Liquid Crystal and Phase-Field models are related by Mathematics

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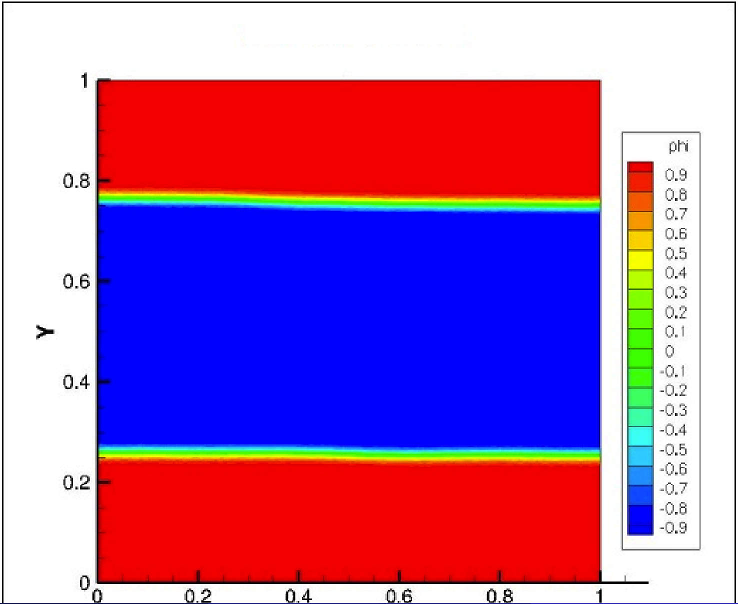
1. Optimization problem and asymptotic as $\varepsilon \to 0$
2. Time-dependent problems
3. Coupling with fluid dynamics
4. Other related models: Membranes, Solidification, Tumors
5. Mixed models: Nematic-Isotropic, Tumor-membranes

1. Optimization problem and asymptotic as $\varepsilon \to 0$

Diffuse-interface Phase-Field



Diffuse-interface Phase-Field

- Situation: Two materials (f.e. two immiscible fluids) or two phases of the same material (f.e. solid-liquid, liquid-gas)
- Assumption: there exists a sharp-interface separating the phases.
- Approximation: Diffuse-interface (with small width ε) approaching sharp interface.
- Scalar Phase variable, $\phi : \Omega \to \mathbf{R}$ (order parameter) s.t. $\begin{cases} \phi = 1 & \text{phase A} \\ \phi = -1 & \text{phase B} \end{cases}$

  and $\phi = 0$ as approximation of the interface Γ.
- Double-well potential function $F(\phi)$, with two stable values ($\phi = \pm 1$) and one unstable ($\phi = 0$). Then, $\int_\Omega F(\phi)$ is a convex-concave functional, but it's essentially convex and bounded from below.
- Examples: polynomial $F(\phi) = (\phi^2 - 1)^2/4$, (singular) logarithmic ....

Area-dependent Energy

Energy [van der Waals]: competition between philic $\frac{1}{2}\int_\Omega |\nabla\phi|^2$ and phobic $\int_\Omega F(\phi)$, averaged by a small width parameter ε:

$$\mathcal{E}(\phi) = \varepsilon\,\frac{1}{2}\int_\Omega |\nabla\phi|^2 + \frac{1}{\varepsilon}\int_\Omega F(\phi)$$

Interface width of order $O(\varepsilon)$, because

1. If width $O(\varepsilon^2)$ then $\varepsilon\displaystyle\int_\Omega |\nabla\phi|^2 >> \frac{1}{\varepsilon}\int_\Omega F(\phi)$.
2. If width $O(\sqrt{\varepsilon})$ then $\displaystyle\frac{1}{\varepsilon}\int_\Omega F(\phi) >> \varepsilon\int_\Omega |\nabla\phi|^2$.

Diffuse-interface towards sharp-interface

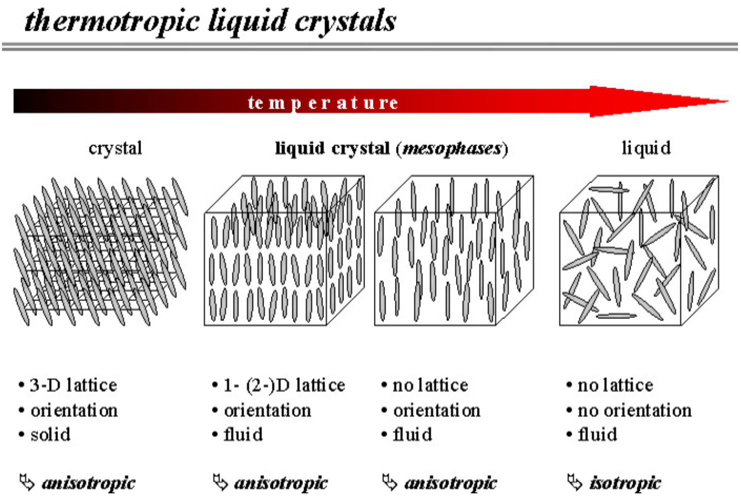
- $\min_{\phi} \mathcal{E}(\phi) = \Big(\int_\Omega \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} \int_\Omega F(\phi) \Big)$ subject to BCs for ϕ: $\phi|_{\partial\Omega_D} = \phi_D$ on $\partial\Omega_D$.
- Euler-Lagrange optimality system ($\frac{\delta \mathcal{E}}{\delta \phi} = 0$):

