PDEs on evolving domains and evolving finite elements

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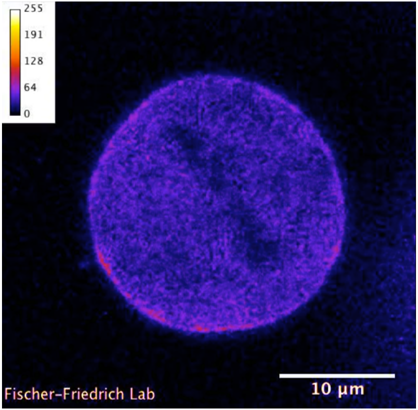
Idea

Develop unified methodology for numerical analysis and simulation of complex of interface and free boundary motion

- Functional analytic framework for abstract PDEs
- Time dependent function spaces
- Approximate time dependent space by evolving finite element spaces
- Evolving bulk and surface domains approximated by fitted triangulated domains
- Avoid unfitted finite elements and level set equations
- Link domain evolution to evolution equation on domains
- In this talk focus on evolving surfaces

A bulk–surface model for cell division via surface diffusion of stress generated surface molecules (myosin II), see [Wittwer and Aland (2022)], [Bonati, Wittwer, Aland, and Fischer-Friedrich (2022)].



Experiment by E. Fischer-Friedrich (TU Dresden).

Motivation I. – cell division by contractile ring formation

A bulk–surface model for cell division via surface diffusion of stress generated surface molecules (myosin II), see [Wittwer and Aland (2022)], [Bonati, Wittwer, Aland, and Fischer-Friedrich (2022)].

Experiment by E. Fischer-Friedrich (TU Dresden).

Chemotaxis

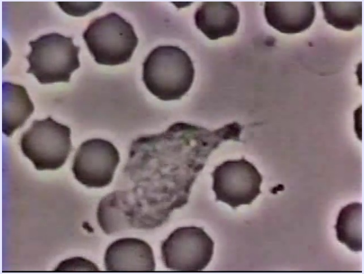


Figure: Neutrophil chasing a bacteria. Rogers Lab [1952]

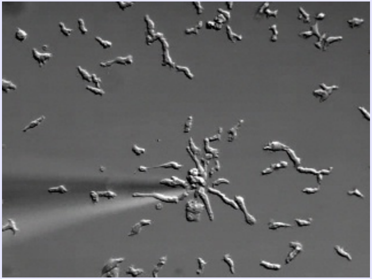


Figure: Multi cell chemotaxis. Firtel Lab.

Surface reaction diffusion and geometric evolution

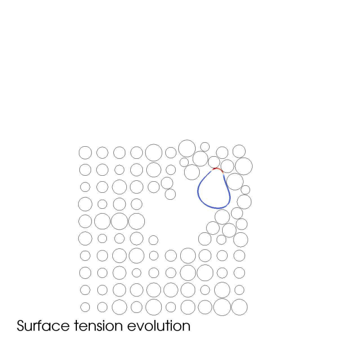


Figure: Simulation of chemotaxis in a field of obstacles : Roy. Soc. Interface [2012]Elliott, Stinner, Venkataraman

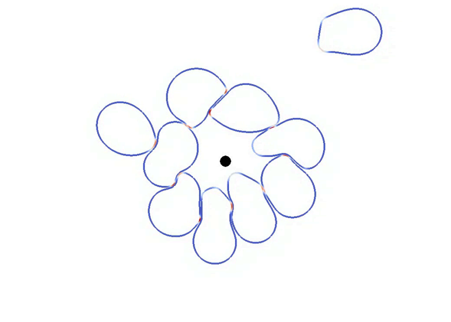


Figure: Simulation of multi-cell chemotaxis: Roy. Soc. Interface [2012] Elliott, Stinner, Venkataraman

Evolving compact hypersurfaces

For each $t \in [0,T]$, let $\Gamma(t) \subset \mathbb{R}^{n+1}$ be a compact (i.e., no boundary) n-dimensional hypersurface of class C^2, and assume the existence of a flow $\Phi\colon [0,T] \times \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$ such that for all $t \in [0,T]$, with $\Gamma_0 := \Gamma(0)$, the map $\Phi_t^0(\cdot) := \Phi(t,\cdot)\colon \Gamma_0 \to \Gamma(t)$ is a C^2-diffeomorphism that satisfies

$$\begin{aligned} \frac{d}{dt}\Phi_t^0(\cdot) &= \mathbf{w}(t,\Phi_t^0(\cdot)) \\ \Phi_0^0(\cdot) &= \mathrm{Id}(\cdot). \end{aligned} \tag{1}$$

We think of the map $\mathbf{w}\colon [0,T] \times \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$ as a velocity field, and we assume that it is C^2 and satisfies the uniform bound

$$|\nabla_{\Gamma(t)} \cdot \mathbf{w}(t)| \leq C \qquad \text{for all } t \in [0,T].$$

A normal vector field on the hypersurfaces is denoted by $\nu\colon [0,T] \times \mathbb{R}^{n+1} \to \mathbb{R}^{n+1}$.
A bulk domain $\Omega(t)$ with boundary $\Gamma(t)$ may be viewed as sub manifold in $\mathbb{R}^{n+2}$.

Parameterised evolving surfaces

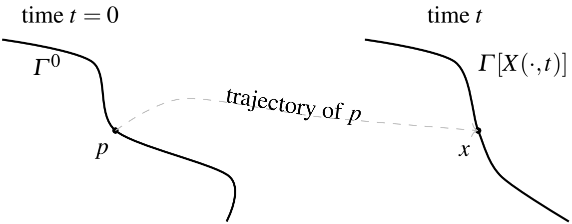
Let $\Gamma(t) \subset \mathbb{R}^3$ be a closed surface parametrised by X over an initial surface Γ^0:

$$\Gamma[X] = \Gamma[X(\cdot,t)] = \{X(p,t) \,:\, p \in \Gamma^0\}.$$

Surface velocity $\mathbf{w}$ satisfies, in $x(t) = X(p,t)$, by

$$\partial_t X(p,t) = \mathbf{w}(X(p,t),t).$$

The surface $\Gamma[X(\cdot,t)]$ is a collection of points x, where
$x = X(p,t)$ is obtained by solving the above ODE from 0 to t for a fixed p.



Material derivative

Normal time derivative Suppose that the velocity field associated to the evolving hypersurface $\{\Gamma(t)\}$ is $\mathbf{w} = \mathbf{w}_\nu + \mathbf{w}_\tau$ where $\mathbf{w}_\nu$ is a normal velocity field and $\mathbf{w}_\tau$ is a tangential velocity field. In this case, the formula

$$\partial^\circ u = u_t + \nabla u \cdot \mathbf{w}_\nu$$

defines the *normal time derivative* $\partial^\circ u$.

For our purposes the **material derivative** is associated with the parameterisation of the hypersurface and depends on the tangential velocity.

$$\partial^\bullet u = \partial^\circ u + \mathbf{w}_\tau \cdot \nabla_\Gamma u$$

A **physical material derivative** would be

$$\dot{u} = \partial^\bullet u + (\mathbf{v}_\tau - \mathbf{w}_\tau) \cdot \nabla_\Gamma u$$

where $\mathbf{v}_\tau$ is a tangential physical material velocity.

