Mathematisches Forschungsinstitut Oberwolfach

Report No. 3/2019

DOI: 10.4171/OWR/2019/3

Surface, Bulk, and Geometric Partial Differential Equations: Interfacial, stochastic, non-local and discrete structures

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20 January – 26 January 2019

Abstract. Partial differential equations in complex domains with free boundaries and interfaces continue to be flourishing research areas at the interfaces between PDE theory, differential geometry, numerical analysis and applications. Main themes of the workshop have been PDEs on evolving domains, phase field approaches, interactions of bulk and surface PDEs, curvature driven evolution equations. Applications particular from biology, such as cell and cancer modelling and fluid as well solid mechanics have been subjects of the conference.

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

Introduction by the Organizers

Partial differential equations involving interfaces and free boundaries continue to be a flourishing field with many new applications. Often these partial differential equations are posed on complex domains and/or involve the geometry of the interface in a complex way. In addition, in many situations stochastic aspects, or the coupling between discrete structures such particles with manifolds or non-local effects also play a role.

The workshop had a focus on methods involving PDE theory, numerical analysis, differential geometry and modelling but also stochastic methods played a role in several talks. Equations coupling surface, bulk and geometry arise from a variety of problems and describe a wealth of phenomena. It was the aim of the proposed workshop to report on recent developments as well as to enhance further

collaboration, in part by extending the focus to include applications and mathematical modelling in order to take into account the importance of such systems in traditional fields like materials science and multi-phase flow as well as emerging applications in the description of biological cells, tumour growth and segregation and learning theory.

The workshop showed that bringing together researchers with different backgrounds such as analysis, computation, and real-life applications is very beneficial not only to individual research areas, but also to advance the general field as a whole. For example, modern analytical techniques for studying questions of existence and uniqueness can form the basis for the development of novel numerical algorithms and help in the corresponding numerical analysis. Indeed, the injection of aspects of differential geometry, partial differential equations theory, classical analysis, and asymptotic analysis have proved instrumental over the past two decades in setting formal underpinnings for proposed numerical methods, establishing ranges of validity, and re-casting vaguely formulated scientific problems as precise models and equations. Practical applications are frequently the driving force for the development of both new mathematical models and new numerical algorithms. Starting with classical (and hard) problems for interface motions in fluid mechanics and materials science, there has been an explosion in the number and nature of applied problems: biological cell mechanics, networks, inverse problems, multi-scale modelling in biological systems random domains and shape optimization under uncertainty.

The workshop was attended by more than 50 participants from Europe, Asia and America with an expertise in analysis of PDEs, modelling, numerical analysis and scientific computing. The scientific programme consisted of 29 plenary talks. In addition nine young researchers was given the opportunity to briefly present their research in ten minutes talks on Wednesday evening.

The workshop had a focus on topics involving problems with interface and complex structures in biological problems, in geometric problems involving interfaces and thin structures and on phase field models. We now briefly discuss the relevant contributions.

Interfaces and complex structures in biology: Venkataraman studied multi-scale models for cell signalling analytically as well as numerically. A hierarchy of PDE models involving diffuse as well as sharp interface models was presented by Berlyand. John King emphasized the role of Stokes flow for tissue growth in contrast to the more often used Darcy models. Interaction of discrete particles with the geometry of membranes was analyzed by Gräser. Rocca studied diffuse interface models for tumour growth and addressed the long time behaviour as well as optimal control problems. Singular limits of coupled bulk-surface models for raft formation were studied by Abels. Agosti combined theoretical analysis and computations to describe the patient specific evolution of brain tumours. Bulk-surface obstacle type problems for polarized cells were analyzed by Röger. A new model for cell blebbing was numerically studied with the help of the surface finite element method by Stinner. Stevens analyzed asymptotic limits for diffusion in

strongly layered domains. These contributions demonstrated that life sciences give rise to a wealth of problems involving surface, bulk, and geometric PDEs.

Curvature driven interface evolution: Eikonal-curvature flow equations with external forces were studied with a viscosity solution approach by Yoshikazu Giga. Bartels introduced and analyzed numerical methods for the flow of elastic knots involving curvature energies which avoid self contact. A new thresholding scheme for codimension two mean curvature flow was analyzed by Laux. Kovács and Lubich studied convergence results for finite element methods for surface evolution equations and in particular could show a first convergence result for a discretization of mean curvature flow in higher dimensions. Pozzi analyzed the long time behavior of elastic networks. The fourth order highly singular crystalline surface diffusion flow has been analyzed by Mi-Ho Giga.

Also in several other talks the geometry and in particular the curvature of interfaces played an important role. Reusken analyzed numerical methods for surface Stokes equations in a stream function formulation. PDEs on curved manifolds involving tangential tensor fields have been studied by Voigt. Walker analyzed a numerical method for the plate equation on curved surfaces and in particular also studied an abstract manifold version of the Kirchoff plate problem. A varifold perspective to weak notions of curvature of a measure were addressed by Masnou. Applications of complex interface evolutions in the context of car painting have been the subject of the talk of Sethian. Surface Navier–Stokes problems have been derived as a singular limit of a bulk Navier–Stokes problem in a curved thin domain by Miura.

Phase field methods: Diffuse interface models appeared in several of the talks involving interfaces in biology. Other contributions involving phase field models are the following. Otto showed optimal relaxation rates for the one-dimensional Cahn–Hilliard equation. Bretin numerically investigated phase field approximations of Steiner and Plateau problems also in higher codimension. Bulk-surface couplings often involve dynamic boundary conditions and such conditions in an Allen–Cahn problem have been analyzed by Lam.

Variational calculus and singular limits have been studied in many of the problems above. In addition, the talk by Thorpe used the notion of Γ-convergence to study discrete-to-continuum limits in semi-supervised learning on graphs. Variational calculus also plays an important role in deriving mathematical models. Liu used an energetic variational approach to derive models involving transport and charged particles in complex biological systems. Variational calculus involving quasi-variational inequalities has been applied by Alphonse to show directional differentiability.

Randomness and uncertainty in surface PDEs and shape optimization have been the subject of talks in the young researchers session. Other themes of talks in the young researchers session involved inverse problems, phase field models, nematic flows, geometric flows and bulk-surface problems in biology.

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-1641185, "US Junior Oberwolfach Fellows".

Workshop: Surface, Bulk, and Geometric Partial Differential Equations: Interfacial, stochastic, non-local and discrete structures

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Abstracts

On the large time behavior of solutions to birth and spread type equations

Yoshikazu Giga
(joint work with Hiroyoshi Mitake, Takeshi Ohtsuka and Hung V. Tran)

We consider a level-set eikonal-curvature flow equation with an external force. Such a problem is considered as a model to describe an evolution of height of crystal surface by two-dimensional nucleation or possibly some class of growths by screw dislocations. For applications, it is important to estimate the growth rate. Without an external source term the solution only spreads horizontally and does not grow vertically so the source term plays a key role for the growth.

Although the large time behavior of parabolic equations is well known, the equations we study are degenerate parabolic equations where no diffusion effect exists in the normal to each level-set of a solution. Thus, very little is known even for the growth rate. Our goal is to describe our recent progress on such type of problems.

Instead of considering a generalequation, we consider

$$u_t - |\nabla u| \left(a \operatorname{div} (\nabla u/|\nabla u|) + 1\right) = r(x) \quad \text{in} \quad \mathbf{R}^N \times (0, \infty)$$

with zero initial data. Here a is a nonnegative constant and r is a given function. Without r, this equation is nothing but the level-set equation of the eikonal-curvature flow of the form $V = a\kappa + 1$, where V denotes the normal velocity and κ denotes the $N-1$ times mean curvature of an evolving surface. In other words, outside of the support $\operatorname{spt} r$ of r each level-set of u spreads by $V = a\kappa + 1$ or u spreads horizontally by this law. The term r plays a role to give a birth if $r > 0$. In the theory of crystal growth, the function $u = u(x,t)$ represents a height function of a crystal at a place x on a flat plane at time t, where N is taken to be equal to two.

We are interested in the large time behavior of a solution u. Namely, we ask to find the asymptotic speed R and asymptotic profile w. In other words, find a real number R and a function w in $\mathbf{R}^N$ such that

$$\sup_{x \in B} |u(x,t) - Rt - w(x)| \to 0 \quad \text{as} \quad t \to \infty$$

for any closed ball B in $\mathbf{R}^N$. Since the problem has various features, we always assume that

$$r \geq 0 \quad \text{and} \quad \operatorname{spt} r \quad \text{is compact.}$$

The unique existence of a global-in-time viscosity solution is standard if r is continuous [7]. However, if r is discontinuous the uniqueness may not be true even if $a = 0$ and we need extra notion to choose a reasonable solution [6].

Theorem ([8]). *If r is moreover Lipschitz, the asymptotic speed*

$$R = \lim_{t\to\infty} u(x,t)/t \geq 0$$

exists. The convergence is locally uniform.

This can be proved by existence of asymptotic speed of $\phi(t) = \sup_x u(x,t)$ and a Lipschitz bound of $u(x,t)$ in x uniformly in $t > 0$. The former is obtained by sub-additivity of ϕ and Fekete's lemma while the latter is obtained by a Bernstein type argument for $|\nabla u|^2$. A similar idea is found in [1] for a different setting.

If $a = 0$, the problem becomes of first order. In this case, it is known that $R = \max_x r$. In fact, we have

Proposition ([9], Scaled limit). *Set $u^\lambda(x,t) = u(\lambda x, \lambda t)/\lambda$ for $\lambda > 0$. Assume that $a = 0$ and r is Lipschitz. Then*

$$\lim_{\lambda\to\infty} u^\lambda(x,t) = R\,(t - |x|)_+ \quad \text{with} \quad R = \max_x r,$$

where $b_+ = \max(b, 0)$. The convergence is locally uniform.

However, if $a > 0$, because of the curvature effect R can be smaller than $\max r$. For example, if $\operatorname{spt} r$ is contained in an interior of a ball of radius $a(N-1)$. R must be zero since a maximal solution with $r(x) = 1_{B_\rho}$, where B_ρ is a ball of radius $\rho < a(N-1)$, grows only in finite time [7]. The question is whether there is an intermediate one.

Theorem ([7], [5]). *There is an explicit example that the asymptotic speed R is positive but less than $\max_x r$ at least in the case $N = 2$.*

This can be proved for example by giving r as a mollified characteristic function of a square not contained in nor containing a unit disk.

We also have a scaled limit for $a > 0$.

Theorem ([5]). *If r is Lipschitz, then*

$$\lim_{\lambda\to\infty} u^\lambda(x,t) = R\,(t - |x|)_+ .$$

The convergence is locally uniform.

This result in particular recovers the result of [10] on large time behavior of the eikonal-curvature flow including an anisotropic version; see [5]. In general, asymptotic speed and asymptotic profile are well-studied for first order Hamilton-Jacobi equations when the Hamiltonian is convex, coercive under spatially periodic setting. The theory started by Fathi [4] and Namah and Roquejoffre [12] is now called a weak KAM (Kalmogonov-Arnold-Moser) theory. See [1], [11] for review. However, when the equation is of second order less is known especially if the parabolicity is degenerate like our problem. In our problem, the parabolicity is degenerate in the direction orthogonal to each level-set of u. If the second order term is of the form $\alpha(x)\Delta u$ with $\alpha \geq 0$, asymptotic profile and speed are given by [2] based on a nonlinear adjoint method [3].

The difficulty to find the asymptotic profile w is based on the fact that the problem called a cell problem of the form

$$R - |\nabla u| \left(\operatorname{div}\left(\nabla w/|\nabla w|\right) + 1\right) = r(x)$$

has many solutions even up to constant. It is not difficult to prove that $u(x,t) - Rt$ converges to some w solving the cell problem by taking a subsequence $t_j \to \infty$. However, full convergence is in general difficult. We only have a partial result for the radial case in our joint work with Mitake and Tran in progress.

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Simulation of elastic knots and inextensible elastic curves

Sören Bartels
(joint work with Philipp Reiter)

Thin elastic bodies like rods and wires tend to minimize their bending energy subject to given boundary conditions and thereby undergo large deformations. The bending energy is given by the integral of the squared curvature of the deformed object which equals the square of the second derivative of the deformation if an inextensibility condition that implies an arclength parametrization is incorporated. To realistically model relaxation dynamics or preserve topological properties of a closed curve, an injectivity condition has to be included in the model. We follow [1, 2] and realize this by adding the tangent-point functional proposed in [3] to the bending energy so that we consider

$$I(u) = \frac{1}{2}\int_0^L |u''(x)|^2 \,\mathrm{d}x + \varrho\,\mathrm{TP}(u)$$

for curves $u \in H^2(0,L;\mathbb{R}^3)$ with $|u'(x)| = 1$ for all $x \in (0,L)$. The evolution is modeled by a corresponding gradient flow which leads to stationary configurations of low energy. We investigate stability and consistency properties of numerical discretization methods. In particular, we consider the discrete time-stepping scheme

$$(d_t u^k, v)_\star + ([u^k]'', v'') = -\varrho\,\delta\mathrm{TP}(u^{k-1})[v]$$

subject to the linearized arclength-conditions

$$[d_t u^k]' \cdot [u^{k-1}]' = 0, \quad v' \cdot [u^{k-1}]' = 0.$$

The numerical scheme is shown to be stable and convergent under moderate conditions on the discretization parameters. In particular, we show that if the step size τ satisfies $\tau \le c$ then we have the energy decay property

$$I(u^L) + (1 - c'\tau)\tau \sum_{k=1}^{L} \|d_t u^k\|_\star^2 \le I(u^0)$$

and the constraint violation bound

$$\max_{k=0,1,\dots,L} \|\,|[u^k]'|^2 - 1\|_{L^1(0,L)} \le c\tau I(u^0)$$

for all $L = 0, 1, \dots, K = \lfloor T/\tau \rfloor$ with a fixed time horizon $T > 0$. The spatial discretization is done using piecewise cubic functions and imposing the constraints at the nodes of the partitioning. Corresponding consistency estimates are derived under minimal regularity conditions. Numerical simulations reported in [1] provide the experimental observation that elastic untwisted knots tend to attain flat configurations. The rigorous dimension reduction from three-dimensional hyperelasticity given in [4] shows that torsion effects are described by considering the functional

$$E(u,b,d) = \frac{1}{2}\int_0^L |u''(x)|^2 \,\mathrm{d}x + \frac{c_t}{2}\int_0^L (b' \cdot d)^2 \,\mathrm{d}x,$$

where we omitted the contribution to avoid self-contact. In this setting the functions $u', b, d : (0, L) \to \mathbb{R}^3$ define a frame for the curve, i.e., for every $x \in (0, L)$ we have that

$$[u'(x), b(x), d(x)] \in SO(3).$$

The discretization of the bending-torsion model has to be done carefully since the coercivity in the variable b arises implicitly. Noting that we have

$$(b' \cdot d)^2 = |b'|^2 - (b \cdot y'')^2$$

and that $c_t \leq 1/2$ we are able to define a discretization with uniform coercivity property. The unit-length constraints are imposed at the nodes of the partitioning while the orthogonality $y' \cdot b = 0$ is enforced via penalization. We eliminate the variable d noting that $d = y' \times b$. Making use of certain delay properties of the discrete product rule we are able to establish the unconditional stability of a decoupled time-stepping scheme for a suitable gradient flow for E.

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Surface Stokes equations in stream function formulation

Arnold Reusken

(joint work with Philip Brandner)

In recent years there has been a strong increase in research on numerical simulation methods for surface (Navier-)Stokes equations, e.g., [1, 2, 3, 4, 5, 6, 7, 8]. By far most of these and other papers on numerical methods for surface flow problems treat the (Navier-)Stokes equations in the primitive velocity and pressure variables. In the paper [1] the Navier-Stokes equations on a stationary smooth closed surface in *stream function* formulation are treated. We are not aware of any other literature in which surface (Navier-)Stokes equations in stream function formulation are studied.

In Euclidean space, the stream function formulation of (Navier-)Stokes is well-known and thoroughly studied, e.g., [9, 10] and the references therein. In numerical simulations of three-dimensional problems this formulation is not often used due to substantial disadvantages. For two-dimensional problems this formulation reduces to a fourth order biharmonic equation for the *scalar* stream function. This formulation has been used in numerical simulations, although it has certain disadvantages related to boundary conditions and regularity ([9, 10]).

In the fields of applications mentioned above, one often deals with smooth simply connected surfaces without boundary. In such a setting there usually are no difficulties related to regularity or boundary conditions and the stream function formulation may be an attractive alternative to the formulation in primitive variables, as already indicated in [1]. This is the main motivation for the study presented in the recent paper [12]. Here we outline the main results of that paper. We give a complete derivation of the surface Helmholtz decomposition, discuss its relation to the surface Hodge decomposition, and derive a well-posed stream function formulation of a class of surface Stokes problems. We consider a smooth connected (not necessarily simply connected) oriented hypersurface $\Gamma \subset \mathbb{R}^3$ without boundary. We introduce the natural surface gradient, divergence, curl and Laplace operators, represented in terms of the standard differential operators of the ambient Euclidean space $\mathbb{R}^3$. These representations, which may differ from the (intrinsic) ones used in differential geometry, are very convenient for the implementation of numerical methods for surface PDEs. Similar representations for surface differential operators are also used in e.g., [11, 6, 8, 5]. We introduce suitable surface $\mathbf{H}(\operatorname{div}_\Gamma)$ and $\mathbf{H}(\operatorname{curl}_\Gamma)$ spaces and derive useful properties of these spaces. A main result of the paper is the derivation of the following Helmholtz decomposition in terms of these surface differential operators.

Theorem. For every $\mathbf{u} \in \mathbf{L}^2_t(\Gamma) = \{\, \mathbf{u} \in L^2(\Gamma)^3 \mid \mathbf{n} \cdot \mathbf{u} = 0 \quad \text{a.e. on } \Gamma \,\}$ there exist unique $\psi, \phi \in H^1_*(\Gamma) := \{\, \phi \in H^1(\Gamma) \mid \int_\Gamma \phi \, ds = 0 \,\}$ and $\boldsymbol{\xi} \in \mathcal{H} = \{\, \mathbf{u} \in \mathbf{L}^2_t(\Gamma) \mid \operatorname{div}_\Gamma \mathbf{u} = 0 \quad \text{and } \operatorname{curl}_\Gamma \mathbf{u} = 0 \,\}$ such that

$$\mathbf{u} = \nabla_\Gamma \psi + \mathbf{curl}_\Gamma \phi + \boldsymbol{\xi}.$$

The range spaces $\nabla_\Gamma(H^1_*(\Gamma))$ and $\mathbf{curl}_\Gamma(H^1_*(\Gamma))$ are closed in $\mathbf{L}^2_t(\Gamma)$ and the direct sum

$$\mathbf{L}^2_t(\Gamma) = \nabla_\Gamma(H^1_*(\Gamma)) \oplus \mathbf{curl}_\Gamma(H^1_*(\Gamma)) \oplus \mathcal{H}$$

is L^2-orthogonal.

The derivation of this result is based on elementary differential calculus. In particular, we do not use the calculus of differential forms. However, we do point out the relation between the Helmholtz decomposition and a Hodge decomposition known from the field of differential forms. As a corollary of this Helmholtz decomposition we obtain that for a simply connected surface, to every tangential divergence free velocity field there corresponds a unique scalar stream function. Using this result the variational form of the Stokes equation can be reformulated as a well-posed variational formulation of a fourth order equation for the stream function. The latter can be rewritten as two coupled second order equations, which form the basis for a finite element discretization. We use quadratic trace finite elements for the discretization of these scalar second order equations. From the finite element approximation of the stream function the velocity field and pressure can be reconstructed. We show results of a numerical experiment that illustrate the convergence properties of this discretization method.

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Thresholding for mean curvature flow in codimension two

Tim Laux

(joint work with Nung Kwan Yip)

The thresholding scheme, first introduced by Merriman, Bence, and Osher in 1992, is an efficient numerical scheme to evolve a hypersurface by mean curvature flow (MCF). It is based on linear diffusion, that is, convolution with the heat kernel G_h at time h, of the characteristic function of the bulk (whose boundary is supposed to evolve by MCF), and pointwise thresholding. The variant in codimension two by Ruuth, Merriman, Xin, and Osher [4] does the same operations on the level of a vector field $u\colon \mathbb{R}^3 \to \mathbb{S}^1 \subset \mathbb{R}^2$ that winds around the filament (or curve) in $\mathbb{R}^3$:

$$v_n := G_h * u_{n-1}, \quad u_n := \frac{v_n}{|v_n|}, \tag{1}$$

which we think of extended in a piecewise constant manner, i.e., $u_h(t) := u_n$ for $t \in \big[nh, (n+1)h\big)$.

Esedoğlu and Otto [1] realized that this scheme respects the gradient-flow structure of mean curvature flow in that it can be viewed as a minimizing movements scheme for an energy which approximates the interfacial area. With Felix Otto,

we realized that thresholding solves a family of localized minimization problems which allows to derive Brakke's inequality for the scheme [2]. The basis of the present work is the following extension of this (localized) minimizing movements principle to surfaces of codimension two: (1) is equivalent to minimizing

$$(2)\quad E_h(u,\zeta)+\frac{1}{h}\int\zeta(u-u_{n-1})\cdot G_h*(u-u_{n-1})\,dx+\int\frac{u-u_{n-1}}{h}\cdot[G_h*,\zeta]\,u\,dx$$

for any localization $\zeta\geq 0$ where $E_h(u,\zeta):=\frac{1}{h}\int\zeta\,(1-u\cdot G_h*u)\,dx$.

