Mathematisches Forschungsinstitut Oberwolfach

Report No. 6/2017

DOI: 10.4171/OWR/2017/6

Emerging Developments in Interfaces and Free Boundaries

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22 January – 28 January 2017

Abstract. The field of the mathematical and numerical analysis of systems of nonlinear partial differential equations involving interfaces and free boundaries is a well established and flourishing area of research. This workshop focused on recent developments and emerging new themes. By bringing together experts in these fields we achieved progress in open questions and developed novel research directions in mathematics related to interfaces and free boundaries. This interdisciplinary workshop brought together researchers from distinct mathematical fields such as analysis, computation, optimisation and modelling to discuss emerging challenges.

Mathematics Subject Classification (2010): 35-XX, 49-XX, 65-XX.

Introduction by the Organisers

The workshop *Emerging Developments in Interfaces and Free Boundaries*, organised by Charles M. Elliott (Warwick), Yoshikazu Giga (Tokyo), Michael Hinze (Hamburg) and Vanessa Styles (Brighton) was attended by 54 participants from Austria, France, Germany, Great Britain, Japan, and the United States, with expertise from three main areas: optimal control of partial differential equations, modelling involving free boundary problems and mathematical and numerical analysis of free boundary problems. Apart from discussing current problems, techniques and issues across the differing communities the focus of the workshop was set on

(1) Diffuse interface methods – modelling, analysis, and optimization,
(2) Analysis and approximation of PDEs on evolving domains,
(3) Evolution of interfaces and free boundaries with applications.

The presentations of Abels, Aland, Blank, Deckelnick, Kahle, Lam, Salgado, Stoll and Wirth concerned modelling, analytical, numerical and optimization approaches to interfaces and free boundaries using diffuse interface methods, while Antil, Bartels, Chambolle, Fritz, van Gennip, Mi-Ho Giga, Hamamuki, Kimura, Lehrenfeld, Nochetto, Ohtsuka, Olshanski, Schulz, Shirakawa and Yamamoto presented talks related to analysis and numerical methods for problems related to evolving shapes and PDEs on evolving domains. Gräser, Kenmochi, King, Liu, Luckhaus, Ranner and Ren gave talks on mathematical modelling of applications related to interfaces and free boundaries.

To offer young researchers a stage for presenting their research, a session for young researchers was organized on Wednesday evening where Tatsu-Hiko Miura, Tatsuya Miura and Siebenborn together with the Oberwolfach Leibniz Graduate Students Alphonse and Djurdjevac took this opportunity and gave talks on their current research results.

Surveys and articles concerning mathematical and numerical approaches to interfaces and free boundary problems may be found in the conference and symposium proceedings [3, 6, 11, 15]. The books [2, 10, 13] contain models, numerical methods and analysis for variational and level set approaches. Modern mathematical concepts of control and optimization with partial differential equation constraints are developed in [14, 16]. Shape optimisation and problems of optimal design are surveyed in [4, 5]. Analysis and numerics for surface PDEs are presented in [1, 9, 17]. Also we mention surveys of models and numerical methods for interface evolution involving curvature, [8, 12]. Finally we remark that many recent references concerning the issues of the workshop are provided at the end of each extended abstract.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1049268, "US Junior Oberwolfach Fellows". Moreover, the MFO and the workshop organizers would like to thank the Simons Foundation for supporting Professor Ricardo Nochetto in the "Simons Visiting Professors" program at the MFO.

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Workshop: Emerging Developments in Interfaces and Free Boundaries

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Abstracts

Sharp Interface Limit for a Stokes/Allen-Cahn System

Helmut Abels
(joint work with Yuning Liu)

We consider the sharp interface limit of a coupled Stokes/Allen-Cahn system, when a parameter $\varepsilon > 0$ that is proportional to the thickness of the diffuse interface tends to zero, in a two dimensional bounded domain $\Omega \subseteq \mathbb{R}^2$. For sufficiently small times we prove convergence of the solutions of the Stokes/Allen-Cahn system to solutions of a sharp interface model, where the interface evolution is given by the mean curvature equation with an additional convection term coupled to a two-phase Stokes system with an additional contribution to the stress tensor, which describes the capillary stress. More precisely, we consider the asymptotic limit $\varepsilon \to 0$ of the following system:

$$-\Delta \mathbf{v}_\varepsilon + \nabla p_\varepsilon = -\varepsilon \operatorname{div}(\nabla c_\varepsilon \otimes \nabla c_\varepsilon) \quad \text{in } \Omega \times (0,T_1), \tag{1}$$

$$\operatorname{div} \mathbf{v}_\varepsilon = 0 \quad \text{in } \Omega \times (0,T_1), \tag{2}$$

$$\partial_t c_\varepsilon + \mathbf{v}_\varepsilon \cdot \nabla c_\varepsilon = \Delta c_\varepsilon - \frac{1}{\varepsilon^2} f'(c_\varepsilon) \quad \text{in } \Omega \times (0,T_1), \tag{3}$$

$$\mathbf{v}_\varepsilon|_{\partial\Omega} = 0 \quad c_\varepsilon|_{\partial\Omega} = -1 \quad \text{on } \partial\Omega \times (0,T_1), \tag{4}$$

$$c_\varepsilon|_{t=0} = c_{0,\varepsilon} \quad \text{in } \Omega \tag{5}$$

for a suitable double well potential f and for suitable "well-prepared" initial data $c_{0,\varepsilon}$ specified below. Here $\mathbf{v}_\varepsilon, p_\varepsilon$ are the velocity and the pressure of the fluid mixture, μ_ε is a chemical potential and c_ε is related to the concentration difference of the fluids. The sharp interface limit of (1)-(5) is the system

$$-\Delta \mathbf{v} + \nabla p = 0 \quad \text{in } \Omega^\pm(t), t \in [0,T_0], \tag{6}$$

$$\operatorname{div} \mathbf{v} = 0 \quad \text{in } \Omega^\pm(t), t \in [0,T_0], \tag{7}$$

$$[2D\mathbf{v} - p\mathbf{I}]\mathbf{n}_{\Gamma_t} = -\sigma H_{\Gamma_t} \mathbf{n}_{\Gamma_t} \quad \text{on } \Gamma_t, t \in [0,T_0], \tag{8}$$

$$[\mathbf{v}] = 0 \quad \text{on } \Gamma_t, t \in [0,T_0], \tag{9}$$

$$\mathbf{v}|_{\partial\Omega} = 0 \quad \text{on } \partial\Omega \times [0,T_0], \tag{10}$$

$$V_{\Gamma_t} - \mathbf{n}_{\Gamma_t} \cdot \mathbf{v}|_{\Gamma_t} = H_{\Gamma_t} \quad \text{on } \Gamma_t, t \in [0,T_0]. \tag{11}$$

Here Ω is the disjoint union of $\Omega^+(t), \Omega^-(t)$, and Γ_t for every $t \in [0,T_0]$, $\Omega^\pm(t)$ are smooth domains, $\Gamma_t = \partial\Omega^+(t)$, $\mathbf{n}_{\Gamma_t}$ is the interior normal of Γ_t with respect to $\Omega^+(t)$. Moreover,

$$[u](p,t) = \lim_{h \to 0+} [u(p + \mathbf{n}_{\Gamma_t}(p)h) - u(p - \mathbf{n}_{\Gamma_t}(p)h)]$$

is the jump of a function $u\colon \Omega \times [0,T_0] \to \mathbb{R}^2$ at Γ_t in direction of $\mathbf{n}_{\Gamma_t}$, H_{Γ_t} and V_{Γ_t} are the curvature and the normal velocity of Γ_t, both with respect to $\mathbf{n}_{\Gamma_t}$.

Furthermore, $D\mathbf{v} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)$ and $\sigma = \int_{\mathbb{R}} \theta_0'(\rho)^2\, d\rho$, where θ_0 is the so-called optimal profile that is the unique solution of

$$-\theta_0''(\rho) + f'(\theta_0(\rho)) = 0 \qquad \text{for all } \rho \in \mathbb{R}, \tag{12}$$

$$\lim_{\rho\to\pm\infty} \theta_0(\rho) = \pm 1, \qquad \theta_0(0) = 0. \tag{13}$$

In the following we assume that $(\mathbf{v}, p, \Gamma)$ is a smooth solution of the limit equation (6)-(11) for some $T_0 > 0$, where $(\Gamma_t)_{t\in[0,T_0]}$ is a family of smoothly evolving compact, non-self-intersecting, closed curves in Ω. More precisely, we assume that

$$\Gamma := \bigcup_{t\in[0,T_0]} \Gamma_t \times \{t\}$$

is a smooth two-dimensional submanifold of $\Omega \times \mathbf{R}$ (with boundary), and $\mathbf{v}|_{\Omega^\pm} \in C^\infty(\overline{\Omega^\pm})^2$, $p|_{\Omega^\pm} \in C^\infty(\overline{\Omega^\pm})$, where

$$\Omega^\pm = \bigcup_{t\in[0,T_0]} \Omega^\pm(t) \times \{t\}.$$

In particular, we assume that $\Gamma_t \subseteq \Omega$ for every $t \in [0, T_0]$, which excludes contact angle problems. Moreover, for $T_1 \geq T_0$ let $(\mathbf{v}_\varepsilon, p_\varepsilon, c_\varepsilon)$ be the (classical) solution of (1)-(5) with smooth initial values $c_{0,\varepsilon}\colon \Omega \to \mathbf{R}$, which will be specified in the main result below.

For the statement of our main result, we need tubular neighborhoods of Γ_t. For $\delta > 0$ and $t \in [0, T_0]$ we defined

$$\Gamma_t(\delta) := \{y \in \Omega : \operatorname{dist}(y, \Gamma_t) < \delta\}, \quad \Gamma(\delta) = \bigcup_{t\in[0,T_0]} \Gamma_t(\delta) \times \{t\}.$$

Moreover, we define the signed distance function

$$d_\Gamma(x,t) := \operatorname{sdist}(\Gamma_t, x) = \begin{cases} \operatorname{dist}(\Omega^-(t), x) & \text{if } x \notin \Omega^-(t) \\ -\operatorname{dist}(\Omega^+(t), x) & \text{if } x \in \Omega^-(t) \end{cases}$$

for all $x \in \Omega, t \in [0, T_0]$. Since Γ is smooth and compact, there is some $\delta > 0$ sufficiently small, such that $d_\Gamma\colon \Gamma(3\delta) \to \mathbf{R}$ is smooth.

Now our main result is:

Theorem (Sharp Interface Limit for Short Times, [1, Theorem 1.1])
Let $N = 2$, $(\mathbf{v}, \Gamma)$ be a smooth solution of (6)-(11) for some $T_0 \in (0, \infty)$ and let

$$c_{A,0}^0(x) = \zeta(d_{\Gamma_0}(x))\theta_0\left(\frac{d_{\Gamma_0}(x)}{\varepsilon}\right) + (1 - \zeta(d_{\Gamma_0}(x)))\left(\chi_{\Omega^+(0)}(x) - \chi_{\Omega^-(0)}(x)\right)$$

for all $x \in \Omega$, where $d_{\Gamma_0} = d_\Gamma|_{t=0}$ is the signed distance function to Γ_0 and $\zeta \in C^\infty(\mathbb{R})$ such that

$$\zeta(s) = 1 \text{ if } |s| \leq \delta;\ \zeta(s) = 0 \text{ if } |s| \geq 2\delta;\ 0 \leq -s\zeta'(s) \leq 4 \text{ if } \delta \leq |s| \leq 2\delta. \tag{14}$$

Moreover, let $c_{0,\varepsilon}\colon \Omega \to \mathbb{R}$, $0 < \varepsilon \leq 1$, be smooth such that

$$\|c_{0,\varepsilon} - c_{A,0}^0\|_{L^2(\Omega)} \leq C\varepsilon^{N+\frac{1}{2}} \qquad \text{for all } \varepsilon \in (0, 1]$$

and some $C > 0$, $\sup_{0<\varepsilon\le 1} \|c_{0,\varepsilon}\|_{L^\infty(\Omega)} < \infty$ *and* $(\mathbf{v}_\varepsilon, c_\varepsilon)$ *be the corresponding solutions of* (1)-(5). *Then there are some* $\varepsilon_0 \in (0,1]$, $R > 0$, $T \in (0, T_0]$, *and* $c_A \colon \Omega \times [0,T_0] \to \mathbb{R}$, $\mathbf{v}_A \colon \Omega \times [0,T_0] \to \mathbb{R}^2$ *(depending on* ε*) such that*

$$\sup_{0\le t\le T} \|c_\varepsilon(t) - c_A(t)\|_{L^2(\Omega)} + \|\nabla(c_\varepsilon - c_A)\|_{L^2(\Omega\times(0,T)\setminus\Gamma(\delta))} \le R\varepsilon^{N+\frac{1}{2}}$$

$$\|\nabla_{\boldsymbol{\tau}}(c_\varepsilon - c_A)\|_{L^2(\Omega\times(0,T)\cap\Gamma(2\delta))} + \varepsilon\|\partial_{\mathbf{n}}(c_\varepsilon - c_A)\|_{L^2(\Omega\times(0,T)\cap\Gamma(2\delta))} \le R\varepsilon^{N+\frac{1}{2}}$$

and for any $q \in [1,2)$

$$\|\mathbf{v}_\varepsilon - \mathbf{v}_A\|_{L^2(0,T;L^q(\Omega))} \le C(q,R)\varepsilon^2 \tag{15}$$

hold true for all $\varepsilon \in (0,\varepsilon_0]$ *and some* $C(q,R) > 0$. *Moreover,*

$$\lim_{\varepsilon\to 0} c_A = \pm 1 \qquad \text{uniformly on compact subsets of } \Omega^\pm.$$

and

$$\mathbf{v}_A = \mathbf{v} + O(\varepsilon) \qquad \text{in} L^\infty(\Omega\times(0,T)) \text{ as } \varepsilon \to 0.$$

We note that the result is comparable to results known for single phase field models like the Allen-Cahn, the Cahn-Hilliard, or the volume preserving Allen-Cahn equation, cf. De Mottoni and Schatzman [5], Alikakos et al. [2], Chen et al. [4], respectively.

More precise information on the approximate solutions $(\mathbf{v}_A, c_A)$ can be found in [1, Theorem 1.3] and its proof. These approximate solutions are constructed with the aid of three levels of terms calculated with the method of formally matched asymptotic expansions. After the construction of these solutions, the main step in the proof of our result is to estimate the difference of approximate and exact solutions with the aid of a suitable refinement of a spectral estimate of the linearized Allen-Cahn operator, which was proven by Chen [3]. Moreover, a careful treatment of the coupling terms is needed.

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Phase-field Modeling of Fluid-Structure-Interaction

Sebastian Aland
(joint work with Dominic Mokbel)

Traditional approaches to Fluid-Structure-Interaction (FSI) use an interface-matched numerical grid where deformations of the solid-fluid interface are realized by a movement of the corresponding grid points. While this methodology provides a sound mathematical description and leads to a very accurate domain representation, it also comes with a some limitations. For example technically complicated re-triangulations are necessary to realize rotations or translations of the two domains with respect to each other.

Consequently, there are some efforts to provide alternative Eulerian formulations of FSI [1]. A first approach for an implicit interface description has been developed for the Level-Set method in [2]. In my talk, we derive an other approach that involves a phase field method for the coupling of a fluid domain with incompressible elastic bodies. The main results are summarized in the following.

Let ϕ denote a phase field that distinguishes between the fluid domain ($\phi \approx 0$) and the solid domain ($\phi \approx 1$). Balance laws for mass and momentum yield the evolution equations

$$\partial^\bullet(\rho(\phi)\mathbf{v}) = \nabla \cdot \mathbb{S}_0(\phi) + \nabla p + \mathbf{F} \qquad \text{in } \Omega \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0 \qquad \text{in } \Omega \tag{2}$$

$$\partial^\bullet \phi = -\nabla \cdot \mathbf{J} \qquad \text{in } \Omega \tag{3}$$

where $\mathbf{v}, p, \mathbb{S}$ denote the (volume-averaged) velocity, pressure and phase- dependent stress. The force $\mathbf{F}$ and flux $\mathbf{J}$ are specified later to meet the requirement of non-increasing energy. The density is chosen as a linear combination of the densities in the two phases: $\rho(\phi) = \phi\rho_1 + (1-\phi)\rho_0$.

To describe the elastic stress in the Eulerian framework we introduce the left Cauchy-Green strain tensor $\mathbb{B}$. In a viscoelastic Maxwell fluid, $\mathbb{S} = \mu(\mathbb{B} - \mathbb{I})$, where μ is the shear modulus of the elastic material. The strain tensor follows the evolution equation

$$\partial^\bullet \mathbb{B} = \nabla \mathbf{v}^T \cdot \mathbb{B} + \mathbb{B} \cdot \nabla \mathbf{v} - \frac{1}{\alpha}(\mathbb{B} - \mathbb{I}) \qquad \text{in } \Omega \tag{4}$$

where α is the relaxation time that controls the dissipation of elastic stress. The limiting case of a purely elastic solid can be described by $1/\alpha = 0$, while $1/\alpha \to \infty$ corresponds to zero elastic stress. Hence, the total phase-dependent stress can we written as

$$\mathbb{S}(\phi) = \nu(\phi)(\nabla \mathbf{v} + \nabla \mathbf{v}^T) + \mu(\phi)(\mathbb{B} - \mathbb{I}) \tag{5}$$

where ν is the viscosity. With this choice, different material laws are obtained depending on the parameters ν, μ, α as shown in the following table. Hence, the modeling of FSI boils down to choosing the physical parameters of the fluid and the elastic domain in the two phases.

material	$\nu(\phi)$	$\mu(\phi)$	$1/\alpha(\phi)$
viscous fluid	> 0	0	*arbitrary*
elastic solid	0	> 0	0
viscoelastic Kelvin-Voigt	> 0	> 0	0
viscoelastic Maxwell	0	> 0	> 0

To close the system of equations, it remains to specify the flux $\mathbf{J}$ and force $\mathbf{F}$ to obtain a thermodynamically consistent evolution. We define the total energy E of the system as sum of kinetic, elastic and surface energy as follows,

$$E = \int_\Omega \frac{\rho\,(\phi)}{2}\,|\mathbf{v}|^2\,\mathrm{d}x + \int_\Omega \frac{\mu\,(\phi)}{2}\mathrm{tr}\,(\mathbb{B} - \ln\mathbb{B} - \mathbb{I})\,\mathrm{d}x + \int_\Omega \sigma\left(\frac{\epsilon}{2}\,|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\right)\,\mathrm{d}x.$$

Here, 'tr' is the trace operator, σ the (scaled) surface tension, ϵ the interface thickness and $W(\phi) = \phi^2(1-\phi)^2$ a double-well potential. Inserting (1)-(5) leads to the energy time evolution

$$\begin{aligned} d_t E = \int_\Omega & -\frac{\nu(\phi)}{2}\left|\nabla\mathbf{v} + \nabla\mathbf{v}^T\right| - \frac{\mu(\phi)}{2\alpha(\phi)}\mathrm{tr}(\mathbb{B} - \mathbb{B}^{-1} - 2\mathbb{I}) \\ & + \mathbf{v}\cdot[\mathbf{F} + \nabla\cdot(\rho'(\phi)\mathbf{v}\otimes\mathbf{J}) + \epsilon\sigma\nabla\cdot(\nabla\phi\otimes\nabla\phi)] \\ & + \mathbf{J}\cdot\nabla\left[\frac{\mu'(\phi)}{2}\mathrm{tr}(\mathbb{B} - \ln\mathbb{B} - \mathbb{I}) + \sigma\left(\frac{1}{\epsilon}W'(\phi) - \epsilon\Delta\phi\right)\right]\,\mathrm{d}x. \end{aligned}$$

Hence, with the choice

$$\mathbf{F} = -\nabla\cdot(\rho'(\phi)\mathbf{v}\otimes\mathbf{J}) - \epsilon\sigma\nabla\cdot(\nabla\phi\otimes\nabla\phi), \tag{6}$$

$$\mathbf{J} = -\gamma W(\phi)\nabla\left[\frac{\mu'(\phi)}{2}\mathrm{tr}(\mathbb{B} - \ln\mathbb{B} - \mathbb{I}) + \sigma\left(\frac{1}{\epsilon}W'(\phi) - \epsilon\Delta\phi\right)\right] \tag{7}$$

for some mobility $\gamma \geq 0$, we obtain non-increasing energy,

$$d_t E = \int_\Omega -\frac{\nu(\phi)}{2}\left|\nabla\mathbf{v} + \nabla\mathbf{v}^T\right| - \frac{\mu(\phi)}{2\alpha(\phi)}\mathrm{tr}(\mathbb{B} - \mathbb{B}^{-1} - 2\mathbb{I}) - |\mathbf{J}|^2\,\mathrm{d}x \;\leq\; 0.$$

If the flux $\mathbf{J}$ is used as defined in Eq. (7), the resulting ϕ does not provide a good description of the interface layer because of the contributions of the elastic strain. Since the primary purpose of ϕ is to track the two-phase interface, we use a modified version of the flux $\mathbf{J}$ without the strain term, which amounts in a classical advected Cahn-Hilliard equation for ϕ.

$$\partial^\bullet\phi = \gamma\nabla\cdot\left[W(\phi)\nabla\left(\frac{1}{\epsilon}W'(\phi) - \Delta\phi\right)\right]. \tag{8}$$

Although the resulting system is no longer variational and does not necessarily decrease the energy, this effect tends to be higher order since away from the interface $W(\phi) \approx 0$ and near the interface ϕ locally equilibrates yielding $W'(\phi) \approx \epsilon^2\Delta\phi$ and thus $\mathbf{J} \approx 0$. Note that if $\mathbf{J} = 0$ then $d_t E = 0$.

In my talk we motivate these modified evolution equations and present first numerical results. A benchmark problem for elastic solids in a flow channel is used to assess the accuracy of the method. We use this problem to address the influence of the interface thickness ϵ and the parameter α that is undetermined in the fluid domain.

Measuring the deformation of the elastic objects, we find very good agreement between our phase field method and an ALE method [3]. This is also confirmed in an experimental comparison to the deformation of elastic beads in a viscous fluid that shows the applicability of our method to real-world problems. We further illustrate the potential of the method to include contact of an elastic object with a rigid wall by simulating a bouncing ball.

