Nonlinear electrokinetics in nematic electrolytes

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Analysis of Nematic Liquid Crystals Flows

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Plan of the Talk

- We study a system of nonlinear PDEs modelling the electrokinetics of a nematic electrolyte material consisting of various ions species contained in a nematic liquid crystal
- The evolution is described by a system coupling a Nernst-Planck system for the ions concentrations with a Maxwell's equation of electrostatics governing the evolution of the electrostatic potential, a Navier-Stokes equation for the velocity field, and a non-smooth Allen-Cahn type equation for the nematic director field
- We focus on the two-species case and prove apriori estimates that provide a weak sequential stability result, the main step towards proving the existence of weak solutions
- Some future perspectives and open problems

The model

We consider a version of the system derived in

[CGLW] M.C. Calderer, D. Golovaty, O. Lavrentovich, and J.N. Walkington, Modeling of nematic electrolytes and nonlinear electroosmosis. *SIAM J. Appl. Math.*, **76** (2016), no. 6, 2260-2285

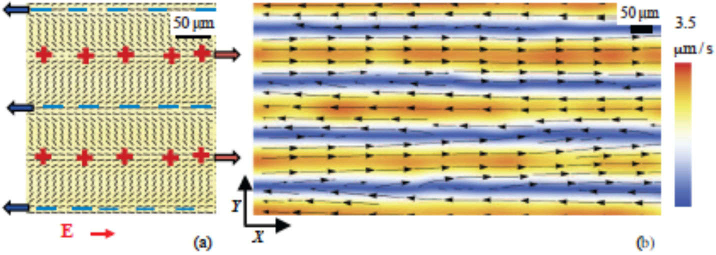
describing the electrokinetics of a nematic electrolyte that consists of ions that diffuse and advect in a nematic liquid crystal environment.

There is a growing interest in nonlinear electrokinetics, in which the flow velocities grow as the square of the applied field.

The studies of the liquid crystal-enabled electrokinetics are a part of a much larger field of liquid crystal colloids that is currently experiencing a great deal of interest partially as a result of the progress in the field of nanotechnology.

Recent experiments demonstrate that when the isotropic electrolyte is replaced with an anisotropic electrolyte, a liquid crystal containing ions, the electrokinetic flow become strongly nonlinear, with the velocities growing as a square of the electric field. For such a flow, if the polarity of the applied fields reversed, the direction of the flow remains unchanged, enabling (alternating current) AC-driven electroosmosis and electrophoresis.

LCs-enabled electroosmotic flows in a flat nematic cell with patterned 1D periodic director field (by [CGLW])



(a) Experimentally imposed director pattern (black dashes) and space charge separation (positive and negative ions marked by + and -) due to director distortions when the electric field is from the left to the right. The director orientation is periodically varying in the vertical direction and an AC field is applied in the horizontal direction. It was observed that spatially periodic horizontal flow proceeds along the "guiding rails" induced by molecular orientation with the direction of the flow independent of the sign of the field.

(b) Experimentally determined map of electroosmotic velocities corresponding to the director pattern in (a).

The variables

The system can be written in terms of the following variables:

- the vector n modelling the local orientation of the nematic liquid crystal molecules,
- the macroscopic velocity v of the liquid crystal molecules,
- the pressure p resulting from the incompressibility constraint on the fluid,
- the electrostatic potential Φ (the electric field $\mathbf{E} = \nabla\Phi$),
- the concentrations c_k, $k = 1, \ldots, N$, with valences $z_k \in \{-1, 1\}$, of the families of charged ions present in the liquid crystal.

Simplifications

We consider a modified version of the system in [CGLW], assuming certain simplifications commonly used in the mathematical literature on liquid crystals:

- we take equal elastic constants in the Oseen-Frank energy
- use a Ginzburg-Landau configuration potential $\mathcal{F}$ of *singular* type in order to avoid introducing the unit length constraint on n (and thus we can correspondingly drop the related Lagrange multiplier term λn in the system in [CGLW])
- we neglect body forces and inertial effects acting on the director field.

Our PDE system

$$\frac{\partial c_k}{\partial t} + v \cdot \nabla c_k = \frac{1}{k_B \theta} \operatorname{div}\left(c_k \mathcal{D}_k \nabla \mu_k\right), \quad \text{for } k = 1, \dots, N,$$

$$-\operatorname{div}(\varepsilon_0 \varepsilon(n) \nabla \Phi) = \sum_{k=1}^{N} q z_k c_k,$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v + \nabla p = -K \operatorname{div}(\nabla n \odot \nabla n) + \operatorname{div} \sigma,$$

$$+ \varepsilon_0 \operatorname{div}\left((\nabla \Phi \otimes \nabla \Phi) \varepsilon(n)\right),$$

$$\operatorname{div} v = 0,$$

$$\gamma_1 (n_t + v \cdot \nabla n - \Omega(v) n) + \gamma_2 D(v) n = K \Delta n + \varepsilon_0 \varepsilon_a \left(\nabla \Phi \otimes \nabla \Phi\right) n - \partial \mathcal{F}$$

μ_k are the electrochemical potentials of the ions associated to the various ions species c_k:

$$\mu_k := k_B \theta (\ln(c_k) + 1) + q z_k \Phi$$

$k_B > 0$ denotes the Boltzmann constant, $\theta > 0$ stands for the absolute temperature, and q denotes the elementary charge.

$$D(v) := \frac{1}{2}(\nabla v + \nabla v^t) \quad \text{and} \quad \Omega(v) := \frac{1}{2}(\nabla v - \nabla v^t)$$

stand for the symmetric and antisymmetric parts of the velocity gradient and $\nabla n \odot \nabla n$ denotes the 3×3 matrix of components $(n_{k,i} n_{k,j})$.

