Liquid crystal flows with free boundary

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Nematic liquid crystal flow in dimension two

We consider the following initial-boundary value problem of nematic liquid crystal flow in a bounded, smooth domain Ω in \mathbb{R}^n $(n \geq 2)$, and T > 0

(NLCF)
$$\begin{cases} \partial_t v + v \cdot \nabla v + \nabla P = \Delta v - \varepsilon_0 \nabla \cdot \left(\nabla u \odot \nabla u - \frac{1}{2} |\nabla u|^2 \mathbb{I}_2 \right) \\ \nabla \cdot v = 0 \\ \partial_t u + v \cdot \nabla u = \Delta u + |\nabla u|^2 u, \end{cases}$$

$$(v,u)\big|_{t=0} = (v_0,u_0)$$
 in Ω ,
 $v=0$ on $\partial\Omega \times (0,T)$, $u=u_0$ on $\partial\Omega \times (0,T)$,

- $v: \Omega \times (0,T) \to \mathbb{R}^n$ fluid velocity
- $P: \Omega \times (0,T) \to \mathbb{R}$ fluid pressure
- ▶ $u: \Omega \times (0,T) \to \mathbb{S}^2$ orientation field of nematic liquid crystal molecules
- $ightharpoonup \varepsilon_0 > 0$: competition between kinetic energy and elastic energy

Nematic liquid crystal flow

(NLCF) is a simplified version of the Ericksen–Leslie model first proposed by Lin 1989. (NLCF) couples two important PDEs:

► Incompressible Navier–Stokes equation

(iNS)
$$\begin{cases} \partial_t v + v \cdot \nabla v + \nabla P = \Delta v & \text{in } \Omega \times (0, T) \\ \nabla \cdot v = 0 & \text{in } \Omega \times (0, T) \end{cases}$$

► Harmonic map heat flow

(HMF)
$$\begin{cases} \partial_t u = \Delta u + |\nabla u|^2 u & \text{in } \Omega \times (0, T) \\ u : \Omega \times (0, T) \to \mathbb{S}^2 \end{cases}$$

Coupling terms

▶ (HMF) provides forcing term to (iNS)

$$-\varepsilon_0 \nabla \cdot \left(\nabla u \odot \nabla u - \frac{1}{2} |\nabla u|^2 \mathbb{I}_2 \right)$$

ightharpoonup (iNS) provides transport term to (HMF) $v \cdot \nabla u$

(iNS) and (HMF)

- ► (iNS)
 - Existence of suitable weak solutions: Leray 1934, Hopf 1951 Leray-Hopf solution is regular in \mathbb{R}^2
 - ▶ Partial regularity results in \mathbb{R}^3 : Caffarelli–Kohn–Nirenberg 1982, Lin 1998

► (HMF)

- ▶ n = 2, Struwe (1985) established the existence of global weak solution, which has at most finitely many singular points
- ▶ $n \ge 3$: existence of global weak solutions Chen–Struwe 1989, Chen–Lin 1993
- ▶ $n \ge 3$: examples of finite time blow-up Coron–Ghidaglia 1989, Chen–Ding 1990
- n = 2: critical dimension. Finite time blow-up Chang-Ding-Ye 1991
 van den Berg-Hulshof-King 2003 (formal analysis)
 Raphaël-Schweyer 2013
 Dávila-del Pino-Wei 2017 (blow-up at multiple points in general domains)

NLCF

- Existence of weak solutions and partial regularity results for n = 2, 3: Lin–Liu 1995, 1996
- ▶ n = 2: Lin-Lin-Wang (2010) proved the global existence of Leray-Hopf type weak solutions for (NLCF) that is smooth away from finitely many points.
- ▶ n = 2: Lin-Wang (2010) proved the uniqueness of Leray-Hopf weak solution to (NLCF)
- ▶ n = 3: Lin-Wang (2016) proved the global existence of weak solutions satisfying the global energy inequality under the assumption that the initial orientation field $d_0(\Omega) \subset \mathbb{S}^2_+$.
- ▶ Blow-solutions in two dimensions at a finite number of points by Lai-Lin-Wei-Wang-Zhou (2021)

