Linear spplitting schemes for a nematic-isotropic model with anchoring effects

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Planning

1. Description of the fluid
   - The model
   - The variational formulation
2. Numerical schemes
   - Nematic-Isotropic. Well-Posedness of the Schemes
3. Numerical simulations

Complex Fluids

It will not be possible to decouple the interactions between microscopic and macroscopic effects.

- Fluids with elastic properties. They possesses intermediate properties between solids and liquids.
  Examples: liquid crystals, polymers (macromolecules), ...
- Phase-field models.
  Examples: multi-fluids (mixture of fluids), multi-phases (solidification), ...

These complex materials have practical utilities because the microstructure can be handled in order to produce good mechanical, optical or thermic properties.

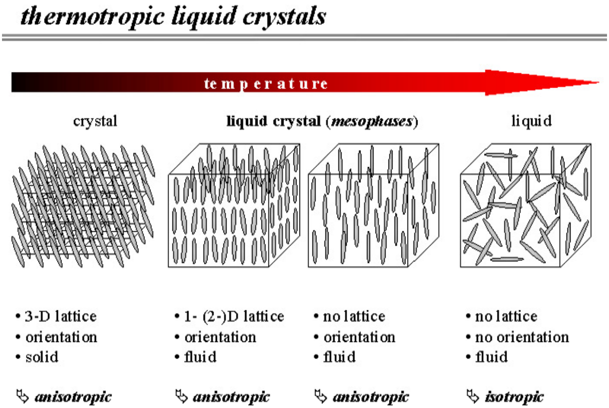


Figure : Types of Liquid Crystals

Types of Liquid Crystals

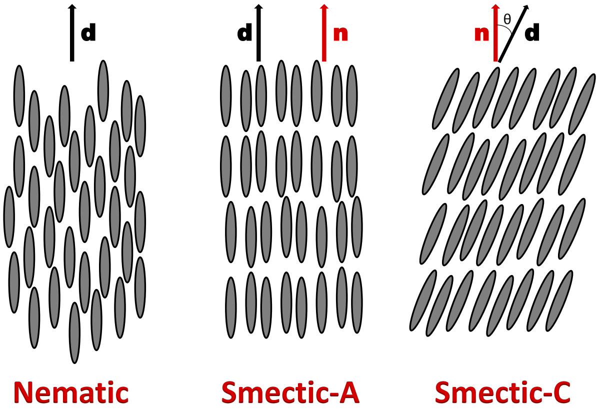
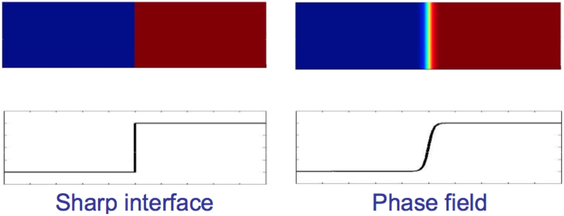


Figure : Types of Liquid Crystals

Phase field or Diffuse interface models



- **Sharp-interface** models
  - PDE for each phase + coupled interface conditions
  - Very difficult numerically (interface tracking)
- **Diffuse interface** Phase-field models
  - Phase function with distinct values (for instance +1 and -1) in each phase, with a smooth change in the interface (of width ε).
  - Surface motion depending on the physical energy dissipation.
  - When interface width ε tends to zero, recover a sharp interface model.

The variables of the problem

The following variable will take part in the description of the model:

- the solenoidal velocity $\mathbf{u}(t, \mathbf{x})$, $t \in (0, T)$, $\mathbf{x} \in \Omega \subset \mathbb{R}^3$
- the pressure of the fluid $p(t, \mathbf{x})$,
- the director field $\mathbf{d}(t, \mathbf{x})$, that represents the average orientation of the liquid crystal molecules,
- the function $c(t, \mathbf{x})$ localizing the two components along the domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) filled by the mixture,

$$c(t, \mathbf{x}) = \begin{cases} -1 & \text{in the Newtonian Fluid part,} \\ \in (-1, 1) & \text{in the interface part,} \\ 1 & \text{in the Nematic Liquid Crystal part.} \end{cases}$$

The total energy

The total energy of the system is given by

$$E_{\text{tot}}(\boldsymbol{u}, \boldsymbol{d}, c) = E_{\text{kin}}(\boldsymbol{u}) + \lambda_{\text{mix}} E_{\text{mix}}(c)$$
$$+\lambda_{\text{nem}} E_{\text{nem}}(\boldsymbol{d}, c) + \lambda_{\text{anch}} E_{\text{anch}}(\boldsymbol{d}, c)$$

The energies

$$E_{\mathrm{kin}}(\boldsymbol{u}) = \frac{1}{2}\int_\Omega |\boldsymbol{u}|^2\,d\boldsymbol{x} \quad \text{kinetic energy},$$

$$E_{\mathrm{mix}}(c) = \int_\Omega \left(\frac{1}{2}|\nabla c|^2 + F(c)\right) d\boldsymbol{x} \quad \text{mixing energy},$$

$$E_{\mathrm{nem}}(\boldsymbol{d}, c) = \int_\Omega I(c)\left(\frac{1}{2}|\nabla \boldsymbol{d}|^2 + G(\boldsymbol{d})\right) d\boldsymbol{x} \quad \text{elastic energy},$$

The double-well potentials

They have their minimums (and consequently their equilibrium states) at ± 1:

$$F(c) = \frac{1}{4\varepsilon^2}(c^2 - 1)^2, \qquad G(\boldsymbol{d}) = \frac{1}{4\eta^2}(|\boldsymbol{d}|^2 - 1)^2,$$

The anchoring effect

At the interface between the nematic and newtonian fluids, liquid crystals prefer to orientate following a certain direction (called as easy direction).

