Stable Approximation of Stefan Problems with fully anisotropic Gibbs–Thomson Law

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Consider a Stefan Problem for Undercooled Solidification.

Container $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3.

Solid-Liquid interface $\Gamma(t)$.

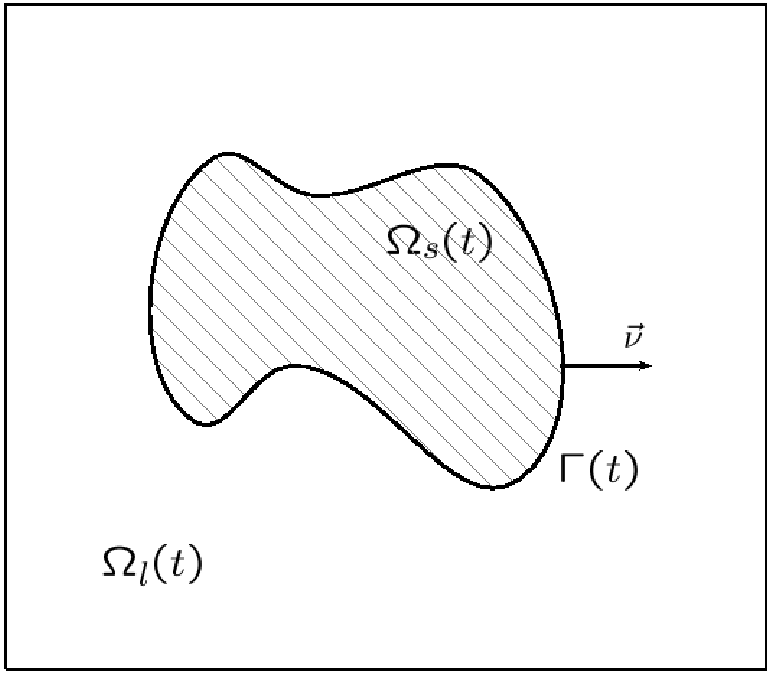
$\Omega_s(t)$, the interior of $\Gamma(t)$, is the solid region.

$\Omega_l(t) := \Omega \setminus \overline{\Omega_s(t)}$ is the liquid region.

Unit normal of $\Gamma(t)$, $\vec{\nu}$, pointing into $\Omega_l(t)$.

Let $\mathcal{V}$ denote normal velocity of $\Gamma(t)$.

$$\left[\frac{\partial \cdot}{\partial \vec{\nu}}\right]_{\Gamma(t)} := \frac{\partial \cdot}{\partial \vec{\nu}}\Big|_{\text{liquid}} - \frac{\partial \cdot}{\partial \vec{\nu}}\Big|_{\text{solid}} .$$



Stefan Problem with Kinetic Undercooling

Find the temperature $u(\cdot, t) : \Omega \to \mathbb{R}$ and the interface $\Gamma(t) \subset \Omega$ such that for $t \in (0, T]$

$$\vartheta\, u_t - \Delta u = f \qquad \text{in } \Omega \setminus \Gamma(t),$$

$$\left[\frac{\partial u}{\partial \vec{\nu}}\right]_{\Gamma(t)} = -\lambda\, \mathcal{V} \qquad \text{on } \Gamma(t), \qquad \text{(Stefan condition)}$$

$$\rho\, \mathcal{V} = \beta(\vec{\nu})\ [\alpha\, \varkappa_\gamma - a\, u] \qquad \text{on } \Gamma(t), \qquad \text{(Gibbs-Thomson condition)}$$

$$u = u_D \qquad \text{on } \partial\Omega$$

with $u(\cdot, 0)$ and $\Gamma(0)$ specified.

Here $\lambda \in \mathbb{R}_{>0}$ is the latent heat, ϑ, ρ, $\alpha \in \mathbb{R}_{\geq 0}$ and $a \in \mathbb{R}_{>0}$.

In addition, $\varkappa_\gamma$ is the weighted mean curvature of Γ, based on a given anisotropy function $\gamma(\cdot)$, and $\beta(\cdot)$ is a given anisotropic mobility.

AIM: Introduce a stable finite element approximation for the Stefan problem.

Crucial: A stable, variational formulation of $\varkappa_\gamma$.

A stable approximation of the Stefan problem with

$$\rho\,\mathcal{V} = \beta(\vec\nu)\ [\alpha\,\varkappa_\gamma - a\,u] \qquad \text{on } \Gamma(t), \qquad \text{(Gibbs-Thomson condition)}$$

hinges on a stable numerical method for the much simpler problem

$$\mathcal{V} = \varkappa_\gamma \qquad \text{on } \Gamma(t), \qquad (\text{MC}_\gamma)$$

i.e. motion by anisotropic mean curvature.

For simplicity, consider first the isotropic case, i.e. $\gamma(\vec\nu) = |\vec\nu| = 1$. Then $\varkappa_\gamma = \varkappa$ and (MC_γ) collapses to

$$\mathcal{V} = \varkappa \qquad \text{on } \Gamma(t), \qquad (\text{MC})$$

i.e. the mean curvature flow.

On noting that $-\varkappa$ can be defined as the first variation of the surface area $|\Gamma|$, (MC) is often interpreted as the L^2-gradient flow of $|\Gamma|$.

For simplicity, let $d = 2$. Let $\vec{x}(\rho, t)$, $\rho \in I := \mathbb{R}/\mathbb{Z}$ (periodic $[0, 1]$), be a parameterization of $\Gamma(t) \subset \mathbb{R}^2$ with unit tangent $\vec{\tau} = \vec{x}_s = \frac{\vec{x}_\rho}{|\vec{x}_\rho|}$ and curvature vector $\vec{\varkappa} = \vec{\tau}_s = \vec{x}_{ss} = \frac{1}{|\vec{x}_\rho|}\left(\frac{\vec{x}_\rho}{|\vec{x}_\rho|}\right)_\rho$. It is easy to see that $\vec{x}_{ss} \,.\, \vec{x}_s = 0$, and so $\vec{\varkappa} = \varkappa\,\vec{\nu}$, where $\varkappa$ denotes curvature and $\vec{\nu} := -\vec{x}_s^{\perp}$ is a chosen unit normal. ($\cdot^\perp$ is clockwise rotation by $\frac{\pi}{2}$)

Then the first variation of

$$|\Gamma(t)| := \int_{\Gamma(t)} 1 \,\mathrm{d}s = \int_I |\vec{x}_\rho| \,\mathrm{d}\rho$$

can be computed as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\Gamma(t)| &= \int_I \frac{\vec{x}_\rho}{|\vec{x}_\rho|} \,.\, \vec{x}_{\rho,t} \,\mathrm{d}\rho = -\int_I \left(\frac{\vec{x}_\rho}{|\vec{x}_\rho|}\right)_\rho \,.\, \vec{x}_t \,\mathrm{d}\rho = -\int_{\Gamma(t)} \vec{x}_{ss} \,.\, \vec{x}_t \,\mathrm{d}s \\ &= -\int_{\Gamma(t)} \varkappa\,(\vec{x}_t \,.\, \vec{\nu}) \,\mathrm{d}s\,.\end{aligned}$$