As a last part of the talk we consider a novel approach for elastic membranes in flow. We present a surface Oldroyd-B model for the in-plane membrane strain along with some first axisymmetric numerical tests. The results of the talk are currently prepared for publication [4].

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A Numerical Method for Fractional Elliptic Quasi-Variational Inequalities

Harbir Antil
(joint work with Carlos N. Rautenberg)

The purpose of this work is twofold: 1) To introduce and show existence, and under certain assumptions, uniqueness of a new class of quasi-variational inequalities (QVIs) involving fractional power, $s \in (0,1)$, of elliptic operators. 2) To develop a solution algorithm suitable for numerical implementation, see [1]. The problem class of interest is the following: Let Ω be an open, bounded and connected domain of $\mathbb{R}^n$, $n \geq 1$, with Lipschitz boundary $\partial\Omega$ and $f \in L^\infty(\Omega)$ non-negative be given. Consider the following *fractional QVI*:

$$(\mathbb{P}) \qquad \text{Find } u \in K(u) : \langle \mathcal{L}^s u, u - v\rangle_{-s,s} \leq \langle f, u - v\rangle_{-s,s} \text{ in } \Omega, \qquad \forall v \in K(u),$$

where $w \mapsto K(w)$ is defined as

$$K(w) := \{v \in \mathbb{H}^s(\Omega) \mid v \leq \Psi(w) \quad \text{a.e. in } \Omega\}, \tag{1}$$

$\mathbb{H}^s(\Omega)$ is defined as

$$\mathbb{H}^s(\Omega) = \Big\{ w = \sum_{k=1}^{\infty} w_k \varphi_k \in L^2(\Omega) : \|w\|^2_{\mathbb{H}^s(\Omega)} := \sum_{k=1}^{\infty} \lambda_k^s |w_k|^2 < \infty \Big\}.$$

Moreover, $\Psi(u) : \Omega \to \mathbb{R}$ is measurable and non-negative for all $u \in \mathbb{H}^s(\Omega)$ and fulfills the assumptions given in the sequel.

The operator $\mathcal{L}^s$, $s \in (0,1)$, is a fractional power of the second order, symmetric and uniformly elliptic operator $\mathcal{L}$, supplemented with homogeneous Dirichlet boundary conditions: $\mathcal{L}w = -\mathrm{div}_{x'}(A\nabla_{x'} w) + cw$, where $0 \le c \in L^\infty(\Omega)$ and $A(x') = A^{ij}(x') = A^{ji}(x')$, $i,j = 1,\dots,n$, is bounded and measurable in Ω and satisfy the uniform ellipticity condition $\Lambda_1|\xi|^2 \le A(x')\xi\cdot\xi \le \Lambda_2|\xi|^2$, for all $\xi \in \mathbb{R}^n$ for almost every $x' \in \Omega$, for some ellipticity constants $0 < \Lambda_1 \le \Lambda_2$.

We emphasize that ($\mathbb{P}$) is nonlocal and the classical techniques dealing with QVIs are not applicable. Indeed existence and uniqueness of solutions for QVIs involve, in general, ordering properties of the associated monotone operator, in this case $\mathcal{L}^s$, and/or compactness properties of the obstacle map Ψ. The former is never available as $\langle \mathcal{L}^s u^+, u^- \rangle_{-s,s} \le 0$ does not hold for all $u \in \mathbb{H}^s(\Omega)$ and we do not assume the latter. A possible alternative is the Caffarelli-Silvestre extension.

The extension idea was introduced by Caffarelli and Silvestre in $\mathbb{R}^n$ [2], see [4] for the bounded domain case. In the nutshell, it says that $\mathcal{L}^s$ can be realized as an operator that maps a Dirichlet boundary condition to a Neumann condition via an extension problem on the semi-infinite cylinder $\mathcal{C} = \Omega \times (0,\infty)$.

Related to the nonlocal QVI given in ($\mathbb{P}$), we introduce the following *extended QVI* problem which is local in nature and includes one extra spatial dimension y:

(P) Find $\mathscr{U} \in \mathcal{K}(\mathscr{U}) : a(\mathscr{U}, \mathscr{U} - \mathscr{V}) \le \langle f, \mathrm{tr}_\Omega(\mathscr{U} - \mathscr{V})\rangle_{-s,s}, \quad \forall \mathscr{V} \in \mathcal{K}(\mathscr{U}),$

where $\mathscr{W} \mapsto \mathcal{K}(\mathscr{W})$ is defined as

$$\mathcal{K}(\mathscr{W}) = \{ \mathscr{V} \in \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C}) \mid \mathrm{tr}_\Omega \mathscr{V} \le \Psi(\mathrm{tr}_\Omega \mathscr{W}) \quad \text{a.e. in } \Omega \}, \tag{2}$$

where $\overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C})$ is defined as

$$\overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C}) = \big\{ w \in H^1(y^\alpha, \mathcal{C}) : w = 0 \text{ on } \partial_L \mathcal{C} \big\} \text{ with } \partial_L \mathcal{C} = \partial\Omega \times [0,\infty).$$

and

$$\mathrm{tr}_\Omega \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C}) = \mathbb{H}^s(\Omega), \qquad \|\mathrm{tr}_\Omega w\|_{\mathbb{H}^s(\Omega)} \lesssim \|w\|_{\overset{\circ}{H}{}^1_L(y^\alpha,\mathcal{C})}.$$

and the bilinear form a is given by

$$a(\mathscr{W}, \mathscr{V}) := \frac{1}{d_s} \int_{\mathcal{C}} y^\alpha \mathbf{A}(x', y) \nabla \mathscr{W} \cdot \nabla \mathscr{V} + y^\alpha c(x') \mathscr{W} \mathscr{V}, \tag{3}$$

for $\mathscr{W}, \mathscr{V} \in \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C})$ with $\alpha = 1 - 2s \in (-1,1)$, and $d_s = 2^\alpha \Gamma(1-s)/\Gamma(s)$. Moreover, $\mathbf{A}(x', y) = \mathrm{diag}\{A(x'), 1\}$. We will construct the solution to ($\mathbb{P}$) by $u = \mathscr{U}|_{\Omega\times\{0\}}$, where $\mathscr{U}$ solves (P); further, in Lemma 1 we prove that the solution set of ($\mathbb{P}$) and (P) have the same cardinality. The result of Lemma 1 is in accordance with [2, 4] but require extra care and does not follow immediately. However, it

has serious consequences: It allows us to transfer the well-posedness of (P) to the intractable ($\mathbb{P}$). This initiates a new paradigm in the field of QVIs.

Towards this end, we consider a function $u : \Omega \to \mathbb{R}$. We then define an α-harmonic extension of u (cf. [2, 4]) to the cylinder $\mathcal{C}$, as the function $\mathscr{U}$ solving

$$\begin{cases} -\operatorname{div}(y^\alpha \mathbf{A}\nabla\mathscr{U}) + y^\alpha c\mathscr{U} = 0 & \text{in } \mathcal{C}, \\ \mathscr{U} = 0 \quad \text{on } \partial_L\mathcal{C}, & \mathscr{U} = u \quad \text{on } \Omega\times\{0\}. \end{cases} \tag{4}$$

Given $u \in \mathbb{H}^s(\Omega)$ this problem has a unique solution $\mathscr{U} \in \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C})$. We define the solution mapping $u \mapsto \mathscr{U}$ of (4) as $H_\alpha : \mathbb{H}^s(\Omega) \to \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C})$, i.e., $\mathscr{U} = H_\alpha u$.

Next we state our main results, we refer to [1] for details.

Lemma 1. Let $\mathbf{S}_\mathbb{P}$ and $\mathbf{S}_P$ denote the set of solutions to ($\mathbb{P}$) and (P), respectively. Then, the maps

$$\operatorname{tr}_\Omega : \mathbf{S}_P \to \mathbf{S}_\mathbb{P}, \qquad \text{and} \qquad H_\alpha : \mathbf{S}_\mathbb{P} \to \mathbf{S}_P,$$

are bijections.

Assumption 2 (first assumption on Ψ)**.**

(i). If $0 \le u_1 \le u_2$, then $0 \le \Psi(u_1) \le \Psi(u_2)$ a.e. in Ω.

(ii). For every non-negative u and $\zeta \in [0, 1)$, there exists $\beta \in (\zeta, 1)$ such that $\Psi(\zeta u) \ge \beta\Psi(u)$ a.e. in Ω.

Theorem 3. *Let the obstacle map Ψ satisfy (i) in Assumption 2. Then, the set of solutions $\mathbf{S}_P$ of (P) is non-empty, it satisfies $\operatorname{tr}_\Omega \mathbf{S}_P \subset L^\infty(\Omega)$. Further, it holds that $\mathbf{S}_\mathbb{P} \equiv \operatorname{tr}_\Omega \mathbf{S}_P \subset L^\infty(\Omega)$ and if $\mathscr{U} \in \mathbf{S}_P$*

$$0 \le \operatorname{tr}_\Omega \mathscr{U} \le u^*, \qquad \text{a.e. in } \Omega$$

where u^* solves (weakly) the problem: Find $u \in \mathbb{H}^s(\Omega)$ such $\mathcal{L}^s u = f$. If in addition to (i), Ψ satisfies also (ii) in Assumption 2, $\mathbf{S}_P$ is a singleton.

Direct discretization of ($\mathbb{P}$), via finite elements, requires to deal with a stiffness matrix $K_{i,j} := \langle \mathcal{L}^s u_i, u_j\rangle_{-s,s}$ which is dense, and hence the dimension of the associated discretized problem is bounded by memory limitations (similar situation occurs when we use the integral definition [2]). In addition, directly using the spectral definition needs access to eigenvalues and eigenvectors of $\mathcal{L}$ which is, again, intractable in general domains. The discretization of problem (P) is a more suitable choice for numerical methods. In this case, although the dimension is increased by one, the stiffness matrix $K_{i,j} := a(\mathscr{U}_i, \mathscr{U}_j)$ is sparse [3]. The evident limitation here is that the domain associated to (P) is not finite. In this vein, we consider a truncation of the domain $\mathcal{C}$, i.e., we define $\mathcal{C}_\tau = \Omega \times (0, \tau)$. For $\mathscr{W} \in \overset{\circ}{H}{}^1_L(y^\alpha, \mathcal{C})$, we define $S(\mathcal{K}^\tau(\mathscr{W}))$ to be the unique solution to the variational inequality

$$\text{Find } \mathscr{U} \in \mathcal{K}^\tau(\mathscr{W}) : a(\mathscr{U}, \mathscr{U} - \mathscr{V}) \le \langle f, \operatorname{tr}_\Omega(\mathscr{U} - \mathscr{V})\rangle_{-s,s}, \tag{5}$$

for all $\mathscr{V} \in \mathcal{K}^\tau(\mathscr{W})$ where $\mathscr{W} \mapsto \mathcal{K}^\tau(\mathscr{W})$ is given by

$$\mathcal{K}^\tau(\mathscr{W}) := \{\mathscr{V} \in \mathcal{K}(\mathscr{W}) \mid \mathscr{V} \le 0 \text{ a.e. in } \Omega \times (\tau, +\infty)\}.$$

Although (5) is posed on the infinite domain $\mathcal{C}$, given that $f \geq 0$, we have that $S(\mathcal{K}^\tau(\mathscr{W})) \equiv 0$ in $\Omega \times (\tau, +\infty)$. Hence, for implementation we only need to solve the problem on the finite domain $\mathcal{C}_\tau$ which is bounded.

The following additional assumption on Ψ allows us to develop a convergent numerical method. The convergence is shown using Mosco convergence of sets.

Assumption 4 (second assumption on Ψ). (*i*). $\Psi(u) \geq \nu > 0$ a.e. in Ω, for all $u \in \mathbb{H}^s(\Omega)$.

(*ii*). For $u_n, u^* \in \mathbb{H}^s(\Omega)$ with $n \in \mathbb{N}$: If $u_n \to u^*$ in $L^p(\Omega)$, for all $p > 1$ then $\Psi(u_n) \to \Psi(u^*)$ in $L^\infty(\Omega)$.

Theorem 5. *Let the obstacle map Ψ satisfy (i) in Assumption 2 and Assumption 4. Further, let $\{\tau_n\}$ be a positive sequence such that $\tau_n \to \infty$ for $n \to \infty$. Then the sequence $\{\mathscr{U}_n\}_{n=0}^\infty$ defined as $\mathscr{U}_n := S(\mathcal{K}^{\tau_n}(\mathscr{U}_{n-1}))$ with $\mathscr{U}_0 \geq 0$ and $n \to \infty$, satisfies*

$$\mathscr{U}_n \to \mathscr{U}, \quad \text{in} \quad \mathring{H}^1_L(y^\alpha, \mathcal{C}),$$

where $\mathscr{U}$ solves (P).

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Numerical methods for optimal transportation

Sören Bartels

(joint work with Stephan Hertzog, Marijo Milicevic and Patrick Schön)

Optimal transport is a classical problem in mathematics that concerns the optimal rearrangement of a given measure $\mu \in \mathcal{M}(X)$ into another measure $\nu \in \mathcal{M}(Y)$ describing, e.g., the transport of available goods from suppliers to recipients under minimal total cost, cf., e.g., [4]. The goal is thus to minimize a cost functional

$$I[s] = \int_X c(x, s(x))\, d\mu(x)$$

among bijections $s : X \to Y$ satisfying

$$\int_X h \circ s\, d\mu = \int_Y h\, d\nu$$

for all $h \in C(Y)$. Existence of solutions is established by considering a relaxation which seeks a transport plan $\pi \in \mathcal{M}(X \times Y)$ whose projections onto X and Y coincide with μ and ν, respectively, and for which

$$J[\pi] = \int_{X\times Y} c(x,y)\, d\pi(x,y)$$

is minimal. Under appropriate conditions on μ and ν optimal transport plans are related to optimal transport maps. The discretization of this formulation leads to large linear programs.

In the case of linear transport costs, e.g., $X = Y = \overline{\Omega}$ and $c(x,y) = |x-y|$, the optimization problem can be reduced to computing a potential $\phi \in C(\overline{\Omega})$ which is maximal for

$$K[\phi] = \int_\Omega f\phi\, dx$$

among functions ϕ that are Lipschitz continuous with constant 1. The function f is the difference of densities for the measures μ and ν. This maximization problem can be discretized with low order $C(\overline{\Omega})$-conforming finite elements and solved iteratively with splitting methods [2]. Due to nonuniqueness of solutions and degeneracy of the functional K error estimates can only be expected for the approximation of the optimal cost. The rate of convergence is formally quadratic in the maximal mesh size. A posteriori error estimates follow from considering the dual formulation and controlling the primal-dual gap [3]. For this to be optimally convergent the dual problem cannot be discretized with piecewise affine vector fields. Instead, higher order $H(\mathrm{div};\Omega)$-conforming methods and related adaptive approximation algorithms turn out to lead to improved experimental convergence rates.

For cost functions $c : X \times Y \to \mathbb{R}$ with superlinear cost we consider discretizations of the relaxed formulation which seek an optimal matrix $\pi_h \in \mathbb{R}^{N\times N}$ for

$$\pi_h \mapsto \sum_{i,j=1}^{N} c(x_i, y_j)\pi_h^{ij}$$

subject to the constraints

$$\pi_h^{ij} \geq 0, \quad \sum_{i=1}^{N} \pi_h^{ij} = \nu^j, \quad \sum_{j=1}^{N} \pi_h^{ij} = \mu^i.$$

We exploit the fact that exact transport plans are sparse, i.e., only $\mathcal{O}(N)$ entries in the matrix π_h are different from zero. Within an active set strategy we activate entries using the optimality conditions. By successively enlarging an activation tolerance we obtain a convergent numerical scheme. Numerical experiments show that the devised method leads to nearly linear complexity with respect to the number N of employed atoms, see [1].

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A phase field ansatz for multi-material topology optimization solved with a variable metric projection type method

Luise Blank

(joint work with Christoph Rupprecht)

Multi-material topology optimization can be formulated with a phase field ansatz. This model allows for areas where there exists a mixture of materials, which makes e.g. the change in topology during the iteration process for finding a solution possible. The phase field $\varphi = (\varphi_i)_{i=1,\dots,N}$ describes the fractions of the materials with φ_i the fraction of the $i-$th material. The weak formulation of the linear elasticity equation then reads as

$$\int_\Omega C(\varphi)\mathcal{E}(\mathbf{u}) : \mathcal{E}(\xi) = \int_{\mathbf{\Gamma_g}} \mathbf{g}\cdot\xi \quad \forall \xi \in \mathbf{H^1}(\mathbf{\Omega};\mathbb{R}^{\mathbf{d}}) \cap \{\xi|_{\mathbf{\Gamma_D}} = \mathbf{0}\},$$

with the displacement field $\mathbf{u} : \Omega \to \mathbb{R}^d$, a stiffness tensor $C(\varphi)$ which is constant in each pure material and the linearized strain tensor $\mathcal{E}(\mathbf{u}) = \frac{1}{2}(D\mathbf{u} + D\mathbf{u}^T)$.

In addition we prescibe the mass of the materials for the optimal distribution of N elastic isotropic homogeneous materials. Here the aim is to minimize the mean compliance $F(\mathbf{u}) := \int_{\Gamma_g} \mathbf{g}\cdot\mathbf{u}$. Due to ill posedness of the problem F is regularized in the sharp interface model with the perimeter. Using phase fields the perimeter is replaced by the Ginzburg-Landau energy

$$E(\varphi) := \int_\Omega \frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}\psi(\varphi)$$

where the potential ψ can be a smooth double well or an obstacle potential with minima at zero and which forces the model to pure phases apart from diffuse interfaces with thickness proportional to $\varepsilon > 0$. This model is analytically studied in [2, 3] including its sharp interface limit.

For interface evolution the phase field approach is well known and analysed. There it is also known that the pure phases are represented by $\varphi \approx 1$ for the double well potential and $\varphi = 1$ in case of the obstacle potential. However, we show in numerical studies that this classification of pure phases does not hold any longer for the double well potential in the topology optimization problem. Here a significant shift of the values giving the pure phases occurs which depend on ε and are not a priori known. Consequently, the given mass constraints $\fint_\Omega \varphi_i = m_i$ do not

result into the property that material i has volume m_i. Therefore, allthough the smooth potential is preferable for numerical optimization due to smoothness and due to the absence of inequality constraints, they cannot be used in this context but leads to missleading numerical results. Hence, the obstacle potential has to be employed.

Considering now the optimization problem reduced to the phase field φ using the solution operator $S : \varphi \longrightarrow \mathbf{u}$ we are faced with a nonlinear problem with convex constraints in function spaces. To obtain a mesh independent, efficient algorithm for the discretized problem one wishes to have a convergent method in function spaces. Moreover, since the topology and in general good initial data are not known, we are interested on a global convergent method. For convexly constrained optimization problem the projected gradient method is well known in Hilbert spaces. However in many PDE constrained problems the differentiability is not given with respect to an Hilbert space. In our problem differentiability is given with respect to $H^1(\Omega, \mathbb{R}^N) \cap L^\infty(\Omega, \mathbb{R}^N)$.

For these kind of problems we present the VMPT (variable metric projection type) method. Here back tracking along a search direction $\mathbf{v}$ is performed, where $\mathbf{v}$ is the minimal solution of a quadratic approximation of the original cost functional with the given convex constraints. The quadratic term can vary from a reflexive Banach space norm (as it would be the case for the projected gradient method) to some positive symmetric bilinear form, which for example may approximate the second derivative. The last allows for superlinear convergence. The following convergence result we obtain in [1] where also the detailed assumptions are given and discussed.

Theorem 1. *Given the problem* $\min j(\varphi)$ *s.t.* $\varphi \in \Phi_{ad}$ *where* Φ_{ad} *is a convex set bounded in* D *and* j *is differentiable in* $X \cap D$ *with a reflexive real Banach space* X *and* D *isometrically isomorphic to a separable real Banach space. Furthermore the bilinear forms in the subproblems for the search directions* $\mathbf{v_k}$ *have to fulfill* $m\|x\|_X^2 \leq a_k(x,x) \leq M_k\|x\|_{X\cap D}^2$. *Let* $\{\varphi_k\} \subseteq \Phi_{ad}$ *be the sequence generated by the VMPT method and under some additional technical assumptions it holds:*
1. $\lim j(\varphi_k)$ *exists.*
2. Every $(X \cap D)$*-accumulation point of* $\{\varphi_k\}$ *is stationary.*
3. Let $\varphi_{k_i} \to \varphi$ *in* $X \cap D$. *Then* $\|v_{k_i}\|_X \to 0$.
4. If $j \in C^{1,\gamma}(\Phi_{ad})$ *for some* $0 < \gamma \leq 1$, *then* $\|v_k\|_X \to 0$.
5. If $j \in C^{1,\gamma}(\Phi_{ad})$ *for some* $0 < \gamma \leq 1$, j *is convex and* $\{a_k\}$ *is uniformly bounded in* X. *Then every* X*-weak accumulation point of* $\{\varphi_k\}$ *is stationary (thus a global minimum).*

We can show that this method can be applied to the given structural optimization problem using $H^1 \cap L^\infty$ and various bilinear forms a_k, as e.g. the H^1-norm or a positive part of the second derivative. Numerically we discuss that the use of scaling the H^1-norm by ε is important to obtain independency of the interface thickness parameter ε. This approach is even more adapted to each iteration for fixed ε taking into account that the interfaces do not necessarily have thickness ε

in the first iterations. We also give evidence and explanations that it is important not to choose a linear interpolation of the elasticity tensor on the diffuse interface. A quadratic interpolation leads to far better numerical results and in combination with appropriate scaling to a speed up for the classical cantilever beam in two dimensions with grid size 2^{-8} from 5d 8h 12m to 2h 44m and with a nested approach even to 17m. Further speed up can be obtained with an L-BFGS update of the bilinear form or with a positive part of the second derivative. With the last choice we obtained always smaller local minimal cost values. We also give examples for 4 phases and in three dimensions.

Comparison with the often used pseudo time stepping, also called gradient flow approach, where either an Allen-Cahn or a Cahn-Hilliard ansatz is employed, is given. The VMPT method is in all tested examples more efficient than these methods even when they are used with appropriate adapted time steps.

Finally also numerical applications of the VMPT method for phase field models in compliant mechanism problems, drag minimization of the Stokes flow and in an inverse problem for a discontinuous diffusion coefficient are given.

