Numerical methods for solving the Cahn-Hilliard equation and its applicability to mixtures of nematic-isotropic flows with anchoring effects

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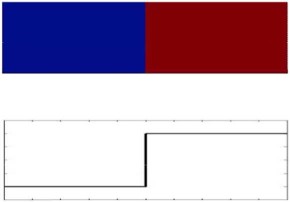
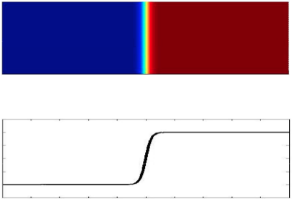
Phase field or Diffuse interface models



Sharp interface



Phase field

- **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.

Motivation

Design numerical schemes for diffuse-interface phase-field problems:

1. Efficient in time (Linear schemes, adaptive time-step).
2. Suitable to use (standard) Finite Elements (mesh adaptation)
3. Mimic properties of the continuous problem: Dissipative Energy law, maximum principle, mass conservation, ...
4. Good finite and large time accuracy (infinite equilibrium states)

Numerical analysis:

1. Large time Energy Stability
2. Unique Solvability of the schemes
3. Convergence of iterative algorithms approximating nonlinear schemes

Allen-Cahn and Cahn-Hilliard models

The **Allen-Cahn** and the **Cahn-Hilliard** models are **gradient flows** for the same **Free Energy** (Liapunov functional):

$$E(\phi) = E_{philic}(\phi) + E_{phobic}(\phi) := \int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + F(\phi) \right) dx$$

where $F(\phi)$ is a **double-well potential** taking two minimum (stable) values:

$F(\phi) = \dfrac{1}{4\varepsilon^2}(\phi^2 - 1)^2$ at $\phi = \pm 1$ (polynomial potential: **Ginzburg-Landau**)

- **Allen-Cahn :** $\phi_t + \gamma \dfrac{\delta E}{\delta \phi} = 0$ $\Rightarrow$ Maximum Principle
- **Cahn-Hilliard:** $\phi_t - \nabla \cdot \left(M(\phi) \nabla \dfrac{\delta E}{\delta \phi} \right) = 0 \Rightarrow$ Mass Conservation

where $\dfrac{\delta E}{\delta \phi} = -\Delta\phi + f(\phi)$ with $f(\phi) = F'(\phi) = \dfrac{1}{\varepsilon^2}(\phi^3 - \phi)$.
In both cases:

$$d_t E(\phi(t)) \leq 0.$$

Weak formulation: Find (ϕ, w) such that

$$\phi \in L^\infty((0,T);H^1(\Omega)) \quad \text{and} \quad w \in L^2((0,T);H^1(\Omega))$$

satisfying

$$\begin{cases} \langle \phi_t, \bar{w} \rangle + \gamma \Big(\nabla w, \nabla \bar{w} \Big) = 0 & \forall\, \bar{w} \in H^1(\Omega) \\ \Big(\nabla \phi, \nabla \bar{\phi} \Big) + \Big(f(\phi), \bar{\phi} \Big) - \Big(w, \bar{\phi} \Big) = 0 & \forall\, \bar{\phi} \in H^1(\Omega). \end{cases}$$

Energy Law:

$$\frac{d}{dt} E(\phi(t)) + \gamma \int_\Omega |\nabla w|^2 dx = 0.$$

Mathematical Analysis: Abels, Garcke, Grasselli, Miranville, Schimperna, ...
Numerical Analysis: Boyer, Elliot, Feng, Gómez, Hughes, Prohl, ...

Generic Second order Finite Difference schemes (Crank-Nicolson for linear terms)

$$\begin{cases} \left(\delta_t\phi^{n+1}, \bar{w}\right) + \gamma\left(\nabla w^{n+\frac{1}{2}}, \nabla \bar{w}\right) = 0 \qquad \forall\, \bar{w} \in H^1(\Omega) \\ \left(\nabla\left(\dfrac{\phi^{n+1}+\phi^n}{2}\right), \nabla\bar{\phi}\right) + \left(f^k(\phi^{n+1},\phi^n), \bar{\phi}\right) - \left(w^{n+\frac{1}{2}}, \bar{\phi}\right) = 0 \;\; \forall\, \bar{\phi} \in H^1(\Omega), \end{cases}$$

where $\delta_t\phi^{n+1} = (\phi^{n+1} - \phi^n)/k$ (discrete time derivative).

Discrete Energy Law: Testing by $(\bar{w}, \bar{\phi}) = (w^{n+\frac{1}{2}}, \delta_t\phi^{n+1})$

$$\delta_t E(\phi^{n+1}) + \gamma\|\nabla w^{n+\frac{1}{2}}\|^2_{L^2} + \cancel{ND_{philic}(\phi^{n+1},\phi^n)} + ND_{phobic}(\phi^{n+1},\phi^n) = 0,$$

where

$$ND_{philic}(\phi^{n+1},\phi^n) := \left(\nabla\left(\frac{\phi^{n+1}+\phi^n}{2}\right), \nabla\delta_t\phi^{n+1}\right) - \delta_t\left(\int_\Omega \frac{1}{2}|\nabla\phi^{n+1}|^2\right) = 0$$

and

$$ND_{phobic}(\phi^{n+1},\phi^n) := \left(f^k(\phi^{n+1},\phi^n), \delta_t\phi^{n+1}\right) - \delta_t\left(\int_\Omega F(\phi^{n+1})\right)$$

Definition

Numerical schemes are energy-stable if

$$\delta_t E(\phi^{n+1}) + \gamma \int_\Omega |\nabla w^{n+\frac{1}{2}}|^2 \leq 0, \quad \forall\, n.$$