This is easy to check: Suppose first that $\zeta=1$ and note that (1) is equivalent to the maximization of the symmetric bilinear form $\int u\cdot v_n dx=\int u\cdot G_h*u_{n-1}dx=:(u,u_{n-1})$ subject to $|u|\leq 1$ a.e., or equivalently, the *minimization* of $-2(u,u_{n-1})=-(u,u)+(u-u_{n-1},u-u_{n-1})+(u_{n-1},u_{n-1})$. Adding the constant $1-(u_{n-1},u_{n-1})$ and dividing by h, one arrives at (2) with $\zeta=1$. If ζ is not constant, the symmetry is lost, which leads to the commutator term in (2).

Note that $[G_h*,\zeta]\,u=\int G_h(z)\,(\zeta(\cdot-z)-\zeta)\,u(\cdot-z)\,dz\approx 2h\,(\nabla\zeta\cdot\nabla)\,G_h*u$. For simplicity, in these notes, we will ignore higher order terms which can be estimated explicitly, cf. [3]. The main result is the following:

Theorem. *Suppose there exists a smooth, embedded MCF $(\Gamma_t)_{t\in[0,T]}$ and suppose the initial conditions u_0 for (1) are well-prepared around Γ_0. Then u_h converges to the smooth MCF in the sense that there exists a subsequence $h\downarrow 0$ and a unit vector field u such that $u_h\to u$ in L^2, and*

- *(i) as $h\downarrow 0$, the energy E_h concentrates only on Γ_t and $\int_U|\nabla u|^2dxdt<\infty$ for every open set U in space time with positive distance to Γ_t;*
- *(ii) away from Γ_t, u is a harmonic map heat flow into $\mathbb{S}^1$.*

While (ii) follows easily, for example by taking outer variations $u_s=\frac{u+s\varphi}{|u+s\varphi|}$ in the minimization problem (2), statement (i) uses a more delicate energy estimate displayed in the proposition below, which exploits the *localized* minimization problems (2), the existence of a smooth mean curvature flow, and *inner* variations $\partial_s u_s+(\xi\cdot\nabla)\,u_s=0$ in the global minimization problem.

Well-preparedness of u_0 means $E_h(u_0,1)\sim|\log h|$ and $E_h(u_0,d^2(\cdot,\Gamma_0))\leq C$. Such u_0 can be constructed easily: For simplicity, think of a filament which is almost parallel to the x_3-axis. On each slice $\{x=(x',x_3)\colon x_3=s\}$ which intersects Γ_0 at the point $(\xi'(s),s)$, $\xi'=(\xi_1,\xi_2)$, set $u_0=\frac{x'-\xi'}{|x'-\xi'|}$. A simple but important back-of-the-envelope computation shows that u_0 is well-prepared.

Proposition. *As $h\to 0$, for any $T'\leq T$*

$$(3)\quad E_h(u_h(T'),\phi_\sigma(T'))+\int_h^{T'}\int\phi_\sigma(t)\left|G_{h/2}*\frac{u_h(t)-u_h(t-h)}{h}\right|^2dx\,dt\leq C(\sigma)E_h(u_0,\phi_\sigma(0))+o(1).$$

Estimate (3) yields the compactness (as the first l.h.s. term controls spatial variations of u_h, and the second l.h.s. term controls variations of $G_{h/2}*u_h$ in time, both localized away from Γ_t). The two main ingredients for the proof of the proposition are pointed out below, followed by a short sketch of the proof of (3).

The first ingredient is to use the squared distance function $\tilde{\phi}(x,t) := \frac{1}{2}d^2(x,\Gamma_t)$ to characterize the motion of the singular set. This was first done in the hypersurface case by Soner and then later extended to higher codimension by Ambrosio-Soner. Lin also established such a fact for the complex Ginzburg-Landau functional; the interested reader is refered to [3] for the precise references. The key observation which we need is that since $\nabla\tilde{\phi}$ solves the heat equation on Γ_t, the Hessian has eigenvalues ≤ 1, i.e.,

$$\nabla^2\tilde{\phi} \leq Id \quad \text{in } A_\sigma := \{(x,t)\colon d(x,\Gamma_t) < \sigma\}, \tag{4}$$

and that since Γ_t has codimension two, precisely two of those eigenvalues are $= 1$, hence $\Delta\tilde{\phi} = 2$ on Γ_t, and since clearly $\partial_t\phi = 0$ on Γ_t, by Taylor's theorem

$$\partial_t\tilde{\phi} - \Delta\tilde{\phi} \leq -2 + \tfrac{1}{2}C(\sigma)d^2(x,\Gamma_t) = -2 + C(\sigma)\tilde{\phi} \quad \text{in } A_\sigma. \tag{5}$$

This function $\tilde{\phi}$ can be extended to a function ϕ, for example (a mollified version of) $\min\{\tilde{\phi}, \frac{1}{2}\sigma^2\}$.

The second ingredient for the proof of the proposition is the following monotonicity formula for E_h:

$$\frac{d}{dh}E_h(u,1) \leq 0 \quad \text{for any unit vector field } u,$$

which is simple to prove, e.g., by spelling out E_h in Fourier space and taking the derivative term by term. This monotonicity formula improves the discrete one known in case of hypersurfaces and it will enter the proof of the proposition below in form of the sharp inequality

$$\int \left|\nabla G_{h/2} * u\right|^2 dx \leq E_h(u,1) \quad \text{for any unit vector field } u. \tag{6}$$

The argument for (3) starts with plugging $u = u_{n-1}$ into (2) with $\zeta = \phi(nh)$:

$$\begin{aligned} E_h(u_n,\phi_n) - E_h(u_{n-1},\phi_{n-1}) \leq & -h\int \phi_n \frac{u_n - u_{n-1}}{h} \cdot G_h * \frac{u_n - u_{n-1}}{h} dx \\ & - h\int \frac{u_n - u_{n-1}}{h} \cdot \frac{1}{h}\left[G_h *, \phi_n\right] u_n \, dx \\ & + hE_h\big(u_{n-1}, \frac{\phi_n - \phi_{n-1}}{h}\big), \end{aligned}$$

where $\phi_n := \phi(t = nh)$. Expanding the commutator on the r.h.s. yields

$$\int \frac{u_n - u_{n-1}}{h} \cdot \frac{1}{h}\left[G_h *, \phi_n\right] u_n \, dx \approx 2\int \frac{u_n - u_{n-1}}{h} \cdot \left(\nabla\phi_n \cdot \nabla\right) G_h * u_n \, dx,$$

which is precisely the (inner) first variation of the metric term (i.e., the second term in (2) with $\zeta = 1$) along the gradient field $\xi = \nabla\phi$. The Euler-Lagrange equation allows us to replace this term by the first variation of $E_h(\cdot, \zeta = 1)$. Then

summing over n and telescoping the l.h.s., this yields

$$\begin{aligned} E_h(u_h(T'),\phi(T')) + \int_0^{T'}\!\!\int \phi \left| G_{h/2} * \frac{u_h(t)-u_h(t-h)}{h}\right|^2 dx\,dt \\ \leq E_h(u_0,\phi(0)) + 2\int_0^{T'}\!\!\int \nabla G_{h/2} * u_h \cdot \nabla^2\phi \nabla\, G_{h/2} * u_h\, dxdt \\ + \int_0^{T'} \frac{1}{h} \int (\partial_t\phi - \Delta\phi)\left(1 - u_h \cdot G_h * u_h\right) dxdt + o(1). \end{aligned}$$

The last r.h.s. term is simply the energy $E_h(u_h, \partial_t\phi - \Delta\phi)$. Over the far-field region A_σ^c, the r.h.s. terms are easily estimated, but the contribution from the near-field region A_σ needs more attention: First, (4) and (5) bound the r.h.s. by

$$E_h(u_0,\phi(0)) + 2\int_0^{T'}\!\!\int \left|\nabla G_{h/2} * u_h\right|^2 dxdt + \int_0^{T'} E_h(u_h, -2 + C(\sigma)\phi)\, dt + o(1).$$

Second, by the monotonicity (6), the two terms without the localization ϕ have the correct sign (≤ 0) so that (3) simply follows from a Gronwall argument.

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Discrete-to-Continuum Limits of p-Laplacian Regularisation in Semi-Supervised Learning on Graphs

Matthew Thorpe

(joint work with Dejan Slepčev and Jeff Calder)

The talk concerns how a family of regression problems in a semi-supervised setting behaves in the large data limit. The task is to assign real-valued labels to a set $X_n = \{x_i\}_{i=1}^n \subset \mathbb{R}^d$ of n sample points, provided a small training subset of N labelled points, i.e. we are given labels $\{y_i\}_{i=1}^N$ on the first N data points. We pose the problem on a graph $G = (X_n, W)$ where X_n form the nodes of the graph and $W = (W_{ij})_{i,j=1}^n$ are edge weights. More precisely, we use random geometric graphs where one defines a connectivity radius ε and weights by

$$W_{ij} = \eta_\varepsilon(|x_i - x_j|) = \frac{1}{\varepsilon^d}\eta\left(\frac{|x_i - x_j|}{\varepsilon}\right).$$

A prototypical example is $\eta(t) = 1$ if $|t| \leq 1$ and $\eta(t) = 0$ for $|t| > 1$, so that the graph has positive weights only when nodes are closer than ε. In order to localise the geometry we choose $\varepsilon = \varepsilon_n$ and let $\varepsilon_n \to 0$ as $n \to \infty$.

We use an objective functional which rewards the regularity of the estimator function and imposes agreement with the training data. In particular, we consider the discrete p-Laplacian regularization defined by

$$\mathcal{E}_n^{(p)}(f) = \frac{1}{\varepsilon_n^p n^2} \sum_{i,j=1}^{n} W_{ij} |f(x_i) - f(x_j)|^p.$$

The variational problem we consider is

$$\text{minimise } \mathcal{E}_n^{(p)}(f) \text{ subject to } f(x_i) = y_i \text{ for all } i \in Z_n$$

where $Z_n \subset \{1, \ldots, n\}$.

If data points x_i are independently sampled from a probability measure $\mu \in \mathcal{P}(\mathbb{R}^d)$ with density ρ then a formal argument shows that the pointwise limit of $\mathcal{E}_n^{(p)}$ is

$$\mathcal{E}_\infty^{(p)}(f) = \sigma \int_{\mathbb{R}^d} |\nabla f(x)|^p \rho^2(x) \, \mathrm{d}x$$

with probability one. For $n \to \infty$ the choice of η in the weights is present only through the constant σ (at least for isotropic weights) defined by

$$\sigma = \int_{\mathbb{R}^d} \eta(x) |x_1| \, \mathrm{d}x.$$

The first question we ask is whether the constrained minimisers of $\mathcal{E}_n^{(p)}$ converge to constrained minimisers of $\mathcal{E}_\infty^{(p)}$ as $n \to \infty$ for $|Z_n| = \{1, \ldots, N\}$ fixed. Clearly the constrained limiting problem only makes sense for $p > d$. It is natural to ask whether this is sufficient. As it turns out one needs to control the length scale ε_n. We uncover a delicate interplay between the regularizing nature of the functionals considered and the nonlocality inherent to the graph constructions. Our first main result is that constrained minimisers of $\mathcal{E}_n^{(p)}$ converge to constrained minimisers of $\mathcal{E}_\infty^{(p)}$ when

$$\varepsilon_n^p n \to 0$$

(the well posed regime) and when

$$\varepsilon_n^p n \to \infty$$

constrained minimisers converge to constants (ill posed regime). The condition $\varepsilon_n^p n \to 0$ implies an upper bound on ε_n.

The proof uses methods from the calculus of variations, namely Γ-convergence, coupled with an optimal transport based metric where one can define the discrete-to-continuum topology necessary to define a notion of convergence for functions on the graph. Precise statements and proofs can be found in [1].

Our second result is to consider the regime where $|Z_n| \to \infty$. Our training data model is that $i \in Z_n$ with probability β_n. In this case our main result is that

constrained minimisers of $\mathcal{E}_n^{(p)}$ converge to constrained minimisers of $\mathcal{E}_\infty^{(p)}$ when $p = 2$,

$$\frac{\varepsilon_n^p}{\beta_n} \to 0 \qquad \text{and} \qquad \frac{\beta_n \varepsilon_n^d n}{\log n} \to +\infty$$

(the well posed regime), and when $p > 1$ and

$$\frac{\varepsilon_n^p}{\beta_n n^c} \to +\infty \quad \text{for any } c > 0$$

constrained minimisers converge to constants (ill posed regime). The proof of the well posed case uses connections between minimisers of the 2-Laplacian and random walks on graphs [2].

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Multiscale modelling, analysis and simulation of cell signalling processes

Chandrasekhar Venkataraman

(joint work with Mariya Ptashnyk)

We consider homogenisation of a model for cell signalling processes in biological tissues. Such signalling processes are the primary mechanism by which cells interact and respond to external stimuli. Hence they play an important role in the majority of cell biological phenomena. The signalling model we consider includes diffusion and nonlinear reactions on the cell surfaces, and both inter- and intracellular signalling. Our main result is to derive, under the assumption of a periodic cell distribution, the equations satisfied in the limit as the cell number tends to infinity with the volume fraction of tissue occupied by the cells constant.

Let $\Omega \subset \mathbb{R}^d$, with $d = 2, 3$ be a Lipschitz domain, representing a part of a biological tissue. To describe the microscopic structure, given by extra- and intracellular spaces separated by cell membranes, we consider a 'unit cell' $Y = [0,1]^d$, and the subdomains $\overline{Y}_i \subset Y$ and $Y_e = Y \setminus Y_i$, together with the boundary $\Gamma = \partial Y_i$. The domain occupied by the intracellular space is given by $\Omega_i^\varepsilon = \bigcup_{\xi \in \Xi^\varepsilon} \varepsilon(Y_i + \xi)$, where $\Xi^\varepsilon = \{\xi \in \mathbb{Z}^n, \quad \varepsilon(Y_i + \xi) \subset \Omega\}$, and the extracellular space is denoted by $\Omega_e^\varepsilon = \Omega \setminus \overline{\Omega}_i^\varepsilon$. The surfaces that describe the cell membranes are denoted by $\Gamma^\varepsilon = \bigcup_{\xi \in \Xi^\varepsilon} \varepsilon(\Gamma + \xi)$.

Signalling molecules (ligands) diffuse in the extracellular space and bind with cell membrane receptors to form receptor-ligand complexes (bound receptors). The signal from the extracellular domain is transduced into the cell through the activation by bound receptors of membrane proteins (co-receptors). Activated co-receptors then interact with signalling molecules in the cell interior. We denote

the concentrations of the extracellular ligands, intracellular ligands, receptors, bound receptors, co-receptors, and activated co-receptors by $c_e^\varepsilon, c_i^\varepsilon, r_f^\varepsilon, r_b^\varepsilon, p_d^\varepsilon$ and p_a^ε respectively. The model for the evolution of the ligand concentration, c_e^ε in the extracellular space Ω_e^ε reads

$$
\begin{aligned}
&\partial_t c_e^\varepsilon - \nabla \cdot (D_e^\varepsilon(x) \nabla c_e^\varepsilon) = F_e(c_e^\varepsilon) && \text{in } \Omega_e^\varepsilon,\ t>0,\\
&D_e^\varepsilon(x) \nabla c_e^\varepsilon \cdot \nu = -\varepsilon G_e(c_e^\varepsilon, r_f^\varepsilon, r_b^\varepsilon) && \text{on } \Gamma^\varepsilon,\ t>0,\\
&D_e^\varepsilon(x) \nabla c_e^\varepsilon \cdot \nu = 0 && \text{on } \partial\Omega,\ t>0,
\end{aligned} \tag{1}
$$

with the nonlinear Robin boundary condition

$$
G_e(c_e^\varepsilon, r_f^\varepsilon, r_b^\varepsilon) = a_e^\varepsilon(x) c_e^\varepsilon r_f^\varepsilon - b_e^\varepsilon(x)\, r_b^\varepsilon,
$$

describing reversible binding of ligands to free receptors creating receptor-ligand complexes. For the receptors and proteins on the cell membrane we obtain the following reaction-diffusion equations

$$
\begin{aligned}
&\partial_t r_f^\varepsilon - \varepsilon^2 D_f \Delta_\Gamma r_f^\varepsilon = F_f(r_f^\varepsilon, r_b^\varepsilon) - G_e(c_e^\varepsilon, r_f^\varepsilon, r_b^\varepsilon) - d_f\, r_f^\varepsilon && \text{on } \Gamma^\varepsilon, t>0,\\
&\partial_t r_b^\varepsilon - \varepsilon^2 D_b \Delta_\Gamma r_b^\varepsilon = \quad G_e(c_e^\varepsilon, r_f^\varepsilon, r_b^\varepsilon) - G_d(r_b^\varepsilon, p_d^\varepsilon, p_a^\varepsilon) - d_b\, r_b^\varepsilon && \text{on } \Gamma^\varepsilon, t>0,\\
&\partial_t p_d^\varepsilon - \varepsilon^2 D_d \Delta_\Gamma p_d^\varepsilon = F_d(p_d^\varepsilon) - G_d(r_b^\varepsilon, p_d^\varepsilon, p_a^\varepsilon) - d_d\, p_d^\varepsilon && \text{on } \Gamma^\varepsilon, t>0,\\
&\partial_t p_a^\varepsilon - \varepsilon^2 D_a \Delta_\Gamma p_a^\varepsilon = \quad G_d(r_b^\varepsilon, p_d^\varepsilon, p_a^\varepsilon) - G_i(p_a^\varepsilon, c_i^\varepsilon) - d_a\, p_a^\varepsilon && \text{on } \Gamma^\varepsilon, t>0,
\end{aligned} \tag{2}
$$

where Δ_Γ denotes the Laplace-Beltrami operator on the surfaces Γ^ε and the binding/dissociation reactions for r_b^ε, p_d^ε, and p_a^ε are defined by

$$
G_d(u,v,w) = a_i^\varepsilon(x)\, u\, v - b_i^\varepsilon(x)\, w,
$$

and the function

$$
G_i(w,v) = \gamma_i^\varepsilon(x) w - \kappa_i^\varepsilon(x) v,
$$

describes the transduction of the signal into the cell inside by activated proteins on the cell membrane. For the molecules involved in the intracellular part of the signalling pathway we consider

$$
\begin{aligned}
&\partial_t c_i^\varepsilon - \varepsilon^2 \nabla \cdot (D_i^\varepsilon(x) \nabla c_i^\varepsilon) = F_i(c_i^\varepsilon) && \text{in } \Omega_i^\varepsilon,\ t>0,\\
&\varepsilon^2 D_i^\varepsilon(x) \nabla c_i^\varepsilon \cdot \nu = \varepsilon G_i(p_a^\varepsilon, c_i^\varepsilon) && \text{on } \Gamma^\varepsilon,\ t>0.
\end{aligned} \tag{3}
$$

In the above, the functions $F_{(\cdot)}$ and the constants $d_{(\cdot)}$ model production and/or decay of the respective species. The model is closed by imposing bounded nonnegative initial data for all the species and Neumann or constant Dirichlet boundary conditions for c_e^ε on $\partial\Omega$.

Under suitable assumptions, see [5] for details, we prove that for every fixed $\varepsilon > 0$ there exists a unique weak solution of the microscopic problem (1)–(3), which is nonnegative and satisfies the following estimates, with C independent of

ε,

$$
\begin{aligned}
&\|c_e^\varepsilon\|_{L^\infty(0,T;L^2(\Omega_e^\varepsilon))} + \|\nabla c_e^\varepsilon\|_{L^2((0,T);L^2(\Omega_e^\varepsilon))} + \sqrt{\varepsilon}\|c_e^\varepsilon\|_{L^2((0,T);L^2(\Gamma^\varepsilon))} \le C,\\
&\|c_i^\varepsilon\|_{L^\infty(0,T;L^2(\Omega_i^\varepsilon))} + \|\varepsilon\nabla c_i^\varepsilon\|_{L^2((0,T);L^2(\Omega_i^\varepsilon))} + \sqrt{\varepsilon}\|c_i^\varepsilon\|_{L^2((0,T);L^2(\Gamma^\varepsilon))} \le C,\\
&\sqrt{\varepsilon}\|r_l^\varepsilon\|_{L^\infty(0,T;L^2(\Gamma^\varepsilon))} + \sqrt{\varepsilon}\|\varepsilon\nabla_\Gamma r_l^\varepsilon\|_{L^2((0,T);L^2(\Gamma^\varepsilon))} \le C, \quad l = f, b,\\
&\sqrt{\varepsilon}\|p_s^\varepsilon\|_{L^\infty(0,T;L^2(\Gamma^\varepsilon))} + \sqrt{\varepsilon}\|\varepsilon\nabla_\Gamma p_s^\varepsilon\|_{L^2((0,T);L^2(\Gamma^\varepsilon))} \le C, \quad s = a, d,\\
&\|c_l^\varepsilon\|_{L^\infty(0,T;L^\infty(\Omega_l^\varepsilon))} + \|r_j^\varepsilon\|_{L^\infty(0,T;L^\infty(\Gamma^\varepsilon))} + \|p_s^\varepsilon\|_{L^\infty(0,T;L^\infty(\Gamma^\varepsilon))} \le C.
\end{aligned} \tag{4}
$$

We use the trace and Gagliardo–Nirenberg inequalities together with an iteration processes to show the above estimates. Similar ideas were used in [2] to show the well-posedness of a system describing nonlinear ligand-receptor interactions for a single cell, whose shape is evolving in time. However due to the multiscale nature of our problem and the corresponding scaling in the microscopic equations, the techniques from [2] cannot be applied directly to obtain uniform a priori estimates.