Choosing w_τ for some purpose of computation or analysis may be appropriate. In numerical methods this is called the *Arbitrary Lagrangian Eulerian (ALE)* approach where it is employed to yield *good meshes*.

Differential operators on $\Gamma[X]$

- Outward normal vector: $\nu = \nu_{\Gamma[X]}$
- Material derivative: $\partial^\bullet u(\cdot,t) = \frac{\mathrm{d}}{\mathrm{d}t}\big(u(X(\cdot,t),t)\big)$
- Tangential gradient: $\nabla_\Gamma u = \nabla_{\Gamma[X]} u = \nabla\bar{u} - (\nabla\bar{u}\cdot\nu)\nu : \Gamma \to \mathbb{R}^3$
- Laplace–Beltrami operator: $\Delta_\Gamma u = \Delta_{\Gamma[X]} u = \nabla_{\Gamma[X]} \cdot \nabla_{\Gamma[X]} u$
- extended Weingarten map (3×3 symmetric matrix)

$$A(x) = \nabla_\Gamma \nu(x)$$

-

$$\text{mean curvature} \qquad H = \mathrm{tr}(A) = \kappa_1 + \kappa_2,$$

$$\text{and} \qquad |A|^2 = \|A\|_F^2 = \kappa_1^2 + \kappa_2^2.$$

Advection-diffusion on an evolving surface

Let $\Gamma(t)$ be a time (t) dependent $n-$dimensional hypersurface in $\mathbb{R}^{n+1}$.

$$\partial^\circ \mathrm{u} + \nabla_\Gamma \cdot (\mathscr{B}_\Gamma \mathrm{u}) - \nabla_\Gamma \cdot (\mathcal{A}_\Gamma \nabla \mathrm{u}) + \mathscr{C}_\Gamma \mathrm{u} = 0 \qquad \text{on } \Gamma(t)$$

$$\mathrm{u}(\cdot, 0) = \mathrm{u}_0 \qquad \text{on } \Gamma_0 := \Gamma(0)$$

$\mathcal{A}_\Gamma$ is a smooth diffusion tensor which maps the tangent space of Γ into itself,
$\mathscr{B}_\Gamma$ is a tangential vector field,
$\mathscr{C}_\Gamma$ is a smooth scalar field.
$\partial^\circ \mathrm{u}$ denotes the normal time derivative
i.e. the time derivative of a function along a trajectory on $\Gamma(t) \times t$ moving in the direction normal to $\Gamma(t)$.

Let $\Gamma(t) = \partial\Omega(t)$where $\Omega(t)$ is a time dependent bulk domain in $\mathbb{R}^{n+1}$.

$$\mathrm{u}_t + \nabla\cdot(\mathscr{B}_\Omega \mathrm{u}) - \nabla\cdot(\mathcal{A}_\Omega \nabla \mathrm{u}) + \mathscr{C}_\Omega \mathrm{u} = 0 \qquad \text{on } \Omega(t)$$

$$(\mathcal{A}_\Omega \nabla \mathrm{u} - \mathscr{B}_\Omega \mathrm{u})\cdot \nu + \alpha \mathrm{u} - \beta \mathrm{v} = 0 \qquad \text{on } \Gamma(t)$$

$$\mathrm{u}(\cdot,0) = \mathrm{u}_0 \qquad \text{on } \Omega_0 := \Omega(0)$$

$$\partial^\circ \mathrm{v} + \nabla_\Gamma\cdot(\mathscr{B}_\Gamma \mathrm{v}) - \nabla_\Gamma(\mathcal{A}_\Gamma \mathrm{v}) + \mathscr{C}_\Gamma \mathrm{v} + (\mathcal{A}_\Omega \nabla \mathrm{u} - \mathscr{B}_\Omega \mathrm{u}) = 0 \qquad \text{on } \Gamma(t)$$

$$\mathrm{v}(\cdot,0) = \mathrm{v}_0 \qquad \text{on } \Gamma_0 := \Gamma(0)$$

where α and β are positive constants.

Surface Navier-Stokes equations

Let $\Gamma(t)$ be a time (t) dependent $2-$dimensional hypersurface in $\mathbb{R}^3$.
Seek a triple (u, p_1, p_2) to the problem:

$$u \cdot \nu_\Gamma = V_\Gamma \qquad \text{on } \cup_{t\in I} \{t\} \times \Gamma(t)$$

$$\partial^\circ u + u \cdot \nabla_\Gamma u + \nabla_\Gamma p_1 + 2\mu_0 \nabla_\Gamma \cdot E(u) = -p_2 \nu + f \qquad \text{on } \cup_{t\in I} \{t\} \times \Gamma(t)$$

$$\nabla_\Gamma \cdot u = 0 \qquad \text{on } \cup_{t\in I} \{t\} \times \Gamma(t)$$

$$E_\Gamma(\mathrm{v}) = \frac{\nabla_\Gamma \mathrm{v} + (\nabla_\Gamma \mathrm{v})^T}{2},.$$

Note: two Lagrange multipliers.
See Miura(2017) for a thin film derivation. Also Reusken et al (2021,2022).

Geometric gradient flow

Concentration dependent energy

$$\mathcal{E}(\Gamma, u) = \int_\Gamma G(u),$$

The (L^2, H^{-1})-gradient flow of $\mathcal{E}$ yields the *coupled geometric flow*:

$$\mathrm{v} = -g(u) H \nu_\Gamma = V \nu_\Gamma,$$

$$\partial^\bullet u + uVH = \Delta_{\Gamma[X]} G'(u),$$

with $g(u) = G(u) - uG'(u)$.

Two phase biomembrane energy:

$$E(\Gamma, \phi : \Gamma \to \mathbb{R}) = \int_\Gamma \underbrace{\frac{k_H(\phi)}{2}\big(H - H_s(\phi)\big)^2 + k_g(\phi) g}_{\text{bending energy}} + \underbrace{\sigma\Big(\frac{\varepsilon}{2}|\nabla_\Gamma \phi|^2 + \frac{1}{\varepsilon} W(\phi)\Big)}_{\text{line energy}}$$

Gradient flow dynamics: Find $\{(\Gamma(t), \phi(t))\}_t$ such that for all (w, η)

$$\big((\mathrm{v}, \partial^\bullet \phi), (w, \eta)\big)_{L^2} := -\big\langle \delta F(\Gamma, \phi), (w, \eta)\big\rangle - \lambda \cdot \big\langle \delta C(\Gamma, \phi), (w, \eta)\big\rangle$$

Theorem: *The strong equations of the gradient flow are*

$$\begin{aligned}
\mathrm{v} = & -\Delta_\Gamma\big(k_H(\phi)(H - H_s(\phi))\big) - |\nabla_\Gamma \nu|^2 k_H(\phi)(H - H_s(\phi)) + \tfrac{1}{2} k_H(\phi)(H - H_s(\phi))^2 H \\
& - \nabla_\Gamma \cdot \big(k_g'(\phi)(HI - \nabla_\Gamma \nu)\nabla_\Gamma \phi\big) \\
& + \sigma\varepsilon \nabla_\Gamma \phi \otimes \nabla_\Gamma \phi : \nabla_\Gamma \nu + \sigma\big(\tfrac{\varepsilon}{2}|\nabla_\Gamma \phi|^2 - \tfrac{1}{\varepsilon} W(\phi)\big) H \\
& - \lambda_V + \big(\lambda_A - \lambda_\phi h(\phi)\big) H, \\
\omega(\varepsilon)\partial^\bullet \phi = & -\tfrac{1}{2}(H - H_s(\phi))^2 k_H'(\phi) + k_H(\phi)(H - H_s(\phi)) H_s'(\phi) - g k_g'(\phi) \\
& + \varepsilon\sigma \Delta_\Gamma \phi - \tfrac{\sigma}{\varepsilon} W'(\phi) - \lambda_\phi h'(\phi),
\end{aligned}$$

plus constraints.