A new model with free boundary (F.H. Lin, Y. S., J. Wei, Y. Zhou)

(LCF)
$$\begin{cases} \partial_t v + v \cdot \nabla v + \nabla P = \Delta v - \varepsilon_0 \nabla \cdot \left(\nabla u \odot \nabla u - \frac{1}{2} |\nabla u|^2 \mathbb{I}_2 \right) \\ \nabla \cdot v = 0 \\ \partial_t u + v \cdot \nabla u = \Delta u + |\nabla u|^2 u, \end{cases}$$

$$(FB) \begin{cases} v \cdot \nu = 0, & \text{on } \partial\Omega \times (0, T), \\ (Sv \cdot \nu)_\tau = 0, & \text{on } \partial\Omega \times (0, T), \\ u(x, t) \in \Sigma, & \text{on } \partial\Omega \times (0, T), \\ \frac{\partial u}{\partial \nu}(x, t) \perp T_{u(x, t)} \Sigma, & \text{on } \partial\Omega \times (0, T), \end{cases}$$

where ν is the unit outer normal of $\partial\Omega$, S is the strain tensor (deformation tensor, shear stress)

$$Sv = \frac{1}{2}(\nabla v + (\nabla v)^T),$$

The blow-up result via parabolic gluing

We construct both interior and boundary bubbling in the half-plane:

Theorem (F.H. Lin, Y. S., J. Wei, Y. Zhou)

For T>0 sufficiently small and any given points in \mathbb{R}^2_+ , there exists initial data (u_0,v_0) such that the solution (u,v) to liquid crystal flow with free boundary conditions blows up at finite time T exactly at these given points. Moreover, u takes the form at leading order of the sharply scaled 1-corotational profile (equivariant harmonic map) with type II rate

$$\lambda(t) \sim \frac{T - t}{|\log(T - t)|^2}.$$

Inner-outer gluing method for parabolic equations

- ightharpoonup good approximation \implies small error
 - perturbation
- $u = \operatorname{approximation} + \underbrace{\eta_R \phi(y, t)}_{\text{inner}} + \underbrace{\psi(x, t)}_{\text{outer}}, \quad y = \frac{x \xi(t)}{\lambda(t)}$
- ► Inner problem: $\lambda^2 \phi_t = L[\phi] + \underbrace{\text{coupling}(\psi) + \text{error}}_{\mathcal{U}}$
- Outer problem (maximum principle): $\psi_t = \Delta_x \psi + \underbrace{(\phi \Delta \eta_R + 2 \nabla \eta_R \cdot \nabla \phi)}_{\text{coupling}} + \text{nonlinear terms} + \text{error}$
- ▶ Orthogonality conditions ($\{Z_j\}$ span the kernel around a "bubble")
- ▶ Fixed point argument: ϕ , ψ , λ , ξ

A crucial tool for the study: estimates of Stokes operator with Navier B.C.

Consider the following Stokes system

$$\begin{cases} \partial_t v + \nabla P = \Delta v + F, & \text{in } \mathbb{R}^2_+ \times (0, \infty), \\ \nabla \cdot v = 0, & \text{in } \mathbb{R}^2_+ \times (0, \infty), \\ \partial_{x_2} v_1 \Big|_{x_2 = 0} = 0, & v_2 \Big|_{x_2 = 0} = 0, \\ v \Big|_{t = 0} = 0, & \end{cases}$$
(0.1)

F is solenoidal:

$$\nabla \cdot F = 0, \quad F_2|_{x_2=0} = 0.$$

Theorem (F.H. Lin, Y. S., J. Wei, Y. Zhou)

