Unfitted finite element methods for surface partial differential equations

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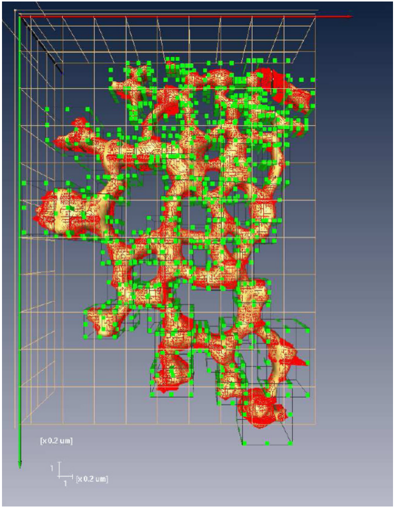
Dune User Meeting 2013

Where do surface partial differential equations come from?



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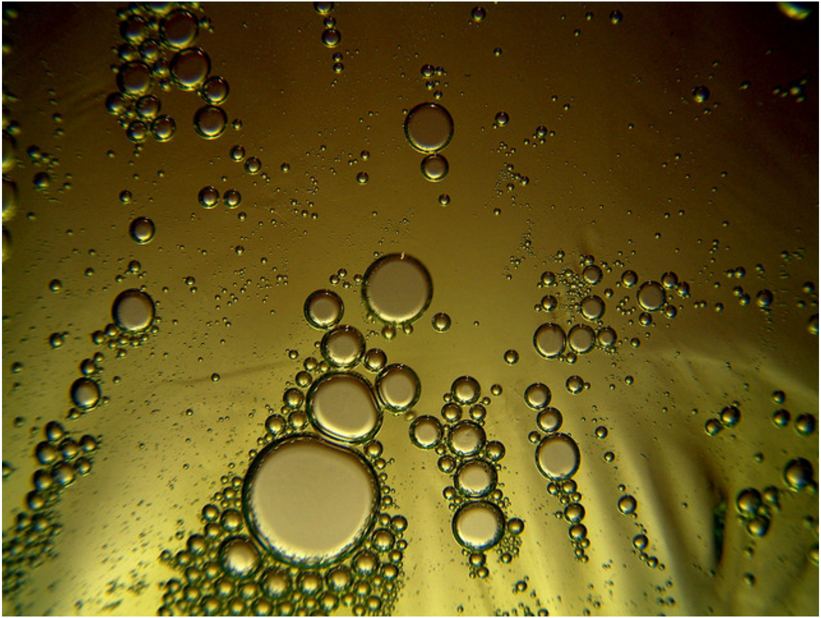
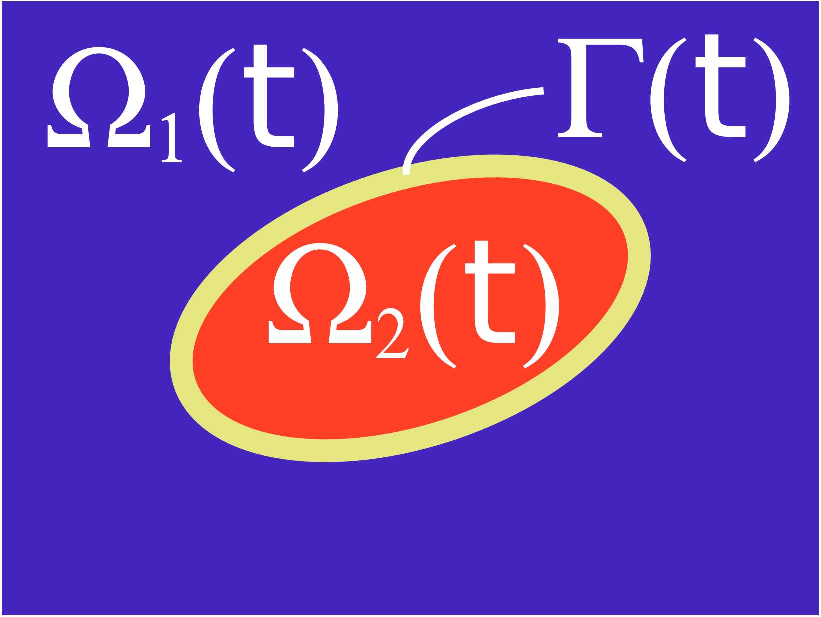