$$-\varepsilon \Delta \phi + \frac{1}{\varepsilon} F'(\phi) = 0 \text{ in } \Omega, \quad \phi|_{\partial\Omega_D} = \phi_D \text{ on } \partial\Omega_D, \quad \varepsilon \nabla \phi \cdot \boldsymbol{n}|_{\partial\Omega_N} = 0 \text{ on } \partial\Omega_N,$$

- Th. Weistrass: Existence of (global) minimum ϕ^ε.
- As $\varepsilon \to 0$, sharp interface limit Γ (zero width), s.t. $\phi^\varepsilon \to \phi^0 = \pm 1$ on $\Gamma_\pm$.
- Γ-convergence results can be obtained [Modica-Mortola'77, Modica'87, ...].
- In fact, the Γ-limit in $L^1(\Omega)$ as $\varepsilon \to 0$ of $\mathcal{E}(\phi^\varepsilon)$ is $C_0 \mathcal{P}(\phi^0)$

  $\mathcal{P}(\phi^0)$ is the "surface-area of $\Gamma = \{\phi^0 = 0\}$ in Ω".

Liquid Crystals



Liquid Crystals

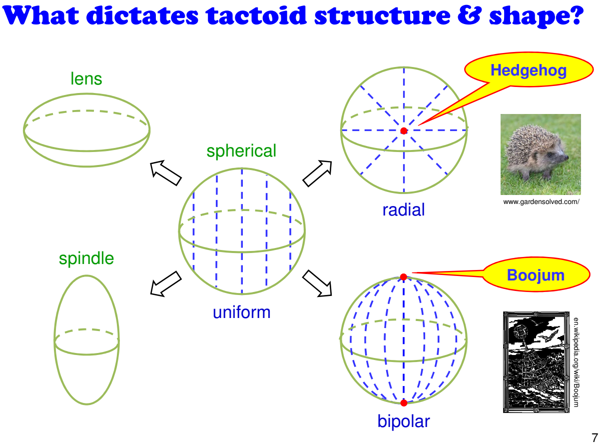
- Situation: An intermediate material between solid and liquid. Microscopically, it's (partially) ordered and macroscopically flows like liquids.
- Assumption: there exists a preferred orientation of molecules
- Director vector variable $\boldsymbol{d} : \Omega \to \mathbb{R}^N$ (order parameter)
- Elastic Energy [Oseen-Frank]: resistance to change the uniform orientation

$$\mathcal{E}(\boldsymbol{d}) = \frac{1}{2}\int_\Omega \Big(K_1(\nabla\cdot\boldsymbol{d})^2 + K_2(\boldsymbol{d}\cdot(\nabla\times\boldsymbol{d}))^2 + K_3|\boldsymbol{d}\times(\nabla\times\boldsymbol{d})|^2 \Big)\, d\boldsymbol{x}$$

K_1, K_2, K_3 splay, twist and bend elastic constants.

- Simplification: equal constant case $\mathcal{E}(\boldsymbol{d}) = \frac{1}{2}\int_\Omega |\nabla \boldsymbol{d}|^2$
- The energy $\mathcal{E}(\boldsymbol{d})$ must be minimized under the non-convex constraint $|\boldsymbol{d}| = 1$.
- Defects: zones where anisotropic orientation is lost, i.e. singularities for the vector field $\boldsymbol{d}$.

Defects are singularities in vector fields. Defect points and BCs. Annihilations.



Penalization

- Approximation by penalization: competition between elastic energy $\frac{1}{2}\int_\Omega |\nabla \boldsymbol{d}|^2$ and constraint $|\boldsymbol{d}| = 1$, averaged by a small penalization parameter ε:

$$\mathcal{E}(\boldsymbol{d}) = \frac{1}{2}\int_\Omega |\nabla \boldsymbol{d}|^2 + \frac{1}{\varepsilon^2}\int_\Omega F(\boldsymbol{d})$$

- $F(\boldsymbol{d})$ is a vectorial double-well potential, with stable points at $|\boldsymbol{d}| = 1$ and unstable at $\boldsymbol{d} = 0$.
- Example: polynomial $F(\boldsymbol{d}) = (|\boldsymbol{d}|^2 - 1)^2/4$.

