Initial-Boundary Value Problem of a Coupled Navier-Stokes/Q-Tensor Model

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Landau-De Gennes Theory of Nematic Liquid Crystals

Three main continuum theories for nematic liquid crystals: **Ossen-Frank theory, Ericksen theory and Landau-De Gennes theory**. In the Landau-De Gennes framework, the state of a nematic liquid crystal is modeled by a symmetric, traceless 3×3 matrix $Q \in M^{3\times3}$, known as the Q-tensor. A nematic liquid crystal is said to be:

- **Isotropic** when $Q = 0$.
- **uniaxial** when Q has two equal non-zero eigenvalues:

$$Q = s\left(n \otimes n - \frac{1}{3}Id\right); \quad s \in \mathbb{R}\backslash\{0\}, \quad n \in \mathbb{S}^2.$$

- **biaxial** when Q has three distinct eigenvalues:

$$Q = s\left(n \otimes n - \frac{1}{3}Id\right) + r\left(m \otimes m - \frac{1}{3}Id\right); \quad s, r \in \mathbb{R}\backslash\{0\}, \quad n, m \in \mathbb{S}^2.$$

Literature: A. Majumdar and A. Zarnescu'2010.

Free Energy of Nematic Liquid Crystals

One of the simplest form of the free energy of nematic liquid crystals under this framework is the following:

$$\mathcal{F}[Q] := \int_\Omega \frac{L}{2} \underbrace{|\nabla Q|^2(x)}_{\text{elastic energy density}} + \underbrace{f_B(Q(x))}_{\text{bulk energy density}} \, \mathrm{d}x.$$

The widely used form of f_B is as follows:

$$f_B(Q) := a\,\mathrm{tr}(Q^2) + b\,\mathrm{tr}(Q^3) + c\left(\mathrm{tr}(Q^2)\right)^2.$$

The boundary condition of Q is supposed to be the strong anchoring:

$$Q|_{\partial\Omega} = Q_b, \quad Q_b \in C^\infty(\partial\Omega; S_0).$$

De Gennes, P.G. '1974, A. Majumdar and A. Zarnescu'2010.

Governing PDE

The system we shall study is proposed by Beris, A.N., Edwards, B.J.:

$$u_t + u \cdot \nabla u - \operatorname{div}(\nu(Q)Du) + \nabla p = -\nabla \cdot \underbrace{(\tau(Q) + \sigma(Q, H(Q)))}_{\text{additional stress tensor}},$$

$$Q_t + u \cdot \nabla Q = -S(u, Q) + H(Q).$$

$$\begin{cases} H(Q) = \Delta Q - Q + \left[QQ - \frac{1}{d}\mathbb{I}\operatorname{tr} Q^2\right] - Q\operatorname{tr} Q^2, \\ \tau(Q) = -\nabla Q \cdot \nabla Q - \frac{1}{d}\mathbb{I}\operatorname{tr} Q^2, \\ \sigma(Q, H(Q)) = Q \cdot \Delta Q - \Delta Q \cdot Q + \cdots, \\ 2S(u, Q) = -(\nabla u - (\nabla u)^T)Q + Q(\nabla u - (\nabla u)^T). \end{cases}$$

Symmetry and Anti-symmetry

If Q is symmetric tensors, then $H(Q)$, $\tau(Q)$ and $S(u, Q)$ are symmetric and $\sigma(Q, H(Q))$ is anti-symmetric.

Energy Dissipation Law

The total energy of the system is composed of two parts:

$$E(t) := \frac{1}{2}\int_{\Omega} |u(t,x)|^2 \mathrm{d}x + \mathcal{F}\left[Q(t)\right].$$

Assuming $(u, Q)_{\partial\Omega} = (0, Q_b(x))$, by testing $(u, -H(Q))$ and integrating over Ω

$$\frac{d}{dt}E(t) + \int_{\Omega} \nu(Q)\left|Du\right|^2 \mathrm{d}x + \int_{\Omega} \left|H(Q)\right|^2 \mathrm{d}x$$

$$= \underbrace{-\int_{\Omega} \nabla\cdot\sigma(Q,H(Q))\cdot u + S(u,Q)H(Q)}_{\text{algebra lemma: } S(u,Q)H(Q)=\sigma(Q,H(Q))\nabla u} \underbrace{-\int_{\Omega} \nabla\cdot\tau(Q)\cdot u - u\cdot\nabla Q H(Q)}_{\text{vanishes by divergence-free condition}}.$$

