Nematic liquid crystal-colloidal interaction

Arnab Roy

Basque Center of Applied Mathematics, Bilbao, Spain

Workshop: Analysis of Nematic Liquid Crystal Flows
April 25 - 29, 2022

Joint work with Zhiyuan Geng, Arghir Dani Zarnescu

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Immersed structure: solids inside fluid

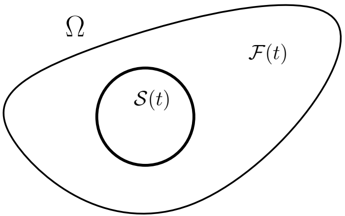

Figure: Rigid body inside a fluid domain

Blood flow problems

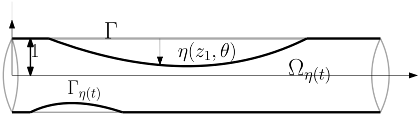

Figure: Deformed domain

Problem Description

- The flow hydrodynamics with incompressible nematic liquid crystals.
- Model colloidal particle as a rigid ball in Ω.
- $\mathcal{S}(t)$: closed, bounded, simply connected, $\mathcal{F}(t)$: fluid domain.

Mathematical set up: fluid domain

Equations defined in $(0, T) \times \mathcal{F}(t)$:

$$\partial_t Q + (u^{\mathcal{F}} \cdot \nabla) Q - S(\nabla u^{\mathcal{F}}, Q) = \Gamma H,$$
$$\partial_t u^{\mathcal{F}} + \left(u^{\mathcal{F}} \cdot \nabla\right) u^{\mathcal{F}} + \nabla p = \mu \Delta u^{\mathcal{F}} + \operatorname{div}(\tau + \sigma),$$
$$\operatorname{div} u^{\mathcal{F}} = 0.$$

$$S(\nabla u^{\mathcal{F}}, Q) = (\Sigma Q - Q \Sigma),$$
$$H = \Delta Q - aQ + b\left(Q^2 - \frac{\operatorname{tr}(Q^2)}{3} \mathbb{I}_d\right) - c\, Q \operatorname{tr}(Q^2).$$

$u^{\mathcal{F}}$: flow velocity, $p^{\mathcal{F}}$: pressure, Q: Landau-de Gennes tensor, traceless and symmetric.

Symmetric and anti-symmetric part of velocity gradient:

$$D = \frac{1}{2}\left(\nabla u^{\mathcal{F}} + (\nabla u^{\mathcal{F}})^{\top}\right), \quad \Sigma = \frac{1}{2}\left(\nabla u^{\mathcal{F}} - (\nabla u^{\mathcal{F}})^{\top}\right).$$

Nematic crystal stress:

$$\tau = -L\nabla Q \odot \nabla Q, \quad \sigma = QH - HQ.$$

Motion: colloidal particle

$$mh'' = -\int_{\partial\mathcal{S}(t)} (2\mu D + \tau + \sigma - p\mathbb{I}_3)n\, d\Gamma,$$

$$J\omega' = -\int_{\partial\mathcal{S}(t)} (x - h) \times \cdot(2\mu D + \tau + \sigma - p\mathbb{I}_3)n\, d\Gamma.$$

n: unit outward normal to the boundary of $\mathcal{F}(t)$.
$h(t)$: centre of mass, $h'(t)$: translational velocity, $\omega(t)$: angular velocity.

$$u^{\mathcal{S}}(t,x) = h'(t) + \omega(t) \times (x - h(t)).$$

Initial-Boundary condition

$$u^{\mathcal{F}} = u^{\mathcal{S}} \quad \text{on } (0,T) \times \partial\mathcal{S}(t), \quad u^{\mathcal{F}} = 0 \quad \text{on } (0,T) \times \partial\Omega,$$
$$Q = 0 \quad \text{on } (0,T) \times \partial\mathcal{S}(t), \quad Q = 0 \quad \text{on } (0,T) \times \partial\Omega.$$

$$\frac{\partial Q}{\partial n} = 0 \quad \text{on } (0,T) \times \partial\mathcal{S}(t), \quad \frac{\partial Q}{\partial n} = 0 \quad \text{on } (0,T) \times \partial\Omega.$$

Results we need

- San Martin et.al (2002): Global weak solution for incompressible fluid + rigid bodies.
- E. Feireisl (2003): motion of rigid bodies in a viscous incompressible fluid.
- M.Paicu, A.Zarnescu (2012): Energy dissipation and regularity for a coupled Navier-Stokes and Q-tensor system.
- F. González, M. Rodríguez (2015): Weak solutions for an initial-boundary Q-tensor problem related to liquid crystals.