Using the estimates (4) along with, now classical, results from the theory of two-scale convergence [1, 4, 3] we prove that a sequence of solutions of problem (1)–(3) converge as $\varepsilon \to 0$ to limits that satisfy the following two-scale macroscopic equations:

$$
\begin{aligned}
\partial_t c_e - \nabla\cdot(D_e^{\hom}(x)\nabla c_e) &= F_e(c_e) - \frac{1}{|Y_e|}\int_\Gamma G_e(c_e, r_f, r_b)d\gamma_y && \text{in } \Omega,\\
D_e^{\hom}(x)\nabla c_e\cdot\nu &= 0 && \text{on } \partial\Omega,\\
\partial_t c_i - \nabla_y\cdot(D_i(y)\nabla_y c_i) &= F_i(c_i) && \text{in } \Omega\times Y_i,\\
D_i(y)\nabla_y c_i\cdot\nu &= G_i(p_a, c_i) && \text{on } \Omega\times\Gamma,
\end{aligned} \tag{5}
$$

where

$$
D_{e,ij}^{\hom}(x) = \frac{1}{|Y_e|}\int_{Y_e}\left[D_{e,ij}(x,y) + \left(D_e(x,y)\nabla_y w^j(y)\right)_i\right]dy,
$$

with w^j being solutions of the unit cell problems

$$
\begin{aligned}
&\operatorname{div}_y(D_e(x,y)(\nabla_y w^j + e_j)) = 0 \quad \text{in } Y_e\times\Omega, \quad \int_{Y_e} w^j(x,y)dy = 0,\\
&D_e(x,y)(\nabla_y w^j + e_j)\cdot\nu = 0 \quad \text{on } \Gamma\times\Omega, \quad w^j(x,\cdot)\ \ Y-\text{periodic},
\end{aligned}
$$

for $x\in\Omega$, where $\{e_j\}_{j=1,\dots,d}$ is the standard basis in $\mathbb{R}^d$, together with the dynamics of receptors and proteins on the cell membrane $\Omega\times\Gamma$

$$
\begin{aligned}
\partial_t r_f - \nabla_{\Gamma,y}\cdot(D_f\nabla_{\Gamma,y} r_f) &= F_r(r_f, r_b) - G_e(c_e, r_f, r_b) - d_f r_f,\\
\partial_t r_b - \nabla_{\Gamma,y}\cdot(D_b\nabla_{\Gamma,y} r_b) &= G_e(c_e, r_f, r_b) - G_d(r_b, p_a, p_d) - d_b r_b,\\
\partial_t p_d - \nabla_{\Gamma,y}\cdot(D_d\nabla_{\Gamma,y} p_d) &= F_p(p_d) - G_d(r_b, p_a, p_d) - d_d p_d,\\
\partial_t p_a - \nabla_{\Gamma,y}\cdot(D_a\nabla_{\Gamma,y} p_a) &= G_d(r_b, p_a, p_d) - G_i(p_a, c_i) - d_a p_a.
\end{aligned} \tag{6}
$$

We approximate the solution to the macroscopic two-scale systems (5) and (6) using a two-scale finite element method (details in [5]). A feature of the numerical approach is that the two-scale systems are treated as parameterised systems in which the macroscopic variables simply play the role of parameters. The upshot

of this treatment is that independent bulk-surface systems are solved in parallel at each node of the triangulation of the macroscopic domain the solutions of which are used in the calculation of the source term in the macroscopic equation for c_e. Benchmark simulations and simulations in a biological regime are reported in [5].

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Hierarchy of PDE Models for Active Gels

Leonid Berlyand

(joint work with Volodimir Rybalko and Jan Fuhrmann)

We consider PDE models of active gels that arise in the studies of motility of eukaryotic cells. Our goal is to capture mathematically the key biological phenomena such as steady motion with no external stimuli, spontaneous breaking of symmetry, and rotation.

We first review our past work on phase field models [2] and then present recent work on the two types of the free boundary models: curvature driven motion [1] and a generalized Hele-Shaw flow for nonlinear PDEs [3].

In the analysis of the above models our focus is on proving existence of the traveling wave solutions that are the signature of the cell motility. We also study breaking of symmetry by proving existence of non-radial steady states. Bifurcation of traveling waves from steady states is established via the Schauder's fixed point theorem for the phase field model and the Leray-Schauder degree theory and Crandal-Rabinowitz theorem for the free boundary problem models.

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Stokes-flow-associated interfacial dynamics and tissue growth

John King

Tissue growth models adopting a Newtonian-fluid constitutive law were described, covering nutrient-rich and nutrient-poor limits. Asymptotic and numerical results were presented, with an emphasis on a buckling instability associated with cell-division-driven compressive stresses and contrasts with conventional fluid dynamics highlighted.

Multi-scale Modeling of Particles in Membranes

Carsten Gräser
(joint work with Luigi Delle Site, Tobias Kies, Ralf Kornhuber, Michael Kozlov)

Particles embedded into biomembranes play a crucial role for membrane function. Due to the inherent multi-scale structure of the problem, the mathematical modeling of coupled particle–membrane systems is a challenging task: At a large scale, the membrane behaves like an elastic shell with bending rigidity. Conversely, the particle–membrane coupling is happening on a much smaller molecular scale. While the mechanical properties can be modeled using Canham–Helfrich type geometric PDEs and a continuum membrane description, the molecular particle–membrane interactions are naturally represented using atomistic or coarse grained molecular dynamics approaches.

To efficiently deal with the multi-scale structure we consider hybrid particle–membrane models [1] combining a continuum membrane description u with discrete particles p_i coupled using the conditions $g_i(u, p_i) = 0$. The latter may, e.g., take the form of an essential boundary condition on the boundary of the particle of given position and orientation $p_i \in \Omega \times [0, 2\pi]$.

In order to investigate the interplay of the mechanical membrane properties and the particle–membrane coupling we consider the joint energy functional

$$\mathcal{E}(u, p) = J(u) + V(p).$$

Here $u \in H$ is a graph representation in a suitable closed subspace $H \subset H^2(\Omega)$ and $\omega \subset (\Omega \times [0, 2\pi])]^N$ is the set of admissible particle configurations. In the so called Monge–Gauge approximation $J(u)$ is a quadratic energy function associated to an $H^2(\Omega)$-elliptic linear differential operator.

Ignoring thermal fluctuations this leads to the coupled minimization problem

$$(u, p) = \operatorname*{arg\,min}_{\substack{(v,q)\in H\times\overline{\omega} \\ \text{s.t. } g_i(v,q_i)=0}} \mathcal{E}(v, q).$$

Associating to each possible particle configuration $q \in \omega$ the optimal membrane shape we arrive at the reduced minimization problem

$$p = \operatorname*{arg\,min}_{q\in\overline{\omega}} \mathcal{E}(q), \qquad \mathcal{E}(q) = \inf_{\substack{v\in H \\ \text{s.t. } g_i(v,q_i)=0}} \mathcal{E}(v, q)$$

for the implicitly given membrane-mediated mechanical particle–particle interaction potential $\mathcal{E}(q)$. Based on the gradient $\nabla\mathcal{E}(q)$ which can be computed using shape calculus we investigate minimizers of $\mathcal{E}(q)$ using a gradient flow approach [3]. To avoid local minimizers this can be combined with simulated annealing techniques. Numerical experiments using this approach showed ring-like clustering of FCHo2 BAR-domain proteins which is supposed to happen at an early stage of clathrin-mediated endocytosis [2].

To go beyond the zero-temperature case modeled by minimizing $\mathcal{E}(q)$ we consider the canonical ensemble for temperature induced particle fluctuations leading to the canonical probability density

$$\rho(q) = \frac{1}{Z} e^{-\beta\mathcal{E}(q)}, \qquad Z = \int_\omega e^{-\beta\mathcal{E}(q)} dq.$$

In order to efficiently compute expectation values $E[A]$ of observables A with respect to ρ we employ a Langevin sampling approach based on the overdamped Langevin equation

$$dq = -\nabla\mathcal{E}(q)dt + \alpha dW$$

to sample from the density ρ. Prototypic numerical experiments indicate that this approach can be a useful and efficient tool to compute observables and free energies for fluctuating particles in the non-zero case. The investigation of how this can be extended to membrane fluctuations is the topic of ongoing research.

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Long-time Dynamics and Optimal Control of a Diffuse Interface Model for Tumor Growth

Elisabetta Rocca

(joint work with Cecilia Cavaterra and Hao Wu)

We investigate the long-time dynamics and optimal control problem of a diffuse interface model that describes the growth of a tumor in presence of a nutrient and surrounded by host tissues. The state system consists of a Cahn-Hilliard type equation for the tumor cell fraction and a reaction-diffusion equation for the nutrient:

$$\phi_t - \Delta\mu = P(\phi)(\sigma - \mu), \qquad \text{in } \Omega \times (0,T), \tag{1}$$

$$\mu = -\Delta\phi + F'(\phi), \qquad \text{in } \Omega \times (0,T), \tag{2}$$

$$\sigma_t - \Delta\sigma = -P(\phi)(\sigma - \mu) + u, \qquad \text{in } \Omega \times (0,T), \tag{3}$$

subject to homogeneous Neumann boundary conditions

$$\partial_\nu \phi = \partial_\nu \mu = \partial_\nu \sigma = 0, \quad \text{on } \partial\Omega \times (0,T), \tag{4}$$

and initial conditions

$$\phi|_{t=0} = \phi_0(x), \quad \sigma|_{t=0} = \sigma_0(x), \quad \text{in } \Omega. \tag{5}$$

Here $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ denotes a bounded domain with smooth boundary $\partial\Omega$ and ν stands for the outward unit normal to $\partial\Omega$. System (1)–(3) is an approximation of the model proposed in [5]. The state variables are reduced to the tumor cell fraction ϕ and the nutrient concentration σ. Typically, $\phi \simeq 1$ and $\phi \simeq -1$ represent the tumor phase and the healthy tissue phase respectively, while $\sigma \simeq 1$ and $\sigma \simeq 0$ indicate in a nutrient-rich or nutrient-poor extracellular water phase. The unknown μ stands for the related chemical potential and the function F is typically a double-well potential with equal minima at $\phi = \pm 1$. P denotes a suitable proliferation function, which is in general a nonnegative and regular function of ϕ. The function u serves as an external source in the equation for σ and can be interpreted as a medication (or a nutrient supply) that serves to eliminate tumor cells in terms of drugs and is introduced into the system through the nutrient.

In [2], the system (1)–(5) with $u = 0$ was rigorously analyzed concerning well-posedness, regularity and long-time behavior (in terms of the global attractor), while in the recent paper [6] the long-time behavior of solutions (in terms of attractors) has been studied for a different system introduced in [4]. Let us indeed notice that, to the best of our knowledge, these are the only two contributions in the literature regarding the long-term dynamics of diffuse interface models for tumor growth.

Here, we consider the problem of "long-time treatment" under a suitable given source under a different perspective, that is convergence of single treajectories, and we prove the convergence of any global solution to a single equilibrium as $t \to +\infty$. Then we consider the "finite-time treatment" of a tumor, which corresponds to an optimal control problem. Here we also allow the objective cost functional to depend on a free time variable, which represents the unknown treatment time to be optimized. We prove the existence of an optimal control and obtain first order necessary optimality conditions for both the drug concentration and the treatment time. One of the main aims of the control problem is to realize in the best possible way a desired final distribution of the tumor cells, which is expressed by the target function ϕ_Ω. By establishing the Lyapunov stability of certain equilibria of the state system (without external source), we see that ϕ_Ω can be taken as a stable configuration, so that the tumor will not grow again once the finite-time treatment is completed.

Let us observe that under the presence of the external source u, we observe that any smooth solution (ϕ, σ) to problem (1)–(5) satisfies the following energy identity:

$$(6)\quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\phi,\sigma)+\int_\Omega \Big[|\nabla\mu|^2+|\nabla\sigma|^2+P(\phi)(\mu-\sigma)^2\Big]\,\mathrm{d}x=\int_\Omega u\sigma\,\mathrm{d}x,\quad \forall\, t>0,$$

which motives the twofold aim of the present contribution.

1: Long-time treatment of medication. For a suitably given external source u, we study the long-term dynamics of problem (1)–(5). We prove that any global weak solution will converge to a single equilibrium as $t\to+\infty$ and provide an estimate on the convergence rate.

In this direction, our result indicates that after certain medication (or even without medication, i.e., $u=0$), the tumor will eventually grow to a steady state as time evolves. However, since the potential function F is nonconvex due to its double-well structure, problem (1)–(5) may admit infinite many steady states so that for the moment one cannot identify which exactly the unique asymptotic limit as $t\to+\infty$ will be.

2: Finite-time treatment of medication. We investigate a more general distributed optimal control problem (cf. [1] and [3]), where we allow the objective cost functional to depend also on a free time variable, representing the unknown treatment time to be optimized. More precisely, denoting by $T\in(0,+\infty)$ a fixed maximal time in which the patient is allowed to undergo a medical treatment, we consider

(CP) *Minimize the cost functional*

$$\begin{aligned}\mathcal{J}(\phi,\sigma,u,\tau)=\frac{\beta_Q}{2}\int_0^\tau\!\!\int_\Omega|\phi-\phi_Q|^2\,\mathrm{d}x\,\mathrm{d}t+\frac{\beta_\Omega}{2}\int_\Omega|\phi(\tau)-\phi_\Omega|^2\,\mathrm{d}x\\+\frac{\alpha_Q}{2}\int_0^\tau\!\!\int_\Omega|\sigma-\sigma_Q|^2\,\mathrm{d}x\,\mathrm{d}t+\frac{\beta_S}{2}\int_\Omega(1+\phi(\tau))\,\mathrm{d}x\\+\frac{\beta_u}{2}\int_0^T\!\!\int_\Omega|u|^2\,\mathrm{d}x\,\mathrm{d}t+\beta_T\tau,\end{aligned}$$

subject to the control constraint

$$u\in\mathcal{U}_{\mathrm{ad}}:=\{u\in L^\infty(Q):\ u_{\min}\le u\le u_{\max}\ \text{a.e. in}\ Q\},\quad \tau\in(0,T),$$

and to the state system (1)–(5), *where* $Q:=\Omega\times(0,T)$.

Here, $\tau\in(0,T]$ represents the treatment time, ϕ_Q and σ_Q represent a desired evolution for the tumor cells and for the nutrient, respectively, while ϕ_Ω stands for desired final distribution of tumor cells. The first three terms of $\mathcal{J}$ are of standard tracking type, as often considered in the literature of parabolic optimal control, and the fourth term of $\mathcal{J}$ measures the size of the tumor at the end of the treatment. The fifth term penalizes large concentrations of the cytotoxic drugs, and the sixth term of $\mathcal{J}$ penalizes long treatment times. As it is presented in $\mathcal{J}$, a large value of $|\phi-\phi_Q|^2$ would mean that the patient suffers from the growth of the tumor, and a large value of $|u|^2$ would mean that the patient suffers from high toxicity of the drug. We shall prove the existence of an optimal control and derive the first-order necessary optimality conditions in terms of a variational inequality involving the adjoint state variables.

The variable τ can be regarded as the necessary treatment time of one cycle, i.e., the amount of time the drug is applied to the patient before the period of rest, or the treatment time before surgery. After the treatment, the ideal situation will be either the tumor is ready for surgery or the tumor will be stable for all time without further medication (i.e., $u = 0$). This goal can be realized by making different choices of the target function ϕ_Ω in the above optimal control problem **(CP)**. For the former case, one can simply take ϕ_Ω to be a configuration that is suitable for surgery. While for the later case, which is of more interest to us, we want to choose ϕ_Ω as a "stable" configuration of the system, so that the tumor does not grow again once the treatment is complete. For this purpose, we prove that any local minimizer of the total free energy $\mathcal{E}$ is Lyapunov stable provided that $u = 0$. As a consequence, these local energy minimizers serve as possible candidates for the target function ϕ_Ω. Then after completing a successful medication, the tumor will remain close to the chosen stable configuration for all time.

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Convergence results for surface evolution coupled to parabolic problems on the surface

Balázs Kovács

(joint work with Buyang Li, Christian Lubich and Christian Power)

Starting from papers of Dziuk and Elliott, much insight into the stability and convergence properties of finite elements on evolving surfaces has been obtained by studying a linear parabolic equation on a given moving closed surface $\Gamma(t)$. The strong formulation of this model problem is to find a solution $u(x,t)$ (for $x \in \Gamma(t)$ and $0 \le t \le T$) with given initial data $u(x,0) = u_0(x)$ to the linear partial differential equation

$$\partial^\bullet u(x,t) + u(x,t)\nabla_{\Gamma(t)} \cdot v(x,t) - \Delta_{\Gamma(t)} u(x,t) = 0, \qquad x \in \Gamma(t),\ 0 < t \le T,$$

where $\partial^\bullet$ denotes the material time derivative, $\Delta_{\Gamma(t)}$ is the Laplace–Beltrami operator on the surface, and $\nabla_{\Gamma(t)} \cdot v$ is the tangential divergence of the *given* velocity v of the surface. The Acta Numerica article of Dziuk and Elliott is an excellent review article (up to 2012) on the numerical analysis of this and related problems.

Beyond the above model problem, there is considerable interest in cases where the velocity of the evolving surface is *not given explicitly*, but depends on the solution u of the parabolic equation; see, e.g. physical and biological models where such situations arise. A further highly interesting problem (for two- or higher-dimensional surfaces) would be to couple mean curvature flow with diffusion on the surface. Studying the convergence of finite elements for these coupled problems, however, remains illusive as long as the convergence of ESFEM for mean curvature flow of closed surfaces is not understood. This has remained an open problem since Dziuk's formulation of such a numerical method for mean curvature flow in his 1990 paper [1]. Contrary to the case of surfaces with prescribed motion, there exists so far no numerical analysis for solution-driven surfaces in $\mathbb{R}^3$, to the best of our knowledge.

We consider different velocity laws for coupling the surface motion with the diffusion on the surface: a *regularized velocity law*:

$$v(x,t) - \alpha \Delta_{\Gamma(t)} v(x,t) = g\big(u(x,t), \nabla_{\Gamma(t)} u(x,t)\big)\, \nu_{\Gamma(t)}(x), \qquad x \in \Gamma(t),$$

with a fixed regularization parameter $\alpha > 0$.

This elliptic regularization allows us to give a complete stability and (optimal-order) convergence analysis of the ESFEM semidiscretisation [2], for finite elements of polynomial degree at least two. The stability and convergence results are extended to full discretisations with linearly implicit backward difference time-stepping [3].

Our approach also applies to the ESFEM discretisation of coupling a *regularized mean curvature flow* and diffusion on the surface:

$$v - \alpha \Delta_{\Gamma(t)} v = \Big(-H + g\big(u, \nabla_{\Gamma(t)} u\big)\Big) \nu_{\Gamma(t)},$$

where H denotes mean curvature on the surface $\Gamma(t)$.

The main difficulty in proving the convergence of the full discretization of the surface-evolution equation is the proof of stability in the sense of bounding errors in terms of defects in the discrete equations, and further establishing, via an inverse inequality, $W^{1,\infty}$ norm bounds for the errors. The proofs require some auxiliary results from [2, 3], which relate different finite element surfaces. The stability proofs use energy estimates (and are performed on the matrix–vector formulation) that become available for BDF methods up to order 5 by the multiplier technique of Nevanlinna & Odeh, which in turn is based on the G-stability theory of Dahlquist. The stability is independent of geometric arguments.

The developed techniques and the mentioned auxiliary results relating different surfaces enable a convergence proof for mean curvature flow [4].

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Convergence of an evolving finite element method for mean curvature flow

Christian Lubich

(joint work with Balász Kovács and Buyang Li)

A proof of convergence was outlined for semi- and full discretizations of mean curvature flow of closed two-dimensional surfaces, based on our paper [4].

Approximating the mean curvature flow by numerical methods was first addressed by Dziuk [1] in 1990. He proposed a finite element method based on a weak formulation of the mean curvature flow as a (formally) heat-like partial differential equation, in which the moving nodes of the finite element mesh determine the approximate evolving surface. However, proving convergence of Dziuk's method or related evolving finite element methods for closed two-dimensional surfaces (or higher-dimensional hypersurfaces) has remained an open problem.

We here consider a different evolving finite element method for mean curvature flow of closed two-dimensional surfaces and prove optimal-order convergence over time intervals on which the evolving surface remains sufficiently regular. We study stability and convergence for both the finite element semi-discretization and the full discretization obtained with a linearly implicit backward difference time discretization. Our approach shares with Dziuk's method the property that the moving nodes of a finite element mesh determine the approximate evolving surface. However, the method presented here discretizes equations that are different from the equation discretized by Dziuk. In his approach, a weak formulation of the quasi-heat equation describing mean curvature flow is discretized, whereas in the present work evolution equations for the normal vector and the mean curvature are discretized, which then yield the velocity of the surface evolving under mean curvature flow. Evolution equations for geometric quantities on a surface evolving under mean curvature flow have been an important tool in the analysis of mean curvature flow ever since Huisken's 1984 paper [2], but apparently they have so far not been used in the numerical approximation of mean curvature flow.

The numerical method based on the discretization of evolution equations of geometric quantities, as presented here, is computationally more expensive than Dziuk's method (roughly by about a factor 2), but on the other hand it provides

full-order approximations to basic geometric quantities — the normal vector and mean curvature — in addition to the position and velocity of the surface.

Our numerical approach is related to our previous paper [3], where we study the convergence of finite elements on an evolving surface driven by diffusion on the surface. The convergence analysis of our method for mean curvature flow uses techniques developed in that previous paper. As in [3], the stability analysis works with the matrix–vector formulation of the method and does not use geometric arguments. The geometry only enters into the analysis of the consistency error. The error analysis combines the stability estimates and consistency estimates to yield optimal-order H^1-norm error bounds for the computed surface position, velocity, normal vector and mean curvature.

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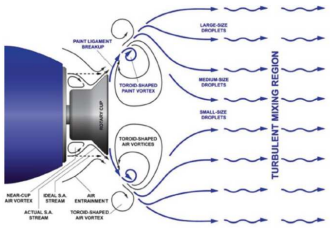
Modeling of Rotary Spray Bell Painting

James A. Sethian

(joint work with Robert I. Saye)

In manufacturing settings, paints are frequently applied by an electrostatic rotary bell atomizer: paint flows to a cup rotating at 10,000-70,000 rpm and is driven by centrifugal forces to form thin sheets and tendrils at the cup edge, where it then atomizes into droplets.