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Recent results on the crystalline curvature flows

Antonin Chambolle

(joint work with Massimiliano Morini, Matteo Novaga and Marcello Ponsiglione)

An anisotropic mean curvature flow is an evolving set $E(t)$ whose boundary evolves with a law of the form

$$V_n = -F(x, t, \nu_E, \kappa_\phi)$$

where F is increasing with respect to κ_ϕ, the "anisotropic divergence" defined by $\kappa_\phi = \mathrm{div}\nabla\phi(\nu_E)$, where ϕ is a norm (a convex, one-homogeneous and even function). We focus on the particular case where $F = \psi(\nu_E)(\kappa_\phi + g(x,t))$ where ψ (the "inverse mobility") is also a norm and g is bounded, Lipschitz in space. Our goal is to study this equation when ϕ is merely Lipschitz, such as the "crystalline case" which is when $\{\phi \le 1\}$ is a polytope. The equation thus reads

$$V_n \in -\psi(\nu_E)\big(\mathrm{div}\partial\phi(\nu_E) + g(x,t)\big). \tag{1}$$

Thanks to a new notion of "distributional super/subflows", which are tubes $E(t)$ such that the distance function to $E(t)$ in the ψ°-norm satisfies an appropriate inequality in the distributional sense, one can establish comparison results for

degenerate geometric equations such as (1) including when ϕ is crystalline. While this notion requires a compatibility condition between ϕ and ψ (namely, that $\phi = \phi' + \varepsilon\psi$ for ϕ' a norm and $\varepsilon > 0$), we are also able to show that the flows generated by this approach converge, as $\varepsilon \to 0$, to a unique limit. The presented paper [3] contains deeper results, such as the convergence, as the discretization step goes to zero, of the anisotropic time-discrete flows built by Almgren-Taylor-Wang [1] to a unique limit, for any ϕ even crystalline.

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Numerical analysis of a diffuse interface approach to an advection–diffusion equation on a moving surface

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(joint work with Vanessa Styles)

Given a family $\{\Gamma(t)\}_{t\in[0,T]}$ of evolving closed hypersurfaces in $\mathbb{R}^{n+1}(n = 1, 2)$ we consider the advection–diffusion equation

$$\partial_t^\bullet u + u\nabla_\Gamma \cdot \mathbf{v} - \Delta_\Gamma u = 0 \quad \text{on } S_T \tag{1}$$

$$u(\cdot, 0) = u_0 \quad \text{on } \Gamma(0). \tag{2}$$

Here, $S_T = \bigcup_{t\in(0,T)} \big(\Gamma(t) \times \{t\}\big)$, $\mathbf{v} : \overline{S_T} \to \mathbb{R}^{n+1}$ is a given velocity field and $\partial_t^\bullet = \partial_t + \mathbf{v} \cdot \nabla$ denotes the material derivative. Furthermore, ∇_Γ is the tangential gradient and $\Delta_\Gamma = \nabla_\Gamma \cdot \nabla_\Gamma$ denotes the Laplace Beltrami operator.

Numerical approaches that have been proposed in the literature in order to approximate solutions of (1), (2) include the evolving surface finite element method ([4, 6, 7]), level set methods based on an extension of the PDE to an open neighbourhood ([1, 13, 5]) as well as trace/cut finite element methods ([10, 11, 9]). In [3, Section 5] a hybrid method combining trace and narrow band techniques is proposed, while diffuse interface approaches have been introduced in [12] and [8]. In this note we propose a variant of the method in [8] and summarize results on the numerical analysis of the resulting scheme. We refer the reader to [2] for a detailed exposition including proofs of the stability and error bounds that we state below.

Let us assume that the hypersurfaces $\{\Gamma(t)\}_{t\in[0,T]}$ are described implicitly, i.e. there exists a smooth function $\phi : \Omega \times [0, T] \to \mathbb{R}$ such that

$$\Gamma(t) = \{x \in \Omega \,|\, \phi(x, t) = 0\} \quad \text{and} \quad \nabla\phi(x, t) \neq 0, x \in \Gamma(t), 0 \leq t \leq T.$$

It can be shown that there are extensions $\mathbf{v}^e$ of $\mathbf{v}$ and u^e of u such that

$$\phi_t + \mathbf{v}^e \cdot \nabla\phi = 0, \quad \nabla u^e \cdot \nabla\phi = 0, \tag{3}$$

$$\partial_t^\bullet u^e + u^e \, \nabla_\phi \cdot \mathbf{v}^e - \Delta_\phi u^e = \phi \, R \tag{4}$$

in a space–time neighbourhood of S_T. In the above, $\nabla_\phi = \big(I - \frac{\nabla\phi}{|\nabla\phi|} \otimes \frac{\nabla\phi}{|\nabla\phi|}\big)\nabla$, $\Delta_\phi = \nabla_\phi \cdot \nabla_\phi$, while R is a smooth function depending on ϕ and u. In order to localize (4) we introduce for small $\epsilon > 0$ the function

$$\rho(x,t) := \begin{cases} \cos^2\left(\frac{\phi(x,t)}{\epsilon}\right), & |\phi(x,t)| \le \frac{\epsilon\pi}{2}, \\ 0, & |\phi(x,t)| > \frac{\epsilon\pi}{2} \end{cases}$$

and a calculation shows that for all $\eta \in H^1(\Omega)$

$$\frac{d}{dt}\int_\Omega u^e \eta \, \rho \, |\nabla\phi| + \int_\Omega \nabla u^e \cdot \nabla\eta \, \rho \, |\nabla\phi| = \int_\Omega u^e \mathbf{v} \cdot \nabla\eta \, \rho \, |\nabla\phi| + \int_\Omega \phi \, R \, \eta \, \rho \, |\nabla\phi|. \tag{5}$$

Next, let $(\mathcal{T}_h)_{0<h<h_0}$ be a regular triangulation of Ω with $h = \max_{T\in\mathcal{T}_h} \mathrm{diam}(T)$ and $0 = t_0 < t_1 < \ldots < t_M = T$ be a partitioning of $[0,T]$ with maximal time step τ. We define our computational domain and the corresponding finite element space at time level m by $D_h^m := \mathrm{supp} I_h\tilde{\rho}(\cdot, t_m)$ and

$$V_h^m := \{\eta_h \in C^0(D_h^m) \,|\, \eta_{h|T} \in P_1(T) \text{ for all } T \subset D_h^m\}.$$

Here, I_h is the usual Lagrange interpolation operator and

$$\tilde{\rho}(x,t) := \begin{cases} \cos^2\left(\frac{\phi(x,t)}{2\epsilon}\right), & |\phi(x,t)| \le \epsilon\pi, \\ 0, & |\phi(x,t)| > \epsilon\pi. \end{cases}$$

Integrating (5) with respect to $t \in [t_{m-1}, t_m]$ and neglecting the perturbation term involving R we are led to the following finite element approximation of (1), (2): Find $u_h^m \in V_h^m$ such that for all $\eta_h \in V_h^m$

$$\begin{aligned} &\int_\Omega u_h^m \, \eta_h \, \rho^m \, |\nabla\phi^m| - \int_\Omega u_h^{m-1} \, \eta_h \, \rho^{m-1} \, |\nabla\phi^{m-1}| + \tau_m \int_\Omega \nabla u_h^m \cdot \nabla\eta_h \, \rho^m \, |\nabla\phi^m| \\ &\quad - \tau_m \int_\Omega u_h^m \, \mathbf{v}^{e,m} \cdot \nabla\eta_h \, \rho^m \, |\nabla\phi^m| + \gamma\tau_m^2 \int_\Omega I_h^m \tilde{\rho}^m \nabla u_h^m \cdot \nabla\eta_h = 0. \end{aligned} \tag{6}$$

Here, I_h^m is the Lagrange interpolation operator for V_h^m. The last term on the left hand side of (6) introduces additional artificial diffusion into the method. The scheme is initialised by choosing $u_h^0 \in V_h^0$ as the L^2-projection of $u^e(\cdot, 0)$ onto V_h^0.

Remark: a) In order to obtain a fully practical scheme the integrals in (6) have to be evaluated using numerical integration. As a result, the method tracks the moving hypersurfaces via the evaluation of the phase–field funtion ρ.

b) Given $u_h^{m-1} \in V_h^{m-1}$, the scheme has a unique solution $u_h^m \in V_h^m$ provided that $0 < h \le h_0, 0 < \tau \le \tau_0$.

c) Conservation of mass for (1), (2) ($\frac{d}{dt}\int_{\Gamma(t)} u(\cdot,t) = 0$) is satisfied at the discrete level in the sense that

$$\frac{2}{\epsilon\pi}\int_\Omega u_h^m\,\rho^m\,|\nabla\phi^m| = \frac{2}{\epsilon\pi}\int_\Omega u_h^0\,\rho^0\,|\nabla\phi^0|, \quad m = 1,\dots,M,$$

where $\frac{2}{\epsilon\pi}\int_\Omega \cdot\,\rho(\cdot,t)\,|\nabla\phi(\cdot,t)|$ can be viewed as an approximation of $\int_{\Gamma(t)}\cdot$.

Our main results are the following stability and error estimates:

Theorem (Stability) There exist $\gamma_1 > 0$ and $\tau_1 \le \tau_0$ such that

$$\max_{m=1,\dots,M}\frac{2}{\epsilon\pi}\int_\Omega |u_h^m|^2\,\rho^m\,|\nabla\phi^m| + \sum_{m=1}^M \tau_m\,\frac{2}{\epsilon\pi}\int_\Omega |\nabla u_h^m|^2\rho^m\,|\nabla\phi^m| \le C\int_{\Gamma(0)}|u_0|^2,$$

provided that $\gamma \ge \gamma_1, h \le c\epsilon$ and $\tau \le \min\bigl(\tau_1,\epsilon^2\bigr)$.

Theorem (Error bounds) Let $e^m := u^e(\cdot,t_m) - u_h^m$, $m = 0,\dots,M$. Then

$$\begin{aligned}\max_{m=1,\dots,M}\frac{2}{\epsilon\pi}\int_\Omega |e^m|^2\,\rho^m\,|\nabla\phi^m| + \sum_{m=1}^M \tau_m\frac{2}{\epsilon\pi}\int_\Omega |\nabla e^m|^2\rho^m\,|\nabla\phi^m| &\le C\epsilon^2,\\ \max_{m=1,\dots,M}\int_{\Gamma(t_m)}|e^m|^2 + \sum_{m=1}^M \tau_m\int_{\Gamma(t_m)}|\nabla_\Gamma e^m|^2 &\le C\epsilon^2,\end{aligned}$$

provided that $\gamma \ge \gamma_1, h \le c\epsilon, \tau \le \min\bigl(\tau_1,\epsilon^2\bigr)$ and that the solution u of (1), (2) is sufficiently smooth.

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On the computation of harmonic maps by unconstrained algorithms based on totally geodesic embeddings

Hans Fritz

The computation of harmonic maps, and respectively, of the harmonic map heat flow between two closed Riemannian manifolds is a challenging problem, since the solution has to satisfy a constraint, which is, in general, non-linear. Different numerical schemes to tackle this problem have been proposed in the last decades, see, for example, [1, 2, 5, 6]. Another interesting approach can be found in [4], where the authors reformulate the original problem in order to remove the constraint. Using an idea by Richard Hamilton from [3], we propose algorithms for the computation of harmonic maps, and respectively, of the harmonic map heat flow between two closed Riemannian manifolds. Our novel approach is based on the totally geodesic embedding of the target manifold into $\mathbb{R}^N$. This approach is widely applicable, since embeddings of Riemannian manifolds into Euclidean spaces can easily be made totally geodesic by extending the Riemannian metric in a certain way. Totally geodesic embeddings allow to reformulate the harmonic map heat flow in a neighbourhood of the embedded target manifold. The extended flow has the important advantages that it is still described by a non-degenerate parabolic PDE and that it is unconstrained at the same time. Instead of assuming a priori that the solution to the flow maps into the target manifold this fact becomes a property of the solution to the extended flow for special initial data. The solution space to the reformulated problem therefore exists of maps which are also allowed to map into the ambient space of the target manifold, that is into $\mathbb{R}^N$. This fact simplifies the discretization of the problem enormously. Our algorithms for the computation of the harmonic map heat flow and of harmonic maps are based on this reformulation. In contrast to previous schemes, we do not make use of projection techniques, tangential deformations, geodesic finite elements or of Lagrange multipliers. Our algorithms are therefore very easy to implement. We have also proved error estimates for harmonic maps into spherical targets. Finally, numerical tests show that the distance to the target remains small.

Our main result is the development of the following new algorithm for the computation of the harmonic map heat flow from a closed d-dimensional hypersurface $\Gamma \subset \mathbb{R}^{d+1}$ into the unit sphere in $\mathbb{R}^{n+1}$ in the time interval $[0,T)$: Let $\Gamma_h \subset \mathbb{R}^{d+1}$ be a polyhedral approximation of Γ and $f_h^0 \in (V_h)^{n+1}$, where V_h is the set of continuous and piecewise affine functions on Γ_h. Suppose that $||f_h^0|-1| < \delta$ on Γ_h for some $\delta \in (0,1)$. Then, for all $m \in \mathbb{N}_0$ with $(m+1)\tau < T$ find $f_h^{m+1} \in (V_h)^{n+1}$

such that

$$\int_{\Gamma_h} \tfrac{f_h^{m+1}-f_h^m}{\tau} \cdot \psi_h \left(\tfrac{1}{2} + \tfrac{1}{2|f_h^m|^4}\right) do + \int_{\Gamma_h} \nabla_{\Gamma_h} f_h^{m+1} : \nabla_{\Gamma_h} \psi_h \left(\tfrac{1}{2} + \tfrac{1}{2|f_h^m|^4}\right) do$$
$$= \int_{\Gamma_h} f_h^m \cdot \psi_h \tfrac{|\nabla_{\Gamma_h} f_h^m|^2}{|f_h^m|^6} do \qquad \text{for all } \psi_h \in (V_h)^{n+1}.$$

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Using evolving interface techniques to solve network problems

Yves van Gennip

(joint work with many people, acknowledged through references in this abstract)

In recent years there has been increasing interest from applied analysts in applying the models and techniques from variational methods and partial differential equations (PDEs) to tackle problems on networks. This talk gave an overview of some of the recent developments in this young and growing area.

For the purposes of the talk, [1] kicked off the research in this area. In this paper the authors use graph versions of the Ginzburg-Landau functional for data clustering, data classification, and image segmentation. Minimisation of the classical continuum Ginzburg-Landau functional,

$$F(u) := \varepsilon \int_\Omega |\nabla u|^2 \, dx + \frac{1}{\varepsilon} \int_\Omega W(u) \, dx,$$

provides a model for phase separation. Here $W(u) = u^2(1-u)^2$ is a double well potential with minima at $u = 0$ and $u = 1$, and u describes the relative presence of the two phases $\{u \approx 0\}$ and $\{u \approx 1\}$ in the domain Ω. When F is minimised under some suitable constraints on u (e.g. a mass constraint of the form $\int_\Omega u \, dx = M$) and for small values of the parameter ε, u will take values close to 0 and 1, with transitions between those values occurring in small regions of width $\mathcal{O}(\varepsilon)$.

In [1] the graph functional

$$f(u) := \sum_{i,j \in V} \omega_{ij}(u_i - u_j)^2 + \frac{1}{\varepsilon} \sum_{i \in V} W(u_i)$$

was introduced. This is a functional whose input argument u is a function on the nodes of a given graph, instead of on a continuum set $\Omega \subset \mathbb{R}^n$ and which serves as a graph counterpart of F. Here V is the node set of the (finite, simple, undirected) graph, ω_{ij} is a nonnegative weight on the edge between nodes i and j in the graph, and u_i is the value of the function u on node i. In [1] this functional was used in combination with either a mass constraint or an additional data fidelity term to cluster or classify the nodes of a graph into two groups ('phases' where $u \approx 0$ and $u \approx 1$) based on the pairwise node similarity encoded in the edge weights ω_{ij}. By treating the pixels of an image as nodes in a graph, data classifcation can be used for image segmentation as well.

We can now ask a number of questions:

(1) Can we find graph analogues of properties of the continuum functional?
(2) Is the continuum functional a limit of the graph functionals in some sense?
(3) What can we say about the resulting algorithm and its usage for data analysis/image processing?
(4) Are there other network problems that can be tackled by a PDE inspired approach?
(5) Are there other PDE/variational systems that have interesting network analogues?
    - If the inspiring PDEs are related, are their graph analogues related?

This talk gave a short overview addressing (some aspects of some of) these questions.

(1) Does f have similar properties as F? In [2] we proved that f Γ-converges, when $\varepsilon \to 0$, to the graph total variation functional

$$TV(u) := \frac{1}{2} \sum_{i,j \in V} \omega_{ij} |u_i - u_j|,$$

with as domain the set of node functions u which take values in $\{0, 1\}$. This mirrors the well-known continuum result [3, 4]. Moreover, for such $\{0, 1\}$-valued functions u, $TV(u)$ reduces to the graph cut [5] of the node partition $V_0 = \{i : u_i = 0\}$, $V_1 = \{i : u_i = 1\}$, i.e. the sum of the edge weights ω_{ij} corresponding to edges that have one node in V_0 and the other in V_1.

(2) Furthermore, when f or TV are defined on certain graphs of which a sensible continuum limit can be defined, they Γ-converge to the continuum total variation in the continuum limit, e.g. on 4-regular graphs obtained by ever finer discretisations of the flat torus [2] and on point clouds obtained by sampling ever more points from an underlying subset of $\mathbb{R}^n$ [6, 7, 8].

(3) Minimisation of f is in practice (approximately) achieved either by solving a gradient flow equation of Allen-Cahn type,

$$\frac{du_i}{dt} = -\sum_{j \in V} \omega_{ij}(u_i - u_j) - \frac{1}{\varepsilon} W'(u_i)$$

(plus additional terms coming from a mass constraint or fidelity term) or by a graph version of the threshold dynamics (or MBO) scheme [9]:

$$u^{k+1} = \begin{cases} 0, & \text{if } \tilde{u}(\tau) < \frac{1}{2}, \\ 1, & \text{if } \tilde{u}(\tau) \geq \frac{1}{2}, \end{cases} \quad \text{where } \tilde{u}(t) \text{ solves } \begin{cases} \tilde{u}(0) = 0, \\ \frac{d\tilde{u}_i}{dt} = -\sum_{j \in V} \omega_{ij}(\tilde{u}_i - \tilde{u}_j). \end{cases}$$

In the (spectral) graph theory literature [5, 10] $(\Delta u)_i := \sum_{j \in V} \omega_{ij}(u_i - u_j)$ is known as the unnormalised or combinatorial graph Laplacian of u. The equations above can also be formulated and solved with normalised versions of the graph Laplacian.

On a given graph, these equations can be solved quickly and accurately using a truncated spectral decomposition based on the eigenfunctions of the graph Laplacian (in combination with a convex splitting scheme in the case of the graph Allen-Cahn equation) [1, 11].

The construction of the underlying graph in the first place can pose a significant computational problem, especially when the number of data points (and thus nodes in the graph) is very large. Matrix completion techniques such as the Nyström extension [12, 13] and fast eigenvalue computation algorithms such as the Rayleigh-Chebychev algorithm [14] make such computations feasible.

This graph Ginzburg-Landau method has found many applications, for example in data clustering and classification and image segmentation [1, 11, 15] and has also been extended to deal with clustering and classification into more than two classes [16, 17, 18, 19, 20]. Recent papers prove convergence of the graph Allen-Cahn algorithm (both the spectrally untruncated and truncated versions) and extend the method to non-smooth potentials and hypergraphs.

This shows that such PDE driven techniques can provide fast approximative alternatives to combinatorial problems whose exact solution is too computationally complex.

(4) Another example of such a problem is the computation of a maximum cut in graphs, i.e. to find a partition of the node set into two sets such that the sum of the edge weights corresponding to edges with one node in each set is maximal. If the graph is bipartite, this corresponds to partitioning the node set according to the bipartite structure. The exact solution of this classical problem is known to be computationally unfeasible for large graphs. Work currently in preparation introduces a fast approximate solution method for this problem using an adaptation of the graph Ginzburg-Landau functional f [21].

(5) The continuum counterparts of both the graph Allen-Cahn equation and graph MBO scheme from point (3) can be viewed as approximating mean curvature flow [22, 23, 24, 25, 26]. This suggests that graph curvature and graph mean curvature flow are interesting concepts to consider as well. In

[27] we introduced both. The graph curvature of a node set S is given by

$$\kappa_i := \begin{cases} \sum_{j\in S^c} \omega_{ij}, & \text{if } i \in S, \\ -\sum_{j\in S} \omega_{ij}, & \text{if } i \in S^c, \end{cases}$$

and the related graph mean curvature flow has a variational formulation along the lines of [28, 29, 30] which leads to a time discrete evolution of node subsets S (given an initial set S_0),

$$S_{n+1} \in \operatorname{argmin}_{\hat{S}} \mathcal{F}(\hat{S}, S_n),$$

where

$$\mathcal{F}(\hat{S}, S_n) := \sum_{i\in S, j\in S^c} \omega_{ij} + \frac{1}{\eth t} \sum_{i\in\hat{S}} d_i s d_i^n.$$

Here d_i is the degree of node i and sd_i^n is the signed graph distance from node i to the boundary of node set S_n. In [27] we started studying the very interesting question if the graph Allen-Cahn equation, graph MBO scheme, and graph mean curvature flow are as intimately connected as their continuum counterparts, but establishing such connections is still mostly an open problem.

Other current work studies a graph version of the Ohta-Kawasaki functional [31], which was originally introduced as a variational model for pattern formation in diblock copolymers [32].

The research on these novel methods has shown that new PDE inspired graph procedures can efficiently (approximately) solve complex graph problems, while at the same time offering fertile ground for proving theoretical connections between the various graph problems (inspired by similar connections their continuum counterparts have) and between the graph problems and their continuum analogues.

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A discrete deterministic game approach for the planer motion by crystalline energy

Mi-Ho Giga
(joint work with Yoshikazu Giga)

Objective: We shall consider a deterministic game in discrete time, so that its value function approximates a solution of a level-set crystalline curvature flow equation ([2], [3], [4]) as the time grid tends to zero. This work is a first nontrivial extension to crystalline case of the approach given by [5] for motion by smooth interfacial energy.