The Maxwell's equation of electrostatics

The diffusion operator in

$$-\operatorname{div}(\varepsilon_0 \varepsilon(n) \nabla \Phi) = \sum_{k=1}^{N} q z_k c_k$$

is ruled by the matrix

$$\varepsilon(n) := \varepsilon_\perp \operatorname{Id} + \varepsilon_a n \otimes n,$$

with constants $\varepsilon_\perp > 0$ and $\varepsilon_a \geq 0$, Id denoting the identity matrix.

Here $\varepsilon_a = \varepsilon_{||} - \varepsilon_\perp$, where $\varepsilon_{||}$ and $\varepsilon_\perp$ denote the electric permittivity when the electric field $\mathbf{E} = \nabla \Phi$ is parallel, respectively, perpendicular to n.

The constant $\varepsilon_0 > 0$ stands for the vacuum dielectric permeability.

The Nernst-Planck type equations

$$\frac{\partial c_k}{\partial t} + v \cdot \nabla c_k = \frac{1}{k_B \theta} \operatorname{div}\left(c_k \mathcal{D}_k \nabla \mu_k\right), \quad \text{for } k = 1, \ldots, N,$$

correspond to the continuity equation for ions

$$\frac{\partial c_k}{\partial t} + \operatorname{div}(c_k u_k) = 0, \quad u_k = v - \frac{1}{k_B \theta} \mathcal{D}_k \nabla \mu_k,$$

with the electrochemical potential of the ions:

$$\mu_k := k_B \theta (\ln(c_k) + 1) + q z_k \Phi$$

and the electric potential Φ satisfying the Maxwell's equation of electrostatics:

$$-\operatorname{div}(\varepsilon_0 \varepsilon(n) \nabla \Phi) = \sum_{k=1}^{N} q z_k c_k.$$

The diffusion matrices $\mathcal{D}_k$ is anisotropic, reflecting the fact that the mobilities of the kth species in the directions parallel and perpendicular to the nematic director are generally different. However $\mathcal{D}_k$ are positive definite, i.e.,

$$(\mathcal{D}_k \xi) \cdot \xi > \alpha |\xi|^2$$

for some $\alpha > 0$ and all $k = 1, \ldots, N$ and $\xi \in \mathbb{R}^3$.

The Navier-Stokes equations

The Navier-Stokes equations

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v + \nabla p = -K \operatorname{div}(\nabla n \odot \nabla n) + \operatorname{div} \sigma + \varepsilon_0 \operatorname{div} \left((\nabla \Phi \otimes \nabla \Phi) \varepsilon(n) \right),$$

with the incompressibility constraint

$$\operatorname{div} v = 0,$$

rule the evolution of the liquid crystal flow.

Note the Korteweg forces on the right hand side being induced by the the director field n and the effects of the electric field, respectively.

As in [Leslie, '92], we assume for the total stress tensor the following general expression:

$$\sigma = \alpha_1 (D(v) n \cdot n) n \otimes n + \alpha_2 \mathring{n} \otimes n + \alpha_3 n \otimes \mathring{n} + \alpha_4 D(v) + \alpha_5 D(v) n \otimes n + \alpha_6 n \otimes D(v) n,$$

where we have denoted $\mathring{n} := \partial_t n + v \cdot \nabla n - \Omega(v) n$ the Lie derivative of n.

The term $\alpha_4 D(v)$ represents the classical Newtonian stress tensor, while the other terms represent the additional stress produced by the interaction of the anisotropic liquid crystal molecules, see [Ericksen, '61].

The director field equation

As mentioned above, we avoid to insert the unit length constraint in

$$\gamma_1(n_t + v \cdot \nabla n - \Omega(v)n) + \gamma_2 D(v)n = K\Delta n + \varepsilon_0\varepsilon_a (\nabla\Phi \otimes \nabla\Phi)\, n - \partial\mathcal{F}$$

and instead require $|n| \leq 1$, (cf. the variable length model proposed by J. L. Ericksen).

Indeed, we enforce the property $|n| \leq 1$ by means of the *singular potential* $\mathcal{F} : \mathbb{R}^3 \to [0, +\infty]$ assumed to be a convex and lower semicontinuous function whose *effective domain* is assumed to coincide with the closed unit ball $\overline{B}_1$ of $\mathbb{R}^3$, with a reference choice being given by

$$\mathcal{F}(n) = \frac{1}{2} F(|n|^2),$$

where F is convex and has the interval $(-\infty, 1]$ as an effective domain. We will actually choose

$$F(r) = (1-r)\log(1-r),$$

but more general choices may be allowed.

Such an idea was introduced by J.L. Ericksen in order to enforce the physicality of a scalar order parameter and has already been applied to liquid crystal models in a number of papers and has the advantage that as soon as we have proved existence of a solution, then the constraint $|n| \leq 1$ is authomatically satisfied.

This helps in the estimates which actually could not be performed in this way in the case of a *classical* double-well potential.

Periodic boundary conditions

In order to avoid complications due to the interaction with the boundary, we will settle the above system on the flat 3-dimensional torus

$$\mathcal{T}^3 = \left([-\pi, \pi]|_{\{-\pi,\pi\}}\right)^3$$

so assuming periodic boundary conditions.

More realistic choices for the boundary conditions could be likely taken.

Nevertheless the above setting, beyond being the simplest one mathematically, is also consistent with the basic physical principles of conservation of charge and of momentum (indeed, we assume no external forces be present), that can be verified respectively by integrating

$$\frac{\partial c_k}{\partial t} + v \cdot \nabla c_k = \frac{1}{k_B \theta} \operatorname{div}\left(c_k \mathcal{D}_k \nabla \mu_k\right), \quad \text{for } k = 1, \dots, N,$$

and

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v + \nabla p = -K \operatorname{div}(\nabla n \odot \nabla n) + \operatorname{div} \sigma, + \varepsilon_0 \operatorname{div}\big((\nabla \Phi \otimes \nabla \Phi)\varepsilon(n)\big),$$

with respect to space variables.