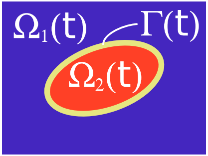
Example problem – surfactants



Example problem – surfactants

- Some fluid flow equations. . .
- Plus surfactant equations:

$$\partial_t w + \vec{v} \cdot \nabla w - \nabla \cdot q_w = 0 \qquad \text{in } \Omega_2(t)$$
$$\partial^\bullet u + u \nabla_\Gamma \cdot \vec{v} - \nabla_\Gamma \cdot q_u = \frac{\partial w}{\partial \nu} \qquad \text{on } \Gamma(t).$$



- with an boundary/interface condition on $\Gamma(t)$:

$$\frac{\partial w}{\partial \nu} = L(w, u).$$

Description of surface

- We assume Γ is a n-dimensional 'nice' hyper surface in $\mathbb{R}^{n+1}$.
- It can be described as the zero level set of a distance function d, which is negative in the interior of Γ and positive outside.
- The normal is given by $\nu = \nabla d$ and the shape operator $\mathcal{H} = \nabla^2 d$.
- The tangential gradient of $z \colon \Gamma \to \mathbb{R}$ is given by

$$\nabla_\Gamma z := \nabla \tilde{z} - (\nu \cdot \nabla \tilde{z})\nu = (\mathrm{Id} - \nu \otimes \nu)\nabla \tilde{z} = P \nabla \tilde{z}$$

  and the Laplace-Beltrami operator by

$$\Delta_\Gamma z := \nabla_\Gamma \cdot \nabla_\Gamma z.$$

- In a narrow band about the surface, each point x has a unique closest point $p = p(x)$ on the surface given by

$$x = p(x) + d(x)\nu(p(x)).$$

Poisson equation on a surface

We will consider the simplest equations we can study.

$$-\Delta_\Gamma u + u = f \quad \text{on } \Gamma.$$

[1] Aubin 1982

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Weak form:

$$\int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma \varphi + u\varphi \, d\sigma = \int_\Gamma f\varphi \quad \text{for all } \varphi \in H^1(\Gamma). \tag{1}$$

Theorem ([1])

There exists a unique solution u to (1) which satisfies the bound:

$$\|u\|_{H^2(\Gamma)} \leq c \, \|f\|_{L^2(\Gamma)} \,. \tag{2}$$

[1] Aubin 1982

Heat equation on an evolving surface

Another simple example:

$$\begin{aligned} \partial^\bullet u + u\nabla_\Gamma \cdot v - \Delta_\Gamma u = 0 \quad & \text{on } \Gamma(t) \\ u(\cdot, 0) = u_0 \quad & \text{on } \Gamma_0. \end{aligned} \tag{3}$$

We assume that the velocity v of $\Gamma(t)$ is known in advance.
$\partial^\bullet z$ denote the material derivative of z calculated by

$$\partial^\bullet z := \partial_t \widetilde{z} + v \cdot \nabla \widetilde{z}.$$

[2] Dziuk and Elliott 2007

Heat equation on an evolving surface

Another simple example:

$$\begin{aligned} \partial^{\bullet} u + u \nabla_{\Gamma} \cdot v - \Delta_{\Gamma} u = 0 \quad & \text{on } \Gamma(t) \\ u(\cdot, 0) = u_0 \quad & \text{on } \Gamma_0. \end{aligned} \tag{3}$$

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$$\partial^{\bullet} z := \partial_t \widetilde{z} + v \cdot \nabla \widetilde{z}.$$

Theorem ([2])

If the evolution of $\Gamma(t)$ is known and 'nice' and $u_0 \in H^1(\Gamma_0)$, then there exists a unique solution to (3).