Background: It is well known that a large class of first order Hamilton-Jacobi equations is obtained as a governing equation of the value function of a control problem or a differential game problem of ODEs. On the other hand a large class of second order elliptic or parabolic equations is obtained as a governing equation of the value function of a stochastic control or stochastic differential game. For example, to derive the level set mean curvature flow, a stochastic game has been proposed by [1], [7] and [8]. A remarkable aspect of the work of [5] is that the level set mean curvature flow, although it is of the second order, is obtained as an equation for a limit of the value function of a time-discrete deterministic game without no stochastic effect. See also [6].

Goal: We would like to extend their result to crystalline flow equations, which have a typical non-local diffusion effect.

Summary: (1) We extend the discrete deterministic two-person game approach by [5] to a smooth anisotropic flow (including degeneracy).
(2) We propose a way of approximation by a discrete deterministic two-person game to the crystalline curvature flow of the form $V = \gamma\kappa_\gamma$ when the Wulff shape of γ is regular polygon rotationally symmetric with respect to the origin. Expected result is the following (work in progress) : Consider a crystalline flow whose crystalline energy has a regular polygonal Wulff shape symmetric with respect to the origin. We approximate the crystalline energy density by an anisotropic energy whose Wullf shape is piecewise circular shape with constant curvature μ. We construct a discrete deterministic game for its anisotropic curvature flow with discrete time grid parameter ε^2 as in [5] with necessary modification. We conclude that if μ tends to zero as ε does i.e. $\mu(\varepsilon) \to 0$ as $\varepsilon \to 0$, then our discrete game approximates the crystalline flow provided that $\mu(\varepsilon) \geq \varepsilon^\beta$ for some $\beta \in (0, 2/3)$. In some sense, we require that approximation parameter tends to zero slowly.

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Moving particles in biological membranes

Carsten Gräser

(joint work with T. Kies, R. Kornhuber and M.-W. Wolf)

We consider a biological membrane composed by a lipid bilayer with embedded particles, like, e.g., transmembrane proteins, BAR-domain proteins, or partially wrapped nano-particles.

The membrane is modeled by a linearized Canham–Helfrich energy for a graph representation over a suitable flat parameter domain $\Omega \subset \mathbb{R}^2$ leading to a biharmonic energy

$$J_{\Omega'}(u) = \frac{\kappa}{2} \int_{\Omega'} |\Delta u|^2 + \frac{\sigma}{2} \int_{\Omega'} |\nabla u|^2.$$

Here, $\Omega' = \Omega \setminus \bigcup_{i=1}^N \overline{B_i}$ is the area incorporated by the membrane, whereas $B_i \subset \Omega$ is the area incorporated by the i-th of N rigid particles. Since particles are allowed to move and rotate freely in the plane, we consider the parameterized particle domains

$$B_i(p_i, \alpha) = \Phi_{p_i,\alpha_i}(B_i^0)$$

obtained by a rigid body motion rotating the reference particle domain B_i^0 by the angle $\alpha_i \in [0, 2\pi]$ and translating it to the position $p_i \in \Omega$. Denoting by $\omega \subset (\Omega, [0, 2\pi])^N$ the set of configurations such that particles do not touch or overlap with each or the boundary we obtain the coupled minimization problem [1]: Find $u \in H^2(\Omega)$ and $(p, \alpha) \in \overline{\omega}$ such that u minimizes $J_{\Omega'(p,\alpha)}$ subject to the coupling conditions

$$u = h_i, \qquad \frac{\partial}{\partial \nu} u = s_i \qquad \text{on } \partial B_i(p_i, \alpha_i). \tag{1}$$

By showing that the reduced functional

$$(p,\alpha) \mapsto E(p,\alpha) = \inf_{v\in H^2(\Omega),\text{s.t.}(1)} J_{\Omega'(p,\alpha)}(v)$$

is lower semi-continuous on $\overline{\omega}$ we establish existence of a minimizer to the coupled problem [3]. Shape calculus allows to compute the gradient $\nabla E(p,\alpha)$ in terms of a deformation field for $\Omega'(p,\alpha)$ and up to second order partial derivatives of the minimizer $u(p,\alpha)$ of J for fixed (p,α). To compute local minimizers we use a scaled gradient flow with explicit Eule time stepping [3].

In oder to avoid remeshing for the stationary problems with varying domain $\Omega'(p,\alpha)$ we follow to approaches: By extending these problem to the whole domain Ω we make them accessible to discretization with simple rectangular Bogner–Fox–Schmitt C^1-finite elements. The former boundary constraints (1) are incorporated by penalization on the now interior curve $\Gamma_i(p_i,\alpha_i) = \partial B_i(p_i,\alpha_i)$. For mesh dependent penalty parameters we are able to show convergence of order $O(h^{1/2})$ which is also numerically observed [2]. The reduced convergence order is due to a lack of regularity of solutions for the extended problem across $\Gamma_i(p_i,\alpha_i)$. As a remedy we introduce a stabilized fictitious domain Nitsche method on $\Omega'(p,\alpha)$ which leads to optimal convergence order $O(h^2)$.

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Two approaches to an approximation of a distance function to moving interfaces

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(joint work with Eleftherios Ntovoris)

On the basis of the theory of viscosity solutions, we introduce two kinds of improved level set equations whose solutions are close to the signed distance function $d(x,t)$ to an evolving interface $\{\Gamma_t\}_t$.

We consider the first order Hamilton-Jacobi equation:

$$w_t(x,t) + H(x,\nabla w(x,t)) = 0 \tag{1}$$

with a geometric Hamiltonian H, and denote by Γ_t the zero level set of a viscosity solution w of the initial value problem of (1); namely, $\Gamma_t = \{w(\cdot,t) = 0\}$. Also, the signed distance function to Γ_t is denoted by $d(\cdot,t)$. An improved equation we introduce is of the form

$$u_t(x,t) + H(x,\nabla u(x,t)) = \beta(u(x,t))G(x,\nabla u(x,t)). \tag{2}$$

Here β is assumed to satisfy $\beta(0) = 0$. It then turns out that this assumption guarantees that the zero level set is not distorted by changing the equation. In other words, we have $\Gamma_t = \{u(\cdot, t) = 0\}$ for the viscosity solution u of the initial value problem of (2). This fact is shown by constructing barrier functions having the same zero level set as Γ_t and applying the comparison principle.

1st approach [1]**:** In the first approach to an approximation of d, we derive an improved equation via Taylor expansion of the equation for d near Γ_t. The equation for d is given by

$$d_t(x,t) + H(x - d(x,t)\nabla d(x,t), \nabla d(x,t)) = 0.$$

Since the difference between $H(x, \nabla d(x,t))$ and the second term on the left-hand side is approximated by $d(x,t)\langle \nabla_x H(x, \nabla d(x,t)), \nabla d(x,t)\rangle$, we take $\beta(u) = u$ and define G on the basis of the inner product above. Under the assumption that d is smooth near Γ_t, we give an upper- and lower bound, which are close to d, for the solution u of (2) near Γ_t. More precisely, we prove that for all $\varepsilon > 0$, there exists $\rho(\varepsilon) > 0$ such that,

$$\begin{cases} e^{-\varepsilon t} d(x,t) \le u(x,t) \le e^{\varepsilon t} d(x,t) & \text{if } 0 \le d(x,t) \le \rho(\varepsilon), \\ e^{\varepsilon t} d(x,t) \le u(x,t) \le e^{-\varepsilon t} d(x,t) & \text{if } -\rho(\varepsilon) \le d(x,t) \le 0. \end{cases}$$

For the proof we show that the functions $e^{\pm \varepsilon t} d(x,t)$ are viscosity sub- and super-solutions of (2) near Γ_t. The time derivatives of them play an important role since they absorb the error term of the Taylor expansion.

2nd approach [2]**:** Our second improved equation is derived by taking the limit of a time step appearing in the so-called reinitialization algorithm. The idea of the reinitialization is, as in [3], to solve the original level set equation (1) and a corrector equation

$$v_t(x,t) = \beta(v(x,t))(1 - |\nabla v(x,t)|) \tag{3}$$

periodically in time. Here a typical choice of β is the (smooth) sign function. We first solve (1) for a period of $k_1 \Delta t$ and then (3) for $k_2 \Delta t$, where k_1, k_2 and Δt are positive constants. Sending $\Delta t \to 0$ and rescaling the time variable, we are led to the equation (2) with $G(x,p) = \theta(1 - |p|)$ ($\theta := k_2/k_1 > 0$). We prove that, as the parameter θ tends to infinity, the solution $u = u^\theta$ of (2) converges to d. When d is continuous as a function of (x,t), this convergence is locally uniform. Our result is applied to more general case where d can be discontinuous. For a possibly discontinuous d we establish

$$\lim_{\substack{(y,s,\theta) \to (x,t,\infty) \\ s \le t}} u^\theta(y,s) = d(x,t) \quad \text{for all } (x,t) \in \mathbf{R}^n \times (0,T).$$

This weak notion of convergence is shown by introducing an upper- and lower half-relaxed limit from below in time.

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Optimal control of two-phase flow with different densities

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(joint work with Harald Garcke and Michael Hinze)

We consider the optimal control of a two-phase fluid that is described by the thermodynamically consistent diffuse interface model proposed in [1]. As key ingredient we present an energy stable scheme introduced in [2]. It allows us to simulate two-phase fluids in an energy stable way and provides enough regularity to apply classic theory from optimal control. More results and references can be found in [3].

1. The governing equations

Let $\Omega \subset \mathbb{R}^n$, $n \in \{2,3\}$, denotes an open, convex and polygonal ($n = 2$) or polyhedral ($n = 3$) bounded domain with outer unit normal ν_Ω, and $I = (0,T]$ with $0 < T < \infty$ is a time interval. The primal variables are the phase field φ, the chemical potential μ, and the solenoidal velocity field v. We state the fully discrete scheme presented in [2] for the numerical approximation of the thermodynamically consistent model for two-phase flow proposed in [1].

Let $0 = t_0 < t_1 < \ldots < t_M = T$ denote an equidistant time grid with mesh size $\tau := t_1 - t_0$. For the spatial discretization we use piecewise linear and globally continuous finite element functions denoted V_m^1 for the phase field and the chemical potential while we use piecewise quadratic and globally continuous finite element functions denoted V_m^2 for the velocity field. Functions from V_m^2 are additionally weakly solenoidal with respect to V_m^1. Then φ_h^m approximates $\varphi(t_m)$, μ_h^m approximates $\mu(t_m)$, and v_h^m approximates $v(t_m)$. The proposed scheme reads:

Given $\varphi_h^{m-2} \in V_{m-2}^1$, $\varphi_h^{m-1} \in V_{m-1}^1$, $\mu_h^{m-1} \in V_{m-1}^1$, $v_h^{m-1} \in V_{m-1}^2$, find $v_h^m \in V_m^2$, $v_h^m|_{\partial\Omega} = \Pi^m(\mathcal{B}_B u_B^m)$, $\varphi_h^m \in V_m^1$, $\mu_h^m \in V_m^1$ such that for all $w \in V_m^2$, $\Psi \in V_m^1$, $\Phi \in V_m^1$ it holds:

$$\frac{1}{\tau}\left(\frac{\rho_h^{m-1}+\rho_h^{m-2}}{2}v_h^m - \rho_h^{m-2}v_h^{m-1}, w\right) + a(\rho_h^{m-1}v_h^{m-1} + J_h^{m-1}, v_h^m, w)$$

$$+(2\eta_h^{m-1}Dv_h^m, Dw) - (\mu_h^m\nabla\varphi_h^{m-1} + \rho_h^{m-1}g, w) - (\mathcal{B}_V u_V^m, w) = 0, \tag{1}$$

$$\frac{1}{\tau}(\varphi_h^m - P^m\varphi_h^{m-1}, \Psi) + (b\nabla\mu_h^m, \nabla\Psi) + (v_h^m\nabla\varphi_h^{m-1}, \Psi) = 0, \tag{2}$$

$$\sigma\epsilon(\nabla\varphi_h^m, \nabla\Phi) + \frac{\sigma}{\epsilon}(W_+'(\varphi_h^m) + W_-'(P^m\varphi_h^{m-1}), \Phi) - (\mu_h^m, \Phi) = 0, \tag{3}$$

where $J_h^{m-1} := -\frac{\rho_2-\rho_1}{2} b \nabla \mu_h^{m-1}$, and for $u \in L^3(\Omega)$, $v, w \in H^1(\Omega)$ we define $a(u,v,w) = \frac{1}{2}\int_\Omega ((u\cdot\nabla)v)w - ((u\cdot\nabla)w)v\,dx$.

The free energy density is denoted by W and is assumed to be of double-well type with exactly two minima at ± 1. For W we use a splitting $W = W_+ + W_-$, where W_+ is convex and W_- is concave. We refer to [3] for the precise assumptions on W. We refer to [4] for optimal control with a non-smooth free energy density. The linear density function is denoted by $\rho = \rho(\varphi)$ with individual densities ρ_1 and ρ_2 for the two different fluids, and the viscosity function is denoted by $\eta = \eta(\varphi)$ while the constant mobility is denoted by b and the gravitational acceleration is denoted by g. By $Dv = \frac{1}{2}(\nabla v + (\nabla v)^t)$ we denote the symmetrized gradient. The scaled surface tension is denoted by σ and the interfacial width is proportional to ϵ. We further apply a volume force $\mathcal{B}_V u_V^m \in L^2(\Omega)^n$ and Dirichlet boundary data $\mathcal{B}_B u_B^m \in H^{1/2}(\partial\Omega)^n$, and require an initial phase field $\varphi_h^0 = u_I \in H^1(\Omega)\cap L^\infty(\Omega)$ and a solenoidal initial velocity field $v_h^0 \in H^1(\Omega)^n \cap L^\infty(\Omega)^n$. The operator $P^m : V_{m-1}^1 \to V_m^1$ denotes an H^1-stable prolongation, e.g. Lagrange interpolation. Further we introduce $V_{m,b}^2 := \{v|_{\partial\Omega} \,|\, v \in V_m^2,\ \int_{\partial\Omega} v|_{\partial\Omega}\cdot\nu_\Omega\,ds = 0\}$ and define Π^m for $m = 1,\dots,M$ as the $L^2(\partial\Omega)$ projection onto the trace space of $V_{m,b}^2$. This projection is used to incorporate the boundary data.

Finally we note that (1)–(3) is a two-step scheme and that an initialization step is required, see [2, 3].

Theorem 1 ([3, Thm. 16])**.** *For given u_I, u_V, u_B, $\varphi^{m-2} \in V_{m-2}^1$, $\varphi^{m-1} \in V_{m-1}^1$, $\mu^{m-1} \in V_{m-1}^1$, $v^{m-1} \in V_{m-1}^2$ there exist unique $v_h^m \in V_m^2$, $v_h^m|_{\partial\Omega} = \Pi^m(\mathcal{B}_B u_B^m)$, $\varphi_h^m \in V_m^1$, and $\mu_h^m \in V_m^1$ solving (1)–(3). It further holds*

$$\begin{aligned}&\|\mu_h^m\|_{W^{1,3}(\Omega)} + \|\varphi_h^m\|_{W^{1,4}(\Omega)} + \|v_h^m\|_{H^1(\Omega)^n}\\ &\le C\left(\|v_h^{m-1}\|_{H^1(\Omega)^n}, \|\mu_h^{m-1}\|_{W^{1,3}(\Omega)}, \|\varphi_h^{m-1}\|_{W^{1,4}(\Omega)}, \|\varphi_h^{m-2}\|_{W^{1,4}(\Omega)},\right.\\ &\left.\|\mathcal{B}_V u_V^m\|_{L^2(\Omega)^n}, \|\mathcal{B}_B u_B^m\|_{H^{\frac{1}{2}}(\partial\Omega)^n}\right),\end{aligned}$$

and the constant depends polynomially on its arguments.

2. The optimal control problem

In the following we consider $u_V \in L^2(0,T;\mathbb{R}^{s_{u_V}})$, $u_B \in L^2(0,T;\mathbb{R}^{s_{u_B}})$, and $u_I \in H^1(\Omega)\cap L^\infty(\Omega)$ as control variables, together with suitable operators $\mathcal{B}_V, \mathcal{B}_B$ and we state the optimal control problem

$$(P_h)\qquad \begin{aligned}\min_{u_V,u_B,u_I,\varphi_h^M} J(u_V,u_B,u_I,\varphi_h^M) &:= \frac{1}{2}\|\varphi_h^M - \varphi_d\|_{L^2(\Omega)}^2\\ &+ \alpha\left(\alpha_I\int_\Omega \frac{\epsilon}{2}|\nabla u_I|^2 + \frac{1}{\epsilon}W_I(u_I)\,dx\right.\\ &\left.+ \frac{\alpha_V}{2}\|u_V\|_{L^2(0,T;\mathbb{R}^{s_{u_V}})}^2 + \frac{\alpha_B}{2}\|u_B\|_{L^2(0,T;\mathbb{R}^{s_{u_B}})}^2\right)\\ &\text{subject to } (1)-(3).\end{aligned}$$

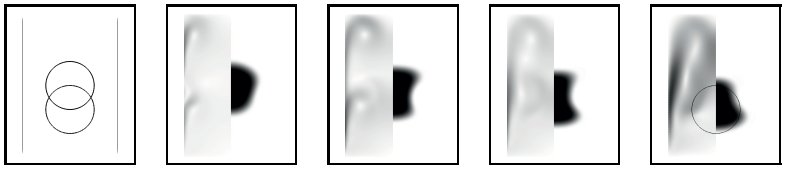

FIGURE 1. Numerical results for the control of a rising bubble.

This is a tracking type functional for minimizing the mismatch between φ_h^M and a desired phase field φ_d. The additional terms penalize strong controls with a parameter $\alpha > 0$, while $\alpha_I + \alpha_V + \alpha_B = 1$ are the positive weights of the different types of control. To obtain a phase field structure for u_I we use the Ginzburg–Landau energy as penalisation for u_I. Here we use a double-obstacle free energy for W_I, i.e. $W_I(\varphi) := \frac{1}{2}(1-\varphi^2)$ if $|\varphi| \leq 1$ and $W_I(\varphi) = +\infty$ else.

Theorem 2 ([3, Thm. 20])**.** *There exists at least one solution to (P_h), i.e. at least one minimizer. First order optimality conditions can be derived by Lagrangian calculus.*

Finally, in [3], the limit $h \to 0$ is considered and we show that in the limit the variables fulfil the time discrete correspondence to (1)–(3). Moreover we show the following strong convergence results:

$$\varphi_h^m \to \varphi^m \text{ in } H^1(\Omega), \qquad \mu_h^m \to \mu^m \text{ in } W^{1,3}(\Omega),$$
$$u_{I,h} \to u_I \text{ in } H^1(\Omega), \qquad v_h^m \to v^m \text{ in } H_1(\Omega)^n, \, (\mathrm{div}(v^m), q) = 0 \, \forall q \in L^2(\Omega).$$

3. A numerical example

We finally support our results by a numerical example. Here, we aim at steering a bubble against buoyancy forces using tangential boundary control. In Figure 1 we show the numerical results. The zero level lines of the initial and desired phase field are shown on the left plot together with the domain of control, which is the left and right boundary. The evolution of the optimally controlled phase field and velocity field at times $t = 0.25, 0.5, 0.75, 1.0$ are the second to fifth plot. The pictures show $|v_h^m|$ on the left and φ_h^m on the right. For $t = 1.0$ we additionally indicate the zero-level line of φ_d by a black line. Note that v_h^m coincides with $B_B u_B^m$ on the boundary.

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Mathematical Model for Biofilm Development (Application of a New Compactness Theorem)

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(joint work with M. Gokieli and M. Niezgódka)

1. Motivation

Our motivation is the completion of mathematical model of biofilm development in a fluid flow and its analysis. This model includes a variational inequality of the Navier-Stokes type with obstacles.

For the solvability of quasi-linaer PDEs we use some compactness theorems in time, for instance, of J.P. Aubin type [1] and J. Simon type [8]. However they are not available for nonlinear variational inequalities of parabolic type with time-dependent convex (interior) constraints, such as $u(x,t) \geq \psi(x,t)$ or $|u(x,t)| \leq \psi(x,t)$.

We discuss a new compactness theorem from this point of view. The main idea is to consider the operator of time-derivative with convex constraints $K(t),\ 0 \leq 1 \leq T$:

$$u \longrightarrow \frac{du(t)}{dt} + \partial I_{K(t)}(u(t)).$$

2. A compactness theorem for variational inequalities

Let H be a Hilbert space, V a Banach space (with strictly convex dual V^*) and W be a Banach space such that V is densely and compactly embedded in $H$and W is continuously embedded in V, and suppose that all spaces are separable and reflexive:

$$W \hookrightarrow V \hookrightarrow (\text{compact})H,\ V \hookrightarrow H = H^* \hookrightarrow W^*,\ \text{compact embeddings.}$$

We are given a family of closed, convex subset $K(t),\ t \in [0,T]$, in V such that $K(t)$ is smooth in t (for instance, $K(t)$ is Lipschitz continuous in $t \in [0,T]$ with respect to the Hausdorff distance in V) and define the the class of test functions

$$\mathcal{K} := \{v \in L^p(0,T;V) \mid v(t) \in K(t) \text{ a.e. } t \in [0,T]\},\ 1 < p < \infty,$$

and the smooth one

$$\mathcal{K}_0 := \{\eta \in \mathcal{K} \mid \eta' \in L^{p'}(0,T;V^*)\},\ \frac{1}{p} + \frac{1}{p'} = 1.$$

Given $u_0 \in \overline{K(0)}^H$, the operator L_{u_0} ($\approx \frac{d}{dt} + \partial I_{K(t)}(\cdot)$) is defined by:

$$f \in L_{u_0}u \Longleftrightarrow \begin{cases} f \in L^{p'}(0,T;V^*),\ u \in \mathcal{K}; \\ \displaystyle\int_0^T \langle \eta' - f, u - \eta\rangle \le \frac{1}{2}|u_0 - \eta(0)|_H^2,\ \forall \eta \in \mathcal{K}_0, \end{cases}$$

where $\langle\cdot,\cdot\rangle$ is the duality between V^* and V. We know [3, 7]that L_{u_0} is maximal monotone from $L^p(0,T;V)$ into $L^{p'}(0,T;V^*)$ and $D(L_{u_0}) \subset \{u \mid u \in \mathcal{K} \cap C([0,T];H),\ u(0) = u_0\}$.