The steps of the proof

Our main aim is to set the ground for proving the existence of weak solutions.

1. *'apriori estimates'*,
2. *'approximation scheme'*,
3. and *'compactness'*.

The apriori estimates are obtained on *presumptive* smooth solutions of the equation.

They allow to control certain norms, sufficiently strong, in order to allow to pass to the limit in the approximation scheme.

Simplification: 2 species

- We focus on a simplified version of the PDE system: beyond setting some physical constants equal to one, the only effective reduction we are actually going to operate concerns the number of species c_k which will be assumed to be equal to 2: c_p and c_m, which denote the density of positive and negative charges, respectively. speaking, this ansatz simplifies the nature of the system and in particular permits us to prove by means of very simple maximum principle arguments the uniform boundedness of c_p and c_m, which is a key ingredient for obtaining the apriori estimates.
- It is worth noting that we expect the same boundedness property to hold also in the general case of N-species, however the proof may be much more involved and require use of more technical results about invariant regions for evolutionary systems (see, e.g., [Cimatti, Fragalà]).
- We also expect that similar arguments could be applied in the more complicated systems where one uses a tensorial order parameter, that is a matrix valued function, i.e. a Q-tensor in the LC terminology, instead of the vector-valued one, n.

Ingredients of the proofs

The main ingredients of the proofs are the following:

- First we perform an energy estimate which is mainly based on a key Lemma providing sufficient conditions on the α_i-coefficients such that the dissipation is non-negative.
- Then, via a maximum-principle technique, we prove pointwise bounds for c_p and c_m.
- The L^∞-estimate on the potential Φ follows instead by a Moser-iteration scheme.
- Moreover we state an L^p-regularity result for n. This result, based on an L^p-estimate for the potential $\partial\mathcal{F}$, is in general new in the framework of non-smooth parabolic systems, while it is quite known in case of scalar equations.
- Finally, an additional regularity result for n is shown in case the anisotropy coefficient ε is sufficiently small.
- The weak sequential stability property result is proved for every $\varepsilon > 0$.

The simplified system (necessary for the maximum principle)

Assume $\varepsilon_\perp = k_B\theta = K = \varepsilon_0 = q = \gamma_1 = \gamma_2 = 1$ and write ε in place of ε_a. Take $\mathcal{D}_p = \mathcal{D}_k = \mathrm{Id} + \varepsilon n \otimes n$.
Then the simplified system takes the form

$$\frac{\partial c_p}{\partial t} + v \cdot \nabla c_p = \operatorname{div}\big((\mathrm{Id} + \varepsilon n \otimes n)(\nabla c_p + c_p \nabla\Phi)\big), \tag{1}$$

$$\frac{\partial c_m}{\partial t} + v \cdot \nabla c_m = \operatorname{div}\big((\mathrm{Id} + \varepsilon n \otimes n)(\nabla c_m - c_m \nabla\Phi)\big), \tag{2}$$

$$-\operatorname{div}\big((\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi\big) = c_p - c_m, \tag{3}$$

$$\begin{aligned}\frac{\partial v}{\partial t} + (v\cdot\nabla)v + \nabla p = {}& \alpha_4 \operatorname{div} D(v) - \operatorname{div}(\nabla n \odot \nabla n) \\ & + \operatorname{div}\big((\nabla\Phi \otimes \nabla\Phi)(\mathrm{Id} + \varepsilon n \otimes n)\big) \\ & + \operatorname{div}\big(\alpha_1 (D(v)n \cdot n) n \otimes n + \alpha_2 \mathring{n} \otimes n + \alpha_3 n \otimes \mathring{n}\big) \\ & + \operatorname{div}\big(\alpha_5 D(v) n \otimes n + \alpha_6 n \otimes D(v) n\big),\end{aligned} \tag{4}$$

$$\operatorname{div} v = 0, \tag{5}$$

$$n_t + v \cdot \nabla n - \Omega(v)n + D(v)n = \Delta n + \varepsilon\,(\nabla\Phi \otimes \nabla\Phi)\, n - \partial\mathcal{F}(n). \tag{6}$$

The singular potential

Note that $\partial\mathcal{F}$ in

$$n_t + v \cdot \nabla n - \Omega(v)n + D(v)n = \Delta n + \varepsilon\,(\nabla\Phi \otimes \nabla\Phi)\, n - \partial\mathcal{F}(n)$$

denotes the *subdifferential* of $\mathcal{F}$

$$\mathcal{F}(n) := \begin{cases} \frac{1}{2}F(|n|^2) - F_*, & \text{if } |n| \leq 1 \\ +\infty, \text{ otherwise} \end{cases}$$

where

$$F(r) := (1-r)\log(1-r) - F_*, \;\; r \in (0,1),$$

and F_* is chosen such that min $F(r) = F(1-1/e) = 0$.

