A non-isothermal model for nematic liquid crystals

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Plan of the Talk

- The objective of our modelling approach: include the temperature dependence in a model describing the evolution of nematic liquid crystal flows.

- Our mathematical results:
  - The results: joint work with Eduard Feireisl (Institute of Mathematics, Czech Academy of Sciences, Prague) and Giulio Schimperna (University of Pavia), accepted for publication on *Nonlinearity*.

- Some future perspectives and open problems.
The motivation

Liquid crystals are a state of matter that have properties between those of a conventional liquid and those of a solid crystal. A liquid crystal may flow like a liquid, but its molecules may be oriented in a crystal-like way. Theoretical studies of these types of materials are motivated by real-world applications: proper functioning of many practical devices relies on optical properties of certain liquid crystalline substances in the presence or absence of an electric field.

At the molecular level, what marks the difference between a liquid crystal and an ordinary, isotropic fluid is that, while the centers of mass of LC molecules do not exhibit any long-range correlation, molecular orientations do exhibit orientational correlations. As a result, in the continuum description of a liquid crystal, at any point in space it is possible to define a preferred direction along which LC molecules tend to be aligned: the unit vector $d$ associated with this direction is called the director, with a term borrowed from optics.
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The modelling literature

There have been numerous attempts to formulate continuum theories describing the behavior of liquid crystals flows:

A static continuum model was proposed by Frank in the 50s of the past century: it is a variational model that posits an elastic free-energy obeying suitable constraints. The corresponding dynamical equations were laid down by Ericksen and Leslie a decade later [Ericksen, Trans. Soc. Rheol., 1961] and [Leslie, Arch. Ration. Mech. Anal., 1963].

An attempt to posit a set of dynamical equations for liquid crystals on a manifold was made a few years ago by [Shkoller, Comm. Part. Diff. Eq., 2002]. He employed the director model proposed by [Lin and Liu, Comm. Pure Appl. Math., 1995], which implies a drastic simplification of the Ericksen-Leslie equations, especially in the description of dissipation.

Several textbooks have been devoted to the presentation of mathematical LC models (cf., e.g., Chandrasekhar (1977), de Gennes (1974)). The survey articles by Ericksen (1976) and Leslie (1978), which present in a very comprehensive fashion the "classical" continuum theories used for static and flow problems.
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The second model is a simplification of the Ericksen-Leslie model and has been introduced in [Lin and Liu, Comm. Pure Appl. Math., 1995], where the authors proved existence and uniqueness of global classical solutions in 2D as well as some corresponding results in 3D (in the case of large viscosity).
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Crystals in the *cholesteric* phase exhibit a twisting of the molecules perpendicular to the director, with the molecular axis parallel to the director. The main difference between the nematic and cholesteric phases is that the former is invariant with respect to certain reflections while the latter is not.
Our main aim

We consider the range of temperatures typical for the nematic phase. The nematic liquid crystals are composed of rod-like molecules, with the long axes of neighboring molecules aligned. It may be described by means of a dimensionless unit vector $d$, the director, that represents the direction of preferred orientation of molecules in a neighborhood of any point of a reference domain. The flow velocity $u$ evidently disturbs the alignment of the molecules and also the converse is true: a change in the alignment will produce a perturbation of the velocity field $u$. Hence, both $d$ and $u$ are relevant in the dynamics, and also the changes of the temperature $\vartheta$ (internal energy).

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$\Rightarrow$ We introduce a very simple \textbf{non-isothermal model for nematic liquid crystals} in the spirit of the simplified version of the Leslie-Ericksen model proposed by Lin and Liu in 1995.
The state variables

- the mean velocity field \( u \)
- the director field \( d \), representing preferred orientation of molecules in a neighborhood of any point of a reference domain
- the absolute temperature \( \vartheta \)
The evolution

The time evolution of the velocity field is governed by the incompressible Navier-Stokes system, with a non-isotropic stress tensor depending on the gradients of the velocity and of the director field $d$, where the transport (viscosity) coefficients vary with temperature.

The dynamics of $d$ is described by means of a parabolic equation of Ginzburg-Landau type, with a suitable penalization term to relax the constraint $|d| = 1$.

The system is supplemented by a heat equation, where the heat flux is given by a variant of Fourier's law, depending also on the director field $d$.

The proposed model is shown compatible with First and Second laws of thermodynamics, and the existence of global-in-time weak solutions for the resulting PDE system is established, without any essential restriction on the size of the data.
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The main difficulties

The existence of weak solutions to the standard incompressible Navier-Stokes system was established in the celebrated paper by [Leray, Acta Math., 1934]. One of the major open problems is to clarify whether or not the weak solutions also satisfy the corresponding total energy balance, more precisely, if the kinetic energy of the system dissipates at the rate given by the viscous stress. To avoid this apparent difficulty, we use the idea proposed in [Feireisl, J. Malek, Differ. Equ. Nonlinear Mech., 2006] replacing the heat equation by the total energy balance and an entropy inequality. Of course, the price to pay is the explicit appearance of the pressure in the total energy balance that must be handled by refined arguments. Apart from the fact that the resulting system is mathematically tractable, such an approach seems much closer to the physical background of the problem, being an exact formulation of the First and Second Laws of thermodynamics.

Another difficulty: the proof of sufficiently strong estimates on the director field $d$ in order to pass to the limit in the approximate problem. In particular, the celebrated Gagliardo-Nirenberg inequality is needed in order to control the strongly nonlinear terms containing $\nabla x d$ in both the momentum equation and the internal energy balance.
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The momentum balance

- The mass conservation reads

$$\frac{\partial}{\partial t} \varrho + \text{div}(\varrho u) = 0.$$ 

- In the context of nematic liquid crystals, we have the incompressibility constraint

$$\text{div} u = 0.$$ 

- By virtue of Newton's second law, the balance of momentum reads

$$\frac{\partial}{\partial t} (\varrho u) + \text{div}(\varrho u \otimes u) = \text{div} T + \varrho f,$$

where $T$ is the Cauchy stress, and $f$ is a given external force.

- Motivated by Lin and Liu, we consider the stress tensor in the form

$$T = S - \varrho \lambda (\vartheta) (\nabla \otimes \nabla d) - p I,$$

where $p$ denotes the pressure and $\nabla \otimes \nabla d := \sum_k \partial_i d_k \partial_j d_k$.

- Moreover, $S$ is the conventional Newtonian viscous stress tensor,

$$S(\vartheta, \nabla \otimes u) = \mu(\vartheta)(\nabla \otimes u + \nabla^T u),$$

$\mu$ is the viscosity coefficient assumed always positive, while $\lambda$ denotes the thermal dilatation coefficient that is an increasing function of $\vartheta$. 
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\( \mu \) is the viscosity coefficient assumed always positive, while \( \lambda \) denotes the thermal dilatation coefficient that is an increasing function of \( \vartheta \).
The director field dynamics

We assume that the driving force governing the dynamics of the director $d$ is of "gradient type" $\partial d J$, where the potential $J$ is given by

$$J(\vartheta, \varrho, d) = W(d) + \frac{1}{\vartheta} G(\vartheta, \varrho)$$

Here $G$ is a regular function of $\vartheta$ and $\varrho$, and $W$ penalizes the deviation of the length $|d|$ from the value 1. $W$ may be a general function that can be written as a sum of a convex (possibly non smooth) part, and a smooth, but possibly non-convex one. A typical example is

$$W(d) = \left( |d|^2 - 1 \right)^2$$

Consequently, $d$ satisfies the following equation

$$\partial_t d + u \cdot \nabla x d + \partial d W(d) = \frac{1}{\varrho} \text{div} \left( \varrho \nabla x d \right)$$
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The internal energy balance

In accordance with the First law of thermodynamics, the internal energy balance reads

$$\frac{\partial}{\partial t} \left( \rho e^{\text{int}} \right) + \text{div} \left( \rho e^{\text{int}} \mathbf{u} \right) + \text{div} \mathbf{q} = T : \nabla \times \mathbf{u},$$

where $e^{\text{int}}$ denotes the internal energy density and $\mathbf{q}$ its flux.