Theorem 1. *Assume:* $\exists \kappa > 0$ *such that*

$$(*)\ \kappa B_W(0) \subset K(t),\ \forall t \in [0,T],\ \textit{where}\ B_W(0) := \{w \in W \mid |w|_W \le 1\}.$$

Then, $\forall M > 0$,

$$Z_M := \{u \in D(L_{u_0}) \mid |u|_{L^p(0,T;V)} \le M,\ \inf_{f \in L_{u_0}u} |f|_{L^{p'}(0,T;V^*)} \le M\}$$

is relatively compact in $L^p(0,T;H)$.

The theorem is proved, based on the uniform estimate of total variation of functions in Z_M, with the help of Helly selection lemma and Riesz representation theorem. See [6] for the detailed proof.

3. Application to biofilm development in a fluid flow

We consider a mathematical model for biofilm development which is governed by three nonlinear evolution equations or inequalities. They are biomass density equation (B), nutrient transport equation (N) and Navier-Stokes variational inequality $(H)^\varepsilon$ including a relaxation parameter ε; in this model ε is a small positive number and fixed. We denote by $u := u(x,t),\ 0 \le u \le 1$, $w := w(x,t),\ 0 \le w \le 1$, and $\mathbf{v} := \mathbf{v}(x,t)$ the biomass density, nutrient concentration and velocity field of the fluid flow.

Let Ω be a bounded smooth domain (container in which biomass growth takes places) in $\mathbf{R}^3$, $Q := \Omega \times (0,T)$, $\Gamma := \partial\Omega$ and Γ_0 a compact subset of Γ. We suppose that

$\beta(\cdot)$ is a maximal (strictly) monotone mapping in $\mathbf{R}$ such that

$$D(\beta) = [0,1),\ \beta(0) = (-\infty, 0],\ \lim_{r \downarrow 0} \frac{\beta(r)}{r} = 0 \text{ (degeneracy)};$$

$d(\cdot)$ is a strictly positive and smooth function on $[0,1]$;
$f(\cdot)$ is of C^1 and Lipschitz continuous on $\mathbf{R}$ with $f(0) \le 0,\ f(1) \ge 1$;
$p_0(\cdot)$ is a non-negative continuous function on $(0,1]$ such that

$$\lim_{r \downarrow 0} p_0(r) = \infty,\ p_0 \text{ is decreasing on } (0,\delta_0),\ p_0(r) = 0, \forall r \in [\delta_0, 1],$$

where δ_0 is a fixed number in $(0,1)$.

With the above data $\beta,\ d,\ p_0$ and appropriate initial data $u_0,\ w_0$ and $\mathbf{v}_0$ our model for biofilm development is formulated as follows.

$$(B)\qquad u' - \Delta\tilde{\beta} + \mathbf{v}\cdot\nabla u + bu = f(w)u \text{ in } V^*_{\Gamma_0},\ \tilde{\beta}\in\beta(u) \text{ in } Q,$$

$$u(0) = u_0,\ \tilde{\beta} = 0 \text{ on } \Gamma_0\times(0,T),\ \frac{\partial\tilde{\beta}}{\partial n} = 0 \text{ on } (\Gamma-\Gamma_0)\times(0,T),$$

$$V_{\Gamma_0} := \{z\in H^1(\Omega)\ |z = 0 \text{ a.e. on } \Gamma_0\},\ V^*_{\Gamma_0} = \text{dual of } V_{\Gamma_0}$$

$$(N)\qquad w' - \mathrm{dvi}(d(u)\nabla w) + \mathbf{v}\cdot\nabla w = -f(w)u \text{ in } H^1(\Omega)^*,\ 0\le w\le 1 \text{ on } Q,$$

$$w(0) = w_0\ (0\le w_0\le 1 \text{ a.e. on } \Omega),\ \frac{\partial w}{\partial n} = 0 \text{ on } \Gamma\times(0,T).$$

On account of the degeneracy of $\beta(u)$ at $u=0$, the biomass front $\partial\{x\mid u(x,t) > 0\}\cap\Omega$ moves slowly in time. In our relaxation model, using the spatial-average

$$u^\varepsilon(x,t) := \int_\Omega \rho_\varepsilon(x-y)u(y,t)dy,\ (\rho_\varepsilon \text{ is the usual spatial} - \text{mollifier}),$$

of biomass density $u(x,t)$, we formulate the hydrodynamics by the following weak variational inequality of the Navier-Stokes type with biomass density dependent obstacle $p_0(u^\varepsilon(x,t))$.

$$(H)^\varepsilon\qquad \mathbf{v}\in L^2(0,T;V)\cap L^\infty(0,T;H),\ |\mathbf{v}|\le p_0(u^\varepsilon) \text{ a.e. on } Q,$$

$$t\to(\mathbf{v}(t),\eta(t))_H \text{ is of BV on } [0,T],\ \forall\eta\in\mathcal{K}_0(u^\varepsilon),$$

$$\mathbf{v}(0) = \mathbf{v}_0 \text{ in } H,$$

$$\int_0^t\int_\Omega \eta'\cdot(\mathbf{v}-\eta) - \nu\int_0^t\int_\Omega \nabla\mathbf{v}\cdot\nabla(\mathbf{v}-\eta) + \int_0^t\int_\Omega(\mathbf{v}\cdot\nabla)\mathbf{v}\cdot(\mathbf{v}-\eta)$$

$$+\frac{1}{2}|\mathbf{v}(t)-\eta(t)|^2_H \le \frac{1}{2}|\mathbf{v}_0-\eta(0)|^2_H,\ \forall t\in[0,T],\ \forall\eta\in\mathcal{K}_0(u^\varepsilon),$$

where

$$\mathcal{K}_0(u^\varepsilon) := \{\eta\in C^1([0,T];W)\mid \mathrm{supp}(\eta)\subset\{p_0(u^\varepsilon) > 0\},\ |\eta|\le p_0(u^\varepsilon) \text{ on } \overline{Q}\}.$$

This coupled system $\{(B),(N),(H)^\varepsilon\}$ is a relaxed version of [2] and it can be solved by the compactness method based on our compactness theorem; see [4,5] for the detailed proof. Major difficulty in the analysis of this system arises from the quasi-variational structure of the coupling (cf. [3]).

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Interface dynamics in biological tissue growth

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(joint work with Joe Eyles and Vanessa Styles)

Biological tissue growth (in its broadest sense – i.e. including populations of single cell organisms (such as in bacterial biofilms), as well as multicellular ones (embryo development, tissue engineering, cancer growth etc.)) exhibits many features not shared by non-biological growth processes. At the macroscale, the most significant of these is probably the presence of cell division (and degradation), leading to the need to encompass sources (and sinks) of material. The simplest spatially structured models for such processes (see e.g. [1] and references therein) introduce an internal velocity field $\boldsymbol{v}(\boldsymbol{x},t)$, whereby within the tissue

$$\nabla\cdot\boldsymbol{v}=k(c)\quad\text{in }\Omega(t) \tag{1}$$

holds, where k is the net growth rate (so will be negative where degradation exceeds division) and $c(\boldsymbol{x},t)$ is the concentration of a generic nutrient. At the tissue edge the kinematic condition

$$V_n=\boldsymbol{v}\cdot\hat{\boldsymbol{n}}\quad\text{on }\partial\Omega(t) \tag{2}$$

holds, where V_n is the outward-normal velocity of the interface and $\hat{\boldsymbol{n}}$ is the unit outward normal. In the radially symmetric case with c prescribed, (1)–(2) suffice to specify moving-boundary evolution, but many effects (notably multi-dimensional instabilities) require a constitutive assumption on $\boldsymbol{v}$ to be formulated in order to close the system (see [2], for example). In many cases, the simplest plausible such assumption is that of Stokes flow, but here we focus on the one which has the longest pedigree historically and is the most tractable mathematically, namely Darcy flow – this is applicable to growth in a porous tissue-engineering scaffold, may be relevant to growth through a relatively static extracellular matrix (for example) and can in rather special circumstances [3] be shown to coincide with Stokes flow. Thus we set

$$\boldsymbol{v}=-K\nabla p\quad\text{in }\Omega(t) \tag{3}$$

for some internal pressure field $p(\boldsymbol{x},t)$ and permeability K, together with

$$p=\gamma\kappa\quad\text{on }\partial\Omega(t), \tag{4}$$

where κ is the mean curvature of the interface and γ is a cell-adhesion parameter.

Our focus here is on the thin-rim limit, relevant in a number of circumstances, whereby growth is confined to a narrow proliferating rim close to the tissue edge, with a necrotic core, in which degradation is taking place, occupying the bulk of the tissue. Applying formal-asymptotic methods to this limit, the rim collapses onto the interface and generates (see [4]) two additional terms in the moving-boundary conditions that replace (2) and (4), namely a constant surface source term Q in (2), giving

$$V_n = Q - K\nabla p \cdot \hat{\boldsymbol{n}} \quad \text{on } \partial\Omega(t), \tag{5}$$

capturing growth within the rim and (in a relevant distinguished limit) an addition regularising term of kinetic-undercooling type in (4), namely

$$p = \gamma\kappa + \nu V_n \quad \text{on } \partial\Omega(t), \tag{6}$$

the constant ν being associated with the mechanical behaviour of the rim. In the simplest case, (1), (3) lead to

$$K\Delta p = \lambda \quad \text{in } \Omega(t), \tag{7}$$

where the constant λ describes degradation (i.e. the volumetric sink) within the core. (5)–(7), together with the specification of the initial tissue domain, describe the moving-boundary problem of interest here. An immediate consequence of the divergence theorem is that

$$\frac{\mathrm{d}V}{\mathrm{d}t} = QA - \lambda V, \tag{8}$$

where V is the tissue volume and A its surface area, so if the tissue is to maximise its growth it should seek to increase its surface area for given volume (i.e. to avoid a spherical morphology): such matters can be clarified by a linear stability analysis. A limit complementary to that of such linearisation about the radially symmetric state is the thin-film limit: the PDE that results from this approach itself exhibits a number of interesting features. In addition, we have obtained extensive numerical solutions (by both sharp- and diffuse-interface methods) to (5)–(7) in both two and three dimensions: these exhibit strong instabilities, reflected in striking surface morphologies, if γ is not too large. There is also considerable scope for further mathematical investigations, with central questions (such as the existence or otherwise of non-radial steady states) being open.

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On Cahn–Hilliard models for tumour growth

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(joint work with Harald Garcke)

In recent years there has been an increased focus on the mathematical modelling of tumour growth with phase field models. In Garcke et al. [7] a Cahn–Hilliard–Darcy system is used to model the evolution of a two-component mixture consisting of tumour and healthy cells, in the presence of a chemical species acting as nutrient. The system of equations reads as follows:

$$\text{(P)}\qquad \begin{aligned} \operatorname{div} \vec{v} &= \mathcal{H}, \\ \vec{v} &= -K(\nabla p - (\mu + \chi\sigma)\nabla\varphi), \\ \partial_t \varphi + \operatorname{div}(\varphi \vec{v}) &= \Delta\mu + \mathcal{M}, \\ \mu &= A\Psi'(\varphi) - B\Delta\varphi - \chi\sigma, \\ \partial_t \sigma + \operatorname{div}(\sigma \vec{v}) &= \Delta\sigma - \chi\Delta\varphi + \mathcal{S}. \end{aligned}$$

Here, φ is an order parameter distinguishing between the tumour ($\{\varphi = 1\}$) and the healthy cells ($\{\varphi = -1\}$), with corresponding chemical potential μ, σ is the nutrient density, $\vec{v}$ is the volume-averaged velocity, and p is the pressure. Ψ is a potential with minima at ± 1. The positive parameters A, B are related to the interfacial thickness and the surface tension, while $K > 0$ is the permeability, and $\chi \geq 0$ is a parameter accounting for the mechanisms of chemotaxis (movement of tumour towards regions of high nutrient density) and active transport (movement of nutrient across the tumour-healthy cell interface that is persistently maintained even in the presence of diffusion). The terms $\mathcal{H}, \mathcal{M}, \mathcal{S}$ model for example nutrient consumption and growth of tumour cells.

Under certain choices of parameters and source terms, many of the previous diffuse interface models for tumour growth in the literature can be recovered. While numerous numerical simulations have been performed, there has been relatively few analytical results. A chief difficulty in the analysis comes from deriving a priori estimates in the presence of source terms in the Cahn–Hilliard equation, and when χ is positive, the nutrient equation contains a cross-diffusion-type term, which seems to an obstacle in applying classical results for second order parabolic equations such as weak comparison principles. Hence, previous works focus on the cases where $\chi = 0$ and the source terms are prescribed functions [8, 9] or chosen such that the total energy is a Lyapunov function [1, 2].

In [5] we studied the system (P) with Neumann boundary conditions for φ and μ, zero velocity $\vec{v} = 0$, positive χ and the following choice of source terms that is motivated from biological intuition:

$$\mathcal{M} = h(\varphi)\mathcal{P}\sigma, \quad \mathcal{S} = -h(\varphi)\mathcal{C}\sigma.$$

Here, h is an interpolation function such that $h(1) = 1$ and $h(-1) = 0$, $\mathcal{P} \geq 0$ is a growth rate and $\mathcal{C} \geq 0$ is a consumption rate. It turns out that the well-posedness of the system can be established only when the potential Ψ has quadratic growth. The result is not applicable to the classical quartic potential $\Psi(s) = (s^2 - 1)^2$

which is often used in diffuse interface models, and is attributed to the fact that the first a priori estimate derived from the energy identity

$$\frac{d}{dt}\int_\Omega A\Psi(\varphi) + \frac{B}{2}|\nabla\varphi|^2 + \frac{1}{2}|\sigma|^2 - \chi\sigma(1-\varphi)\,dx + \int_\Omega |\nabla\mu|^2 + |\nabla(\sigma-\chi\varphi)|^2\,dx = \int_\Omega \mu\mathcal{M} + (\sigma-\chi\varphi)\mathcal{S}\,dx$$

requires control on the square of the mean of μ in order to control the right-hand side with the left-hand side. In the case of Dirichlet boundary conditions, this restriction on the potential can be overcome by the Poincaré inequality, and well-posedness of the system for potentials of higher polynomial growth and also singular potentials has been established in [3].

For the system with Darcy's flow, the source term $\mathcal{H}$ is typically related to the term $\mathcal{M}$. Furthermore, the choice of boundary conditions for the velocity or the pressure may impose compatibility conditions on $\mathcal{H}$. For instance, Neumann boundary conditions for φ and p require that $\mathcal{H}$ must have mean zero. However, if $\mathcal{H}$ depends on φ or σ, then the zero mean condition may not be satisfied in general. In [4] the global weak existence in 2D and 3D for (P) with prescribed function $\mathcal{H}$ and source terms $\mathcal{M}$ and $\mathcal{S}$ that can be functions of φ, μ and σ with at most linear growth is established. Asymptotic limits $K \to 0$ and $\chi \to 0$ are also investigated, which serve to recover previous weak existence results in the literature. To allow for $\mathcal{H}$ to be a function also depending on φ and σ, in [6] we studied (P) with Robin and Dirichlet boundary conditions for the pressure, and showed the existence of weak solutions in 3D.

The above analytical results serve as a foundation for future in-depth analysis of diffuse interface models of tumour growth, as well as applications towards optimal control and parameter estimation.

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Higher order unfitted finite element methods for interface problems

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(joint work with A. Reusken)

In the recent decade *unfitted finite element methods* have drawn an increasing amount of attention. The possibility to handle complex geometries without the need for complex and time consuming mesh generation is very appealing. The methodology of unfitted finite element methods, i.e. methods which are able to cope with interfaces or boundaries which are not aligned with the grid, has been investigated for different problems. However, The development of numerical methods which are flexible with respect to the geometrical configuration, robust and *higher order accurate* at the same time is still challenging.

In unfitted finite element methods, for the representation of the geometry most often an implicit description with a scalar indicator function, e.g. a level set functions, is used. One major issue in the design and realization of higher order finite element methods is the problem of accurate and stable numerical integration on arising level set domains.

We present a new approach which allows for a higher order accurate and robust numerical treatment of domains that are prescribed by level set functions. The approach is based on isoparametric mappings that are specifically tailored. Adding together components from isoparametric (fitted) finite element methods and low order (second order) unfitted finite element methods we obtain a method that is robust and fairly simple to implement. The method is geometry-based and can be applied to unfitted interface or boundary value problems as well as to partial differential equations on surfaces. We outline the main aspects of the method for the following elliptic interface model problem. Let Ω be a polygonal domain and $\Omega_1 \cup \Omega_2 = \Omega$ a nonoverlapping partitioning with $\Gamma = \bar{\Omega}_1 \cap \bar{\Omega}_2$ a smooth interface. We seek for a solution u to the PDE:

$$\begin{aligned} -\mathrm{div}(\alpha \nabla u) &= f && \text{in } \Omega_i,\ i = 1, 2, \\ [\![\alpha \nabla u \cdot n]\!]_\Gamma &= 0 && \text{on } \Gamma, \quad [\![u]\!]_\Gamma = 0 \quad \text{on } \Gamma, \end{aligned}$$

where α is domain-wise constant and $[\![\cdot]\!]_\Gamma$ denotes the usual jump operator on Γ. We assume that the interface is described via a level set function ϕ as $\Gamma = \{\phi = 0\}$.

1. The construction of the isoparametric mapping

The basic idea of the new isoparametric method is the application of a mapping that improves the approximation quality of a robust but only low order accurate geometry approximation, the reference configuration. On simplicial meshes a

piecewise linear approximation $\hat{\phi}_h$ (which can be obtained by nodal interpolation) provides a geometry approximation $\Gamma^{\text{lin}} := \{\hat{\phi}_h = 0\}$ which is planar on each element T of a triangulation $\mathcal{T}_h$ of Ω. Exploiting that an *explicit* representation of Γ^{lin} is easily obtained, for this kind of geometry approximation numerical integration (of arbitrary high order) has been developed based on a decomposition of cut elements into simple geometries, e.g. simplices. This integration approach forms the basis for the new method.

With a mesh transformation Θ_h we improve the quality of the approximation corresponding to Γ^{lin} so that $\Gamma_h := \Theta_h(\Gamma^{\text{lin}})$ defines the new geometry approximation with an *explicit* representation. A detailed description of the construction of Θ_h can be found in [1]. The crucial properties of Θ_h are the following:

- $\hat{\phi}_h \circ \Theta_h^{-1} \approx \phi$ in a small (mesh-dependent) neighborhood of Γ.
- Θ_h is a homeomorphism on Ω.
- $\Theta_h = \text{id}$ away from Γ^{lin}, i.e. the most part of the mesh remains untouched.
- Θ_h is a finite element function, i.e. Θ_h and $D\Theta_h$ are efficiently computable.
- $\Theta_h(x_V) = x_V$ for all vertices x_V in the mesh as $\hat{\phi}(x_V) = \phi(x_V)$.
- The transformation is a perturbation to the identity, $\|D\Theta_h\|_{L^\infty(\Omega)} \leq h$.
- Higher derivatives are uniformly bounded, $\max_{T\in\mathcal{T}_h} \|D^m\Theta_h\|_{L^\infty(T)} \leq 1$, $m = 1, .., k+1$.

We note that the *cut topology does not change* under the transformation, this means that the triangulation consisting of curved elements $\{\Theta_h(T)\}_{T\in\mathcal{T}_h}$ has the same cut configuration as $\mathcal{T}_h$. Further, we note that the first property ensures $\Theta_h(\Gamma^{\text{lin}}) \approx \Gamma$.

2. An unfitted isoparametric finite element method for the elliptic interface model problem

According to the mesh transformation we adapt the usual unfitted finite element spaces. Let V_h^Γ be an appropriate (possibly higher order) finite element space for a stable discretization of a PDE problem with respect to the geometry approximation Γ^{lin}. Then, we define the finite element space for the discretization with respect to the geometry approximation to Γ_h as $\mathcal{V}_h^\Gamma := \{\varphi \circ \Theta_h^{-1}, \varphi \in V_h^\Gamma\}$.

For the elliptic interface model problem we take the usual cut finite element space with respect to the piecewise planar geometry approximation Γ^{lin}, $V_h^\Gamma := V_h|_{\Omega_1^{\text{lin}}} \oplus V_h|_{\Omega_2^{\text{lin}}}$ where V_h is the space of continuous piecewise polynomial functions of degree $k > 0$ and Ω_i^{lin}, $i = 1, 2$ are the piecewise planar approximations to Ω_i, $i = 1, 2$.

Using Nitsche's method in the context of unfitted finite element methods to weakly impose the interface conditions, cf. [2], we obtain an unfitted isoparametric

finite element discretization: Find $u_h \in \mathcal{V}_h^\Gamma$ such that

$$\sum_{i=1,2} \int_{\Theta_h(\Omega_i^{\mathrm{lin}})} \alpha_i \nabla u_h \nabla v_h \, dx - \int_{\Theta_h(\Gamma^{\mathrm{lin}})} \{\!\{\alpha \nabla u_h \cdot n\}\!\} [\![v_h]\!] \, ds$$
$$- \int_{\Theta_h(\Gamma^{\mathrm{lin}})} \{\!\{\alpha \nabla v_h \cdot n\}\!\} [\![u_h]\!] \, ds + \frac{\lambda}{h} \int_{\Theta_h(\Gamma^{\mathrm{lin}})} [\![u_h]\!][\![v_h]\!] \, ds = \int_\Omega f v \, dx \quad \text{for all } v_h \in \mathcal{V}_h^\Gamma,$$

where $\{\!\{\cdot\}\!\}$ is the averaging operator also taken in [2] and λ is a sufficiently large stabilization parameter the choice of which depends only on α, k and the shape regularity of the underlying triangulation $\mathcal{T}_h$ of Ω. We note that in an implemenation of the method the integration in the discrete variational formulation can be transformed to integrals on the reference domains Γ^{lin}, Ω_i^{lin}, $i = 1, 2$ which (only) involve additional factors depending on Θ_h which are explicitly computable.

In the analyses [3, 4] of the method we derived higher order (a priori) error bounds for the discretization error based on Strang-type estimates. To this end, we needed to ensure the above mentioned properties of the transformation Θ_h.