Integrating over $[0,t]$ gives

$$E(t) + \int_{Q_t} \nu(Q)|Du(\tau,x)|^2 + |H(\tau,x)|^2 \mathrm{d}x\mathrm{d}\tau = E(0), \quad t \in [0,T]$$

Known Results

The **Cauchy problem** of this system (and a more general one) was investigated in M. Paicu and A. Zarnescu' 2011 and 2012. The main results they obtained are the following:

- The existence of global weak solutions.
- The existence of global strong solutions in two dimension.
- More regular solution with more regular initial data.
- $\cdots$

Global Weak Solutions

In the first step, we assume the 0-Dirichlet boundary conditions for (u, Q):

Theorem

For any $u_0 \in L^2_\sigma(\Omega)$ and $Q_0 \in H^1_0(\Omega)$, there exists

$$u \in L^\infty(0, T; L^2_\sigma(\Omega)) \cap L^2(0, T; H^1_{0,\sigma}(\Omega)),$$
$$Q \in L^\infty(0, T; H^1_0(\Omega)) \cap L^2(0, T; H^1_0(\Omega) \cap H^2(\Omega))$$

solving the initial-boundary value problem **in the sense of distribution** and the energy dissipation law holds.

Steps of the Proof:

1. Adapt the generalized Galerkin approximation used in F.H.Lin and C.Liu'1995.
2. Show that the approximating systems admits an energy dissipation law, which implies a priori estimates for solution series.
3. Passing to the limit using Aubin-Lions compactness.

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Local Strong Solution

For the coupled system, we impose the following initial-boundary conditions

$$\begin{cases} u = 0, & (t,x) \in (0,T) \times \partial\Omega, \\ Q = 0, & (t,x) \in (0,T) \times \partial\Omega, \\ u(0,x) = u_0, & x \in \Omega, \\ Q(0,x) = Q_0, & x \in \Omega. \end{cases}$$

Theorem (H.Abels, G.Dolzman and Y.Liu)

For any $u_0 \in H^1_{0,\sigma}(\Omega)$ and $Q_0 \in H^1_0(\Omega) \cap H^2(\Omega)$, there exists $T > 0$ such that there is a unique solution

$$u \in H^1(0,T; L^2_\sigma(\Omega)) \cap L^2(0,T; H^1_{0,\sigma}(\Omega) \cap H^2(\Omega)),$$
$$Q \in H^1(0,T; H^1_0(\Omega)) \cap L^2(0,T; H^1_0(\Omega) \cap H^3(\Omega))$$

solving the initial-boundary value problem.

Linearization around a given trajectory

Let $\tilde{Q}$ be such that

$$\tilde{Q} \in L^2(0,T;H^3(\Omega)) \cap C([0,T];H^2(\Omega) \cap H_0^1(\Omega)) \cap H^1(0,T;H_0^1(\Omega))$$

We then linearize the nonlinear system around $\tilde{Q}$ by introducing the following linear operator:

$$\mathcal{T}(\tilde{Q})\begin{pmatrix} u \\ Q \end{pmatrix} = \begin{pmatrix} u_t - P_\sigma\left(\operatorname{div}(\nu(\tilde{Q})Du)\right) - P_\sigma\nabla\cdot\overbrace{(\tilde{Q}\Delta Q - \Delta Q\tilde{Q})}^{\sigma(\tilde{Q},\Delta Q)} \\ Q_t - \Delta Q \underbrace{-\frac{1}{2}(\nabla u - (\nabla u)^T)\tilde{Q} + \frac{1}{2}\tilde{Q}(\nabla u - (\nabla u)^T)}_{S(u,\tilde{Q})} \\ (u,Q)\big|_{t=0} \end{pmatrix}.$$