Three effects can be described:

- the parallel case, where all directions are easy,
- the homeotropic case, where the direction is the normal to the interface,
- no anchoring.

The anchoring energy

$$E_{\text{anch}}(\mathbf{d}, c) = \frac{1}{2}\int_\Omega \left(\delta_1\, |\mathbf{d}|^2 |\nabla c|^2 + \delta_2\, |\mathbf{d}\cdot\nabla c|^2\right) dx$$

where the anchoring energy will take different forms depending on the anchoring effect considered, that is,

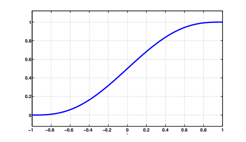
$$(\delta_1, \delta_2) = \begin{cases} (0,0) & \text{no anchoring,} \\ (0,1) & \text{parallel anchoring,} \\ (1,-1) & \text{homeotropic anchoring.} \end{cases} \tag{1}$$

The localizing functional $I(c)$

It represents the volume fraction of liquid crystal at each point $x \in \Omega$ and its derivative will be denoted by $i(c) := I'(c)$. It could take different forms but any admissible form must satisfy the following properties:

$$I \in C^2(\mathbb{R}), \qquad I(c) = \begin{cases} 0 & \text{if } c \le -1, \\ \in (0,1) & \text{if } c \in (-1,1), \\ 1 & \text{if } c \ge 1. \end{cases}$$

$$I(c) := \begin{cases} 0 & \text{if } c \le -1, \\ \dfrac{1}{16}(c+1)^3(3c^2 - 9c + 8) & \text{if } c \in (-1,1), \\ 1 & \text{if } c \ge 1, \end{cases}$$



The model

Combining the Least Action Principle (LAP) and the Maximum Dissipation Principle (MDP), we arrive to the following PDE system, fulfilled in the time space domain $(0, T) \times \Omega$:

$$\left\{ \begin{array}{l} \boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p - \nabla \cdot \sigma_{\mathrm{tot}} = 0, \quad \nabla \cdot \boldsymbol{u} = 0, \\ \boldsymbol{d}_t + (\boldsymbol{u} \cdot \nabla) \boldsymbol{d} + \gamma_{\mathrm{nem}} \boldsymbol{w} = 0, \quad \boldsymbol{w} = \dfrac{\delta E_{\mathrm{tot}}}{\delta \boldsymbol{d}}, \\ c_t + \boldsymbol{u} \cdot \nabla c - \nabla \cdot (\gamma_{\mathrm{mix}} \nabla \mu) = 0, \quad \mu = \dfrac{\delta E_{\mathrm{tot}}}{\delta c}. \end{array} \right. \tag{2}$$

The total stress tensor

$$\sigma_{\rm tot} = \sigma_{\rm vis} + \sigma_{\rm mix} + \sigma_{\rm nem} + \sigma_{\rm anch},$$

being:

$$\begin{aligned} \sigma_{\rm vis} &= 2\nu \boldsymbol{D}\boldsymbol{u} \quad \text{viscosity}, \\ \sigma_{\rm mix} &= -\lambda_{\rm mix} \nabla c \otimes \nabla c \quad \text{mixing tensor}, \\ \sigma_{\rm nem} &= -\lambda_{\rm nem} I(c) (\nabla \boldsymbol{d})^t \nabla \boldsymbol{d} \quad \text{nematic tensor}, \end{aligned}$$

and the anchoring tensor $\sigma_{\rm anch}$ has the form:

$$(\sigma_{\rm anch})_{ij} = \lambda_{\rm anch} \left[\delta_1 \, |\boldsymbol{d}|^2 \, \nabla c \otimes \nabla c + \delta_2 \, (\boldsymbol{d} \cdot \nabla c) \, (\nabla c \otimes \boldsymbol{d}) \right]$$

The expression for w

The variational derivative of E_{tot} with respect to the nematic part, w, is

$$w = \frac{\delta E_{\text{tot}}}{\delta d} = \lambda_{\text{nem}}[-\nabla \cdot (I(c)\nabla d) + I(c)\, G'(d)] + \lambda_{\text{anch}} \frac{\delta E_{\text{anch}}}{\delta d}.$$

The chemical potential of the phase-field function, μ

$$\mu = \frac{\delta E_{\text{tot}}}{\delta c} = \lambda_{\text{mix}}[-\Delta c + F'(c)] + \lambda_{\text{nem}} I'(c) \left(\frac{1}{2}|\nabla d|^2 + G(d)\right) + \lambda_{\text{anch}} \frac{\delta E_{\text{anch}}}{\delta c}.$$

The PDE system (2) is closed with the following initial and boundary conditions:

$$\begin{aligned} &\boldsymbol{u}|_{t=0} = \boldsymbol{u}_0, \quad \boldsymbol{d}|_{t=0} = \boldsymbol{d}_0, \quad c|_{t=0} = c_0 \quad \text{in } \Omega, \\ &\boldsymbol{u}|_{\partial\Omega} = \big(I(c)\nabla \boldsymbol{d}\big)\boldsymbol{n}\big|_{\partial\Omega} = \mathbf{0} \quad \text{in } (0,T), \\ &\left.\frac{\partial c}{\partial \boldsymbol{n}}\right|_{\partial\Omega} = (\nabla \mu)\cdot \boldsymbol{n}|_{\partial\Omega} = 0 \quad \text{in } (0,T). \end{aligned} \tag{3}$$