Assumptions for the energy estimate

In order to prove the energy estimate, let us suppose that there exists $\delta > 0$ such that the coefficients in

$$\sigma = \alpha_1 (D(v)n \cdot n) n \otimes n + \alpha_2 \mathring{n} \otimes n + \alpha_3 n \otimes \mathring{n} + \alpha_4 D(v) + \alpha_5 D(v) n \otimes n + \alpha_6 n \otimes D(v) n,$$

satisfy

$$\alpha_4 > 0, \quad \alpha_4 - |\alpha_1| - |\alpha_5| - |\alpha_6| - \frac{1}{1-\delta} > 0.$$

Finally, we assume the initial data to satisfy the following conditions, where $\bar{c} > 0$ is a given constant:

$$\begin{aligned}
&c_{p,0}, c_{m,0} \in L^\infty(\mathcal{T}^3), \quad 0 \le c_{p,0}, c_{m,0} \le \bar{c} \text{ a.e. in } \mathcal{T}^3, \\
&v_0 \in L^2(\mathcal{T}^3), \quad \operatorname{div} v_0 = 0, \\
&n_0 \in H^1(\mathcal{T}^3), \quad |n_0(x)| \le 1, \forall x \in \mathcal{T}^3.
\end{aligned}$$

The *weak sequential stability* theorem

Theorem (Main result)

Let us assume that there exists a family $(c_p^{(k)}, c_m^{(k)}, \Phi^{(k)}, v^{(k)}, n^{(k)})_{k\in\mathbb{N}}$ *of smooth solutions of the system* (1)–(6) *on the flat 3-dimensional torus* $\mathcal{T}^3$ *subject to corresponding initial data*

$$c_p^{(k)}(0) = c_{p,0}^{(k)}, \quad c_m^{(k)}(0) = c_{m,0}^{(k)}, \quad n^{(k)}(0) = n_0^{(k)},$$

with $(c_{p,0}^{(k)}, c_{m,0}^{(k)}, n_0^{(k)}) \in (C^\infty(\mathcal{T}^3))^3$. *Moreover we assume that there exists a constant* $\tilde{C}$, *independent of* $k \in \mathbb{N}$, *such that*

$$\|c_{p,0}^{(k)}\|_{L^\infty}, \|c_{m,0}^{(k)}\|_{L^\infty}, \|n_0^{(k)}\|_{H^1(\mathcal{T}^3)}, \|v_0\|_H \leq \tilde{C} \quad \text{and } c_{i,0}^k \to c_{i,0}, \quad n_0^k \to n_0,$$

the latter convergence relations holding, e.g., in the sense of distributions.

Then there exists a (non-relabelled) sequence of the family $(c_p^{(k)}, c_m^{(k)}, \Phi^{(k)}, v^{(k)}, n^{(k)})$ *tending, in a suitable weak sense, to a quintuple* (c_p, c_m, Φ, v, n) *solving the weak formulation of system* (1)-(6).

The Energy estimate

Proposition (Energy law)

Let $(c_m, c_p, \Phi, v, n) : \Omega \to \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}^3$ *be a sufficiently smooth solution of system* (1)-(6) *on* $\mathcal{T}^3 \times (0, T)$ *complemented with initial conditions and satisfying the coefficient relations that ensure the non-negativity of the dissipation. Then there holds the energy inequality*

$$E(t) + \int_0^t \int_\Omega \left(\frac{1}{c_p} |\nabla c_p + c_p \nabla \Phi|^2 + \frac{1}{c_m} |\nabla c_m - c_m \nabla \Phi|^2 \right)$$

$$+ \int_0^t \int_\Omega \underbrace{\left(\alpha_4 |D(v)|^2 + \alpha_1 (n \cdot D(v) n)^2 + 2(\mathring{n} \cdot D(v) n) + (\alpha_5 + \alpha_6) |D(v) n|^2 + |\mathring{n}|^2 \right)}_{\geq 0}$$

$$\leq E(0)$$

where the energy functional is defined as

$$E(t) = \int_\Omega \left(\frac{1}{2} |v|^2 + \frac{1}{2} |\nabla n|^2 + \mathcal{F}(n) + c_p \ln c_p + c_m \ln c_m + \frac{1}{2} (1 + \varepsilon n \otimes n) \nabla \Phi \cdot \nabla \Phi \right).$$

Nonnegativity of the Dissipation

The energy estimate implies a number of apriori bounds for the solutions of system (1)-(6), provided that the dissipation term is nonnegative.this results as a restriction on the choice of the parameters α_j. following

Lemma

If $\alpha_4 > 0$, $\quad \alpha_4 - |\alpha_1| - |\alpha_5| - |\alpha_6| - \frac{1}{1-\delta} > 0$, *then we have, for some* $\delta' > 0$,

$$\alpha_4 |D|^2 + \alpha_1 (n \cdot Dn)^2 + 2(\mathring{n} \cdot Dn) + (\alpha_5 + \alpha_6)|Dn|^2 + |\mathring{n}|^2 \geq \delta' \left(|Dn|^2 + |\mathring{n}|^2 \right)$$

for arbitrary $\mathring{n} \in \mathbb{R}^3, n \in \mathbb{R}^3$, $D \in \mathbb{R}^{3\times3}$ *with* $|n| \leq 1$ *and the matrix D symmetric and traceless.*

Proof.

Noting that we have (where we use that $|n| \leq 1$):

$$(n \cdot Dn)^2 \leq |n|^2 |Dn|^2 \leq |D|^2, \quad |2(\mathring{n} \cdot Dn)| \leq 2|\mathring{n}||Dn| \leq (1-\delta)|\mathring{n}|^2 + \frac{1}{1-\delta}|D|^2$$

we immediately deduce that assumptions $\alpha_4 > 0$, $\alpha_4 - |\alpha_1| - |\alpha_5| - |\alpha_6| - \frac{1}{1-\delta} > 0$ implies the claimed positivity of dissipation. □

Consequences of the Energy Estimate

As a consequence of the energy estimate, using also the positive definiteness of the matrix $n \otimes n$ and the assumptions on F, we can obtain a number of apriori bounds holding for any hypothetical solution of the system and independently of any eventual approximation or regularization parameter.

Namely, we have

$$
\begin{aligned}
&\|v\|_{L^\infty(0,T;H)} + \|v\|_{L^2(0,T;V)} \leq c, \\
&\|n\|_{L^\infty(0,T;V)} \leq c, \qquad |n| \leq 1 \quad \text{a.e. in } (0,T) \times \mathcal{T}^3, \\
&c_p, c_m \geq 0 \quad \text{a.e. in } (0,T) \times \mathcal{T}^3, \\
&\|\nabla \Phi\|_{L^\infty(0,T;H)} \leq c.
\end{aligned}
$$

where c is a constant depeding only on $E(0)$.