Hence the L^2-gradient flow of $|\Gamma|$ is: $\qquad \vec{x}_t \,.\, \vec{\nu} = \varkappa\,. \qquad$ (MC)

Weak formulation of (MC)

Based on

$$\vec{x}_t \,.\, \vec{\nu} = \varkappa \qquad \text{and} \qquad \varkappa\, \vec{\nu} = \vec{x}_{ss}\,.$$

Given $\Gamma(0)$, for $t \in (0,T]$ find $\vec{x}(t) \in \underline{V} := H^1(I;\mathbb{R}^2)$ and $\varkappa(t) \in V := H^1(I;\mathbb{R})$ such that

$$\int_\Gamma \vec{x}_t \,.\, \vec{\nu}\, \varphi \,\mathrm{d}s - \int_\Gamma \varkappa\, \varphi \,\mathrm{d}s = 0 \quad \forall\ \varphi \in V\,,$$

$$\int_\Gamma \varkappa\, \vec{\nu} \,.\, \vec{\varphi} \,\mathrm{d}s + \int_\Gamma \vec{x}_s \,.\, \vec{\varphi}_s \,\mathrm{d}s = 0 \quad \forall\ \vec{\varphi} \in \underline{V}\,.$$

"Stability": Choose $\varphi = \varkappa$ and $\vec{\varphi} = \vec{x}_t$ to obtain

$$\begin{aligned} 0 &= \int_\Gamma \varkappa^2 \,\mathrm{d}s + \int_\Gamma \vec{x}_s \,.\, \vec{x}_{t,s} \,\mathrm{d}s \\ &= \int_\Gamma \varkappa^2 \,\mathrm{d}s + \int_I \frac{\vec{x}_\rho}{|\vec{x}_\rho|} \,.\, \vec{x}_{\rho,t} \,\mathrm{d}\rho \\ &= \int_\Gamma \varkappa^2 \,\mathrm{d}s + \frac{\mathrm{d}}{\mathrm{d}t} |\Gamma(t)|\,. \end{aligned}$$

Semidiscrete Finite Element Approximation

Let $I \equiv \mathbb{R}/\mathbb{Z} = \cup_{j=1}^{N} J_j$, $N \geq 3$, partitioned into intervals $J_j = [q_{j-1}, q_j]$.

$\underline{V}^h := \{\vec{\chi} \in C(I, \mathbb{R}^2) : \vec{\chi}|_{J_j}$ is linear $\forall\ j = 1 \to N\} =: [V^h]^2 \subset H^1(I, \mathbb{R}^2)$.

Let $\{\phi_j\}_{j=1}^{N}$ denote the standard basis of V^h.

$\vec{X}^h(t) \in \underline{V}^h$ approximating $\vec{x}(t) \Rightarrow$ a polygonal approximation, $\Gamma^h(t)$, to $\Gamma(t)$.

Given $\Gamma^h(0)$, for $t \in (0, T]$ find $\vec{X}^h(t) \in \underline{V}^h$ and $\kappa^h(t) \in V^h$ such that

$$\langle \vec{X}^h_t, \chi\, \vec{\nu}^h \rangle^h_{\Gamma^h} - \langle \kappa^h, \chi \rangle^h_{\Gamma^h} = 0 \qquad \forall\ \chi \in V^h;$$

$$\langle \kappa^h\, \vec{\nu}^h, \vec{\eta} \rangle^h_{\Gamma^h} + \langle \vec{X}^h_s, \vec{\eta}_s \rangle_{\Gamma^h} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}^h;$$

where

$$\langle f, g \rangle_{\Gamma^h} := \int_{\Gamma^h(t)} f \,.\, g \,\mathrm{d}s = \int_I f \,.\, g\, |\vec{X}^h_\rho(t)| \,\mathrm{d}\rho$$

with $\langle \cdot, \cdot \rangle^h_{\Gamma^h}$ the mass lumped inner product.

Stability: Choose $\chi = \kappa^h$ and $\vec{\eta} = \vec{X}^h_t$ to obtain

$$0 = \langle \kappa^h, \kappa^h \rangle^h_{\Gamma^h} + \langle \vec{X}^h_s, \vec{X}^h_{t,s} \rangle_{\Gamma^h} = \langle \kappa^h, \kappa^h \rangle^h_{\Gamma^h} + \frac{\mathrm{d}}{\mathrm{d}t} |\Gamma^h(t)| \,.$$

Let $0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = T$ be a partitioning of $[0,T]$, $\tau_m := t_{m+1} - t_m$, $m = 0 \to M-1$, and $\tau := \max_{m=0\to M-1} \tau_m$.

Given $\Gamma^0 = \vec{X}^0(I)$, $\vec{X}^0 \in \underline{V}^h$, for $m = 0 \to M-1$ find $\vec{X}^{m+1} \in \underline{V}^h$ and $\kappa^{m+1} \in V^h$ such that

$$\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \rangle^h_{\Gamma^m} - \langle \kappa^{m+1}, \chi \rangle^h_{\Gamma^m} = 0 \qquad \forall\ \chi \in V^h;$$

$$\langle \kappa^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle^h_{\Gamma^m} + \langle \vec{X}^{m+1}_s, \vec{\eta}_s \rangle_{\Gamma^m} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}^h.$$

Stability: Choose $\chi = \kappa^{m+1}$ and $\vec{\eta} = \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}$ to obtain

$$0 = \tau_m\, \langle \kappa^{m+1}, \kappa^{m+1} \rangle^h_{\Gamma^m} + \langle \vec{X}^{m+1}_s, (\vec{X}^{m+1} - \vec{X}^m)_s \rangle_{\Gamma^m}\,,$$

where, on letting $\vec{h}^m_j := \vec{X}^m(q_{j+1}) - \vec{X}^m(q_j)$,

$$\langle \vec{X}^{m+1}_s, (\vec{X}^{m+1} - \vec{X}^m)_s \rangle_{\Gamma^m} = \sum_{j=1}^N \left[\frac{|\vec{h}^{m+1}_j|^2 - \vec{h}^{m+1}_j \,.\, \vec{h}^m_j}{|\vec{h}^m_j|} \right]$$

$$= \sum_{j=1}^N \left[\frac{(|\vec{h}^{m+1}_j| - |\vec{h}^m_j|)^2 + |\vec{h}^{m+1}_j|\,|\vec{h}^m_j| - \vec{h}^{m+1}_j \,.\, \vec{h}^m_j}{|\vec{h}^m_j|} + |\vec{h}^{m+1}_j| - |\vec{h}^m_j| \right]$$

$$\geq \sum_{j=1}^N \left[|\vec{h}^{m+1}_j| - |\vec{h}^m_j| \right] = |\Gamma^{m+1}| - |\Gamma^m|\,.$$

$$|\Gamma|_\gamma := \int_\Gamma \gamma(\vec\nu)\,\mathrm{d}s$$

where $\gamma : \mathbb{R}^d \setminus \{\vec{0}\} \to \mathbb{R}_{>0}$ is a given anisotropy function, which we will assume is positively homogeneous of degree one, i.e.