In particular, the discrete energy decreases,

$$E(\phi^{n+1}) \leq E(\phi^n), \quad \forall\, n.$$

Eyre's decomposition

[Eyre]
Splitting the potential term

$F(\phi) = F_c(\phi) + F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave)

Taking implicitly the convex term and explicitly the non-convex one, i.e.

$$f^k(\phi^{n+1}, \phi^n) = f_c(\phi^{n+1}) + f_e(\phi^n) = \frac{1}{\varepsilon^2}((\phi^{n+1})^3 - \phi^n),$$

Properties:

- First order accurate
- Nonlinear scheme
- Unconditionally unique solvable
- Unconditionally energy-stable

Midpoint (MP)

Midpoint approximation of the potential term **[Elliot], [Du], [Lin],...**

$$f^k(\phi^{n+1},\phi^n) = \frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n}$$

Then

$$ND_{phobic}(\phi^{n+1},\phi^n) = 0 \quad \Rightarrow \quad \delta_t E(\phi^{n+1}) + \gamma \|\nabla w^{n+\frac{1}{2}}\|^2_{L^2} = 0$$

Properties:

- Second order accurate
- Nonlinear scheme
- Conditionally unique solvable ($k < \varepsilon^4/\gamma$)
- Unconditionally energy-stable

Midpoint (MP). Newton Scheme

Theorem

- *Solvability hypothesis*

$$k < \frac{4\varepsilon^4}{\gamma}$$

- *Convergence hypothesis*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \text{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

[Wang et al.]
Splitting the potential term $F(\phi) = F_c(\phi) + F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave), Taking **MP** for the convex term and **BDF2** for the non-convex:

$$f^k(\phi^{n+1}, \phi^n, \phi^{n-1}) = \frac{F_c(\phi^{n+1}) - F_c(\phi^n)}{\phi^{n+1} - \phi^n} + \frac{1}{2}\Big(3 f_e(\phi^n) - f_e(\phi^{n-1})\Big) .$$

Properties:

- Second order accurate
- Nonlinear scheme
- Unconditionally unique solvable
- Unconditionally energy-stable for a perturbed energy

$$\widetilde{E}(\phi^{n+1}) = E(\phi^{n+1}) + k^2 \int_\Omega \frac{1}{4\varepsilon^2} |\delta_t \phi^{n+1}|^2 dx,$$

Theorem

- *Unconditionally unique solvable*
- *Convergence hypothesis (Idem* **MP***)*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \textit{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

Optimal Dissipation Scheme (OD2)

Aim: Design $f^k(\phi^{n+1},\phi^n)$, linear, second order accurate and

$$ND_{phobic}(\phi^{n+1},\phi^n) = O(k^2)$$

Idea: Using a Hermite quadrature formula,

$$\frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n} = \frac{1}{\phi^{n+1} - \phi^n} \int_{\phi^n}^{\phi^{n+1}} f(\phi) d\phi$$

$$= f(\phi^n) + \frac{f'(\phi^n)}{2}(\phi^{n+1} - \phi^n) + C\, f''(\phi^{n+\zeta})\, (\phi^{n+1} - \phi^n)^2$$

We define

$$f^k(\phi^{n+1},\phi^n) := f(\phi^n) + \frac{1}{2}(\phi^{n+1} - \phi^n) f'(\phi^n)$$

Properties:

- Second order
- Linear scheme
- Conditionally solvable ($k < 8\varepsilon^4/\gamma$)

Remark: We can not control the sign of $ND_{phobic}(\phi^{n+1},\phi^n)$

Splitting the potential term $F(\phi) = F_c(\phi) + F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave), **OD2** approximation of the convex term and **BDF2** the non-convex one,

$$f^k(\phi^{n+1}, \phi^n, \phi^{n-1}) = f_c(\phi^n) + \frac{1}{2}(\phi^{n+1} - \phi^n) f_c'(\phi^n) + \frac{1}{2}\left(3 f_e(\phi^n) - f_e(\phi^{n-1})\right).$$

Properties:

- Second order
- Linear scheme
- Unconditionally solvable

Remark: We can not control the sign of $ND_{phobic}(\phi^{n+1}, \phi^n)$

Time step adaptivity.

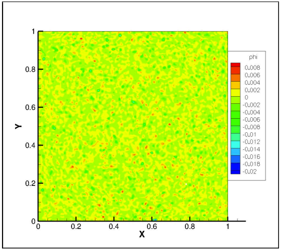
We have developed a new adaptive-in-time algorithm by using a criterion related to the 'residual energy law'.

Generic Algorithm:

Given $\phi^n, \phi^{n-1}, dt^{n-1}$, dt^n, **resmax** and **resmin**:

1. Compute ϕ^{n+1} and
$$RE^{n+1} := \frac{E(\phi^{n+1}) - E(\phi^n)}{dt^n} + \|\nabla w^{n+1/2}\|^2_{L^2}.$$
2. If $|RE^{n+1}| > $ **resmax**, take $dt^n = dt^n/\theta$ and go to 1). $(\theta > 1)$
3. If $|RE^{n+1}| < $ **resmin**, take $dt^{n+1} = \theta dt^n$.
4. Take $t^{n+1} = t^n + dt^n$ and go to next time step.

- $\mathcal{P}_1$-cont. FE for ϕ_h, w_h.
- $\Omega = [0,1]^2$, $h = 1/90$, $\gamma = 10^{-4}$, $\varepsilon = 10^{-2}$, **resmax** $= 10$ and **resmin** $= 1$.
- In Newton's method, a tolerance parameter $tol = 10^{-3}$. The time-step is reduced in the case that the method does not converge in 10 iterations.
- Random initial data (the same for all the schemes).