Rotary Bell: Schematic of paint flow and air currents

The goal of computational modeling of this process is to both understand the dynamics, and to optimize flow characteristics. This includes

- Optimizing the atomization process for higher paint flow rates, in particular trying to obtain more uniform and consistent atomization in the 30,000 to 60,000 rpm range.
- Studying the atomization process as a function of paint fluid properties (such as density, viscosity, and surface tension) and physical properties, such as inflow rates, bell rotation speeds and shaping air currents.
- Analyzing film dynamics, particularly in the immediate atomization zone right past the cup edge, including the dynamics of filament formation and droplet size, distribution and trajectories.

However, the fluid mechanics of this problem make it particularly challenging:

- The cup is rotating fast (50,000 rpm).
- Interfaces are contorted and complex.
- Thin sheets of paint roll off, and then break into droplets.
- The flow is not axisymmetric: Three-dimensional effects are what cause droplets to break off, into tiny tendrils and droplets.
- Paint is non-Newtownian.

From a computational point of view, these challenges dictate several requirements. First, we need appropriate equations of motion in a moving, rotating coordinate system referencing curved surfaces. Second, hybrid interface solvers which coupled interface jump conditions with highly contorted interfaces are required. Third, highly accurate fluid solvers are needed to deal with the sharp density jumps between the paint fluid dynamics and fast moving shaping air currents. Fourth, adaptive mesh refinement is needed, because of the vast scales between the smallest droplets and the extent of the computational domain. And fifth, the sheer scale of the time step and space discretization require use of advanced high performance computing capabilities, replete with attention to massively parallel processing on multi-core architectures.

To meet these needs, we have been working on building a numerical methodology that can accurately compute the underlying dynamics. Our methodology combines (1) level set methods to track the paint/air fluid interface, in a way that is able to deal with significant distortions, tearing, breakup and merger [1, 2]; (2) implicit mesh discontinuous Galerkin methods for high order accurate computation of the underlying flow and interface dynamics, employing temporary body-fitted DG meshes in order to impose complex interface jump conditions [3]; (3) an adaptive mesh refinement scheme to resolve fluid droplets, in which subdivision criteria are based on width/thickness of paint film, as well as curvature; and (4) advanced efficient parallel implementation on high performance multi-core architectures.

Results so far have been promising, and we plan to report on them in the near future.

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A Coupled Bulk-Surface Model for Lipid Raft Formation in Cell Membranes

Helmut Abels

(joint work with Johannes Kampmann)

We consider a model, which describes the formation of so-called lipid rafts on cell membranes. The model was derived by Garcke et al. in [2] and leads to the following bulk–surface system:

$$\partial_t u = D\Delta u \qquad \text{in } B\times(0,T], \tag{1}$$

$$-D\nabla u\cdot\nu = q \qquad \text{on } \Gamma\times(0,T], \tag{2}$$

$$\partial_t\varphi = \Delta_\Gamma\mu \qquad \text{on } \Gamma\times(0,T], \tag{3}$$

$$\mu = -\varepsilon\Delta_\Gamma\varphi + \varepsilon^{-1}W'(\varphi) - \delta^{-1}(2v-1-\varphi) \qquad \text{on } \Gamma\times(0,T], \tag{4}$$

$$\partial_t v = \Delta_\Gamma\theta + q = \frac{4}{\delta}\Delta_\Gamma v - \frac{2}{\delta}\Delta_\Gamma\varphi + q \qquad \text{on } \Gamma\times(0,T], \tag{5}$$

$$\theta = \frac{2}{\delta}(2v-1-\varphi) \qquad \text{on } \Gamma\times(0,T] \tag{6}$$

with initial conditions for u, φ and v. Here $B\subseteq\mathbb{R}^3$ is a bounded smooth domain with boundary $\Gamma := \partial B$ and outer unit normal ν, and $T,\varepsilon,D,\delta>0$ are arbitrary. q is an exchange term for the cytosolic and membrane-bound cholesterol and will be specified later. Here (3) and (5) are mass balance equations for the surface quantities. (1) and (2) model the evolution of the cytosolic cholesterol by a simple diffusion equation with diffusion coefficient $D>0$. Equation (5) also includes a cross-diffusion, which stems from the cholesterol-lipid affinity in the surface energy $\mathcal{F}$. Finally, equations (3) and (4) constitute Cahn-Hilliard dynamics for the lipid concentration and allow for a contribution from the cholesterol evolution via the last term. We note that the parameter δ controls how much the preferred binding between saturated lipids and cholesterol influences the system.

We note that sufficiently smooth solutions of the system satisfy

$$\frac{d}{dt}\left(\mathcal{F}(v(\cdot,t),\varphi(\cdot,t)) + \frac{1}{2}\int_B u(\cdot,t)^2\right) \le \int_\Gamma q(\theta-u)\,d\mathcal{H}^2 \quad \text{for all } t\in(0,T]. \tag{7}$$

It is possible to prove that the energy stays bounded on finite time intervals under suitable growth assumptions on q. This is a key ingredient for our following existence proof.

Theorem (Existence of Weak Solutions)**.**
Let $T \in (0,\infty)$. Let $\varphi_0 \in H^1(\Gamma), v_0 \in H^1(\Gamma)$ and $u_0 \in L^2(B)$. Moreover, assume that the exchange term $q : \mathbb{R}^2 \to \mathbb{R}$ is continuous and fulfills

$$|q(u,v)| \le C(1+|u|+|v|) \qquad \forall\ u,v \in \mathbb{R} \tag{8}$$

for some $C > 0$. Then there exist functions $(u,\varphi,v,\mu,\theta) \in \mathcal{W}_B \times \mathcal{W}_\Gamma^1 \times \mathcal{W}_\Gamma^1 \times \mathcal{W}_\Gamma^2 \times \mathcal{W}_\Gamma^2$ which are a weak solution to problem (1)–(6), where

$$\mathcal{W}_B := L^2\left(0,T;H^1(B)\right) \cap H^1\left(0,T;\left(H^1(B)\right)'\right),$$
$$\mathcal{W}_\Gamma^1 := L^2(0,T;H^1(\Gamma)) \cap H^1(0,T;H^{-1}(\Gamma)),\ \text{and}\ \mathcal{W}_\Gamma^2 := L^2(0,T;H^1(\Gamma)).$$

We refer to [1] or [3] for the proofs and details of this and the following results.

Since the diffusion in the bulk is often much higher than the lateral diffusion on the cell membrane, it is reasonable to consider $D \to \infty$ in (1)–(6). Formally, one derives

$$\partial_t u = -\frac{1}{|B|}\int_\Gamma q(u,v) \qquad \text{for } t \in (0,T], \tag{9}$$
$$\partial_t \varphi = \Delta_\Gamma \mu \qquad \text{on } \Gamma \times (0,T], \tag{10}$$
$$\mu = -\varepsilon\Delta_\Gamma\varphi + \varepsilon^{-1}W'(\varphi) - \delta^{-1}(2v-1-\varphi) \qquad \text{on } \Gamma \times (0,T], \tag{11}$$
$$\partial_t v = \Delta_\Gamma \theta + q(u,v) \qquad \text{on } \Gamma \times (0,T], \tag{12}$$
$$\theta = \frac{2}{\delta}(2v-1-\varphi) \qquad \text{on } \Gamma \times (0,T]. \tag{13}$$

Here u is spatially constant and its evolution in time is governed by the ordinary differential equation (9). More precisely, we can show:

Proposition. *Let $\{D_n\}_{n\in\mathbb{N}} \subset (0,\infty)$ be such that $\lim_{n\to\infty} D_n = \infty$ and let $(u^{D_n},\varphi^{D_n},\mu^{D_n},\theta^{D_n},v^{D_n})$ be weak solutions from the above Theorem with $D = D_n$ and initial data independent of n. Then there exists a subsequence (again denoted by $\{D_n\}_{n\in\mathbb{N}}$) such that*

$$u^{D_n} \rightharpoonup u \text{ in } L^2(0,T;H^1(B)) \cap H^1\Big(0,T;\big(H^1(B)\big)'\Big) \text{ with } u(t) \in \mathbb{R} \forall t \in (0,T),$$
$$(\varphi^{D_n},v^{D_n}) \rightharpoonup (\varphi,v) \text{ in } L^2(0,T;H^1(\Gamma)) \cap H^1(0,T;H^{-1}(\Gamma)),$$
$$(\mu^{D_n},\theta^{D_n}) \rightharpoonup (\mu,\theta) \text{ in } L^2(0,T;H^1(\Gamma)),$$

and such that the limit functions are weak solution to the reduced problem (9)–(13).

The inequality (7) allows to identify two different classes of constitutive laws for the exchange term q. Every constitutive law which implies that $\int_\Gamma q(\theta-u)$ is non-positive also implies that the energy of the coupled system is decreasing. This is called the equilibrium case. But this might not be true in general. One

possible approach is to see the cholesterol attachment to the membrane as a "reaction" between free sites on the membrane, namely regions of low membrane-bound cholesterol concentration v and the cytosolic cholesterol, whereas the detachment from the membrane can be considered to be proportional to v. This leads to

$$q(u,v) := c_1 u(1-v) - c_2 v \tag{14}$$

with positive constants $c_1, c_2 \in \mathbb{R}$, cf. [2]. In [2], the authors present numerical simulations which allow to compare the qualitative behavior for the reduced model in the equilibrium and non-equilibrium case. In the equilibrium case, the simulations display the saturated lipids clustered in one connected domain, in contrast to the complex patterns observed in the formation of lipid rafts. On the other hand, the non-equilibrium case (14) exhibits the emergence of patterns similar to the formation of lipid rafts, see [2, Figures 3 and 11]. Furthermore, it turns out that the reduced system in the non-equilibrium case displays a surprising relationship to the so-called Ohta-Kawasaki system arising in the modeling of diblock copolymers. Based on further numerical experiments it was conjectured in [2, Section 3.4] that as $\delta \to 0$, solutions to the reduced model in the case (14) should approach solutions to the Ohta-Kawasaki equations.

By the following Theorem, this is actually true for the mean value free parts of the solutions and a slight modification of the Otha-Kawasaki equation. In the following, P_Γ denotes the projection onto the mean value free part, i.e. $P_\Gamma f := f - \frac{1}{|\Gamma|}\int_\Gamma f := f_\Gamma$.

Theorem (Convergence to a Modified Ohta-Kawasaki Equation)**.**
Let q be as in (14)and let $\{\delta_n\}_{n\in\mathbb{N}} \subset (0,\infty)$ be a sequence with $\lim_{n\to\infty}\delta_n = 0$. Let $(u^{\delta_n}, \varphi^{\delta_n}, \mu^{\delta_n}, \theta^{\delta_n}, v^{\delta_n})$ be weak solutions of (9)–(13) with $\delta = \delta_n$. We assume that the initial data is independent of δ_n and in addition that the initial data for u belongs to $[0, M|B|^{-1}]$. Then there exists a subsequence (again denoted by $\{\delta_n\}_{n\in\mathbb{N}}$) such that $\{u^{\delta_n}\}_{n\in\mathbb{N}}$ and $(\varphi_\Gamma^{\delta_n}, \mu_\Gamma^{\delta_n}, \theta_\Gamma^{\delta_n})$ fulfil

$$\begin{aligned} u^{\delta_n} &\rightharpoonup u \text{ in } H^1(0,T), \\ \varphi_\Gamma^{\delta_n} &\rightharpoonup \varphi_\Gamma \text{ in } L^2(0,T;H^1(\Gamma)) \cap H^1(0,T;H^{-1}(\Gamma)), \\ (\mu_\Gamma^{\delta_n}, \theta_\Gamma^{\delta_n}) &\rightharpoonup (\mu_\Gamma, \theta_\Gamma) \text{ in } L^2(0,T;H^1(\Gamma)) \end{aligned}$$

and $(u, \varphi_\Gamma, \mu_\Gamma, \theta_\Gamma)$ is a weak solution to the modified Ohta-Kawasaki equation

$$\begin{aligned} &\partial_t \varphi_\Gamma = \Delta_\Gamma \mu_\Gamma, \quad \frac{5}{4}\mu_\Gamma = -\varepsilon\Delta_\Gamma\varphi_\Gamma + \frac{1}{\varepsilon}P_\Gamma W'(\varphi_\Gamma) - \frac{1}{2}\sigma, \\ &\Delta_\Gamma \sigma = \frac{c_1 u(t) + c_2}{2}\varphi_\Gamma, \qquad \int_\Gamma \sigma = 0, \end{aligned}$$

where $\sigma := \theta_\Gamma - \frac{1}{2}\mu_\Gamma$, together with

$$\frac{d}{dt}\int_B u(t) = -\frac{c_1}{|B|}\left(\int_B u(t)\right)^2 + \left(c_1\frac{M-|\Gamma|}{|B|} - c_2\right)\int_B u(t) + c_2 M \text{ on } (0,T].$$

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Weak and approximate curvatures of a measure: a varifold perspective

Simon Masnou

(joint work with Blanche Buet and Gian Paolo Leonardi)

We introduce in [5] a new approach for the computation of second-order extrinsic properties (curvatures) for a very general class of geometric objects, including both smooth or piecewise smooth d-submanifolds and discrete datasets in the Euclidean n-space. The generality and potentialities of our method can be mostly appreciated on unstructured datasets, like point clouds, for which the determination of curvatures is a very important, but extremely delicate task. Indeed, the need of efficient and robust techniques for the analysis of geometric features of general datasets is today of primary importance, due to the variety of both data sources and applications of data analysis, in particular in high dimensions.

The proposed framework relies on a suitable extension of the theory of *varifolds*. Varifolds represent very natural generalizations of classical d-surfaces, as they encode, loosely speaking, a joint distribution of mass and tangents. More technically, varifolds are Radon measures defined on the Grassmann bundle $\mathbb{R}^n \times \mathbb{G}_{d,n}$ whose elements are pairs specifying a position in space and an unoriented d-plane. Varifolds have been proposed more than 50 years ago by Almgren [3] as a mathematical model for soap films, bubble clusters, crystals, and grain boundaries. After Allard's fundamental work [1], they have been successfully used in the context of Geometric Measure Theory, Geometric Analysis, and Calculus of Variations. Within the classical theory of varifolds, a generalized notion of curvature is encoded in the *first variation* operator, see [1, 2, 9]. The so–called *Allard varifolds*, i.e., varifolds whose first variation is a Radon measure, constitute a very important class of measures. More than a decade after Allard's work, a theory of *curvature varifolds* was proposed by Hutchinson [7, 6]. This theory provides a notion of *generalized second fundamental form* (extended by Mantegazza in [8] to the case of varifolds with boundary), together with existence and regularity results for solutions to variational problems involving curvature–dependent functionals.

As we already pointed out in our previous work [4], the theory of varifolds has seen no substantial applications in the fields of applied mathematics. A possible explanation is that some key tools, like the first variation operator, are not directly applicable to general varifolds, and in particular to varifolds arising from discrete

datasets. For example, the first variation of a point cloud varifold is not a measure, but only a distribution resulting from a directional/tangential derivative of a finite sum of weighted Dirac's deltas. Therefore, the standard first variation of a point cloud varifold does not directly provide any consistent notion of (mean) curvature for that kind of dataset. In [4] we have shown how to define consistent notions of approximate mean curvature for any varifold, including those of discrete type. In [5] we extend the theory and define *approximate second fundamental forms* for the whole class of varifold measures.

More precisely, we first introduce a suitable family of variation operators and obtain from them a notion of *weak second fundamental form* which appears to be weaker than (but fully consistent with) the tensor defined by Hutchinson. Using a regularization technique, we show how to define approximate second fundamental forms for general varifolds. These approximate curvature tensors depend on a parameter which controls the approximation scale. We prove in [5] various compactness, consistency, and convergence results, typically we compare the approximate second fundamental forms of a sequence of varifolds with the second fundamental form of its weak-$*$ limit.

We also show in [5] several numerical tests on point clouds that illustrate the robustness of the method. In particular, some examples of 2-dimensional point clouds in $\mathbb{R}^3$ are considered. For them, we compute the approximate principal curvatures also in presence of noise and singularities to illustrate the stability of our approach.

We believe that our notion of approximate second fundamental form constitutes a general, robust, and easily-computable tool for extracting curvature information from very general geometric objects. Several promising research directions are thus opened. Only to name a few: the development of a theory of discrete geometric evolutions (e.g., the discrete mean curvature flow) for point clouds, with application to shape smoothing and segmentation; the use of curvature estimators for data analysis and classification *in any dimension and codimension*; the determination of intrinsic properties of unstructured datasets (like the density of a point cloud) via curvature–related properties.

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Optimal L^1-relaxation rates for the Cahn-Hilliard equation on the line

Felix Otto
(joint work with Sebastian Scholtes and Maria Westdickenberg)

We study the relaxation of the Cahn-Hilliard equation on the line

$$u_t - (W'(u) - u_{xx})_{xx} = 0 \tag{1}$$

with $\lim_{x\to\pm\infty} u = \pm 1$, where for simplicity we take $W = \frac{1}{4}(u^2-1)^2$ to be the standard double-well potential. The only stationary solutions are the translates $\{v_c := v(\cdot - c)\}_{c\in\mathbb{R}}$ of the kink $v = \tanh\frac{x}{\sqrt{2}}$. It is well known that equation (1) preserves mass:

$$\frac{d}{dt}\int (u-v) = 0 \quad \text{so that w. l. o. g.} \quad \int (u-v) = 0. \tag{2}$$

Furthermore, (1) dissipates energy: $\dot{E} = -D$, where

$$E := \int \big((W(u) + \frac{u_x^2}{2}) - (W(v) + \frac{v_x^2}{2})\big), \quad D := \int (W'(u) - u_{xx})_x^2. \tag{3}$$

Our goal is to quantify the rate at which $u \to v$ as $t \uparrow \infty$.

For a given configuration u, let

$$c := \operatorname{argmin}_c \int (u - v_c)^2 \quad \text{and} \quad f_c := u - v_c \tag{4}$$

and note that by mass conservation, cf. (2), there holds

$$2c = \int f_c. \tag{5}$$

We start with heuristics: Linearizing (1) around v_c and appealing to the Euler-Lagrange equation for (4), we obtain

$$(f_{ct} - \dot{c}v_{cx}) - (W''(v_c)f_c - f_{cxx})_{xx} = 0, \quad \int f_c v_{cx} = 0, \tag{6}$$

which in on large spatial scales is approximated by

$$(f_{ct} - 2\dot{c}\delta(\cdot - c)) - (W''(1)f_c)_{xx} = 0, \quad f_c(x = c) = 0, \tag{7}$$

also known as the Stefan problem. From this we learn that the free boundary $x = c$ acts as a sink for the diffusing excess mass f_c. The anti-derivative

$$F_c(x) := \left\{ \begin{array}{ll} \int_{-\infty}^{c} f_c & x < c \\ -\int_{c}^{+\infty} f_c & x > c \end{array} \right\}$$

satisfies the diffusion equation with homogeneous Neumann data on the (moving) half space, so that we expect $\sup_x |F_c| \lessapprox \frac{1}{\sqrt{4\pi W''(1)t}} \int |F_{0c}|$, where the index 0 indicates initial data. By volume conservation, cf. (5), in the form $2c = [F_c]$, this yields the algebraic relaxation $|2c| \lessapprox \frac{1}{\sqrt{4\pi W''(1)t}} \int |F_{0c}|$, a scaling we exactly capture:

THEOREM. Suppose that for any $\delta > 0$

$$E_0 \leq 2 \int (W(v) + \frac{v_x^2}{2}) - \delta. \tag{8}$$

Then

$$tc^2 + t^{\frac{3}{2}} E \lesssim_\delta \Big(\int |F_{0c}| + 1 \Big)^2 \quad \text{and} \quad c^2 + t^{\frac{1}{2}} E \lesssim_\delta \Big(\int |f_{0c}| + 1 \Big)^2.$$

Assumption (8), which ensures that there is not enough energy to form three (and thus even two) transition layers, is necessary to rule out the slow-coarsening scenario. As opposed to the above, prior results have been perturbative. Setting $f := u - v$, Bricmont et. al. showed that $\sup_x \frac{|f_0|}{(1+|x|)^{3+}} \ll 1$ implies $tc^2 \lesssim 1$; Howard could weaken the assumption to $\sup_x \frac{|f_0|}{(1+|x|)^2} \ll 1$ (note that $\sup_x \frac{|f_0|}{(1+|x|)^2}$ has the same scaling as $\int |F_{0c}|$). Carlen et. al. established that $\int x^2 f_0^2 \leq 1$ and $\int f_0^2 \ll 1$ implies the (suboptimal) $t^{\frac{9}{13}} E \lesssim 1$. (Two of the present authors established the optimal $tE \lesssim 1$ under the scaling-wise similar assumption $\int F_0^2 \leq 1$ and (8).)

To give an idea of the proof, we focus on $t^{\frac{1}{2}} E \lesssim (\int |f_{0c}| + 1)^2$. At the core, there is a Nash-type argument based on $V := \int |f_c|$. The argument is simple on the level of the Stefan problem (7), where it is easy to see

$$\dot{V} \leq 0 \quad \text{and thus} \quad V \leq V_0, \tag{9}$$

while the dissipation of energy, cf. (3), assumes the simple form

$$\dot{E} = -D \quad \text{where } E = \int \frac{W''(1)}{2} f_c^2, \;\; D = \int (W''(1) f_{cx})^2.$$

In combination with the elementary interpolation estimate

$$E \lesssim D^{\frac{1}{3}} V^{\frac{4}{3}}, \text{ which amounts to } \|f_c\|_{L^2} \lesssim \|f_{cx}\|_{L^2}^{\frac{1}{3}} \|f_c\|_{L^1}^{\frac{2}{3}}, \tag{10}$$

this yields the desired $t^{\frac{1}{2}} E \lesssim V_0^2$ by an elementary ODE argument.