[2] Dziuk and Elliott 2007

Computational challenges

- solve pdes on curved domains

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- large changes in curvatures and no symmetry assumptions

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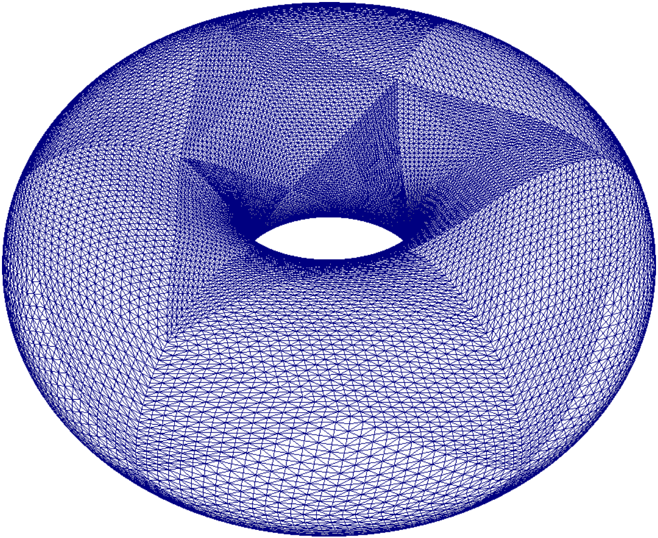
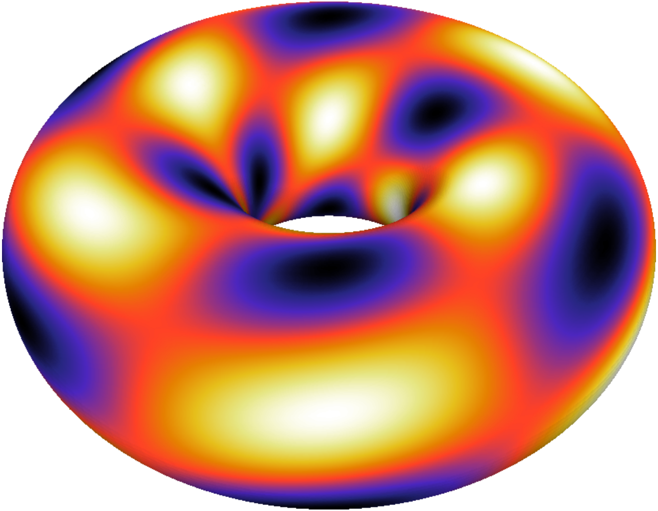
- time-dependent domains
- coupled to equations/methods for the location of the surface
- combined with bulk effects
- nonlinear equations
- stable, accurate, efficient and practical methods

Surface finite element method



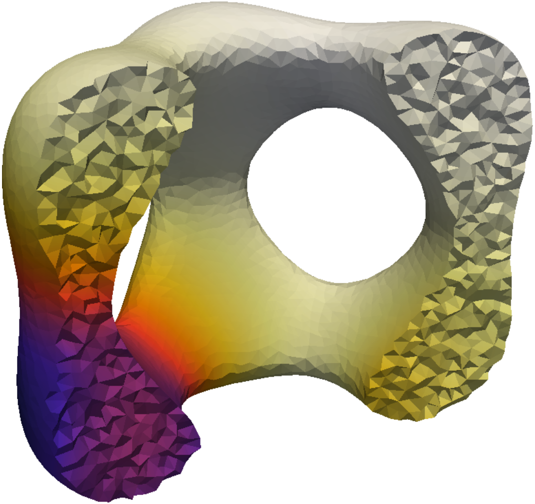
Solution on a torus



Error table

h	L^2 error	(eoc)
1.60000	4.36707	—
$9.82540 \cdot 10^{-1}$	1.57587	2.090335
$5.41335 \cdot 10^{-1}$	$5.66160 \cdot 10^{-1}$	1.717298
$2.77856 \cdot 10^{-1}$	$1.66560 \cdot 10^{-1}$	1.834542
$1.39856 \cdot 10^{-1}$	$4.37702 \cdot 10^{-2}$	1.946719
$7.00447 \cdot 10^{-2}$	$1.10891 \cdot 10^{-2}$	1.985583
$3.50370 \cdot 10^{-2}$	$2.78139 \cdot 10^{-3}$	1.996469
$1.75203 \cdot 10^{-2}$	$6.95862 \cdot 10^{-4}$	1.999229

Extensions I: a coupled bulk–surface problem[3]



[3] Elliott and TR 2013b

Extensions II: evolving surfaces[4]

This can be used to solve a Cahn-Hilliard equation on an evolving surface:

[video removed]

[4] Dziuk and Elliott 2007; Elliott and TR 2013a

Triangulated surfaces: summary

Advantages:

- these computations calculate the solution to a Poisson equation (symmetric) at each time
- error estimate: $\sup_{t\in(0,T)} \|u - u_h\|_{L^2(\Gamma(t))} \leq C(u_0)h^2$
- efficient with respect to degrees of freedom
- simple to implement

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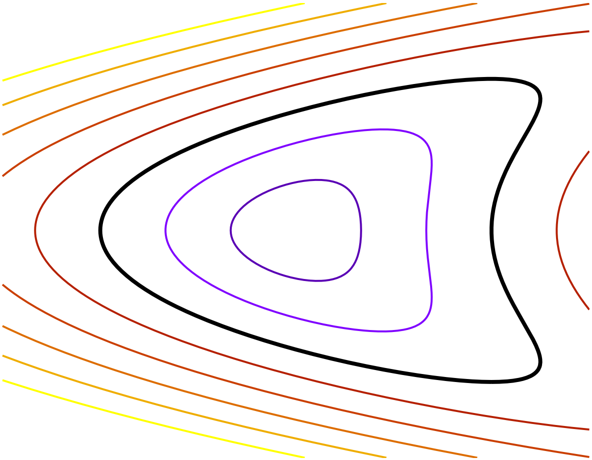
- simple to implement

Disadvantages:

- construction of triangulation can be difficult
- evolving triangulations can distort
- explicit tracking of interface in equations for surface

Level set methods[5]?



5 Bertalmío, Cheng, Osher, and Sapiro 2001

Eulerian formulation

Given $d \colon \mathbb{R}^{n+1} \to \mathbb{R}$ (distance function), such that $\Gamma = \{d = 0\}$ the (stationary) surface heat equation

$$u_t = \Delta_\Gamma u \quad \text{on } \Gamma \times (0, T),$$

becomes:

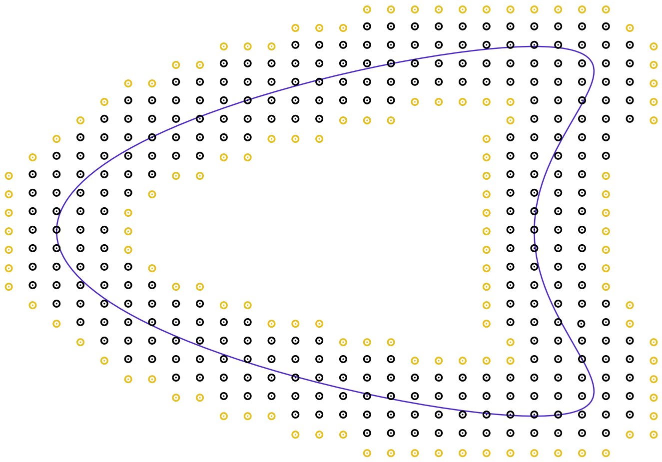
$$u_t = \nabla \cdot (P \nabla u) \quad \text{on } \mathbb{R}^{n+1} \times (0, T).$$

where

$$P(x) = \mathrm{Id} - \nu(x) \otimes \nu(x) \qquad \nu(x) = \frac{\nabla d(x)}{|\nabla d(x)|} \quad \text{for } x \in \mathbb{R}^{n+1}.$$

This method has been extended to many other equations including evolving surfaces.

The closest point method[6]



6 Ruuth and Merriman 2008

The closest point method

For the surface heat equation, we solve

$$\partial_t u(p) - \Delta(u(p)) = 0$$

on a narrow band about the surface.

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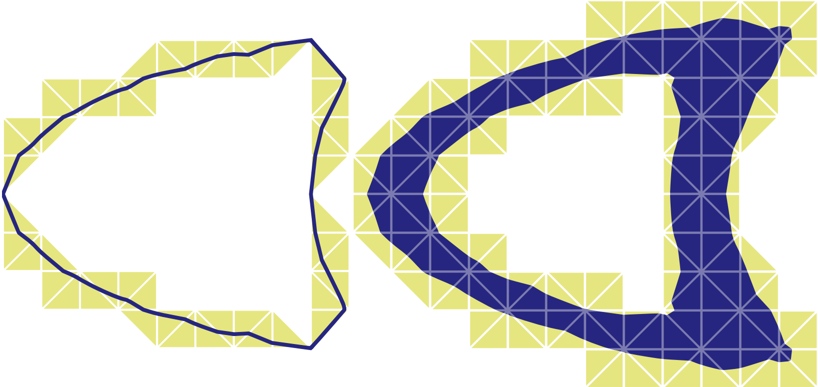
on a narrow band about the surface.
The idea is: for $u\colon \Gamma \to \mathbb{R}$

$$\nabla(u \circ p)(y) = \nabla_\Gamma u(y), \quad y \in \Gamma.$$

Unfitted finite element methods[7]