$\varepsilon \to 0$

- $\min_{\boldsymbol{d}} \mathcal{E}(\boldsymbol{d})\Big(= \frac{1}{2}\int_\Omega |\nabla \boldsymbol{d}|^2 + \frac{1}{\varepsilon^2}\int_\Omega F(\boldsymbol{d})\Big)$ subject to Dirichlet BCs for $\boldsymbol{d}$
- Euler-Lagrange optimality system ($\frac{\delta \mathcal{E}}{\delta \boldsymbol{d}} = 0$):

$$-\Delta \boldsymbol{d} + \frac{1}{\varepsilon^2} F'(\boldsymbol{d}) = 0 \text{ in } \Omega, \quad \boldsymbol{d}|_{\partial\Omega_D} = \boldsymbol{d}_D \text{ on } \partial\Omega_D, \quad \nabla \boldsymbol{d} \cdot \boldsymbol{n}|_{\partial\Omega_N} = 0 \text{ on } \partial\Omega_N,$$

- Th. Weistrass: Existence of (global) minimum $\boldsymbol{d}^\varepsilon$.
- Limit of penalization problem as $\varepsilon \to 0$. Harmonic functions with values in the unit sphere surface $\mathcal{S}^1$ [F. Bethuel, H. Brezis, F. Helein], [J.Ball,A.Zarnescu]

Theorem

$\boldsymbol{d}^\varepsilon \to \boldsymbol{d}^0$ s.t. $|\boldsymbol{d}^0| = 1$ in Ω solution of

$$-\Delta \boldsymbol{d}^0 - |\nabla \boldsymbol{d}^0|^2 \boldsymbol{d}^0 = 0 \text{ in } \Omega, \quad \boldsymbol{d}^0|_{\partial\Omega_D} = \boldsymbol{d}_D \text{ on } \partial\Omega_D, \quad \nabla \boldsymbol{d}^0 \cdot \boldsymbol{n}|_{\partial\Omega_N} = 0 \text{ on } \partial\Omega_N.$$

In fact, $\lambda = |\nabla \boldsymbol{d}^0|^2 \boldsymbol{d}^0$ is the Lagrange multiplier related to $|\boldsymbol{d}^0| = 1$

2. Time-dependent problems

- Idea: ODE $c_t + F'(c) = 0$ with $F(c) = (c^2 - 1)^2$.
- Critical points: $c = \pm 1$ (stables) and $c = 0$ (unstable)
- Energy's law: $\dfrac{d}{dt}F(c(t)) + c_t(t)^2 = 0$, hence $F(c)$ is a Lyapunov functional.

Phase-Field

- Phase variable : $\phi = \phi(t, \boldsymbol{x})$. Energy : $\mathcal{E}(\phi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi)$
- Chemical potential : $\frac{\delta\mathcal{E}}{\delta\phi} = \mu = -\varepsilon\Delta\phi + \frac{1}{\varepsilon}F'(\phi)$, + BCs
- (AC) Allen-Cahn eq: $\partial_t\phi + \gamma\frac{\delta\mathcal{E}}{\delta\phi} = 0$ in Ω ($\gamma > 0$ relaxation time).
  - Maximum principle: If data take values in $[-1, 1]$ then $\phi(t, \boldsymbol{x}) \in [-1, 1]$.
  - No conservative: $\frac{d}{dt}\int_\Omega \phi(t) = \gamma\,\varepsilon\int_{\partial\Omega} \nabla\phi\cdot\boldsymbol{n} - \frac{\gamma}{\varepsilon}\int_\Omega F'(\phi(t)) \neq 0$
- (CH) Cahn-Hilliard eq: $\partial_t\phi - \nabla\cdot(m\nabla(\frac{\delta\mathcal{E}}{\delta\phi})) = 0$ in Ω.
  - Flux: $m\nabla(\frac{\delta\mathcal{E}}{\delta\phi})$, with $m = m(\phi) \geq 0$ the mobility.
  - Conservative: $\frac{d}{dt}\int_\Omega \phi(t) = 0$ (if $m\nabla\mu\cdot\boldsymbol{n}|_{\partial\Omega} = 0$).
  - Not maximum principle in general.

