}^{x}(T) + k_{j}^{y}(T) + \|\overline{b}\|)\Big], \\ k_{j+1}^{y}(T) &\leq k_{0}^{y}(T) \\ &\quad + CC_{2,T}\Big[k_{j}^{u}(T)k_{j}^{\nabla y}(T) + k_{j}^{\nabla y}(T)^{2}(k_{j}^{x}(T) + k_{j}^{y}(T) + \|\overline{b}\|)\Big] \\ k_{j+1}^{x}(T) &\leq CC_{3,T}k_{j}^{\nabla y}(T)^{2}(k_{j}^{x}(T) + k_{j}^{y}(T) + \|\overline{b}\|). \end{split}$$

Let $\tilde{C}_T := \max\{C_{1,T}, C_{2,T}, C_{3,T}\}$. We note that $\lim_{T\to 0} \tilde{C}_T = 0$ and if $T = +\infty$, \tilde{C}_T is a constant independent of T.

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Let $\tilde{C}_{\mathcal{T}} := \max\{C_{1,\mathcal{T}}, C_{2,\mathcal{T}}, C_{3,\mathcal{T}}\}$. We note that $\lim_{T\to 0} \tilde{C}_{\mathcal{T}} = 0$ and if $T = +\infty$, $\tilde{C}_{\mathcal{T}}$ is a constant independent of T.

For $3 \le p \le a \le 3 + \varepsilon$.

$$\begin{split} \|u_{j+1}\|_{L^{q}_{\sigma}(\Omega)} &\leq \|u_{0}\|_{L^{q}_{\sigma}(\Omega)} + \left\| \int_{0}^{t} e^{-(t-s)A_{\mathbb{P}\text{div}}(u_{j} \otimes u_{j}) + e^{-(t-s)A_{\mathbb{P}\text{div}}([\nabla y_{j}]^{\top} \nabla y_{j}) \, \mathrm{d}s} \right\|_{L^{q}_{\sigma}(\Omega)} \\ &\leq \|u_{0}\|_{L^{q}_{\sigma}(\Omega)} \\ &+ C \int_{0}^{t} e^{-(t-s)\omega} (t-s)^{-\frac{1}{2} - \frac{3}{2q}} (\|u_{j} \otimes u_{j}\|_{L^{q/2}_{\sigma}(\Omega)} + \|[\nabla y_{j}]^{\top} \nabla y_{j}\|_{L^{q/2}(\Omega)^{3 \times 3}}) \, \mathrm{d}s \\ &\leq \|u_{0}\|_{L^{q}_{\sigma}(\Omega)} + C \int_{0}^{t} e^{-t\omega} (t-s)^{-\frac{1}{2} - \frac{3}{2q}} s^{-3(\frac{1}{p} - \frac{1}{q})} \\ &\qquad \qquad \left\{ \left(e^{\frac{s\omega}{2}} s^{\frac{3}{2}(\frac{1}{p} - \frac{1}{q})} \|u_{j}\|_{L^{q}_{\sigma}(\Omega)} \right)^{2} + \left(e^{\frac{s\omega}{2}} s^{\frac{3}{2}(\frac{1}{p} - \frac{1}{q})} \|\nabla y_{j}\|_{L^{q}(\Omega)^{3 \times 3}} \right)^{2} \right\} \, \mathrm{d}s \\ &\leq \|u_{0}\|_{L^{q}_{\sigma}(\Omega)} + C \left(e^{-t\omega} \int_{0}^{t} (t-s)^{-\frac{1}{2} - \frac{3}{2q}} s^{-3(\frac{1}{p} - \frac{1}{q})} \, \mathrm{d}s \right) [k_{j}^{u}(\tau)^{2} + k_{j}^{\nabla y}(\tau)^{2}] \end{split}$$

which implies, multiplying by the factor e $\frac{\omega t}{2} \frac{3}{t} (\frac{1}{p} - \frac{1}{q})$ and taking $\sup_{0 < t < T}$, that