There are two challenges in passing from the Stefan problem (7) to the Cahn-Hilliard equation (1). The first challenge is to find a substitute for the elementary interpolation estimate (10). It relies on the quantitative linearization

$$(8) \quad \Longrightarrow \quad E \sim \int (f_c^2 + f_{cx}^2), \quad D \sim \int (f_{cx}^2 + f_{cxxx}^2),$$

which allows one to easily establish (10) in the form $E \lesssim D^{\frac{1}{3}} (V+1)^{\frac{4}{3}}$.

The second challenge is to find a substitute for (9). We establish $V \stackrel{<}{\sim} V_0 + 1$ by a duality argument: Given a time T, one first shows on the basis of the simple energy estimate for $t \in [0, T]$, that

$$(11) \quad c(t) - c(T) \stackrel{<}{\sim} (T-t)^{\frac{1}{4}} + 1 \text{ so that } c(t) \leq \bar{c}(t) := c(T) + C((T-t)^{\frac{1}{4}} + 1).$$

One then solves the linear homogeneous equation

$$\begin{aligned} -\zeta_t - (W''(1)\zeta - \zeta_{xx})_{xx} = 0 \quad &\text{for } x > \bar{c}, \\ \zeta = \zeta_{xx} = 0 \quad &\text{for } x = \bar{c} \end{aligned}$$

backwards in time with terminal data $\zeta = \text{sign} f_c$ at $t = T$. Because of (11), the moving domain $\{x > \bar{c}(t)\}$ stays solidly to the right of the free boundary. Note that $-\zeta_t - (W''(1)\zeta - \zeta_{xx})_{xx} = 0$ is dual to $f_{ct} - (W''(1)f_c - f_{cxx})_{xx} = 0$, which is a good approximation to (6) away from the free boundary. Equation (6) in turn was the linearization of (1). This allows one to relate $\int |f_c(t = T)| = \int (f_c \zeta)(t = T)$ to $\int f_{0c}\zeta(t = 0)$. In order to deal with the approximation and linearization errors, we use the semi-group estimate

$$|\zeta| + \max\{T-t, (T-t)^{\frac{1}{2}}\}|\zeta_{xx}| + \max\{(T-t)^2, T-t\}|\zeta_{xxxx}| \stackrel{<}{\approx} \sup_x |\zeta(t = T)|,$$

and the challenge in deriving this comes from the moving domain. However, the latter is a subcritical perturbation. This can be seen by the change of variables $y = x - \bar{c}(t)$ and appealing to Schauder theory for the (parabolic) operator

$$\partial_t - \partial_y^2 + \partial_y^4 \quad \text{with Dirichlet b. c. on } \{y > 0\}.$$

This maximal regularity theory in Hölder spaces has to be based on the Carnot-Carathéodory metric

$$|t - t'|^{\frac{1}{4}} + \min\{|y - y'|^{\frac{1}{2}}, |y - y'|\},$$

where the presence of the (formally lower order) expression $|y - y'|^{\frac{1}{2}}$ is crucial for capturing the correct large-scale behavior dominated by (second-order) diffusion.

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Tangential tensor fields - modeling, numerics and applications

Axel Voigt

(joint work with Michael Nestler, Ingo Nitschke and Sebastian Reuther)

Over the last decade a huge interest has been developed for surface PDEs in both numerical analysis and applications. To deal with PDEs defined on curved manifolds requires to combine various mathematical disciplines, e.g., differential geometry, variational methods, numerics and even topology. Although some numerical approaches exist, which rely on a geometric framework, the important breakthrough in the development of numerical methods for this type of PDEs is the avoidance of charts and atlases. Either the methods are based on a triangulated surface and require information on the manifold solely through knowledge of the vertices, or an implicit surface representation is used and the problem is extended to the embedding space. Most of this work until today is concerned with scalar-valued surface PDEs, see [1] for a review. In this case the coupling between the geometry of the surface and the PDE is weak and thus allows to solve these problems with small modifications of established numerical approaches in flat space. For vector- and tensor-valued surface PDEs this coupling becomes much stronger. We provide an approach, which is based on a reformulation of the problem in Cartesian coordinates and allows for a componentwise solution using tools for scalar-valued surface PDEs. The approach does not require any assumptions on the extension of the surface quantities in the embedding space. Starting with the manifold and the covariant derivative ∇, we extend the manifold and the quantities on it to an embedding thin film with the corresponding embedding space/thin film derivative $\underline{\nabla}$. By using thin film coordinates we can separate tangential and normal contributions, which enables to identify the tangential parts with ∇ and to express $\underline{\nabla}$ in terms of partial derivatives along the Euclidean basis. This reformulation maintains physical invariance and allows to rewrite any manifold bound, vector- or tensor-valued PDE into a set of scalar-valued PDEs along an Euclidean basis. In this form the problem can be solved for each component by established finite element methods. We numerically demonstrate optimal order of convergence for different examples and provide all necessary tools to solve general vector- and tensor-valued surface PDEs within a numerical framework for scalar-valued surface PDEs. In particular we obtain for 0-tensors (scalars) and 1-tensors (vectors)

$$
\begin{aligned}
&d=0, s:\mathcal{M}\mapsto \mathrm{T}^0(\mathcal{M}) \qquad [\nabla s]_i = \partial_i s \qquad\qquad [\nabla s] = \Pi[\underline{\nabla}\,\underline{s}]\\
&d=1, \boldsymbol{p}:\mathcal{M}\mapsto \mathrm{T}^1(\mathcal{M}) \quad [\nabla \boldsymbol{p}]_{ij} = \partial_j p_i - \Gamma^k_{ij} p_k \quad [\nabla \boldsymbol{p}] = \Pi[\underline{\nabla}\,\underline{\boldsymbol{p}}] + (\underline{\boldsymbol{p}}\cdot\boldsymbol{\nu})\boldsymbol{B},
\end{aligned}
$$

where $\mathcal{M}\subset\mathbb{R}^3$ denotes the manifold, $\mathrm{T}^d(\mathcal{M})$ the tangent d-tensors bundle on $\mathcal{M}$, Π the projection to $\mathrm{T}^d(\mathcal{M})$, ∂_i partial derivatives, Γ^k_{ij} the Christoffel symbols, $\boldsymbol{\nu}$ the manifold normal and $\boldsymbol{B}$ the shape operator. While the description of the covariant derivative for scalar quantities, i. e. $[\nabla s] = \Pi[\underline{\nabla}\,\underline{s}] = \underline{\nabla}\,\underline{s} - \boldsymbol{\nu}(\boldsymbol{\nu}\cdot\underline{\nabla}\,\underline{s})$, is well established, see e.g. Def. 2.3 in [1], the description in Cartesian coordinates for tensors depends on the degree d and requires additional coupling terms with

geometric quantities, which increase with the degree d. The Cartesian descriptions can now be used to derive a generic componentwise finite element formulation for vector- and tensor-valued surface PDEs. For 1-tensors (vectors) similar approaches have been considered for specific applications. However, besides [2], all use $[\nabla \boldsymbol{p}] = \Pi[\underline{\nabla}\,\underline{\boldsymbol{p}}]$, which only holds if $\boldsymbol{\nu} \cdot \underline{\boldsymbol{p}} = 0$. In [3, 4] this is enforced by a penalty approach and in [5] by using a Lagrange multiplier. To demonstrate the approach we consider a vector-Helmholtz problem on a manifold without boundary embedded in $\mathbb{R}^3$. The variational formulation reads: Find $\boldsymbol{p} \in \mathbb{H}^{1,1}_{tan}(\mathcal{M})$, s.t.

$$a(\boldsymbol{p}, \boldsymbol{\psi}) = l(\boldsymbol{\psi}) \quad \forall \boldsymbol{\psi} \in \mathbb{H}^{1,1}_{tan}(\mathcal{M}) \tag{1}$$

with $a(\boldsymbol{p}, \boldsymbol{\psi}) = \langle \nabla \boldsymbol{p}, \nabla \boldsymbol{\psi} \rangle_2 + \langle \boldsymbol{p}, \boldsymbol{\psi} \rangle_1$ and $l(\boldsymbol{\psi}) = \langle \boldsymbol{f}, \boldsymbol{\psi} \rangle_1$, with $\mathbb{H}^{1,1}_{tan}(\mathcal{M})$ the Sobolev space of tangent tensor fields of degree 1 on $\mathcal{M}$ with covariant gradient and an appropriate norm $\langle \boldsymbol{p}, \boldsymbol{\psi} \rangle_d = \langle \Pi[\boldsymbol{p}], \Pi[\boldsymbol{\psi}] \rangle_{(\mathbb{R}^3)^d}$ for d-tensor fields. Using the derived identities, this can be rewritten in the extended space and the problem can be expressed in Cartesian coordinates. This extended formulation reads: Find $\underline{\boldsymbol{p}} \in [H^1(\mathcal{M})]^3$, s.t.

$$a(\underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}}) = l(\underline{\boldsymbol{\psi}}) \quad \forall \underline{\boldsymbol{\psi}} \in [H^1(\mathcal{M})]^3 \tag{2}$$

with $a(\underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}}) = \langle \underline{\nabla}\,\underline{\boldsymbol{p}} + (\underline{\boldsymbol{p}} \cdot \boldsymbol{\nu})\boldsymbol{B}, \underline{\nabla}\,\underline{\boldsymbol{\psi}} + (\underline{\boldsymbol{\psi}} \cdot \boldsymbol{\nu})\boldsymbol{B} \rangle_2 + \langle \underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}} \rangle_1$ and $l(\boldsymbol{\psi}) = \langle \underline{\boldsymbol{f}}, \underline{\boldsymbol{\psi}} \rangle_1$ and $[H^1(\mathcal{M})]^3$ the embedded product Sobolev space of 1-tensor fields on $\mathcal{M}$. The space $[H^1(\mathcal{M})]^3 \supset \mathbb{H}^{1,1}_{tan}(\mathcal{M}) \cong \Pi\left[[H^1(\mathcal{M})]^3\right]$ is orthogonal decomposable into $[H^1(\mathcal{M})]^3 = \mathbb{H}^{1,1}_{tan}(\mathcal{M}) \oplus \mathbb{H}^{1,1}_{nor}(\mathcal{M})$ w.r.t. the projection operator Π. Since $\mathbb{H}^{1,1}_{nor}(\mathcal{M})$ is located in the kernel of the symmetric bilinear form a, the solution of (2) is not unique. To overcome this issue and preserve also the well-posedness of problem (1) in the bigger space $[H^1(\mathcal{M})]^3 \supset \mathbb{H}^{1,1}_{tan}(\mathcal{M})$, the problem has to be modified: Find $\underline{\boldsymbol{p}} \in [H^1(\mathcal{M})]^3$, s.t.

$$\tilde{a}(\underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}}) = l(\underline{\boldsymbol{\psi}}) \quad \forall \underline{\boldsymbol{\psi}} \in [H^1(\mathcal{M})]^3 \tag{3}$$

with $\tilde{a}(\underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}}) = a(\underline{\boldsymbol{p}}, \underline{\boldsymbol{\psi}}) + \langle \mathcal{P}(\underline{\boldsymbol{p}}), \underline{\boldsymbol{\psi}} \rangle_{\mathbb{R}^3}$ where $\mathcal{P}$ is an appropriate penalization function, e.g. $\mathcal{P}(\underline{\boldsymbol{p}}) = \omega_t \, (\boldsymbol{\nu} \otimes \boldsymbol{\nu}) \cdot \underline{\boldsymbol{p}}$, with $\omega_t > 0$. The weak formulation reads

$$\begin{aligned}
&\int_{\mathcal{M}} \left(\Pi \cdot [\underline{\nabla}\,\underline{\boldsymbol{p}}]\right) : \left([\underline{\nabla}\,\underline{\boldsymbol{\psi}}] \cdot \Pi\right) + \left(\boldsymbol{B} : [\underline{\nabla}\,\underline{\boldsymbol{p}}]\right) \left(\boldsymbol{\nu} \cdot \underline{\boldsymbol{\psi}}\right) + \left(\boldsymbol{\nu} \cdot \underline{\boldsymbol{p}}\right) \left(\boldsymbol{B} : [\underline{\nabla}\,\underline{\boldsymbol{\psi}}]\right) \, \mathrm{d}\mathcal{M} \\
&+ \int_{\mathcal{M}} \left(\mathcal{H}^2 - 2\mathcal{K}\right) \left(\boldsymbol{\nu} \cdot \underline{\boldsymbol{p}}\right) \left(\boldsymbol{\nu} \cdot \underline{\boldsymbol{\psi}}\right) + \underline{\boldsymbol{p}} \cdot \Pi \cdot \underline{\boldsymbol{\psi}} + \omega_t \left(\underline{\boldsymbol{p}} \cdot \boldsymbol{\nu}\right) \left(\underline{\boldsymbol{\psi}} \cdot \boldsymbol{\nu}\right) \, \mathrm{d}\mathcal{M} \\
&= \int_{\mathcal{M}} \boldsymbol{f} \cdot \Pi \cdot \underline{\boldsymbol{\psi}} \, \mathrm{d}\mathcal{M} \quad \forall \underline{\boldsymbol{\psi}} \in [H^1(\mathcal{M})]^3
\end{aligned}$$

where we have used several geometric identities. The problem is solved on an ellipsoid with major axis $A = 1$, $B = 0.5$ and $C = 1.5$ and $\boldsymbol{f} = -\operatorname{div}(\nabla \boldsymbol{p}^*) + \boldsymbol{p}^*$, with $\boldsymbol{p}^* = \mathrm{Rot}(xyz)$. We consider a surface triangulation $\mathcal{M}_h$ and construct a surface finite element discretization for each component with piecewise linear Lagrange elements. We consider both the analytically available geometric quantities and numerically computed once from the surface triangulation. The resulting linear system is assembled and solved in the finite element toolbox AMDiS [6] using a

BiCGstab(l) solver. As error measure we use a componentwise averaged L^2-norm. Convergence properties regarding the number of degrees of freedom (DOFs) and the strength of the penalty parameter ω_t are shown in figure 1. The results indicate

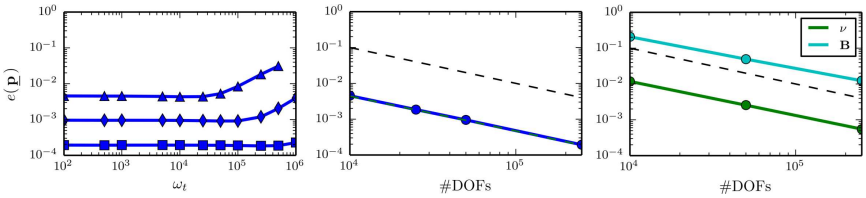

FIGURE 1. L^2 error (left) as function of ω_t, with 10k (triangles), 50k (diamonds) and 250k (squares) DOFs. (middle) with numerically approximated surface quantities (solid) w.r.t. the number of DOFs for fixed $\omega_t = 1000$. Dashed line indicates linear rate of convergence. (right) for numerical approximation of surface quantities w.r.t. the number of DOFs for fixed $\omega_t = 1000$.

almost no dependency on ω_t, which reflects the behavior of the analytical solution, up to values where the penalty term begins to dominate the numerical solution behavior. We further see linear convergence in the geometric properties and also a linear convergence behavior in the considered error, which does not depend on the used approximation of the geometric terms. As the geometry is approximated by a surface triangulation better than linear convergence properties could not be expected, as it is shown to be optimal for a surface finite element approach with piecewise linear Lagrange elements for a scalar-valued surface Laplace problem [1, 7]. Further details on the approach and its extension to general tensor-valued surface PDEs can be found in [8].

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Thermal Effects in General Diffusion: An Energetic Variational Approach

Chun Liu

(joint work with Francesco De Anna, Pei Liu and Hao Wu)

Almost all biological activities involve transport and distribution of ions and charged particles in complicated biological environments. The complicated coupling and competition between different ionic solutions in various biological environments give the intricate specificity and selectivity in these systems. These systems are often associated with complicated, but special biological and chemical conditions, such as the high concentration of specific species in solutions, which make most of the "ideal" assumptions in classical and conventional approaches irrelevant or unsuitable in the studies of biological problems.

In the talk, I will explore the underlying mechanism governing various diffusion processes [4]. We will employ a general framework of energetic variational approaches, consisting of, in particular, Onsager's Maximum Dissipation Principles [1, 2, 3], and their specific applications in biology and physiology [5]. I will discuss several extended general diffusion systems motivated by the study of ion channels and ionic solutions in biological cells. In particular, I will focus on our recent results in studying the interactions between different species, the boundary effects [8] and in some cases, the thermal effects [6, 7].

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A diffuse interface model for the patient specific evolution of Glioblastoma Multiforme.

Abramo Agosti
(joint work with Pasquale Ciarletta and Maurizio Grasselli)

This presentation concerns the study of diffuse-interface models based on mixture theory to describe tumor growth dynamics. In particular, using thermodynamic principles, a Cahn-Hilliard type equation with degenerate mobility is derived, coupled with nutrient diffusion, chemotaxis, proliferation and apoptosis dynamics. A single-well potential of Lennard-Jones type is used in this model to describe the cell-cell and cell-matrix mechanical interactions. This model was recently used to describe the patient-specific evolution of a highly malignant brain tumour, the glioblastoma multiforme (GBM).

We have derived some analytical results regarding the existence of different classes of weak solutions of the model for the cases of spatial dimension $d = 1$ and $d = 2, 3$ separately. In particular, energy estimates ensure the separation property from the pure phase corresponding to the singularity of the potential almost everywhere in spacetime, whereas entropy estimates ensure the positivity property of the solution almost everywhere in spacetime. The solution can be equal to zero on sets with positive measure. The existence of compactly supported solutions makes the problem ill-posed, since on the free boundary of their support no sufficient boundary conditions for well-posedness are specified, and the presence of both solutions with a moving support with finite speed of velocity and of solutions with fixed support characterizes the non-uniqueness for solutions of the model.

We have studied the well-posedness and the convergence of different finite element approximations of the problem which preserve the analytical properties of the continuous solutions. The discrete schemes are formulated in order to ensure the mass conservation (in the absence of nutrients), gradient stability, the separation and positivity properties of the discrete solution, and the selection of the physical solutions with compact support and moving boundary from the ones with fixed support.

Numerical simulations have been investigated on real brain geometries, in which the preferential directions of the chemotactic movement along white matter fiber tracts are defined by proper anisotropic diffusion and chemotactic tensors. These tensors are obtained by elaborating patient-specific Diffusion Tensor Imaging (DTI) data.

In this talk I will compare the observed in-vitro evolution of a culture of glioblastoma cells to the growth and coarsening dynamics described by the model. Moreover, feding the model by clinical neuroimaging data that provide the anatomical and microstructural characteristics of a patient brain, I will show its predictive ability by comparing the results of numerical simulations with the clinical data from one patient collected at given times of key clinical interest, from the first diagnosis of glioblastoma to its surgical removal and the subsequent radiation therapies.

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A bulk-surface obstacle type problem as a model for polarized cells

Matthias Röger

(joint work with Barabara Niethammer and Juan Velázquez)

The polarization of a biological cell, for example characterized by a heterogenous distribution of certain proteins, is key to many functions. We study here a simple polarization module with two types of a certain protein on the cell surface, which are either in an active or in an inactive state. We denote the first surface concentration as u and the second as v. Furthermore, the inactive proteins can move to the interior of the cell and vice versa, we denote the corresponding concentration by w. We are interested in the response to a given signal, in the form of a concentration c of a certain chemical messenger on the surface.

This setup leads to a system of bulk diffusion and surface reaction–diffusion equations. The coupling is via a Robin-type boundary condition for w and a source term in the v equation. To give a more precise formulation let a open, bounded set $\Omega \subset \mathbb{R}^3$ with smooth boundary $\Gamma := \partial\Omega$ describe the cell interior and cell surface. We then consider the following system.

$$\partial_t u = \Delta u + cv - \frac{a_4 u}{1+u} \qquad \text{on } \Gamma \times (0,T) \tag{1}$$

$$\partial_t v = \Delta v - cv + \frac{a_4 u}{1+u} - a_5 v + a_6 w \qquad \text{on } \Gamma \times (0,T) \tag{2}$$

$$\partial_t w = D\Delta w \qquad \text{in } \Omega \times (0,T) \tag{3}$$

$$-D\frac{\partial w}{\partial n} = -a_5 v + a_6 w \qquad \text{on } \Gamma \times (0,T). \tag{4}$$

For the parameters we assume $a_3, a_4, a_5, a_6 > 0$, $D \geq 1$ and for the messenger concentration that $c\colon \Gamma \to \mathbb{R}_+$ is continuous and strictly positive. With some abuse of notation Δu and Δv denote the Laplace-Beltrami operator on the surface Γ, while Δw is the usual Laplacian.

Solutions satisfy the mass conservation property

$$\int_\Omega w(x,t)\,dx + \int_\Gamma (u(y,t)+v(y,t))\,d\mathcal{H}^2(y) \;=\; M \qquad \text{for all } t \geq 0.$$

Our goal is to study for given $c = c(x)$ stationary states of (1)-(4) in certain parameter regimes and to examine when polarization patterns appear.