Nonlinear Terms and Functional Spaces

Using the above defined $\tilde{Q}$, we can also define a nonlinear operator $\mathcal{N}$ by

$$\mathcal{N}(\tilde{Q})\begin{pmatrix} u \\ Q \end{pmatrix} = \begin{pmatrix} P_\sigma\left[\operatorname{div}\left(\left(\nu(Q)-\nu(\tilde{Q})\right)Du\right)+\nabla\cdot\left(\tau(Q)+\sigma(Q-\tilde{Q},\Delta Q)-u\otimes u\right)\right] \\ -u\cdot\nabla Q - S(u,Q-\tilde{Q})-L(Q) \\ (u_0,Q_0) \end{pmatrix}$$

We define two Banach spaces $X_T = X_T^1 \times X_T^2$ and Y_T by

$$X_T^1 = \left\{u \in L^2(0,T;H^2(\Omega)\cap H^1_{0,\sigma}(\Omega))\cap H^1(0,T;L^2(\Omega))\right\}$$

$$X_T^2 = \left\{Q \in L^2(0,T;H^3(\Omega))\cap H^1(0,T;H^1_0(\Omega)),\ \Delta Q|_{\partial\Omega}=0\right\}$$

$$Y_T = L^2(0,T;L^2_\sigma(\Omega))\times L^2(0,T;H^1_0(\Omega))\times H^1_{0,\sigma}(\Omega)\times\left(H^2(\Omega)\cap H^1_0(\Omega)\right)$$

Proof of the existence of local strong solution

- The linear operator $\mathcal{T}(\tilde{Q}) : X_T \to Y_T$ is an isomorphism.
- The nonlinear operator $\mathcal{N}(\tilde{Q}) : X_T \to Y_T$ is locally Lipschitz with arbitrarily small Lipschitz constant when $T > 0$ is sufficiently small.

Then the proof amounts to showing the existence of $(u, Q) \in X_T$ such that

$$\mathcal{T}(\tilde{Q}) \begin{pmatrix} u \\ Q \end{pmatrix} = \mathcal{N}(\tilde{Q}) \begin{pmatrix} u \\ Q \end{pmatrix}$$

and this is equivalent to the assertion that the nonlinear mapping

$$\mathcal{F}(\tilde{Q}) := \mathcal{T}^{-1}\mathcal{N} : X_T \to X_T$$

has a fixed point. To this end, we choose $\tilde{Q}$ to be the solution to:

$$\begin{cases} \tilde{Q}_t &= \Delta \tilde{Q}, & (x,t) \in Q_T, \\ \tilde{Q} &= 0, & (x,t) \in \partial\Omega \times (0,T), \\ \tilde{Q} &= Q_0, & (x,t) \in \Omega \times \{0\}. \end{cases}$$

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The Analysis of the Linear Operator: I

To prove $\mathcal{T}(\tilde{Q}) : X_T \to Y_T$ is an isomorphism is equivalent to show the strong wellposedness of the following linear system:

$$\begin{cases} u_t - \operatorname{div}\left(\nu(\tilde{Q})Du\right) + \nabla p - \nabla \cdot (\tilde{Q}\Delta Q - \Delta Q\tilde{Q}) = f, \\ Q_t - \Delta Q - \frac{1}{2}(\nabla u - (\nabla u)^T)\tilde{Q} + \frac{1}{2}\tilde{Q}(\nabla u - (\nabla u)^T) = g, \\ u = 0, \; x \in \partial\Omega, \\ Q = 0, \; x \in \partial\Omega, \\ (u, Q)|_{t=0} = (u_0, Q_0). \end{cases}$$

with $(f, g, u_0, Q_0) \in Y_T$ and $(u, Q) \in X_T$.

- Testing the equations by u and ΔQ respectively will give an energy dissipation law, which implies the existence of global weak solutions.
- Testing the equations by $\left(P_\sigma \operatorname{div}\left(\nu(\tilde{Q})Du\right), \Delta^2 Q\right)$ will give the a priori estimate for strong solution.

