Phase-field approximation to Willmore flows with constraints

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Motivation I

Cell membrane: living cell/environment. Made of lipids, proteins, ...
Model: lipid bilayer in which lipid molecules move freely and proteins are embedded. Thickness usually small $\rightarrow$ surface.
Configuration and deformation of elastic lipid bilayers:
Canham-Helfrich's model (1973). Curvature/bending energy:

$$\mathcal{E}_H := \int_\Sigma \left(\frac{k_c}{2} (\mathcal{H} - \mathcal{H}_0)^2 + \frac{k_g}{2} \mathcal{K} \right) ds$$

where

- k_c, k_g: bending rigidities,
- $\mathcal{H}$: mean curvature,
- $\mathcal{H}_0$: spontaneous curvature,
- $\mathcal{K}$: Gauß curvature.

Motivation II

Equilibrium shape for a closed surface:

$$\min \int_{\Sigma} \left(\frac{k_c}{2} \left(\mathcal{H} - \mathcal{H}_0\right)^2 \right) \, ds$$

Constraints: fixed area and volume.

$$k_c \left(\mathcal{H} + \mathcal{H}_0\right) \left(\mathcal{H}^2 - \mathcal{H}_0 \, \mathcal{H} - \mathcal{K}\right) + k_c \, \Delta_{\Sigma}\mathcal{H} = \lambda \, \mathcal{H} - \mu \, ,$$

with Lagrange multipliers λ and μ.
Highly nonlinear PDE + sharp interface: drawbacks for numerical simulations.

Results on the FBP

- Existence of minimisers without constraints and $\mathcal{H}_0 = 0$. Simon (1993), Rivière (2008)
- Existence of minimisers with constraints: axisymmetric geometry. Choksi & Veneroni
- Existence of critical points bifurcating from a sphere. Nagasawa & Takagi (2003)
- Existence of minimisers with isoperimetric constraint and $\mathcal{H}_0 = 0$. Schygulla (2012)
- Local existence for the evolution equation. Nagasawa & Yi (2012)

Phase-field approximation I

Regularize the interface. Du, Liu & Wang (2004)

Order parameter: v.

- $\{x \; : \; v(x) = 0\}$ represents the membrane,
- $\{x \; : \; v(x) > 0\}$ represents the inside of the membrane,
- $\{x \; : \; v(x) < 0\}$ represents the outside of the membrane.

Simplifying assumption: homogeneous membrane and $\mathcal{H}_0 = 0$.

$$\mathcal{E}_H = \frac{k_c}{2} \int_\Sigma \mathcal{H}^2 \, ds \quad \longrightarrow \quad E = k \int_\Omega \left[\Delta v - \frac{1}{\varepsilon^2} \left(v^2 - 1 \right) v \right]^2 dx$$

Phase-field approximation II

$$\mathcal{E}_H = \frac{k_c}{2} \int_\Sigma \mathcal{H}^2 \, ds \quad \longrightarrow \quad E = k \int_\Omega \left[\Delta v - \frac{1}{\varepsilon^2} \left(v^2 - 1 \right) v \right]^2 dx \,,$$

$$\text{volume} \longrightarrow \int_\Omega v \, dx \,,$$

$$\text{area} \longrightarrow F = \int_\Omega \left[\frac{\varepsilon}{2} |\nabla v|^2 + \frac{1}{4\varepsilon} \left(v^2 - 1 \right)^2 \right] dx \,.$$

Phase-field approximation III ($\varepsilon = 1$)

$$\partial_t v = \frac{\delta E}{\delta v} + A + B\,\frac{\delta F}{\delta v}\,,$$

with

$$\frac{\delta F}{\delta v} = \mu := -\Delta v + W'(v)\,,$$

and

$$\frac{\delta E}{\delta v} = \Delta\mu - W''(v)\,\mu\,.$$

$$W(r) := \frac{1}{4}\,\left(r^2 - 1\right)^2\,, \qquad r \in \mathbb{R}\,,$$

Outline

1. Volume constraint

Outline

Outline

Phase-field approximation

Let Ω be an open bounded subset of $\mathbb{R}^N$, $1 \leq N \leq 3$.

$$\begin{aligned} \partial_t v &- \Delta\mu + W''(v)\,\mu - \overline{W''(v)\,\mu} = 0\,, \quad (t,x) \in (0,\infty)\times\Omega\,, \\ \mu &= -\Delta v + W'(v)\,, \quad (t,x) \in (0,\infty)\times\Omega\,, \\ \nabla v\cdot\nu &= \nabla\mu\cdot\nu = 0\,, \quad (t,x)\in(0,\infty)\times\Gamma\,, \\ v(0) &= v_0\,, \quad x\in\Omega\,, \end{aligned}$$

with

$$W(r) := \frac{1}{4}\,\left(r^2-1\right)^2\,, \qquad r\in\mathbb{R}\,,$$

and

$$\overline{f} := \frac{1}{|\Omega|}\int_\Omega f(x)\,dx\,, \qquad f\in L^1(\Omega)\,.$$