Note that the second bound on n directly follows from our choice of the potential F.

The maximum principle

Proposition (Maximum principle)

If (c_p, c_m, Φ) *solve equations* (1), (2), (3) *subject to periodic boundary conditions and initial data* c_p^0, c_m^0 *as above, then there follows*

$$|c_p(x,t)|, |c_m(x,t)| \le \bar{c}, \quad a.e. \text{ in } (0,T) \times \mathcal{T}^3.$$

Proof of the maximum principle 1

We multiply

$$\frac{\partial c_p}{\partial t} + v \cdot \nabla c_p = \operatorname{div}\left((\mathrm{Id} + \varepsilon n \otimes n)(\nabla c_p + c_p \nabla \Phi)\right)$$

by $(c_p - \bar{c})^+$ and integrate over $\mathcal{T}^3$ and by parts, to obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |(c_p - \bar{c})^+|^2 + \frac{1}{2}\int_\Omega v \cdot \nabla((c_p - \bar{c})^+)^2$$
$$+ \int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)\nabla(c_p - \bar{c})^+ \cdot \nabla(c_p - \bar{c})^+$$
$$+ \int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi \cdot \nabla\left(\frac{1}{2}((c_p - \bar{c})^+)^2 + \bar{c}(c_p - \bar{c})^+\right) = 0.$$

Similarly, we get from the equation for c_m:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega |(c_m - \bar{c})^+|^2 + \frac{1}{2}\int_\Omega v \cdot \nabla((c_m - \bar{c})^+)^2$$
$$+ \int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)\nabla(c_m - \bar{c})^+ \cdot \nabla(c_m - \bar{c})^+$$
$$- \int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi \cdot \nabla\left(\frac{1}{2}((c_m - \bar{c})^+)^2 + \bar{c}(c_m - \bar{c})^+\right) = 0.$$

Proof of the maximum principle 2

We now define

$$M(r) := \begin{cases} 0 & \text{if } r \le \bar{c}, \\ \frac{1}{2}((r-\bar{c})^+)^2 + \bar{c}(r-\bar{c})^+ & \text{if } r \ge \bar{c}. \end{cases}$$

Then, summing the two inequalities and using incompressibility, we deduce

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(|(c_p-\bar{c})^+|^2 + |(c_m-\bar{c})^+|^2\right) \le -\int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi \cdot \nabla(M(c_p) - M(c_m)).$$

The integral on the right-hand side can be computed by using equation

$$-\operatorname{div}\left((\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi\right) = c_p - c_m.$$

This leads to

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left(|(c_p-\bar{c})^+|^2 + |(c_m-\bar{c})^+|^2\right) \le -\int_\Omega (c_p - c_m)(M(c_p) - M(c_m)) \le 0,$$

the inequality following from the monotonicity of the function M. Noting that the initial conditions implies that the left-hand side is null at $t = 0$, we obtain the claimed estimate.

Further estimates on c_p and c_m

We have obtained the additional bound

$$\|c_p\|_{L^\infty(0,T;L^\infty(\mathcal{T}^3))} + \|c_m\|_{L^\infty(0,T;L^\infty(\mathcal{T}^3))} \leq c,$$

where the constant c depends just on the L^∞ norm of $c_p(0)$ and $c_m(0)$.
We can then test (1):

$$\frac{\partial c_p}{\partial t} + v \cdot \nabla c_p = \operatorname{div}\left((\mathrm{Id} + \varepsilon n \otimes n)(\nabla c_p + c_p \nabla \Phi)\right)$$

by c_p. Using once more the positive definiteness of the matrix $n \otimes n$, we may note that

$$\left| \int_\Omega c_p \nabla \Phi \cdot \nabla c_p \right| \leq \|c_p\|_{L^\infty(\mathcal{T}^3)} \|\nabla \Phi\|_H \|\nabla c_p\|_H \leq c \|\nabla c_p\|_H \leq c + \frac{1}{2} \|\nabla c_p\|_H^2,$$

with an analogous relation holding for c_m and where the constants $c > 0$ are independent of time. Analogously we can estimate the term $-\int_\Omega \varepsilon (n \otimes n) c_p \nabla \Phi \cdot \nabla c_p$.

Then, it is not difficult to deduce the parabolic regularity estimate

$$\|c_p\|_{L^2(0,T;V)} + \|c_m\|_{L^2(0,T;V)} \leq c.$$

Further estimates on Φ

In view of the fact that Φ is defined up to an additive constant, it is not restrictive to assume that

$$\Phi_\Omega = \int_\Omega \Phi(t) = 0 \quad \text{for a.e. } \ t \in (0,T).$$

Of course, such a normalization property implies

$$\|\Phi\|_{L^\infty(0,T;V)} \le c.$$

We have, however, a better property which is given by the following

Lemma (Uniform boundedness of Φ)

We have the additional estimate

$$\|\Phi\|_{L^\infty(0,T;L^\infty(\mathcal{T}^3))} \le c.$$

Proof of the boundedness of Φ - Part 1

The proof follows by applying a Moser iteration argument on equation

$$-\operatorname{div}\left((\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi\right) = c_p - c_m,$$

and using the uniform boundedness of the right-hand side.
We multiply it by $(\Phi)^{p-1} := |\Phi|^{p-1}\operatorname{sign}\Phi$ where the exponent p will be taken larger and larger. This gives

$$\begin{aligned}(p-1)\int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)|\Phi|^{p-2}\nabla\Phi\cdot\nabla\Phi &= \int_\Omega (c_p - c_m)|\Phi|^{p-1}\operatorname{sign}\Phi \\ &\le c\int_\Omega |\Phi|^{p-1} \le c\int_\Omega\left(\frac{1}{p} + \frac{p-1}{p}|\Phi|^p\right) \\ &\le \frac{c}{p} + c\int_\Omega |\Phi|^p.\end{aligned}$$