Reformulation of the stress tensor

The following relation holds:

$$-\nabla \cdot \sigma_{\text{mix}} - \nabla \cdot \sigma_{\text{nem}} - \nabla \cdot \sigma_{\text{anch}} = -\mu \nabla c - (\nabla \boldsymbol{d})^t \boldsymbol{w} + \nabla \varphi$$

where

$$\varphi = \lambda_{\text{nem}} I(c) \left(\frac{1}{2} |\nabla \boldsymbol{d}|^2 + G(\boldsymbol{d}) \right) + \lambda_{\text{mix}} \left(\frac{1}{2} |\nabla c|^2 + F(c) \right) + \frac{\lambda_{\text{anch}}}{2} W(\boldsymbol{d}, c),$$

with $W(\boldsymbol{d}, c) = \left(\delta_1 |\boldsymbol{d}|^2 |\nabla c|^2 + \delta_2 |\boldsymbol{d} \cdot \nabla c|^2 \right)$.

$$\langle \mathbf{u}_t, \bar{\mathbf{u}}\rangle + ((\mathbf{u}\cdot\nabla)\mathbf{u}, \bar{\mathbf{u}}) + (\nu(c)D\mathbf{u}, D\bar{\mathbf{u}}) - (\widetilde{p}, \nabla\cdot\bar{\mathbf{u}})$$

$$- ((\nabla \mathbf{d})^t \mathbf{w}, \bar{\mathbf{u}}) + (c\,\nabla\mu, \bar{\mathbf{u}}) = 0,$$

$$\widetilde{p} = p + \varphi, \qquad (\nabla\cdot\mathbf{u}, \bar{p}) = 0,$$

$$\langle \mathbf{d}_t, \bar{\mathbf{w}}\rangle + ((\mathbf{u}\cdot\nabla)\mathbf{d}, \bar{\mathbf{w}}) + \gamma_{\rm nem}(\mathbf{w}, \bar{\mathbf{w}}) = 0,$$

$$\lambda_{\rm nem}(I(c)\nabla\mathbf{d}, \nabla\bar{\mathbf{d}}) + \lambda_{\rm nem}(I(c)\,\mathbf{g}(\mathbf{d}), \bar{\mathbf{d}}) + \lambda_{\rm anch}\frac{\delta E_{\rm anch}}{\delta \mathbf{d}} = (\mathbf{w}, \bar{\mathbf{d}}),$$

$$(c_t, \bar{\mu}) - (c\,\mathbf{u}, \nabla\bar{\mu}) + \gamma_{\rm mix}(\nabla\mu, \nabla\bar{\mu}) = 0,$$

$$\lambda_{\rm mix}(\nabla c, \nabla\bar{c}) + \lambda_{\rm mix}(f(c), \bar{c})$$

$$+\lambda_{\rm nem}\left(i(c)\left[\frac{|\nabla\mathbf{d}|^2}{2} + G(\mathbf{d})\right], \bar{c}\right) + \lambda_{\rm anch}\frac{\delta E_{\rm anch}}{\delta c} = (\mu, \bar{c}),$$

for each $(\bar{\mathbf{u}}, \bar{p}, \bar{\mathbf{w}}, \bar{\mathbf{d}}, \bar{\mu}, \bar{c}) \in \mathbf{H}_0^1(\Omega)\times L_0^2(\Omega)\times \mathbf{H}^1(\Omega)\times \mathbf{H}^1(\Omega)\times H^1(\Omega)\times H^1(\Omega)$.

Continuous energy law

Using adequate test functions, we can prove that (2)-(3) satisfies the following (dissipative) energy law:

$$\frac{d}{dt}E_{\mathrm{tot}}(\boldsymbol{u}, \boldsymbol{d}, c) + \int_\Omega \nu(c)|\boldsymbol{D}\boldsymbol{u}|^2\, d\boldsymbol{x} + \gamma_{nem}\int_\Omega |\boldsymbol{w}|^2\, d\boldsymbol{x}$$
$$+ \gamma_{mix}\int_\Omega |\nabla \mu|^2\, d\boldsymbol{x} = 0.$$

From the energy law, we deduce the following regularity for a (possible) solution:

$$\left\{\begin{array}{l} \boldsymbol{u} \in L^\infty(0,T;\mathbf{L}^2(\Omega)) \cap L^2(0,T;\mathbf{H}^1(\Omega)),\\ \boldsymbol{w} \in L^2(0,T;\mathbf{L}^2(\Omega)),\\ \nabla c \in L^\infty(0,T;\mathbf{L}^2(\Omega)),\\ \nabla \mu \in L^2(0,T;\mathbf{L}^2(\Omega)),\\ \displaystyle\int_\Omega F(c)d\boldsymbol{x} \in L^\infty(0,T),\\ \displaystyle\int_\Omega I(c)\left(\frac{1}{2}|\nabla \boldsymbol{d}|^2 + G(\boldsymbol{d})\right)d\boldsymbol{x} \in L^\infty(0,T)\\ E_{anch}(c,\boldsymbol{d}) \in L^\infty(0,T),\\ c \in L^\infty(0,T;H^1(\Omega)),\\ \displaystyle\int_\Omega I(c)\,|\boldsymbol{d}|^4 \in L^\infty(0,T),\\ \boldsymbol{d} \in L^\infty(0,T;\mathbf{L}^2(\Omega)). \end{array}\right. \tag{4}$$

For simplicity, we describe our numerical scheme using an uniform partition of the time interval: $t_n = nk$, where $k > 0$ denotes the (fixed) time step. Moreover, hereafter we denote

$$\delta_t a^{n+1} := \frac{a^{n+1} - a^n}{k}.$$

The concept of energy-stability, introduced for other energy-based systems by F. Guillén-González & Tierra