$$k_{j+1}^{u}(T) \le k_{0}^{u}(T) + C\left(\sup_{0 < t < T} e^{-\frac{\omega t}{2}} t^{\frac{3}{2}\left(\frac{1}{p} - \frac{1}{q}\right)} \int_{0}^{t} (t - s)^{-\frac{1}{2} - \frac{3}{2q}} s^{-3\left(\frac{1}{p} - \frac{1}{q}\right)} ds\right) [k_{j}^{u}(T)^{2} + k_{j}^{\nabla y}(T)^{2}]. \tag{4}$$

Since $3 \le \rho < q < 3 + \varepsilon$, it follows that $\frac{1}{2} - \frac{3}{2\rho} \ge 0$, $1 - 3(\frac{1}{\rho} - \frac{1}{q}) > 0$, $\frac{1}{2} - \frac{3}{2q} > 0$, and hence

$$\begin{split} \sup_{0 < t < \mathcal{T}} e^{-\frac{\omega t}{2} \frac{3}{t^{\frac{3}{2}}} (\frac{1}{p} - \frac{1}{q})} \int_{0}^{t} (t - s)^{-\frac{1}{2} - \frac{3}{2q}} s^{-3} (\frac{1}{p} - \frac{1}{q})_{ds} \\ &= \left(\sup_{0 < t < \mathcal{T}} e^{-\frac{\omega t}{2}} t^{\frac{1}{2} - \frac{3}{2p}} \right) B (1 - 3(\frac{1}{p} - \frac{1}{q}), \frac{1}{2} - \frac{3}{2q}), \end{split}$$

where B(x,y) denotes the beta function for x,y>0. Therefore, setting $C_{1,T}:=\sup_{0< t< T}e^{-\frac{\omega t}{2}}t^{\frac{1}{2}-\frac{3}{2p}}$, equation (4) turns into

$$k_{j+1}^{u}(T) \le k_0^{u}(T) + CC_{1,T}[k_j^{u}(T)^2 + k_j^{\nabla y}(T)^2].$$
 (5)

Nematic Liquid Crystals in Lipschitz —— domains

Similarly for the differences we can write

$$\begin{split} \delta_{j}^{u}(T) &\leq C \, \tilde{C}_{T} \Big[\delta_{j-1}^{u}(T) (k_{j}^{q}(T) + k_{j-1}^{q}(T)) + \delta_{j-1}^{\nabla y}(T) (k_{j}^{q}(T) + k_{j-1}^{q}(T)) \Big], \\ \delta_{j}^{\nabla y}(T) &\leq C \, \tilde{C}_{T} \Big[\delta_{j-1}^{u}(T) k_{j}^{q}(T) + k_{j-1}^{q}(T) \delta_{j-1}^{\nabla y}(T) \\ &\quad + (\delta_{j-1}^{\nabla y}(T) k_{j}^{q}(T) + k_{j-1}^{q}(T) \delta_{j-1}^{\nabla y}(T)) (k_{j}^{\infty}(T) + k_{j}^{\infty}(T) + \|\overline{b}\|) \\ &\quad + k_{j-1}^{q}(T)^{2} (\delta_{j-1}^{x}(T) + \delta_{j-1}^{y}(T)) \Big], \\ \delta_{j}^{y}(T) &\leq C \, \tilde{C}_{T} \Big[\delta_{j-1}^{u}(T) k_{j}^{q}(T) + k_{j-1}^{q}(T) \delta_{j-1}^{\nabla y}(T) \\ &\quad + (\delta_{j-1}^{\nabla y}(T) k_{j}^{q}(T) + k_{j-1}^{q}(T) \delta_{j-1}^{\nabla y}(T)) (k_{j}^{\infty}(T) + k_{j}^{\infty}(T) + \|\overline{b}\|) \\ &\quad + k_{j-1}^{q}(T)^{2} (\delta_{j-1}^{x}(T) + \delta_{j-1}^{y}(T)) \Big], \\ \delta_{j}^{x}(T) &\leq C \, \tilde{C}_{T} \Big[(\delta_{j-1}^{\nabla y}(T) k_{j}^{q}(T) + k_{j-1}^{q}(T) \delta_{j-1}^{\nabla y}(T)) (k_{j}^{\infty}(T) + k_{j}^{\infty}(T) \\ &\quad + \|\overline{b}\|) + k_{j-1}^{q}(T)^{2} (\delta_{j-1}^{x}(T) + \delta_{j-1}^{y}(T)) \Big]. \end{split}$$