As a first step, we take $p = p_0 = 6$. Then, controlling the right-hand side by the Poincaré-Wirtinger inequality we deduce

$$c\int_\Omega |\Phi|^6 = c\|\Phi - \Phi_\Omega\|_6^6 \le c\|\nabla\Phi\|_2^6 \le c.$$

Proof of the boundedness of Φ - Part 2

Here and below, we note by $\|\cdot\|_q$ the norm in $L^q(\mathcal{T}^3)$, $1 \leq q \leq \infty$. Hence, noting that

$$(p-1)\int_\Omega (\mathrm{Id} + \varepsilon n \otimes n)|\Phi|^{p-2}\nabla\Phi \cdot \nabla\Phi \geq \frac{4(p-1)}{p^2}\int_\Omega \left|\nabla(\Phi)^{p/2}\right|^2$$

at the first iteration, i.e. for $p = 6$, we deduce

$$\left\|\nabla\Phi^3\right\|_2 \leq c$$

whence, using Sobolev's embeddings,

$$\|\Phi\|_{18}^3 \leq c(\left\|\nabla|\Phi|^3\right\|_2 + \|\Phi\|_6^3) \leq c.$$

Now we take care of further iterations: for $p \geq 2$ we have

$$\int_\Omega \left|\nabla(\Phi)^{p/2}\right|^2 \leq \frac{cp}{(p-1)} + \frac{cp^2}{p-1}\int_\Omega |\Phi|^p \leq c + c(p+2)\int_\Omega |\Phi|^p$$

where c is independent of p.
Adding also $\|\Phi\|_p^p$ to both hand sides and using the Sobolev embedding, we then deduce

$$\begin{aligned}\|\Phi\|_{3p}^p &= \left\|(\Phi)^{p/2}\right\|_6^2 \leq c\left\|(\Phi)^{p/2}\right\|_V^2 \\ &\leq c\left\|(\Phi)^{p/2}\right\|_2^2 + c\int_\Omega \left|\nabla(\Phi)^{p/2}\right|^2 \leq c + c(p+3)\|\Phi\|_p^p \leq c + cp\|\Phi\|_p^p,\end{aligned}$$

where c is still independent of p.

Proof of the boundedness of Φ - Part 3

We define $b_p = \max(1, \|\Phi\|_p)$. Then, assuming without loss of generality that $c \geq 1$ the last inequality implies:

$$b_{3p}^p \leq cp b_p^p$$

with $c > 1$ a constant independent of p. Then, since $\ln b_{3p} \leq \frac{\ln(cp)}{p} + \ln b_p$, we get

$$\begin{aligned} \ln b_{3^n p} &\leq \frac{\ln(c3^{(n-1)}p)}{3^{n-1}p} + \ln b_{3^{n-1}p} \\ &\leq \frac{\ln(c3^{(n-1)}p)}{3^{n-1}p} + \frac{\ln(c3^{(n-2)}p)}{3^{n-2}p} + \cdots + \ln b_p. \end{aligned}$$

and hence

$$\ln b_{3^n p} \leq \sum_{k=1}^{n-1} \frac{\ln(c3^k p)}{c3^k p} + \ln b_p.$$

Noting that constant c is independent of n and p and letting $n \nearrow \infty$ we obtain the estimate.

Additional regularity

Lemma (Additional regularity estimate)

The following additional regularity conditions hold:

$$\|\nabla\Phi\|_{L^\infty(0,T;L^{p_M}(\mathcal{T}^3))} \leq c_{p_M}, \qquad \text{for some } p_M > 2$$

$$\|n_t\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} + \|\Delta n\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} \leq c, \qquad \text{for some } p_0 > 1$$

$$\|\partial\mathcal{F}(n)\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} \leq c \qquad \text{for some } p_0 > 1.$$

Proof - Step 1

The key point stands in the application of refined elliptic regularity result to equation

$$-\operatorname{div}\big((\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi\big) = c_p - c_m.$$

- In view of the bound $|n| \leq 1$ and of the positive definiteness of $n \otimes n$, the matrix $\mathrm{Id} + \varepsilon n \otimes n$ is strongly elliptic and has bounded coefficients.
- Since the right hand side is uniformly bounded, we can then apply the integrability result by Meyers, which implies

$$\|\nabla\Phi\|_{L^\infty(0,T;L^{p_M}(\mathcal{T}^3))} \leq c_{p_M} \quad \text{for some } p_M > 2.$$

- At least in 3D, there is no quantitative control of p_M but we know that $p_M > 2$.

As a consequence the n-equation can be rearranged in the form

$$n_t - \Delta n + \partial\mathcal{F}(n) = \underbrace{-v \cdot \nabla n + \Omega(v)n - D(v)n + \varepsilon\left(\nabla\Phi \otimes \nabla\Phi\right) n}_{:=f},$$

where a simple check based on the previous estimates shows that, at least,

$$v \cdot \nabla n + \Omega(v)n - D(v)n \in L^{\frac{3}{2}}(0, T; L^{\frac{3}{2}}(\mathcal{T}^3))$$

which implies

$$f \in L^p(0, T; L^p(\mathcal{T}^3)) \quad \text{for all } p \leq p_0 \text{ where } p_0 := \min\left(\tfrac{3}{2}, \tfrac{p_M}{2}\right).$$