Numerical Simulations. Dynamic

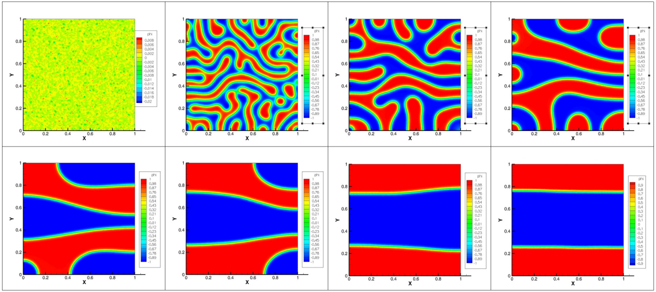


Figura: Dynamic of the model for the random initial condition

Mixing energy

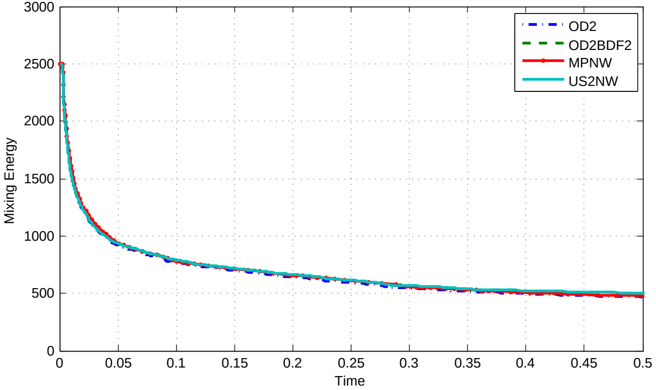


Figura: Mixing energy in [0, 0.5]

Mixing energy

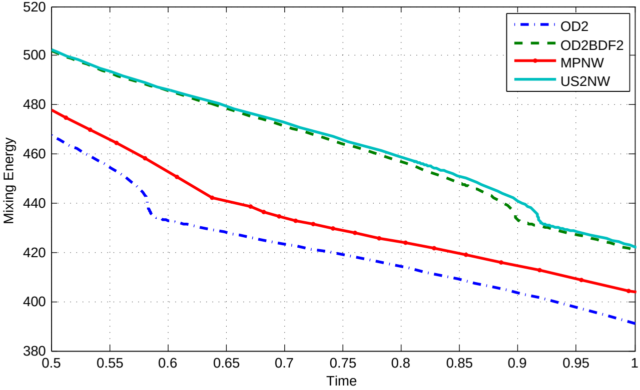


Figura: Mixing energy in [0.5, 1]

Mixing energy

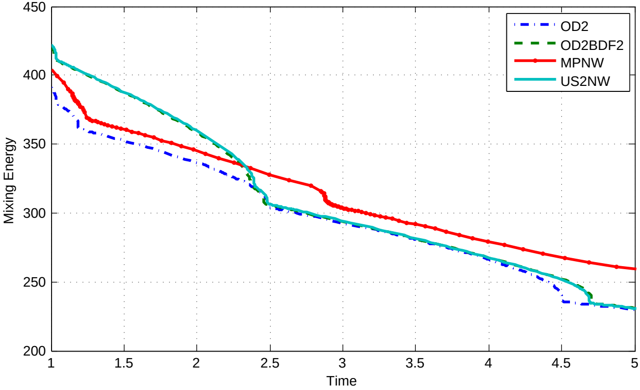


Figura: Mixing energy in [1, 5]

Mixing energy

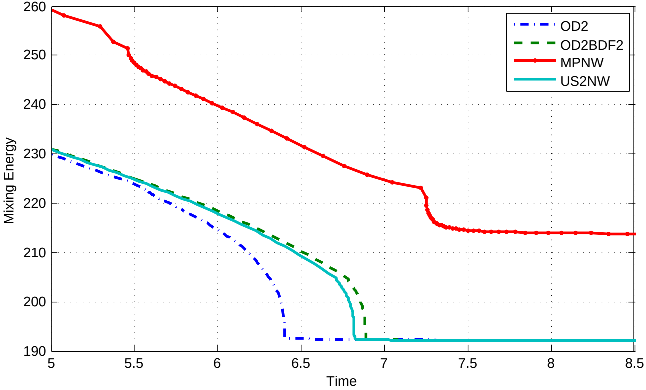


Figura: Mixing energy in [5, 8.5]

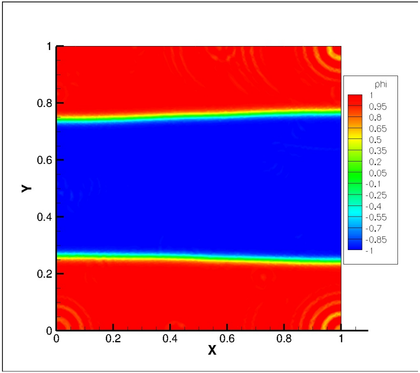


Figura: Equilibrium solution of MP

Time steps

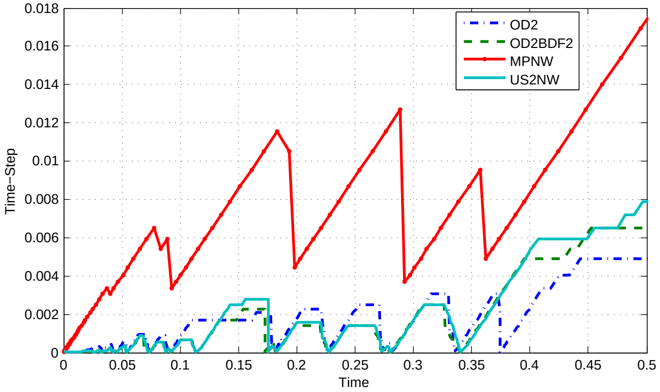


Figura: Time steps in [0, 0.5]