Notation

- $V := \{w \in H^2(\Omega) \; : \; \nabla w \cdot \nu = 0 \quad \text{on} \quad \Gamma\}$,
- $V_\alpha := \{w \in V \; : \; \overline{w} = \alpha\}$, where $\alpha \in \mathbb{R}$.
- Energy functional:

$$E(v) := \frac{1}{2} \int_\Omega \left[-\Delta v + W'(v)\right]^2 \, dx \, .$$

Well-posedness

Given $\alpha \in \mathbb{R}$ and $v_0 \in V_\alpha$, there is a unique solution v satisfying for all $T > 0$

- $v \in \mathcal{C}([0,T]; L^2(\Omega)) \cap L^\infty(0,T; V_\alpha)$,
- $\mu := -\Delta v + W'(v) \in L^2(0,T; V)$,
- $t \longmapsto E(v(t)) = ||\mu(t)||_2^2/2$ is a non-increasing function,
- $$\int_0^\infty \left\| -\Delta\mu(t) + W''(v(t))\,\mu(t) - \overline{W''(v)\,\mu}(t) \right\|_2^2 \, dt \le 2E(v_0)$$

Colli & L. (2011)

Proof

- Variational approach: time step $\tau \in (0,1)$. Define $(v_n^\tau)_{n\geq 0}$ by:
- $v_0^\tau := v_0$,
- for $n \geq 1$,

$$v_n^\tau \in \operatorname{argmin} \left\{ \frac{1}{2} \|w - v_{n-1}^\tau\|_2^2 + \tau\, E(w) \;:\; w \in V_\alpha \right\}.$$

- Euler-Lagrange equation.
- Piecewise constant interpolation: $v^\tau(t) := v_n^\tau$ for $t \in [n\tau, (n+1)\tau)$ and $n \geq 0$.
- Estimates for v^τ in $L^\infty(0,T;H^2(\Omega))$ and for $\mu^\tau := -\Delta v^\tau + W'(v^\tau)$ in $L^2(0,T;H^2(\Omega))$ + time equicontinuity.

Outline

Notation

- $V := \{w \in H^2(\Omega) \ : \ \nabla w \cdot \nu = 0 \quad \text{on} \quad \Gamma\}$,
- Free energy functional:

$$F(v) := \int_\Omega \left[\frac{1}{2}\,|\nabla v|^2 + W(v)\right]\,dx\,, \quad I(v) := \overline{v}\,, \qquad v \in H^1(\Omega)\,.$$

- $\beta_\alpha := \inf\{F(w) \ : \ w \in H^1(\Omega)\,,\ I(w) = \alpha\}$, $\alpha \in \mathbb{R}$.
- $\mathcal{M}^1_{\alpha,\beta} := \{w \in H^1(\Omega) \ : \ I(w) = \alpha\,,\ F(w) = \beta\}$, $\alpha, \beta \in \mathbb{R}$.
- Clearly, $\mathcal{M}^1_{\alpha,\beta} = \emptyset$ if $\beta < \beta_\alpha$.
- Energy functional:

$$E(v) := \frac{1}{2}\int_\Omega \left[-\Delta v + W'(v)\right]^2\,dx\,.$$

$\mathcal{M}^1_{\alpha,\beta}$

$\mathcal{M}^1_{\alpha,\beta} := \{w \in H^1(\Omega) \ : \ \overline{w} = \alpha\,, \ F(w) = \beta\}$, $\alpha, \beta \in \mathbb{R}$.

- $\mathcal{M}^1_{\alpha,\beta} = \emptyset$ if $\beta < \beta_\alpha$.
- $\mathcal{M}^1_{\alpha,\beta_\alpha} \neq \emptyset$.
- If $\beta > \beta_\alpha$, $w \in \mathcal{M}^1_{\alpha,\beta_\alpha}$, and $\varphi \in H^1(\Omega)$ with $\overline{\varphi} = 0$, there is $\lambda_\varphi > 0$ such that $w + \lambda_\varphi\, \varphi \in \mathcal{M}^1_{\alpha,\beta}$.

$\mathcal{M}^2_{\alpha,\beta} := \{w \in H^2_N(\Omega) \ : \ \overline{w} = \alpha\,, \ F(w) = \beta\}$, $\alpha, \beta \in \mathbb{R}$.