Functional framework

$$H(\Omega) = \left\{ v \in L^2(\Omega) \mid \operatorname{div} v = 0, \quad v \cdot n = 0 \text{ in } H^{-1/2}(\partial\Omega) \right\},$$

$$V(\Omega) = \left\{ v \in H^1(\Omega) \mid \operatorname{div} v = 0 \right\}.$$

If χ is the characteristic function of a subset in Ω, we define

$$K(\chi) = \left\{ v \in V(\Omega) \mid \chi D(v) = 0 \text{ in } L^2(\Omega) \right\}.$$

$$S(\chi) = \{ x \in \Omega \mid \chi(x) = 1 \}.$$

$$M = \{ Q \in SO(d) \mid \mathrm{tr}(Q) = 0 \}.$$

Uniform velocity field in $(0, T) \times \Omega$:

$$u = \begin{cases} u^{\mathcal{F}} \text{ in } \mathcal{F}(t), \\ u^{\mathcal{S}} \text{ in } \mathcal{S}(t). \end{cases}$$

Weak solution

Let $u_0 \in H(\Omega)$, $Q_0 \in H^1_0(\mathcal{F}_0)$ and φ_0 be characteristic function of $\mathcal{S}_0$. The triplet (u, Q, φ) satisfying $u \in L^\infty(0,T; H(\Omega)) \cap L^2(0,T; K(\varphi))$, $Q \in L^\infty(0,T; H^1(\mathcal{F}(t))) \cap L^2(0,T; H^2(\mathcal{F}(t)))$, $\varphi \in$ Char (Ω) is said to be a weak solution if the following holds:

$$\int_0^T \int_{\mathcal{F}(t)} [-Q \cdot \partial_t \psi - \Gamma \Delta Q \cdot \psi - (u \cdot \nabla)\psi \cdot Q - \Sigma Q \cdot \psi + Q\Sigma \cdot \psi]$$

$$= \int_{\mathcal{F}_0} Q_0 \cdot \psi(0) + \Gamma \int_0^T \int_{\mathcal{F}(t)} \left[-aQ + b\left(Q^2 - \frac{\mathrm{tr}(Q^2)}{3}\mathbb{I}_3\right) - c\, Q\, \mathrm{tr}(Q^2)\right] \cdot \psi,$$

$$\int_0^T \int_\Omega \left[-u\partial_t\zeta - u_\alpha u_\beta \partial_\alpha \zeta_\beta + \mu D(u) : D(\zeta)\right] \, dx \, dt - \int_\Omega u_0 \cdot \zeta(0) \, dx$$
$$= \int_0^T \int_{\mathcal{F}(t)} \left[Q_{\gamma\delta,\alpha} Q_{\gamma\delta,\beta} \zeta_{\alpha,\beta} - Q_{\alpha\gamma} \Delta Q_{\gamma\beta} \zeta_{\alpha,\beta} + \Delta Q_{\alpha\gamma} Q_{\gamma\beta} \zeta_{\alpha,\beta}\right] \, dx \, dt,$$

$$\int_0^T \int_\Omega \varphi \left[\partial_t \eta + (u \cdot \nabla)\eta\right] \, dx \, dt = - \int_\Omega \varphi_0 \cdot \eta(0) \, dx,$$

for any functions $\psi \in C_c^\infty([0,T) \times \mathcal{F}(t); M)$, $\zeta \in H^1((0,T) \times \Omega) \cap L^2(0,T; K(\varphi))$, $\zeta(T) = 0$, $\eta \in C^1((0,T) \times \Omega)$, $\eta(T) = 0$.

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Main result

Assume that $u_0 \in H(\Omega)$, $Q_0 \in H^1_0(\mathcal{F}_0)$, φ_0 is the characteristic function of $\mathcal{S}_0$ and the boundaries $\partial\Omega$, $\partial\mathcal{S}$ are of class C^2. Then there exists at least a solution to the system. Moreover,

$$E(u,Q)(t) + \mu \int_0^t \int_\Omega |Du|^2 + \Gamma \int_0^t \int_{\mathcal{F}(t)} \mathrm{tr}\Big(L\Delta Q - aQ + b[Q^2 - \frac{\mathrm{tr}(Q^2)}{3} Id] - cQ\mathrm{tr}(Q^2) \Big)^2 \leqslant E(u_0, Q_0),$$

where

$$E(t) \stackrel{def}{=} \frac{1}{2}\int_\Omega |u|^2 + \int_{\mathcal{F}(t)} \Big[\frac{1}{2}|\nabla Q|^2 + \frac{a}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}(\mathrm{tr}(Q^2))^2 \Big].$$

Difficulties

- The fluid domain depends on time.
- Appropriate test function space.
- Approximate problem: a penalized problem where we approximate the rigid bodies by very viscous fluids.
- Passing to the limit.