- ▶ Let us denote $\delta_j(T) := \delta_j^u(T) + \delta_j^{\nabla_y}(T) + \delta_i^y(T) + \delta_j^x(T)$.
- ► Then if

$$144C\tilde{C}_{T}K(1+\|b\|_{L^{\infty}(\Omega)^{3}})<1,$$
(6)

where $K = \max\{k_0^q(T), k_0^q(T)^2\}$, we have a contraction in terms of δ_j , which gives us the existence.

Nematic Liquid Crystals in Lipschitz domains

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We give a short summary of the conditions that provide the validity of (6).

- (a) In the case $T=+\infty$, if $\|a\|_{L^p_\sigma(\Omega)}+\|\nabla b\|_{L^p(\Omega)^{3\times 3}}$ is small enough, the validity of (6) can be inferred. This implies eventually the global existence under a suitable smallness condition on the initial data a and ∇b .
- (b) If p>3, then (6) follows from the fact that $\lim_{T\to 0} \tilde{C}_T=0$. This will imply local existence of solutions without any smallness assumptions on the initial data.
- (c) If p=3, then (6) follows for small times T using a similar argument to that of p>3. Again this will imply local existence of solutions without any smallness assumption on the initial data.

Computational and Applied Mathematics

- Let us denote $\delta_i(T) := \delta_i^u(T) + \delta_i^{\nabla y}(T) + \delta_i^y(T) + \delta_i^x(T)$.
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► The above estimates are not enough because we cannot take q=p. Therefore, using the estimates we need to extend our consideration to L^s with time weight $\sigma'=\frac{3}{2}(\frac{1}{p}-\frac{1}{s})$ where

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Using similar strategy we can prove that the solutions are BC with respect to time.

Nematic Liquid Crystals in Lipschitz —— domains

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Applied Mathematics

Retrieving the condition |d| = 1

- Let u and d be mild solutions to our problem such that the initial conditions satisfy $a \in L^p_\sigma(\Omega)$ and $b \in W^{1,p}(\Omega; \mathbb{C}^3)$ with |b| = 1 in Ω for some $3 \le p < 3 + \varepsilon$.
- ▶ Assume further, that for every $p < q < 3 + \varepsilon$

$$\begin{split} t &\mapsto t^{\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}u(t) \in \mathrm{BC}([0,T);\mathrm{L}^q_\sigma(\Omega)), \\ t &\mapsto t^{\frac{3}{2}(\frac{1}{p}-\frac{1}{q})}\nabla d(t) \in \mathrm{BC}([0,T);\mathrm{L}^q_\sigma(\Omega)), \\ d &\in \mathrm{BC}([0,T);\mathrm{L}^\infty(\Omega;\mathbb{C}^3)). \end{split}$$

▶ Then for all $\vartheta \in W^{1,(p/2)'}(\Omega; \mathbb{C}^3)$,

$$\int_{\Omega} d_{t}(t) \cdot \overline{\vartheta} \, dx + \int_{\Omega} \nabla d(t) \cdot \overline{\nabla \vartheta} \, dx = - \int_{\Omega} (u(t) \cdot \nabla) d(t) \cdot \overline{\vartheta} \, dx
+ \int_{\Omega} |\nabla d(t)|^{2} d(t) \cdot \overline{\vartheta} \, dx.$$
(7