Model abstract problem

Abstract problem

$$
\begin{aligned}
\text{Find} \;\; u(t) &\in \mathcal{V}(t) \\
u(0) = u_0 &\in \mathcal{V}(0) \\
\partial^\bullet u + \mathcal{A}(t)u = f \;\; &\in \mathcal{V}^*(t)
\end{aligned}
$$

written in a variational form as

$$
\langle \partial^\bullet u, v \rangle_{\mathcal{V}^*(t),\mathcal{V}(t)} + a(t;u,v) = \langle f, v \rangle_{\mathcal{V}^*(t),\mathcal{V}(t)}
$$
$$
u(0) = u_0
$$

with associated (arbitrary) family of Hilbert triples

$$
\mathcal{V}(t) \subset \mathcal{H}(t) \subset \mathcal{V}^*(t), \; t \in [0,T]
$$

parametrised by $t \in [0,T]$.

Alphonse, E., Stinner (2015) Port. Math. + I.F.B.

Model abstract problem: Saddle point problem

For $t \in \mathbb{R}_+$ let $Y(t)$ and $X(t)$ be, respectively, given families of evolving Hilbert and Banach spaces. We denote the dual $X(t)$ as $X^*(t)$ and assume we have the *Gelfand triple* structure:

$$X(t) \subset Y(t) \subset X^*(t).$$

where we refer to $Y(t)$ as the pivot space. Let $Z(t)$ be an evolving Banach family. We are concerned with the *linear saddle-point* problem:

$$\begin{aligned} \partial^{\bullet} u(t) + A(t)u(t) + B^*(t)p(t) = f(t) \quad &\in X^*(t), \\ B(t)u(t) = g(t) \quad &\in Z^*(t), \\ u(0) = u_0 \in Y(0). \end{aligned}$$

with $\partial_t^{\bullet} u$ denoting the material derivative and we seek a pair of solutions (u, p).

Spaces

$$\mathcal{Z}(t) \subset \mathcal{Z}_0(t) \subset \mathcal{V}(t) \subset \mathcal{H}(t)$$

- $\mathcal{H}(t)$ pivot space
- $\mathcal{V}(t)$ solution spaces
- $\mathcal{Z}_0(t)$ regularity space for dual problem
- $\mathcal{Z}(t)$ higher regularity space for solution with specific data

Collaborators

Gerd Dziuk

Bjoern Stinner, Tom Ranner, Hans Fritz

Amal Alphonse, Ana Djurdjevac, Diogo Caetano,

Balas Kovacs, Harald Garcke

Pierre Stepanov,

PDE and Finite Element setting

- Domain and function spaces
- PDE: Initial value problem
- Bilinear forms and transport formulae
- Variational formulation
- Verify assumptions

- Evolving bulk finite element spaces
- Lifted bulk finite element spaces
- Evolving surface finite element spaces
- Lifted surface finite element spaces
- Discrete material derivatives and transport formulae

All these require precise definitions.

ABC Methodology

- Construct finite dimensional spaces as analogues of the continuous spaces
- Approximation theory
- Construct discrete analogues of bilinear forms in variational setting
- Well posedness of discrete problem
- Perturbation bounds for bilinear forms
- Error analysis via well posedness of continous problem and consistency

Model abstract discrete problem

Abstract problem

$$\text{Find } u_h(t) \in \mathcal{V}_h(t)$$
$$u_h(0) = u_0^h \in \mathcal{V}_h(0)$$
$$\partial_h^\bullet u_h + \mathcal{A}_h(t) u_h = f_h \quad \in \mathcal{V}_h^*(t)$$

written in a variational form as

$$\langle \partial_h^\bullet u_h, \mathrm{v} \rangle_{\mathcal{V}_h^*(t),\mathcal{V}_h(t)} + a_h(t; u_h, \mathrm{v}) = \langle f_h, \mathrm{v} \rangle_{\mathcal{V}_h^*(t),\mathcal{V}_h(t)}$$
$$u_h(0) = u_0^h$$

with associated (arbitrary) family of Hilbert triples

$$\mathcal{V}_h(t) \subset \mathcal{H}_h(t) \subset \mathcal{V}_h^*(t),\ t \in [0,T]$$

parametrised by $t \in [0,T]$.

Dziuk+E. (2007) ESFEM

Model abstract lifted discrete problem

Abstract lifted problem

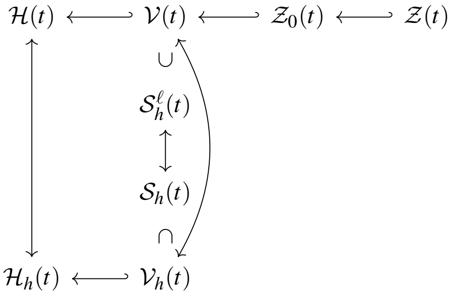
$$\text{Find } u_h^\ell(t) \in \mathcal{V}_h^\ell(t)$$
$$u_h^\ell(0) = u_0^{h,\ell} \in \mathcal{V}_h^\ell(0)$$
$$\partial_h^{\bullet,\ell} u_h^\ell + \mathcal{A}_h^\ell(t) u_h^\ell = f_h^\ell$$

written in a variational form as

$$\langle \partial_h^{\bullet,\ell} u_h^\ell, \mathrm{v} \rangle_{\mathcal{V}^*(t),\mathcal{V}(t)} + a_h^\ell(t; u_h, \mathrm{v}) = \langle f_h^\ell, \mathrm{v} \rangle_{\mathcal{V}^*(t),\mathcal{V}(t)}, \forall \mathrm{v} \in \mathcal{V}_h^\ell(t)$$
$$u_h^\ell(0) = u_0^{h,\ell}$$

$$\mathcal{V}_h^\ell(t) \subset \mathcal{V}(t)$$

Dziuk+E.(2013), E.+Ranner(2021)



$\subset$ denotes subspace inclusion

$\hookrightarrow$ denotes continuous embedding

$\leftrightarrow$ denotes that the lift is a bijection between these spaces.