The solution to (0.1) with solenoidal forcing can be expressed in the form

$$v(x,t) = \int_0^t \int_{\mathbb{R}^2_+} \mathcal{G}^0(x,y,t-\tau) F(y,\tau) dy d\tau +$$

$$\int_0^t \int_{\mathbb{R}^2_+} \mathcal{G}^*(x,y,t-\tau) \int_0^\tau F(y,s) ds dy d\tau \qquad (0.2)$$

$$P(x,t) = \int_0^t \int_{\mathbb{R}^2_+} \mathcal{P}(x,y,t-\tau) \cdot F(y,\tau) dy d\tau$$

$$|\partial_t^s D_x^k D_y^m P_j(x,y,t)| \lesssim t^{-1-s-\frac{m_2}{2}} (|x-y^*|^2 + t)^{-\frac{1+|k|+|m'|}{2}} e^{-\frac{cy_2^2}{t}},$$

$$|\partial_t^s D_x^k D_y^m G_{ij}^*(x,y,t)| \lesssim t^{-1-s-\frac{m_2}{2}} (|x-y^*|^2 + t)^{-\frac{2+|k|+|m'|}{2}} e^{-\frac{cy_2^2}{t}}.$$
(0.3)

See Solonnikov for others B.C.

Heat flow of harmonic maps with free boundary

Let (M, g) be an m-dimensional smooth Riemannian manifold with boundary ∂M and N be another smooth compact Riemannian manifold without boundary. Suppose Σ is a k-dimensional submanifold of N without boundary. Any continuous map $u_0: M \to N$ satisfying $u_0(\partial M) \subset \Sigma$ defines a relative homotopy class in maps from $(M, \partial M)$ to (N, Σ) . A map $u: M \to N$ with $u(\partial M) \subset \Sigma$ is called homotopic to u_0 if there exists a continuous homotopy $h:[0,1]\times M\to N$ satisfying $h([0,1] \times \partial M) \subset \Sigma$, $h(0) = u_0$ and h(1) = u. An interesting problem is that whether or not each relative homotopy class of maps has a representation by harmonic maps, which is equivalent to the following problem:

$$\begin{cases}
-\Delta u = \Gamma(u)(\nabla u, \nabla u), \\
u(\partial M) \subset \Sigma, \\
\frac{\partial u}{\partial \nu} \perp T_u \Sigma.
\end{cases}$$
(0.4)

Here ν is the unit normal vector of M along the boundary ∂M , $\Delta \equiv \Delta_M$ is the Laplace-Beltrami operator of (M,g), Γ is the second fundamental form of N (viewed as a submanifold in \mathbb{R}^{ℓ} via Nash's isometric embedding), T_pN is the tangent space in \mathbb{R}^{ℓ} of N at p and \perp means orthogonal in \mathbb{R}^{ℓ} . (0.4) is the Euler-Lagrange equation for critical points of the Dirichlet energy functional

$$E(u) = \int_{M} |\nabla u|^2 \, dv_g$$

defined over the space of maps

$$H^1_{\Sigma}(M,N) = \{ u \in H^1(M,N) : u(x) \subset \Sigma \text{ a.e. } x \in \partial M \}.$$

Existence by flow (see Eells-Sampson for standard harmonic maps)

$$\begin{cases} \partial_t u - \Delta u = \Gamma(u)(\nabla u, \nabla u) & \text{on } M \times [0, \infty), \\ u(x, t) \in \Sigma & \text{on } \partial M \times [0, \infty), \\ \frac{\partial u}{\partial \nu}(x, t) \perp T_{u(x, t)} \Sigma & \text{on } \partial M \times [0, \infty) \\ u(\cdot, 0) = u_0 & \text{on } M. \end{cases}$$
(0.5)

Weak solutions of the harmonic map heat flow with FB

Take $M = \mathbb{R}^{n+1}_+$ and $N = \mathbb{R}^{\ell}$. We will try to solve the following regularized version of the heat flow (extrinsic version):

$$\begin{cases}
\partial_t u - \Delta u = 0 & \text{in } \mathbb{R}^{n+1}_+ \times \mathbb{R}_+, \\
u(x,0,t) \in \Sigma & x \in \mathbb{R}^n, t > 0, \\
-\lim_{y \to 0^+} \frac{\partial u}{\partial y}(x,y,t) \perp T_{u(x,0,t)} \Sigma & x \in \mathbb{R}^n, t > 0, \\
u(x,y,0) = u_0(x,y) & (x,y) \in \mathbb{R}^{n+1}_+.
\end{cases}$$
(0.6)