Retrieving the condition |d| = 1

Define

$$\varphi:=|d|^2-1.$$

Note that by assumption $\varphi(t) \in L^{\infty}(\Omega)$ for every $t \in (0, T)$ and that

$$\partial_k \varphi(t) = 2\overline{d(t)} \cdot \partial_k d(t) \in L^p(\Omega), \varphi_t(t) = 2\overline{d(t)} \cdot d_t(t) \in L^{p/2}(\Omega).$$
(8)

- ▶ It follows from (8) that for almost every $t \in (0, T)$ we have $\varphi(t) \in W^{1,p}(\Omega) \subset W^{1,(p/2)'}(\Omega)$.
- \blacktriangleright Therefore, φ itself is an admissible test function and we can deduce

$$\int_{\Omega} \varphi_{t} \varphi \, dx + \int_{\Omega} |\nabla \varphi|^{2} \, dx = -\int_{\Omega} u \cdot \nabla \varphi \varphi \, dx + 2 \int_{\Omega} |\nabla d|^{2} \varphi^{2} \, dx.$$
(9)

▶ Then for any t < T we find that

$$\frac{1}{2}\int_{\Omega}\phi(t)^2\ dx+\int_0^t\int_{\Omega}|\nabla\phi(s)|^2\ dx\ ds=2\int_0^t\int_{\Omega}|\nabla d(s)|^2\phi(s)^2\ dx\ ds.$$

- ▶ We shall now show that Gronwall's inequality can be applied and we can infer that $\phi = 0$.
- lackbox For $0 < ilde{t} < t$ to be chosen appropriately, we write

$$\underbrace{\int_{0}^{t} \int_{\Omega} |\nabla d(s)|^{2} \phi(s)^{2} dx ds}_{A} = \underbrace{\int_{0}^{\tilde{t}} \int_{\Omega} |\nabla d(s)|^{2} \phi(s)^{2} dx ds}_{I} + \underbrace{\int_{\tilde{t}}^{t} \int_{\Omega} |\nabla d(s)|^{2} \phi(s)^{2} dx ds}_{I}.$$
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Retrieving the condition |d| = 1

We estimate the integral II in the following way.

$$\begin{split} \int_{\tilde{t}}^{t} \int_{\Omega} & |\nabla d(s)|^{2} \phi(s)^{2} \ dx \ ds \leq \int_{\tilde{t}}^{t} \||\nabla d(s)|^{2}\|_{L^{\frac{q}{2}}} \|\phi(s)^{2}\|_{L^{(\frac{q}{2})'}} \ ds \\ &= \int_{\tilde{t}}^{t} \|\nabla d(s)\|_{L^{q}}^{2} \|\phi(s)\|_{L^{2 \cdot (\frac{q}{2})'}}^{2} \ ds \\ &\leq C \int_{\tilde{t}}^{t} s^{-3(\frac{1}{p} - \frac{1}{q})} \|\phi(s)\|_{L^{2-\frac{q}{q-2}}}^{2} \ ds \\ &\stackrel{\text{interpolation}}{\leq} C \int_{\tilde{t}}^{t} s^{-3(\frac{1}{p} - \frac{1}{q})} \|\phi(s)\|_{L^{2}}^{2(1-\alpha)} \|\phi(s)\|_{L^{6}}^{2\alpha} \ ds \\ &\leq C \int_{\tilde{t}}^{t} s^{-3(\frac{1}{p} - \frac{1}{q})} \|\phi(s)\|_{L^{2}}^{2(1-\alpha)} \|\phi(s)\|_{H^{1}}^{2\alpha} \ ds \\ &\stackrel{\text{Young's}}{\leq} \int_{\tilde{t}}^{t} \frac{\left[Cs^{-3(\frac{1}{p} - \frac{1}{q})} \|\phi(s)\|_{L^{2}}^{2(1-\alpha)}\right]^{\frac{1}{1-\alpha}}}{\frac{1}{1-\alpha}} + \frac{\|\phi(s)\|_{H^{1}}^{\frac{2\alpha}{\alpha}}}{\frac{1}{\alpha}} \\ &\leq \int_{\tilde{t}}^{t} \left[(1-\alpha)C^{\frac{1}{1-\alpha}}\tilde{t}^{-\frac{3}{1-\alpha}(\frac{1}{p} - \frac{1}{q})} + \alpha\right] \|\phi(s)\|_{L^{2}}^{2} \ ds \\ &+ \alpha \int_{\tilde{t}}^{t} \|\nabla \phi(s)\|_{L^{2}}^{2} \ ds. \end{split}$$