Pullback and pushforward maps

Definition (Compatibility)

For $t \in [0,T]$, let $\mathcal{X}(t)$ be a separable Hilbert space and denote by $\mathcal{X}_0 := \mathcal{X}(0)$. Let $\phi_t : \mathcal{X}_0 \to \mathcal{X}(t)$ be a family of invertible, linear homeomorphisms, with inverse $\phi_{-t} : \mathcal{X}(t) \to \mathcal{X}_0$, such that there exists $C_{\mathcal{X}} > 0$ such that for every $t \in [0,T]$

$$||\phi_t \eta||_{\mathcal{X}(t)} \le C_{\mathcal{X}} ||\eta||_{\mathcal{X}_0} \qquad \text{for all } \eta \in \mathcal{X}_0$$

$$||\phi_{-t} \eta||_{\mathcal{X}_0} \le C_{\mathcal{X}}^{-1} ||\eta||_{\mathcal{X}(t)} \qquad \text{for all } \eta \in \mathcal{X}(t),$$

and such that the map $t \mapsto ||\phi_t \eta||_{\mathcal{X}(t)}$ is continuous for all $\eta \in \mathcal{X}_0$. Under these circumstances, we call the pair $(\mathcal{X}(t), \phi_t)_{t\in[0,T]}$ compatible. We call the map ϕ_t the push-forward operator and ϕ_{-t} the pull-back operator.

Remark

If $\mathcal{S}(t)$ be a closed subspace in $\mathcal{H}(t)$ for each $t \in [0,T]$ and ϕ_t maps $\mathcal{S}_0 := \mathcal{S}(0) \to \mathcal{S}(t)$, then $(\mathcal{S}(t), \phi_t|_{\mathcal{S}_0})_{t\in[0,T]}$ form a compatible pair.

Evolving Bochner spaces

Definition (Bochner-type spaces)

Define the spaces

$$L^2_X = \{u : [0,T] \to \bigcup_{t\in[0,T]} X(t) \times \{t\}, t \mapsto (\bar{u}(t),t) \mid \phi_{-(\cdot)}\bar{u}(\cdot) \in L^2(0,T;X_0)\}$$
$$L^2_{X^*} = \{f : [0,T] \to \bigcup_{t\in[0,T]} X^*(t) \times \{t\}, t \mapsto (\bar{f}(t),t) \mid \phi^*_{(\cdot)}\bar{f}(\cdot) \in L^2(0,T;X^*_0)\}.$$

More precisely, these spaces consist of equivalence classes of functions agreeing almost everywhere in $[0,T]$*, just like ordinary Bochner spaces.*

For $u \in L^2_X$, we will make an abuse of notation and identify $u(t) = (\bar{u}(t),t)$ with $\bar{u}(t)$ (and likewise for $f \in L^2_{X^*}$).

Theorem

The spaces L^2_X *and* $L^2_{X^*}$ *are Hilbert spaces with the inner products*

$$\begin{aligned}(u,v)_{L^2_X} &= \int_0^T (u(t),v(t))_{X(t)}\, \mathrm{d}t \\ (f,g)_{L^2_{X^*}} &= \int_0^T (f(t),g(t))_{X^*(t)}\, \mathrm{d}t.\end{aligned} \tag{2}$$

Pushed-forward continuously differentiable functions

Definition (Spaces of pushed-forward continuously differentiable functions)

Define the spaces

$$C^k_X = \{\xi \in L^2_X \mid \phi_{-(\cdot)}\xi(\cdot) \in C^k([0,T];X_0)\} \quad \text{for } k \in \{0,1,\dots\}$$

$$\mathcal{D}_X(0,T) = \{\eta \in L^2_X \mid \phi_{-(\cdot)}\eta(\cdot) \in \mathcal{D}((0,T);X_0)\}$$

$$\mathcal{D}_X[0,T] = \{\eta \in L^2_X \mid \phi_{-(\cdot)}\eta(\cdot) \in \mathcal{D}([0,T];X_0)\}.$$

Since $\mathcal{D}((0,T);X_0) \subset \mathcal{D}([0,T];X_0)$, we have

$$\mathcal{D}_X(0,T) \subset \mathcal{D}_X[0,T] \subset C^k_X.$$

Abstract strong and weak material derivatives

Definition (Strong material derivative)

For $\xi \in C^1_X$ define the strong material derivative $\dot{\xi} \in C^0_X$ by

$$\dot{\xi}(t) := \phi_t \left(\frac{d}{dt} (\phi_{-t} \xi(t)) \right).$$

- We see that the space C^1_X is the space of functions with a strong material derivative, justifying the notation.
-

Definition (Weak material derivative)

For $u \in L^2_{\mathcal{V}}$, if there exists a function $g \in L^2_{\mathcal{V}^*}$ such that

$$\int_0^T \langle g(t), \eta(t) \rangle_{\mathcal{V}^*(t), \mathcal{V}(t)} = - \int_0^T (u(t), \dot{\eta}(t))_{\mathcal{H}(t)} - \int_0^T \lambda(t; u(t), \eta(t))$$

holds for all $\eta \in \mathcal{D}_{\mathcal{V}}(0,T)$, then we say that g is the weak material derivative of u, and we write $\dot{u} = g$ or $\partial^{\bullet} u = g$.

The form λ is identified using the push forward map. This concept of a weak material derivative is indeed well-defined: if it exists, it is unique, and every strong material derivative is also a weak material derivative.

Theorem (Transport theorem and formula of partial integration)

For all u, $v \in W(\mathcal{V}, \mathcal{V}^*)$, the map

$$t \mapsto (u(t), v(t))_{\mathcal{H}(t)}$$

is absolutely continuous on $[0,T]$ *and*

$$\frac{d}{dt}(u(t), v(t))_{\mathcal{H}(t)t} = \langle \partial^\bullet u(t), v(t) \rangle_{\mathcal{V}^*, \mathcal{V}(t)} + \langle \partial^\bullet v(t), u(t) \rangle_{\mathcal{V}^*(t), \mathcal{V}(t)}$$

$$+ \lambda(t; u(t), v(t))$$

for almost every $t \in [0,T]$. *For all u,* $v \in W(\mathcal{V}, \mathcal{V}^*)$, *the following formula of partial integration holds*

$$(u(T), v(T))_{\mathcal{H}(T)} - (u(0), v(0))_{\mathcal{H}_0}$$
$$= \int_0^T \langle \partial^\bullet u(t), v(t) \rangle_{\mathcal{V}^*(t)\mathcal{V}(t)} + \langle \partial^\bullet v(t), u(t) \rangle_{\mathcal{V}^*(t)\mathcal{V}(t)}$$
$$+ \lambda(t; u(t), v(t)) \, \mathrm{d}t.$$