Following Ericksen's model, the flux can be taken in the form

$$\mathbf{q} = -\kappa (\vartheta) \nabla \times \vartheta - (\kappa || - \kappa \perp) (\vartheta) \cdot \nabla (\nabla \times \vartheta),$$

where $\kappa, \kappa || - \kappa \perp$ are positive functions of the temperature. Finally, we take $e^{\text{int}} = c_v \vartheta$, where $c_v > 0$ is the specific heat at constant volume.
The internal energy balance

In accordance with the First law of thermodynamics, the internal energy balance reads

\[ \partial_t (\rho e_{\text{int}}) + \text{div}(\rho e_{\text{int}} \mathbf{u}) + \text{div} \mathbf{q} = \mathbf{T} : \nabla \mathbf{u}, \]

where \( e_{\text{int}} \) denotes the internal energy density and \( \mathbf{q} \) its flux.
In accordance with the **First law of thermodynamics**, the internal energy balance reads
\[
\partial_t (\varrho e_{\text{int}}) + \text{div}(\varrho e_{\text{int}} u) + \text{div} q = \mathbb{T} : \nabla_x u,
\]
where $e_{\text{int}}$ denotes the internal energy density and $q$ its flux.

Following **Ericksen’s model**, the flux can be taken in the form
\[
q = -\kappa(\vartheta) \nabla_x \vartheta - (\kappa_{||} - \kappa_{\perp})(\vartheta) \mathbf{d}(\mathbf{d} \cdot \nabla_x \vartheta),
\]
where $\kappa$, $\kappa_{||} - \kappa_{\perp}$ are positive functions of the temperature. Finally, we take $e_{\text{int}} = c_v \vartheta$, where $c_v > 0$ is the specific heat at constant volume.
The PDEs: assuming $\rho = c_v = 1$, we get the following system:

\[
\begin{align*}
\text{div } u &= 0, \\
\partial_t u + \text{div}(u \otimes u) + \nabla_x p &= \text{div } \mathbb{S} - \text{div } (\lambda(\vartheta)(\nabla_x d \otimes \nabla_x d)) + f, \\
\partial_t \vartheta + \text{div}(\vartheta u) + \text{div } q &= \mathbb{S} : \nabla_x u - \lambda(\vartheta)(\nabla_x d \otimes \nabla_x d) : \nabla_x u, \\
\partial_t d + u \cdot \nabla_x d + \partial W(d) &= \text{div } \nabla_x d.
\end{align*}
\]
**The PDEs**: assuming $\rho = c_v = 1$, we get the following system:

\[
\begin{align*}
\text{(INC)} & \quad \text{div} \, \mathbf{u} = 0, \\
\text{(MOM)} & \quad \partial_t \mathbf{u} + \text{div} (\mathbf{u} \otimes \mathbf{u}) + \nabla_x p &= \text{div} \mathbb{S} - \text{div} (\lambda(\vartheta) (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d})) + \mathbf{f}, \\
\text{(INT)} & \quad \partial_t \vartheta + \text{div} (\vartheta \mathbf{u}) + \text{div} \mathbf{q} = \mathbb{S} : \nabla_x \mathbf{u} - \lambda(\vartheta)(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) : \nabla_x \mathbf{u}, \\
\text{(EQD)} & \quad \partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d} + \partial \mathcal{W}(\mathbf{d}) = \text{div} \nabla_x \mathbf{d}.
\end{align*}
\]

**The boundary conditions**: in order to avoid the occurrence of boundary layers, we suppose that the boundary is impermeable and perfectly smooth imposing the complete slip boundary conditions:

\[
\mathbf{u} \cdot \mathbf{n}|_{\partial \Omega} = 0, \quad [\mathbb{T} \mathbf{n}] \times \mathbf{n}|_{\partial \Omega} = 0,
\]

together with the no-flux boundary condition for the temperature

\[
\mathbf{q} \cdot \mathbf{n}|_{\partial \Omega} = 0,
\]

and the Neumann boundary condition for the director field

\[
\nabla_x d_i \cdot \mathbf{n}|_{\partial \Omega} = 0 \quad \text{for} \quad i = 1, 2, 3.
\]

The last relation accounts for the fact that there is no contribution to the surface force $\mathbb{T} \mathbf{n}$ from the director $\mathbf{d}$. It is also suitable for implementation of a numerical scheme.
The total energy balance

Multiplying momentum equation (MOM) by $u$ and adding the resulting expression to (INT) we deduce the total energy balance in the form

$$\partial_t \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) \right) + \text{div} \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) u \right) + \text{div}(p u) + \text{div} q = \text{div} (S u) - \text{div} \left( \lambda (\vartheta) \left( \nabla x d \right) \odot \left( \nabla x d \right) \right) + f \cdot u.$$

Moreover, using the boundary conditions and integrating the last equation over $\Omega$ we obtain

$$\partial_t \int_\Omega \left( \frac{1}{2} |u|^2 + \vartheta \right) = \int_\Omega f \cdot u,$$

in particular, the total energy is a constant of motion as soon as $f \equiv 0$. 
The total energy balance

Multiplying momentum equation (MOM) by $\mathbf{u}$ and adding the resulting expression to (INT) we deduce the total energy balance in the form

$$ \partial_t \left( \left( \frac{1}{2} |\mathbf{u}|^2 + \vartheta \right) \right) + \text{div} \left( \left( \frac{1}{2} |\mathbf{u}|^2 + \vartheta \right) \mathbf{u} \right) + \text{div}(\rho \mathbf{u}) + \text{div} \mathbf{q} $$

$$ = \text{div}(S \mathbf{u}) - \text{div} \left( \lambda(\vartheta) (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) \mathbf{u} \right) + \mathbf{f} \cdot \mathbf{u}. $$
The total energy balance

Multiplying momentum equation (MOM) by \( u \) and adding the resulting expression to (INT) we deduce the **total energy balance** in the form

\[
\partial_t \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) \right) + \text{div} \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) u \right) + \text{div}(\rho u) + \text{div} q \\
= \text{div}(S u) - \text{div} \left( \lambda(\vartheta) (\nabla_x d \odot \nabla_x d) u \right) + f \cdot u.
\]

Moreover, using the boundary conditions and integrating the last equation over \( \Omega \) we obtain

\[
\partial_t \int_{\Omega} \left( \frac{1}{2} |u|^2 + \vartheta \right) = \int_{\Omega} f \cdot u,
\]

in particular, the total energy is a constant of motion as soon as \( f \equiv 0 \).
The entropy production

Let us denote by $\Lambda(\vartheta)$ a primitive of $\frac{1}{\lambda(\vartheta)}$. Testing (INT) by $\frac{1}{\lambda(\vartheta)}$ and (EQD) by $(\text{div} \nabla x d - \partial W(d))$, integrating the sum over $\Omega$, we get:

$$\int_{\Omega} \left( \partial_t d + u \cdot \nabla x d \right) (\text{div} \nabla x d - \partial W(d)) + \partial_t \int_{\Omega} \left( \Lambda(\vartheta) + \int_{\Omega} q \cdot \nabla x \vartheta \lambda'(\vartheta) (\lambda(\vartheta))^2 \right) = \int_{\Omega} |\text{div} (\varrho \nabla x d - \partial W(d))|^2 + \int_{\Omega} 1/\lambda(\vartheta) S : \nabla x u$$