[7] Olshanskii, Reusken, and Grande 2009; Deckelnick, Dziuk, Elliott, and Heine 2009

Construction of domains

- Let U be a (polyhedral) domain containing $\Gamma = \{\Phi(x) = 0\}$
- Let $\mathcal{T}_h$ be a (regular) triangulation of U, h the mesh size
- Let X_h the space of piecewise bulk linear finite element on U
- We write $z^e(x) = z(p(x))$, for $x \in U$.

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Let $I_h \colon C(\bar{U}) \to X_h$ denote the usual Lagrangian interpolation operator. We have for $T \in \mathcal{T}_h$,

$$\|d - I_h d\|_{L^\infty(T)} + h \|\nabla(d - I_h d)\|_{L^\infty(T)} \leq ch^2 \|d\|_{W^{2,\infty}(T)} .$$

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$$\|d - I_h d\|_{L^\infty(T)} + h \|\nabla(d - I_h d)\|_{L^\infty(T)} \leq ch^2 \|d\|_{W^{2,\infty}(T)}.$$

Define

$$\Gamma_h := \{x \in U : I_h d(x) = 0\}$$
$$D_h := \{x \in U : |I_h d(x)| < h\},$$

Method one: sharp interface method

We define

$$\widetilde{\mathcal{T}}_h^I := \{T \in \mathcal{T}_h : |T \cap \Gamma_h| > 0\}.$$

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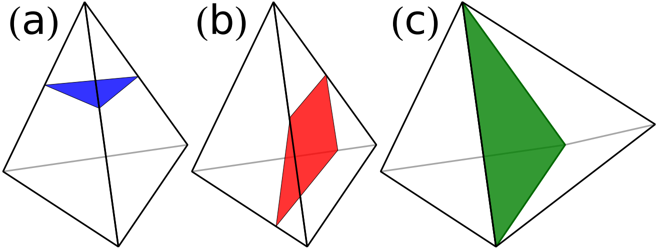

$$\mathcal{T}_h^I := \{ T \in \widetilde{\mathcal{T}}_h^I : T \text{ has not been disregarded because of (c)} \}.$$

Method one: sharp interface method

- Let $U_h^I = \bigcup_{T \in \mathcal{T}_h^I} T$.
- We define the space element space V_h^I as the space of piecewise linear functions on U_h^I.

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This space has the following interpolation result:

Lemma

$$\|z^e - I_h z^e\|_{L^2(\Gamma_h)} + h \|\nabla(z^e - I_h z^e)\|_{L^2(\Gamma_h)} \leq ch^2 \|z\|_{H^2(\Gamma)}.$$

Method one: sharp interface method

- Let $U_h^l = \bigcup_{T \in \mathcal{T}_h^l} T$.
- We define the space element space V_h^l as the space of piecewise linear functions on U_h^l.

This space has the following interpolation result:

Lemma

$$\|z^e - I_h z^e\|_{L^2(\Gamma_h)} + h \|\nabla(z^e - I_h z^e)\|_{L^2(\Gamma_h)} \leq ch^2 \|z\|_{H^2(\Gamma)}.$$

The finite element problem is: find $u_h \in V_h^l$ such that

$$\int_{\Gamma_h} \nabla u_h \cdot \nabla \phi_h + u_h \phi_h \, d\sigma_h = \int_{\Gamma_h} f^e \phi_h \, d\sigma_h \quad \text{for all } \phi_h \in V_h^l. \tag{4}$$

Method one: sharp interface method

Using a variant of Strang lemma and interpolation lemma we have the following error bound:

Theorem

$$\|u^e - u_h\|_{L^2(\Gamma_h)} + h \|\nabla(u^e - u_h)\|_{L^2(\Gamma_h)} \leq ch^2 \|f\|_{L^2(\Gamma)} . \quad (5)$$

Proof.
The key step in the proof is to notice that

$$\nabla_\Gamma u(p(x)) = (\mathrm{Id} - d\mathcal{H})^{-1} \nabla u^e(x).$$

□

Method two: narrow band method

Define

$$\mathcal{T}_h^B := \{ T \in \mathcal{T}_h : |T \cap D_h| > 0\},$$

and

$$U_h^B := \bigcup_{T \in T_h^B} T.$$

We define the space element space V_h^B as the space of piecewise linear functions on U_h^B.