The Analysis of the Linear Operator: II

We shall first establish the wellposedness of the following $\varepsilon-$ regularized system:

$$\begin{cases} u_t - \text{div}\left(\nu(\tilde{Q})Du\right) + \nabla p - \nabla \cdot (\tilde{Q}\Delta Q - \Delta Q\tilde{Q}) = f, \\ Q_t + \varepsilon\Delta^2 Q - \Delta Q - \frac{1}{2}(\nabla u - (\nabla u)^T)\tilde{Q} + \frac{1}{2}\tilde{Q}(\nabla u - (\nabla u)^T) = g, \\ u = 0, \ x \in \partial\Omega, \\ Q = 0, \ \Delta Q = 0, \ x \in \partial\Omega, \\ (u, Q)|_{t=0} = (u_0, Q_0). \end{cases}$$

1. The local strong solution by a fixed point argument.
2. The global strong solution by testing procedure and an uniform a priori estimate.
3. send $\varepsilon \to 0$ to get rid of $-\varepsilon\Delta^2 Q$ in the equations and the boundary condition $\Delta Q|_{\partial\Omega} = 0$ **becomes a compatibility condition** for a second-order parabolic equation.
4. Show that the weak $\varepsilon-$ limit is the strong solution of the original linear system.

More about the Testing Procedure: I

Testing: $u \rightsquigarrow P_\sigma \,\mathrm{div}\, \big(\nu(\tilde Q) Du\big)$ and $Q \rightsquigarrow \Delta^2 Q$:

$$\overbrace{u_t - \mathrm{div}\, \big(\nu(\tilde Q)Du\big) + \nabla p}^{\text{Testing by } P_\sigma\,\mathrm{div}\big(\nu(\tilde Q)Du\big)} - \overbrace{\nabla\cdot\big(\tilde Q\Delta Q - \Delta Q\tilde Q\big)}^{\text{Testing by } \mathrm{div}\big(\nu(\tilde Q)Du\big)} = f,$$

$$\underbrace{Q_t + \varepsilon\Delta^2 Q - \Delta Q}_{\text{Testing by } \Delta^2 Q} \underbrace{- \frac{1}{2}(\nabla u - (\nabla u)^T)\tilde Q + \frac{1}{2}\tilde Q(\nabla u - (\nabla u)^T)}_{\text{Testing by } \Delta^2 Q} = g,$$

Testing by $P_\sigma \,\mathrm{div}\, \big(\nu(\tilde Q)Du\big)$ is equivalent to testing by $\mathrm{div}\, \big(\nu(\tilde Q)Du\big)$ for the second part of the equations of u !

$$P_\sigma \,\mathrm{div}\, \big(\nu(\tilde Q)Du\big) = \mathrm{div}\, \big(\nu(\tilde Q)Du\big) - \nabla q, \quad q \in H^1_{(0)}(\Omega),$$

$$\int_\Omega \nabla\cdot(\tilde Q\Delta Q - \Delta Q\tilde Q)\nabla q = -\int_\Omega \underbrace{(\tilde Q\Delta Q - \Delta Q\tilde Q)}_{anti-symmetric} \underbrace{\nabla^2 q}_{symmetric} = 0.$$

More about the testing procedure: II

The additional boundary conditions $\Delta Q|_{\partial\Omega} = 0$ will eliminate all the boundary integral possibly arising due to the integrate by parts:

$$\left.\begin{array}{l}\overbrace{\nabla\cdot(\tilde{Q}\Delta Q - \Delta Q\tilde{Q})}^{\text{Testing by } \operatorname{div}\left(\nu(\tilde{Q})Du\right)} \\ \underbrace{-\frac{1}{2}(\nabla u - (\nabla u)^T)\tilde{Q} + \frac{1}{2}\tilde{Q}(\nabla u - (\nabla u)^T)}_{\text{Testing by } \Delta^2 Q}\end{array}\right\} \rightsquigarrow \text{lower order terms}$$

Estimates on the lower order terms gives:

$$\|u\|^2_{L^\infty(0,T;H^1)} + \|Q\|^2_{L^\infty(0,T;H^2)} + \varepsilon\|Q\|^2_{L^2(0,T;H^4)} + \|u\|^2_{L^2(0,T;H^2)} + \|Q\|^2_{L^2(0,T;H^3)} \leqslant C(\Omega,\tilde{Q})\left(\|Q_0\|^2_{H^2} + \|u_0\|^2_{H^1} + \|f\|^2_{L^2(Q_T)} + \|g\|^2_{L^2(0,T;H^1)}\right).$$

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Testing procedure again !