3. Extensions and future work

The idea of applying isoparametric unfitted method based on the mesh transformation Θ_h is also applicable to other problems, e.g. unfitted Stokes interface problems [5] and PDEs on surfaces [6]. Extensions to problems with moving domains are still missing, they are the topic of current research. A combination of space-time unfitted finite element methods [7] with the isoparametric mesh transformation (in space) seems a reasonable approach which could lead to robust and higher order accurate methods in space and time. The investigation of such methods is planned for the future. Another topic related to higher order unfitted finite element method is the question of efficiently solving arising linear systems which are typically very ill-conditioned. The question of optimal solution strategies is open and requires further attention.

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Nematic Liquid Crystals with Variable Degree of Orientation

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(joint work with Shawn S. Walker and Wujun Zhang)

Complex fluids are ubiquitous in nature and industrial processes and are critical for modern engineering systems. An important difficulty in modeling and simulating complex fluids is their inherent microstructure. Manipulating the microstructure via external forces can enable control of the mechanical, chemical, optical, or thermal properties of the material. Liquid crystals are a relatively simple example of a material with microstructure that may be immersed in a fluid with a free interface.

There are three basic models with increasing degree of mathematical complexity for the equilibrium state of liquid crystals: the Ossen-Frank model [12], the Ericksen-Leslie model [8, 12], and the Q-tensor model [7, 12]. The former leads to so-called harmonic maps and consists of minimizing the Dirichlet integral for a director field $\boldsymbol{n}$, namely a unit vector field:

$$E[\boldsymbol{n}] = \int_\Omega |\nabla \boldsymbol{n}|^2 dx.$$

Several numerical methods have been proposed for this problem [1, 4, 6]. However, $E[\boldsymbol{n}]$ does not allow for point defects of $\boldsymbol{n}$ in dimension $d = 2$ or line defects for $d = 3$, which dictate the material properties of liquid crystals.

The Ericksen-Leslie model, or one-constant model, is a compromise between the two extreme models and reduces to minimizing the bulk energy

$$E[s, \boldsymbol{n}] = \underbrace{\int_\Omega \Big(\kappa |\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2\Big) dx}_{=E_1[s,\boldsymbol{n}]} + \underbrace{\int_\Omega \psi(s) dx}_{=E_2[s]}$$

over a bounded domain $\Omega \subset \mathbb{R}^d$, with $d \geq 2$, where $s : \Omega \to (-\frac{1}{2}, 1)$ is a scalar order parameter that represents the degree of orientation of the rod-like molecules of the liquid crystal, ψ is a double-well potential that confines s to lie in the interval $(-\frac{1}{2}, 1)$, and $\kappa > 0$ is the only model parameter. The case $s \approx 1$ corresponds to perfect alignment of molecules with the director $\boldsymbol{n}$, $s \approx -\frac{1}{2}$ signifies a right angle between them, and $s = 0$ is the state of isotropic distribution of molecules or no preferred direction. The zero level set of s determines the location of *defects*, which are typically sets of dimension 1 and 2 for $d = 3$ where $|\nabla \boldsymbol{n}|$ blows up.

Since the director field $\boldsymbol{n} \notin [H^1(\Omega)]^d$, the existence and structure of minimizers of $E[s, \boldsymbol{n}]$ is far from obvious. A fundamental observation, made in [2, 9], reveals a hidden regularity in the auxiliary variable $\boldsymbol{u} = s\boldsymbol{n}$. In fact, since $\nabla |\boldsymbol{n}|^2 = 2\mathbf{n}^{\mathbf{T}} \nabla \boldsymbol{n} = \mathbf{0}$, we obtain the pointwise equality

$$|\nabla \boldsymbol{u}|^2 = |\boldsymbol{n} \otimes \nabla s + s \nabla \boldsymbol{n}|^2 = |\nabla s|^2 + s^2 |\nabla \boldsymbol{n}|^2,$$

because $\boldsymbol{n} \otimes \nabla s$ and $\nabla \boldsymbol{n}$ are orthogonal. This yields the equivalent form of $E_1[s, \boldsymbol{n}]$

$$\widetilde{E}_1[s, \boldsymbol{n}] = \int_\Omega \Big((\kappa - 1)|\nabla s|^2 + |\nabla \boldsymbol{u}|^2\Big) dx,$$

which shows that $\boldsymbol{u} \in [H^1(\Omega)]^d$ but $\widetilde{E}_1[s, \boldsymbol{n}]$ contains a negative term provided $\kappa < 1$; this is the most important regime responsible for defects.

Converging numerical methods to approximate $E[s, \boldsymbol{n}]$ require regularization [3]. We present a novel structure preserving discretization of $E[s, \boldsymbol{n}]$ within the space of continuous piecewise linear finite elements $\mathbb{V}_h$ which circumvents regularization altogether. If $\{\phi_i\}$ is the canonical basis of hat functions of $\mathbb{V}_h$, the idea is to write the Dirichlet integral for $v_h = \sum_i v_i \phi_i \in \mathbb{V}_h$ as

$$\int_\Omega |\nabla v_h|^2 = \frac{1}{2} \sum_{i,j} k_{ij} (v_i - v_j)^2, \quad k_{ij} = -\int_\Omega \nabla \phi_i \cdot \nabla \phi_j$$

and then define the approximate energy $E_1^h[s_h, \boldsymbol{n}_h]$ to be

$$E_1^h[s_h, \boldsymbol{n}_h] = \frac{\kappa}{2} \sum_{ij} k_{ij} (s_i - s_j)^2 + \frac{1}{2} \sum_{ij} \frac{s_i^2 + s_j^2}{2} |\boldsymbol{n}_i - \boldsymbol{n}_j|^2.$$

We show that this method is consistent and stable provided the underlying mesh is weakly acute: $k_{ij} \geq 0$ for all $i \neq j$. We prove Γ-convergence of discrete global minimizers to continuous ones as the mesh size h goes to zero [5]. We develop a quasi-gradient flow scheme for computing discrete equilibrium solutions and prove that it has a strictly monotone energy decreasing property. We illustrate the method's ability to handle non-trivial line and plane defects for $d = 3$ via several simulations implemented within the software platform [13]. Moreover, we extend both theory and numerical experiments to model colloidal and electric effects, such as the Freedericksz transition and the so-called Saturn ring defect.

Our results are contained in [10, 11]. A music video summarizing them is also available on YouTube: *Mathematical Modeling and Simulation of Nematic Liquid Crystals (A Montage)*, `http://www.youtube.com/watch?v=pWWw7_6cQ-U`.

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Minimizing movement approach for spirals evolving by crystalline curvature using level set functions

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(joint work with Yen-Hsi Richard Tsai)

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with smooth boundary, and $a_1, a_2, \ldots, a_N \in \Omega$. We consider evolution of spirals Γ_t associated with $a_1, \ldots, a_N$ in Ω by the crystalline curvature and eikonal equation.

It is well-known that, the anisotropic curvature H_γ of the interfacial curve $\Gamma = \{x \in \Omega;\ u(x) = c\}$ with level set formulation $u(x)$ is defined as the first variation of the anisotropic perimeter functional

$$J_\gamma(u) = \int_\Omega \gamma(\nabla u) dx$$

with a density function $\gamma\colon \mathbb{R}^2 \to [0, \infty)$, which is convex and positively homogeneous of degree 1. If γ is smooth, then $H_\gamma = -\mathrm{div} D\gamma(\nabla u)$ in the sense of L^2. In particular, if $\gamma(p) = |p|$, then H_γ is the isotropic curvature of Γ. It is well-known that the set $\mathcal{W}_\gamma = \{p \in \mathbb{R}^2;\ \gamma^\circ(p) \le 1\}$, which is called "Wulff shape", satisfies that $H_\gamma = 1$ on ∂W_γ under some suitable assumptions, where $\gamma^\circ(p) = \sup\{p \cdot q;\ \gamma(q) \le 1\}$. The crystalline curvature is defined as the anisotropic curvature such that $\mathcal{W}_\gamma$ is convex polygon. Therefore, we here assume that

(A1) γ is convex,
(A2) γ is positively homogeneous of degree 1,
(A3) there exists $\Lambda > 0$ such that $\Lambda^{-1} \le \gamma \le \Lambda$ on S^1,
(A4) γ is piecewise linear.

Under these hypothesis, we consider evolution of spiral curves Γ_t by

$$V_\gamma = f - H_\gamma \quad \text{on } \Gamma_t, \tag{1}$$

where V_γ is the normal velocity of Γ_t with anisotropic *distance* $\mathrm{dist}_\gamma(x, y) = \gamma^\circ(x - y)$. For evolution of interfacial curve by (1), Chambolle [1] introduced a time-discrete approximation algorithm with level set method using signed distance function from the evolving interfaces. Oberman, Osher, Takei and Tsai [3] introduced a numerical method for Chambolle's algorithm. On the other hand, Y.-H. R. Tsai, Giga and the author [4, 5] introduced a level set method for evolving

spirals. Therefore, we propose the methods combining the Chambolle's algorithm with the level set method for evolving spirals.

To present our method we now introduce the level set method for spirals by [4, 5]. Let us set $W = \Omega \setminus \bigcup_{j=1}^{N} \overline{B_\rho(a_j)}$ with $\rho > 0$, where $B_\rho(a) = \{x \in \mathbb{R}^2;\ |x - a| < \rho\}$. We assume that $\overline{B_\rho(a_i)} \cap \overline{B_\rho(a_j)} = \emptyset$ if $i \neq j$, and $\overline{B_\rho(a_j)} \subset \Omega$ for $j = 1, \ldots, N$. Define $\theta \colon \overline{W} \to \mathbb{R}$ as

$$\theta(x) = \frac{1}{L\pi} \sum_{j=1}^{N} m_j \arg(x - a_j),$$

where $m_j \in \mathbb{Z} \setminus \{0\}$ is a signed number of spirals associated with a_j (see [5] for details), and $L \geq 1$ is a numerical cofficient choosing for stability of numerical simulations. Then, we represent spiral curves Γ_t at time $t \geq 0$ and whose direction $\mathbf{n} \in S^1$ of the evolution as

$$\Gamma_t = \{x \in \overline{W};\ u(t,x) - \theta(x) \equiv 0 \mod (2/L)\mathbb{Z}\}, \quad \mathbf{n} = -\frac{\nabla(u-\theta)}{|\nabla(u-\theta)|}. \tag{2}$$

For example, evolution of Γ_t by (1) with smooth γ is represented as

$$u_t - \gamma(\nabla(u-\theta))\{\mathrm{div} D\gamma(\nabla(u-\theta)) + f\} = 0. \tag{3}$$

See [2] for derivation of the level set equation.

In [1] we consider a minimizing problem for a functional of anisotropic perimeter and the distance between the original curve and its deformation to approximate the motion by (1) in discrete time interval $[t, t+h]$. By the analogue from the curvature term in (3), the functional for the evolution of spirals is of the form

$$F_\gamma(u;\Gamma) = \int_W \gamma(\nabla(u-\theta))dx - \int_W fudx + \frac{1}{2h}\|u - g_\Gamma\|_{L^2}^2. \tag{4}$$

Note that the second term of the above denotes the driving force term. In [1] the function g_Γ should be chosen as the signed distance function $d_\gamma(x,\Gamma)$ of the form

$$d_\gamma(x,\Gamma) := \begin{cases} -\inf_{y\in\Gamma} \gamma^\circ(x-y) & \text{in } \mathbf{n}\text{-side of } \Gamma, \\ \inf_{y\in\Gamma} \gamma^\circ(x-y) & \text{otherwise} \end{cases}$$

if Γ is interfacial curve. However, if Γ is spiral curve, the signed distance function does not work well since Γ does not divide the domain into the $\pm\mathbf{n}$-side regions.

To overcome this difficulty, we introduce two methods. The first one is to construct a signed distance function only in a neighborhood of Γ. For this purpose, we first construct $\mathbf{n}$-side and $-\mathbf{n}$-side distance functions of Γ. The simplest way is to solve two eikonal equations $V_\gamma = \pm 1$, i.e.,

$$u_t = \gamma(\nabla(u-\theta)), \quad v_t = -\gamma(\nabla(v-\theta))$$

with $u(0,\cdot) = v(0,\cdot) = u_0 \in C(\overline{W})$, where u_0 is such that $\Gamma = \{x \in \overline{W};\ u_0(x) - \theta(x) \equiv 0 \mod (2/L)\mathbb{Z}\}$. Then, we define $t_u(x)$ for $x \in \overline{W}$ as the time such that

$$\begin{aligned} u(t_u(x),x) - \theta(x) &\equiv 0 \mod (2/L)\mathbb{Z}, \\ u(\cdot,x) - \theta(x) &\not\equiv 0 \mod (2/L)\mathbb{Z} \text{ on } [0, t_u(x)) \end{aligned}$$

if $u_0(x) - \theta(x) \not\equiv 0 \mod (2/L)\mathbb{Z}$, and $t_u(x) = 0$ if $u_0(x) - \theta(x) \equiv 0 \mod (2/L)\mathbb{Z}$. We also define $t_v(x)$ using v in the same manner. Note that t_u and t_v is the $\mathbf{n}$-side and $-\mathbf{n}$-side distance function for Γ, respectively. Then, we now define $g_\Gamma(x)$ as

$$g_\Gamma(x) = \begin{cases} \theta_\Gamma(x) - \min\{Mt_u(x), \dfrac{1}{L}\} & \text{if } t_u(x) < t_v(x), \\ \theta_\Gamma(x) - \dfrac{2}{L} + \min\{Mt_v(x), \dfrac{1}{L}\} & \text{otherwise} \end{cases} \tag{5}$$

with a constant $M \geq 1$, where θ_Γ is a branch of θ whose $(2/L)$-jump discontinuity is only on Γ. One can find that

$$g_\Gamma(x) - \theta(x) = Md_\gamma(x, \Gamma) \quad \text{for } x \in \{y \in \overline{W};\ |d_\gamma(x, \Gamma)| \leq 1/(LM)\}.$$

The constant $M \geq 1$ should be chosen so that g_Γ has no discontinuity on far away region from Γ; note that g_Γ may have discontinuity on $\{x \in \overline{W};\ t_u(x) = t_v(x) > 0\}$ if M is small. Then, we consider the minimizer u^* of (4) with above g_Γ, and set

$$T_1(\Gamma) = \{x \in \overline{W};\ u^* - \theta \equiv 0 \mod (2/L)\mathbb{Z}\}.$$

For given initial curve Γ, the evolution of spirals by (1) at $t > 0$ which is denoted by Γ_t is defined as

$$\Gamma_t = T_1^{[t/(Mh)]}(\Gamma).$$

Note that the iteration number of this method to fixed time $t > 0$ is $M \times [t/h]$ because of the coefficient $M \geq 1$ in front of d_γ.

The second method is just using a level set function. If $\Gamma = \{x \in \overline{W};\ w(x) - \theta(x) \equiv 0 \mod (2/L)\mathbb{Z}\}$ with $w \in C(\overline{W})$, then we consider the minimizing problem of (4) with $g_\Gamma = w$. Then, we define

$$\begin{aligned} T_2(\Gamma) &= \{x \in \overline{W};\ w^{**} - \theta \equiv 0 \mod (2/L)\mathbb{Z}\}, \\ w^{**} &:= w + \gamma(\nabla(w^* - \theta))(w^* - w). \end{aligned}$$

For given initial curve $\Gamma = \{x \in \overline{W};\ w_0 - \theta \equiv 0 \mod (2/L)\mathbb{Z}\}$ with $w_0 \in C(\overline{W})$, the evolution of spirals Γ_t by (1) at $t > 0$ with the second method is defined as

$$\begin{aligned} \Gamma_t = T_2^{[t/h]}(\Gamma) &= \{x \in \overline{W};\ w^{**}_{[t/h]}(x) - \theta(x) \equiv 0 \mod (2/L)\mathbb{Z}\}, \\ w^{**}_{n+1} &= w^{**}_n + \gamma(\nabla(w^*_{n+1} - \theta))(w^*_{n+1} - w^{**}_n), \\ w^*_{n+1} &= \arg\min_w F_\gamma(w, \Gamma_n)|_{g_\Gamma = w^{**}_n},\ w^{**}_0 = w_0. \end{aligned}$$

The numerical results of the above two method are also presented in this talk.

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Unfitted finite element methods for PDEs on evolving surfaces

Maxim Olshanskii
(joint work with Arnold Reusken and Xianmin Xu)

Partial differential equations posed on evolving surfaces appear in a number of applications such as two-phase incompressible flows (surfactant transport on the interface) and flow and transport phenomena in biomembranes. Numerical approaches discussed in this report are based on Eulerian description of the surface PDE problem and employ a time-independent background mesh that is not fitted to the surface. The time-dependent surface $\Gamma(t) \subset \mathbb{R}^3$ is assumed smooth and closed for all $t \in [0,T]$. The evolution of the surface may be given implicitly, for example, by the level set method. As an example of the surface PDE we consider the transport–diffusion equation modelling the conservation of a scalar quantity u with a diffusive flux on $\Gamma(t)$, which is passively advected by a given smooth velocity field $\mathbf{w} : \mathbb{R}^3 \times [0,T] \to \mathbb{R}^3$,

$$\dot{u} + (\operatorname{div}_\Gamma \mathbf{w})u - \nu \Delta_\Gamma u = f \quad \text{on } \Gamma(t),\ t \in (0,T], \tag{1}$$

with initial condition $u(\mathbf{x},0) = u_0(\mathbf{x})$ for $\mathbf{x} \in \Gamma_0 := \Gamma(0)$. Here $\dot{u}$ denotes the advective material derivative, $\operatorname{div}_\Gamma$ is the surface divergence, Δ_Γ is the Laplace–Beltrami operator, and $\nu > 0$ is the constant diffusion coefficient.

In the report, we discuss two unfitted finite element methods based on restrictions of outer (bulk, volumetric) finite element functions to the surface. This methodology is known as the trace finite element method (TraceFEM), see the recent review article [4]. In the first approach from [1, 2] to problems posed on time-dependent surfaces, one considers a space–time manifold

$$\mathcal{S} = \bigcup_{t\in(0,T)} \Gamma(t) \times \{t\}, \quad \mathcal{S} \subset \mathbb{R}^4,$$

and a weak formulation of (1) as a surface PDE on $\mathcal{S}$: Find $u \in W$ such that

$$\langle \dot{u}, v \rangle_{H' \times H} + \int_0^T \int_{\Gamma(t)} (uv \operatorname{div}_\Gamma \mathbf{w} + \nu_d \nabla_\Gamma u \cdot \nabla_\Gamma v)\, ds\, dt = \int_0^T \int_{\Gamma(t)} f v\, ds\, dt. \tag{2}$$

for all $v \in H$, $u(\cdot,0) = u_0(\mathbf{x})$. Here the trial and test spaces are the following Hilbert spaces of functions defined on $\mathcal{S}$:

$$H = \{\, v \in L^2(\mathcal{S}) \mid \|\nabla_\Gamma v\|_{L^2(\mathcal{S})} < \infty \,\}, \quad (u,v)_H = (u,v)_{L^2(\mathcal{S})} + (\nabla_\Gamma u, \nabla_\Gamma v)_{L^2(\mathcal{S})};$$
$$W = \{\, u \in H \mid \dot{u} \in H' \,\}, \quad \|u\|_W^2 := \|u\|_H^2 + \|\dot{u}\|_{H'}^2.$$

Now the space–time trace finite element method builds on the weak formulation (2). In particular, one considers space–time prismatic elements and defines finite

element counterparts of W and H as traces of outer space–time polynomial finite element spaces on a tetrahedral reconstruction of $\mathcal{S}$. It turns out that the resulting method can be implemented in an efficient time-marching way. It has been also proved to be of the optimal first order (in space and time) in an energy norm and of the second order convergence in a weaker norm.

Another unfitted finite element method we discuss is the one recently proposed in [3]. The main motivation for this method is to avoid space–time elements or any reconstruction of the space–time manifold. Assume that the surface is defined implicitly as the zero level of a smooth level set function ϕ on $\Omega \times (0,T)$: $\Gamma(t) = \{\mathbf{x} \in \mathbb{R}^3 \,:\, \phi(t,\mathbf{x}) = 0\}$, such that $|\nabla\phi| \geq c_0 > 0$ in a suitable neighborhood of $\mathcal{S}$. One obtains the following equivalent formulation of (1),

$$(3) \qquad \left\{ \begin{array}{ll} \dfrac{\partial u}{\partial t} + \mathbf{w}\cdot\nabla u + (\operatorname{div}_\Gamma \mathbf{w})u - \nu\Delta_\Gamma u = f & \text{on } \Gamma(t), \\ \nabla u \cdot \nabla\phi = 0 & \text{in } \mathcal{O}(\Gamma(t)). \end{array} \right. \quad t \in (0,T].$$

Here $\mathcal{O}(\Gamma(t))$ is a $\mathbb{R}^3$ neighborhood of $\Gamma(t)$ for any fixed $t \in (0,T]$. Assuming $\Gamma(t_n)$ lies in the neighborhood of $\Gamma(t_{n-1})$, where $u(t_{n-1})$ is defined, one may discretize (3) in time using, for example, the implicit Euler method (higher order differences are equally suitable):

$$(4) \qquad \frac{u^n - u(t_{n-1})}{\Delta t} + \mathbf{w}^n \cdot \nabla u^n + (\operatorname{div}_\Gamma \mathbf{w}^n)u^n - \nu\Delta_\Gamma u^n = f^n \quad \text{on } \Gamma(t_n),$$

$\Delta t = t_n - t_{n-1}$. Now one applies the trace finite element method to discretize (4) only in space. A numerical extension procedure, $u_h^n \to u_h^{ext,n}$, and the finite element formulation of (4) define the fully discrete numerical method. To find a suitable extension, one can consider a numerical solver for hyperbolic systems and apply it to the second equation in (3). Numerical results from [3] suggest that the Fast Marching Method is suitable for building extensions in narrow bands of tetrahedra containing Γ_h, but other (higher order) numerical methods can be also used.

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Geometric variational problems with nonlocal interaction

Xiaofeng Ren

We discuss some geometric variational problems arising from the studies of diblock copolymers, triblock copolymers, and the FitzHugh-Nagumo system. Common in these problems the free energy is a sum of a local energy (the perimeter of Caccioppoli sets) and a nonlocal energy given in terms of the Green's functions of the Poisson equation or the Helmholtz equation. Both binary systems (of two constituents) and ternary systems (of three constituents) will be discussed. For a binary system we show the existence of droplet assemblies as stationary points [2] and explain the impact of the domain shape on the locations of the droplets in an assembly [1]. For a ternary system we prove the existence of a new morphological phase: the double bubble phase, as a stable stationary point [3].