Finite element space

- For each $h \in (0, h_0)$, numerical method is based in a finite dimensional subspace $\mathcal{S}_h(t)$ with constructed Hilbert spaces $(\mathcal{H}_h(t), ||\cdot||_{\mathcal{H}_h(t)})$ and $(\mathcal{V}_h(t), ||\cdot||_{\mathcal{V}_h(t)})$ for all $t \in [0, T]$ and
$$\mathcal{S}_h(t) \subset \mathcal{V}_h(t) \subset \mathcal{H}_h(t).$$
- Push forward map $\phi_t^h \colon \mathcal{H}_{h,0} := \mathcal{H}_h(0) \to \mathcal{H}_h(t)$.
$\{\mathcal{S}_h(t)\}_{t\in[0,T]}$, evolving, finite-dimensional space subspace of $\mathcal{V}_h(t)$ satisfying $\phi_t^h(\mathcal{S}_{h,0}) = \mathcal{S}_h(t)$ (where $\mathcal{S}_{h,0} = \mathcal{S}_h(0)$).
- $$\|\eta_h\|_{\mathcal{H}_h(t)} \leq c\,\|\eta_h\|_{\mathbb{V}_h(t)} \qquad \text{for all } \eta_h \in \mathcal{V}_h(t).$$
- $(\mathcal{H}_h(t), \phi_t^h)_{t\in[0,T]}$ and $(\mathcal{V}_h(t), \phi_t^h|_{\mathcal{V}_{h,0}})_{t\in[0,T]}$ are compatible pairs uniformly in h:
$$c^{-1}\,\|\eta_h\|_{\mathcal{H}_{h,0}} \leq \left\|\phi_t^h \eta_h\right\|_{\mathcal{H}_h(t)} \leq c\,\|\eta_h\|_{\mathcal{H}_{h,0}} \qquad \text{for all } \eta_h \in \mathcal{H}_{h,0}$$
$$c^{-1}\,\|\eta_h\|_{\mathcal{V}_{h,0}} \leq \left\|\phi_t^h \eta_h\right\|_{\mathcal{V}_h(t)} \leq c\,\|\eta_h\|_{\mathbb{V}_{h,0}} \qquad \text{for all } \eta_h \in \mathcal{V}_{h,0}.$$

Discrete material derivative

- Since $\mathcal{S}_h(t)$ is a closed subspace of $\mathbb{V}_h(t)$ it is a Hilbert space and forms a compatible pair $(\mathcal{S}_h(t), \phi_t^h|_{\mathcal{S}_{h,0}})_{t\in[0,T]}$.
- Well defined spaces $L^2_{\mathcal{S}_h}$ and $C^1_{\mathcal{S}_h}$ and the material derivative $\partial_h^\bullet \chi_h$ is well defined for $\chi_h \in C^1_{\mathcal{S}_h}$.
- Defines the spaces $L^2_{\mathcal{H}_h}, L^2_{\mathcal{V}_h}$ and $C^1_{\mathcal{H}_h}, C^1_{\mathcal{V}_h}$. For $\eta_h \in C^1_{\mathcal{H}_h}$, we denote by $\partial_h^\bullet \eta_h$ the (strong) material derivative) with respect to the push-forward map ϕ_t^h defined by

$$\partial_h^\bullet \eta_h := \phi_t^h\left(\frac{d}{dt}\phi_{-t}^h \eta_h\right).$$

Basis functions and transport property

Let $\{\chi_i(\cdot,0)\}_{i=1}^N$ be a basis of $\mathcal{S}_{h,0}$ and push-forward to construct a time dependent basis $\{\chi_i(\cdot,t)\}_{i=1}^N$ of $\mathcal{S}_h(t)$ by

$$\chi_i(\cdot,t) = \phi_t^h(\chi_i(\cdot,0)).$$

It follows that

$$\partial_h^\bullet \chi_i = 0$$

so that for a decomposition

$$\chi_h(t) := \sum_{i=1}^N \gamma_i(t)\chi_i(t) \qquad \text{for all } \chi_h \in \mathcal{S}_h(t),$$

we compute that

$$\partial_h^\bullet \chi_h = \sum_{i=1}^N \dot{\gamma}_i(t)\chi_i(t) \qquad \text{for all } \chi_h \in C^1_{\mathcal{S}_h}.$$

Another discrete material derivative appropriate for analysis

$\partial_\ell^\bullet \eta$ denotes the material derivative for the push-forward map ϕ_t^ℓ.

$$\partial_\ell^\bullet \eta := \phi_t^\ell \frac{d}{dt}(\phi_{-t}^\ell \eta) \qquad \text{for all } \eta \in C^1_{(\mathcal{H},\phi^\ell)}.$$

This is a different material derivative to the material derivative defined with respect to the push-forward map ϕ_t^h.

Important observation of Dziuk and Elliott, the following commutation result holds:

$$\partial_\ell^\bullet(\eta_h^\ell) = (\partial_h^\bullet \eta_h)^\ell \qquad \text{for all } \eta_h \in C^1_{\mathcal{H}_h}.$$

Indeed:

$$\partial_\ell^\bullet(\eta_h^\ell) = \phi_t^\ell \frac{\mathrm{d}}{\mathrm{d}t}(\phi_{-t}^\ell(\eta_h^\ell)) = \left(\phi_t^h\left(\left(\frac{\mathrm{d}}{\mathrm{d}t}(\phi_{-t}^h \eta_h)^\ell\right)^{-\ell}\right)\right)^\ell = \left(\phi_t^h\left(\frac{\mathrm{d}}{\mathrm{d}t}(\phi_{-t}^h \eta_h)\right)\right)^\ell = (\partial_h^\bullet \eta_h)^\ell,$$

since the lift at time $t = 0$ and time derivative commute and $(\cdot)^\ell$ and $(\cdot)^{-\ell}$ are inverses.

Lemma

$\eta_h \in C^1_{\mathcal{H}_h}$ if, and only if, $\eta_h^\ell \in C^1_{(\mathcal{H},\phi^\ell)}$, and $\eta_h \in C^1_{\mathcal{V}_h}$ if, and only if, $\eta_h^\ell \in C^1_{(\mathcal{V},\phi^\ell)}$.

Tasks for realisation of abstract theory

Define

- Evolving finite element
- Evolving triangulation
- Evolving finite element space

Establish

- Approximation properties
- Lifted evolving spaces

Realise

- $\Omega_h(t)$ and $\Gamma_h(t)$ by interpolation, for example.
  Evolving nodes on initial triangulations by velocity field
- $\mathcal{S}_h(t)$

Establish

- Discrete bilinear forms
- Approximation estimates
- Ritz projection and for material derivative

Surface finite elements

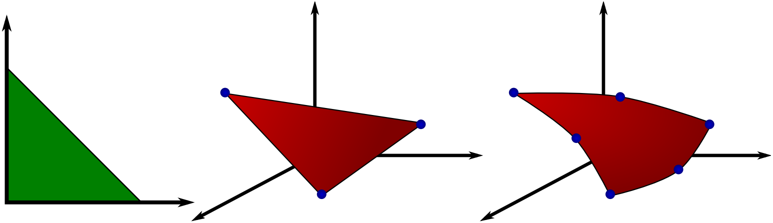


Figure: Examples of different surface finite elements in the case $n = 2$. Left shows a reference finite element (in green), centre shows an affine finite element and right shows an isoparametric surface finite element with a quadratic F_K. The plot shows the element domains in red and the location of nodes in blue.