Time steps

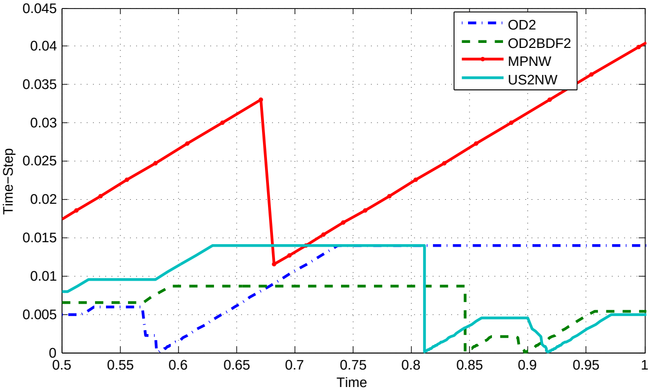


Figura: Time steps in [0.5, 1]

Time steps

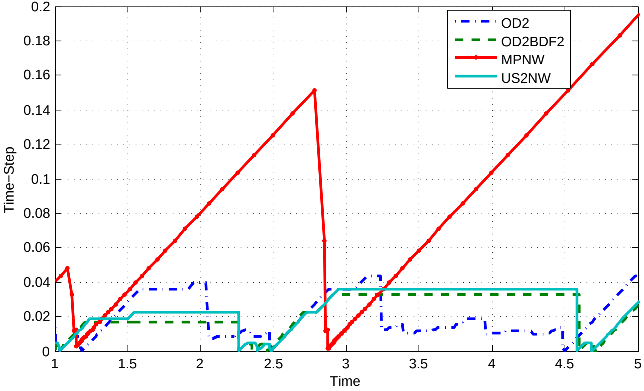


Figura: Time steps in [1, 5]

Time steps

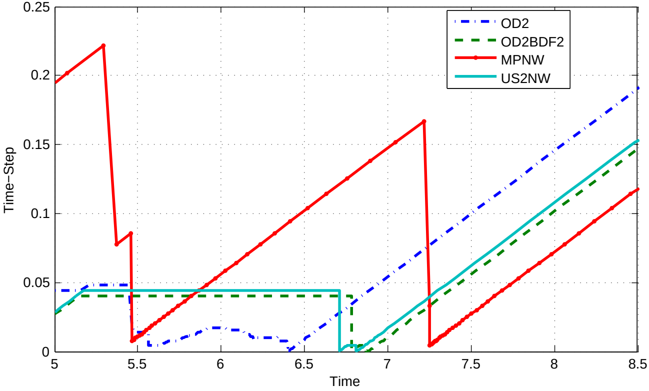


Figura: Time steps in [5, 8.5]

Time steps

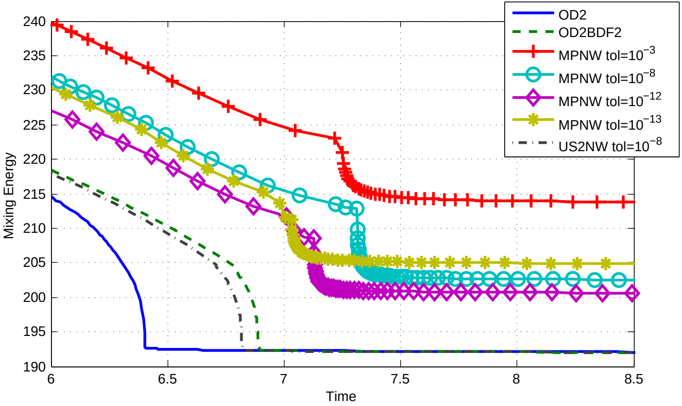


Figura: Mixing energy in [6, 8.5]

Computational cost:

	MP	OD2	OD2-BDF2	US2
# Time steps	339	2642	4340	3691
# Linear systems solved	3896	3533	5687	12812

(**OD2** with constant time step $k = 10^{-4} \Rightarrow \simeq$ 80000 iterations)

Conclusions:

	MP	OD2	OD2-BDF2	US2	LM2
Linear	X	✓	✓	X	✓
Unconditionally Unique Solvable	X	X	✓	✓	✓
Conditionally Unique Solvable	✓	✓			
Unconditionally Energy-Stable $E(\phi)$	✓	X	X	X	X
Uncond. (Modified-Energy)-Stable $\widetilde{E}(\phi)$		X	X	✓	✓
One-Step Algorithm	✓	✓	X	X	X
Time-step Adaptivity	X	✓	✓	✓	X

Figura: Features of schemes

$3D$ Numerical Simulations.

- **OD2** time scheme.
- Finite element discretization in space, with ϕ_h and w_h in $\mathcal{P}_1$-cont. FE
- $\Omega = [0, 1]^3$, $h = 1/30$, $\gamma = 10^{-4}$, $\varepsilon = 10^{-2}$, **resmax** $= 10$ and **resmin** $= 1$.
- Random initial data.

View I

View II

LINEAR UNCONDITIONAL ENERGY-STABLE SPLITTING SCHEMES FOR A PHASE-FIELD MODEL FOR NEMATIC-ISOTROPIC FLOWS WITH ANCHORING EFFECTS