A numerical scheme is energy-stable if it satisfies

$$\delta_t E_{\rm tot}(\boldsymbol{u}^{n+1}, \boldsymbol{d}^{n+1}, c^{n+1}) + \int_\Omega \nu(c^{n+1})|\boldsymbol{D}\boldsymbol{u}^{n+1}|^2\,dx$$
$$+\gamma_{\rm nem}\int_\Omega |\boldsymbol{w}^{n+1}|^2\,dx + \gamma_{\rm mix}\int_\Omega |\nabla \mu^{n+1}|^2\,dx \le 0, \quad \forall n.$$

In particular, energy-stable schemes satisfy the energy decreasing in time property, i.e.,

$$E_{\rm tot}(\boldsymbol{u}^{n+1}, \boldsymbol{d}^{n+1}, c^{n+1}) \le E_{\rm tot}(\boldsymbol{u}^{n}, \boldsymbol{d}^{n}, c^{n}), \quad \forall n.$$

Nematic-Isotropic. Coupled Nonlinear Implicit Scheme

Given $(u^n, p^n, d^n, w^n, c^n, \mu^n)$, find $(u^{n+1}, p^{n+1}, d^{n+1}, w^{n+1}, c^{n+1}, \mu^{n+1})$ such that,

$$\begin{aligned}
\left(\frac{u^{n+1}-u^n}{k}, \bar{u}\right) + \left((u^{n+1}\cdot\nabla)u^{n+1}, \bar{u}\right) - (p^{n+1}, \nabla\cdot\bar{u}) + 2(\nu D u^{n+1}, D\bar{u}) \\
- \left((\nabla d^{n+1})^t w^{n+1}, \bar{u}\right) + (c^{n+1}\,\nabla\mu^{n+1}, \bar{u}) = 0\,, \\
(\nabla\cdot u^{n+1}, \bar{p}) = 0\,, \\
\left(\frac{d^{n+1}-d^n}{k}, \bar{w}\right) + \left((u^{n+1}\cdot\nabla)d^{n+1}, \bar{w}\right) + \gamma_{nem}(w^{n+1}, \bar{w}) = 0\,, \\
\lambda_{nem}(I(c^{n+1})\nabla d^{n+1}, \nabla\bar{d}) + \lambda_{nem}(I(c^{n+1})\, g(d^{n+1}), \bar{d}) + \lambda_{anch}\left(\frac{\delta E_{anch}}{\delta d}(c^{n+1}, d^{n+1}), \bar{d}\right) - (w^{n+1}, \bar{d}) = 0\,, \\
\left(\frac{c^{n+1}-c^n}{k}, \bar{\mu}\right) - (c^{n+1}\, u^{n+1}, \nabla\bar{\mu}) + \gamma_{mix}(\nabla\mu^{n+1}, \nabla\bar{\mu}) = 0\,, \\
\lambda_{mix}(\nabla c^{n+1}, \nabla\bar{c}) + \lambda_{mix}(f(c^{n+1}), \bar{c}) + \lambda_{nem}\left(i(c^{n+1})\left[\frac{|\nabla d^{n+1}|^2}{2} + G(d^{n+1})\right], \bar{c}\right) \\
+\lambda_{anch}\left(\frac{\delta E_{anch}}{\delta c}(c^{n+1}, d^{n+1}), \bar{c}\right) - (\mu^{n+1}, \bar{c}) = 0\,,
\end{aligned} \tag{5}$$

Disadvantages of this scheme:

- High computational cost (Coupled + Nonlinear system)
- it is not clear that any iterative method to approximate the nonlinear scheme will converge(several nonlinearities)
- Energy-stability ?

The splitting schemes

We have designed two splitting first-order schemes (inspired in Cabrales, Guillén-González & Gutiérrez-Santacreu and Guillén-González & Tierra, denoted by

$$(\boldsymbol{d}^{n+1}, \boldsymbol{w}^{n+1}) \quad \to \quad (c^{n+1}, \mu^{n+1}) \quad \to \quad (\boldsymbol{u}^{n+1}, p^{n+1}),$$

or

$$(c^{n+1}, \mu^{n+1}) \quad \to \quad (\boldsymbol{d}^{n+1}, \boldsymbol{w}^{n+1}) \quad \to \quad (\boldsymbol{u}^{n+1}, p^{n+1}),$$

decoupling computations for nematic part $(\boldsymbol{d}, \boldsymbol{w})$ from the phase-field part (c, μ) (or the contrary in the second case) and from the fluid part $(\boldsymbol{u}, p)$.

Step 1: Find $(\boldsymbol{d}^{n+1}, \boldsymbol{w}^{n+1}) \in \boldsymbol{D}_h \times \boldsymbol{W}_h$ s. t, for each $(\bar{\boldsymbol{d}}, \bar{\boldsymbol{w}}) \in \boldsymbol{D}_h \times \boldsymbol{W}_h$

$$\left\{ \begin{aligned} &\left(\frac{\boldsymbol{d}^{n+1}-\boldsymbol{d}^n}{k}, \bar{\boldsymbol{w}}\right) + ((\boldsymbol{u}^\star \cdot \nabla)\boldsymbol{d}^n, \bar{\boldsymbol{w}}) + \gamma_{\rm nem}(\boldsymbol{w}^{n+1}, \bar{\boldsymbol{w}}) = 0, \\ &\lambda_{\rm nem}\left(I(c^n)\nabla \boldsymbol{d}^{n+1}, \nabla \bar{\boldsymbol{d}}\right) + \lambda_{\rm nem}\left(I(c^n)\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n), \bar{\boldsymbol{d}}\right) \\ &+\lambda_{\rm anch}\left(\Lambda_{\boldsymbol{d}}(\boldsymbol{d}^{n+1}, c^n), \bar{\boldsymbol{d}}\right) - (\boldsymbol{w}^{n+1}, \bar{\boldsymbol{d}}) = 0, \end{aligned} \right.$$

$$\text{where} \qquad \boldsymbol{u}^\star := \boldsymbol{u}^n + 2\,k\,(\nabla \boldsymbol{d}^n)^t\,\boldsymbol{w}^{n+1},$$