Phase-field approximation

Let Ω be an open bounded subset of $\mathbb{R}^N$, $1 \leq N \leq 3$, and $v_0 \in \mathcal{M}^2_{\alpha,\beta}$.

$$\begin{aligned} \partial_t v &- \Delta\mu + W''(v)\,\mu = A + B\,\mu\,, \quad (t,x) \in (0,\infty) \times \Omega\,, \\ \mu &= -\Delta v + W'(v)\,, \quad (t,x) \in (0,\infty) \times \Omega\,, \\ \nabla v \cdot \nu &= \nabla\mu \cdot \nu = 0\,, \quad (t,x) \in (0,\infty) \times \Gamma\,, \\ v(0) &= v_0\,, \quad x \in \Omega\,, \end{aligned}$$

with

$$W(r) := \frac{1}{4}\,\left(r^2 - 1\right)^2\,, \qquad r \in \mathbb{R}\,,$$

and A and B are time-depending functions and the Lagrange multipliers corresponding to the volume and area constraints

$$\overline{v(t)} = \alpha = \overline{v_0} \quad \text{and} \quad F(v(t)) = \beta = F(v_0)\,, \qquad t \geq 0\,.$$

Computing the Lagrange multipliers

$$\mu = -\Delta v + W'(v)$$

$$\begin{aligned} A + B\,\overline{\mu} &= \overline{W''(v)\mu}\,, \\ B\,\|\mu - \overline{\mu}\|_2^2 &= \|\nabla\mu\|_2^2 + \int_\Omega W''(v)\,\mu^2\,dx \\ &\quad - \overline{W''(v)\mu}\,\int_\Omega \mu\,dx\,. \end{aligned}$$

$\mu =$ const.?

Variational scheme

- $\alpha \in \mathbb{R}$, $\beta > \beta_\alpha$.
- Variational approach: time step $\tau \in (0,1)$. Define $(v_n^\tau)_{n\geq 0}$ by:
- $v_0^\tau := v_0$,
- for $n \geq 1$,

$$v_n^\tau \in \operatorname{argmin} \left\{ \frac{1}{2} \|w - v_{n-1}^\tau\|_2^2 + \tau\, E(w) \ : \ w \in \mathcal{M}^1_{\alpha,\beta} \right\} .$$

- v_n^τ is well-defined.
- Euler-Lagrange equation.

Euler-Lagrange equation

- Euler-Lagrange equation for v_n^τ:

$$\frac{v_n^\tau - v_{n-1}^\tau}{\tau} + \frac{\delta E}{\delta v}(v_n^\tau) = A\,\frac{\delta I}{\delta v}(v_n^\tau) + B\,\frac{\delta F}{\delta v}(v_n^\tau)\,.$$

- Problem to identify the Euler-Lagrange equation if

$$\mu_n^\tau := \frac{\delta F}{\delta v}(v_n^\tau) = -\Delta v_n^\tau + W'(v_n^\tau) = \text{ const. } = |\Omega| \text{ const. } \frac{\delta I}{\delta v}(v_n^\tau)$$

Lagrange multipliers

$$\mu_n^\tau = -\Delta v_n^\tau + W'(v_n^\tau)\,.$$

$$\begin{aligned} A + B\,\overline{\mu_n^\tau} &= \overline{W''(v_n^\tau)\mu_n^\tau}\,, \\ B\,\|\mu_n^\tau - \overline{\mu_n^\tau}\|_2^2 &= \|\nabla\mu_n^\tau\|_2^2 + \int_\Omega W''(v_n^\tau)\,(\mu_n^\tau)^2\,dx \\ &\quad - \overline{W''(v_n^\tau)\mu_n^\tau}\,\int_\Omega \mu_n^\tau\,dx\,. \end{aligned}$$

Restriction on (α, β)

Steady states:

$$\mathcal{Z}_{\alpha,\beta} := \left\{ w \in \mathcal{M}^2_{\alpha,\beta} \;:\; -\Delta w + W'(w) - \overline{W'(w)} = 0 \text{ in } \Omega \right\} .$$

Assumption:

$$\mathcal{Z}_{\alpha,\beta} = \emptyset \, .$$

- Given $\alpha \in \mathbb{R}$, the set $\{\beta \in (\beta_\alpha, \infty) \;:\; \mathcal{Z}_{\alpha,\beta} = \emptyset\}$ is open and contains a neighbourhood of infinity.
- Functional inequality.

Convergence

- Piecewise constant interpolation: $v^\tau(t) := v_n^\tau$ for $t \in [n\tau, (n+1)\tau)$ and $n \geq 0$. Similar definitions for μ^τ, A^τ, and B^τ.
- Estimates for v^τ in $L^\infty(0, T; H^2(\Omega))$ and for μ^τ in $L^2(0, T; H^2(\Omega))$ + time equicontinuity.
- Estimates for A^τ and B^τ in $L^2(0, T)$, the latter being the most delicate point (functional inequality).
- Convergence $\longrightarrow$ existence.
- Uniqueness.

Colli & L.

Further questions

- Behaviour as $\varepsilon \to 0$: formal approach for E with volume and area constraints.

  Du, Liu, Ryham, & Wang (2005), Wang (2008).

- Behaviour as $\varepsilon \to 0$: rigorous approach without or with constraints.

  Bellettini & Mugnai (2010)

- Phase-field approximations for non-homogeneous membranes.

  Wang & Du (2008), Lowengrub, Rätz, & Voigt (2009), Elliott & Stinner (2010), Givli, Giang, & Bhattacharya (2012)

- Coupling with Navier-Stokes equations but no constraints.

  Wu & Xu