Evolving isoparametric surface finite element

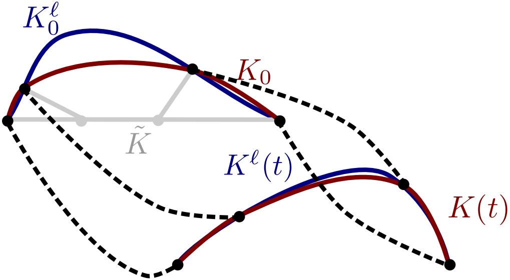


Figure: Examples of construction of an isoparametric evolving surface finite element for $k = 3$. The Lagrange nodes $a_i(t)$ follow the dashed black trajectories from the initial element $K_0 \subset \Gamma_{h,0}$ to a element $K(t) \subset \Gamma_h(t)$.

Weak and variational formulation of the advection diffusion equation

For every $\varphi(\cdot,t) \in H^1(\Gamma(t))$

Weak form

$$\int_{\Gamma(t)} \partial^\bullet u \varphi + \int_{\Gamma(t)} u\varphi \nabla_\Gamma \cdot v + \int_{\Gamma(t)} \nabla_\Gamma u \cdot \nabla_\Gamma \varphi = 0$$

Variational form

$$\frac{d}{dt}\int_{\Gamma(t)} u\varphi + \int_{\Gamma(t)} \nabla_\Gamma u \cdot \nabla_\Gamma \varphi = \int_{\Gamma(t)} u \partial^\bullet \varphi$$

Abstract variational form

$$\frac{d}{dt} m(u,\varphi) + a(u,\varphi) = m(u, \partial^\bullet \varphi).$$

Finite element space

For each t we have the finite element spaces

Space on triangulated surface

$$S_h(t) = \left\{ \phi_h \in C^0(\Gamma_h(t)) \,|\, \phi_h|_E \text{ is linear affine for each } E \in \mathcal{T}_h(t) \right\}$$

Lifted space on smooth surface

$$S_h^l(t) = \left\{ \varphi_h = \phi_h^l \,|\, \phi_h \in S_h(t) \right\}$$

Note that $S_h^l(t) \subset H^1(\Gamma(t))$ and that for each $\varphi_h \in S_h^l$ there is a unique $\phi_h \in S_h$ such that $\varphi_h = \phi_h^l$.

Discrete surface

$$\frac{d}{dt}\int_{\Gamma_h(t)} f = \int_{\Gamma_h(t)} \partial_h^\bullet f + f\,\nabla_{\Gamma_h}\cdot V_h.$$

Abstract form: discrete surface

$$\frac{d}{dt}m_h(\phi,W_h) = m_h(\partial_h^\bullet\phi,W_h) + m_h(\phi,\partial_h^\bullet W_h) + g_h(V_h;\phi,W_h)$$

$$\frac{d}{dt}a_h(\phi,W_h) = a_h(\partial_h^\bullet\phi,W_h) + a_h(\phi,\partial_h^\bullet W_h) + b_h(V_h;\phi,W_h)$$

Finite element method

$$\frac{d}{dt} m_h(U_h, \phi_h) + a_h(U_h, \phi_h) = m_h(U_h, \partial_h^{\bullet} \phi_h), \quad U_h(\cdot, 0) = U_{h0}. \tag{3}$$

Evolving mass matrix

$$M(t)_{jk} = \int_{\Gamma_h(t)} \chi_j \chi_k,$$

Evolving stiffness matrix

$$\mathcal{S}(t)_{jk} = \int_{\Gamma_h(t)} \nabla_{\Gamma_h} \chi_j \nabla_{\Gamma_h} \chi_k,$$

$U_h = \sum_{j=1}^{N} \alpha_j \chi_j$, $\alpha = (\alpha_1, \ldots, \alpha_N)$

Algebraic form

$$\frac{d}{dt}(M(t)\alpha) + \mathcal{S}(t)\alpha = 0, \tag{4}$$

which does not explicitly involve the velocity of the surface.

Error analysis: Not quite but near!!

$$\frac{1}{2}\frac{d}{dt}m_h(\theta,\theta)+a_h(\theta,\theta)=F_h(\theta).$$

Theorem

Let u be a sufficiently smooth solution satisfying

$$\int_0^T \|u\|^2_{H^2(\Gamma)}+\|\partial^\bullet u\|^2_{H^2(\Gamma)}dt<\infty$$

and let $u_h(,t)=U_h^l(\cdot,t), t\in[0,T]$ *be the spatially discrete solution with initial data* $u_{h0}=U_{h0}^l$ *satisfying*

$$\|u(\cdot,0)-u_{h0}\|_{L^2(\Gamma(0))}\leq ch^2.$$

Then the error estimate

$$\sup_{t\in(0,T)}\|u(\cdot,t)-u_h(\cdot,t)\|_{L^2(\Gamma(t))}\leq ch^2$$

holds for a constant c independent of h.

Following [Huisken (1984)], for a regular evolving surface $\Gamma[X]$ the identities hold:

$$\nabla_\Gamma H = \Delta_\Gamma \nu + |A|^2 \nu, \qquad \text{and} \tag{5}$$

$$\partial^\bullet \nu = -\nabla_\Gamma V, \tag{6}$$

$$\tag{7}$$

For example:

$$\begin{aligned} V &= -H, \\ \partial^\bullet \nu &\overset{(2)}{=} -\nabla_\Gamma V \\ &\overset{(4a)}{=} -\nabla_\Gamma (-H) \\ &\overset{(1)}{=} \Delta_\Gamma \nu + |A|^2 \nu. \end{aligned} \tag{4a}$$

MCF and Dziuk's algorithm

A regular surface $\Gamma[X]$ moving under mean curvature flow satisfies:

$$\partial_t X = v \circ X,$$
$$v = -H\nu.$$

Heat-like equation, using that on any Γ: $-H\nu = \Delta_\Gamma x_\Gamma$ (where $x_\Gamma = \mathrm{id}_\Gamma$):

$$\partial_t X(p,t) = \Delta_{\Gamma[X]} x_{\Gamma[X]}.$$

[Dziuk (1990)]

Simple and elegant algorithm;
computes all geometry from surface via evolving surface finite elements.

A coupled system for mean curvature flow

Inspired by [Huisken (1984)], consider the coupled system:

$$\mathrm{v} = -H\nu,$$

$$\partial^\bullet \nu = \Delta_{\Gamma[X]} \nu + |A|^2 \nu,$$
$$\partial^\bullet H = \Delta_{\Gamma[X]} H + |A|^2 H,$$

$$\partial_t X = \mathrm{v} \circ X.$$

The equations for ν and H are solved using evolving surface finite element formulation on a surface computed

---

First convergence proof for MCF in [Kovacs Li, and Lubich (2019)]: optimal-order H^1 norm error estimates (for evolving surface FEM of order $k \geq 2$ and BDF of order 2 to 5).

Leads to a less simple, but natural algorithm;
computes all geometry from evolution equations.

A geometric gradient flow involving diffusion on surface

Consider the energy

$$\mathcal{E}(\Gamma[X], u) = \int_{\Gamma[X]} G(u),$$

where

- $\Gamma[X]$ is an evolving surface;
- u is a concentration on the surface $\Gamma[X]$.

The (L^2, H^{-1})-gradient flow of $\mathcal{E}$ yields the *coupled geometric flow*:

$$v = -g(u) H \nu_\Gamma = V \nu_\Gamma,$$
$$\partial^\bullet u + uVH = \Delta_{\Gamma[X]} G'(u),$$

with $g(u) = G(u) - uG'(u)$.