$\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n)$ is a 1st order approximation of $\boldsymbol{g}(\boldsymbol{d}(t_{n+1}))$ and $\Lambda_{\boldsymbol{d}}(\boldsymbol{d}^{n+1}, c^n)$ is the discrete approximation of $\frac{\delta E_{\rm anch}}{\delta \boldsymbol{d}}(\boldsymbol{d}(t_{n+1}), c(t_{n+1}))$:

$$\Lambda_{\boldsymbol{d}}(\boldsymbol{d}^{n+1}, c^n) := \delta_1\,|\nabla c^n|^2\,\boldsymbol{d}^{n+1} + \delta_2\,(\boldsymbol{d}^{n+1}\cdot\nabla c^n)\,\nabla c^n$$

Step 2: Find $(c^{n+1}, \mu^{n+1}) \in C_h \times M_h$ s. t., for $(\bar{c}, \bar{\mu}) \in C_h \times M_h$

$$
\left\{
\begin{aligned}
&\left(\frac{c^{n+1} - c^n}{k}, \bar{\mu}\right) - (c^n \boldsymbol{u}^{\star\star}, \nabla \bar{\mu}) + \gamma_{\mathrm{mix}}(\nabla \mu^{n+1}, \nabla \bar{\mu}) = 0, \\
&\lambda_{\mathrm{mix}}(\nabla c^{n+1}, \nabla \bar{c}) + \lambda_{\mathrm{mix}}(f_k(c^{n+1}, c^n), \bar{c}) \\
&+\lambda_{\mathrm{nem}} \left(i_k(c^{n+1}, c^n) \left[\frac{1}{2} |\nabla \boldsymbol{d}^{n+1}|^2 + G(\boldsymbol{d}^{n+1}) \right], \bar{c} \right) \\
&+\lambda_{\mathrm{anch}} \left(\Lambda_c(\boldsymbol{d}^{n+1}, c^{n+1}), \nabla \bar{c} \right) - (\mu^{n+1}, \bar{c}) = 0,
\end{aligned}
\right.
$$

where $\boldsymbol{u}^{\star\star} := \boldsymbol{u}^n - 2\,k\,c^n \nabla \mu^{n+1}$,

$f_k(c^{n+1}, c^n)$ and $i_k(c^{n+1}, c^n)$ are 1st order approximations of $f(c(t_{n+1}))$ and $i(c(t_{n+1}))$, resp., $\Lambda_c(\boldsymbol{d}^{n+1}, c^{n+1})$ is the discrete approximation of $\dfrac{\delta E_{\mathrm{anch}}}{\delta c}(\boldsymbol{d}(t_{n+1}), c(t_{n+1}))$:

$$
\Lambda_c(\boldsymbol{d}^{n+1}, c^{n+1}) := \delta_1 \, |\boldsymbol{d}^{n+1}|^2 \, \nabla c^{n+1} + \delta_2 \, (\boldsymbol{d}^{n+1} \cdot \nabla c^{n+1}) \, \boldsymbol{d}^{n+1}
$$

Step 3: Find $(\boldsymbol{u}^{n+1}, p^{n+1}) \in \boldsymbol{V}_h \times P_h$ s. t., for each $(\bar{\boldsymbol{u}}, \bar{p}) \in \boldsymbol{V}_h \times P_h$

$$\begin{cases} \left(\dfrac{\boldsymbol{u}^{n+1} - \widehat{\boldsymbol{u}}}{k}, \bar{\boldsymbol{u}}\right) + c(\boldsymbol{u}^n, \boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}) - (p^{n+1}, \nabla \cdot \bar{\boldsymbol{u}}) \\ \qquad + (\nu(c^{n+1}) \boldsymbol{D} \boldsymbol{u}^{n+1}, \boldsymbol{D} \bar{\boldsymbol{u}}) = 0, \\ (\nabla \cdot \boldsymbol{u}^{n+1}, \bar{p}) = 0, \end{cases}$$

where

$$\widehat{\boldsymbol{u}} := \frac{\boldsymbol{u}^{\star} + \boldsymbol{u}^{\star\star}}{2}.$$

Local (in time) discrete energy law:

Scheme given by **Step1-3** satisfies the following local discrete energy law:

$$
\begin{aligned}
&\delta_t E(\mathbf{d}^{n+1}, c^{n+1}, \mathbf{u}^{n+1}) + \gamma_{\text{nem}} \|\mathbf{w}^{n+1}\|_{L^2}^2 \\
&\quad + \gamma_{\text{mix}} \|\nabla \mu^{n+1}\|_{L^2}^2 + \|\nu(c^{n+1})^{1/2} \mathbf{D}\mathbf{u}^{n+1}\|_{L^2}^2 \\
&\quad + ND_{\mathbf{u}}^{n+1} + ND_{\text{elast}}^{n+1}(c^n) + ND_{\text{penal}}^{n+1}(c^n) \\
&\quad + ND_{\text{philic}}^{n+1} + ND_{\text{phobic}}^{n+1} + ND_{\text{interp}}^{n+1} + ND_{\text{anch}}^{n+1} = 0
\end{aligned}
$$