Thus, finally, we arrive at:

$$\partial_t \int_{\Omega} \left( \Lambda(\vartheta) - |\nabla x d|^2/2 - W(d) \right) = \int_{\Omega} |\text{div} (\varrho \nabla x d - \partial W(d))|^2 + \int_{\Omega} 1/\lambda(\vartheta) S : \nabla x u - \int_{\Omega} q \cdot \nabla x \vartheta \lambda'(\vartheta) (\lambda(\vartheta))^2,$$

where the entropy density of the system is $S = (\Lambda(\vartheta) - |\nabla x d|^2/2 - W(d))$ and, if $\lambda' \geq 0$, then the Second law of thermodynamics is satisfied.
The entropy production

Let us denote by $\Lambda(\vartheta)$ a primitive of $1/\lambda(\vartheta)$. Testing (INT) by $1/\lambda(\vartheta)$ and (EQD) by $(\text{div} \nabla_x \mathbf{d} - \partial W(\mathbf{d}))$, integrating the sum over $\Omega$, we get

$$
\int_\Omega (\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d}) (\text{div} \nabla_x \mathbf{d} - \partial W(\mathbf{d})) + \partial_t \int_\Omega (\Lambda(\vartheta)) + \int_\Omega \mathbf{q} \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2}
$$

$$
= \int_\Omega |\text{div} \nabla_x \mathbf{d} - \varrho \partial W(\mathbf{d})|^2 + \int_\Omega \frac{1}{\lambda(\vartheta)} \mathbb{S} : \nabla_x \mathbf{u} - \int_\Omega (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) : \nabla_x \mathbf{u},
$$

and

$$
\int_\Omega (\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla_x \mathbf{d}) (\text{div} \nabla_x \mathbf{d} - \partial W(\mathbf{d})) = \partial_t \int_\Omega \left( - \frac{|\nabla_x \mathbf{d}|^2}{2} - W(\mathbf{d}) \right) - \int_\Omega (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) : \nabla_x \mathbf{u}
$$

Thus, finally, we arrive at

$$
\partial_t \int_\Omega \left( \Lambda(\vartheta) - \frac{|\nabla_x \mathbf{d}|^2}{2} - W(\mathbf{d}) \right) = \int_\Omega |\text{div} (\varrho \nabla_x \mathbf{d}) - \partial W(\mathbf{d})|^2
$$

$$
+ \int_\Omega \frac{1}{\lambda(\vartheta)} \mathbb{S} : \nabla_x \mathbf{u} - \int_\Omega \mathbf{q} \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2},
$$

where the entropy density of the system is $S = (\Lambda(\vartheta) - |\nabla_x \mathbf{d}|^2/2 - W(\mathbf{d}))$ and, if $\lambda' \geq 0$, then the Second law of thermodynamics is satisfied.
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the momentum equations \((\forall \varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3), \varphi \cdot n|_{\partial \Omega} = 0)\):
  \[
  \int_{\Omega} u(t, \cdot) \cdot \nabla \psi = 0 \quad \text{for a.a. } t \in (0, T) \forall \psi \in C_\infty(\Omega).
  \]
  \[
  \int_{T_0} \int_{\Omega} (u \cdot \partial_t \varphi + u \otimes u : \nabla \varphi) = \int_{T_0} \int_{\Omega} \Delta \varphi + \int_{\Omega} u_0 \cdot \varphi(0, \cdot).
  \]
- the equation for \(d\) holding in the strong sense:
  \[
  \partial_t d + u \cdot \nabla d + \partial W(d) = \Delta d \quad \text{a.e. in } (0, T) \times \Omega, \quad \nabla d \cdot n|_{\partial \Omega} = 0, \quad i = 1, 2, 3;
  \]
- the total energy balance (for any \(\varphi \in C_0^\infty([0, T] \times \bar{\Omega}; \mathbb{R}^3)\)):
  \[
  \int_{T_0} \int_{\Omega} \left( \frac{1}{2} |u|^2 + \vartheta \right) \partial_t \varphi + \left( \frac{1}{2} |u|^2 + \vartheta \right) u \cdot \nabla \varphi + q \cdot \nabla \varphi
  \]
  \[
  = \int_{T_0} \int_{\Omega} S - \lambda(\vartheta) \left( \nabla d \otimes \nabla d \right) - p I u \cdot \nabla \varphi - \int_{\Omega} \left( \frac{1}{2} |u_0|^2 + \vartheta_0 \right) \varphi(0, \cdot);
  \]
- the entropy production inequality (in the sense of distributions):
  \[
  \partial_t \left( \Lambda(\vartheta) - |\nabla d|^2 - W(d) \right) \geq - \text{div} (u \Lambda(\vartheta) + q \lambda(\vartheta) + u \cdot \nabla d \otimes \nabla d - u W(d)) + |\Delta d - \partial W(d)|^2 + \frac{1}{\lambda(\vartheta)} S : \nabla u - q \cdot \nabla \vartheta \lambda'(\vartheta)(\lambda(\vartheta))^2
  \]
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the momentum equations \((\forall \varphi \in C_0^\infty([0, T] \times \overline{\Omega}; \mathbb{R}^3), \varphi \cdot n|_{\partial \Omega} = 0)\):

  \[
  \int_{\Omega} u(t, \cdot) \cdot \nabla_x \psi = 0 \text{ for a.a. } t \in (0, T) \quad \forall \psi \in C^\infty(\overline{\Omega}),
  \]

  \[
  \int_0^T \int_{\Omega} \left( u \cdot \partial_t \varphi + u \otimes u : \nabla_x \varphi \right) = \int_0^T \int_{\Omega} \mathbf{T} : \nabla_x \varphi - \int_{\Omega} u_0 \cdot \varphi(0, \cdot);
  \]
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the **momentum equations** \((\forall \varphi \in C^\infty_0([0, T) \times \Omega; \mathbb{R}^3), \varphi \cdot n|_{\partial \Omega} = 0):\)

\[
\int_{\Omega} u(t, \cdot) \cdot \nabla_x \psi = 0 \text{ for a.a. } t \in (0, T) \quad \forall \psi \in C^\infty_0(\Omega),
\]

\[
\int_0^T \int_{\Omega} \left( u \cdot \partial_t \varphi + u \otimes u : \nabla_x \varphi \right) = \int_0^T \int_{\Omega} \mathbb{T} : \nabla_x \varphi - \int_{\Omega} u_0 \cdot \varphi(0, \cdot);
\]

- the **equation for** \(d\) **holding in the strong sense:**

\[
\partial_t d + u \cdot \nabla_x d + \partial W(d) = \Delta d \text{ a.e. in } (0, T) \times \Omega, \quad \nabla_x d_i \cdot n|_{\partial \Omega} = 0, \ i = 1, 2, 3;
\]
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the **momentum equations** \((\forall \varphi \in C_0^\infty([0, T] \times \overline{\Omega}; \mathbb{R}^3), \varphi \cdot n|_{\partial \Omega} = 0)\):
  \[
  \int_{\Omega} u(t, \cdot) \cdot \nabla_x \varphi = 0 \text{ for a.a. } t \in (0, T) \quad \forall \varphi \in C^\infty(\overline{\Omega}),
  \]
  \[
  \int_0^T \int_{\Omega} \left( u \cdot \partial_t \varphi + u \otimes u : \nabla_x \varphi \right) = \int_0^T \int_{\Omega} \mathbb{T} : \nabla_x \varphi - \int_{\Omega} u_0 \cdot \varphi(0, \cdot);
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  \]

- the **total energy balance** (for any \(\varphi \in C_0^\infty([0, T] \times \overline{\Omega})):\)
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the **momentum equations** \((\forall \varphi \in C_0^\infty([0, T) \times \overline{\Omega}; \mathbb{R}^3), \varphi \cdot n|_{\partial\Omega} = 0)\):
  
  \[
  \int_{\Omega} u(t, \cdot) \cdot \nabla_x \psi = 0 \text{ for a.a. } t \in (0, T) \quad \forall \psi \in C^\infty(\overline{\Omega}),
  \]

  \[
  \int_0^T \int_{\Omega} \left( u \cdot \partial_t \varphi + u \otimes u : \nabla_x \varphi \right) = \int_0^T \int_{\Omega} \nabla \cdot \varphi - \int_{\Omega} u_0 \cdot \varphi(0, \cdot);
  \]