Dissipative models

Energy's law: $\dfrac{d}{dt}\mathcal{E}(t) + DISS = 0$ where $DISS = \begin{cases} \gamma \displaystyle\int_\Omega \left(\frac{\delta \mathcal{E}}{\delta \phi}\right)^2 & \text{for (AC),} \\ \displaystyle\int_\Omega \left| m \nabla \left(\frac{\delta \mathcal{E}}{\delta \phi}\right)\right|^2 & \text{for (CH)} \end{cases}$

Theorem (Analysis of the initial-boundary problem)

- *Weak solutions. Regularity.*
- *Time-periodicity for periodic time-dependent BCs.*

Theorem (Asymptotic behavior as $t \to +\infty$)

- *Existence of attractor.*
- *Convergence of trajectories to a (steady) equilibrium with polynomial decay:*

$$\phi(t) \to \phi^\infty \quad \textit{and} \quad \|\phi(t) - \phi^\infty\| \le C \frac{1}{(1+t)^p}.$$

- *Stability of local minima. In general, not asymptotic stability ("continuous" of critical points with the same energy).*

- Energy $\mathcal{E}(\boldsymbol{d}) = \frac{1}{2}\int_\Omega |\nabla \boldsymbol{d}|^2 + \frac{1}{\varepsilon^2}\int_\Omega F(\boldsymbol{d})$
- Equilibrium system: $\frac{\delta \mathcal{E}}{\delta \boldsymbol{d}} = -\Delta \boldsymbol{d} + \frac{1}{\varepsilon^2} F'(\boldsymbol{d}),$ + BCs
- Allen-Cahn system. $\partial_t \boldsymbol{d} + \gamma \frac{\delta \mathcal{E}}{\delta \boldsymbol{d}} = 0,$ +ICs, BCs.
- Maximum principle: If $|data| \le 1$ then $|\boldsymbol{d}(t, \boldsymbol{x})| \le 1$.
- Energy's law: $\frac{d}{dt}\mathcal{E}(t) + \gamma \int_\Omega \left| \frac{\delta \mathcal{E}}{\delta \boldsymbol{d}} \right|^2 = 0.$

3. Coupling with fluid dynamics

Navier-Stokes for incompressible fluids

- Linear momentum balance and incompressibility constraint):

$$\partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} - \nabla\cdot\Sigma = \boldsymbol{f}, \quad \nabla\cdot\boldsymbol{v} = 0 \quad + ICs, BCs,$$

- Viscous newtonian fluids: Stress tensor $\Sigma = -p\, Id + 2\nu D\boldsymbol{v}$, with $p = p(t,\boldsymbol{x})$ the pressure (normal force), $\nu > 0$ viscosity coeff. and $D\boldsymbol{v} = (\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^t)/2$ the deformation tensor.
- In particular, for constant viscosity

$$\partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} + \nabla p - \nu\Delta\boldsymbol{v} = \boldsymbol{f}, \quad \nabla\cdot\boldsymbol{v} = 0 \quad + ICs, BCs,$$

- Dissipative energy's law: $\dfrac{d}{dt}\mathcal{E}_{kin}(\boldsymbol{v}) + DISS = \displaystyle\int_\Omega \boldsymbol{f}\cdot\boldsymbol{v}$ where
$\mathcal{E}_{kin}(\boldsymbol{v}) = \dfrac{1}{2}\displaystyle\int_\Omega |\boldsymbol{v}|^2$ (Kinetic's energy) and
$DISS = \displaystyle\int_\Omega \nu|\nabla\boldsymbol{v}|^2 \geq 0$ (viscosity's dissipation)

Some results

Theorem (Analysis of the initial-boundary problem)

Existence of weak solutions. Regularity and uniqueness (local in time in 3D, global in time near of regular stationary solutions).

Theorem (Asymptotic behavior as $t \to +\infty$)

When $\mathbf{f} = \nabla q$ *then* $\mathbf{v}(t) \to 0$ *with exponential decay.*

Theorem (Numerical approx.)

- *Finite-Element space approx, compatibility between velocity and pressure approx., “inf-sup" stability cond.*
- *Energy-stable time approx. and Large-time stability. Time-splitting schemes. Time adaptation.*

- Situation: Two immiscible fluids (A and B) with matched densities (and viscosities), assuming a mixed diffuse-interface between them, of width $O(\varepsilon)$.
- Conservative phenomena: NS fluids + CH phase
- Stress tensor: $\Sigma = -p\, Id + 2\nu D\mathbf{v} + \Sigma_{phase}$ with $\Sigma_{phase} = -\lambda\varepsilon(\nabla\phi \otimes \nabla\phi)$. Then

$$-\nabla \cdot \Sigma_{phase} = \lambda\varepsilon\, \Delta\phi\nabla\phi + \nabla\left(\frac{\lambda\varepsilon}{2}|\nabla\phi|^2\right)$$

i.e. capillary effects (= surface tension coefficient (λ) $\times$ curvature ($\Delta\phi$) $\times$ normal direction to the interface ($\nabla\phi$) + normal force changing the pressure).