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We define the space element space V_h^B as the space of piecewise linear functions on U_h^B.

Lemma

$$\frac{1}{\sqrt{h}} \left\| (z^e - I_h z) \left| \nabla I_h d \right| \right\|_{L^2(D_h)} + \sqrt{h} \left\| \nabla (z^e - I_h z^e) \left| \nabla I_h d \right| \right\|_{L^2(D_h)} \\ \leq c h^2 \left\| z \right\|_{H^2(\Gamma)} .$$

Method two: narrow band method

The second finite element scheme is: find $u_h \in V_h$ such that

$$\frac{1}{2h}\int_{D_h}(\nabla u_h \cdot \nabla \phi_h + u_h\phi_h)\,|\nabla I_h d|\ dx = \frac{1}{2h}\int_{D_h} f^e\phi_h\,|\nabla I_h d|\ dx. \tag{6}$$

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Applying the same techniques again, we have

Theorem

$$\|u^e - u_h\|_{L^2(\Gamma_h)} + h \left(\frac{1}{2h} \int_{D_h} |\nabla(u^e - u_h)|^2 |\nabla I_h d| \, dx \right)^{\frac{1}{2}} \leq ch^2 \|f\|_{L^2(\Gamma)}.$$

The proof follows in the same way.

Implementation

Mesh $\mathcal{T}_h$	`ALUGrid CONFORM`

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Important elements $\mathcal{T}_h^{I/B}$	`Dune::Fem::FilteredGridPart`

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Approximate level set descriptions Φ_h	`Dune::Fem::DiscreteFunction` + closest point operator for extensions

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Integrals $\int_{\Gamma_h \cap T} \cdot \, d\sigma_h$ or $\frac{1}{2h} \int_{D_h \cap T} \cdot \lvert \nabla \Phi_h \rvert \, dx$	SubElementQuadrature: takes an element and discrete level set function, triangulates integration domain (using Triangle or Tetgen), and sums quadrature rules over each domain

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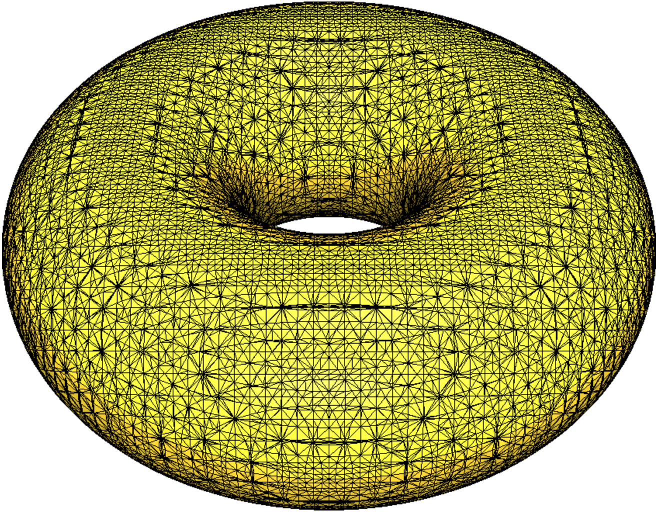
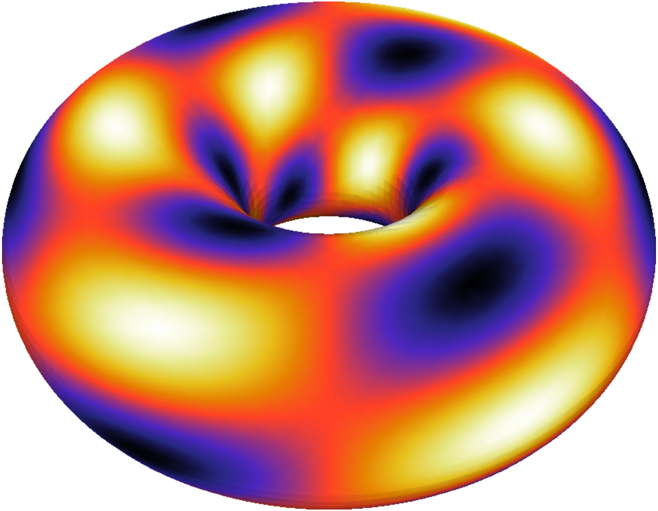
Integrals $\int_{\Gamma_h \cap T} \cdot \, d\sigma_h$ or $\frac{1}{2h} \int_{D_h \cap T} \cdot \, \lvert \nabla \Phi_h \rvert \, dx$	`SubElementQuadrature`: takes an element and discrete level set function, triangulates integration domain (using `Triangle` or `Tetgen`), and sums quadrature rules over each domain
Linear solver	`Dune::Fem::ISTLCGOp` with Jacobi preconditioning.