We focus on the study of (0.6) for

$$\Sigma = \mathbb{S}^{\ell-1}$$

Intrinsic version: Hamilton, Struwe, Chen-Lin

Harmonic maps with free boundary and their geometric interest

$$\begin{cases}
-\Delta u = \Gamma(u)(\nabla u, \nabla u), \\
u(\partial M) \subset \Sigma, \\
\frac{\partial u}{\partial \nu} \perp T_u \Sigma.
\end{cases}$$

- ► Existence and regularity: Nitsche, Hildebrandt, Jost, Duzaar-Steffen, Hardt-Lin, etc...
- ► New point of view via half-harmonic maps: Da Lio-Rivière, Millot-S., Da Lio-Rivière-Laurain
- ▶ Branched minimal immersions with free boundary and spectral geometry of extremal Steklov eigenvalues: Fraser-Schoen, Karpukhin, Laurain-Petrides, etc..

Ginzburg-Landau approximation

Given $U_0 \in \dot{H}^1(\mathbb{R}^{n+1}_+, \mathbb{S}^{\ell-1})$ and $\varepsilon > 0$, consider

$$\begin{cases} (\partial_t - \Delta) U_{\varepsilon}(x, y, t) = 0 & \text{in } \mathbb{R}^{n+1}_+ \times (0, \infty), \\ U_{\varepsilon}(x, y, 0) = U_0(x, y) & \text{in } \mathbb{R}^{n+1}_+, \\ \frac{\partial U_{\varepsilon}}{\partial y} = -\frac{1}{\varepsilon^2} (1 - |U_{\varepsilon}|^2) U_{\varepsilon} & \text{on } \partial \mathbb{R}^{n+1}_+ \times (0, \infty). \end{cases}$$
(0.7)

For fixed $\varepsilon > 0$, (0.7) is the gradient flow of

$$E_{\varepsilon}(U) = \int_{\mathbb{R}^{n+1}_{\perp}} \frac{1}{2} |\nabla U|^2 dx dy + \int_{\partial \mathbb{R}^{n+1}_{\perp}} \frac{(1 - |U|^2)^2}{4\varepsilon^2} dx.$$

There exist smooth solutions $U_{\varepsilon}: \mathbb{R}^{n+1}_+ \times (0, \infty) \to \mathbb{R}^L$ of (0.7):

$$E_{\varepsilon}(U_{\varepsilon})(t) + \int_{0}^{t} \int_{\mathbb{R}^{n+1}_{+}} |\partial_{t}U_{\varepsilon}|^{2} dx dy dt$$

$$\leq E_{\varepsilon}(U_{0}) = \int_{\mathbb{R}^{n+1}_{+}} \frac{1}{2} |\nabla U_{0}|^{2} dx dy. \tag{0.8}$$

For $U_0 \in H^1(\mathbb{R}^{n+1}_+, \mathbb{S}^{L-1})$, let $u_0 = U_0|_{\partial \mathbb{R}^{n+1}_+}$. Let \mathcal{P}^k denote the k-dimensional Hausdorff measure on $\mathbb{R}^{n+1} \times \mathbb{R}$ with respect to

$$\delta((X,t),(Y,s)) = \max\{|X-Y|,\sqrt{|t-s|}\}.$$

Theorem (A. Hyder, A. Segatti, Y. S., C. Wang)