$$\gamma(\lambda\,\vec p) = \lambda\,\gamma(\vec p) \quad \forall\ \vec p \in \mathbb{R}^d \setminus \{\vec{0}\},\ \forall\ \lambda \in \mathbb{R}_{>0}\,.$$

Let $\Gamma(\varepsilon) := \{\vec z + \varepsilon\,\vec g(\vec z) : \vec z \in \Gamma\}$. First variation of this energy yields

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,|\Gamma(\varepsilon)|_\gamma\,|_{\varepsilon=0} = -\int_\Gamma \vec\varkappa_\gamma\,.\,\vec g\,\mathrm{d}s\,;$$

where

Weighted mean curvature vector: $\vec\varkappa_\gamma := \varkappa_\gamma\,\vec\nu$,

Weighted mean curvature: $\varkappa_\gamma := -\nabla_s\,.\,\vec\nu_\gamma$,

Cahn–Hoffmann vector: $\vec\nu_\gamma := \gamma'(\vec\nu)$ Cahn, Hoffmann (74).

In the case $d = 2$ it holds that $\varkappa_\gamma \vec{\nu} = [\gamma'(\vec{\nu})]_s^\perp = [\gamma'(-\vec{x}_s^\perp)]_s^\perp$ since

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Gamma(t)|_\gamma = \frac{\mathrm{d}}{\mathrm{d}t}\int_I \gamma(-\vec{x}_\rho^\perp)\,\mathrm{d}\rho = \int_I \gamma'(-\vec{x}_\rho^\perp)\,.\,(-\vec{x}_{\rho,t}^\perp)\,\mathrm{d}\rho = \int_I [\gamma'(-\vec{x}_s^\perp)]^\perp\,.\,\vec{x}_{\rho,t}\,\mathrm{d}\rho$$
$$= -\int_I [\gamma'(-\vec{x}_s^\perp)]_\rho^\perp\,.\,\vec{x}_t\,\mathrm{d}\rho = -\int_{\Gamma(t)} [\gamma'(-\vec{x}_s^\perp)]_s^\perp\,.\,\vec{x}_t\,\mathrm{d}s\,.$$

Weak formulation of

$$\mathcal{V} = \varkappa_\gamma \qquad \text{on } \Gamma(t) \qquad (\mathrm{MC}_\gamma)$$

is then: Given $\Gamma(0)$, for $t \in (0,T]$ find $\vec{x}(t) \in \underline{V}$ and $\varkappa_\gamma(t) \in V$ such that

$$\langle \vec{x}_t, \vec{\nu}\,\varphi\rangle_\Gamma - \langle \varkappa_\gamma, \varphi\rangle_\Gamma = 0 \quad \forall\ \varphi \in V\,,$$

$$\langle \varkappa_\gamma\,\vec{\nu}, \vec{\varphi}\rangle_\Gamma - \langle \gamma'(\vec{\nu}), \vec{\varphi}_s^\perp\rangle_\Gamma = 0 \quad \forall\ \vec{\varphi} \in \underline{V}\,.$$

“Stability”: Choose $\varphi = \varkappa_\gamma$ and $\vec{\varphi} = \vec{x}_t$ to obtain

$$0 = \langle \varkappa_\gamma, \varkappa_\gamma\rangle_\Gamma - \langle \gamma'(\vec{\nu}), \vec{x}_{s,t}^\perp\rangle_\Gamma = \langle \varkappa_\gamma, \varkappa_\gamma\rangle_\Gamma + \frac{\mathrm{d}}{\mathrm{d}t}|\Gamma(t)|_\gamma\,.$$

Given $\Gamma^h(0)$, for $t \in (0,T]$ find $\vec{X}^h(t) \in \underline{V}^h$ and $\kappa_\gamma^h(t) \in V^h$ such that

$$\langle \vec{X}_t^h, \chi\, \vec{\nu}^h \rangle_{\Gamma^h}^h - \langle \kappa_\gamma^h, \chi \rangle_{\Gamma^h}^h = 0 \qquad \forall\ \chi \in V^h;$$

$$\langle \kappa_\gamma^h\, \vec{\nu}^h, \vec{\eta} \rangle_{\Gamma^h}^h - \langle \gamma'(\vec{\nu}^h), \vec{\eta}_s^\perp \rangle_{\Gamma^h} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}^h.$$

Stability: Choose $\chi = \kappa_\gamma^h$ and $\vec{\eta} = \vec{X}_t^h$ to obtain

$$0 = \langle \kappa_\gamma^h, \kappa_\gamma^h \rangle_{\Gamma^h}^h - \langle \gamma'(\vec{\nu}^h), [\vec{X}_{t,s}^h]^\perp \rangle_{\Gamma^h} = \langle \kappa_\gamma^h, \kappa_\gamma^h \rangle_{\Gamma^h}^h + \frac{\mathrm{d}}{\mathrm{d}t} |\Gamma^h(t)|_\gamma \,.$$

Problem: For a general anisotropy γ it does not appear possible to derive a (linear) semi-implicit fully discrete finite element approximation that mimicks this behaviour, i.e. that satisfies

$$|\Gamma^{m+1}|_\gamma + \tau_m \langle \kappa_\gamma^{m+1}, \kappa_\gamma^{m+1} \rangle_{\Gamma^m}^h \leq |\Gamma^m|_\gamma$$

and so is **unconditionally stable**.

IDEA: Restrict class of admissible anisotropies.

Example Anisotropy

As the simplest example, take the following "elliptic" anisotropy:

$$\gamma(\vec{p}) := \sqrt{\vec{p}\,.\,G\,\vec{p}},$$

where $G \in \mathbb{R}^{2\times 2}$ is symmetric and positive definite.

Note that

$$\gamma'(\vec{p}) = [\gamma(\vec{p})]^{-1}\,G\,\vec{p}.$$

For the semi-implicit fully discrete scheme we then approximate $\gamma'(\vec{\nu}^h)$ by

$$[\gamma(\vec{\nu}^m)]^{-1}\,G\,\vec{\nu}^{m+1} = -[\gamma(\vec{\nu}^m)]^{-1}\,G\,[\vec{X}_s^{m+1}]^{\perp}$$

to obtain a linear, unconditionally stable approximation.