Proof - Step 2

Componentwise, the n-equation takes form:

$$\partial_t n_i - \Delta n_i + F'(|n|^2)n_i = f_i,$$

where F' is monotone because F is convex.
Take from now on $p =: p_0$ (for simplicity of notation). We then test

$$\partial_t n_i - \Delta n_i + F'(|n|^2)n_i = f_i,$$

by the function $G_i(n) = |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)n_i$ to obtain

$$\frac{1}{2}\int_\Omega |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)\frac{\mathrm{d}}{\mathrm{d}t}|n_i|^2 + \int_\Omega |F'(|n|^2)|^p n_i^2$$
$$+ \int_\Omega |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)|\nabla n_i|^2 + \mathcal{M}_i = \int_\Omega f_i \; F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)n_i,$$

where the "mixed" term $\mathcal{M}$ is given by

$$\mathcal{M}_i = (p-1)\int_\Omega |F'(|n|^2)|^{p-2}F''(|n|^2)n_i\nabla|n|^2 \cdot \nabla n_i$$
$$= \frac{(p-1)}{2}\int_\Omega |F'(|n|^2)|^{p-2}F''(|n|^2)\nabla|n|^2 \cdot \nabla n_i^2.$$

Summing up for $i = 1, 2, 3$. It is then easy to check that (due to convexity of F)

$$\sum_{i=1}^{3}\mathcal{M}_i = \frac{(p-1)}{2}\int_\Omega |F'(|n|^2)|^{p-2}F''(|n|^2)\nabla|n|^2 \cdot \nabla|n|^2 \geq 0.$$

Proof - Step 3

We now split the term $\int_\Omega |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)|\nabla n|^2$ over two subsets of $\mathcal{T}^3$, namely

$$\mathcal{T}^3_+ := \left\{x \in \mathcal{T}^3, |n|^2(x) \geq 1 - \frac{1}{e}\right\}, \text{ respectively } \mathcal{T}^3_- := \left\{x \in \mathcal{T}^3, |n|^2(x) < 1 - \frac{1}{e}\right\},$$

where we neglect the dependence on t for simplicity.
Then, taking into account that

$$F'(r) \geq 0 \text{ for } r \in (1 - \frac{1}{e}, 1),$$

neglecting the positive term $\int_{\mathcal{T}^3_+} |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)|\nabla n|^2$ on the l.h.s., and using

$$F'(|n|^2(x)) \in (-1, 0) \text{ for } x \in \mathcal{T}^3_-$$

we deduce (also by Hölder's and Young's inequalities):

$$\begin{aligned}
&\frac{1}{2}\int_\Omega |F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)\frac{\mathrm{d}}{\mathrm{d}t}|n|^2 + \int_\Omega |F'(|n|^2)|^p |n|^2 \\
&\quad \leq \int_\Omega F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2) f \cdot n + \int_{\mathcal{T}^3_-} |F'(|n|^2)|^{p-1} |\nabla n|^2 \\
&\quad \leq \left\| F'(|n|^2)|^{p-1} \operatorname{sign} F'(|n|^2)\right\|_{p/(p-1)} \|f \cdot n\|_p + \int_\Omega |\nabla n|^2 \\
&\quad \leq c\left\| F'(|n|^2)|\right\|_p^{p-1} \|f\|_p + c \leq \sigma \left\| F'(|n|^2)|\right\|_p^p + c_\sigma \|f\|_p^p + c.
\end{aligned}$$

Proof - Step 4

Now, note that

$$\frac{1}{2}\int_\Omega |F'(|n|^2)|^{p-1}\,\mathrm{sign}\,F'(|n|^2)\frac{\mathrm{d}}{\mathrm{d}t}|n|^2 = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \Gamma_p(|n|^2),$$

where the function Γ_p is defined by the right hand side above and it is bounded from below. Notice that $\lim_{r\to 1^-}\Gamma_p(r) < +\infty$ and that

$$\int_\Omega |F'(|n|^2)|^p|n|^2 \geq \frac{1}{2}\int_\Omega |F'(|n|^2)|^p - c.$$

Hence, taking $\sigma < 1/2$, we see that the first term on the right hand side of

$$\frac{1}{2}\int_\Omega |F'(|n|^2)|^{p-1}\,\mathrm{sign}\,F'(|n|^2)\frac{\mathrm{d}}{\mathrm{d}t}|n|^2 + \int_\Omega |F'(|n|^2)|^p|n|^2 \\ \leq \sigma\left\|F'(|n|^2)\right\|_p^p + c_\sigma\|f\|_p^p + c.$$

is controlled. On the other hand, integrating in time, we may note that the latter term is also controlled. As a consequence, we obtain first

$$\|F'(|n|^2)\|_{L^p((0,T)\times\mathcal{T}^3)} \leq c \quad \text{and, as a consequence, } \|\partial\mathcal{F}(n)\|_{L^p((0,T)\times\mathcal{T}^3)} \leq c\,.$$

By comparison and elliptic regularity results of Agmon-Douglis-Nirenberg type, we get

$$\|n_t\|_{L^p(0,T;L^p(\mathcal{T}^3))} + \|\Delta n\|_{L^p(0,T;L^p(\mathcal{T}^3))} \leq c.$$

Additional regularity for small ε

In the case when the anisotropy coefficient ε in

$$-\operatorname{div}\left((\mathrm{Id} + \varepsilon n \otimes n)\nabla\Phi\right) = c_p - c_m$$

is small enough compared to the other parameters, we can prove some additional estimates.This is stated in the following

Lemma (H^2-estimates)

Let us assume that the initial data satisfy the previous assumptions. Furthermore, let $\varepsilon > 0$ be small enough. Then, we have

$$\|\Phi\|_{L^2(0,T;H^2(\mathcal{T}^3))} + \|n\|_{L^2(0,T;H^2(\mathcal{T}^3))} \leq c.$$