Our main results then concern the following rescaled stationary system

$$0 = \Delta u_\varepsilon + c v_\varepsilon - \frac{a_4 u_\varepsilon}{\varepsilon + u_\varepsilon} \qquad \text{on } \partial\Omega \times (0,T) \tag{5}$$

$$0 = \varepsilon \Delta v_\varepsilon - c v_\varepsilon + \frac{a_4 u_\varepsilon}{\varepsilon + u_\varepsilon} - a_5 v_\varepsilon + a_6 w_\varepsilon \qquad \text{on } \partial\Omega \times (0,T) \tag{6}$$

$$0 = D\Delta w_\varepsilon \qquad \text{in } \Omega \times (0,T) \tag{7}$$

$$-D\frac{\partial w_\varepsilon}{\partial n} = -a_5 v_\varepsilon + a_6 w_\varepsilon \qquad \text{on } \partial\Omega \times (0,T), \tag{8}$$

with the property

$$\int_\Gamma (u_\varepsilon + \varepsilon v_\varepsilon) + \int_B \varepsilon w_\varepsilon = m.$$

From a mathematical point of view, the most remarkable feature is the convergence to a generalized obstacle problem. Responsible for this feature is the presence of the Michaelis-Menten reaction term, see [1] for a corresponding result for a standard reaction–diffusion system.

Theorem. *Consider a sequence $(w_\varepsilon, u_\varepsilon, v_\varepsilon)$ of solutions to (5)-(8) with total mass m. Then there exists a subsequence $\varepsilon \to 0$ and nonnegative functions (w,u,v) such that*

$$u_\varepsilon \rightharpoonup u \quad \text{in } H^2(\Gamma), \qquad v_\varepsilon \rightharpoonup v \quad \text{in } L^2(\Gamma), \qquad w_\varepsilon \rightharpoonup w \quad \text{in } H^1(\Omega).$$

Moreover there exists $\xi \in L^\infty(\Gamma)$ with $0 \leq \xi \leq 1$ such that

$$0 = \Delta u + cv - a_4\xi \qquad \text{on } \Gamma, \tag{9}$$

$$0 = -cv + a_4\xi - a_5 v + a_6 w \qquad \text{on } \Gamma, \tag{10}$$

$$0 = D\Delta w \qquad \text{in } \Omega, \tag{11}$$

$$-D\frac{\partial w}{\partial n} = -a_5 v + a_6 w \qquad \text{on } \Gamma \tag{12}$$

and such that $u\xi = u$ and $\int_\Gamma u = m$ hold. Moreover, w, u and v are all nonnegative, $u \in W^{2,p}(\Gamma)$ for any $1 \leq p < \infty$, $w \in C^\infty(\Omega) \cap C^0(\overline{\Omega})$, and $v \in L^\infty(\Gamma)$.

We can give a rather precise analysis of the polarization property of the model in two cases: first the infinite cytosolic diffusion limit $D \to \infty$ and second the case of spherical shell shape, i.e. $\Omega = B(0,1)$. Let us restrict ourselves in the following to the second case. We then can reformulate the problem (9)-(12) as a generalized obstacle problem that involves the Dirichlet to Neumann operator N.

Proposition. *Let* $\ell = \frac{a_6}{D}$ *and define*

$$g(x) = \frac{c(x)}{c(x) + a_5} \in (0,1)\,, \qquad x \in \Gamma\,.$$

Then (u, v, w, ξ) *satisfies* (9)-(12) *if and only if* (u, ξ, α), $\alpha \in \mathbb{R}$, *is a solution of*

$$0 = \Delta u - a_4(1-g)\xi + \alpha g - g\ell\big(N(u) + u - \bar{u}\big)\,, \qquad u \geq 0\,, \tag{13}$$

$$u\xi = u \text{ almost everywhere on } \Gamma\,, \qquad 0 \leq \xi \leq 1, \tag{14}$$

and if

$$w = \frac{1}{a_6}\Big(\alpha - \ell\big(N(u) + u - \bar{u}\big)\Big), \qquad v = \frac{1}{a_5}(1-g)(a_6 w + a_4 \xi).$$

Observe that we obtain by integration over Γ that

$$\alpha = \frac{1}{\int_\Gamma g} \int_\Gamma \Big(a_4(1-g)\xi + \ell g\big(N(u) + u - \bar{u}\big)\Big).$$

We finally turn to a characterization of polarization in terms of the limit problem. We therefore characterize a concentration u as a polarized state if both the set $\{u = 0\}$ and the set $\{u > 0\}$ have positive measure. The final outcome of our analysis is a threshold for the occurrence of polarized states in terms of a certain critical mass. To identify this value we first prove that there exists a unique value α_* for which

$$0 = \Delta u - a_4(1-g) + \alpha_* g - g\ell\big(N(u) + u - \bar{u}\big)$$

can be solved. Moreover, there exists a unique solution u_* with

$$\min_\Gamma u_* = 0.$$

We then define the critical mass as

$$m_* := \int_\Gamma u_*.$$

The following theorem now characterizes the onset of polarized states.

Theorem. *For* $m > 0$ *consider the solution* (u, ξ, α) *of* (13), (14). *If* $m > m_*$ *we have that* $u > 0$ *in* Γ *and* $\alpha = \alpha_*$. *Moreover* $u = u_* + (m - m_*)|\Gamma|$. *If* $m < m_*$ *we have* $|\{u = 0\}| > 0$ *and* $\alpha < \alpha_*$.

For details and additional results for a slightly extended system we refer to our forthcoming work [2].

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On a surface finite element method for cell blebbing

Björn Stinner
(joint work with Adam Nixon and Andreas Dedner)

In some environments, cells resort to the formation of blebs at the front end in order to migrate. These are spherical protrusions of the cell's membrane, which detaches from the cortex. Subsequently, the cortex is disintegrated and reformed at the membrane, followed by a retraction stage that can be exploited by the cell to alter its position.

In this study, the focus is on the detachment. It is motivated by the results in [2], which is based on the computational approach in [8]. There, a chain of springs models the membrane in 2D. Its movement is governed by a force balance accounting for the effects of pressure within the cell, the membrane's elastic properties (tension and bending resistance), the linker molecules (also modelled as elastic springs), and a drag force due to the viscous environment. Computational results then are compared with image data to validate the model and quantify parameters.

Given these findings, the objectives of this investigation have been

- to extend the membrane model to surfaces in 3D and the derivation of an abstract continuum model in variational form that allows for some flexibility in the definitions of the forces,
- to develop a robust and efficient numerical method, for which we chose triangulated surfaces and surface finite elements,
- and to provide software that enables a convenient access to the numerical method in the sense that steering in data, changing parameters, but also amending definitions of forces is convenient.

The membrane is modelled as an evolving surface. It is parametrised over the initial surface by a field $\boldsymbol{u} : \Gamma^0 \times [0,T) \to \mathbb{R}^3$, in which the forces are expressed. Specific choices lead to the surface partial differential equation

$$\begin{aligned}\omega\partial_t \boldsymbol{u} = &- k_b \Delta_{\Gamma^0}^2 \boldsymbol{u} + k_\psi \nabla_{\Gamma^0} \cdot \Big(\nabla_{\Gamma^0} \boldsymbol{u} - x_0 \frac{\nabla_{\Gamma^0} \boldsymbol{u}}{|\nabla_{\Gamma^0} \boldsymbol{u}|} \Big) \\ &- k(|\boldsymbol{u} - \boldsymbol{u}_c|) \Big((\boldsymbol{u} - \boldsymbol{u}_c) - l_0 \frac{\boldsymbol{u} - \boldsymbol{u}_c}{|\boldsymbol{u} - \boldsymbol{u}_c|} \Big) + \frac{p^0}{V^0} \boldsymbol{\nu}\end{aligned}$$

where $\omega, k_b, k_\psi, x_0, l_0, p^0, V^0$ are positive material parameters, $\boldsymbol{u}_c$ is a field on Γ^0 modelling the position of the cortex, and $\boldsymbol{\nu}$ is the external unit normal. The function $k(|\boldsymbol{u}-\boldsymbol{u}_c|)$ models the breakage of linker molecules when stretched beyond a given length. A restriction of this model to two spatial dimensions followed by a discretisation with standard finite difference stencils yields the model in [8].

An abstract variational problem is derived using operator splitting for the fourth order term. Introducing $\boldsymbol{w} = -\Delta_{\Gamma^0} \boldsymbol{u}$ the problem reads: Find $\boldsymbol{u}, \boldsymbol{w} \in L^2(0,T; H^1(\Gamma^0))$ with $\partial_t \boldsymbol{u} \in L^2(0,T; L^2(\Gamma^0))$ such that for all $\boldsymbol{\phi}, \boldsymbol{\eta} \in H^1(\Gamma^0)$ and

almost all $t \in (0,T)$

$$m(\partial_t \boldsymbol{u}, \boldsymbol{\phi}) + s(id; \boldsymbol{w}, \boldsymbol{\phi}) + s(\psi'; \boldsymbol{u}, \boldsymbol{\phi}) + m(\boldsymbol{k}(\boldsymbol{u}), \boldsymbol{\phi}) = 0,$$
$$s(\boldsymbol{u}, \boldsymbol{\eta}) - m(\boldsymbol{w}, \boldsymbol{\eta}) = 0,$$

where

$$s(\boldsymbol{A}; \boldsymbol{x}, \boldsymbol{y}) := \int_\Gamma^0 \boldsymbol{A}(\nabla_{\Gamma^0} \boldsymbol{x}) : \nabla_{\Gamma^0} \boldsymbol{y} d\sigma, \qquad m(\boldsymbol{b}(\boldsymbol{x}), \boldsymbol{y}) := \int_\Gamma^0 \boldsymbol{b}(\boldsymbol{x}) \cdot \boldsymbol{y} d\sigma.$$

Here, $\psi : \Gamma^0 \times \mathbb{R}^{3\times 3} \to [0,\infty)$ is assumed bounded and measurable in the first and continuously differentiable in the second argument with Lipschitz partial derivative,

$$|\psi'(\boldsymbol{x}, \boldsymbol{A}) - \psi'(\boldsymbol{x}, \boldsymbol{B})| \le C_\psi |\boldsymbol{A} - \boldsymbol{B}| \quad \forall \boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{3\times 3},\ \boldsymbol{x} \in \Gamma^0.$$

The field $\boldsymbol{k} : \Gamma^0 \times \mathbb{R}^3 \to \mathbb{R}^3$ is assumed bounded and measurable in the first and Lipschitz in the second argument,

$$|\boldsymbol{k}(\boldsymbol{x}, \boldsymbol{a}) - \boldsymbol{k}(\boldsymbol{x}, \boldsymbol{b})| \le C_k |\boldsymbol{a} - \boldsymbol{b}| \quad \forall \boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3,\ \boldsymbol{x} \in \Gamma^0.$$

For the discretisation we assume an approximation of Γ^0 by a h-family of triangulated surfaces

$$\Gamma_h^0 = \bigcup_{T \in \mathcal{T}_h} T$$

interpolating Γ^0, on which we consider the finite element spaces

$$S_h := \Big\{ \phi_h \in C^0(\Gamma_h^0) \,\Big|\, \phi_h|_T \text{ linear } \forall T \in \mathcal{T}_h \Big\}.$$

In practice, data such as the cortex position $\boldsymbol{u}_c$ usually are only approximately known. We assume that, quantitatively, this uncertainty is similar to the uncertainty of the initial membrane position. In the abstract context we thus assume that the $\boldsymbol{k}$ is approximated by a function $\boldsymbol{k}_h$, which is Lipschitz with the same constant C_k. Moreover, we assume that the approximation is consistent, i.e., there is a constant $C > 0$ such that for all h and all $\boldsymbol{a} \in \mathbb{R}$

$$\|\boldsymbol{k}(\cdot, \boldsymbol{a}) - \boldsymbol{k}_h(\cdot, \boldsymbol{a})\|_{L^\infty(\Gamma^0)} \le C(1 + |\boldsymbol{a}|)h. \tag{1}$$

Similarly, an approximation of ψ by some ψ_h can be handled.

A semi-discrete problem is obtained in a straightforward way by replacing the surface and test and trial functions in the abstract problem with finite element versions. We can show the following result:

Theorem. The semi-discrete problems are well-posed.
Their solutions $(\boldsymbol{u}_h, \boldsymbol{w}_h)$ converge to some functions $(\boldsymbol{u}, \boldsymbol{w})$ as $h \to 0$ that uniquely solve the abstract variational problem and satisfy

$$\|\boldsymbol{u}\|^2_{L^\infty(H^1(\Gamma^0))} + \|\boldsymbol{w}\|^2_{L^2(H^1(\Gamma^0))} \le C.$$

If $\boldsymbol{u}, \partial_t \boldsymbol{u}, \boldsymbol{w} \in L^2_{H^2}$ then

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|^2_{L^\infty_{L^2}} + \|\boldsymbol{w} - \boldsymbol{w}_h\|^2_{L^2_{L^2}} + \|\nabla_{\Gamma^0}(\boldsymbol{u} - \boldsymbol{u}_h)\|^2_{L^2_{L^2}} \le Ch^2.$$

Some comments on the proof:

- For the general procedure, we can follow the lines of [7], which treats the Cahn-Hilliard equation including the operator splitting. In particular, suitable a priori estimates are obtained this way.
- The approximation of the surface has been analysed in [6] and subsequent work. Here, an additional variational crime consists of the data approximation (e.g., $\boldsymbol{k}$ by $\boldsymbol{k}_h$). But its treatment is relatively straightforward thanks to the consistency assumption (1).
- The nonlinearity in the gradient required some more significant investigation. Strong convergence of the gradient turns out to be sufficient. It can be obtained exploiting the linearity of the problem in the fourth order term and a suitable Ritz-projection [6].

A couple of numerical tests confirm the convergence result. Some remarks on the software:

- The Unified Form Language (UFL) [1] provides a convenient way to formulate variational problems. It is implemented in `python`, and also parameters can be set and data such as the initial mesh can be steered in with relative ease.
- The variational problem formulation is translated into some `C++` code, which then binds to the `DUNE` software [4] as a backend. In particular, the functionality of the software backend is made available in python.
- For further details we refer to [5] with regards to the `python` interface to `DUNE`, and to [3] for the `UFL` bindings.

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The Plate Equation on Curved Domains and Surfaces

Shawn W. Walker
(joint work with Douglas N. Arnold)

The classic HHJ method has been analyzed from various viewpoints in several papers [5, 7, 6, 2, 1, 8, 4, 12], with some recent results [10, 11] on decompositions of the HHJ method.

To the best of our knowledge, no analysis has been done for HHJ on curved, parametric elements which is needed to ensure optimal order of the HHJ method on curved domains. Indeed, curved elements allow for more accurate approximation of boundary conditions. This paper provides a convergence analysis for curved HHJ elements for solving a non-conforming formulation of the Kirchhoff plate equation; optimal convergence is obtained when appropriate order curved elements are used near the piecewise C^{k+1} boundary for $k \geq 1$. Moreover, we demonstrate that the lowest order HHJ scheme on a polygonal approximation of the disk converges with optimal order despite the well-known Babuska paradox [3].

Our analysis follows the framework of [2] and [4], where we use mesh-dependent norms in a non-conforming formulation of the Kirchhoff plate problem. A highlight of the analysis in [7, 2, 4] is the use of convenient Fortin-like interpolation operators. The main issues to address in the curved element setting are: (i) extending the Fortin-like operators to the curved element setting (in an appropriate sense); (ii) analyzing the geometric error in the domain approximation; (iii) proving a new kind of Poincaré inequality in the mesh dependent norms for thin domains to avoid sub-optimal convergence results; and (iv) approximation of the variety of boundary conditions that occur in plate problems. The results we present here should be of relevance to simulating plate problems on curved domains (in general).

We also illustrate how one can use the HHJ method to solve an *abstract manifold version* of the Kirchoff plate problem. For instance, the standard Kirchhoff plate model is as follows. Denote the scalar displacement by w, let $\mathcal{S}^2$ be the set of symmetric 2×2 tensors, and define the symmetric bending moment $[\sigma^{\alpha\beta}]_{\alpha,\beta=1}^2 \equiv \boldsymbol{\sigma} \in \mathcal{S}^2$ as

$$\sigma^{\alpha\beta}(w) := C^{\alpha\beta\mu\rho}\partial_\mu\partial_\rho w = D\left[(1-\nu)\delta^{\alpha\mu}\delta^{\beta\rho}\partial_\mu\partial_\rho w + \nu\delta^{\alpha\beta}(\partial_\gamma\partial_\gamma w)\right], \tag{1}$$

where $D = E/(1-\nu^2) > 0$ is the bending modulus (E is the Young's modulus), and $\nu \in (-1, 1)$ is Poisson's ratio. Note that $C^{\alpha\beta\mu\rho}$ (and its inverse) can be written as

$$C^{\alpha\beta\mu\rho} = 2\bar{\mu}\delta^{\alpha\mu}\delta^{\beta\rho} + \bar{\lambda}\delta^{\alpha\beta}\delta^{\mu\rho}, \qquad K_{\gamma\omega\alpha\beta} = \frac{1}{2\bar{\mu}}\delta_{\gamma\alpha}\delta_{\omega\beta} - \frac{\nu}{E}\delta_{\gamma\omega}\delta_{\alpha\beta}, \tag{2}$$

where $\delta^{\beta\rho}$, $\delta_{\gamma\alpha}$ are the standard "Kronecker delta."

Moreover, we assume that $\Theta := \partial U$ partitions into four mutually disjoint components Θ_{c} (clamped), Θ_{s} (simply supported), Θ_{f} (free), and Θ_{a} (alternate) which

indicate the boundary conditions to impose on Θ, namely:

(3)
$$w = 0, \text{ on } \Theta_c \cup \Theta_s, \qquad \mathbf{n} \cdot \nabla w = 0, \text{ on } \Theta_c \cup \Theta_a, \qquad \mathbf{n}^\dagger \boldsymbol{\sigma} \mathbf{n} = 0, \text{ on } \Theta_s \cup \Theta_f,$$
$$n_\alpha(\partial_\beta \sigma^{\alpha\beta}) + \boldsymbol{t} \cdot \nabla \left(\mathbf{n}^\dagger \boldsymbol{\sigma} \boldsymbol{t}\right) = 0, \text{ on } \Theta_f \cup \Theta_a,$$

where $\mathbf{n}$ is the (covariant) outer unit normal vector on Θ, $\boldsymbol{t}$ is the (contravariant) positively oriented unit tangent vector on Θ. The strong form of the Kirchoff plate equation is then

$$\partial_\alpha \partial_\beta \sigma^{\alpha\beta} = f, \quad \text{on } U, \tag{4}$$

with load f and boundary conditions given by (3).

The *manifold* version of the plate problem introduces a Riemannian metric $g_{\mathfrak{ab}} \equiv \boldsymbol{g}$ on $U \subset \mathbb{R}^2$. Moreover, we replace partial derivatives by *covariant* derivatives, and $\boldsymbol{\sigma}$ is viewed as a *contravariant* tensor:

$$\sigma^{\alpha\beta} := C^{\alpha\beta\mu\rho} \nabla_\mu \nabla_\rho w = D\left[(1-\nu)\nabla^\alpha \nabla^\beta w + \nu g^{\alpha\beta}(\nabla_\gamma \nabla^\gamma w)\right], \tag{5}$$

where we use the inverse metric $g^{\mathfrak{ab}} \equiv \boldsymbol{g}^{-1}$. The elasticity tensor (and its inverse) takes the form

$$C^{\alpha\beta\mu\rho} = 2\bar{\mu} g^{\alpha\mu} g^{\beta\rho} + \bar{\lambda} g^{\alpha\beta} g^{\mu\rho}, \qquad K_{\gamma\omega\alpha\beta} = \frac{1}{2\bar{\mu}} g_{\gamma\alpha} g_{\omega\beta} - \frac{\nu}{E} g_{\gamma\omega} g_{\alpha\beta}, \tag{6}$$

where the metric clearly appears.

Furthermore, this leads to solving the plate problem on a *parametrized surface*. The *surface version* is obtained by taking the metric as being induced by a parametrization $\boldsymbol{\Phi}$. In addition, the variables are expressed in an extrinsic way. For example, the symmetric (covariant) Hessian becomes the *surface Hessian* given by:

$$\operatorname{hess}_\Gamma w = (\partial_\alpha \boldsymbol{\Phi}) g^{\alpha\beta} (\nabla_\beta \nabla_\gamma w) g^{\gamma\mu} (\partial_\mu \boldsymbol{\Phi})^\dagger, \tag{7}$$

where $\Gamma \subset \mathbb{R}^3$ is a smooth embedded surface, and $\boldsymbol{\Phi}$ is the parametrization of Γ. Hence, HHJ (originally meant for solving the Kirchoff plate problem on a domain in $\mathbb{R}^2$) gives a method for solving 4th order problems on surfaces (the surface biharmonic equation is a specific example).

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On the flow of elastic networks

Paola Pozzi
(joint work with Anna Dall'Acqua and Chun-Chi Lin)

Networks arise naturally in the study of multiphase systems and the dynamics of their interfaces. The study of planar networks moving according to curve shortening flow (a second order flow) has been thoroughly investigated in recent years (see for instance the survey paper [1]). Much less is known when the evolution is elastic (a fourth order flow).

We provide a long-time existence result for the elastic flow of a three-network, a triod, in $\mathbb{R}^n$, see [2]. A triod $\Gamma = \{f_1, f_2, f_3\}$ is given by the union of three regular smooth curves parametrized by maps $f_i : [0,1] \to \mathbb{R}^n$, $i = 1,2,3$, such that they share the same origin in the point $f_1(0) = f_2(0) = f_3(0)$ (a so called concurrency point, that will be allowed to move in time) and end in some given fixed distinct points P_i, $i = 1,2,3$, that is $f_j(1) = P_j$ for $j = 1,2,3$. A typical example is given by the well-known Mercedez-Benz symbol. Since the curves f_i are immersed and self-intersection might occur, more interesting configurations are of course allowed.

The energy associated to the network Γ (and that will be decreased along the flow) is given by

$$\mathcal{E}(\Gamma) = \sum_{i=1}^{3} \left(\int_I |\vec{\kappa}_i|^2 ds_i + \lambda_i \int_I ds_i \right)$$

where $I = (0,1)$, $ds_i = |\partial_x f_i| dx$ denotes the arc-length element and $\vec{\kappa}_i$ the curvature vector of each curve f_i. The parameters $\lambda_i \geq 0$ are given fixed constants and induce a penalization of the growth of the length of the given curve when strictly positive.