The numerical dissipation terms are:

$$ND_{\mathbf{u}}^{n+1} = \frac{1}{2k}\left(\|\mathbf{u}^{n+1} - \widehat{\mathbf{u}}\|_{L^2}^2 + \frac{\|\widehat{\mathbf{u}} - \mathbf{u}^{\star}\|_{L^2}^2 + \|\widehat{\mathbf{u}} - \mathbf{u}^{\star\star}\|_{L^2}^2}{2} + \frac{\|\mathbf{u}^{\star} - \mathbf{u}^{n}\|_{L^2}^2 + \|\mathbf{u}^{\star\star} - \mathbf{u}^{n}\|_{L^2}^2}{2} \right)$$

$$ND_{\rm elast}^{n+1}(c^n) = \lambda_{\rm nem}\,\frac{k}{2}\int_\Omega i(c^n)\left|\delta_t \nabla \mathbf{d}^{n+1}\right|^2 d\mathbf{x},$$

$$ND_{\rm penal}^{n+1}(c^n) = \lambda_{\rm nem}\int_\Omega i(c^n)\left(\mathbf{g}_k(\mathbf{d}^{n+1},\mathbf{d}^n)\cdot\delta_t \mathbf{d}^{n+1} - \delta_t G(\mathbf{d}^{n+1})\right) d\mathbf{x},$$

$$ND_{\rm philic}^{n+1} = \lambda_{\rm mix}\,\frac{k}{2}\int_\Omega \left|\delta_t \nabla c^{n+1}\right|^2 d\mathbf{x},$$

$$ND_{\rm phobic}^{n+1} = \lambda_{\rm mix}\int_\Omega \left(f_k(c^{n+1},c^n)\,\delta_t c^{n+1} - \delta_t F(c^{n+1})\right) d\mathbf{x},$$

$$ND^{n+1}_{\mathrm{interp}} = \lambda_{\mathrm{nem}} \int_\Omega \left(\frac{|\nabla \boldsymbol{d}^{n+1}|^2}{2} + G(\boldsymbol{d}^{n+1}) \right) \times \left(i_k(c^{n+1}, c^n)\, \delta_t c^{n+1} - \delta_t I(c^{n+1}) \right) d\boldsymbol{x},$$

and

$$ND^{n+1}_{\mathrm{anch}} = \lambda_{\mathrm{anch}} \frac{k}{2} \int_\Omega \Big(\delta_1 \left(|\delta_t \boldsymbol{d}^{n+1}|^2 |\nabla c^n|^2 + |\boldsymbol{d}^{n+1}|^2 |\delta_t \nabla c^{n+1}|^2 \right) + \delta_2 \left(|\delta_t \boldsymbol{d}^{n+1} \cdot \nabla c^n|^2 + |\boldsymbol{d}^{n+1} \cdot \nabla \delta_t c^{n+1}|^2 \right) \Big) d\boldsymbol{x}.$$

with (δ_1, δ_2) defined in (1) depending on the type of anchoring.

The function f_k

$$f_k(c^{n+1}, c^n) := \widetilde{f}(c^n) + \frac{1}{2}\,\|\widetilde{f}'\|_\infty\,(c^{n+1} - c^n),$$

in our case reduces to

$$f_k(c^{n+1}, c^n) = \widetilde{f}(c^n) + (c^{n+1} - c^n) \tag{6}$$

where $\widetilde{f}(c)$ is the C^1-truncation of $F'(c)$:

$$\widetilde{f}(c) = \begin{cases} \dfrac{2}{\varepsilon^2}(c+1) & \text{if } c \le -1, \\ \dfrac{1}{\varepsilon^2}(c^2-1)\,c & \text{if } c \in [-1,1], \\ \dfrac{2}{\varepsilon^2}(c-1) & \text{if } c \ge 1, \end{cases} \tag{7}$$

The function g_k

$$g_k(d^{n+1}, d^n) = \widetilde{g}(d^n) + \frac{\sqrt{51}}{2}\,(d^{n+1} - d^n), \tag{8}$$

where $\widetilde{g}(d)$ is the C^1-truncation of $g(d)$:

$$\widetilde{g}(d) = \begin{cases} 2\,(|d| - 1)\,\dfrac{d}{|d|} & \text{if } |d| \geq 1, \\ (|d|^2 - 1)\,d & \text{if } |d| \leq 1, \end{cases}$$

The function i_k

$$i_k(c^{n+1}, c^n) = i(c^n) + \frac{5\sqrt{3}}{12}\,(c^{n+1} - c^n). \tag{9}$$

Lemma

If $\mathbf{D}_h \subseteq \mathbf{W}_h$, then there exist a unique solution $(\mathbf{d}^{n+1}, \mathbf{w}^{n+1})$ of ***STEP 1*** *using the potential approximation (8) for $\mathbf{g}_k(\mathbf{d}^{n+1}, \mathbf{d}^n)$.*

Lemma

If $1 \in C_h$, then there exist a unique solution (c^{n+1}, μ^{n+1}) of ***STEP 2*** *using the potential approximations (6) and (9) for $f_k(c^{n+1}, c^n)$ and $i_k(c^{n+1}, c^n)$, respectively.*

Lemma

If the pair of FE spaces $(\boldsymbol{V}_h, P_h)$ *satisfies the discrete inf-sup condition*

$$\exists\, \beta > 0 \quad \textit{such that} \quad \|p\|_{L^2} \leq \beta \sup_{\bar{\boldsymbol{u}} \in V_h \setminus \{\Theta\}} \frac{(p, \nabla \cdot \bar{\boldsymbol{u}})}{\|\bar{\boldsymbol{u}}\|_{H^1}} \quad \forall\, p \in P_h\,, \tag{10}$$

then there exist a unique solution $(\boldsymbol{u}^{n+1}, p^{n+1})$ *of* ***STEP 3****.*

We propose the following choice for the discrete spaces:

$$(\boldsymbol{u}, p) \sim P_2 \times P_1 \,, \qquad (c, \mu) \sim P_1 \times P_1 \qquad \text{and} \qquad (\boldsymbol{d}, \boldsymbol{w}) \sim P_1 \times P_1 \,, \tag{11}$$

that satisfy the assumptions of Lemmas 1, 2 and 3.