Nematic Liquid Crystals in Lipschitz domains

To estimate the integral I we choose an approximating sequence $\{b_j\}$ (of smooth functions) to b in $W^{1,3}$ and proceed as follows. We write

$$\begin{split} \int_0^{\tilde{t}} \int_{\Omega} |\nabla d(s)|^2 \phi(s)^2 \ dx \ ds &\leq C \int_0^{\tilde{t}} \int_{\Omega} |\nabla d(s) - \nabla b|^2 \phi(s)^2 \ dx \ ds \\ &+ C \int_0^{\tilde{t}} \int_{\Omega} |\nabla b - \nabla b_j|^2 \phi(s)^2 \ dx \ ds \\ &+ C \int_0^{\tilde{t}} \int_{\Omega} |\nabla b_j|^2 \phi(s)^2 \ dx \ ds. \end{split}$$

Now choosing j such that $\|\nabla(b-b_j)\|_{L^3} \leq \sqrt{\epsilon}$, we can write

$$C \int_{0}^{\tilde{t}} \int_{\Omega} |\nabla b - \nabla b_{j}|^{2} \phi(s)^{2} dx ds$$

$$\leq C \int_{0}^{\tilde{t}} ||\nabla (b - b_{j})||_{L^{3}}^{2} ||\phi(s)||_{L^{6}}^{2} ds \qquad (12)$$

$$\leq C \epsilon \int_{0}^{\tilde{t}} ||\phi(s)||_{L^{2}}^{2} ds + C \epsilon \int_{0}^{\tilde{t}} ||\nabla \phi(s)||_{L^{2}}^{2} ds.$$

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Nematic Liquid Crystals in Lipschitz domains

Retrieving the condition |d| = 1

Similarly if \tilde{t} is chosen small enough, we have

$$C\int_{0}^{\tilde{t}}\int_{\Omega}|\nabla d(s)-\nabla b|^{2}\phi(s)^{2} dx ds \leq C\epsilon\int_{0}^{\tilde{t}}\|\phi(s)\|_{L^{2}}^{2} ds + C\epsilon\int_{0}^{\tilde{t}}\|\nabla\phi(s)\|_{L^{2}}^{2} ds.$$

$$(13)$$

Again

$$\begin{split} C \int_0^{\tilde{t}} \int_{\Omega} |\nabla b_j|^2 \phi(s)^2 \ dx \ ds &\leq C \int_0^{\tilde{t}} \|\nabla b_j\|_{L^q}^2 \|\phi(s)\|_{\frac{2q}{q-2}}^2 \ ds \\ &\leq C \int_0^{\tilde{t}} \|\phi(s)\|_{L^2}^{2(1-\alpha)} \|\phi(s)\|_{H^1}^{2\alpha} \ ds \\ &\leq \int_0^{\tilde{t}} (1-\alpha)C^{\frac{1}{1-\alpha}} \|\phi(s)\|_{L^2}^2 \ ds + \alpha \int_0^{\tilde{t}} \|\phi(s)\|_{H^1}^2 \ ds \\ &\leq \int_0^{\tilde{t}} \left[(1-\alpha)C^{\frac{1}{1-\alpha}} + \alpha \right] \|\phi(s)\|_{L^2}^2 \ ds \\ &+ \alpha \int_0^{\tilde{t}} \|\nabla \phi(s)\|_{L^2}^2 \ ds. \end{split}$$