Given $\Gamma^0 = \vec{X}^0(I)$, $\vec{X}^0 \in \underline{V}^h$, for $m = 0 \to M-1$ find $\vec{X}^{m+1} \in \underline{V}^h$ and $\kappa_\gamma^{m+1} \in V^h$ such that

$$\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\,\vec{\nu}^m\rangle_{\Gamma^m}^h - \langle \kappa_\gamma^{m+1}, \chi\rangle_{\Gamma^m}^h = 0 \qquad \forall\ \chi \in V^h;$$

$$\langle \kappa_\gamma^{m+1}\,\vec{\nu}^m, \vec{\eta}\rangle_{\Gamma^m}^h + \langle [\gamma(\vec{\nu}^m)]^{-1}\,G\,[\vec{X}_s^{m+1}]^{\perp}, \vec{\eta}_s^{\perp}\rangle_{\Gamma^m} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}^h.$$

$$\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \rangle^h_{\Gamma^m} - \langle \kappa_\gamma^{m+1}, \chi \rangle^h_{\Gamma^m} = 0 \qquad \forall\ \chi \in V^h;$$

$$\langle \kappa_\gamma^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle^h_{\Gamma^m} + \langle [\gamma(\vec{\nu}^m)]^{-1}\, G\, [\vec{X}_s^{m+1}]^\perp, \vec{\eta}_s^\perp \rangle_{\Gamma^m} = 0 \qquad \forall\ \vec{\eta} \in \underline{V}^h.$$

Stability: Choose $\chi = \kappa_\gamma^{m+1}$ and $\vec{\eta} = \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}$ and observe that

$$\langle [\gamma(\vec{\nu}^m)]^{-1} G\, [\vec{X}_s^{m+1}]^\perp, [\vec{X}^{m+1} - \vec{X}^m]_s^\perp \rangle_{\Gamma^m} = \sum_{j=1}^N \frac{[\vec{h}_j^{m+1}]^\perp . G\,(\,[\vec{h}_j^{m+1}]^\perp - [\vec{h}_j^m]^\perp\,)}{\gamma([\vec{h}_j^m]^\perp)}$$

$$= \sum_{j=1}^N \frac{(\gamma([\vec{h}_j^{m+1}]^\perp) - \gamma([\vec{h}_j^m]^\perp))^2}{\gamma([\vec{h}_j^m]^\perp)}$$

$$+ \sum_{j=1}^N \frac{\gamma([\vec{h}_j^{m+1}]^\perp)\,\gamma([\vec{h}_j^m]^\perp) - [\vec{h}_j^{m+1}]^\perp . G\,[\vec{h}_j^m]^\perp}{\gamma([\vec{h}_j^m]^\perp)}$$

$$+ \sum_{j=1}^N \left[\gamma([\vec{h}_j^{m+1}]^\perp) - \gamma([\vec{h}_j^m]^\perp)\right]$$

$$\geq \sum_{j=1}^N \left[\gamma([\vec{h}_j^{m+1}]^\perp) - \gamma([\vec{h}_j^m]^\perp)\right] = \int_{\Gamma^{m+1}} \gamma(\vec{\nu}^{m+1})\, \mathrm{d}s - \int_{\Gamma^m} \gamma(\vec{\nu}^m)\, \mathrm{d}s.$$

Note: Inequality also holds element-wise.

Idea: Consider an l_r-norm of such "elliptic" anisotropies.

$$\gamma(\vec{p}) = \left(\sum_{\ell=1}^{L} [\gamma_\ell(\vec{p})]^r\right)^{\frac{1}{r}}, \qquad \gamma_\ell(\vec{p}) := \sqrt{\vec{p}\,.\,G_\ell\,\vec{p}}, \qquad r \in [1,\infty),$$

where $G_\ell \in \mathbb{R}^{2\times 2}$, $\ell = 1 \to L$, are symmetric and positive definite.

Note that

$$\gamma'(\vec{p}) = [\gamma(\vec{p})]^{1-r} \sum_{\ell=1}^{L} [\gamma_\ell(\vec{p})]^{r-1}\,\gamma'_\ell(\vec{p})\,.$$

For the semi-implicit fully discrete scheme we then approximate $\gamma'(\vec{\nu}^h)$ by

$$\sum_{\ell=1}^{L}\left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} [\gamma_\ell(\vec{\nu}^m)]^{-1}\,G_\ell\,\vec{\nu}^{m+1}$$
$$= -\sum_{\ell=1}^{L}\left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} [\gamma_\ell(\vec{\nu}^m)]^{-1}\,G_\ell\,[\vec{X}_s^{m+1}]^\perp$$

to obtain an unconditionally stable approximation that is linear for $r = 1$.

Given $\Gamma^0 = \vec{X}^0(I)$, $\vec{X}^0 \in \underline{V}^h$, for $m = 0 \to M-1$ find $\vec{X}^{m+1} \in \underline{V}^h$ and $\kappa_\gamma^{m+1} \in V^h$ such that

$$\langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \rangle_{\Gamma^m}^h - \langle \kappa_\gamma^{m+1}, \chi \rangle_{\Gamma^m}^h = 0 \quad \forall\ \chi \in V^h;$$

$$\langle \kappa_\gamma^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle_{\Gamma^m}^h + \sum_{\ell=1}^{L} \langle \left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} [\gamma_\ell(\vec{\nu}^m)]^{-1} G_\ell\, [\vec{X}_s^{m+1}]^\perp, \vec{\eta}_s^\perp \rangle_{\Gamma^m} = 0 \quad \forall\ \vec{\eta} \in \underline{V}^h.$$

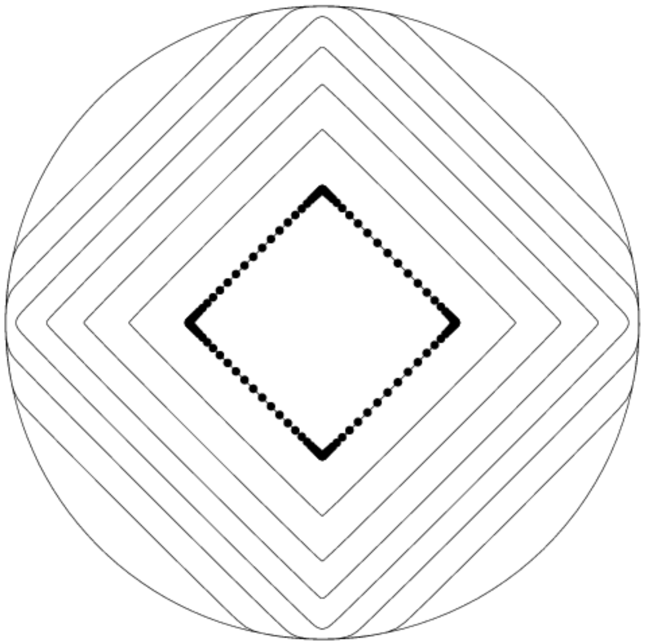
Stability: Choose $\chi = \kappa_\gamma^{m+1}$ and $\vec{\eta} = \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}$, use element-wise inequality for each γ_ℓ and apply Hölder to obtain that