- the **equation for \(d\)** holding in the strong sense:
  
  \[
  \partial_t d + u \cdot \nabla_x d + \partial W(d) = \Delta d \text{ a.e. in } (0, T) \times \Omega, \quad \nabla_x d_i \cdot n|_{\partial\Omega} = 0, \quad i = 1, 2, 3;
  \]

- the **total energy balance** (for any \(\varphi \in C_0^\infty([0, T) \times \overline{\Omega})\)):
  
  \[
  \int_0^T \int_{\Omega} \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) \partial_t \varphi + \left( \frac{1}{2} |u|^2 + \vartheta \right) u \cdot \nabla_x \varphi + q \cdot \nabla_x \varphi \right)
  \]

  \[
  = \int_0^T \int_{\Omega} \left( S - \lambda(\vartheta) (\nabla_x d \otimes \nabla_x d) - pI \right) u \cdot \nabla_x \varphi - \int_{\Omega} \left( \frac{1}{2} |u_0|^2 + \vartheta_0 \right) \varphi(0, \cdot);
  \]

- the **entropy production inequality** (in the sense of distributions):
A weak solution is a triple \((u, d, \vartheta)\) satisfying:

- the **momentum equations** \((\forall \varphi \in C_0^\infty([0, T] \times \overline{\Omega}; \mathbb{R}^3), \varphi \cdot n|_{\partial \Omega} = 0)\):
  \[
  \int_{\Omega} u(t, \cdot) \cdot \nabla_x \psi = 0 \text{ for a.a. } t \in (0, T) \quad \forall \psi \in C^\infty(\overline{\Omega}),
  \]
  \[
  \int_0^T \int_{\Omega} \left( u \cdot \partial_t \varphi + u \otimes u : \nabla_x \varphi \right) = \int_0^T \int_{\Omega} \mathbb{T} : \nabla_x \varphi - \int_{\Omega} u_0 \cdot \varphi(0, \cdot);
  \]

- the **equation for d** holding in the strong sense:
  \[
  \partial_t d + u \cdot \nabla_x d + \partial W(d) = \Delta d \text{ a.e. in } (0, T) \times \Omega, \quad \nabla_x d_i \cdot n|_{\partial \Omega} = 0, \ i = 1, 2, 3; \]

- the **total energy balance** (for any \(\varphi \in C_0^\infty([0, T] \times \overline{\Omega}))\):
  \[
  \int_0^T \int_{\Omega} \left( \frac{1}{2} |u|^2 + \vartheta \right) \partial_t \varphi + \left( \frac{1}{2} |u|^2 + \vartheta \right) u \cdot \nabla_x \varphi + q \cdot \nabla_x \varphi \right)
  \]
  \[
  = \int_0^T \int_{\Omega} (\mathbb{S} - \lambda(\vartheta) (\nabla_x d \otimes \nabla_x d) - p \mathbb{I}) u \cdot \nabla_x \varphi - \int_{\Omega} \left( \frac{1}{2} |u_0|^2 + \vartheta_0 \right) \varphi(0, \cdot);
  \]

- the **entropy production inequality** (in the sense of distributions):
  \[
  \partial_t \left( \Lambda(\vartheta) - \frac{|\nabla_x d|^2}{2} - W(d) \right) \geq - \text{div} \left( u \Lambda(\vartheta) + \frac{q}{\lambda(\vartheta)} + u \cdot (\nabla_x d \otimes \nabla_x d) - u W(d) \right)
  \]
  \[
  + |\Delta d - \partial W(d)|^2 + \frac{1}{\lambda(\vartheta)} \mathbb{S} : \nabla_x u - q \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{\lambda(\vartheta)}^2
  \]
The assumptions

We assume that $W \in C^2(\mathbb{R}^3)$, $W \geq 0$, $\partial W(d) \cdot d \geq 0$ for all $|d| \geq D_0$ for a certain $D_0 > 0$.

The transport coefficients are continuously differentiable functions of the absolute temperature satisfying $0 < \mu \leq \mu(\vartheta) \leq \mu$, $0 < \kappa \leq \kappa(\vartheta)$, $(\kappa || - \kappa \perp)(\vartheta) \leq \kappa$ for all $\vartheta \geq 0$ for suitable constants $\kappa$, $\kappa$, $\mu$, $\mu$.

$s \in C_1([0, +\infty))$ be such that $s'(\vartheta) \geq 0$, $s'(0) > 0$, $s(0) = 0$, $s(\vartheta) \leq s$ for all $\vartheta \geq 0$ for a certain $s > 0$. 

E. Rocca (University of Milan)
The assumptions

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The assumptions

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- The transport coefficients are continuously differentiable functions of the absolute temperature satisfying

  \[
  0 < \mu \leq \mu(\vartheta) \leq \bar{\mu}, \quad 0 < \kappa \leq \kappa(\vartheta), \quad (\kappa_{||} - \kappa_{\perp})(\vartheta) \leq \bar{\kappa} \quad \text{for all } \vartheta \geq 0
  \]

for suitable constants \( \kappa, \bar{\kappa}, \mu, \bar{\mu} \)
The assumptions

We assume that

1. \( W \in C^2(\mathbb{R}^3) \), \( W \geq 0 \), \( \partial W(d) \cdot d \geq 0 \) for all \( |d| \geq D_0 \) for a certain \( D_0 > 0 \)

2. The transport coefficients are continuously differentiable functions of the absolute temperature satisfying

   \[ 0 < \mu \leq \mu(\vartheta) \leq \bar{\mu}, \quad 0 < \kappa \leq \kappa(\vartheta), \quad (\kappa_{||} - \kappa_{\perp})(\vartheta) \leq \bar{\kappa} \]

   for all \( \vartheta \geq 0 \)

   for suitable constants \( \kappa, \bar{\kappa}, \mu, \bar{\mu} \)

3. \( \lambda \in C^1([0, +\infty)) \) be such that

   \[ \lambda'(\vartheta) \geq 0, \quad \lambda'(0) > 0, \quad \lambda(0) = 0, \quad \lambda(\vartheta) \leq \bar{\lambda} \]

   for all \( \vartheta \geq 0 \)

   for a certain \( \bar{\lambda} > 0 \).
The existence theorem

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain of class $C^{2+\nu}$ for some $\nu > 0$. Assume that the previous hypotheses are satisfied. Finally, let the initial data be such that $u_0 \in L^2(\Omega; \mathbb{R}^3)$, $\text{div} u_0 = 0$, $d_0 \in L^\infty \cap W^{1,2}(\Omega; \mathbb{R}^3)$, $\vartheta_0 \in L^1(\Omega)$, $\text{ess inf}_{\Omega} \vartheta_0 > 0$.

Then our problem possesses a weak solution $(u, d, \vartheta)$ in $(0, T) \times \Omega$ belonging to the class $u \in L^\infty (0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2 (0, T; W^{1,2}(\Omega))$, $d \in L^\infty ((0, T) \times \Omega; \mathbb{R}^3) \cap L^\infty (0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^2 (0, T; W^{2,2}(\Omega; \mathbb{R}^3))$, $\vartheta \in L^\infty (0, T; L^1(\Omega)) \cap L^p (0, T; W^{1,p}(\Omega))$, $1 \leq p < 5/4$, $\vartheta > 0$ a.e. in $(0, T) \times \Omega$, with the pressure $p \in L^{5/3}((0, T) \times \Omega)$. 