We aslo consider recently discovered toroidal assemblies in block copolymers, and find a solution, called a torus profile, that is a set enclosed by an approximate torus of the major radius 1 and the minor radius q, to the profile problem of diblock copolymers. There is a way to set up the profile problem in a function space as a integro-partial differential equation. The linearized operator $\mathcal{L}$ of the problem at the torus profile is decomposed into a family of linear integro-ordinary differential operators $\mathcal{L}^m$ where the index $m = 0, 1, 2, ...$ is called a mode. The spectrum of $\mathcal{L}$ is the union of the spectra of the $\mathcal{L}^m$'s. It is proved that for each m, when q is sufficiently small, $\mathcal{L}^m$ is positive definite. (0 is an eigenvalue for both $\mathcal{L}^0$ and $\mathcal{L}^1$, due to the translation and rotation invariance.) As q tends to 0, more and more $\mathcal{L}^m$'s become positive definite. However no matter how small q is, there is always a mode m of which $\mathcal{L}^m$ has a negative eigenvalue. This mode grows to infinity like $q^{-3/4}$ as $q \to 0$ [4].

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A Diffuse Interface Model for Two-Phase Ferrofluid Flows

Abner J. Salgado

(joint work with Ricardo H. Nochetto and Ignacio Tomas)

A ferrofluid is a liquid which becomes strongly magnetized in the presence of applied magnetic fields. It is a colloid made of nanoscale monodomain ferromagnetic particles suspended in a carrier fluid. These particles are suspended by Brownian motion and will not precipitate nor clump under normal conditions. Ferrofluids

are dielectric and paramagnetic. They find applications in magnetic manipulation of microchannel flows, microvalves, magnetically guided transport and other fields. We consider the Rosensweig [Ros97] model of ferrofluids, which reads

(1)
$$\begin{aligned} &\mathsf{u}_t + \mathsf{u}\cdot\nabla\mathsf{u} - (\nu+\nu_r)\Delta\mathsf{u} + \nabla\mathsf{p} = 2\nu_r\nabla\times\mathsf{w} + \mu_0\mathsf{m}\cdot\nabla\mathsf{h}, \qquad \nabla\cdot\mathsf{u} = 0,\\ &\jmath\mathsf{w}_t + \jmath\mathsf{u}\cdot\nabla\mathsf{w} - c_1\Delta\mathsf{w} - c_2\nabla\nabla\cdot\mathsf{w} + 4\nu_r\mathsf{w} = 2\nu_r\nabla\times\mathsf{u} + \mu_0\mathsf{m}\times\mathsf{h},\\ &\mathsf{m}_t + \mathsf{u}\cdot\nabla\mathsf{m} + \frac{1}{\mathcal{T}}(\mathsf{m} - \varkappa_0\mathsf{h}) = \mathsf{w}\times\mathsf{m}, \qquad -\Delta\varphi = \nabla\cdot(\mathsf{h}_a - \mathsf{m}). \end{aligned}$$

Here, u and w represent the linear and angular velocity, respectively, p is the pressure. The magnetization is denoted by m and we model the magnetic field by means of a scalar potential φ. The externally applied field is denoted by h_a. The constitutive parameters $\nu, \nu_r, c_1, c_2, \varkappa_0, \mathcal{T}$ and $\jmath$ are assumed constant and positive. The constant $\varkappa_0$ is known as the magnetic susceptibility and μ_0 is the permeability of vacuum.

The Rosensweig model (1) couples the micropolar Navier-Stokes equations with a transport equation for the magnetization and Maxwell's equations for the magnetic field. The PDE literature for this model is rather scarce, and the existing works add a convenient diffusion term to the magnetization equation, the physical validity of which is questionable.

In [NST16b] we studied system (1) without the addition of any nonphysical terms. The starting point is the realization that by multiplying the linear momentum equation by u, the angular momentum by w and the magnetization equation by m we get

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\mathsf{u}\|_{\mathbf{L}^2}^2 + \jmath\|\mathsf{w}\|_{\mathbf{L}^2}^2 + \mu_0\|\mathsf{m}\|_{\mathbf{L}^2}^2\right) + \nu\|\nabla\mathsf{u}\|_{\mathbf{L}^2}^2 + c_1\|\nabla\mathsf{w}\|_{\mathbf{L}^2}^2 + c_2\|\nabla\cdot\mathsf{w}\|_{\mathbf{L}^2}^2\\ &+ 4\nu_r\|\mathsf{w} - \frac{1}{2}\nabla\times\mathsf{u}\|_{\mathbf{L}^2}^2 + \frac{\mu_0}{\mathcal{T}}\|\mathsf{m}\|_{\mathbf{L}^2}^2 = \mu_0 b(\mathsf{m},\mathsf{h},\mathsf{u}) + \mu_0\left\langle\mathsf{m}\times\mathsf{h},\mathsf{w}\right\rangle + \frac{\mu_0\varkappa_0}{\mathcal{T}}\left\langle\mathsf{h},\mathsf{m}\right\rangle. \end{aligned}$$

To control the terms on the right hand side we must multiply the magnetization equation by $\mathsf{h} = \nabla\varphi$, which yields

$$\left\langle\mathsf{m}_t,\mathsf{h}\right\rangle + b(\mathsf{u},\mathsf{m},\mathsf{h}) + \frac{1}{\mathcal{T}}\left\langle\mathsf{m} - \varkappa_0\mathsf{h},\mathsf{h}\right\rangle = \left\langle\mathsf{w}\times\mathsf{m},\mathsf{h}\right\rangle. \tag{2}$$

After some manipulations this allows us to obtain an energy law.

Any reasonable numerical scheme must preserve this feature, and this implies that identity (2) must be reproducible at the discrete level. This imposes, in particular, the requirement that if we denote by $\mathbb{X}$ and $\mathbb{M}$ the discretization spaces for the magnetic potential and magnetization, respectively, they must obey the relation $\nabla\mathbb{X} \subset \mathbb{M}$. In accordance, the space $\mathbb{M}$ must consist of discontinuous functions and the discretization of the magnetization equation and all the terms that contain a magnetization must be carried out appropriately.

We developed, in [NST16b], a numerical scheme for (1) that has all the aforementioned properties. We showed that the discrete scheme always has a solution and is unconditionally stable. In addition, under the simplifying assumption that $\mathsf{h} = \mathsf{h}_a$, which is valid when $\varkappa_0$ is small, we showed that our scheme converges, as

the discretization parameters tend to zero, to a solution of (1). To obtain convergence we must additionally require that $\mathbb{M} = \mathbb{P}^d$, where $\mathbb{P}$ is the pressure space. This, in particular, implies that the pressure space $\mathbb{P}$ is discontinuous. Finally we must also assume that $\mathbb{P} \cap C(\bar{\Omega}) \neq \emptyset$, which imposes a requirement on the polynomial degree of $\mathbb{P}$.

While the Rosensweig model is of interest by itself, most technologically relevant applications of ferrofluids involve the interaction of a ferrofluid and a regular one. For this reason, in [NST16a], we developed a diffuse interface model for two phase ferrofluid flows. Instead of trying to derive the model from energy variational frameworks we just assemble its components based on the following principles:

1. We want the simplest PDE model, which captures the essence of partially miscible, almost matching density, two phase flows: one is a ferrofluid and the other a non magnetizable one.
2. The Kelvin (magnetic) force — which is $\mu_0 \mathsf{m}\cdot\nabla\mathsf{h}$ in the first equation of (1) — and capillary forces dominate the dynamics. Thus, gravity plays a secondary role.
3. The magnetization m and magnetizing field h are close to equilibrium. This implies that there are no torques or angular momentum.

With these guidelines in mind, we propose

(3)
$$
\begin{aligned}
\theta_t + \mathsf{u}\cdot\nabla\theta &= \gamma\Delta\psi, & \psi &= \frac{1}{\epsilon} f(\theta) - \epsilon\Delta\theta,\\
\mathsf{u}_t + \mathsf{u}\cdot\nabla\mathsf{u} - \nabla\cdot\left(\nu(\theta)\mathbf{T}(\mathsf{u})\right) + \nabla\mathsf{p} &= \mu_0\mathsf{m}\cdot\nabla\mathsf{h} + \frac{\sigma}{\epsilon}\theta\nabla\psi, & \nabla\cdot\mathsf{u} &= 0,\\
\mathsf{m}_t + \mathsf{u}\cdot\nabla\mathsf{m} + \frac{1}{\mathcal{T}}(\mathsf{m} - \varkappa(\theta)\mathsf{h}) &= 0, & -\Delta\varphi &= \nabla\cdot(\mathsf{h}_a - \mathsf{m}).
\end{aligned}
$$

The variables θ and ψ are the order parameter and chemical potential, respectively, and the interfacial density is denoted by ϵ. As usual, $\mathbf{T}(\mathsf{u})$ denotes the symmetric gradient of u. Notice also that the material parameters ν and $\varkappa$ are now phase dependent. For (3) we can show that, provided $\varkappa(\theta) \leq \varkappa_0 \leq 4$, we have the following energy law:

$$
\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Bigg(\|\mathsf{u}\|^2_{\mathbf{L}^2} + \mu_0\|\mathsf{m}\|^2_{\mathbf{L}^2} + \mu_0\|\mathsf{h}\|^2_{\mathbf{L}^2} + \epsilon\sigma\|\nabla\theta\|^2_{\mathbf{L}^2} + \frac{2\sigma}{\epsilon}\int_\Omega F(\theta)\Bigg) &\frac{\mu_0}{\mathcal{T}}\left(1 - \frac{\varkappa_0}{4}\right)\|\mathsf{m}\|^2_{\mathbf{L}^2}\\
+ \frac{\mu_0}{4\mathcal{T}}\|\mathsf{h}\|^2_{\mathbf{L}^2} + \|\sqrt{\nu(\theta)}\mathbf{T}(\mathsf{u})\|^2_{\mathbf{L}^2} + \gamma\sigma\|\nabla\psi\|^2_{\mathbf{L}^2} &\leq \mu_0\mathcal{T}\|\partial_t\mathsf{h}_a\|^2_{\mathbf{L}^2} + \frac{\mu_0}{\mathcal{T}}\|\mathsf{h}_a\|^2_{\mathbf{L}^2}.
\end{aligned}
$$

As in the one phase case, an identity like (2) must be obtained. It is particular to notice that, for commercial grade ferrofluids, $\varkappa_0 \in [0.5, 4.3]$, so the obtained energy law almost covers the whole range of interest.

We also propose numerical schemes for (3). As in the one phase case, we must require that $\nabla\mathbb{X} \subset \mathbb{M}$. With this structural condition, and again under the assumption that $\varkappa(\theta) \leq \varkappa_0 \leq 4$, we can show existence of discrete solutions and their unconditional stability. To obtain convergence, we once again must assume that $\mathsf{h} = \mathsf{h}_a$, thus showing the existence of solutions for a simplified version of (3).

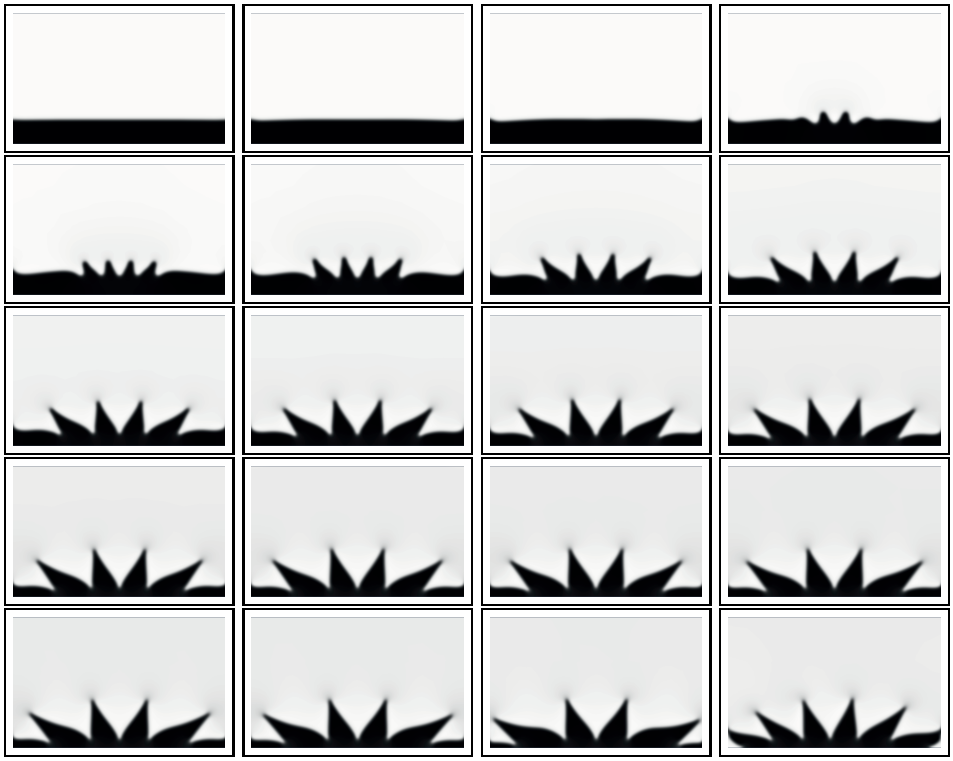

FIGURE 1. The Rosensweig instability

Model (3) is extremely simple minded, yet it is able to reproduce many of interesting phenomena that one can see in ferrofluids. For instance, Figure 1 shows a simulation of the so-called Rosensweig instability, that was obtained with the numerical scheme we developed for (3).

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On Novel Approaches Towards Shape Optimization by Usage of Shape Manifolds

Volker Schulz

Diffuse interfaces maybe an appropriate approach towards shape optimization problems in certain cases. However, in many practical applications, sharp interfaces are required, e.g., in the presence of convection dominated flow regimes. This talk addresses methods for carrying over SQP methods from nonlinear programming in vector spaces to shape spaces. Since shapes are not defining a vector space structure, this poses certain challenges. These can be partly relieved by exploiting the shape manifold structure as developed earlier in the field of differential geometry. In [1], the foundations for interpreting shape optimization as optimization on shape manifolds have been laid. The publication [2] addresses first approaches towards shape-SQP methods and [3] presents efficient methods for sharp interface optimization problems based on the standard Hadamard form of shape drivatives. A central question is the proper choice of a Riemannian metric on shape manifolds. It is demonstrated [4, 5] that certain Steklov-Poincareé type metrics are of advantage, when combining volumetric and boundary formulations of the shape derivative, as well as for numerical accuracy. The relevant exterior bilinear elasticity form is chosen in a way to preserve mesh quality. Practical experiences with an inverse diffusion problem are discussed.

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Energy-dissipations for gradient systems associated with anisotropic grain boundary motions

Ken Shirakawa
(joint work with Salvador Moll and Hiroshi Watanabe)

Summary of the results

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a smooth boundary $\partial\Omega$. Let $Q := (0,\infty)\times\Omega$ be the product space of the time-interval $(0,\infty)$ and the spatial domain Ω, and let $\Sigma := (0,\infty)\times\partial\Omega$.

In this talk, we consider the following system of PDEs.

$$
(1)\qquad \begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)\gamma(R(\theta)D\theta) = 0 \text{ in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\big(\alpha(\eta)R(-\theta)\partial\gamma(R(\theta)D\theta) + \nu D\theta\big) \\ \qquad\qquad +\alpha(\eta)\partial\gamma(R(\theta)D\theta)\cdot R(\theta+\tfrac{\pi}{2})D\theta \ni 0 \text{ in } Q, \\ \big(\alpha(\eta)R(-\theta)\partial\gamma(R(\theta)D\theta) + \nu D\theta\big)\cdot n_{\partial\Omega} = 0 \text{ on } \Sigma, \\ \eta(0,x) = \eta_0(x),\ \theta(0,x) = \theta_0(x),\ x\in\partial\Omega. \end{cases}
$$

This system is derived as a gradient system of the following functional $\mathscr{F} : L^2(\Omega)^2 \to [0,\infty)$, which is a modified version of the free-energy of grain boundary motion, proposed by Kobayashi et -al. [6]:

$$
(2)\qquad \begin{aligned} [\eta,\theta]\in L^2(\Omega)^2 \quad\mapsto\quad \mathscr{F}(\eta,\theta) &:= \frac{1}{2}\int_\Omega |D\eta|^2\,dx + \int_\Omega \hat{g}(\eta)\,dx \\ &\quad + \int_\Omega \alpha(\eta)\gamma(R(\theta)D\theta)\,dx + \frac{\nu}{2}\int_\Omega |D\theta|^2\,dx \in [0,\infty]. \end{aligned}
$$

In the context, $\nu > 0$ is a fixed positive (small) constant, and $n_{\partial\Omega}$ is the unit outer normal on $\partial\Omega$. $R \in C^\infty(\mathbb{R};\mathbb{R}^{2\times 2}) \cap W^{1,\infty}(\mathbb{R};\mathbb{R}^{2\times 2})$ is a matrix-valued function of rotation defined as:

$$
R : \vartheta\in\mathbb{R} \mapsto R(\vartheta) := \begin{bmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{bmatrix} \in \mathbb{R}^{2\times 2}.
$$

Besides, the following conditions are settled as the assumptions in (1)–(2).

- (A1): $0 \le \hat{g} \in C^3(\mathbb{R})$, $g := \frac{d}{d\eta}\hat{g} \in C^2(\mathbb{R})$, and $g(0) \le 0$ and $g(1) \ge 0$.
- (A2): $\alpha_0 \in W^{1,\infty}_{\mathrm{loc}}(\mathbb{R}^2)$, $\alpha \in C^2(\mathbb{R})$ is convex, $\alpha'(0) = 0$, and $\delta_* := \inf \alpha_0(\mathbb{R}) \cup \alpha(\mathbb{R}) > 0$.
- (A3): $\gamma : \mathbb{R}^2 \to [0,\infty)$ is a two-dimensional norm which provides an equivalent topology to that by the standard Euclidean norm $|\cdot|$, and $\partial\gamma : \mathbb{R}^2 \to 2^{\mathbb{R}^2}$ is its subdifferential which is possibly multi-valued.
- (A4): $\eta_0, \theta_0 \in L^2(\Omega)$ are given initial data, and the pair of these $[\eta_0,\theta_0]$ belongs to a class D_0, prescribed as follows:

$$
D_0 := \big\{\ [\tilde{\eta},\tilde{\theta}] \in H^1(\Omega)^2 \ \big|\ 0 \le \tilde{\eta} \le 1 \text{ a.e. in } \Omega,\ \tilde{\theta}\in L^\infty(\Omega)\ \big\}.
$$

In this study, we propose the system (1) as an expansive version of the mathematical model by Kobayashi et -al [6], and then, the principal modification is in the point that we take into account the anisotropy of crystalline structures. Here, the variables $\eta, \theta \in L^2(\Omega)$ are order parameters, which indicate, respectively, the orientation order and the orientation angle in the polycrystal.

In (1)–(2), the norm γ is called "anisotropic metric", and it is supposed to involve the effect of anisotropy. In particular, the sublevel set $W_\gamma := \{\gamma^\circ \le 1\}$ of the polar function γ° is called "Wulff shape", which is supposed to reproduce the unit of stable crystalline structure. The convex functions similar to γ have been adopted in a number of previous works [1, 2, 3, 4, 5, 7] as mathematical expressions of anisotropic metrics, and hence, the use of such function is now one of dominant methods to analyze various anisotropic phenomena.

However, in the cases of grain boundaries, the presence of γ would not be enough for the reproduction of anisotropy, because the Wulff shape would possibly rotate in response to the variation of the orientation angle θ. The rotation $R = R(\theta)$ as in (1)–(2) is to enable the reproductions of such dynamical changes of the crystalline structures, and similar idea has been adopted in several previous works, e.g. [3]. Alternatively, the presence of $R = R(\theta)$ brings additional difficulty in mathematics, because it brings two multi-valued terms $-\mathrm{div}\big(\alpha(\eta)R(-\theta)\partial\gamma(R(\theta)D\theta)+\nu D\theta\big)$ and $\alpha(\eta)\partial\gamma(R(\theta)D\theta)\cdot R(\theta+\frac{\pi}{2})D\theta$ in (1), together with the lack of convexity of the principal part $\int_\Omega \alpha(\eta)\gamma(R(\theta)D\theta)\,dx$ in (2).

The objective of this report is to show the qualitative properties of the system (1) under the following definition of solutions.

Definition of solution. A pair of functions $[\eta,\theta] \in L^2_{\mathrm{loc}}([0,\infty);L^2(\Omega)^2)^2$ is called a solution to (1), iff. the following conditions are fulfilled.

(S1)**:** $[\eta,\theta] \in W^{1,2}_{\mathrm{loc}}([0,\infty);L^2(\Omega))^2 \cap L^\infty(0,\infty;H^1(\Omega))^2$, $0 \le \eta \le 1$ a.e. in Q, and $[\eta(0),\theta(0)] = [\eta_0,\theta_0]$ in $L^2(\Omega)^2$.

(S2)**:** η solves the following evolution equation:

$$\eta_t(t) - \Delta_N\eta(t) + g(\eta(t)) + \alpha'(\eta(t))\gamma(R(\theta(t))D\theta(t)) = 0 \ \text{ in } L^2(\Omega), \ \text{ a.e. } t>0,$$

where Δ_N is the Laplacian operator with the Neumann-zero boundary condition.

(S3)**:** There exists a function $\omega^* \in L^\infty(Q)^2$ such that $\omega^* \in \partial\gamma(R(\theta)D\theta)$ in $\mathbb{R}^2$, a.e. in Q, and

$$\begin{aligned}&\big(\alpha_0(\eta)\theta_t(t),\theta(t)-\varphi\big)_{L^2(\Omega)} + \big(\alpha(\eta(t))\omega^*(t)\cdot R(\theta(t)+\tfrac{\pi}{2})D\theta(t),\theta(t)-\varphi\big)_{L^2(\Omega)}\\ &\quad+\nu\big(D\theta(t),D(\theta(t)-\varphi)\big)_{L^2(\Omega)^2} + \int_\Omega \alpha(\eta(t))\gamma(R(\theta(t))D\theta(t))\,dx\\ &\le \int_\Omega \alpha(\eta(t))\gamma(R(\theta(t))D\varphi)\,dx, \quad \text{for any } \varphi\in H^1(\Omega), \ \text{a.e. } t>0.\end{aligned}$$

Based on these, we report the following Theorems 1–2, associated with the *energy-dissipation property* in (1), as the most advanced results at the present time.