$$\sum_{\ell=1}^{L} \langle \left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} [\gamma_\ell(\vec{\nu}^m)]^{-1}\, G_\ell\, [\vec{X}_s^{m+1}]^\perp, [\vec{X}^{m+1} - \vec{X}^m]_s^\perp \rangle_{\Gamma^m}$$
$$\geq \sum_{\ell=1}^{L} \int_{\Gamma^{m+1}} \left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} \gamma_\ell(\vec{\nu}^{m+1})\ \mathrm{d}s - \sum_{\ell=1}^{L} \int_{\Gamma^m} \left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r-1} \gamma_\ell(\vec{\nu}^m)\ \mathrm{d}s$$
$$\geq \int_{\Gamma^{m+1}} \sum_{\ell=1}^{L} \left[\frac{\gamma_\ell(\vec{\nu}^{m+1})}{\gamma(\vec{\nu}^{m+1})}\right]^{r} \gamma(\vec{\nu}^{m+1})\ \mathrm{d}s - \int_{\Gamma^m} \left(\sum_{\ell=1}^{L} [\gamma_\ell(\vec{\nu}^m)]^r\right)^{\frac{1}{r}}\ \mathrm{d}s$$
$$= \int_{\Gamma^{m+1}} \gamma(\vec{\nu}^{m+1})\ \mathrm{d}s - \int_{\Gamma^m} \gamma(\vec{\nu}^m)\ \mathrm{d}s\,.$$

Numerical Results for (MC$_\gamma$)

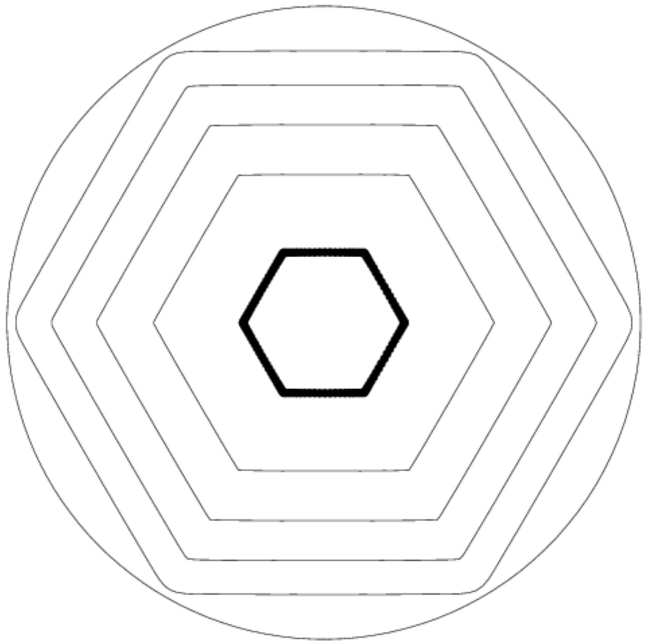
$$G_\ell := R(-\theta_\ell)D(\varepsilon_\ell)R(\theta_\ell), \quad \text{where } D(\varepsilon) := \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon^2 \end{pmatrix}, \ R(\theta) := \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$

$\varepsilon_\ell \equiv 10^{-2}$, $(\theta_1,\ldots,\theta_L) = (\frac{\pi}{4}, \frac{3\pi}{4})$



$N = 128$, $\tau = 10^{-3}$,
$t = 0,\ 0.05, \ldots, T = 0.35$

$\varepsilon_\ell \equiv 10^{-2}$, $(\theta_1,\ldots,\theta_L) = (0, \frac{\pi}{3}, \frac{2\pi}{3})$



$N = 128$, $\tau = 10^{-3}$,
$t = 0,\ 0.05, \ldots, T = 0.25$

Extension to 3d

Extending the approximation from 2d to 3d is **not straightforward**.

But using ideas from differential geometry, Barrett, Garcke, Nürnberg (08) reformulated the anisotropic mean curvature $\varkappa_\gamma$ in a way that lends itself to a stable variational approximation for $d = 2$ and $d = 3$.

In particular, for

$$\gamma(\vec{p}) = \left(\sum_{\ell=1}^{L} [\gamma_\ell(\vec{p})]^r \right)^{\frac{1}{r}}, \qquad \gamma_\ell(\vec{p}) := \sqrt{\vec{p} \, . \, G_\ell \, \vec{p}}, \qquad r \in [1, \infty),$$

where $G_\ell \in \mathbb{R}^{d \times d}$, $\ell = 1 \to L$, are symmetric and positive definite, we obtain the identity

$$\varkappa_\gamma \, \vec{\nu} = \sum_{\ell=1}^{L} \gamma_\ell(\vec{\nu}) \, \widetilde{G}_\ell \, \nabla_s^{\widetilde{G}_\ell} \, . \left[\left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})} \right]^{r-1} \nabla_s^{\widetilde{G}_\ell} \, \vec{x} \right].$$

Here

$$\widetilde{G}_\ell := [\det G_\ell]^{\frac{1}{2}} \, G_\ell^{-1}, \qquad \ell = 1 \to L,$$

and $\nabla_s^{\widetilde{G}_\ell}$, $\nabla_s^{\widetilde{G}_\ell} .$ are anisotropic surface gradient and divergence operators induced by the inner product

$$(\vec{u}, \vec{v})_{\widetilde{G}_\ell} := \vec{u} \, . \, \widetilde{G}_\ell \, \vec{v} \qquad \forall \, \vec{u}, \, \vec{v} \in \mathbb{R}^d.$$

Note: In contrast to

$$\varkappa_\gamma\,\vec\nu = -\nabla_s\,.\,(\vec\nu\,[\gamma'(\vec\nu)]^T) + \nabla_s\,.\,(\gamma(\vec\nu)\,\nabla_s\,\vec x) - \gamma(\vec\nu)\,\Delta_s\,\vec x\,,$$

which is based on the standard, isotropic differential operators, the identity

$$\varkappa_\gamma\,\vec\nu = \sum_{\ell=1}^{L} \gamma_\ell(\vec\nu)\,\widetilde G_\ell\,\nabla_s^{\widetilde G_\ell}\,.\,\left[\left[\frac{\gamma_\ell(\vec\nu)}{\gamma(\vec\nu)}\right]^{r-1}\nabla_s^{\widetilde G_\ell}\,\vec x\right]\,,$$

gives rise to a symmetric formulation. In particular, we obtain:

Find $\{\vec X^{m+1}, \kappa_\gamma^{m+1}\} \in \underline{V}^h(\Gamma^m)\times V^h(\Gamma^m)$ such that

$$\langle\frac{\vec X^{m+1}-\vec X^m}{\tau_m}, \chi\,\vec\nu^m\rangle^h_{\Gamma^m} - \langle\kappa_\gamma^{m+1},\chi\rangle^h_{\Gamma^m} = 0 \qquad \forall\;\chi\in V^h(\Gamma^m),$$

$$\langle\kappa_\gamma^{m+1}\,\vec\nu^m,\vec\eta\rangle^h_{\Gamma^m} + \langle\nabla_s^{\widetilde G}\,\vec X^{m+1},\nabla_s^{\widetilde G}\,\vec\eta\rangle_{\gamma,\Gamma^m} = 0 \qquad \forall\;\vec\eta\in\underline{V}^h(\Gamma^m)\,,$$

where

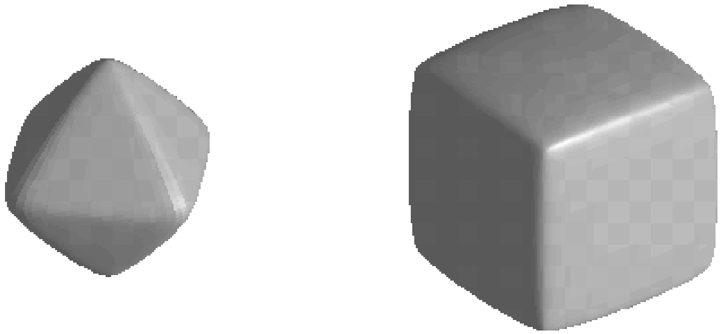
$$\langle\nabla_s^{\widetilde G}\,\vec X^{m+1},\nabla_s^{\widetilde G}\,\vec\eta\rangle_{\gamma,\Gamma^m} := \sum_{\ell=1}^{L}\int_{\Gamma^m}\left[\frac{\gamma_\ell(\vec\nu^{m+1})}{\gamma(\vec\nu^{m+1})}\right]^{r-1}(\nabla_s^{\widetilde G_\ell}\,\vec X^{m+1},\nabla_s^{\widetilde G_\ell}\,\vec\eta)_{\widetilde G_\ell}\,\gamma_\ell(\vec\nu^m)\;\mathrm{d}s\,.$$

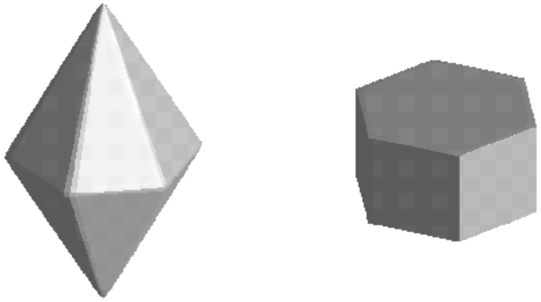
$r=1$: Linear system. Existence, uniqueness and stability.

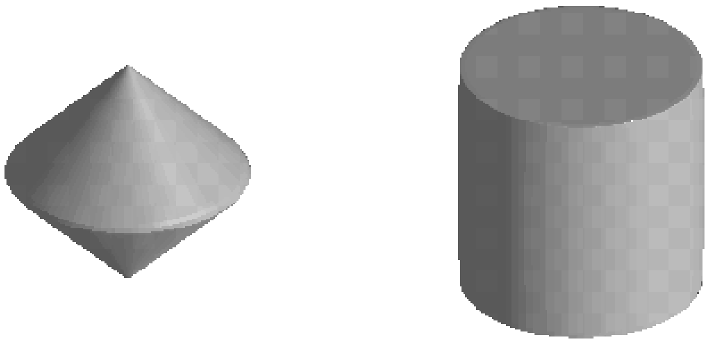
$r>1$: Nonlinear system. Stability.

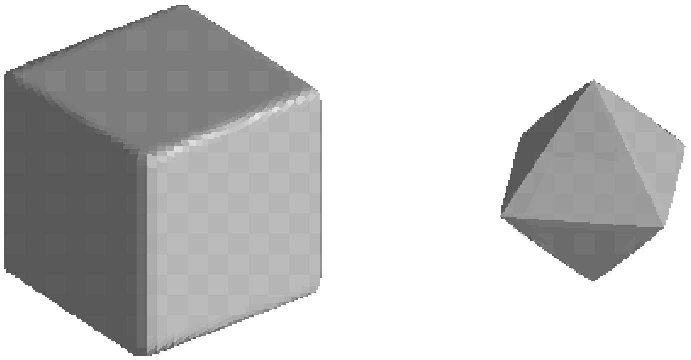
Example Anisotropies, $d = 3$

Examples of Frank diagrams $\mathcal{F}$ and associated Wulff shapes $\mathcal{W}$:









Find the temperature $u(\cdot,t) : \Omega \to \mathbb{R}$ and the interface $\Gamma(t) \subset \Omega$ such that for $t \in (0,T]$

$$\vartheta\, u_t - \Delta u = f \qquad \text{in } \Omega \setminus \Gamma(t),$$

$$\left[\frac{\partial u}{\partial \vec{\nu}}\right]_{\Gamma(t)} = -\lambda\, \mathcal{V} \qquad \text{on } \Gamma(t), \qquad \text{(Stefan condition)}$$

$$\rho\, \mathcal{V} = \beta(\vec{\nu})\; [\alpha\, \varkappa_\gamma - a\, u] \qquad \text{on } \Gamma(t), \qquad \text{(Gibbs-Thomson condition)}$$

$$u = u_D \qquad \text{on } \partial\Omega$$

with $u(\cdot,0)$ and $\Gamma(0)$ specified.

Here $\lambda \in \mathbb{R}_{>0}$ is the latent heat, ϑ, ρ, $\alpha \in \mathbb{R}_{\geq 0}$ and $a \in \mathbb{R}_{>0}$.

In addition, $\varkappa_\gamma$ is the weighted mean curvature of Γ, based on a given anisotropy function $\gamma(\cdot)$, and $\beta(\cdot)$ is a given anisotropic mobility.

Let $(\eta, \phi) := \int_\Omega \eta\, \phi \, \mathrm{d}\vec{z}$. For a test function φ with $\varphi = 0$ on $\partial\Omega$, we have that

$$\vartheta\,(u_t, \varphi) + (\nabla u, \nabla \varphi) - (f, \varphi) = - \int_{\Gamma(t)} \left[\frac{\partial u}{\partial \vec{\nu}}\right]_{\Gamma(t)} \varphi \, \mathrm{d}s = \lambda \int_{\Gamma(t)} (\vec{x}_t \,.\, \vec{\nu})\, \varphi \, \mathrm{d}s \,. \quad (1)$$

Moreover

$$\rho\,(\vec{x}_t \,.\, \vec{\nu}) = \beta(\vec{\nu})\; [\alpha\, \varkappa_\gamma - a\, u] \qquad (2)$$

and

$$\varkappa_\gamma\, \vec{\nu} = \sum_{\ell=1}^{L} \gamma_\ell(\vec{\nu})\, \widetilde{G}_\ell\, \nabla_s^{\widetilde{G}_\ell} \,.\, \left[\left[\frac{\gamma_\ell(\vec{\nu})}{\gamma(\vec{\nu})}\right]^{r-1} \nabla_s^{\widetilde{G}_\ell}\, \vec{x}\right] . \qquad (3)$$