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Non-isothermal liquid crystal model
Prague, December 2010
The existence theorem

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain of class $C^{2+\nu}$ for some $\nu > 0$. Assume that the previous hypotheses are satisfied. Finally, let the initial data be such that

$$u_0 \in L^2(\Omega; \mathbb{R}^3), \; \text{div} \, u_0 = 0, \; d_0 \in L^\infty \cap W^{1,2}(\Omega; \mathbb{R}^3),$$

$$\vartheta_0 \in L^1(\Omega), \; \text{ess inf}_\Omega \vartheta_0 > 0.$$
The existence theorem

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$$\vartheta_0 \in L^1(\Omega), \quad \text{ess inf}_\Omega \vartheta_0 > 0.$$

Then our problem possesses a weak solution $(u, d, \vartheta)$ in $(0, T) \times \Omega$ belonging to the class

$$u \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega)),$$

$$d \in L^\infty((0, T) \times \Omega; \mathbb{R}^3) \cap L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{2,2}(\Omega; \mathbb{R}^3)),$$

$$\vartheta \in L^\infty(0, T; L^1(\Omega)) \cap L^p(0, T; W^{1,p}(\Omega)), \quad 1 \leq p < 5/4, \quad \vartheta > 0 \text{ a.e. in } (0, T) \times \Omega,$$

with the pressure $p$,

$$p \in L^{5/3}((0, T) \times \Omega).$$
An idea of the proof

We perform suitable a-priori estimates which coincide with the regularity class stated in the Theorem. It can be shown that the solution set of our problem is weakly stable (compact) with respect to these bounds, namely, any sequence of (weak) solutions that complies with the uniform bounds established above has a subsequence that converges to some limit. Hence, we construct a suitable family of approximate problems (via Faedo-Galerkin scheme + regularizing terms in the momentum equation) whose solutions weakly converge (up to subsequences) to limit functions which solve the problem in the weak sense.
An idea of the proof

- We perform suitable **a-priori estimates** which coincide with the regularity class stated in the Theorem.
An idea of the proof

- We perform suitable **a-priori estimates** which coincide with the regularity class stated in the Theorem.

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An idea of the proof

- We perform suitable a-priori estimates which coincide with the regularity class stated in the Theorem.

- It can be shown that the solution set of our problem is weakly stable (compact) with respect to these bounds, namely, any sequence of (weak) solutions that complies with the uniform bounds established above has a subsequence that converges to some limit.

- Hence, we construct a suitable family of approximate problems (via Faedo-Galerkin scheme + regularizing terms in the momentum equation) whose solutions weakly converge (up to subsequences) to limit functions which solve the problem in the weak sense.
Total dissipation balance

Combining the energy balance (multiplied by a positive constant $K > 0$) with the entropy inequality we obtain the total dissipation balance in the form

$$\int_{\Omega} \left( K^2 |u|^2 + (K \vartheta - \Lambda(\vartheta)) + |\nabla x d|^2 + W(d) \right) \leq \int_{\Omega} \left( K^2 |u_0|^2 + (K \vartheta_0 - \Lambda(\vartheta_0)) + |\nabla x d_0|^2 + W(d_0) \right).$$

For $K$ sufficiently large, the terms on the left hand side turn out to be non-negative, and the integral on the right-hand side is bounded; hence we deduce the a priori bounds $u \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^{10/3}((0, T) \times \Omega; \mathbb{R}^3)$, $\vartheta, \log(\vartheta) \in L^\infty(0, T; L^1(\Omega))$, $d \in L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3))$. Moreover, we also get $\Lambda(\vartheta) \in L^\infty(0, T; L^1(\Omega))$, $(\Lambda(\vartheta) + \epsilon) \in L^2(0, T; W^{1,2}(\Omega))$. 

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Non-isothermal liquid crystal model

Prague, December 2010
**Total dissipation balance**

Combining the energy balance (multiplied by a positive constant $K > 0$) with the entropy inequality we obtain the **total dissipation balance** in the form

$$\int_\Omega \left( \frac{K}{2} |\mathbf{u}|^2 + (K \vartheta - \Lambda(\vartheta)) + \frac{1}{2} |\nabla_x \mathbf{d}|^2 + W(\mathbf{d}) \right) (\tau, \cdot)$$

$$+ \int_0^\tau \int_\Omega \left( |\Delta \mathbf{d} - \partial W(\mathbf{d})|^2 + \frac{1}{\lambda(\vartheta)} \mathbf{S} : \nabla_x \mathbf{u} - \mathbf{q} \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{\lambda^2(\vartheta)} \right)$$

$$\leq \int_\Omega \left( \frac{K}{2} |\mathbf{u}_0|^2 + (K \vartheta_0 - \Lambda(\vartheta_0)) + \frac{1}{2} |\nabla_x \mathbf{d}_0|^2 + W(\mathbf{d}_0) \right) .$$
Total dissipation balance

Combining the energy balance (multiplied by a positive constant $K > 0$) with the entropy inequality we obtain the **total dissipation balance** in the form

\[
\int_{\Omega} \left( \frac{K}{2} |u|^2 + (K\vartheta - \Lambda(\vartheta)) + \frac{|\nabla x d|^2}{2} + W(d) \right) (\tau, \cdot) \\
+ \int_{0}^{\tau} \int_{\Omega} \left( |\Delta d - \partial W(d)|^2 + \frac{1}{\chi(\vartheta)} \mathbb{S} : \nabla x u - q \cdot \nabla x \vartheta \frac{\lambda'(\vartheta)}{\lambda^2(\vartheta)} \right) \\
\leq \int_{\Omega} \left( \frac{K}{2} |u_0|^2 + (K\vartheta_0 - \Lambda(\vartheta_0)) + \frac{|\nabla x d_0|^2}{2} + W(d_0) \right).
\]

For $K$ sufficiently large, the terms on the left hand side turn out to be non-negative, and the integral on the right-hand side is bounded; hence we deduce the **a priori bounds**

\[
\begin{align*}
    u & \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^{10/3}((0, T) \times \Omega; \mathbb{R}^3), \\
    \vartheta, \log(\vartheta) & \in L^\infty(0, T; L^1(\Omega)), \\
    d & \in L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3)).
\end{align*}
\]

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Total dissipation balance

Combining the energy balance (multiplied by a positive constant $K > 0$) with the entropy inequality we obtain the **total dissipation balance** in the form

$$
\int_{\Omega} \left( \frac{K}{2} |u|^2 + (K \vartheta - \Lambda(\vartheta)) + \frac{|\nabla \times d|^2}{2} + W(d) \right) (\tau, \cdot) \\
+ \int_{0}^{\tau} \int_{\Omega} \left( |\Delta d - \partial W(d)|^2 + \frac{1}{\lambda(\vartheta)} S : \nabla_x u - q \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{\lambda^2(\vartheta)} \right) \\
\leq \int_{\Omega} \left( \frac{K}{2} |u_0|^2 + (K \vartheta_0 - \Lambda(\vartheta_0)) + \frac{|\nabla \times d_0|^2}{2} + W(d_0) \right).
$$

For $K$ sufficiently large, the terms on the left hand side turn out to be non-negative, and the integral on the right-hand side is bounded; hence we deduce the **a priori bounds**

$$u \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^3)) \cap L^2(0, T; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^{10/3}((0, T) \times \Omega; \mathbb{R}^3),$$

$$\vartheta, \ \log(\vartheta) \in L^\infty(0, T; L^1(\Omega)),$$

$$d \in L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3)).$$

Moreover, we also get

$$\Lambda(\vartheta) \in L^\infty(0, T; L^1(\Omega)), \quad (\Lambda(\vartheta))^+ \in L^2(0, T; W^{1,2}(\Omega)).$$
Direct field estimate

\[
\text{Take the scalar product of the } d \text{-equation with } d \text{ yielding}
\]
\[
\partial_t |d|^2 + u \cdot \nabla x |d|^2 + 2 \partial W(d) \cdot d = \Delta |d|^2 - 2 |\nabla x d|^2.
\]

By means of our assumptions on \(W\), we may apply the standard maximum principle to \(|d|^2\) obtaining \(d \in L^\infty((0,T) \times \Omega; \mathbb{R}^3)\) and so also \(d \in L^2(0,T; W^{2,2}(\Omega; \mathbb{R}^3))\), which, together with Gagliardo-Nirenberg interpolation inequality
\[
\|\nabla x d\|_{L^4(\Omega)} \leq c_1 \|\Delta d\|_{L^2(\Omega)}^{1/2} \|d\|_{L^\infty(\Omega)}^{1/2} + c_2 \|d\|_{L^\infty(\Omega)},
\]
gives rise to \(\nabla x d \in L^4((0,T) \times \Omega)\).