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Approximate problem

Given $u_0 \in H(\Omega)$, $Q_0 \in L^2(\Omega)$ and $\tau_0 \in L^\infty(\Omega) \cap \mathrm{Char}(\Omega)$, we want to find $(u^n, Q^n, \varphi^n, \tau^n)$ such that $u^n \in L^\infty(0,T;H(\Omega)) \cap L^2(0,T;V(\Omega))$,

$$Q^n \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)),$$

$$\varphi^n,\ \tau^n \in \text{Char } (\Omega) \text{ with } S(\varphi^n) = (S(\tau^n))_\delta,$$

and the following relations hold

$$\int_0^T \int_\Omega \Big[- Q^n \cdot \partial_t \psi - (\Gamma + n\varphi^n)\Delta Q^n \cdot \psi - (u^n \cdot \nabla)\psi \cdot Q^n$$

$$- \Sigma^n Q^n \cdot \psi + Q^n \Sigma^n \cdot \psi \Big] = \int_\Omega Q_0 \cdot \psi(0)$$

$$+ \int_0^T \int_\Omega (\Gamma + n\varphi^n) \Big[-aQ^n + b\left((Q^n)^2 - \frac{\mathrm{tr}((Q^n)^2)}{3} \mathbb{I}_3 \right) - c\, Q^n \,\mathrm{tr}((Q^n)^2) \Big] \cdot \psi,$$

$$\int_0^T \int_\Omega \left[-u^n \partial_t \zeta - u^n_\alpha u^n_\beta \partial_\alpha \zeta_\beta + (\mu + n\varphi^n) D(u^n) : D(\zeta)\right] - \int_\Omega u_0 \cdot \zeta(0)$$

$$= \int_0^T \int_\Omega \left[Q^n_{\gamma\delta,\alpha} Q^n_{\gamma\delta,\beta} \zeta_{\alpha,\beta} - Q^n_{\alpha\gamma} \Delta Q^n_{\gamma\beta} \zeta_{\alpha,\beta} + \Delta Q^n_{\alpha\gamma} Q^n_{\gamma\beta} \zeta_{\alpha,\beta}\right],$$

$$\int_0^T \int_{\Omega_\delta} \tau^n \left[\partial_t \theta + (\overline{u^n} \cdot \nabla)\theta\right] = -\int_{\Omega_\delta} \tau_0 \cdot \theta(0),$$

for any functions $\psi \in C_c^\infty([0,T) \times \Omega; M)$, $\zeta \in H^1((0,T) \times \Omega) \cap L^2(0,T; V(\Omega))$, $\zeta(T) = 0$, $\theta \in C^1((0,T) \times \Omega_\delta)$, $\theta(T) = 0$.

Existence: Approximate problem

For any $n \in \mathbb{N}$, $u_0 \in H(\Omega)$, $\tau_0 \in L^\infty(\Omega) \cap \text{Char}(\Omega)$, there exists at least a solution of the penalized problem. Moreover, we have the following energy estimate: for a.e. $x \in \Omega$, $t \in (0,T)$

$$E(u^n, Q^n)(t) + \int_0^t \int_\Omega (\mu + n\varphi^n)|Du^n|^2 \\ + \int_0^t \int_\Omega (\Gamma + n\varphi^n)\mathrm{tr}\Big(L\Delta Q^n - aQ^n + b[(Q^n)^2 - \frac{\mathrm{tr}((Q^n)^2)}{3}Id] \\ - cQ^n \mathrm{tr}((Q^n)^2)\Big)^2 \leqslant E(u_0, Q_0).$$

Convergences

$$
\begin{aligned}
u^n \to u \text{ weakly in } L^2(0,T;V(\Omega)) \text{ and weakly}^* \text{ in } L^\infty(0,T;H(\Omega)),\\
Q^n \to Q \text{ weakly in } L^2(0,T;H^2(\Omega)) \text{ and weakly}^* \text{ in } L^\infty(0,T;H^1(\Omega)),\\
H^n \to H \text{ weakly in } L^2(0,T;L^2(\Omega)),\\
\tau^n \to \tau \text{ weakly}^* \text{ in } L^\infty(0,T;L^\infty(\Omega_\delta)).
\end{aligned}
$$

Strategy

- Passing the limit in the transport equation: the compactness result due to Diperna and Lions.
- Strong convergences: $\{Q^n\}$ converges strongly to Q in $L^2(0,T;H^1(\mathcal{F}(t)))$, $\{u^n\}$ converges strongly to u in $L^2(0,T;L^2(\Omega))$.
- Passing the limit in the Q-tensor equation: test function $\psi \in C_c^1([0,T] \times (\Omega \setminus \mathcal{S}_\delta(\varphi(t))), M)$, then due to the fact that $\mathcal{S}(\varphi^n(t)) \subset \mathcal{S}_\delta(\varphi(t))$, we have $\varphi^n \psi = 0$.

- Passing the limit in the momentum equation:

$$\int_0^T \int_{\mathcal{F}(t)} [\nabla Q^n \otimes \nabla Q^n : D(\zeta) + (H^n Q^n - Q^n H^n) : \nabla \zeta]$$

$$+ \lim_{n\to\infty} \int_0^T \int_{\mathcal{S}(\varphi^n(t))} [(H^n Q^n - Q^n H^n) : \nabla \zeta]$$

- Behaviour of H^n in the solid domain.

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Future Direction

- The Neumann boundary condition at the interface: test function space, appropriate approximate problem, recovery of interface condition.
- Several colloidal particles.

Thank You