Testing (1) with $\varphi = u - u_D$, (2) with $\chi = \frac{\lambda}{a}\, \vec{x}_t \,.\, \vec{\nu}$ and (3) with $\vec{\eta} = \frac{\alpha\,\lambda}{a}\, \vec{x}_t$ yields that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\vartheta}{2}\, |u - u_D|_\Omega^2 + \frac{\alpha\,\lambda}{a}\, |\Gamma(t)|_\gamma + \lambda\, u_D \, \mathrm{vol}(\Omega_s(t))\right) + |\nabla u|_\Omega^2 + \frac{\lambda\,\rho}{a} \int_{\Gamma(t)} \frac{\mathcal{V}^2}{\beta(\vec{\nu})}\, \mathrm{d}s$$
$$= (f, u - u_D)\,.$$

We will directly discretize (1)–(3), resulting in a coupled system, and obtain a discrete analogue of this energy bound.

Based on continuous piecewise linear approximations of u, Γ and $\varkappa_\gamma$.

For $m \geq 0$, given $U^m \in S^h_D$ and $\vec{X}^m \in \underline{V}^h(\Gamma^m)$,
find $U^{m+1} \in S^h_D$, $\vec{X}^{m+1} \in \underline{V}^h(\Gamma^m)$ and $\kappa_\gamma^{m+1} \in W^h(\Gamma^m)$ such that for all $\varphi \in S^h_0$, $\chi \in W^h(\Gamma^m)$, $\vec{\eta} \in \underline{V}^h(\Gamma^m)$

$$\vartheta \left(\frac{U^{m+1} - U^m}{\tau_m}, \varphi \right)^h + (\nabla U^{m+1}, \nabla \varphi) - \lambda \left\langle \pi^m \left[\frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m} . \vec{\omega}^m \right], \varphi \right\rangle_{\Gamma^m} = (f^{m+1}, \varphi)^h ,$$

$$\rho \left\langle [\beta(\vec{\nu}^m)]^{-1} \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \right\rangle^h_{\Gamma^m} - \alpha \langle \kappa_\gamma^{m+1}, \chi \rangle^h_{\Gamma^m} + a \langle U^{m+1}, \chi \rangle_{\Gamma^m} = 0 ,$$

$$\langle \kappa_\gamma^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle^h_{\Gamma^m} + \langle \nabla_s^{\widetilde{G}}\, \vec{X}^{m+1}, \nabla_s^{\widetilde{G}}\, \vec{\eta} \rangle_{\gamma,\Gamma^m} = 0 .$$

Coupled system of equations.

$r = 1$: Linear system. Existence, uniqueness and stability.

$r > 1$: Nonlinear system. Stability.

$$\vartheta \left(\frac{U^{m+1}-U^m}{\tau_m}, \varphi\right)^h + (\nabla U^{m+1}, \nabla \varphi) - \lambda \left\langle \pi^m \left[\frac{\vec X^{m+1}-\vec X^m}{\tau_m} \,.\, \vec\omega^m\right], \varphi \right\rangle_{\Gamma^m} = (f^{m+1}, \varphi)^h \,,$$

$$\rho \left\langle [\beta(\vec\nu^m)]^{-1} \frac{\vec X^{m+1}-\vec X^m}{\tau_m}, \chi\, \vec\omega^m \right\rangle^h_{\Gamma^m} - \alpha\, \langle \kappa_\gamma^{m+1}, \chi\rangle^h_{\Gamma^m} + a\, \langle U^{m+1}, \chi\rangle_{\Gamma^m} = 0\,,$$

$$\langle \kappa_\gamma^{m+1}\, \vec\omega^m, \vec\eta\rangle^h_{\Gamma^m} + \langle \nabla_s^{\widetilde G}\, \vec X^{m+1}, \nabla_s^{\widetilde G}\, \vec\eta\rangle_{\gamma,\Gamma^m} = 0\,.$$

Stability: Choose $\varphi = U^{m+1} - u_D$, $\chi = \frac{\lambda}{a}\,\pi^m[(\vec X^{m+1}-\vec X^m)\,.\,\vec\omega^m]$ and $\vec\eta = \frac{\alpha\,\lambda}{a}\,(\vec X^{m+1}-\vec X^m)$ yields, on recalling that

$$\langle \nabla_s^{\widetilde G}\, \vec X^{m+1}, \nabla_s^{\widetilde G}\, (\vec X^{m+1}-\vec X^m)\rangle_{\gamma,\Gamma^m} \geq |\Gamma^{m+1}|_\gamma - |\Gamma^m|_\gamma\,,$$

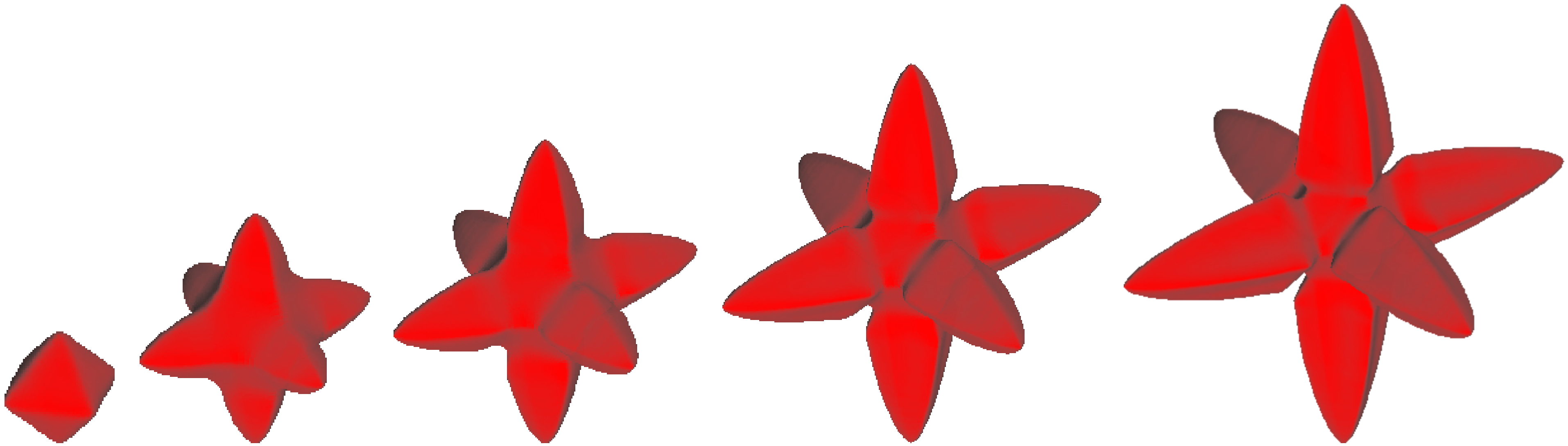
that

$$\mathcal{E}(U^{m+1}, \vec X^{m+1}) + \lambda\, u_D\, \langle \vec X^{m+1}-\vec X^m, \vec\nu^m\rangle^h_{\Gamma^m} + \frac{\vartheta}{2}\, |U^{m+1}-U^m|^2_{\Omega,h}$$
$$+ \tau_m\, |\nabla U^{m+1}|^2_\Omega + \tau_m\, \frac{\lambda\,\rho}{a} \left| [\beta(\vec\nu^m)]^{-\frac12} \frac{\vec X^{m+1}-\vec X^m}{\tau_m} \,.\, \vec\omega^m \right|^2_{\Gamma^m,h}$$
$$\leq \mathcal{E}(U^m, \vec X^m) + (f^{m+1}, U^{m+1}-u_D)^h\,;$$