Recall that, the previous argument gives the local wellposedness the following system:

$$
\begin{aligned}
&u_t + u \cdot \nabla u - \operatorname{div}(\nu(Q) Du) + \nabla p = -\nabla \cdot (\tau(Q) + \sigma(Q, H(Q))),\\
&Q_t + u \cdot \nabla Q = S(u, Q) + H(Q).
\end{aligned}
$$

with the following boundary conditions:

$$
\begin{cases}
u = 0, & (t, x) \in (0, T) \times \partial\Omega,\\
Q = 0, \quad \Delta Q = 0, & (t, x) \in (0, T) \times \partial\Omega.
\end{cases}
$$

Testing the system by $\left(P_\sigma \operatorname{div}(\nu Du), \Delta H(Q)\right)$ will not give rise to non-vanishing boundary integral due to $\Delta Q|_{\partial\Omega} = 0$, which is a **compatibility condition** for local strong solution.

Uniform estimate for the global strong solution

Proposition

For constant viscosity, the local strong solution satisfies the following uniform estimate:

- $\frac{1}{2}\frac{d}{dt}\mathcal{A}(t) + \mathcal{B}(t) \leqslant C(\Omega)\mathcal{A}(t)\left(\mathcal{A}(t)+1\right), \quad d=2,$
- $\frac{1}{2}\frac{d}{dt}\mathcal{A}(t) + \mathcal{B}(t) \leqslant C(\Omega)\mathcal{A}(t)\left(\mathcal{A}^3(t)+1\right), \quad d=3.$

where

$$\mathcal{A}(t) := \|H(Q(\cdot,t))\|^2_{L^2(\Omega)} + \|\nabla u(\cdot,t)\|^2_{L^2(\Omega)},$$
$$\mathcal{B}(t) := \|\nabla_x H(Q(\cdot,t))\|^2_{L^2(\Omega)} + \|P_\sigma \Delta u(\cdot,t)\|^2_{L^2(\Omega)}.$$

The energy dissipation gives $\mathcal{A}(t) \in L^1(0,T)$. Applying Gronwall's inequality (and continuity argument for $d=3$) gives the uniform estimate.

Global strong solution

For the moment, we only work out the result for a constant viscosity ν:

Theorem (H.Abels, G.Dolzman and Y.Liu)

When $d = 2$, the local strong solution doesn't blow up at any finite $T > 0$.
When $d = 3$, let $Q^* \in H^2(\Omega) \cap H_0^1(\Omega)$ be an absolute minimizer of the free energy. Then there exist $\delta > 0$ such that for any

$$(u_0, Q_0) \in H_0^1(\Omega) \times \left(H^2(\Omega) \cap H_0^1(\Omega)\right)$$

satisfying $\|u_0\|_{H^1(\Omega)} + \|Q_0 - Q^*\|_{H^2(\Omega)} < \delta$, the initial-boundary value problem admits a unique global strong solution.

Similar Results: H.Wu, X.Xu and C.Liu'2011.

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Conclusion

We obtained the following results for system with 0-Dirichlet boundary conditions:

1. Global weak solutions.
2. Local strong solution.
3. Global strong solution in 2d.
4. Global strong solution in 3d with initial data near the equilibrium.

Future work

1. (Local) Wellposedness for strong anchoring boundary condition for Q.
   Linearize the system around $\tilde{Q}$ verifying:

$$\begin{cases} \tilde{Q}_t = \Delta \tilde{Q} + \cdots, & (x,t) \in Q_T, \\ \tilde{Q} = Q_b(x), & (x,t) \in \partial\Omega \times (0,T), \\ \tilde{Q} = Q_0, & (x,t) \in \Omega \times \{0\}. \end{cases}$$

2. Wellposedness for Neuman boundary condition for Q.

Thank you

Thank you for your attention!