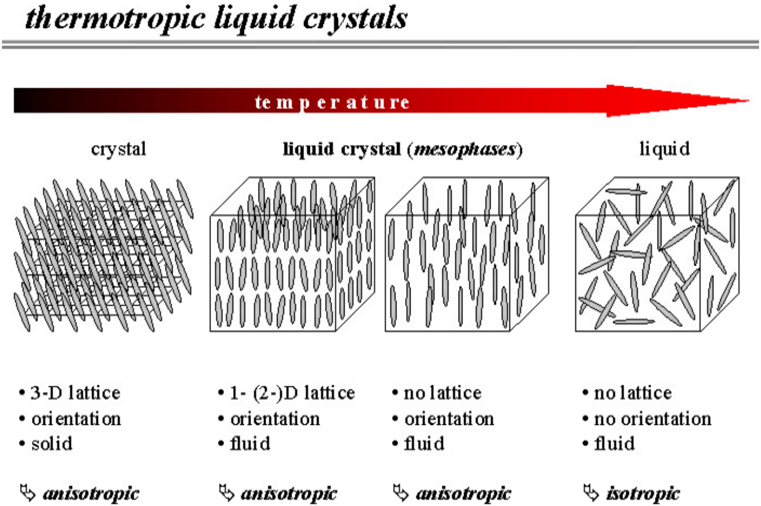


Figura: Types of Liquid Crystals

Types of Liquid Crystals

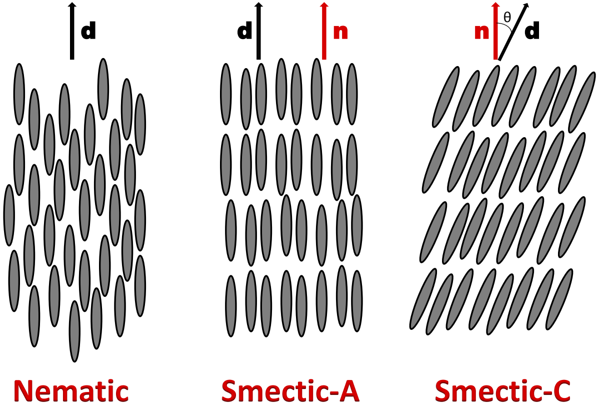


Figura: Types of Liquid Crystals

Nematic Liquid Crystals

Ginzburg-Landau formulation (penalized version of Ericksen-Leslie system):

$$\left\{\begin{array}{l} \boldsymbol{u}_t + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p - \nabla\cdot\sigma_{\rm vis} - \nabla\cdot\sigma_{\rm nem} = 0, \\ \nabla\cdot\boldsymbol{u} = 0\,, \\ \boldsymbol{d}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{d} + \gamma_{\rm nem}\boldsymbol{w} = 0\,, \\ \boldsymbol{w} = \frac{\delta E_{\rm nem}}{\delta \boldsymbol{d}}\,, \end{array}\right. \tag{1}$$

where $(\delta\cdot/\delta\boldsymbol{d})$ denotes the variational derivative with respect to $\boldsymbol{d}$, $\gamma_{nem} > 0$ is the relaxation time coefficient,

$$\begin{array}{rcl} \sigma_{\rm vis} & = & 2\nu\boldsymbol{D}\boldsymbol{u}\,, \\ \sigma_{\rm nem} & = & -\lambda_{\rm nem}(\nabla\boldsymbol{d})^t\nabla\boldsymbol{d}\,, \end{array}$$

and

$$E_{\rm nem}(\boldsymbol{d}) = \int_\Omega \left(\frac{1}{2}|\nabla\boldsymbol{d}|^2 + G(\boldsymbol{d})\right)\,d\boldsymbol{x} \qquad \text{with} \qquad G(\boldsymbol{d}) = \frac{1}{4\eta^2}(|\boldsymbol{d}|^2-1)^2\,.$$

It is known that this system satisfies the following energy law,

$$\frac{d}{dt}\left[E_{kin}(\boldsymbol{u}) + \lambda_{nem}E_{nem}(\boldsymbol{d})\right] + 2\int_\Omega \nu|\boldsymbol{D}\boldsymbol{u}|^2 d\boldsymbol{x} + \lambda_{nem}\int_\Omega \gamma_{nem}\left|\frac{\delta E_{nem}}{\delta\boldsymbol{d}}\right|^2 d\boldsymbol{x} = 0\,.$$

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,

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

Nematic-Isotropic. Energy

The total energy of the system is given by

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

with

$$\begin{aligned} E_{\text{kin}}(\boldsymbol{u}) &= \frac{1}{2}\int_\Omega |\boldsymbol{u}|^2 \, d\boldsymbol{x} \quad \text{kinetic energy}, \\ E_{\text{mix}}(c) &= \int_\Omega \left(\frac{1}{2}|\nabla c|^2 + F(c)\right) d\boldsymbol{x} \quad \text{mixing energy}, \\ E_{\text{nem}}(\boldsymbol{d}, c) &= \int_\Omega I(c)\left(\frac{1}{2}|\nabla \boldsymbol{d}|^2 + G(\boldsymbol{d})\right) d\boldsymbol{x} \quad \text{elastic energy}, \end{aligned}$$

where

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

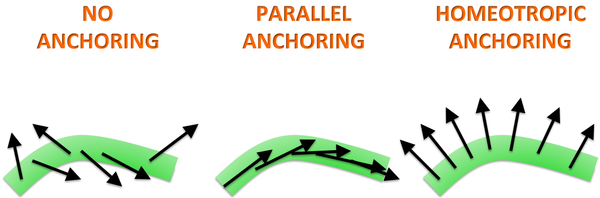
and we represent their derivatives as $f(c) := F'(c)$ and $\boldsymbol{g}(\boldsymbol{d}) := G'(\boldsymbol{d})$.

Nematic-Isotropic. 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 the director vector is parallel to the interface,
- the homeotropic case, where the director vector is normal to the interface,
- no anchoring.



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

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

$$(\delta_1, \delta_2) = \begin{cases} (0,0) & \text{no anchoring,} \\ (0,1) & \text{parallel anchoring,} \\ (1,-1) & \text{homeotropic anchoring.} \end{cases} \qquad (2)$$

Nematic-Isotropic. 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:

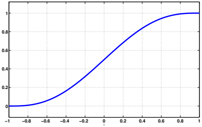
- $I \in C^2(\mathbb{R})$,
- $I(c) = 0$ if $c \leq -1$,
- $I(c) = 1$ if $c \geq 1$,
- $I(c) \in (0,1)$ if $c \in (-1,1)$.