Derivation and analytic theory in [Bürger (2021)].

Properties of MCF and the gradient flow

(i) Conservation of mean-convexity: **[both]**

$$\text{if } H(\cdot,0) \geq 0, \text{ then } H(\cdot,t) > 0, \ \forall t.$$

(i) Loss of convexity: **[MCF preserves]**

$$\text{if } \Gamma^0 \text{ is convex, then } \Gamma[X(\cdot,t)] \text{ is not necessarily convex.}$$

(iii) Formation of self-intersections are possible. **[not for MCF]**

(iv) Concentration properties: **[irrelevant for MCF]**

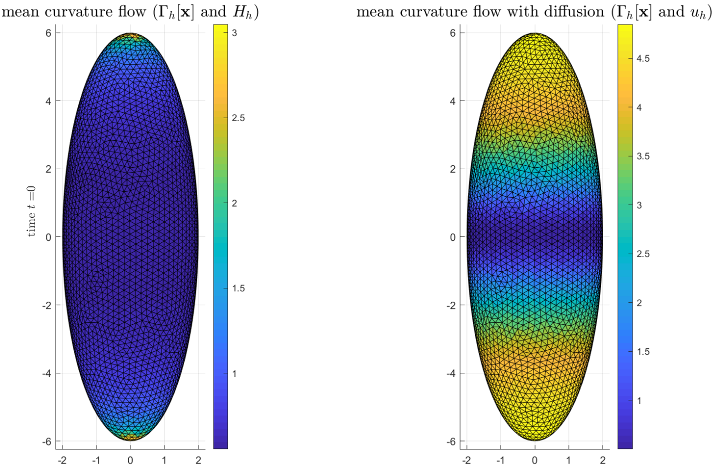
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Gamma[X]} u = 0, \qquad u(\cdot,0) \geq 0 \Rightarrow u(\cdot,t) \geq 0, \ \forall t, \qquad \min\{u\} \nearrow .$$

[Huisken (1984)]

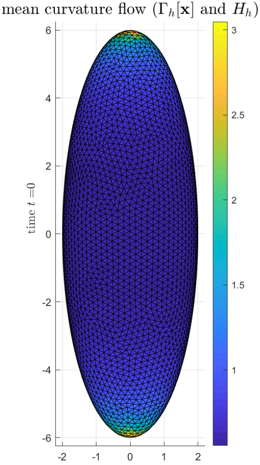
[Bürger (2021)]

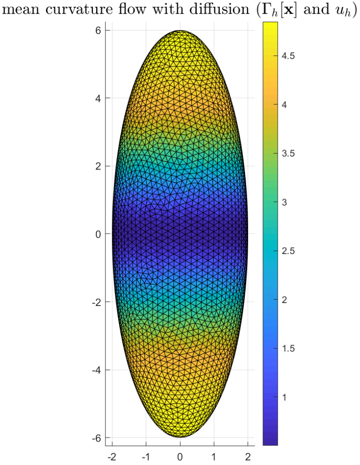
All observable in numerical experiments.

Mean curvature flow and the coupled geometric flow



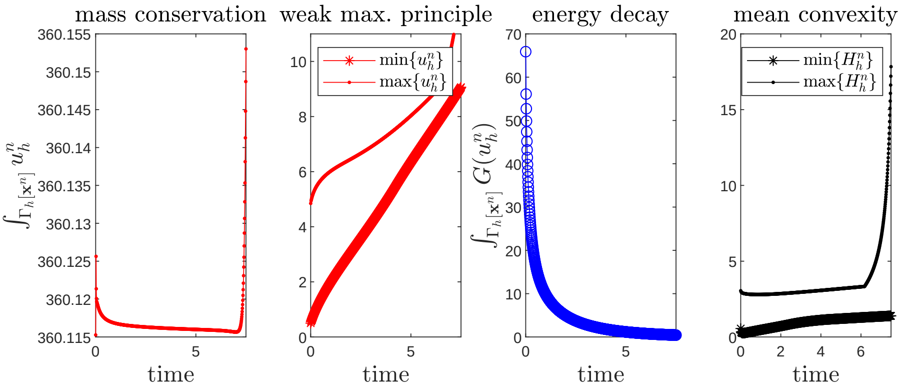
Loss of convexity, while preserving mean convexity



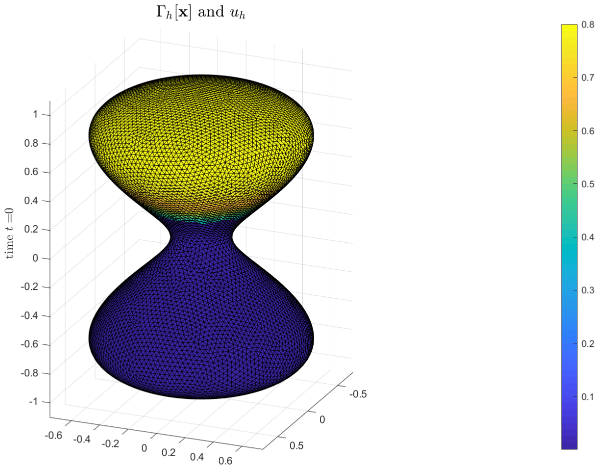


Loss of convexity, while preserving mean convexity

Qualitative properties of the fully discrete solution



Slow diffusion through a tight neck



cf. [Ecker (2008)]

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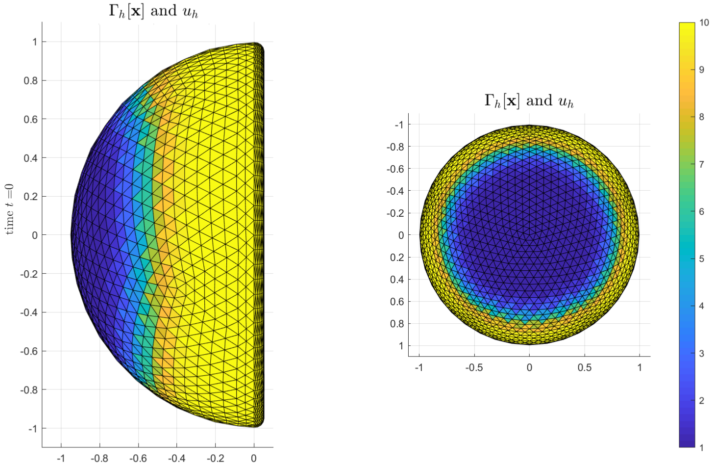
$\Gamma_h[\mathbf{x}]$ and u_h
time $t = 0$
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1
-0.8
-0.6
-0.4
-0.2
0
$\Gamma_h[\mathbf{x}]$ and u_h
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
-1
-0.5
0
0.5
1
10
9
8
7
6
5
4
3
2
1

Self-intersection

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Coupled system for

the interaction of mean curvature flow and diffusion

Instead of mean curvature flow

$$v = (-H)\nu_\Gamma,$$

consider now the generalised mean curvature flow

$$v = V\nu_\Gamma \quad \text{with} \quad V = -F(u,H),$$

with a given function F.