An L^2-gradient flow of the above energy induces the following geometric problem (P): Find $f_i : [0,T) \times I \to \mathbb{R}^n$, $i = 1,2,3$, such that

$$\partial_t f_i - \langle \partial_t f_i, \partial_s f_i \rangle \partial_s f_i = -\nabla_s^2 \vec{\kappa}_i - \frac{1}{2} |\vec{\kappa}_i|^2 \vec{\kappa}_i + \lambda_i \vec{\kappa}_i \text{ on } (0,T) \times I \text{ for } i = 1,2,3,$$

with boundary conditions

$$\begin{cases} f_i(t,1) = P_i, & \text{for all } t \in (0,T), i = 1,2,3, \\ \vec{\kappa}_i(t,1) = 0 = \vec{\kappa}_i(t,0) & \text{for all } t \in (0,T),\ i = 1,2,3, \\ f_1(t,0) = f_2(t,0) = f_3(t,0) & \text{for all } t \in (0,T), \\ \quad \text{and } \sum_{i=1}^{3} (\nabla_s \vec{\kappa}_i(t,0) - \lambda_i \partial_s f_i(t,0)) = 0 & \text{for all } t \in (0,T), \end{cases}$$

and initial value

$$\Gamma(t=0) = \{f_1(0,\cdot), f_2(0,\cdot), f_3(0,\cdot)\} = \Gamma_0, \text{ in } I.$$

Note that the boundary conditions are natural in the sense of calculus of variations. Also, for each curve f_i and a given vector field $\phi : I \to \mathbb{R}^n$ we denote by $\nabla_s \phi := \partial_s \phi - \langle \partial_s \phi, \partial_s f_i \rangle \partial_s f_i$ the normal component of the derivative with respect to arc-length (and for simplicity of notation we write s instead of s_i).

We remark that the triple junction is allowed to move in time and that, unlike the network flow by mean curvature, there is no prescription of angles at the junction.

It turns out that for the evolution of the network, we need to have some control over the following conditions:

> A) the length of each curve f_i, $i = 1,2,3$, is bounded away from zero,
> B) at the triple junction, at least two unit tangents $\partial_s f_i$ and $\partial_s f_j$ form a positive angle.

Our result, whose proof is given in [2], can be summarized as follows: provided the initial network Γ_0 of smooth regular curves fulfills the necessary boundary and compatibility conditions, and provided the network $\Gamma(t)$ satisfies A) and B) on any compact time interval $[0,T]$, then our problem (P) admits an eternal smooth solution.

The overall proof strategy is similar to many other results on long-time existence for the elastic flow of a single open curve with fixed boundary points (see for instance [3] and reference in there). Starting from a short-time existence result and assuming that the maximal existence time T is finite, uniform estimates for the curvatures and their derivatives are derived so that the flow can be extended up to the maximal time. A contradiction is achieved by restarting the flow at time T.

The main difficulties arising when dealing with networks lie in the treatment of the boundary conditions and the choice of tangential components. Note that for the formulation of the geometric problem, tangential components do not play a role, but when the problem is tackled analytically they do. Also, unlike the evolution of a single curve, some choice of non-zero tangential component is necessary in order to allow the triple junction to freely move in space. A thorough discussion of these issues and how they are overcome is given in [2].

Finally, note that the problem presented here has been treated recently with other techniques in [4].

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Singular limit problem for the Navier–Stokes equations in a curved thin domain

Tatsu-Hiko Miura

A thin domain is a domain with very small width in one or several directions. Fluid flows in thin domains frequently appear in problems of natural sciences like the ocean and atmosphere dynamics. In the study of the Navier–Stokes equations in a three-dimensional thin domain we naturally expect to get the global-in-time existence of a strong solution for large data depending on the smallness of the width of the domain since a thin domain with very small width can be seen as almost two-dimensional. We are also interested in the behavior of a solution to the bulk Navier–Stokes equations in a thin domain as the thickness of the domain tends to zero. When a thin domain degenerates into a lower dimensional set, it is important to find limit equations on the limit set and compare the bulk and limit equations to understand the effects of the thin direction and the limit set on the original problem in the thin domain.

Raugel and Sell [2] first studied such problems for the Navier–Stokes equations in a flat product thin domain $\Omega_\varepsilon = Q \times (0, \varepsilon)$ with a rectangle Q and a sufficiently small $\varepsilon > 0$. Since then many researchers have studied the Navier–Stokes equations with various boundary conditions in a flat thin domain of the form

$$\Omega_\varepsilon = \{x = (x', x_3) \in \mathbb{R}^3 \mid x' \in \omega,\, x_3 \in (\varepsilon g_0(x'), \varepsilon g_1(x'))\}$$

with a two-dimensional domain ω and functions g_0 and g_1 on ω (see e.g. [3, 4, 13]). Also, Temam and Ziane [14] considered the case of a thin spherical shell

$$\Omega_\varepsilon = \{x \in \mathbb{R}^3 \mid a < |x| < a + \varepsilon a\}, \quad a > 0$$

to give a mathematical justification of derivation of the primitive equations for the ocean and atmosphere (see [5, 6]). However, there is no result on the Navier–Stokes equations in a curved thin domain around a general closed surface since the shapes of the thin domain and its limit surface make analysis of vector fields on the curved thin domain very difficult (we refer to [11] for the study of a reaction-diffusion equation in a curved thin domain around a lower dimensional manifold).

In the recent work [9] we studied the Navier–Stokes equations in a curved thin domain to investigate the effects of the shapes of the thin domain and its limit surface and to provide mathematical tools for analysis of vector fields on the curved

thin domain. Let Γ be a closed (i.e. compact and without boundary), connected, oriented, and smooth surface in $\mathbb{R}^3$ with unit outward normal vector field n and g_0 and g_1 smooth functions on Γ satisfying $g := g_1 - g_0 \geq c$ on Γ with a constant $c > 0$. For a sufficiently small $\varepsilon > 0$ we define a curved thin domain in $\mathbb{R}^3$ by

$$\Omega_\varepsilon := \{y + rn(y) \mid y \in \Gamma,\, r \in (\varepsilon g_0(y), \varepsilon g_1(y))\}$$

and consider the Navier–Stokes equations with Navier's slip boundary conditions

$$\text{(1)} \qquad \begin{cases} \partial_t u^\varepsilon + (u^\varepsilon \cdot \nabla)u^\varepsilon - \nu\Delta u^\varepsilon + \nabla p^\varepsilon = f^\varepsilon & \text{in} \quad \Omega_\varepsilon \times (0,\infty), \\ \operatorname{div} u^\varepsilon = 0 & \text{in} \quad \Omega_\varepsilon \times (0,\infty), \\ u^\varepsilon \cdot n_\varepsilon = 0 & \text{on} \quad \Gamma_\varepsilon \times (0,\infty), \\ 2\nu P_\varepsilon D(u^\varepsilon) n_\varepsilon + \gamma_\varepsilon u^\varepsilon = 0 & \text{on} \quad \Gamma_\varepsilon \times (0,\infty), \\ u^\varepsilon|_{t=0} = u_0^\varepsilon & \text{in} \quad \Omega_\varepsilon. \end{cases}$$

Here Γ_ε is the boundary of Ω_ε that is the union of the inner and outer boundaries Γ_ε^0 and Γ_ε^1 given by $\Gamma_\varepsilon^i := \{y + \varepsilon g_i(y) n(y) \mid y \in \Gamma\}$, $i = 0, 1$ and n_ε is the unit outward normal vector field of Γ_ε. Also, $\nu > 0$ is the viscosity coefficient independent of ε, $\gamma_\varepsilon \geq 0$ is the friction coefficient given by $\gamma_\varepsilon := \gamma_\varepsilon^i$ on Γ_ε^i, $i = 0, 1$ with γ_ε^0 and γ_ε^1 nonnegative constants depending on ε, and

$$P_\varepsilon := I_3 - n_\varepsilon \otimes n_\varepsilon, \quad D(u^\varepsilon) := \frac{\nabla u^\varepsilon + (\nabla u^\varepsilon)^T}{2}$$

are the orthogonal projection onto the tangent plane of Γ_ε and the strain rate tensor, where I_3 is the 3×3 identity matrix and $n_\varepsilon \otimes n_\varepsilon$ is the tensor product of n_ε with itself. Under suitable assumptions we established in [9] the global existence of a strong solution to (1) for large data $\|u_0^\varepsilon\|_{H^1(\Omega_\varepsilon)}, \|f^\varepsilon\|_{L^\infty(0,\infty;L^2(\Omega_\varepsilon))} = O(\varepsilon^{-1/2})$ as in the previous works [2, 3, 4, 13] on flat thin domains. Moreover, we proved that the tangential component of the average in the thin direction

$$M_\tau u^\varepsilon(y) := \frac{1}{\varepsilon g(y)} \int_{\varepsilon g_0(y)}^{\varepsilon g_1(y)} P(y) u^\varepsilon(y + rn(y))\, dr, \quad y \in \Gamma \quad (P := I_3 - n \otimes n)$$

of a strong solution u^ε to (1) converges weakly in appropriate function spaces on Γ as $\varepsilon \to 0$ and characterized the weak limit as a unique weak solution to

$$\text{(2)} \quad g\Big(\partial_t v + \overline{\nabla}_v v\Big) - 2\nu \left\{ P \operatorname{div}_\Gamma [g D_\Gamma(v)] - \frac{1}{g}(\nabla_\Gamma g \otimes \nabla_\Gamma g) v \right\} + (\gamma^0 + \gamma^1) v + g \nabla_\Gamma q = gf \quad \text{on} \quad \Gamma \times (0,\infty)$$

and

$$\text{(3)} \qquad \operatorname{div}_\Gamma(gv) = 0 \quad \text{on} \quad \Gamma \times (0,\infty), \quad v|_{t=0} = v_0 \quad \text{on} \quad \Gamma.$$

Here ∇_Γ and $\operatorname{div}_\Gamma$ are the tangential gradient and surface divergence on Γ, $\overline{\nabla}_v v$ is the covariant derivative of v along itself, γ^0 and γ^1 are nonnegative constants corresponding to the limits of $\varepsilon^{-1}\gamma_\varepsilon^0$ and $\varepsilon^{-1}\gamma_\varepsilon^1$ as $\varepsilon \to 0$, and

$$D_\Gamma(v) := P \left(\frac{\nabla_\Gamma v + (\nabla_\Gamma v)^T}{2} \right) P$$

is the surface strain rate tensor. We also derived estimates for the difference between solutions to (1) and (2)–(3) and established strong convergence results.

When $g \equiv 1$ and $\gamma^0 = \gamma^1 = 0$ our limit equations (2)–(3) are of the form

$$\partial_t v + \overline{\nabla}_v v - 2\nu P \mathrm{div}_\Gamma[D_\Gamma(v)] + \nabla_\Gamma q = f, \quad \mathrm{div}_\Gamma v = 0 \quad \text{on} \quad \Gamma \times (0,\infty). \tag{4}$$

It is shown in [8, Lemma 2.5] that $2P\mathrm{div}_\Gamma[D_\Gamma(v)] = \Delta_B v + Kv$ on Γ for a tangential and surface divergence-free vector field v on Γ, where Δ_B and K are the Bochner Laplacian on Γ and the Gaussian curvature of Γ. Also, since Γ is two-dimensional, K agrees with the Ricci curvature Ric of Γ, i.e. $Kv = \mathrm{Ric}(v)$ for a tangential vector field v on Γ. Hence the equations (4) read

$$\partial_t v + \overline{\nabla}_v v - \nu\{\Delta_B v + \mathrm{Ric}(v)\} + \nabla_\Gamma q = f, \quad \mathrm{div}_\Gamma v = 0 \quad \text{on} \quad \Gamma \times (0,\infty). \tag{5}$$

Note that these equations are described only in terms of the intrinsic quantities of the Riemannian manifold Γ. The equations (5) were called the "correct" Navier–Stokes equations on a Riemannian manifold in [1, 12] and studied by Mitrea–Taylor [7], Nagasawa [10], and Taylor [12]. Therefore, our limit equations (2)–(3) can be seen as the damped and weighted Navier–Stokes equations on a manifold.

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Diffusion in strongly layered domains

Angela Stevens
(joint work with Benedikt Jost)

We analyze the diffusion equation in two dimensional domains which are perforated by an ondulating structure consisting of horizontal bars and vertical connections distributed in an arbitrary periodic fashion on the lateral boundary of the horizontal bars. The main aim is to find critical structures of this type, which give rise to different homogenization limits. Our homogenization limit results in multicomponent systems, where the coupling of the different components is via the boundary instead of the bulk. Additionally, a reduction of diffusivity from two to one dimension is obtained. Allowing further for two-dimensional weakly connected domains, where the above obstacles include additional small pathways and concentration traps, the limiting equations are coupled in the bulk by memory terms and at the boundary via concentration gaps.
Our motivation to study diffusion in such geometries originates from the peculiar shapes of cell organelles like mitochondria and the endoplasmic reticulum, which exhibit strongly layered structures.

Domains, disconnected by horizontal bars, have already been considered by Cioranescu and Saint Jean Paulin, by Corbo Esposito, Donato, Gaudiello and Picard, by Mel'nyk, by Andreucci, Bisegna and DiBenedetto, as well as by Blanchard, Gaudiello and Mossino. Homogenization of domains with small pathways and traps have been studied by Khruslov, by Briane, as well as by Amaziane and Pankratov. Results for small pathways in surfaces or strips have been analyzed by Marcenko and Khruslov, as well as by Del Vecchio. Strongly oscillating structures have also been dealt with by Mel'nyk et al. in the context of thick periodic junctions, and in the context of oscillating boundaries by Arrieta et al., by Hale and Raugel, by Mel'nyk and Popov, as well as by Chechkin, Friedman and Piatnitski.

To the best of our knowledge, the basic domains considered in [1] are the first examples for a multi-component limiting model combined with reduction of two dimensional diffusion to one dimension. Even though the different components are all existing on the same domain, their coupling is only at the boundary. The geometry of the domain requires continuity conditions for the test functions. In order to obtain a reasonable weak formulation, a two-scale compactness result is proved, which yields continuity of the systems' components. Uniqueness holds due to classical theory. Further, the weakly connected domains considered in [1] seem to be the first examples which combine reduction to one dimensional diffusion with concentration gaps at the boundary and coupling via memory terms. The geometry of our obstacles possess two different and distinct traps. Hence, in comparison to Amaziane and Pankratov, we get two coupling memory terms in each equation instead of one.

The main difficulty in [1] was to find a reasonable geometry that can produce all the desired effects and to obtain the different related compactness results. Usually weak convergence in H^1 is needed for traps and for concentration gaps, when

considering suitable extensions of the solution. However, for a domain with disconnected parts, weak convergence in H^1 can only be achieved by restricting the set of initial conditions. In [1] this problem was overcome by providing a two-scale result for an H^1 extension, which turns out to be strong enough for the given setting. Therefore more general initial conditions can be considered, than those needed for weak convergence in H^1. Examples for initial data are given which are admissible for our proof, but not possible to assume for the usual approach. For the concentration gaps we adapt the technique from Briane in order to be able to only use two-scale convergence, whereas the proof by Del Vecchio and the one by Marcenko and Khruslov strictly need weak H^1 convergence. Moreover, the method for homogenization of oscillating boundaries by Corbo Esposito et al. does not apply for our geometies. We adapt techniques for homogenization of completely disconnected domains. Uniqueness can be shown by classical approaches, see Ladyzenskaja et al.

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Phase field approximation of the Steiner and Plateau problems: a numerical investigation

Elie Bretin

We analyze in this talk the ability of different phase field models to approximate solutions to the Steiner and Plateau problems. Recall that the Steiner problem consists in finding, for a given collection of points $a_0, \cdots, a_N \in \mathbb{R}^2$, a compact connected set $K \subset \mathbb{R}^2$ containing all the a_i's and having minimal length. In a joint work with M. Bonnivard and A. Lemenant, we first focus on the phase field model they have recently introduced together with F. Santambrogio in [1]. This model is defined as

$$F_\varepsilon(u) \quad = \quad P_\varepsilon(u) + \frac{1}{\lambda_\varepsilon} \sum_{i=1}^{N} \mathbf{D}(u^2 + \delta_\varepsilon; a_0, a_i),$$

where $P_\varepsilon(u) = \displaystyle\int_{\mathbb{R}^2} \varepsilon |\nabla u|^2 + \frac{1}{\varepsilon}(1-u)^2 dx$ is a Cahn-Hilliard type functional and

$$\mathbf{D}(w; a, b) := \inf_{\Gamma : a \rightsquigarrow b} \int_\Gamma w \, d\mathcal{H}^1 \in [0, +\infty].$$

The second term of the functional aims to force the connectedness of the limit set.

A major issue with the discretization of this phase field model comes from the lack of regularity of a critical point u, which appears to be only $C^{0,\alpha}$ for all $\alpha \in (0,1)$. As a result, u is not smooth enough to be discretized in space with a sufficient precision, which globally reduces the rate of convergence of the numerical scheme.

We therefore propose to improve the regularity by considering a higher-order derivative in the Cahn-Hilliard functional

$$P_\varepsilon(u) = \int_\Omega \varepsilon^3 |\Delta u|^2 + \frac{1}{\varepsilon}(1-u)^2 dx,$$

and we justify in [2] the Γ-convergence of this slightly modified version of the functional. We also introduce a numerical scheme which approximates fairly the associated gradient flow. A major novelty of our work is the extension of these results to space dimension 3 (see the numerical example in Figure 1).

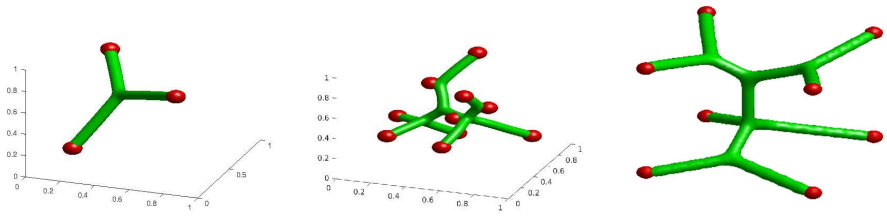

FIGURE 1. Numerical approximation of solutions to the Steiner problem in space dimension 3.

The second part of my contribution is a comparison of the previous results with those obtained using a numerical approximation of the approach introduced by Chambolle, Ferrari, and Merlet in [3]. Their model is defined as

$$F_\varepsilon(\sigma, u) = \int_\Omega \varepsilon |\nabla u|^2 + \frac{1}{\varepsilon}(1-u)^2 dx + \frac{1}{\varepsilon}\int_\Omega u|\sigma|^2 dx$$

where $a\varepsilon^2 \leq u \leq 1$ $(a > 0)$ and the vector field σ satisfies the constraint

$$div(\sigma) = (\delta_{x_0} - \frac{1}{N}\sum_i \delta_{a_i}) * \rho_\varepsilon.$$

The two models seem to be similar in the sense that

$$\sum_{i=1}^N \mathbf{D}(u^2 + \delta_\varepsilon; x_0, x_i) = \min_\sigma \left\{ \int_\Omega (u^2 + \delta_\varepsilon)|\sigma| : div(\sigma) = \delta_{x_0} - \frac{1}{N}\sum_i \delta_{x_i} \right\},$$

however we show an advantage of Chambolle-Ferrari-Merlet's model: it can be easily extended to tackle the Plateau problem by simply considering a curl constraint instead of a divergence constraint.

In the last part of our contribution we introduce a perturbed Allen-Cahn equation which forces the preservation of the evolving set's topology, and we illustrate how it can be used to approximate solutions to both Steiner and Plateau problems.

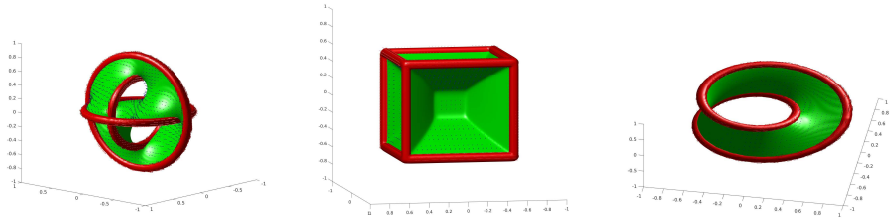

FIGURE 2. Numerical approximation of solutions to the Plateau problem based on the approach of [3].

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Crystalline surface diffusion flow for graph-like curves

MI-HO GIGA
(joint work with Yoshikazu Giga)

We are interested in motion of curves governed by singular interfacial energy (density), especially the surface diffusion flow by "crystalline energy" which is introduced by Cater, Roosen, Cahn, Taylor [2], with a numerical simulation.

We focus on an initial value problem of 4th order gradient flow type partial differential equation for curves described by the graph of a piecewise linear function called a "strictly admissible crystal".

Our major concern is to show that strictly admissibility is preserved for a short time in a rigorous way, based on subdifferential theory. For this purpose, we derive a system of ordinary differential equations (ODEs) for lengths of facets and solve it to show that strictly admissibility is preserved.