We consider the following interpolation function

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

and its derivative is defined as

$$i(c) := I'(c) = \begin{cases} \dfrac{15}{16}\,(c+1)^2\,(c-1)^2 & \text{if } c \in (-1,1)\,, \\ 0 & \text{otherwise}\,. \end{cases}$$



Nematic-Isotropic. 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 $(0, T) \times \Omega$:

$$\begin{cases} \boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p - \nabla \cdot \sigma_{\text{tot}} = 0, \\ \nabla \cdot \boldsymbol{u} = 0, \\ \boldsymbol{d}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{d} + \gamma_{\text{nem}} \boldsymbol{w} = 0, \\ \boldsymbol{w} = \frac{\delta E_{\text{tot}}}{\delta \boldsymbol{d}}, \\ c_t + \boldsymbol{u} \cdot \nabla c - \nabla \cdot (\gamma_{\text{mix}} \nabla \mu) = 0, \\ \mu = \frac{\delta E_{\text{tot}}}{\delta c}. \end{cases} \tag{3}$$

Nematic-Isotropic. The total stress tensor

The total tensor reads,

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

being:

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

and the anchoring tensor σ_{anch} has the form:

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

Nematic-Isotropic. The expression for w and μ

Taking into account that the total energy of the system is given by

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

then the variational derivatives of $E_{\rm tot}$ are

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

and

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

where the anchoring terms will depend on each case:

$$\frac{\delta E_{anch}}{\delta \boldsymbol{d}} = \begin{cases} 0 & \text{No anchoring}\,, \\ (\boldsymbol{d}\cdot\nabla c)\,\nabla c & \text{Parallel anch.}\,, \\ |\nabla c|^2 \boldsymbol{d} - (\boldsymbol{d}\cdot\nabla c)\,\nabla c & \text{Homeotropic anch.}\,. \end{cases} \tag{4}$$

and

$$\frac{\delta E_{anch}}{\delta c} = \begin{cases} 0 & \text{No anchoring}\,, \\ -\nabla\cdot[(\boldsymbol{d}\cdot\nabla c)\,\boldsymbol{d}] & \text{Parallel anch.}\,, \\ -\nabla\cdot[|\boldsymbol{d}|^2\nabla c - (\boldsymbol{d}\cdot\nabla c)\,\boldsymbol{d}] & \text{Homeotropic anch.} \end{cases} \tag{5}$$

Nematic-Isotropic. The model

The PDE system (3) is closed with the following initial and boundary conditions:

$$\begin{aligned}
&\boldsymbol{u}|_{t=0} = \boldsymbol{u}_0, \quad \boldsymbol{d}|_{t=0} = \boldsymbol{d}_0, \quad c|_{t=0} = c_0 && \text{in } \Omega,\\
&\boldsymbol{u}|_{\partial\Omega} = \big(I(c)\nabla \boldsymbol{d}\big)\boldsymbol{n}\big|_{\partial\Omega} = \boldsymbol{0} && \text{in } (0,T),\\
&\left.\frac{\partial c}{\partial \boldsymbol{n}}\right|_{\partial\Omega} = \left.\left(\nabla \frac{\delta E_{tot}}{\delta c}\right)\cdot \boldsymbol{n}\right|_{\partial\Omega} = 0 && \text{in } (0,T),
\end{aligned} \tag{6}$$

Nematic-Isotropic. Reformulation of the stress tensor

Lemma

The following relation holds:

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

where

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

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

$$\langle \boldsymbol{u}_t, \bar{\boldsymbol{u}}\rangle + ((\boldsymbol{u}\cdot\nabla)\boldsymbol{u}, \bar{\boldsymbol{u}}) + (\nu(c)\boldsymbol{D}\boldsymbol{u}, \boldsymbol{D}\bar{\boldsymbol{u}}) - (\widetilde{p}, \nabla\cdot\bar{\boldsymbol{u}}) - \left((\nabla \boldsymbol{d})^t \boldsymbol{w}, \bar{\boldsymbol{u}}\right) + (c\nabla\mu, \bar{\boldsymbol{u}}) = 0,$$

$$(\nabla\cdot\boldsymbol{u}, \bar{p}) = 0,$$

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

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

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

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

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

Nematic-Isotropic. Continuous energy law

Using adequate test functions, we can prove that the previous system satisfies the following (dissipative) energy law:

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

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

$$\left\{\begin{array}{l}
\boldsymbol{u} \in L^\infty(0,T;\mathbf{L}^2(\Omega)) \cap L^2(0,T;\mathbf{H}^1(\Omega)),\\
\boldsymbol{w} \in L^2(0,T;\mathbf{L}^2(\Omega)),\\
\nabla c \in L^\infty(0,T;\mathbf{L}^2(\Omega)),\\
\nabla\mu \in L^2(0,T;\mathbf{L}^2(\Omega)),\\
\int_\Omega F(c)d\boldsymbol{x} \in L^\infty(0,T),\\
\int_\Omega I(c)\left(\frac{1}{2}|\nabla\boldsymbol{d}|^2 + G(\boldsymbol{d})\right)d\boldsymbol{x} \in L^\infty(0,T)\\
E_{anch}(c,\boldsymbol{d}) \in L^\infty(0,T),\\
c \in L^\infty(0,T;H^1(\Omega)),\\
\int_\Omega I(c)\,|\boldsymbol{d}|^4 \in L^\infty(0,T),\\
\boldsymbol{d} \in L^\infty(0,T;\mathbf{L}^2(\Omega)).
\end{array}\right. \qquad (7)$$