1) $\exists U_* \in L^{\infty}(\mathbb{R}_+, H^1(\mathbb{R}_+^{n+1}, \mathbb{S}^{\ell-1}))$ with $\partial_t U_* \in L^2(\mathbb{R}_+^{n+1} \times \mathbb{R}_+)$ solving

$$\begin{cases} (\partial_t - \Delta)U_* = 0 & \text{in } \mathbb{R}^{n+1}_+ \times (0, \infty), \\ U_*|_{t=0} = U_0 & \text{on } \mathbb{R}^{n+1}_+, \\ U_*(x, 0, t) \in N; & \frac{\partial U_*}{\partial y}(x, 0, t) \perp T_{U_*(x, 0, t)} N & \text{on } \mathbb{R}^n \times (0, \infty). \end{cases}$$

such that $U_{\varepsilon} \rightharpoonup U_{*}$ in $H^{1}(\mathbb{R}^{n+1}_{+} \times \mathbb{R}_{+})$. 2) $\exists \Sigma \subset \partial \mathbb{R}^{n+1}_{+} \times (0,\infty)$, with $\mathcal{P}^{n+1}(\Sigma) < \infty$, such that

$$U_{\varepsilon} \to U_* \in C^2_{loc}(\overline{\mathbb{R}^{n+1}_+} \times (0,\infty) \setminus \Sigma).$$

Theorem (Continued)

3) Set $u_* = U_*|_{\partial \mathbb{R}^{n+1}_+ \times [0,\infty)}$. Then $u_* \in C^{\infty}(\mathbb{R}^n \times (0,\infty) \setminus \Sigma)$ solves the $\frac{1}{2}$ -harmonic map heat flow:

$$\begin{cases} (\partial_t - \Delta)^{\frac{1}{2}} u_* \perp T_{u_*} \mathbb{S}^{L-1} & \text{in } \mathbb{R}^n \times (0, \infty), \\ u_*(x, 0) = u_0(x) & \text{in } \mathbb{R}^n. \end{cases}$$
(0.9)

4) For any $C_0 > 0$, $\exists \epsilon_0 > 0$ such that if

$$\|\nabla U_0\|_{L^{\infty}(\mathbb{R}^{n+1})} \le C_0, \quad E(U_0) \le \epsilon_0,$$

$$U_* \in C^{\infty}\big(\overline{\mathbb{R}^{n+1}_+} \times (0,\infty)\big) \ (\Rightarrow u_* = U_*\big|_{\partial \mathbb{R}^{n+1}_+ \times [0,\infty)} \in C^{\infty}\big).$$

Why is the LCF with FB model physical?

We first derive the energy law. Multiply by v and integrate over Ω :

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega}|v|^2+\int_{\Omega}(v\cdot\nabla v)\cdot v+\int_{\Omega}\nabla P\cdot v=-\int_{\Omega}|\nabla v|^2-\int_{\Omega}(\Delta u\cdot\nabla u)\cdot v,$$

where we have used

$$\nabla \cdot \left(\nabla u \odot \nabla u - \frac{1}{2} |\nabla u|^2 \mathbb{I}_2 \right) = \Delta u \cdot \nabla u.$$

And

$$\int_{\Omega} (v \cdot \nabla v) \cdot v = \int_{\Omega} \nabla P \cdot v = 0.$$

So we have

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega}|v|^2 = -\int_{\Omega}|\nabla v|^2 - \int_{\Omega}(\Delta u \cdot \nabla u) \cdot v. \tag{0.10}$$

Multiply with $\Delta u + |\nabla u|^2 u$ and integrate over Ω

$$-\frac{1}{2}\frac{d}{dt}\int_{\Omega}|\nabla u|^2 + \int_{\Omega}(v\cdot\nabla u)\cdot(\Delta u + |\nabla u|^2u) = \int_{\Omega}|\Delta u + |\nabla u|^2u|^2.$$

Since

$$\int_{\Omega} (v \cdot \nabla u) \cdot (|\nabla u|^2 u) = \int_{\Omega} |\nabla u|^2 v \cdot \frac{\nabla (|u|^2)}{2} = 0,$$

we obtain

$$-\frac{1}{2}\frac{d}{dt}\int_{\Omega}|\nabla u|^2 + \int_{\Omega}(\Delta u \cdot \nabla u) \cdot v = \int_{\Omega}|\Delta u + |\nabla u|^2 u|^2. \quad (0.11)$$

Combining (0.10) and (0.11), we get

Combining (0.10) and (0.11), we get
$$\frac{1}{2}\frac{d}{dt}\left(\int_{\Omega}|v|^2+|\nabla u|^2\right) = -\int_{\Omega}|\nabla v|^2 - \int_{\Omega}\left|\Delta u + |\nabla u|^2u\right|^2 (0.12)$$

which is called *the basic energy law* (energy dissipation).