This estimate turns out to be "crucial" in order to obtain a bound for the pressure and, in general, for the proof of existence of solutions.
Director field estimate

Take the scalar product of the \(d\)-equation equation with \(d\) yielding

\[
\partial_t |d|^2 + u \cdot \nabla_x |d|^2 + 2 \partial W(d) \cdot d = \Delta |d|^2 - 2 |\nabla_x d|^2.
\]
**Director field estimate**

Take the scalar product of the $d$-equation equation with $d$ yielding

$$
\partial_t |d|^2 + u \cdot \nabla_x |d|^2 + 2 \partial W(d) \cdot d = \Delta |d|^2 - 2|\nabla_x d|^2.
$$

By means of our assumptions on $W$, we may apply the standard **maximum principle to $|d|^2$** obtaining

$$d \in L^\infty((0, T) \times \Omega; \mathbb{R}^3)$$

and so also

$$d \in L^2(0, T; W^{2,2}(\Omega; \mathbb{R}^3)),$$

which, together with **Gagliardo-Nirenberg interpolation inequality**

$$
\|\nabla_x d\|_{L^4(\Omega)} \leq c_1 \|\Delta d\|_{L^2(\Omega)}^{1/2} \|d\|_{L^\infty(\Omega)}^{1/2} + c_2 \|d\|_{L^\infty(\Omega)},
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**Director field estimate**

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\]

and so also

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d \in L^2(0, T; W^{2,2}(\Omega; \mathbb{R}^3)),
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\[
\|\nabla_x d\|_{L^4(\Omega)} \leq c_1 \|\Delta d\|_{L^2(\Omega)}^{1/2} \|d\|_{L^\infty(\Omega)}^{1/2} + c_2 \|d\|_{L^\infty(\Omega)},
\]

gives rise to

\[
\nabla_x d \in L^4((0, T) \times \Omega).\]

This estimate turns out to be “crucial” in order to obtain a bound for the pressure and, in general, for the proof of existence of solutions.
Pressure estimate

Thanks to our choice of the slip boundary conditions for the velocity, the pressure $p$ can be "computed" directly from our equations as the unique solution of the elliptic problem

$$\Delta p = \text{div div} \left( S - \lambda (\vartheta) \nabla x d \odot \nabla x d - u \otimes u \right),$$

supplemented with the boundary condition

$$\partial_n p = \text{div} \left( S - \lambda (\vartheta) \nabla x d \odot \nabla x d - u \otimes u \right) \cdot n \text{ on } \partial \Omega.$$

To be precise, the last two relations have to be interpreted in a "very weak" sense. Namely, the pressure $p$ is determined through a family of integral identities

$$\int_\Omega p \Delta \phi = \int_\Omega \left( S - \lambda (\vartheta) \nabla x d \odot \nabla x d - u \otimes u \right) : \nabla^2 x \phi$$

for any test function $\phi \in C^\infty(\Omega)$, $\nabla x \phi \cdot n |_{\partial \Omega} = 0$.

Consequently, the bounds already established may be used, together with the standard elliptic regularity results, to conclude that $p \in L^{5/3}((0, T) \times \Omega)$. 

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Pressure estimate

Thanks to our choice of the slip boundary conditions for the velocity, the pressure $p$ can be “computed” directly from our equations as the unique solution of the elliptic problem

$$
\Delta p = \text{div} \text{div} \left( \mathbb{S} - \lambda(\vartheta) \nabla_x d \odot \nabla_x d - u \otimes u \right),
$$

supplemented with the boundary condition

$$
\partial_n p = (\text{div} (\mathbb{S} - \lambda(\vartheta) \nabla_x d \odot \nabla_x d - u \otimes u)) \cdot n \quad \text{on} \quad \partial \Omega.
$$
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$$\int_{\Omega} p \Delta \varphi = \int_{\Omega} \left( S - \lambda(\vartheta) \nabla_x d \otimes \nabla_x d - u \otimes u \right) : \nabla_x^2 \varphi$$

for any test function $\varphi \in C^\infty(\overline{\Omega})$, $\nabla_x \varphi \cdot n |_{\partial\Omega} = 0$. 
Pressure estimate

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To be precise, the last two relations have to be interpreted in a “very weak” sense. Namely, the pressure $p$ is determined through a family of integral identities

$$\int_{\Omega} p \Delta \varphi = \int_{\Omega} \left( \mathbb{S} - \lambda(\vartheta) \nabla x d \odot \nabla x d - u \otimes u \right) : \nabla^2 x \varphi$$

for any test function $\varphi \in C^\infty(\overline{\Omega})$, $\nabla x \varphi \cdot n|_{\partial \Omega} = 0$. Consequently, the bounds already established may be used, together with the standard elliptic regularity results, to conclude that

$$p \in L^{5/3}((0, T) \times \Omega).$$
Entropy estimate

Multiplying the $\vartheta$-equation by $H'(\vartheta)$ (for a generic $H \in C^2([0, +\infty])$) we deduce its "renormalized" form

$$\partial_t H(\vartheta) + \text{div}(H(\vartheta)u) + \text{div}(H'(\vartheta)q) + H''(\vartheta)(\kappa(\vartheta)|\nabla x\vartheta|)^2 + (\kappa|\bullet| - \kappa_\perp(\vartheta)|d\cdot\nabla x\vartheta|)^2 = H'(\vartheta)(S - \lambda(\vartheta)\nabla x d \odot \nabla x d): \nabla x u \in D'((0, T) \times \Omega).$$

The choice $H(\vartheta) = (1 + \vartheta)^\eta$, $\eta \in (0, 1)$, together with the uniform bounds obtained before, yield $\nabla x (1 + \vartheta)^\nu \in L^2((0, T) \times \Omega; \mathbb{R}^3)$ for any $0 < \nu < 1/2$.

Now, we apply an interpolation argument between $\vartheta \in L^\infty(0, T; L^1(\Omega))$ and $\vartheta^\nu \in L^1(0, T; L^3(\Omega))$, for $\nu \in (0, 1]$, getting $\vartheta \in L^q((0, T) \times \Omega)$ for any $1 \leq q < 5/3$.

Further, observing that, for all $p \in [1, 5/4)$ and $\nu > 0$,

$$\int (0, T) \times \Omega |\nabla x \vartheta|^p \leq \left( \int (0, T) \times \Omega |\nabla x \vartheta|^{2\nu} \right)^{\frac{p}{2}} \left( \int (0, T) \times \Omega \vartheta^{1-\nu} \right)^{\frac{2p-2p}{2}} \leq \left( \int (0, T) \times \Omega \vartheta \right)^{2p-2p} \leq \left( \int (0, T) \times \Omega \vartheta^p \right)^{\frac{2p}{2p-2} - p},$$

we conclude that $\nabla x \vartheta \in L^p((0, T) \times \Omega; \mathbb{R}^3)$, $\nabla x (\Lambda(\vartheta)) \in L^p((0, T) \times \Omega; \mathbb{R}^3)$ for any $1 \leq p < 5/4$. 