- Phase energy: $\mathcal{E}_{phase}(\phi) = \int_\Omega E_{phase}(\phi) = \lambda \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} F(\phi) \right)$
- By using $F'(\phi)\nabla\phi = \nabla(F(\phi))$, the phase tensor can be rewritten as

$$-\nabla \cdot \Sigma_{phase} = -\mu \, \nabla \phi + \nabla \left(E_{phase}(\phi) \right)$$

- PDE coupled system (Model H) [Hohenberg and Halperin'77]:

$$\begin{cases} \text{NS}: \quad \partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla \widetilde{p} - \nu \Delta \boldsymbol{v} = \mu \, \nabla \phi, \quad \nabla \cdot \boldsymbol{v} = 0, \quad (\widetilde{p} = p + E_{phase}(\phi)) \\ \text{CH}: \quad \partial_t \phi + \boldsymbol{v} \cdot \nabla \phi - \nabla \cdot (m \nabla \mu) = 0, \quad \mu = \dfrac{\delta \mathcal{E}_{phase}}{\delta \phi} = \lambda(-\varepsilon \Delta \phi + \dfrac{1}{\varepsilon} F'(\phi)) \end{cases}$$

- Conservation of phase: $\dfrac{d}{dt} \displaystyle\int_\Omega \phi = 0 \quad$ (if $\boldsymbol{v} \cdot \boldsymbol{n}|_{\partial\Omega} = 0$ and $m \nabla \mu \cdot \boldsymbol{n}|_{\partial\Omega} = 0$)
- Dissipative problem: $\dfrac{d}{dt} \Big(\mathcal{E}_{kin}(\boldsymbol{v}) + \mathcal{E}_{phase}(\phi) \Big) + \displaystyle\int_\Omega \nu |\nabla \boldsymbol{v}|^2 + \int_\Omega m |\nabla \mu|^2 = 0,$

Theorem ((Analysis) [Abels, Garcke, Grasselli, Gal, ...)

Existence of weak solutions. Global in time regularity of the phase. Regularity of velocity and uniqueness (local in time in 3D or global in time for dominant viscosity). Asymptotic $\varepsilon \to 0$

Theorem (($t \to +\infty$), [Feiresl, Miranville, Grasselli, Wu, Schimperna, ...)

$(\mathbf{v}(t), \phi(t)) \to (0, \phi^\infty)$ *with polynomial decay, where* $\nabla \mu^\infty = 0$ *with* $\mu^\infty = \frac{\delta \mathcal{E}_{phase}}{\delta \phi}(\phi^\infty)$.
Stability of local minima.

Theorem ((Numeric), [Elliot, Boyer, Wise, Eyre, Shen, Grun, FGG-Tierra,...)

Unique-solvable and Energy-stable first order numerical schemes. Convergence. Error estimates. Time-splitting.

Open problems

1. Global regular solutions near of regular stationary solutions $(0, \phi^\infty)$.
2. Second order time-splitting schemes

Liquid crystal fluids

1. Situation: Fluid dynamic of a nematic liquid crystal.
2. Vector director $\boldsymbol{d}$, with $|\boldsymbol{d}| \approx 1$.
3. Nematic (elastic) stress tensor: $\Sigma_{nem} = -\lambda((\nabla \boldsymbol{d})^t \nabla \boldsymbol{d})$
4. Nematic energy: $\mathcal{E}_{nem}(\boldsymbol{d}) = \int_\Omega E_{nem}(\boldsymbol{d}) = \lambda \int_\Omega \left(\frac{1}{2} |\nabla \boldsymbol{d}|^2 + \frac{1}{\varepsilon^2} F(\boldsymbol{d}) \right)$
5. PDE coupled system (Lin's model) [F.H.Lin] as a simplification of the Erickseen-Leslie's model (NS-AC):

$$\begin{cases} NS: & \partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla \widetilde{p} - \nu \Delta \boldsymbol{v} = (\nabla \boldsymbol{d})^t \boldsymbol{w}, \quad \nabla \cdot \boldsymbol{v} = 0, \quad (\widetilde{p} = p + E_{nem}(\boldsymbol{d})) \\ AC: & \partial_t \boldsymbol{d} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{d} + \gamma\, \boldsymbol{w} = 0, \quad \boldsymbol{w} = \lambda(-\Delta \boldsymbol{d} + \frac{1}{\varepsilon^2} F'(\boldsymbol{d})) \end{cases}$$

6. Dissipative problem: $\frac{d}{dt}\Big(\mathcal{E}_{kin}(\boldsymbol{v}) + \mathcal{E}_{nem}(\boldsymbol{d}) \Big) + \int_\Omega \nu |\nabla \boldsymbol{v}|^2 + \gamma \int_\Omega |\boldsymbol{w}|^2 = 0$

Theorem ((Analysis), Lin-Liu, FGG-Rguez Bellido-Rojas Medar, ...)