The discrete and physical parameters

The newtonian fluid is represented by blue color while the nematic fluid is represented by red one.
For simplicity we are considering constant viscosity $\nu(c) = \nu_0$.

Ω	$[0, T]$	h	dt	ν_0	η
$[-1, 1]^2$	$[0, 10]$	$2/90$	0.001	1.0	0.075

λ_{nem}	λ_{mix}	λ_{anch}	γ_{nem}	γ_{mix}	ε
0.1	0.01	0.1	0.5	0.01	0.05

Table : Parameters

Nematic-Isotropic. Circular droplet and director field parallel to the y-axis

Circular droplet and director field parallel to the y-axis

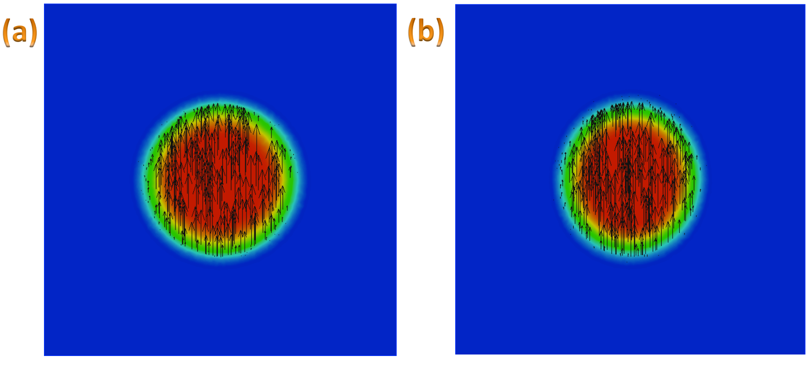


Figure : (a) initial configuration, (b) state at $t = 10$ without considering anchoring effects.

Circular droplet and director field parallel to the y-axis

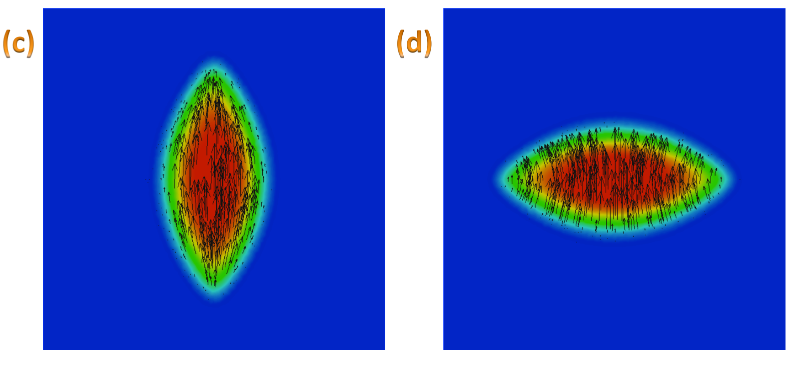
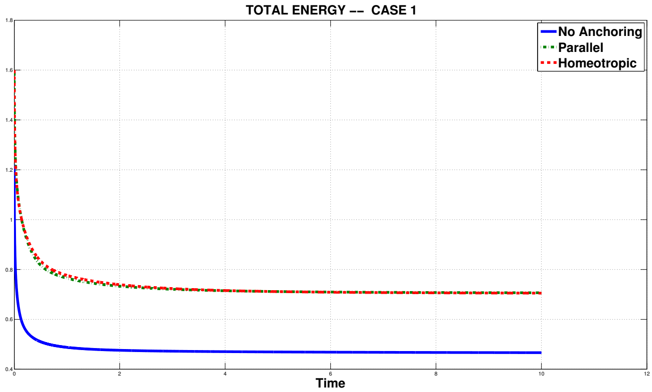


Figure : (c) state at $t = 10$ considering parallel anchoring, (d) state at $t = 10$ considering homeotropic anchoring.

Nematic-Isotropic. Circular droplet and director field parallel to the y-axis



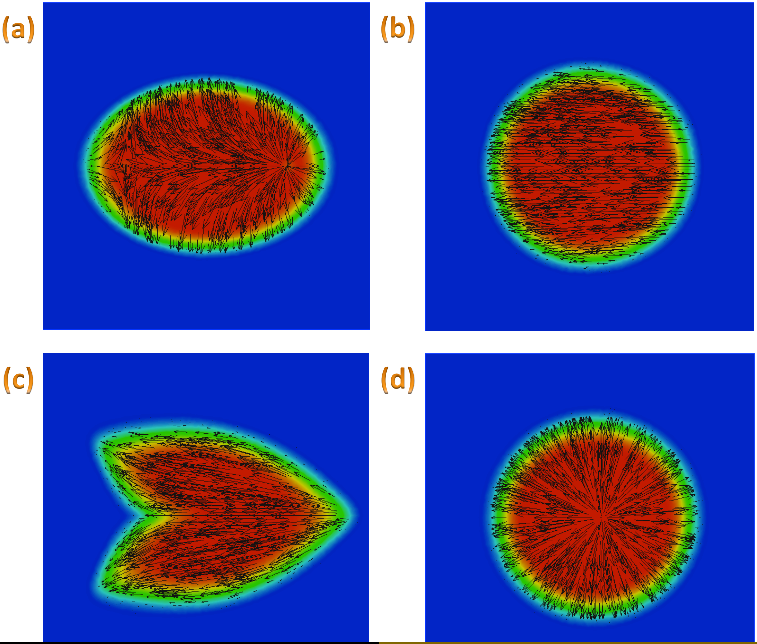
Elliptic droplet with two points defects at $(\pm 1/2, 0)$