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Entropy estimate

Multiplying the $\vartheta$-equation by $H'(\vartheta)$ (for a generic $H \in C^2([0, +\infty)))$ we deduce its "renormalized" form

$$
\partial_t H(\vartheta) + \text{div}(H(\vartheta)u) + \text{div}(H'(\vartheta)q) \\
+ H''(\vartheta)\left(\kappa(\vartheta)|\nabla_x \vartheta|^2 + (\kappa_{||} - \kappa_{\perp})(\vartheta)|d \cdot \nabla_x \vartheta|^2\right) \\
= H'(\vartheta)\left(S - \lambda(\vartheta)\nabla_x d \odot \nabla_x d\right) : \nabla_x u \quad \text{in } D'(0, T \times \Omega).
$$
Entropy estimate

Multiplying the $\vartheta$-equation by $H'(\vartheta)$ (for a generic $H \in C^2([0, +\infty)))$ we deduce its “renormalized” form

$$\partial_t H(\vartheta) + \text{div}(H(\vartheta)u) + \text{div}(H'(\vartheta)q)$$

$$+ H''(\vartheta)\left(\kappa(\vartheta)|\nabla_x \vartheta|^2 + (\kappa_\parallel - \kappa_\perp)(\vartheta)|d \cdot \nabla_x \vartheta|^2\right)$$

$$= H'(\vartheta)\left(\mathcal{S} - \lambda(\vartheta)\nabla_x d \odot \nabla_x d\right) : \nabla_x u \quad \text{in } D'((0, T) \times \Omega).$$

The choice $H(\vartheta) = (1 + \vartheta)^\eta$, $\eta \in (0, 1)$, together with the uniform bounds obtained before, yield

$$\nabla_x (1 + \vartheta)^\nu \in L^2((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } 0 < \nu < \frac{1}{2}.$$
Entropy estimate

Multiplying the \(\vartheta\)-equation by \(H'(\vartheta)\) (for a generic \(H \in C^2([0, +\infty))\)) we deduce its “renormalized” form

\[
\partial_t H(\vartheta) + \text{div}(H(\vartheta)u) + \text{div}(H'(\vartheta)q) \\
+ H''(\vartheta) \left( \kappa(\vartheta)|\nabla_x \vartheta|^2 + (\kappa \parallel - \kappa \perp)(\vartheta)|d \cdot \nabla_x \vartheta|^2 \right) \\
= H'(\vartheta) \left( S - \lambda(\vartheta) \nabla_x d \odot \nabla_x d \right) : \nabla_x u \quad \text{in} \ D'( (0, T) \times \Omega ).
\]

The choice \(H(\vartheta) = (1 + \vartheta)^\eta, \ \eta \in (0, 1)\), together with the uniform bounds obtained before, yield

\[
\nabla_x (1 + \vartheta)^\nu \in L^2((0, T) \times \Omega; \mathbb{R}^3) \quad \text{for any} \ 0 < \nu < \frac{1}{2}.
\]

Now, we apply an interpolation argument between \(\vartheta \in L^\infty(0, T; L^1(\Omega))\) and \(\vartheta^\nu \in L^1(0, T; L^3(\Omega))\), for \(\nu \in (0, 1]\), getting

\[
\vartheta \in L^q((0, T) \times \Omega) \quad \text{for any} \ 1 \le q < 5/3.
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Entropy estimate

Multiplying the $\vartheta$-equation by $H'(\vartheta)$ (for a generic $H \in C^2([0, +\infty)))$ we deduce its “renormalized” form

$$\partial_t H(\vartheta) + \text{div}(H(\vartheta)u) + \text{div}(H'(\vartheta)q)
+ H''(\vartheta) \left( \kappa(\vartheta)|\nabla_x \vartheta|^2 + (\kappa_\parallel - \kappa_\perp)(\vartheta)|d \cdot \nabla_x \vartheta|^2 \right)
= H'(\vartheta) \left( S - \lambda(\vartheta) \nabla_x d \odot \nabla_x d \right) : \nabla_x u \quad \text{in } \mathcal{D}'((0, T) \times \Omega).$$

The choice $H(\vartheta) = (1 + \vartheta)^\eta$, $\eta \in (0, 1)$, together with the uniform bounds obtained before, yield

$$\nabla_x (1 + \vartheta)^\nu \in L^2((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } 0 < \nu < \frac{1}{2}.$$

Now, we apply an interpolation argument between $\vartheta \in L^\infty(0, T; L^1(\Omega))$ and $\vartheta^\nu \in L^1(0, T; L^3(\Omega))$, for $\nu \in (0, 1]$, getting

$$\vartheta \in L^q((0, T) \times \Omega) \text{ for any } 1 \leq q < \frac{5}{3}.$$

Further, observing that, for all $p \in [1, 5/4)$ and $\nu > 0$,

$$\int_{(0, T) \times \Omega} |\nabla_x \vartheta|^p \leq \left( \int_{(0, T) \times \Omega} |\nabla_x \vartheta|^{2\nu - 1} \right)^{\frac{p}{2}} \left( \int_{(0, T) \times \Omega} \vartheta^{(1-\nu)\frac{p}{2-p}} \right)^{\frac{2-p}{2}},$$

we conclude that

$$\nabla_x \vartheta \in L^p((0, T) \times \Omega; \mathbb{R}^3), \quad \nabla_x (\Lambda(\vartheta)) \in L^p((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } 1 \leq p < \frac{5}{4}.$$
The passage to the limit

On the approximated problem, we get

\[
\left| u \right|^2 + p u \text{ bounded in } L^1((0, T) \times \Omega; \mathbb{R}^3) \text{ for some } \iota > 1,
\]

\[
\vartheta u, \Lambda(\vartheta) u \text{ bounded in } L^q((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } q \in \left[1, \frac{10}{9}\right),
\]

\[
S u, \lambda(\vartheta) (\nabla x d \otimes \nabla x d) u \text{ bounded in } L^{5/4}(0, T; L^{5/4}(\Omega; \mathbb{R}^3)),
\]

\[
q \lambda(\vartheta) \text{ bounded in } L^s((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } s \in \left[1, \frac{5}{4}\right).
\]

We pass to the limit in the total energy balance and to the \( \lim \sup \) in the entropy inequality (thanks also to the positivity and convexity of some terms).

\[
\int_0^T \int_\Omega \left( \frac{1}{2} \left| u \right|^2 + \vartheta \partial_t \phi + \left| u \right|^2 u \cdot \nabla x \phi + q \cdot \nabla x \phi \right) \, dt \, dx = \int_0^T \int_\Omega \left( S - \lambda(\vartheta) (\nabla x d \otimes \nabla x d) - p I \right) u \cdot \nabla x \phi - \int_\Omega \left( \frac{1}{2} \left| u_0 \right|^2 + \vartheta_0 \right) \phi(0, \cdot) \, dx.
\]

\[
\partial_t \left( \Lambda(\vartheta) - \left| \nabla x d \right|^2 - W(d) \right) \geq - \text{div} \left( u \Lambda(\vartheta) + q \lambda(\vartheta) + u \cdot (\nabla x d \otimes \nabla x d) - u W(d) \right) + \left| \Delta d - \partial W(d) \right|^2 + \frac{1}{\lambda(\vartheta)} S: \nabla x u - q \cdot \nabla x \vartheta \lambda'(\vartheta) (\lambda(\vartheta))^2.
\]
The passage to the limit

On the approximated problem, we get

\[
|u|^2 + p \leq \text{bounded in } L^\infty((0, T) \times \Omega; \mathbb{R}^3) \quad \text{for some } \infty > 1,
\]

\[
\vartheta u, \Lambda(\vartheta) \leq \text{bounded in } L^q((0, T) \times \Omega; \mathbb{R}^3) \quad \text{for any } q \in [1, 10/9],
\]

\[
S u, \lambda(\vartheta) (\nabla x d \odot \nabla x d) u \leq \text{bounded in } L^{5/4}(0, T; L^{5/4}(\Omega; \mathbb{R}^3)),
\]

\[
\lambda(\vartheta) \text{ bounded in } L^s((0, T) \times \Omega; \mathbb{R}^3) \quad \text{for any } s \in [1, 5/4].
\]