Theorem 1 (Existence of solutions with energy-dissipations). *Under (A1)–(A4), the system* (1) *admits at least one solution which fulfills the following inequality, implying the energy-dissipation:*

$$\int_s^t |\eta_t(\tau)|^2_{L^2(\Omega)}\,d\tau + \delta_* \int_s^t |\theta_t(\tau)|^2_{L^2(\Omega)}\,d\tau + \mathscr{F}(\eta(t),\theta(t)) \le \mathscr{F}(\eta(s),\theta(s)),\ \text{for a.e. } s>0 \text{ and all } t \ge s. \tag{3}$$

Theorem 2 (Large-time behavior). *Let us assume (A1)–(A4), and for a solution* $[\eta,\theta]$ *to* (1) *fulfilling* (3)*, let us define the* ω*-limit set of* $[\eta,\theta]$ *by putting*

$$\omega(\eta,\theta) := \left\{ [\eta_\infty,\theta_\infty] \;\middle|\; \begin{array}{l} \text{there exists } \{t_n\} \subset (0,\infty) \text{ such that } t_n \uparrow \infty \text{ and} \\ [\eta(t_n),\theta(t_n)] \to [\eta_\infty,\theta_\infty] \text{ in } L^2(\Omega)^2,\ \text{as } n\to\infty \end{array} \right\}.$$

Then, the following items hold.

*(I)***:** $\omega(\eta,\theta)$ *is nonempty and compact in* $L^2(\Omega)^2$.
*(II)***:** *Any* ω*-limit point* $[\eta_\infty,\theta_\infty] \in \omega(\eta,\theta)$ *satisfies that:*

$$-\Delta_N \eta_\infty + g(\eta_\infty) = 0 \text{ in } L^2(\Omega),\ \text{ and }\ \theta_\infty \equiv \text{Const. on } \Omega.$$

Acknowledgement: This study is supported by Grant-in-Aid No. 25800086, No. 26400138 and No. 16K05224, JSPS.

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Preconditioning for Cahn-Hilliard equations

Martin Stoll
(joint work with Jessica Bosch and Christian Kahle)

The solution of vector-valued Cahn-Hilliard equations is an important task with applications across the sciences. After a suitable discretization and the choice of an appropriate nonlinear solver, one typically has to solve a large linear system of equations. This process typically uses up most of the computing time and making it robust and fast is a key challenge. We here address the numerical solution of a Cahn-Hilliard system

$$\partial_t u_i = (L\Delta \mathbf{w})_i, \tag{1}$$

$$w_i = f(u_i) + \beta(\mathbf{u}) - \varepsilon^2 \Delta u_i, \tag{2}$$

$$\nabla u_i \cdot \mathbf{n} = (L\nabla \mathbf{w})_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \tag{3}$$

for $i = 1, \dots, N$, which is obtained using a smooth potential $\psi(\mathbf{u})$ and $\beta(\mathbf{u}) := -\frac{1}{N}\sum_{i=1}^{N} f(u_i)$. The matrix $L = (L_{ij})_{i,j=1,\dots,N} \in \mathbb{R}^{N\times N}$ is the mobility matrix and

$$\mathbf{f}(\mathbf{u}) = (f(u_1), \dots, f(u_N))^T := \left(\frac{\partial \psi}{\partial u_1}, \dots, \frac{\partial \psi}{\partial u_N}\right)^T = \frac{\partial \psi}{\partial \mathbf{u}}.$$

the fully discrete linear systems for both smooth and nonsmooth potentials reads in matrix form as

$$\begin{bmatrix} I \otimes M & -\mathcal{B} \\ \tau L \otimes K & I \otimes M \end{bmatrix} \begin{bmatrix} \mathbf{w}^{(k+1)} \\ \mathbf{u}^{(k+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ (I \otimes M)\,\mathbf{u}^{(n-1)} \end{bmatrix}, \tag{4}$$

where k denotes the Newton step, τ the time step size, and $n-1$ denotes the time step. Note that we neglect the index for the current time step n. The first right hand side is

$$\mathbf{b} = (I \otimes M)\left(-2\left(\mathbf{u}^{(k)}\right)^3 + \frac{3}{2}\left(\mathbf{u}^{(k)}\right)^2\right) + \frac{1}{N}(I \otimes M)\left(\sum_{j=1}^{N} 2\left(u_j^{(k)}\right)^3 - \frac{3}{2}\left(u_j^{(k)}\right)^2\right)\mathbf{1}$$

for the use of the smooth potential and

$$\mathbf{b} = \mathbf{0}$$

for the use of the nonsmooth potential. Further, $K := ((\nabla\varphi_i, \nabla\varphi_j))_{i,j=1,\dots,m} \in \mathbb{R}^{m\times m}$ is the stiffness matrix, $M := ((\varphi_i, \varphi_j)_h)_{i,j=1,\dots,m} \in \mathbb{R}^{m\times m}$ is the lumped mass matrix and $I \in \mathbb{R}^{N\times N}$ is the identity matrix. M is a symmetric positive definite diagonal matrix and K is symmetric and positive semidefinite. The matrix $\mathcal{B}$ is a block matrix reflecting the contributions from the nonlinear potential for both the smooth and nonsmooth potential. We propose the block-triangular preconditioner

$$\mathcal{P} = \begin{bmatrix} I \otimes M & 0 \\ \tau L \otimes K & -\hat{\mathcal{S}} \end{bmatrix},$$

where $\hat{\mathcal{S}}$ is an approximation of the Schur complement $\mathcal{S} = I \otimes M + \tau(L \otimes K)(I \otimes M)^{-1}\mathcal{B}$ (see [2]). In the smooth potential case, we showed that the linear system (4) is close to

$$\mathcal{K}_0 = \begin{bmatrix} I \otimes M & -\varepsilon^2 I \otimes K \\ \tau L \otimes K & I \otimes M \end{bmatrix}, \tag{5}$$

for which we can derive a robust Schur-complement approach based on a matching argument [5]. Unfortunately, such a close-ness result for the nonsmooth case is very restrictive on the time-step, which makes this technique infeasible. Therefore, we directly approximate the Schur-complement of (4) for which we obtain

$$\begin{aligned} \hat{\mathcal{S}} &= \hat{\mathcal{S}}_1 (I \otimes M)^{-1} \hat{\mathcal{S}}_2 \\ &= \left(\frac{N}{\sqrt{\epsilon}(N-1)} (I \otimes M) + \sqrt{\tau}(L \otimes K) \right) (I \otimes M)^{-1} \left(\frac{\sqrt{\epsilon}(N-1)}{N} (I \otimes M) + \sqrt{\tau}\mathcal{B} \right) \\ &= I \otimes M + \tau(L \otimes K)(I \otimes M)^{-1}\mathcal{B} + \frac{\sqrt{\tau}\, N}{\sqrt{\epsilon}(N-1)}\mathcal{B} + \frac{\sqrt{\tau\epsilon}(N-1)}{N}(L \otimes K). \end{aligned} \tag{6}$$

While this approach provides fairly robust results in practice, we currently are not able to prove any satisfying eigenvalue bounds for reasonable step-sizes. Additionally, we presented how such a preconditioner can be embedded into a coupled Navier-Stokes-Cahn-Hilliard system [4] where one obtains a structured linear system of the form

$$\mathcal{A} = \left(\begin{array}{c|c} \boldsymbol{A}_{\mathrm{NS}} & \boldsymbol{C}_I \\ \hline \boldsymbol{C}_T & \boldsymbol{A}_{\mathrm{CH}} \end{array} \right),$$

with $\boldsymbol{A}_{\mathrm{NS}}$ representing the Navier-Stokes contributions, $\boldsymbol{A}_{\mathrm{CH}}$ the Cahn-Hilliard contributions, and $\boldsymbol{C}_I$,$\boldsymbol{C}_T$ the coupling matrices. Using both the state-of-the-art preconditioner for the Navier-Stokes equations [3] as well as the above described Cahn-Hilliard preconditioners one can obtain robust preconditioners for the coupled system [1]. While in many cases the performance was very satisfying there are still many interesting questions left such as the consideration of logarithmic potentials, nonlocal derivatives, and the solution of optimization problems subject to Cahn-Hilliard constraints.

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Models for transport networks and their relation to inpainting

Benedikt Wirth
(joint work with Alessio Brancolini)

Classical optimal transport aims to identify the most cost-efficient transportation scheme to move material from a prescribed initial spatial distribution to a prescribed final spatial distribution, both given as probability measures on some compact $\Omega \subset \mathbb{R}^n$,

$$\mu_+, \mu_- \in \mathcal{P}(\Omega)\,.$$

The cost of a transportation scheme can here be thought of as the accumulated cost for transporting each single mass particle, which only depends on initial and final particle position.

In contrast, models of transportation networks assign each transported mass particle a cost that does not only depend on start and end point, but also on the path taken in between and on how many particles were transported together (the cost per mass particle in general decreases the more particles travel together, modelling some kind of efficiency gain or bulk discount). This automatically leads to optimal transportation schemes in which many particles use the same travel routes so that mass transport happens along a common flow network. Therefore, those models lend themselves for describing for example logistic or street networks as well as the vasculature in biological organisms.

Transportation network models have for instance been studied by Xia [1], by Maddalena, Morel, and Solimini [2], or by Brancolini and Buttazzo [3], all based on very different model formulations. Since the former two model formulations are known to be equivalent [4] and the latter was found to allow a very similar formulation [5], it seems worth generalizing the different models to a common framework in which one can switch between the different formulations. This entails repeating the analysis of the above-mentioned works for more general transportation costs as defined below.

Definition 1 (Transportation cost)**.** The *transportation cost* is a function $\tau : [0,\infty) \to [0,\infty)$, $\tau \not\equiv 0$, such that

$$(1)\ \tau(0) = 0, \qquad (2)\ \tau \text{ is non-decreasing}, \qquad (3)\ \tau \text{ is concave}.$$

The transportation cost $\tau(w)$ has the interpretation of the cost per transport distance for transporting an amount of mass w. The analysis in [1, 2] exploits the fact that their choice $\tau(w) = w^\alpha$ for some $\alpha \in (0,1)$ is strictly concave with infinite slope at the origin, which we now no longer assume. Below we summarize the different resulting model formulations and their relation.

Eulerian formulation. In this formulation, which repeats and generalizes Xia's work [1], we may even replace the requirement of concave τ by merely subadditivity. Here, transportation schemes are described by weighted graphs or their limit objects.

Definition 2 (Transport paths and cost functional)**.** (1) A *discrete transport path* is a weighted directed graph $G = (V, E, w)$, where the weight $w(e)$ for any edge $e \in E$ can be thought of as the mass flux through e.

(2) The *flux* associated with the discrete transport path G is given by the vector-valued Radon measure $\mathcal{F}_G = \sum_{e\in E} w(e)\frac{\vec{e}}{|\vec{e}|}(\mathcal{H}^1 \llcorner e)$, where $\vec{e}$ stands for the vector along the edge.

(3) The *cost function* of the discrete transport path G is $J^\tau_{\mathrm{F}}(G) = \sum_{e\in E} \tau(w(e))\,|\vec{e}|$.

(4) The *cost function* of a *transport path* $\mathcal{F}$ (a vector-valued Radon measure on $\mathbb{R}^n$) for given initial and final measure $\mu_+, \mu_- \in \mathcal{P}(\Omega)$ is defined as

$$\mathcal{J}^{\tau,\mu_+,\mu_-}[\mathcal{F}] = \inf\left\{ \liminf_{k\to\infty} J^\tau_{\mathrm{F}}(G_k) \;:\; (\mu^k_+, \mu^k_-, \mathcal{F}_{G_k}) \overset{*}{\rightharpoonup} (\mu_+, \mu_-, \mathcal{F}), \right.$$
$$\left. \mu^k_+, \mu^k_- \in \mathcal{P}(\mathbb{R}^n),\ \operatorname{div} \mathcal{F}_{G_k} = \mu^k_+ - \mu^k_- \right\},$$

where the infimum of the empty set shall be infinite. Obviously, this is the infimum cost of approximating the flux $\mathcal{F}$ by finite transportation networks transporting mass from μ^k_+ to μ^k_-.

(5) The *transport problem* is to find the solution $\mathcal{F}$ of

$$d_\tau(\mu_+, \mu_-) = \min_{\mathcal{F}} \mathcal{J}^{\tau,\mu_+,\mu_-}[\mathcal{F}]\,.$$

(6) We shall call τ *admissible*, if there exists a concave function $\beta \geq \tau$ with $\int_0^1 \beta(w) w^{\frac{1}{n}-2}\,\mathrm{d}w < \infty$.

The following properties of the cost function can now be derived essentially by standard variational arguments and by construction of appropriate hierarchical discrete transport paths.

Theorem 3 (Properties of cost distance)**.** *If τ is admissible,*

(1) *$\mathcal{J}^{\tau,\mu_+,\mu_-}$ admits minimizers,*
(2) *d_τ metrizes weak-* convergence in $\mathcal{P}(\Omega)$,*
(3) *$(\mathcal{P}(\Omega), d_\tau)$ is a length space.*

Lagrangian formulation. This formulation follows [2]. In the following we set $\Gamma = [0, 1]$ to be the set of transported particles with the Lebesgue measure as mass distribution $P_\Gamma = \mathcal{L}\llcorner\Gamma$.

Definition 4 (Irrigation patterns)**.** (1) An *irrigation pattern* is a measurable function $\chi : \Gamma \to \mathrm{AC}([0, 1]; \mathbb{R}^n)$, where the absolutely continuous function $\chi_p : [0, 1] \to \mathbb{R}^n$ indicates the travel path of particle $p \in \Gamma$. The *irrigating measure* μ^χ_+ and the *irrigated measure* μ^χ_- are defined as the pushforward of P_Γ under $p \mapsto \chi_p(0)$ and $p \mapsto \chi_p(1)$, respectively.

(2) The *flux through* $x \in \mathbb{R}^n$ is $m_\chi(x) = P_\Gamma(\{p \in \Gamma : x \in \chi_p([0, 1])\})$.

(3) The *cost function* for given initial and final mass $\mu_+, \mu_- \in \mathcal{P}(\Omega)$ is

$$\mathcal{J}^{\tau,\mu_+,\mu_-}[\chi] = \begin{cases} \int_\Gamma \int_0^1 \frac{\tau(m_\chi(\chi_p(t)))}{m_\chi(\chi_p(t))} |\dot\chi_p(t)|\,\mathrm{d}t\mathrm{d}P_\Gamma(p) & \text{if } \mu^\chi_\pm = \mu_\pm, \\ \infty & \text{else.} \end{cases}$$

Static formulation. This formulation can be thought of as an extension of the model in [3].

Definition 5 (Networks). (1) The *maintenance cost* $\varepsilon(b)$ for a network with flow resistance $b \in [0,\infty)$ is defined as

$$\varepsilon(b) = (-\tau)^*(-b) = \sup_w\{-bw + \tau(w)\}.$$

(2) Let $a_\varepsilon = \inf \varepsilon^{-1}(\{0\}) = \tau'(0)$. For a rectifiable set $\Sigma \subset \mathbb{R}^n$ (the *network*) and a function $b : \Sigma \to [0,\infty)$ we define the *network distance*

$$d_{\Sigma,b}(x,y) = \inf\left\{\int_{\Sigma\cap\gamma} b(z)\,\mathrm{d}\mathcal{H}^1(z) + a_\varepsilon \mathcal{H}^1(\gamma\setminus\Sigma) : \gamma \text{ Lipschitz curve from } x \text{ to } y\right\}.$$

(3) Given initial and final measure $\mu_+, \mu_- \in \mathcal{P}(\Omega)$, the *cost function* is

$$\mathcal{J}^{\varepsilon,\mu_+,\mu_-}[\Sigma,b] = \mathrm{W}_{\Sigma,b}(\mu_+,\mu_-) + \int_\Sigma \varepsilon(b(x))\,\mathrm{d}\mathcal{H}^1(x) \text{ with Wasserstein distance}$$

$$\mathrm{W}_{\Sigma,b}(\mu_+,\mu_-) = \inf\left\{\int_{\Omega\times\Omega} d_{\Sigma,b}(x,y)\,\mathrm{d}\pi(x,y) : \pi\in\mathcal{P}(\Omega\times\Omega), \begin{Bmatrix}\pi(A\times\Omega)=\mu_+(A)\\ \pi(\Omega\times A)=\mu_-(A)\end{Bmatrix}\forall A \text{ meas.}\right\}.$$

All these formulations can be shown to describe the same network structures.

Theorem 6 (Model equivalence). *It holds* $\min_{\mathcal{F}}\mathcal{J}^{\tau,\mu_+,\mu_-}[\mathcal{F}] = \min_\chi \mathcal{J}^{\tau,\mu_+,\mu_-}[\chi] = \min_{\Sigma,b}\mathcal{J}^{\tau,\mu_+,\mu_-}[\Sigma,b]$*, and the minimizers can be related with each other.*

As a last formulation variant, in 2D under some additional restrictions on μ_+ and μ_-, one can rewrite those models as versions of Mumford–Shah inpainting problems, which are well-known in image processing. Furthermore, quite efficient convexifications are known for these Mumford–Shah problems which allow numerical computation of optimal inpaintings (see right), whose discontinuity lines correspond to the network.

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Emerging Developments in Interfaces and Free Boundaries

Masahiro Yamamoto

We discuss three inverse problems related to free boundaries or moving boundaries.

1. Nucleation - Cahn's time-cone method

This is a joint work with Dr. Yikan Liu (The Univ. of Tokyo) and Prof. Daijung Jiang (Central China Normal Univ.).

As a model for nucleation, we consider Cahn' time cone method:

$$u(x,t) = \int_{\Omega_\rho(x,t)} \Psi(y,s)dyds. \tag{1}$$

Here $\Psi(x,t)$ and $\rho(t)$ denote the nucleation rate and the growth speed respectively, and $u(x,t)$ is the expected number of transformation events, and we set

$$\Omega_\rho(x,t) := \left\{ (y,s);\, y \in \mathbb{R}^n,\, 0 < s < t,\, |y-x| < \int_s^t \rho(\tau)d\tau \right\}.$$

Given Ψ and ρ, we can calculate $u(x,t)$ by (1). However the calcuations are not light and discussions on the design and the parameter identifications look not simple for the integration form. By a procedure similar to the D'Alembert formula of the one dimensional wave equation, we derive a multiple hyperbolic equation for the solution u to (1), and establish the foundation for discussing numerics and inverse problems, control problems.

Reference: Liu, Yikan, Jiang, Daijun and Yamamoto, Masahiro, Inverse source problem for a double hyperbolic equation describing the three-dimensional time cone model, SIAM J. Appl. Math. **75** (2015), 2610–2635.

2. Stability for inverse obstacle scattering problem

This is a joint work with Dr. Johannes Elschner and Prof. Guanghui Hu (Chinese Academy of Sciences).

Let $D \subset \mathbb{R}^n$ be a bounded domain. By $u(x)$ we denote the total field and we set $u^{in}(x) = e^{ik\alpha\cdot x}$ with $\alpha \in S^{n-1}$ and $k > 0$. Let $u^S(x) = u(x) - u^{in}(x)$ be the scattering field. Then

$$\begin{cases} (\Delta + k^2)u = 0 \quad \text{in } \mathbb{R}^n \setminus \overline{D} \\ u|_{\partial D} = 0 \quad \text{sound-soft} \\ \lim_{|x|\to\infty} |x|^{\frac{n-1}{2}}(\partial_{|x|}u^S - iku^S) = 0 \quad \text{(Sommerfeld radiation condition).} \end{cases}$$

Then we have asymptotics:

$$u^S(x) = |x|^{\frac{1-n}{2}} e^{ik|x|} \left(u_\infty(D,k,\alpha)\left(\frac{x}{|x|}\right) + O\left(\frac{1}{x}\right)\right)$$

and we call $u_\infty(D,k,\alpha)$ the far field pattern. Then we discuss

Inverse obstacle scattering problem: Determine D from $u_\infty(D,k,\alpha)(\xi)$, $\xi \in S^{n-1}$.

As for the the uniqueness, there are many works and we refer only to Kirsch-Kress (1993) and Colton-Sleeman (1983) for smooth D, and Cheng-Yamamoto (2004), Alessandrini-Rondi (2005), Liu-Zou (2006), Elschner-Yamamoto (2006, 2008), Elschner-Hu (2016) for polygonal D.

As for the conditional stability, we refer to Isakov (1993) and Sincich and Sini (2008).

We proposed a novel method for proving the conditional stability which is applicable to a wide class of partial differential equations, not only to the Helmholtz equations.

3. Uniqueness of moving boundary related to continuous casting

This is a joint project with Prof. Jin Cheng (Fudan Univ.).

In practice such as continuous casting, it is difficult to assume the Stefan condition and thus our governing system is

$$\begin{cases} \partial_t u = \partial_x^2 u(x,t), \quad Q := \{(x,t);\, 0 < x < \ell(t),\, 0 < t < T\}, \\ u(\ell(t),t) = 0, \quad t > 0. \end{cases}$$

Then we discuss:

Inverse problem: Determine $\ell(t)$, $0 < t < T$ from $u(0,t), \partial_x u(0,t)$, $0 < t < T$.

We have proved:

Case A: $\ell_1(0) = \ell_2(0)$: The uniqueness holds.

Case B: unknown $\ell_1(0)$, $\ell_2(0)$:

If $u_1(0,t) = u_2(0,t)$, $\partial_x u_1(0,t) = \partial_x u_2(0,t)$, $0 < t < T$, then we have either

- uniqueness
- joining of ℓ_1, ℓ_2 after one time when $\ell_1' \ell_2' > 0$, and then never separated
- $\ell_1(t) > \ell_2(t)$, $0 \le t \le T$ or $\ell_1(t) < \ell_2(t)$, $0 \le t \le T$.

The proof is based on the unique continuation, backward uniqueness in t for heat equation.

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