Weak sequential stability - Part 1

- We assume: $(c_{p,k}, c_{m,k}, \Phi_k, v_k, n_k)$ is family of approximating solutions complying with the estimates derived before uniformly with respect to the parameter $k \in \mathbb{N}$
- The aim is now to prove that there exists a (non-relabelled) sequence of the above sequence tending, in a suitable way, to a quintuple (c_p, c_m, Φ, v, n) solving system (1)-(6) in a weak sense

Weak sequential stability - Part 2

To this aim, we start deducing some convergence properties arising as a consequence of the previous bounds. that there exists $\lambda \in L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))$ such that

$$
\begin{aligned}
&v_k \to v \quad \text{weakly star in } \; L^\infty(0,T;H) \cap L^2(0,T;V),\\
&n_k \to n \quad \text{weakly star in } \; L^\infty(0,T;V) \cap L^\infty(0,T;L^\infty(\mathcal{T}^3)),\\
&\Phi_k \to \Phi \quad \text{weakly star in } \; L^\infty(0,T;V) \cap L^\infty(0,T;L^\infty(\mathcal{T}^3)),\\
&c_{p,k},\ c_{m,k} \to c_p,\ c_m \quad \text{weakly star in } \; L^2(0,T;V) \cap L^\infty(0,T;L^\infty(\mathcal{T}^3)),\\
&\nabla\Phi_k \to \nabla\Phi \quad \text{weakly star in } L^\infty(0,T;L^{p_M}(\mathcal{T}^3)),\\
&\partial_t n_k,\, \Delta n_k,\, \partial\mathcal{F}(n_k) \to n_t,\, \Delta n,\, \lambda \quad \text{weakly in } L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3)),
\end{aligned}
$$

where p_0, p_M are the exponents introduced in the previous:

Lemma

The following additional regularity conditions hold:

$$
\begin{aligned}
&\|\nabla\Phi\|_{L^\infty(0,T;L^{p_M}(\mathcal{T}^3))} \le c_{p_M}, \qquad \text{for some } p_M > 2\\
&\|n_t\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} + \|\Delta n\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} \le c, \qquad \text{for some } p_0 > 1\\
&\|\partial\mathcal{F}(n)\|_{L^{p_0}(0,T;L^{p_0}(\mathcal{T}^3))} \le c \qquad \text{for some } p_0 > 1.
\end{aligned}
$$

Weak sequential stability - Part 3

Of course this implies in particular:

- $\Phi_\Omega = 0$,
- $0 \le c_p \le \bar{c}$, $0 \le c_m \le \bar{c}$, $|n| \le 1$ almost everywhere in $\mathcal{T}^3$,
- if ε is sufficiently small we also get:

$$\Phi_k,\ n_k \to \Phi,\ n \quad \text{weakly in } L^2(0,t;H^2(\mathcal{T}^3)).$$

We show now how to treat the passing to the limit for the most difficult terms.

$$\|v_k\|_{L^4(0,T;L^3(\mathcal{T}^3))} \le c,$$

whence, by $\|c_p\|_{L^2(0,T;V)} + \|c_m\|_{L^2(0,T;V)} \le c$, there follows

$$\|v_k \cdot \nabla c_{p,k}\|_{L^{4/3}(0,T;L^{6/5}(\mathcal{T}^3))} + \|v_k \cdot \nabla c_{m,k}\|_{L^{4/3}(0,T;L^{6/5}(\mathcal{T}^3))} \le c.$$

Then it is not difficult to deduce from equations (1), (2) for $c_{p,k}$ and $c_{m,k}$ that

$$\|\partial_t c_{p,k}\|_{L^{4/3}(0,T;V')} + \|\partial_t c_{m,k}\|_{L^{4/3}(0,T;V')} \le c.$$

Hence, the Aubin-Lions lemma with the uniform boundedness property gives

$$c_{p,k},\ c_{m,k},\ n_k \to c_p,\ c_m,\ n \quad \text{strongly in } L^q(0,T;L^q(\mathcal{T}^3)) \ \ \forall\, q \in [1,\infty).$$

Weak sequential stability - Part 4

Then, using the monotonicity of $\partial\mathcal{F}$, and the classical result by Barbu we get $\lambda = \partial\mathcal{F}(n)$. Moreover, we get

$$\|c_{p,k}\nabla\Phi_k\|_{L^\infty(0,T;H)} + \|c_{m,k}\nabla\Phi_k\|_{L^\infty(0,T;H)} \leq c,$$

whence

$$c_{p,k}\nabla\Phi_k \to c_p\nabla\Phi, \quad c_{m,k}\nabla\Phi_k \to c_m\nabla\Phi \quad \text{weakly star in } L^\infty(0,T;H).$$

Using the Gagliardo-Nirenberg inequality and the fact that $|n_k| \leq 1$, we get

$$\|\nabla n_k \odot \nabla n_k\|_{L^s(0,T;L^s(\mathcal{T}^3))} \leq c \quad \text{for some exponent } s > 1.$$

Finally, using the bound on $\partial_t n_k$ and again the Gagliardo-Nirenberg inequality interpolating between the spaces $L^\infty(0,T;L^\infty(\mathcal{T}^3))$ and $L^{p_0}(0,T;W^{2,p_0}(\mathcal{T}^3))$ at place $1/2$, we also get the convergence

$$\nabla n_k \odot \nabla n_k \to \nabla n \odot \nabla n \quad \text{weakly in } L^s(0,T;L^s(\mathcal{T}^3)),$$

which is sufficient in order to conclude the passage to the limit as $k \to \infty$ in order to obtain the claimed weak solutions.

Many thanks to all of you for the attention!

The content of the talk is contained in

[Feireisl, Rocca, Schimperna, Zarnescu, DCDS-S, 2021,14(1): 219-241]