The real question is:
How robust is our approach from [KLL (2019)]?

Brief answer: Very!!

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$$V = -H. \tag{4a}$$

For example:

$$\begin{aligned} \partial^\bullet \nu &\overset{(2)}{=} -\nabla_\Gamma V \\ &\overset{(4a)}{=} -\nabla_\Gamma(-H) \\ &\overset{(1)}{=} \Delta_\Gamma \nu + |A|^2 \nu. \end{aligned}$$

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$$V = F(u,H) = -g(u)H. \tag{4b}$$

For example

$$\begin{aligned} \partial^\bullet \nu &\overset{(2)}{=} -\nabla_\Gamma V \\ &\overset{(4b)}{=} -\nabla_\Gamma\big(-g(u)H\big) \\ &= g(u)\nabla_\Gamma H + H\nabla_\Gamma(g(u)) \\ &\overset{(1)}{=} g(u)\Big(\Delta_\Gamma \nu + |A|^2 \nu\Big) + H\nabla_\Gamma(g(u)). \qquad (/g(u) > 0) \end{aligned}$$

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Evolving surface finite elements
and matrix–vector formulation

Key observations

We use dynamic variables to determine
the geometric quantities in the surface velocity $v_h \approx V_h \nu_h$.

	exact solution	approximation	geometry
surface:	$X(\cdot,t) : \Gamma^0 \to \mathbb{R}^3$	$X_h(\cdot,t) : \Gamma_h^0 \to \mathbb{R}^3$ (collected into $\mathbf{x}(t)$)	
velocity:	$\mathrm{v} : \Gamma[X] \to \mathbb{R}^3$	$\mathrm{v}_h : \Gamma_h[\mathbf{x}] \to \mathbb{R}^3$	
surface normal:	$\nu : \Gamma[X] \to \mathbb{S}^3$	$\nu_h : \Gamma_h[\mathbf{x}] \to \mathbb{R}^3$	$\neq \nu_{\Gamma_h[\mathbf{x}]} \in \mathbb{S}^3$
normal velocity:	$V : \Gamma[X] \to \mathbb{R}$	$V_h : \Gamma_h[\mathbf{x}] \to \mathbb{R}$	$\neq V_{\Gamma_h[\mathbf{x}]}$

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surface normal:	$\nu : \Gamma[X] \to \mathbb{S}^3$	$\nu_h : \Gamma_h[\mathbf{x}] \to \mathbb{R}^3$	$\neq \nu_{\Gamma_h[\mathbf{x}]} \in \mathbb{S}^3$
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Semi-discrete problem

$$V = -F(u,H), \;\; H = -K(u,V), \mathbf{w} = (\nu, \mathbf{V})$$

Evolving surface FEM [Dziuk and Elliott], [Demlow (2009)];
nodal values $z_h \rightsquigarrow \mathbf{z}$ (for all finite element functions).

$$\partial_t X_h = v_h \circ X_h,$$

with $$v_h = \widetilde{I}_h(V_h \nu_h),$$

for $w_h = (\nu_h, V_h)$

$$\int_{\Gamma_h[\mathbf{x}]} \partial_2 K_h \, \partial_h^\bullet w_h \cdot \varphi_h^w + \int_{\Gamma_h[\mathbf{x}]} \nabla_{\Gamma_h[\mathbf{x}]} w_h \cdot \nabla_{\Gamma_h[\mathbf{x}]} \varphi_h^w$$
$$= \int_{\Gamma_h[\mathbf{x}]} |A_h|^2 w_h \cdot \varphi_h^w + \int_{\Gamma_h[\mathbf{x}]} f(\partial_1 K_h, w_h, u_h; \partial_h^\bullet u_h) \cdot \varphi_h^w,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\int_{\Gamma_h[\mathbf{x}]} u_h \, \varphi_h^u\Big) + \int_{\Gamma_h[\mathbf{x}]} D(u_h) \nabla_{\Gamma_h[\mathbf{x}]} u_h \cdot \nabla_{\Gamma_h[\mathbf{x}]} \varphi_h^u = \int_{\Gamma_h[\mathbf{x}]} u_h \, \partial_h^\bullet \varphi_h^u,$$

Matrix–vector formulation

Upon setting $\mathbf{w} = \big(\mathbf{n}, \mathbf{V}\big)^T \in \mathbb{R}^{4N}$, the semi-discrete problem is equivalent to the following differential algebraic system:

$$\dot{\mathbf{x}} = \mathbf{v},$$

$$\mathbf{v} = \mathbf{V} \bullet \mathbf{n},$$

$$\mathbf{M}(\mathbf{x}, \mathbf{u}, \mathbf{w})\dot{\mathbf{w}} + \mathbf{A}(\mathbf{x})\mathbf{w} = \mathbf{f}(\mathbf{x}, \mathbf{w}, \mathbf{u}; \dot{\mathbf{u}}),$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\mathbf{M}(\mathbf{x})\mathbf{u}\Big) + \mathbf{A}(\mathbf{x}, \mathbf{u})\mathbf{u} = 0.$$

Used for computation and analysis.

Stability via energy estimates

A key issue is to compare different quantities on different meshes.
For this we need pointwise $W^{1,\infty}$ norm bound on the position errors.

(i) Obtain pointwise H^1 norm stability estimates over $[0, T^*]$,

using **energy estimates**,
testing with time derivatives of the errors

(ii) Using an inverse estimate to establish bounds in the $W^{1,\infty}$ norm.

(iii) Prove that in fact $T^* = T$.

Similarly to [Kovacs, Li, and Lubich (2019,2020)]
and [Binz and Kovacs (2021)]

Consider the semi-discretisation of the coupled system for the interaction of mean curvature flow and diffusion using ESFEM of polynomial degree $k \geq 2$.
Let the solutions (X, v, ν, V, u) be sufficiently smooth.
Then for sufficiently small h the following estimates hold for $0 \leq t \leq T$:

$$
\begin{aligned}
\|(x_h(\cdot,t_n))^L - \mathrm{id}_{\Gamma(t_n)}\|_{H^1(\Gamma(t_n))^3} &\leq Ch^k, \\
\|(v_h(\cdot,t_n))^L - v(\cdot,t_n)\|_{H^1(\Gamma(t_n))^3} &\leq Ch^k, \\
\|(\nu_h(\cdot,t_n))^L - \nu(\cdot,t_n)\|_{H^1(\Gamma(t_n))^3} &\leq Ch^k, \\
\|(V_h(\cdot,t_n))^L - V(\cdot,t_n)\|_{H^1(\Gamma(t_n))} &\leq Ch^k, \\
\|(u_h(\cdot,t_n))^L - u(\cdot,t_n)\|_{H^1(\Gamma(t_n))} &\leq Ch^k.
\end{aligned}
$$

The constant $C > 0$ is independent of h, but depends on the solution and on T.

E.+Garcke+ Kovacs (2022)

Outlook

- Extend theory for systems of PDEs on prescribed evolving domains
- Nonlinear equations
- Coupling of bulk surface fluid problems in prescribed evolving domains
- General approach to coupling PDE equations to flow of function spaces
- Finding flow maps ϕ allowing good discrete flows