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

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

Definition

A numerical scheme is energy-stable if it satisfies

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

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

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

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

$$
\left\{
\begin{aligned}
&\left(\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{k}, \bar{\boldsymbol{u}}\right) + \left((\boldsymbol{u}^{n+1}\cdot\nabla)\boldsymbol{u}^{n+1}, \bar{\boldsymbol{u}}\right) - (p^{n+1}, \nabla\cdot\bar{\boldsymbol{u}}) + 2(\nu \boldsymbol{D}\boldsymbol{u}^{n+1}, \boldsymbol{D}\bar{\boldsymbol{u}}) \\
&\qquad - \left((\nabla \boldsymbol{d}^{n+1})^t \boldsymbol{w}^{n+1}, \bar{\boldsymbol{u}}\right) + (c^{n+1}\nabla\mu^{n+1}, \bar{\boldsymbol{u}}) = 0\,, \\
&(\nabla\cdot\boldsymbol{u}^{n+1}, \bar{p}) = 0\,, \\
&\left(\frac{\boldsymbol{d}^{n+1}-\boldsymbol{d}^n}{k}, \bar{\boldsymbol{w}}\right) + \left((\boldsymbol{u}^{n+1}\cdot\nabla)\boldsymbol{d}^{n+1}, \bar{\boldsymbol{w}}\right) + \gamma_{nem}(\boldsymbol{w}^{n+1}, \bar{\boldsymbol{w}}) = 0\,, \\
&\lambda_{nem}(I(c^{n+1})\nabla\boldsymbol{d}^{n+1}, \nabla\bar{\boldsymbol{d}}) + \lambda_{nem}(I(c^{n+1})\,\boldsymbol{g}(\boldsymbol{d}^{n+1}), \bar{\boldsymbol{d}}) + \lambda_{anch}\left(\frac{\delta E_{anch}}{\delta \boldsymbol{d}}(c^{n+1}, \boldsymbol{d}^{n+1}), \bar{\boldsymbol{d}}\right) - (\boldsymbol{w}^{n+1}, \bar{\boldsymbol{d}}) = 0\,, \\
&\left(\frac{c^{n+1}-c^n}{k}, \bar{\mu}\right) - (c^{n+1}\boldsymbol{u}^{n+1}, \nabla\bar{\mu}) + \gamma_{mix}(\nabla\mu^{n+1}, \nabla\bar{\mu}) = 0\,, \\
&\lambda_{mix}(\nabla c^{n+1}, \nabla\bar{c}) + \lambda_{mix}(f(c^{n+1}), \bar{c}) + \lambda_{nem}\left(i(c^{n+1})\left[\frac{|\nabla\boldsymbol{d}^{n+1}|^2}{2} + G(\boldsymbol{d}^{n+1})\right], \bar{c}\right) \\
&\qquad + \lambda_{anch}\left(\frac{\delta E_{anch}}{\delta c}(c^{n+1}, \boldsymbol{d}^{n+1}), \bar{c}\right) - (\mu^{n+1}, \bar{c}) = 0\,,
\end{aligned}
\right.
\tag{8}
$$

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 ?

We have designed two splitting first-order schemes, denoted by

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

or

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

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 $(\bar{\boldsymbol{d}}, \bar{\boldsymbol{w}}) \in \boldsymbol{D}_h \times \boldsymbol{W}_h$

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

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

$\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n)$ is an 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 $(\bar{c}, \bar{\mu}) \in C_h \times M_h$

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

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

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

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

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

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

where

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

and

$$c(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) := \Big((\boldsymbol{u} \cdot \nabla)\boldsymbol{v}, \boldsymbol{w}\Big) + \frac{1}{2}\Big(\nabla \cdot \boldsymbol{u}, \boldsymbol{v} \cdot \boldsymbol{w}\Big).$$

Scheme given by **STEPS 1-3** satisfies the following local discrete energy law:

$$\delta_t E(\boldsymbol{d}^{n+1}, c^{n+1}, \boldsymbol{u}^{n+1}) + \gamma_{\text{nem}} \|\boldsymbol{w}^{n+1}\|_{L^2}^2$$

$$+\gamma_{\text{mix}}\|\nabla \mu^{n+1}\|_{L^2}^2 + \|\nu(c^{n+1})^{1/2}\boldsymbol{D}\boldsymbol{u}^{n+1}\|_{L^2}^2$$

$$+ND_{\boldsymbol{u}}^{n+1} + ND_{\text{elast}}^{n+1}(c^n) + ND_{\text{penal}}^{n+1}(c^n)$$

$$+ND_{\text{philic}}^{n+1} + ND_{\text{phobic}}^{n+1} + ND_{\text{interp}}^{n+1} + ND_{\text{anch}}^{n+1} = 0.$$

The numerical dissipation terms are:

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

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

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

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

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

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

and

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

with (δ_1, δ_2) defined in (2) depending on the type of anchoring.

QUESTION:
How to define $f_k(c^{n+1}, c^n)$, $\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n)$, $i_k(c^{n+1}, c^n)$ to obtain linear unconditionally energy-stable schemes ?