a Hedgehog defect at $(1/2, 0)$ and an Antihedgehog defect at $(-1/2, 0)$

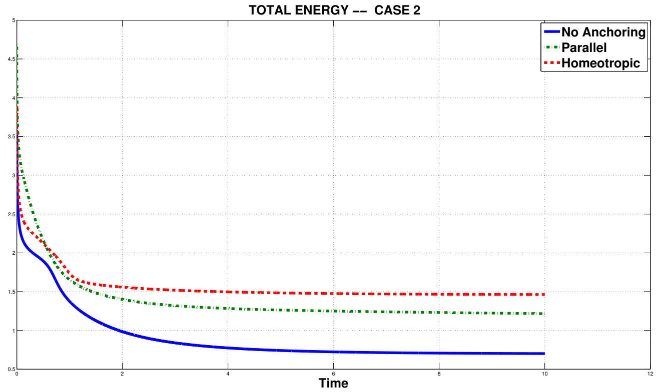
$$d_0(x) = \widehat{d}/\sqrt{|\widehat{d}|^2 + 0.05^2}, \text{ with } \widehat{d} = (x^2 + y^2 - 0.25, y)\,.$$

Defect annihilation in Nematic Liquid Crystals

Defect annihilation in Nematic Liquid Crystals Drops


(a)
(b)
(c)
(d)

Nematic-Isotropic. Circular droplet and director field parallel to the y-axis

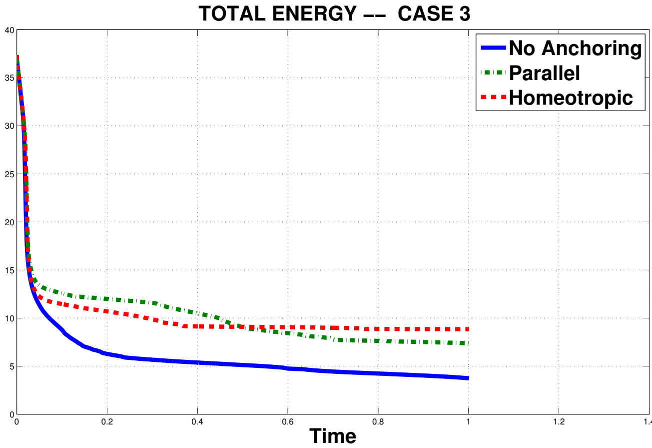


Nematic-Isotropic. Spinodal Decomposition

- Random initial data for c, i.e., $c \in [-10^{-2}, 10^{-2}]$ in $\Omega = [0,1] \times [0,1]$, $t \in [0,1]$ and $dt = 10^{-4}$.
- The initial director vector is computed using the function:

$$\boldsymbol{d} = I(c)\left(\sin(x\,y)\sin(x\,y), \cos(x\,y)\cos(x\,y)\right).$$

Nematic-Isotropic. Spinodal Decomposition



R. C. Cabrales, F. Guillén-González, J. V. Gutiérrez-Santacreu, *A Time-Splitting Finite-Element Stable Approximation for the Ericksen-Leslie Equations*. SIAM J. Sci. Comput. **37** (2015), no. 2, B261–B282.

F. Guillén-González, G. Tierra, *On linear schemes for a Cahn Hilliard diffuse interface model.* J. Comput. Physics **234** (2013), 140-171.

F. Guillén-González, G. Tierra, *Splitting schemes for a Navier-Stokes-Cahn-Hilliard model for two fluids with different densities.* J. Comput. Math. 32 (2014), no. 6, 643–664.

F. Guillén-González, G. Tierra, *Second order schemes and time-step adaptivity for Allen-Cahn and Cahn-Hilliard models.* Computers & Mathematics with Applications **68** (2014), 821-846

Guillén-González F, Rodríguez-Bellido MA, Tierra G. Linear unconditional energy-stable splitting schemes for a phase-field model for nematic-isotropic flows with anchoring effects. *Int. J. Numer. Meth. Engng* 2016;

J. Shen, X. Yang, *Decoupled energy stable schemes for phase field models of two-phase complex fluids.* SIAM J. Sci. Comput. **36** (2014), 122-145.

G. Tierra, F. Guillén-González, 2015 *Numerical methods for solving the Cahn-Hilliard equation and its applicability to related Energy-based models.* Arch. Computat. Methods Eng. **22**, 269-289

X. Yang, M. Forest, H. Li, C. Liu, J. Shen, Q. Wang, F. Chen, *Modeling and simulations of drop pinch-off from liquid crystal filaments and the leaky liquid crystal faucet immersed in viscous fluids. J. Comput. Phys.* **236** (2013), 1–14.

P. Yue, J. J. Feng, C. Liu, J. Shen, *A diffuse-interface method for simulating two-phase flows of complex fluids. J. Fluid Mech.* **515** (2004), 293–317.

P. Yue, J. J. Feng, C. Liu, J. Shen, *Interfacial forces and Marangoni flow on a nematic drop retracting in an isotropic fluid*. *Journal of Colloid and Interface Science* **290** (2005), 281–288.

Acknowledgments

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Thank you very much for your attention!