where $\mathcal{E}(U^m, \vec X^m) := \frac{\vartheta}{2}\,|U^m-u_D|^2_{\Omega,h} + \frac{\alpha\,\lambda}{a}\,|\Gamma^m|_\gamma$.

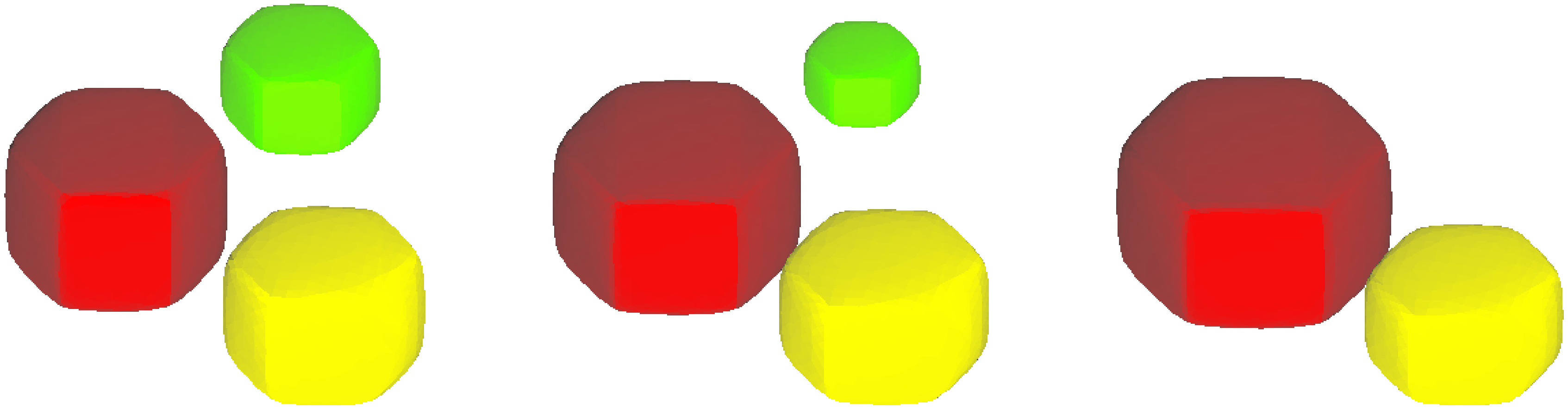
$\gamma(\vec{\nu})$ is a cubic anisotropy ($\{G_\ell\}_{\ell=1}^3$, with $r = 9$ and reg. $\varepsilon = 0.6$).

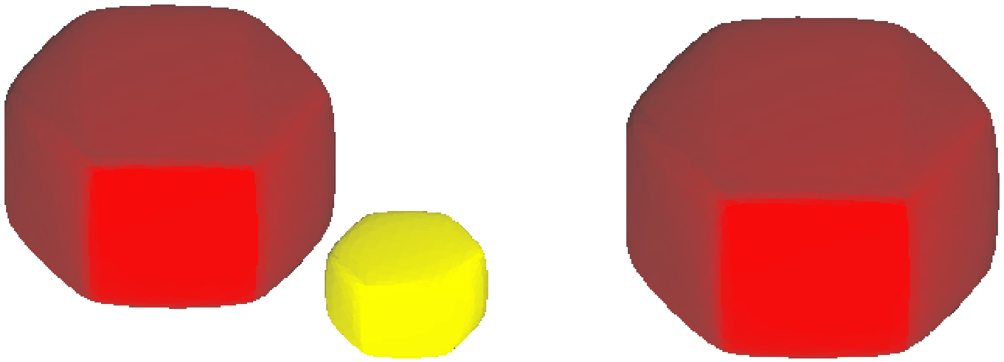
$\beta(\vec{\nu}) = \gamma(\vec{\nu})$, $u_D = -1$, $\Omega = (-4, 4)^3$, $\Gamma(0)$ sphere radius $\frac{1}{10}$.

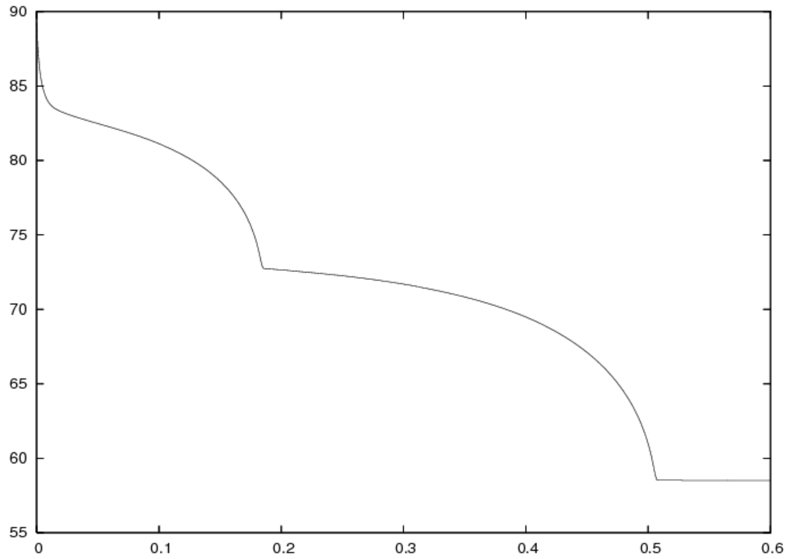


$\vec{X}(t)$ at times $t = 0.1, 0.2, 0.25, 0.3, 0.34$.
Mesh parameters $N_f = 512$, $N_c = 32$ for Ω,
$J_\Gamma^0 = 768$ for Γ and uniform time step $\tau = 2 \times 10^{-4}$.

Anisotropic Mullins–Sekerka ($\vartheta = \rho = 0,\ \lambda = a = \alpha = 1$)







$\vec{X}(t)$ at times $t = 0.05$, 0.15 0.3, 0.45, $T = 0.6$, and the energy $|\Gamma^m|$.

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