Assume that the interfacial energy W is a piecewise linear convex function with coercivity: $\lim_{|p|\to\infty} W(p)/|p| = +\infty$. On $H^{-1}_{\mathrm{av}}(\mathbf{T})$ consider a functional

$$\Phi(v) = \begin{cases} \int_{\mathbf{T}} W\left(v_x(x)\right) dx, & v \in W^{1,1}(\mathbf{T}) \cap H^{-1}_{\mathrm{av}}(\mathbf{T}), \\ \infty, & \text{otherwise.} \end{cases}$$

We consider an H^{-1}_{av} gradient flow equation:

$$\begin{aligned} &\frac{du}{dt}(t) \in -\partial_{H^{-1}} \Phi\left(u(t)\right) \quad \text{a.e.} \quad t > 0, \\ &u|_{t=0} = u_0 \in H^{-1}_{\mathrm{av}}(\mathbf{T}). \end{aligned}$$

Here $H^1_{\rm av}(\mathbf{T})$ denotes the average free subspace of $H^1(\mathbf{T})$ of the form

$$H^1_{\rm av}(\mathbf{T}) = \left\{ f \in H^1(\mathbf{T}) \;\middle|\; \int_{\mathbf{T}} f dx = 0 \right\}$$

with $\mathbf{T} = \mathbf{R}/\omega\mathbf{Z}$. Let $H^{-1}_{\rm av}(\mathbf{T})$ be the dual space of $H^1_{\rm av}(\mathbf{T})$. Its inner product is denoted by $((\ ,\ ))_{-1}$. Here $\partial_{H^{-1}}\Phi$ denotes the subdifferential of Φ in $H^{-1}_{\rm av}(\mathbf{T})$, i.e.,

$$\partial_{H^{-1}}\Phi(v) = \left\{ f \in H^{-1}_{\rm av}(\mathbf{T}) \mid \Phi(v+h) - \Phi(v) \geq ((h,f))_{-1} \text{ for all } h \in H^{-1}_{\rm av}(\mathbf{T}) \right\}.$$

Since Φ is lower semicontinous and convex, an abstract theory (initiated by Kōmura) yields a unique solution $u \in C\left([0,\infty), H^{-1}_{\rm av}(\mathbf{T})\right)$ of the $H^{-1}_{\rm av}(\mathbf{T})$ gradient flow equation which is absolutely continuous in any compact interval in $(0,\infty)$ with values in $H^{-1}_{\rm av}(\mathbf{T})$. This solution is called a variational solution of $u_t = -\Delta\left(W'(u_x)_x\right)$.

Definition. *We consider a piecewise linear function v on $\mathbf{T}$. The interval where v is an affine function is called a faceted region. We say that v is admissible if the slope of v in each faceted region is in a jump of W' and the slope of v in an adjacent faceted region is in an adjacent jump of W'. We say that $v = v(x)$ is a strictly admissible crystal with η if there exists $\eta \in C^2(\mathbf{R})$ such that*

(1) $\eta(x) \in \partial W\left(v_x(x)\right)$ a.e. $x \in \mathbf{R}$;
(2) η is piecewise polynomial of degree 3 on each faceted region;
(3) $\eta_x \neq 0$ at the ends of each faceted region;
(4) $\eta(x) \in \operatorname{int}\left\{\partial W\left(v_x(x)\right)\right\}$ on the interior of each faceted region.

Main Theorem (M.-H. G. & Y. Giga)**.** *Assume coercivity: $\lim_{|p|\to\infty} W(p)/|p| = +\infty$. If $u = u(x,t)$ is initially strictly admissible, then a variational solution u is strictly admissible at least for a short time. The lengths of facets of the solution u are determined by a system of ODEs as long as u stays strictly admissible.*

For the proof, we need a characterization of a subdifferential. The following type of result is known when $W(p) = |p| + a|p|^r$, $r > 1$ with $a > 0$ by Y. Kashima [6], [7] and when $W(p) = |p|$ by [5].

Theorem. *For $v \in D(\Phi)$ with $\partial_{H^{-1}_{\rm av}}\Phi(v) \neq \emptyset$, we have*

$$\partial_{H^{-1}_{\rm av}}\Phi(v) = \left\{ \eta_{xxx} \mid \eta \in CH(v) \right\},$$

where

$$CH(v) := \left\{ \eta \in C^1(\mathrm{T}) \mid \eta_x \in H^1_{\rm av}(\mathrm{T}),\ \eta(x) \in \partial W\left(v_x(x)\right) \text{ a.e. } \mathbf{T} \right\}.$$

Remark. *An element of $CH(v)$ is called a Cahn-Hoffman (vector) field.*

We next recall that the variational solution u is actually right differentiable for all $t > 0$ and $d^+u/dt = -\partial^0_{H^{-1}}\Phi\left(u(t)\right)$ where $\partial^0_{H^{-1}}\Phi$ is the minimal section defined by

$$\partial^0_{H^{-1}}\Phi(v) = \arg\min\left\{ \|f\|_{H^{-1}_{av}(T)} \;\middle|\; f \in \partial_{H^{-1}}\Phi(v) \right\}.$$

We then calculate the minimal section.

Proposition. *For $\zeta \in CH(v)$,*

$$\zeta_{xxx} = \partial^0_{H^{-1}_{\mathrm{av}}} \Phi(v)$$

if and only if $\zeta = \arg\min \left\{ \|\eta_{xx}\|^2_{L^2_{\mathrm{av}}(T)} \;\middle|\; \eta \in CH(v) \right\}$.

Remark. *This is an obstacle problem. The field ζ is called the minimal Cahn-Hoffman field. We are able to show that such ζ is unique.*

The proof is similar to that of [5].

Key Lemma. *Assume that v is admissible. Let ζ be a minimal Cahn-Hoffman field for v. Then $\zeta \in C^2(\mathrm{T})$ and ζ is a piecewise polynomial of degree 3.*

This is proved by calculating the Euler-Lagrange inequality for ζ.

Sketch of the proof of the Main Theorem. If initially v is strictly admissible, there is a unique minimal Cahn-Hoffman field η which lies in the interior of $\partial W(v)$ except at the end points of a faceted region. Moreover, it is a cubic polynominal in each faceted region. At the end points the derivative of η is not zero. The profile of v is essentially determined by the set of lengths of faceted regions $\ell = (\ell_1, \dots, \ell_m)$. By the transport equation $d\ell/dt$ is determined by the second derivative b of $\eta(x,t)$ at end points of each faceted region and ℓ. Unfortunately, b is determined by ℓ implicitly. More precisely,

$$M(\ell)b = f(\ell),$$

where $M(\ell)$ is an $m \times m$ symmetric matrix and f is $\mathbf{R}^m$-valued function. Fortunately, M is positive definite so the ODEs for ℓ can be written of a normal form. Fortunately, the strict admissibility is an open property so at least in a short time strictly admissibility is preserved. This is a short sketch of the proof of the Main Theorem.

Remark. *The second order problem is easy to handle because the minimal Cahn-Hoffman vector field is affine so it is easy to derive ODEs for ℓ for an admissible crystal as proposed by* [1], [9]. *The relation to the abstract theory was explained in* [3]. *The fourth order problem is quite different since it does not enjoy comparison principle. Several differences are explained in a review paper* [4].

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Directional differentiability for elliptic quasi-variational inequalities

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(joint work with Michael Hintermüller and Carlos N. Rautenberg)

We study the differentiability of the solution map associated to the quasi-variational inequality (QVI)

$$\begin{aligned} y \in &\mathbf{K}(y): \quad \langle Ay - f, v - y\rangle \geq 0 \quad \forall v \in \mathbf{K}(y) \\ &\mathbf{K}(y) := \{v \in V : v \leq \Phi(y)\}, \end{aligned} \tag{1}$$

in particular, the multi-valued mapping taking the source term f into the set of solutions y. Showing that this map is differentiable (in a suitable sense) is not only an interesting analytical problem in its own right but is also of use for optimal control, numerics and applications. Based on our work [1], we give a first result for the directional differentiability for QVIs in the infinite-dimensional setting (the corresponding theory for variational inequalities (VIs) has been thoroughly investigated, eg. [2, 3]).

1. Functional framework and background

Let X be a locally compact topological space, countable at infinity, with ξ a Radon measure on X. Suppose $V \subset L^2(X;\xi) =: H$ is a Hilbert space with the embedding continuous and dense and such that $|u| \in V$ whenever $u \in V$, and let $A\colon V \to V'$ be a bounded, linear, coercive and T-monotone operator. Assume also that

$$V \cap C_c(X) \subset C_c(X) \quad \text{and} \quad V \cap C_c(X) \subset V \quad \text{are dense embeddings.}$$

Define $V'_+ := \{g \in V' : \langle g, v\rangle \geq 0 \quad \forall v \in V_+\}$ which arises from the cone V_+ which is the set of almost everywhere (a.e.) non-negative elements of V. Precisely, we study the directional differentiability of the map $\mathbf{Q}\colon V'_+ \rightrightarrows V$ taking $f \mapsto y$ in (1).

Before proceeding, let us recall the sensitivity result for VIs. Given an obstacle $\phi \in V_+$, define the set

$$\mathbf{K} := \{w \in V : w \leq \phi\},$$

and given a source term $f \in V'$, define by $S\colon V' \to V$ the mapping such that $S(f)$ solves the inequality in (1) with $\mathbf{K}(y)$ replaced by $\mathbf{K}$ (and hence the QVI simplifies into a VI). The *tangent cone* and the *critical cone* associated to $\mathbf{K}$ are given respectively by

$$T_{\mathbf{K}}(y) := \{\varphi \in V : \varphi \leq 0 \text{ q.e. on } \{y = \phi\}\} \text{ and } \mathcal{K}_{\mathbf{K}}(y) := T_{\mathbf{K}}(y) \cap [f - Ay]^{\perp},$$

where the notation 'q.e.' means quasieverywhere. Given $f \in V'$ and $d \in V'$, Theorem 3.3 of [3] yields that the map S is directionally differentiability in the sense that there exists a function $S'(f)(d) \in V$ such that

$$S(f + td) = S(f) + tS'(f)(d) + o(t) \quad \forall t > 0$$

where $t^{-1}o(t) \to 0$ as $t \to 0^+$ in V and $\delta := S'(f)(d)$ is positively homogeneous in d and it satisfies the VI

$$\delta \in \mathcal{K}_{\mathbf{K}}(y) : \langle A\delta - d, v - \delta\rangle \geq 0 \quad \forall v \in \mathcal{K}_{\mathbf{K}}(y), \text{ where } y = S(f).$$

2. Directional differentiability for QVIs

To formulate the QVI case, consider (1) with $\Phi\colon V \to V$ an increasing map with $\Phi(0) \geq 0$. The idea in [1] is the following: approximate a QVI solution $q(t) \in \mathbf{Q}(f + td)$ by a sequence $q_n(t)$ of solutions of VIs, obtain suitable differential formulae for those $q_n(t)$ and then pass to the limit in those formulae to obtain an expansion formula relating elements of $\mathbf{Q}(f + td)$ to elements of $\mathbf{Q}(f)$. There are some delicacies in this procedure:

(1) **derivation of the expansion formulae** for the above-mentioned VI iterates $q_n(t)$; they must relate $q(t)$ to a $y \in \mathbf{Q}(f)$, and recursion plays a highly nonlinear role in the relationship between the iterates
(2) **obtaining uniform bounds on the directional derivatives of the iterates**; even though the derivatives satisfy a VI, one has to handle a recurrence inequality (unless some regularity is available [1, §4.3] which allows some simplification)
(3) **identifying the limit of the higher-order terms as a higher-order term**; this procedure involves two limits: one as $t \to 0^+$ and one as $n \to \infty$, and commutation of limits in general requires an additional uniform convergence.

The main difficulty is indeed the final point here. The iteration scheme alluded to above requires some further restrictions on the data f and the direction d, namely $f, d \in V'_+$. Since we study the differentiability of implicit obstacle problems defined through the obstacle mapping Φ, it is clear that at least some differentiability is required of Φ and we introduce these further assumptions below. First, let us fix some notation. Define $\bar{y} \in V$ as the weak solution of the unconstrained problem $A\bar{y} = f$. In a similar fashion, define $\bar{q}(t) \in V$ as the solution of the unconstrained problem with right hand side $f + td$: $A\bar{q}(t) = f + td$. The following set can be thought as a *translated* critical cone:[1]

$$\mathcal{K}_{\mathbf{K}(y)}(y, \alpha) := \Phi'(y)(\alpha) + \mathcal{K}_{\mathbf{K}(y)}(y).$$

The main result of [1] is the following.

Theorem (Theorem 1.6 of [1])**.** *Let $f, d \in V'_+$. Given $y \in \mathbf{Q}(f) \cap [0, \bar{y}]$, assume the following:*

[1]Explicitly, this set is $\{\varphi \in V : \varphi \leq \Phi'(y)(w)$ q.e. on $\{y = \Phi(y)\}$ and $\langle Ay - f, \varphi - \Phi'(y)(w)\rangle = 0\}$.

(1) the map $\Phi\colon V \to V$ is Hadamard directionally differentiable
(2) either
  (a) $\Phi\colon V \to V$ is completely continuous, or
  (b) $V = H^1(\Omega)$, $X = \overline{\Omega}$ where Ω is a bounded Lipschitz domain, $\Phi\colon L^\infty_+(\Omega) \to L^\infty_+(\Omega)$ is concave with $\Phi(0) \geq c > 0$, and $f, d \in L^\infty_+(\Omega)$
(3) the map $\Phi'(v)\colon V \to V$ is completely continuous (for fixed $v \in V$)
(4) for any $b \in V$, $h\colon (0,T) \to V$ and $\lambda \in [0,1]$,

$$\frac{\|\Phi'(y + tb + \lambda h(t))h(t)\|_V}{t} \to 0 \text{ as } t \to 0^+ \text{ if } \frac{h(t)}{t} \to 0 \text{ as } t \to 0^+$$

(5) given $T_0 \in (0,T)$ small, if $z\colon (0,T_0) \to V$ satisfies $z(t) \to y$ as $t \to 0^+$, then

$$\|\Phi'(z(t))b\|_V \leq C_\Phi \|b\|_V \quad \text{where } C_\Phi < \frac{1}{1 + c^{-1}C}$$

for all $t \in (0,T_0)$, where C and c are (respectively) the constants of boundedness and coercivity of A.

Then there exists $q(t) \in \mathbf{Q}(f + td) \cap [y, \bar{q}(t)]$ and $\alpha = \alpha(d) \in V_+$ such that

$$q(t) = y + t\alpha + o(t) \quad \forall t > 0$$

holds where $t^{-1}o(t) \to 0$ as $t \to 0^+$ in V and α satisfies the QVI

$$\alpha \in \mathcal{K}_{\mathbf{K}(y)}(y,\alpha) : \langle A\alpha - d, v - \alpha\rangle \geq 0 \quad \forall v \in \mathcal{K}_{\mathbf{K}(y)}(y,\alpha).$$

The directional derivative $\alpha = \alpha(d)$ is positively homogeneous in d.

It should be emphasized that the assumptions 4 and 5 depend on the specific function y, i.e., these are *local* conditions. The result in the general multi-valued setting given in Theorem 2 is a differentiability result for a specific selection mechanism that associates to a function $y \in \mathbf{Q}(f)$ a function $q(t) \in \mathbf{Q}(f + td)$. A useful variant of the theorem would be to obtain the result for the mapping that selects the minimal or maximal solution to the QVI, i.e., if $\mathsf{M}(f) \in \mathbf{Q}(f)$ is the maximal solution of the QVI with source term f, is M directionally differentiable?

Theorem (Theorem 1.7 of [1])**.** *In the context of Theorem 2, if the set $\mathcal{K}_{\mathbf{K}(y)}(y,w)$ simplifies to*

$$\mathcal{S}_{\mathbf{K}(y)}(y,w) := \{\varphi \in V : \varphi = \Phi'(y)(w) \text{ q.e. on } \{y = \Phi(y)\}\},$$

then the derivative α satisfies

$$\alpha \in \mathcal{S}_{\mathbf{K}(y)}(y,\alpha) : \langle A\alpha - d, \alpha - v\rangle = 0 \quad \forall v \in \mathcal{S}_{\mathbf{K}(y)}(y,\alpha).$$

In this case, if $h \mapsto \Phi'(v)(h)$ is linear, $\alpha = \alpha(d)$ satisfies $\alpha(c_1d_1 + c_2d_2) = c_1\alpha(d_1) + c_2\alpha(d_2)$ for constants $c_1, c_2 > 0$ and directions $d_1, d_2 \in V'_+$.

An application of the above to a model of thermoforming can be found in [1]. Ongoing work involves deriving strong stationarity conditions for optimal control problems with QVI constraints and sensitivity for the parabolic QVI case.

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Affine linear transmission conditions in equations and dynamic boundary conditions of Allen-Cahn type and their approximation by Robin boundary conditions

Kei Fong Lam

(joint work with Pierluigi Colli, Takeshi Fukao and Hao Wu)

We consider a system of equations and dynamic boundary conditions with Allen–Cahn characteristics for a pair of functions u (denoting the bulk variable) and ϕ (denoting the surface variable) as follows:

$$\begin{aligned} u_t - \Delta u + f(u) &= 0 \text{ in } \Omega, \\ \phi_t - \Delta_\Gamma \phi + f_\Gamma(\phi) + h'(\phi)\partial_n u &= 0 \text{ on } \Gamma := \partial\Omega, \\ u|_\Gamma &= h(\phi) \text{ on } \Gamma, \end{aligned} \tag{1}$$

furnished with initial conditions $u(0) = u_0$ in Ω and $\phi(0) = \phi_0$ on Γ. In the above $\Omega \subset \mathbb{R}^3$ denotes a bounded domain with smooth boundary Γ, ∂_n is the normal derivative on Γ, Δ_Γ is the Laplace–Beltrami operator, while f and f_Γ are the derivatives of double well potentials F and F_Γ, respectively, and $h : \mathbb{R} \to \mathbb{R}$ is a smooth function.

The above system (1) generalises the equations studied by Calatroni and Colli [1], who considered the case $h(s) = s$, along with nonlinearities f and f_Γ that are sums of maximal monotone mappings and Lipschitz perturbations. In general, it is not immediately clear whether (1) is well-posed, and from the corresponding weak formulation (where we denote by g the inverse of h, i.e., $\phi = g(u)$)

$$\begin{aligned} 0 = &\int_\Omega (u_t + f(u))\zeta + \nabla u \cdot \nabla \zeta \, dx \\ &+ \int_\Gamma g'(u)\Big((g(u))_t + f_\Gamma(g(u))\Big)\zeta + \nabla_\Gamma g(u) \cdot \nabla_\Gamma \Big(g'(u)\zeta\Big) \, dS \end{aligned}$$

holding for all test functions $\zeta \in H^1(\Omega)$ such that $\zeta|_\Gamma \in H^1(\Gamma)$, we observe that for an approximation scheme such as Faedo–Galerkin the main difficulty in deducing the existence of weak solutions lies in passing to the limit in the possibly highly nonlinear term $\nabla_\Gamma(g'(u)\zeta)$. However, we believe that recent progress in the theory of maximal L^p regularity may prove useful in establishing well-posedness for regular nonlinearities.

Another approach, motivated from numerical analysis, is to approximate the complicated Dirichlet boundary condition $u|_\Gamma = h(\phi)$ with a Robin boundary condition. This motivates us to consider the approximation system

$$\begin{aligned} u_t^K - \Delta u^K + f(u^K) &= 0 \text{ in } \Omega, \\ \phi_t^K - \Delta_\Gamma \phi^K + f_\Gamma(\phi^K) + h'(\phi^K)\partial_n u^K &= 0 \text{ on } \Gamma, \\ K\partial_n u^K &= h(\phi^K) - u^K \text{ on } \Gamma. \end{aligned} \tag{2}$$

In the formal limit $K \to 0$, if $u^K \to u$ and $\phi^K \to \phi$, then the Robin boundary condition yields $u|_\Gamma = h(\phi)$. Furthermore (2) can be interpreted as the L^2-gradient flow of the energy functional

$$E(u,\phi) = \int_\Omega \frac{1}{2}|\nabla u|^2 + F(u)\,dx + \int_\Gamma \frac{1}{2}|\nabla_\Gamma \phi|^2 + F_\Gamma(\phi) + \frac{1}{2K}|u - h(\phi)|^2\,dS,$$

so that a standard Faedo–Galerkin approximation can be deployed to infer the strong well-posedness of (2). This is done in [4] along with a Moreau–Yosida approximation for non-smooth maximal monotone nonlinearities. Moreover, for analytical F, F_Γ and h, an extended Łojasiewicz–Simon inequality for E can be derived. This is used in [7] to show that the unique global strong solution of (2) converges to a single steady state as time tends to infinity at an algebraic rate. New difficulties arise since we have a pair of variables (u,ϕ) in the definition of the energy E, as oppose to earlier works where ϕ is the trace value of u. Hence, the framework introduced in [2] cannot be applied directly, and we have to adapt the arguments in [9] to derive the Łojasiewicz–Simon inequality.

For the crucial question concerning the rigorous limit $K \to 0$, the identity from the gradient flow characteristic of (2) provides sufficient uniform estimates to pass to the limit in the special case $h(s) = \alpha s + \beta$ for $\alpha \neq 0$ and $\beta \in \mathbb{R}$. In other words, for affine linear h, the unique strong solution of (2) converges weakly to a solution of (1), and as a consequence leads to a weak well-posedness result for (1) when h is affine linear. By adopting a similar abstract formulation used in [3], we establish strong well-posedness to (1) with non-smooth maximal monotone nonlinearities in [4], and allows us to further derive error estimates between the strong solutions of (1) and (2) for affine linear h, which read as follows

$$\begin{aligned} &\|u^K - u\|_{L^\infty(0,T;L^2(\Omega))\cap L^2(0,T;H^1(\Omega))} + \|\phi^K - \phi\|_{L^\infty(0,T;L^2(\Gamma))\cap L^2(0,T;H^1(\Gamma))} \\ &\quad + K^{-1/2}\|\alpha\phi^K + \beta - u^K\|_{L^2(0,T;L^2(\Gamma))} \leq CK^{1/2}\|\partial_n u\|_{L^2(0,T;L^2(\Gamma))}. \end{aligned}$$

We see that the affine linear relation $u|_\Gamma = \alpha\phi + \beta$ is achieved at a linear rate in K. In a forthcoming work [6] we plan to apply a similar Robin penalty approach to study a modification of the coupled bulk-surface Cahn–Hilliard system proposed by [8] and further analysed by [5].

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