We pass to the limit in the total energy balance and to the lim sup in the entropy inequality (thanks also to the positivity and convexity of some terms).

\[
\int_0^T \int_\Omega \left( \frac{1}{2} |u|^2 + \vartheta \right) \partial_t \phi + \left( \frac{1}{2} |u|^2 + \vartheta \right) u \cdot \nabla x \phi + q \cdot \nabla x \phi = \int_0^T \int_\Omega \left( S - \lambda(\vartheta) (\nabla x d \odot \nabla x d) - p I \right) u \cdot \nabla x \phi - \int_\Omega \left( \frac{1}{2} |u_0|^2 + \vartheta_0 \right) \phi(0, \cdot)
\]

\[
\partial_t (\Lambda(\vartheta) - |\nabla x d|^2 - W(d)) \geq -\text{div} \left( u \Lambda(\vartheta) + q \lambda(\vartheta) + u \cdot (\nabla x d \odot \nabla x d) - u W(d) \right) + |\Delta d - \partial W(d)|^2 + \lambda(\vartheta) S : \nabla x u - q \cdot \nabla x \vartheta \lambda'(\vartheta) \left( \lambda(\vartheta) \right)^2.
\]
The passage to the limit

On the approximated problem, we get

\[
\left( \frac{|u|^2}{2} + p \right) u \text{ bounded in } L^\iota((0, T) \times \Omega; \mathbb{R}^3) \text{ for some } \iota > 1 ,
\]

\[
\vartheta u, \ \Lambda(\vartheta)u \text{ bounded in } L^q((0, T) \times \Omega; \mathbb{R}^3)) \text{ for any } q \in [1, 10/9) ,
\]

\[
\mathcal{S}u, \ \lambda(\vartheta)(\nabla_x d \otimes \nabla_x d)u \text{ bounded in } L^{5/4}(0, T; L^{5/4}(\Omega; \mathbb{R}^3)) ,
\]

\[
\frac{q}{\lambda(\vartheta)} \text{ bounded in } L^s((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } s \in [1, 5/4) .
\]
The passage to the limit

On the approximated problem, we get

\[
\left( \frac{|u|^2}{2} + p \right) u \text{ bounded in } L^\iota((0, T) \times \Omega; \mathbb{R}^3) \text{ for some } \iota > 1,
\]

\[\vartheta u, \ \Lambda(\vartheta)u \text{ bounded in } L^q((0, T) \times \Omega; \mathbb{R}^3)) \text{ for any } q \in [1, 10/9),\]

\[Su, \ \lambda(\vartheta)(\nabla_x d \odot \nabla_x d)u \text{ bounded in } L^{5/4}(0, T; L^{5/4}(\Omega; \mathbb{R}^3)),\]

\[\frac{q}{\lambda(\vartheta)} \text{ bounded in } L^s((0, T) \times \Omega; \mathbb{R}^3) \text{ for any } s \in [1, 5/4).\]

We pass to the limit in the **total energy balance** and to the lim sup in the **entropy inequality** (thanks also to the positivity and convexity of some terms)

\[
\int_0^T \int_\Omega \left( \left( \frac{1}{2} |u|^2 + \vartheta \right) \partial_t \varphi + \left( \frac{1}{2} |u|^2 + \vartheta \right) u \cdot \nabla_x \varphi + q \cdot \nabla_x \varphi \right)
\]

\[
= \int_0^T \int_\Omega \left( S - \lambda(\vartheta) (\nabla_x d \odot \nabla_x d) - pI \right) u \cdot \nabla_x \varphi - \int_\Omega \left( \frac{1}{2} |u_0|^2 + \vartheta_0 \right) \varphi(0, \cdot);
\]

\[
\partial_t \left( \Lambda(\vartheta) - \frac{|\nabla_x d|^2}{2} - W(d) \right) \geq - \text{div} \left( u \Lambda(\vartheta) + \frac{q}{\lambda(\vartheta)} + u \cdot (\nabla_x d \odot \nabla_x d) - u W(d) \right)
\]

\[
+ |\Delta d - \partial W(d)|^2 + \frac{1}{\lambda(\vartheta)} S : \nabla_x u - q \cdot \nabla_x \vartheta \frac{\lambda'(\vartheta)}{(\lambda(\vartheta))^2}.
\]
Remarks on the modelling approach

Similarly to the simplified models proposed by Lin and Liu, we ignore the stretching of the director field induced by straining of the fluid producing an extra term $-\nabla x u \cdot d$ in the $d$-equation. Such a situation was treated by Coutand and Shkoller (2001) where local well-posedness is established for the model without thermal effects for the PDE system

$$
\begin{align*}
\begin{cases}
\frac{\partial u}{\partial t} - \text{div}(u \otimes u) - \nu \Delta u &= \text{div} S, \\
S &= -p I - L(\nabla d \otimes \nabla d) - \delta (L \Delta d - f(d)) \otimes d,
\end{cases}
\end{align*}
$$

where we have set $f(d) := \frac{1}{2} \partial_d (\hat{\psi}(|d|^2) - |d|^2)$ and the coefficient $\nu, L, \delta$ satisfy $\nu, L > 0$ and $\delta \geq 0$.

In [Sun and Liu, Disc. Conti. Dyna. Sys., 2009] global well-posedness is proved in the 2D case or in 3D under the condition that the viscosity coefficient is sufficiently large. To the best of our knowledge, global-in-time existence for this 3D model is entirely open, even within the class of weak solutions. The case of Dirichlet boundary conditions both for $u$ and $d$ are under study in a recent joint work with C. Cavaterra and E. Rocca (University of Milan).
Remarks on the modelling approach

- Similarly to the simplified models proposed by Lin and Liu, we ignore the stretching of the director field induced by straining of the fluid producing an extra term $-\nabla_x u \cdot d$ in the d-equation. Such a situation was treated by Coutand and Shkoller (2001) where local well-posedness is established for the model without thermal effects for the PDE system

\[
\begin{align*}
    u_t - \text{div}(u \otimes u) - \nu \Delta u &= \text{div} \mathcal{S}, \\
    \mathcal{S} &= -pI - L(\nabla d \otimes \nabla d) - \delta(L\Delta d - f(d)) \otimes d, \\
    \text{div} u &= 0, \\
    d_t + u \cdot \nabla d - \delta d \cdot \nabla u - L\Delta d + f(d) &= 0,
\end{align*}
\]

where we have set

\[
f(d) := (\psi(|d|^2) - 1) d = \frac{1}{2} \partial_d \left( \hat{\psi}(|d|^2) - |d|^2 \right)
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\text{div} \mathbf{u} &= 0, \\
d_t + \mathbf{u} \cdot \nabla d - \delta d \cdot \nabla \mathbf{u} - L\Delta d + f(d) &= 0,
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Open problems and perspectives

- The study of the long-time behaviour of solutions: there are papers on the non-isothermal simplified model or for the full model in 2D or for large viscosity (cf. [Wu, Xu, Liu, 2010]).
- The complete isothermal 3D model is the subject of a joint work with E. Feiresl, G. Schimperna and H. Petzeltová where we characterize the ω-limit set as a singleton under a number of different conditions (e.g. in case ψ is analytic).
- The study of non-isothermal models for other phases of liquid crystals: in 1888, a botanical physiologist Friedrich Reinitzer (at the Charles University in Prague) examined the physico-chemical properties of various derivatives of cholesterol, known as cholesteric liquid crystals. He found that cholesteryl benzoate has two melting points. At 145.5 °C (293.9 °F) it melts into a cloudy liquid, and at 178.5 °C it melts again and the cloudy liquid becomes clear.
- The study the singular limit of our system with $W_\varepsilon(d) = \frac{1}{\varepsilon^2}(|d|^2 - 1)^2$, where the physically meaningful condition $|d| = 1$ is obtained: non convex problem (cf. [Chen, Math. Z. (1989)] for nematic liquid crystals).
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