Existence of weak solutions. Regularity and uniqueness (local in time in 3D or global in time for dominant viscosity). Uniqueness and regularity criteria. Time-periodic.

Theorem (($t \to +\infty$), Climent-FGG-Rguez Bellido, Petzeltova-Rocca-Schimperna, Grasselli-Wu,.....)

$(\boldsymbol{v}(t)\boldsymbol{d}(t)) \to (0, \boldsymbol{d}^\infty)$ *s.t.* $\dfrac{\delta \mathcal{E}_{nem}}{\delta \boldsymbol{d}}(\boldsymbol{d}^\infty)$ *with polynomial decay. Stability of local minima.*

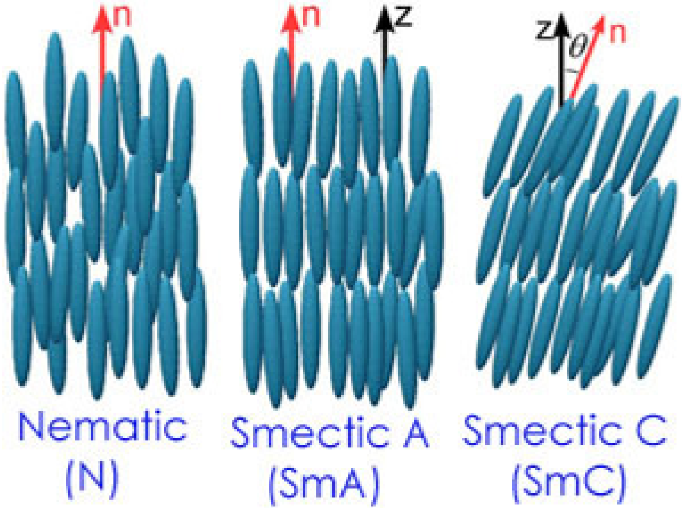
Theorem ((Numeric), Walkington, Liu, Prohl, Shen, Badia, Cabrales-FGG-Santacreu, ...)

Energy-stable numerical schemes, Unconditional (nonlinear) or conditional (linear). Convergence. Error estimates. Time-splitting.

Open problems

1. Asymptotic $\varepsilon \to 0$. Problem: how to control the limit of $(\nabla \boldsymbol{d}_\varepsilon)^t \nabla \boldsymbol{d}_\varepsilon$
2. For models with stretching: Time-periodic, Attractors, Stability of local minima.

Smectic-A LCs



- [E, Liu, FGG-Climent, FGG-Tierra]
- Layer variable: $\boldsymbol{n} = \boldsymbol{d} = \nabla\varphi$
- Smectic energy + penalization: $\mathcal{E}_{sm} = \lambda \int_\Omega \left(\frac{1}{2}|\Delta\varphi|^2 + \frac{1}{\varepsilon^2} F(\nabla\varphi) \right)$
- PDE coupled system (E's model) [E] (NS-AC):

$$\begin{cases} \text{NS}: & \partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} + \nabla\widetilde{p} - \nu\Delta\boldsymbol{v} = \mu\nabla\varphi, \quad \nabla\cdot\boldsymbol{v} = 0, \\ \text{AC}: & \partial_t\varphi + \boldsymbol{v}\cdot\nabla\varphi + \gamma\,\mu = 0, \quad \mu = \dfrac{\delta\mathcal{E}_{sm}}{\delta\varphi} = \lambda(\Delta\varphi - \dfrac{1}{\varepsilon^2}\nabla\cdot F'(\nabla\varphi)) \end{cases}$$

- Energy's law:

$$\frac{d}{dt}\Big(\mathcal{E}_{kin}(\boldsymbol{v}) + \mathcal{E}_{sm}(\varphi)\Big) + \int_\Omega \nu|D\boldsymbol{v}|^2 + \gamma\int_\Omega |\mu|^2 = 0$$

4. Other related models: Membranes, Solidification, Tumors

Membranes

- Elastic curvature-dependent energy: Willmore or bending energy

$$\mathcal{E}_b(\phi) = \frac{\lambda}{2}\int_\Omega (-\varepsilon\Delta\phi + \frac{1}{\varepsilon}F'(\phi))^2 = \frac{\lambda}{2}\int_\Omega w^2$$

- Conservative CH problem + Surface Area constraint: $B(\phi) = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2\right)$
- As $\varepsilon \to 0$, $\mathcal{E}_b(\phi^\varepsilon)$ Γ-conv. to the square of the curvature [Belletini'97]
- The elastic bending energy is modified to penalize the area:

$$\mathcal{E}(\phi) = \mathcal{E}_b(\phi) + \frac{1}{\eta}\frac{1}{2}(B(\phi) - \beta)^2$$