On the other hand, the physical compatibility condition should be satisfied

be satisfied
$$\left\langle \left(\frac{\nabla v + (\nabla v)^T}{2} - P \mathbb{I}_2 - \nabla u \odot \nabla u \right) \nu, \tau \right\rangle = 0, \quad \text{on } \partial \Omega,$$
(0.13)

where

$$\nabla \cdot \left(\frac{\nabla v + (\nabla v)^T}{2} - P \mathbb{I}_2 - \nabla u \odot \nabla u \right)$$
 is called *stress tensor*. It is easy to see that $\langle P \mathbb{I}_2 \nu, \tau \rangle = 0$ as

 $\langle \nu, \tau \rangle = 0$. Also,

$$\left\langle \frac{\nabla v + (\nabla v)^T}{2} \nu, \tau \right\rangle = 0$$

,

 $0 = \langle (\nabla u \odot \nabla u) \nu, \tau \rangle = \langle \nabla_{\nu} u, \nabla_{\tau} u \rangle$

implies the free boundary condition

 $\frac{\partial u}{\partial \nu} \perp T_u \Sigma$ on $\partial \Omega \times (0,T)$.

Symmetry encoded in the free boundary condition

Since on $\partial \mathbb{R}^2_+$ one has

$$\begin{cases}
 u(x,t) \in \Sigma, \\
 \frac{\partial u}{\partial \nu}(x,t) \perp T_{u(x,t)}\Sigma, \\
 \frac{\partial u}{\partial \nu}(x,t) = 0, \\
 u_3 = 0,
\end{cases}$$
(0.14)

and

$$\begin{cases} v \cdot \nu = 0, \\ (Sv \cdot \nu)_{\tau} = 0, \end{cases} \implies \begin{cases} \partial_{x_2} v_1 = 0, \\ v_2 = 0, \end{cases}$$
 (0.15)

then even reflection for u_1 , u_2 , v_1 and odd reflection for u_3 , v_2 :

$$\tilde{u}(x_1,x_2,t) = \begin{pmatrix} u_1(x_1,-x_2,t) \\ u_2(x_1,-x_2,t) \\ -u_3(x_1,-x_2,t) \end{pmatrix}, \quad \tilde{v}(x_1,x_2,t) = \begin{pmatrix} v_1(x_1,-x_2,t) \\ -v_2(x_1,-x_2,t) \end{pmatrix},$$

is such that the free boundary conditions are satisfied.

(0.16)

With the previous reflections and

$$\tilde{P}(x_1, x_2, t) = P(x_1, -x_2, t),$$
(0.17)

the structure of the equation is preserved, i.e.,

$$\begin{cases}
\partial_{t}\tilde{u} + \tilde{v} \cdot \nabla \tilde{u} = \Delta \tilde{u} + |\nabla \tilde{u}|^{2} \tilde{u}, \\
\partial_{t}\tilde{v} + \tilde{v} \cdot \nabla \tilde{v} + \nabla \tilde{P} = \Delta \tilde{v} - \nabla \cdot \left(\nabla \tilde{u} \odot \nabla \tilde{u} - \frac{1}{2} |\nabla \tilde{u}|^{2} \mathbb{I}_{2}\right), \\
\nabla \cdot \tilde{v} = 0.
\end{cases}$$
(0.18)

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Open problems

- ➤ Caffarelli-Kohn-Nirenberg partial regularity of suitable solutions in two dimensions
- ▶ Global Weak solutions in three dimensions
- ➤ Coupling surface diffusion with heat flows of harmonic maps (Vorticity formulation with compensated-compactness phenomena with the Hopf differential)
- ▶ (Heat flow of) Harmonic maps with free boundary: Rigidity à la Siu-Sampson for manifolds with boundary, singular domains/targets, Teichmuller flow on moduli space of hyperbolic metrics on surfaces with boundary

THANK YOU