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$$\leq C \int_{0}^{\tilde{t}} ||\phi(s)||_{L^{2}}^{2(1-\alpha)} ||\phi(s)||_{H^{1}}^{2\alpha} ds$$

$$\leq \int_{0}^{\tilde{t}} (1-\alpha) C^{\frac{1}{1-\alpha}} ||\phi(s)||_{L^{2}}^{2} ds + \alpha \int_{0}^{\tilde{t}} ||\phi(s)||_{H^{1}}^{2} ds$$

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Nematic Liquid Crystals in Lipschitz domains

Combining (12)-(14) with (11) we can write

$$A \leq I + II$$

$$\leq \int_0^t \underbrace{\left[(1 - \alpha)C^{\frac{1}{1 - \alpha}} \tilde{t}^{-\frac{3}{1 - \alpha}(\frac{1}{\rho} - \frac{1}{q})} + \alpha + (1 - \alpha)C^{\frac{1}{1 - \alpha}} + C\epsilon \right]}_{\text{constant function and therefore continuous}} \|\phi(s)\|_{L^2}^2 ds$$

$$+ (C\epsilon + \alpha) \int_0^t \|\nabla \phi(s)\|_{L^2}^2 ds.$$
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Let ϵ be such that $C\epsilon + \alpha < 1$ and we choose \tilde{t} such that $\|\nabla d(s) - \nabla b\|_{L^3} < \sqrt{\epsilon}, \ s \in (0, \tilde{t}).$

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Further regularity

Let $\Phi: [L^{p'}_{\sigma}(\Omega)]^* \to L^p_{\sigma}(\Omega)$ denote the canonical isomorphism between $[L^{p'}_{\sigma}(\Omega)]^*$ and $L^p_{\sigma}(\Omega)$, and recall the duality pairing

$$(\Phi^{-1}u)(v) = \langle \Phi^{-1}u, v \rangle_{[L^{p'}_{\sigma}]^*, L^{p'}_{\sigma}} = \langle u, v \rangle_{L^p_{\sigma}, L^{p'}_{\sigma}} = \int_{\Omega} u \cdot \overline{v} \, dx.$$

We regard Φ^{-1} also as the canonical inclusion of $L^p_\sigma(\Omega)$ into $W^{-1,p}_\sigma(\Omega)$ by

$$\langle \Phi^{-1}u, v \rangle_{W_{\sigma}^{-1,p}, W_{0,\sigma}^{1,p'}} = \langle u, v \rangle_{L_{\sigma}^p, L_{\sigma}^{p'}}, \quad u \in L_{\sigma}^p(\Omega), \ v \in W_{0,\sigma}^{1,p'}(\Omega).$$

In this sense, we define the weak Stokes operator \mathcal{A}_{ρ} in $W_{\sigma}^{-1,\rho}(\Omega)$ by $\mathrm{dom}(\mathcal{A}_{\rho}) := \Phi^{-1}W_{0,\sigma}^{1,\rho}(\Omega)$ and

$$\mathcal{A}_{\rho}: \operatorname{dom}(\mathcal{A}_{\rho}) \subset W_{\sigma}^{-1,\rho}(\Omega) \to W_{\sigma}^{-1,\rho}(\Omega),$$

$$w \mapsto \left[v \mapsto \int_{\Omega} \nabla \Phi w \cdot \overline{\nabla v} \, \mathrm{d}x \right]. \tag{16}$$

▶ The proof of regularity follows by interpreting the integral equations as linear equations with a known right-hand side and using the maximal regularity properties of the weak Stokes and Neumann operators.