- Chemical potential:

$$\mu = \frac{\delta\mathcal{E}(\phi)}{\delta\phi} = -\varepsilon\lambda\Delta w + \frac{\lambda}{\varepsilon}w\,F''(\phi) + \frac{1}{\eta}(B(\phi) - \beta)(-\varepsilon\Delta\phi)$$
$$= \varepsilon^2\lambda\,\Delta^2\phi + G(\phi)$$

- PDE coupled system:

$$\begin{cases} \text{NS}: & \partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} + \nabla\widetilde{p} - \nu\Delta\boldsymbol{v} = \mu\,\nabla\phi, \quad \nabla\cdot\boldsymbol{v} = 0, \\ \text{CH}: & \partial_t\phi + \boldsymbol{v}\cdot\nabla\phi - \nabla\cdot(m\nabla\mu) = 0, \quad \mu = \varepsilon^2\lambda\,\Delta^2\phi + G(\phi) \end{cases}$$

- Conservation of phase: $\dfrac{d}{dt}\displaystyle\int_\Omega \phi = 0 \quad$ (if $\boldsymbol{v}\cdot\boldsymbol{n}|_{\partial\Omega} = 0$ and $m\nabla\mu\cdot\boldsymbol{n}|_{\partial\Omega} = 0$)
- Dissipative problem, satisfying the energy's law:

$$\frac{d}{dt}\Big(\mathcal{E}_{kin}(\boldsymbol{v}) + \mathcal{E}(\phi)\Big) + \int_\Omega \nu|\nabla\boldsymbol{v}|^2 + \int_\Omega m|\nabla\mu|^2 = 0$$

Open problems:

Asymptotic as $t \to +\infty$

Analysis for the non-penalized problem, via Lagrange multiplier [Colli-Laurencot'11,'12]

Solidification: Canigalp's model

- Phase: $\phi(t, \boldsymbol{x}) \in [0, 1]$ fraction of solid ($\phi = 1$ solid, $\phi = 0$ liquid).
- Latent heat effect; energy vs temperature is a multivalued function.
- Dendrite increasing vs anisotropic energy
- Models coupling convection in the liquid part are free-boundary models (limit of models with degenerate viscosity).
- Open problem: To obtain a diffuse-interface model (in the whole domain) with convection in the liquid part

[Calsavara-FGG]

Energy functional:

$$\mathcal{E} = \mathcal{E}_{kin}(\boldsymbol{v}) + \mathcal{E}_{heat}(\theta) + \mathcal{E}_{phase}(\phi),$$

$$\mathcal{E}_{kin}(v) = \frac{1}{2}\int_\Omega |\boldsymbol{v}|^2, \quad \mathcal{E}_{heat}(\theta) = \frac{1}{2\,l}\int_\Omega (\theta - \theta_{melting})^2,$$

$$\mathcal{E}_{phase}(\phi) = \lambda \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi)\right), \quad F(\phi) = \phi^2(1-\phi)^2.$$

where $l > 0$ (latent heat), $\lambda > 0$ (capillarity).

Solidification (free-boundary problem)

$$
\begin{cases}
(\theta + l\, g(\phi))_t + \boldsymbol{v}\cdot\nabla\left(\theta + l\, g(\phi)\right) - \nabla\cdot(k(\phi)\nabla\theta) = f & \text{in } Q,\\
\phi_t + \boldsymbol{v}\cdot\nabla\phi + \gamma\left(\dfrac{\delta\mathcal{E}_{phase}}{\delta\phi} - g'(\phi)(\theta - \theta_{melting})\right) = 0 & \text{in } Q,\\
\boldsymbol{v}_t + \boldsymbol{v}\cdot\nabla\boldsymbol{v} - \nabla\cdot(2\nu(\phi)D\boldsymbol{v}) + \nabla p - \dfrac{\delta\mathcal{E}_{phase}}{\delta\phi}\nabla\phi = G(\theta,\phi) & \text{in } Q_{ml},\\
\nabla\cdot\boldsymbol{v} = 0 & \text{in } Q_{ml},\\
D\boldsymbol{v} = 0 & \text{in } Q_s,
\end{cases}
$$

$$
Q_{ml} = \{(x,t)\in Q \,:\, \phi(x,t) < 1\} \ \text{ and } \ Q_s = \{(x,t)\in Q \,:\, \phi(x,t) = 1\}.
$$

The function $g = g(\phi)$ will be an interpolation function, with $g(1) = 0$ (solid phase), $g(0) = 1$ (liquid phase) and $0 < g < 1$ in the mushy zone.

$\nu(\phi) \in [\nu_L, +\infty]$. A classical Carman-Kozeny term is $\nu(\phi) = \nu_L\phi^2/(1-\phi)^3$.