That is, we want $f_k(c^{n+1}, c^n)$, $\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n)$, $i_k(c^{n+1}, c^n)$ linear such that

$$ND^{n+1}_{\text{penal}}(c^n) \geq 0, \quad ND^{n+1}_{\text{phobic}} \geq 0, \quad \text{and } ND^{n+1}_{\text{interp}} \geq 0\,.$$

Nematic-Isotropic. The function f_k

$$f_k(c^{n+1}, c^n) := \widetilde{f}(c^n) + \frac{1}{2} \|\widetilde{f}'\|_\infty (c^{n+1} - c^n), \qquad (9)$$

in our case reduces to

$$f_k(c^{n+1}, c^n) = \widetilde{f}(c^n) + (c^{n+1} - c^n) \qquad (10)$$

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

$$\widetilde{f}(c) = \begin{cases} \frac{2}{\varepsilon^2}(c+1) & \text{if } c \leq -1, \\ \frac{1}{\varepsilon^2}(c^2-1)\, c & \text{if } c \in [-1,1], \\ \frac{2}{\varepsilon^2}(c-1) & \text{if } c \geq 1, \end{cases} \qquad (11)$$

$$\boldsymbol{g}_k(\boldsymbol{d}^{n+1}, \boldsymbol{d}^n) = \widetilde{\boldsymbol{g}}(\boldsymbol{d}^n) + \frac{\sqrt{51}}{2}(\boldsymbol{d}^{n+1} - \boldsymbol{d}^n), \qquad (12)$$

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

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

and we also take

$$i_k(c^{n+1}, c^n) = i(c^n) + \frac{5\sqrt{3}}{12}(c^{n+1} - c^n). \qquad (13)$$

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* (12) *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* (10) *and* (13) *for $f_k(c^{n+1}, c^n)$ and $i_k(c^{n+1}, c^n)$, respectively.*

Lemma

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

$$\exists\, \beta > 0 \quad \textit{such that} \quad \|p\|_{L^2} \leq \beta \sup_{\bar{\mathbf{u}} \in V_h \setminus \{\Theta\}} \frac{(p, \nabla \cdot \bar{\mathbf{u}})}{\|\bar{\mathbf{u}}\|_{H^1}} \quad \forall\, p \in P_h\,, \tag{14}$$

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

We propose the following choice for the discrete spaces:

$$(\mathbf{u}, p) \sim P_2 \times P_1\,, \qquad (c, \mu) \sim P_1 \times P_1 \qquad \text{and} \qquad (\mathbf{d}, \mathbf{w}) \sim P_1 \times P_1\,, \tag{15}$$

that satisfy the assumptions of Lemmas 6, 7 and 8.

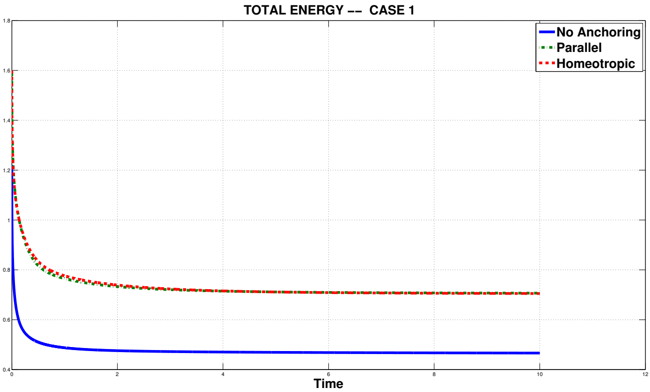
The newtonian fluid is represented by blue color while the nematic fluid is represented by red one.
For simplicity we are considering constant viscosity $\nu(c) = \nu_0$.

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

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

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



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

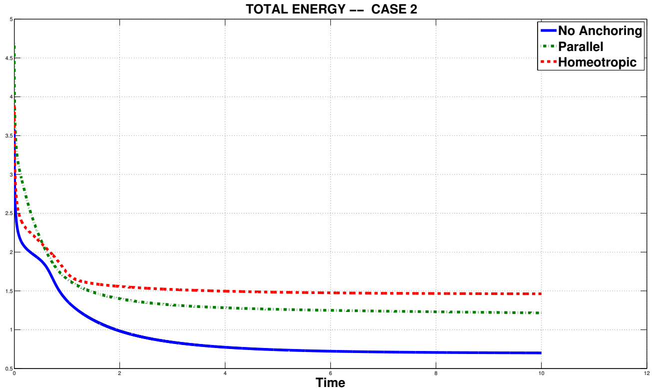
- A Hedgehog defect at $(1/2, 0)$ and an Antihedgehog defect at $(-1/2, 0)$

$$\boldsymbol{d}_0(x) = \widehat{\boldsymbol{d}} / \sqrt{|\widehat{\boldsymbol{d}}|^2 + 0{,}05^2}, \text{ with } \widehat{\boldsymbol{d}} = (x^2 + y^2 - 0{,}25, y) \, .$$

Defect annihilation in Nematic Liquid Crystals

Defect annihilation in Nematic Liquid Crystals Drops

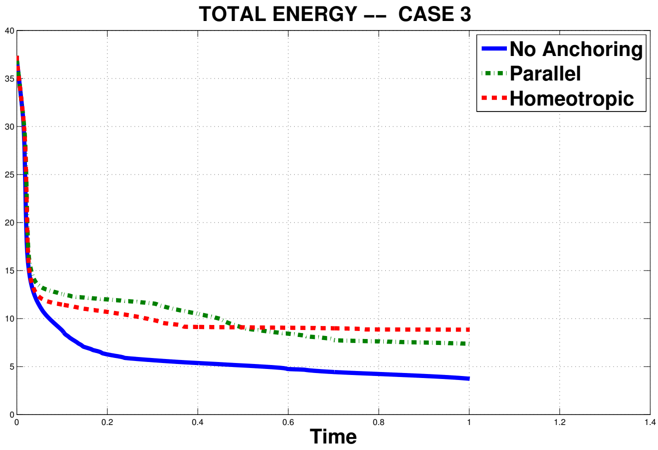
Nematic-Isotropic. Circular droplet and director field parallel to the y-axis



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:

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


TOTAL ENERGY -- CASE 3
No Anchoring
Parallel
Homeotropic
Time
0
5
10
15
20
25
30
35
40
0
0.2
0.4
0.6
0.8
1
1.2
1.4

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THANK YOU FOR YOUR ATTENTION!