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Crystals in Lipschitz domains Anupam Pal Choudhury Johann Radon Institute for Computational and

Nematic Liquid

The case of Dirichlet boundary data

- ▶ In the case of Lipschitz domains, the global existence and uniqueness (under suitable smallness assumptions) can be studied using the semilinear approach.
- ▶ Let us denote $\delta = d e$. Then we can rewrite the system as

$$\begin{aligned} \partial_t u + \big(u \cdot \nabla \big) u - \Delta u + \nabla \pi &= -\mathsf{div}([\nabla \delta]^\top \nabla \delta) \text{ in } (0, T) \times \Omega, \\ \partial_t \delta + \big(u \cdot \nabla \big) \delta &= \Delta \delta + |\nabla \delta|^2 \delta + |\nabla \delta|^2 e \text{ in } (0, T) \times \Omega, \\ \text{div } u &= 0 \text{ in } (0, T) \times \Omega, \\ \big(u, \delta \big) &= (0, 0) \text{ on } (0, T) \times \partial \Omega, \\ \big(u, \delta \big) \Big|_{t=0} &= (a, \tilde{b}) \text{ in } \Omega, \end{aligned}$$

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where $\tilde{b} = b - e$.

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Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, then there exists $\varepsilon > 0$ such that given initial conditions $a \in L^p_{\sigma}(\Omega)$ and $b \in W^{1,p}(\Omega)^3 \cap L^{\infty}(\Omega)^3$ with b = e on $\partial \Omega$ for some $e \in \mathbb{S}^2$ where $3 , the following hold true for <math>q \in (p, 3 + \varepsilon)$.

(a) There exists T > 0 depending on the initial data such that equation (17) with Dirichlet boundary conditions has a local mild solution (u, δ) satisfying

$$u \in S_q^u(T) \cap BC([0,T); L_{\sigma}^p(\Omega)),$$

$$\delta \in S_q^d(T) \cap BC([0,T); W_0^{1,p}(\Omega)^3) \cap BC([0,T); L^{\infty}(\Omega)^3),$$

where in the limit $s \to 0+$, one has

$$\|u(s)-\mathsf{a}\|_{L^p_{\sigma}(\Omega)}\to 0, \|\delta(s)-\tilde{b}\|_{L^\infty(\Omega)^3}\to 0, \|\nabla[\delta(s)-\tilde{b}]\|_{L^p(\Omega)^{3\times 3}}\to 0$$

(b) In the limit $s \to 0+$, the solutions satisfy

$$s^{\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|u(s)\|_{L^q_\sigma(\Omega)}\to 0\quad \text{and}\quad s^{\frac{3}{2}\left(\frac{1}{p}-\frac{1}{q}\right)}\|\nabla\delta(s)\|_{L^q(\Omega)^{3\times 3}}\to 0.$$

(c) If a and ∇b are sufficiently small, then the solution exists globally in the class

$$u \in S_q^u(\infty) \cap BC([0,\infty); L_\sigma^p(\Omega)),$$

$$\delta \in S_q^d(\infty) \cap BC([0,\infty); W_0^{1,p}(\Omega)^3) \cap BC([0,\infty); L^\infty(\Omega)^3).$$

- (d) The solution is unique in the class given in (a) provided p > 3, and in the case p = 3, it is unique in the subset of this class satisfying in addition the limit conditions (b).
- (e) The condition |d| = 1 is preserved if |d(0)| = |b| = 1.

Theorem

For every $s \in (1,2)$, the solution has the following additional regularity properties

$$u \in W^{1,s}(0,T;W_{\sigma}^{-1,\frac{p}{2}}(\Omega)) \cap L^{s}(0,T;W_{0,\sigma}^{1,\frac{p}{2}}(\Omega)),$$
$$\delta \in W^{1,s}(0,T;L^{\frac{p}{2}}(\Omega)^{3}) \cap L^{s}(0,T;dom(B_{\frac{p}{2}})).$$

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$$u \in S_q^u(\infty) \cap BC([0,\infty); L_p^{\sigma}(\Omega)),$$

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Existence:

- In this case, we do not need to split the director field as the homogeneous Dirichlet boundary conditions ensure exponential decay.
- ▶ The proof then follows, as in the previous case, by considering the integral formulations for u, δ and $\nabla \delta$.