- Phase eq. is of Allen-Cahn type for the modified free energy:

$$\mathcal{E}_{mod}(\phi, \theta) = \lambda \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} F(\phi) \right) - \int_\Omega g(\phi)(\theta - \theta_{melting})$$

- The modified double-well potential $\dfrac{\lambda}{\varepsilon} F(\phi) - g(\phi)(\theta - \theta_{melting})$ has the same two minimum points at $\phi = 0$ and $\phi = 1$, but modifying its values in these wells depending on the temperature.
- Maximum principle: $0 \leq \phi \leq 1$
- Energy's law:

$$\frac{d\mathcal{E}}{dt} + \int_\Omega 2\nu(\phi)|D\boldsymbol{v}|^2 + \frac{1}{l} \int_\Omega k(\phi)|\nabla(\theta - \theta_{melting})|^2 + \frac{1}{\gamma} \int_\Omega (\phi_t + \boldsymbol{v} \cdot \nabla \phi)^2 = forces$$

Tumors [Wu, van Zwieten, van der Zee'13]

- Phases: concentration of tumor (or necrotic or quiescent) and health cells + Convection-Diffusion of nutrients (oxygen).
- $c(t, \boldsymbol{x})$ fraction of tumor cells, $n(t, \boldsymbol{x})$ concentration of nutrients:

$$
\begin{aligned}
&c_t - \Delta\mu_c = P(c)(\mu_n - \mu_c), \quad \mu_c = -\varepsilon^2\Delta c + F'(c), \\
&n_t - \Delta\mu_n = -P(c)(\mu_n - \mu_c), \quad \mu_n = \tfrac{1}{\delta} n,
\end{aligned}
$$

- $P(c)$ is a nonnegative proliferation function: $\begin{cases} P(c) = \delta\,\widehat{P}\,c(1-c) & \text{if } c \in [0,1], \\ P(c) = 0 & \text{otherwise} \end{cases}$
- The total "mass" is conserved, i.e. $\dfrac{d}{dt}\displaystyle\int_\Omega (c+n) = \int_\Omega \Delta(\mu_c + \mu_n) = 0$
- Dissipative system, wrt. the energy $\mathcal{E}(c,n) = \displaystyle\int_\Omega \left(\frac{\varepsilon^2}{2}|\nabla c|^2 + F(c) + \frac{1}{2\,\delta} n^2 \right)$:

$$
\frac{d}{dt}\mathcal{E}(c,n) + \int_\Omega \left(|\nabla\mu_c|^2 + |\nabla\mu_n|^2 + P(c)(\mu_n - \mu_c)^2 \right) = 0
$$

4. Mixed models: Nematic-Isotropic, Tumor-membranes

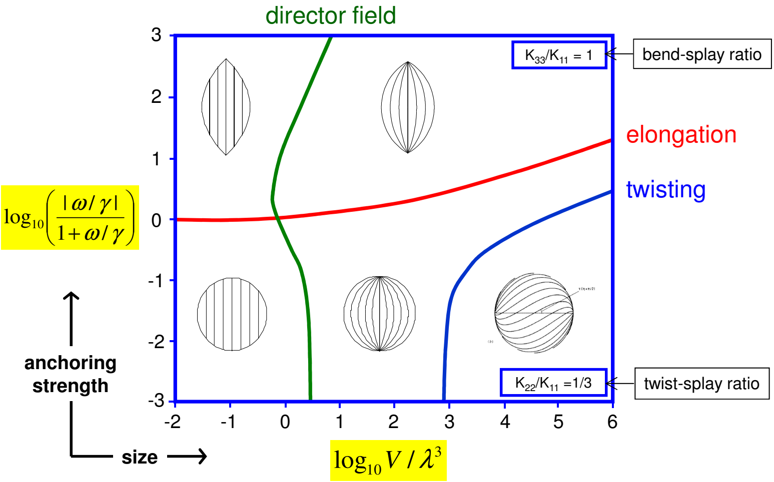
Nematic-Isotropic

- Two-fluids + elastic energy in the nematic part (via interpolation function) + anchoring forces on Nematic-Isotropic interface
- CH phase + NS fluids + AC nematic + interpolation function
- [Liu, Yang, Shen, Wang, ...] Modelization and numerical simulations
- [FGG-Rguez Bellido-Tierra] Stable decoupled numerical scheme + numerical simulations

Open Problems:

- Mathematical analysis
- Splitting second-order schemes
- Capture the experimental phase diagram of different defects

Theoretical phase diagram



Tumors and membranes: [Chen, Wise, Shenoy, Lowengrub'14]

- Competition between tumor increasing and elasticity of biologic membranes
- Open Problem: To study models with
  - (CH + source terms) for tumors
  - (CH + Area constraint) for membranes

THANK YOU FOR YOUR ATTENTION