Retrieving the unit modulus condition for the director field:

- Once we have proved the existence of δ , we can go back to the original variable d which satisfies the same regularity.
- We can then proceed as in the proof in the previous case. The only point to notice is that we can use $\phi := |d|^2 1$ as a test function and this vanishes on the boundary.
- ▶ The discussion on regularity remains the same.

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Concluding remarks and Future directions

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In the case of a smooth domain Ω our approach yields similar results as has been obtained by Hieber et al. using quasilinear techniques.

More concretely, their approach requires initial data in Besov spaces

$$a \in B_{qp}^{2\mu - 2/p}(\Omega)^3 \cap L_{\sigma}^p(\Omega),$$

$$b \in B_{qp}^{2\mu - 2/p}(\Omega)^3, \quad \frac{2}{p} + \frac{3}{q} < 1, \frac{1}{2} + \frac{1}{p} + \frac{3}{2q} < \mu \le 1,$$

using the fact that the embedding $B_{qp}^{2\mu-2/p}(\Omega)\hookrightarrow C^1(\overline{\Omega})$ holds. These initial data are much more regular than the ones assumed by us.

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 Note that there are also other versions of the simplified Ericksen-Leslie model.

For instance, some authors drop the assumption $\left|d\right|=1$ and replace the dynamical equation for the director field d by

$$\partial_t d - \Delta d + (u \cdot \nabla) d = -\gamma f(d), \quad \gamma > 0,$$

for a bounded vector valued penalty function f.

The method we presented here can be adapted for this setting as well.

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$$\begin{split} \partial_t u + (u \cdot \nabla) u &= \text{Div } \sigma \text{ in } J \times \Omega, \\ \text{div } u &= 0 \text{ in } J \times \Omega, \\ d \times \left(g + \text{Div}(\frac{\partial W^{OF}(d, \nabla d)}{\partial (\nabla d)}) - \frac{\partial W^{OF}(d, \nabla d)}{\partial d} \right) &= 0 \text{ in } J \times \Omega, \\ |d| &= 1 \text{ in } J \times \Omega, \\ \left(u, d \right) \Big|_{t=o} &= (u_0, d_0) \text{ in } \Omega. \end{split}$$

- \triangleright u velocity, σ stress, d director field
- ▶ The Oseen-Frank density

$$W^{OF} = \frac{1}{2} \Big[k_1 (div \ d)^2 + k_2 |d \times (\nabla \times d)|^2 + k_3 |d \cdot (\nabla \times d)|^2 + (k_2 + k_4) (tr(\nabla d)^2 - (div \ d)^2) \Big]$$

where $k_1, \dots, k_4 \subset \mathbb{R}$ are elasticity coefficients.

$$\sigma = -\pi Id - \left[\frac{\partial W^{OF}(d, \nabla d)}{\partial \nabla d}\right]^T \nabla d + \sigma_L,$$

where

$$\sigma_L := \alpha_1 [dd^T : D] dd^T + \alpha_2 dN^T + \alpha_3 Nd^T + \alpha_4 D + \alpha_5 d[Dd]^T + \alpha_6 [Dd] d^T,$$

$$D = \frac{1}{2}([\nabla u]^T + \nabla u), \ V = \frac{1}{2}([\nabla u]^T - \nabla u)$$
 and $N = \partial_t d + (u \cdot \nabla)d - Vd$.

Nematic Liquid Crystals in Lipschitz domains

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- ► The major question is if the semilinear approach might be suitable for more complex models even in smooth domains.
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Thank You