Method one: underlying mesh



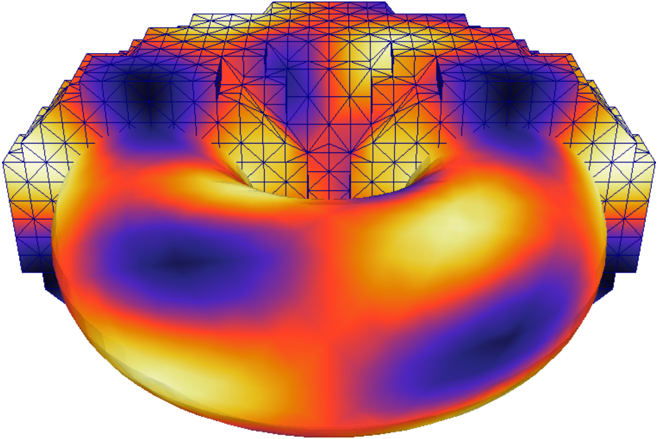
Method one: numerical results



Method one: numerical results

h	$\|u^e - u_h\|_{L^2(\Gamma_h)}$	eoc
$2^{-1}\sqrt{3}$	6.03053	—
$2^{-2}\sqrt{3}$	1.67739	1.846067
$2^{-3}\sqrt{3}$	$7.10825 \cdot 10^{-1}$	1.238652
$2^{-4}\sqrt{3}$	$1.90004 \cdot 10^{-1}$	1.903465
$2^{-5}\sqrt{3}$	$4.73865 \cdot 10^{-2}$	2.003482
$2^{-6}\sqrt{3}$	$1.19721 \cdot 10^{-2}$	1.984800
$2^{-7}\sqrt{3}$	$3.01376 \cdot 10^{-3}$	1.990040

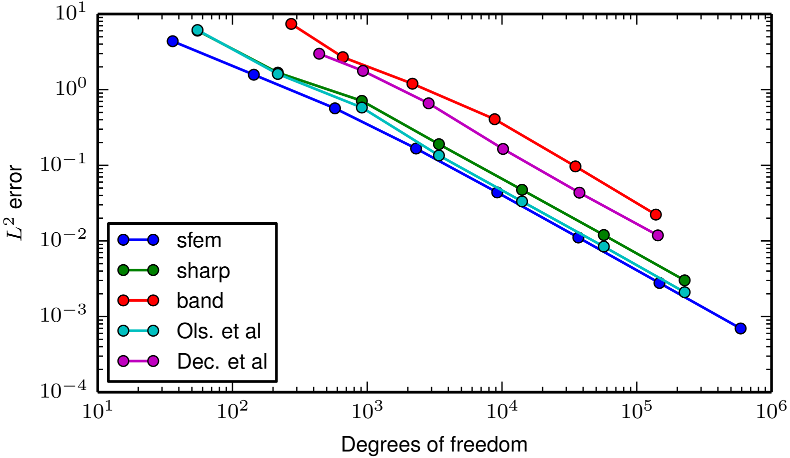
Method two: numerical results



Numerical results: method two

h	$\|u^e - u_h\|_{L^2(\Gamma_h)}$	eoc
$2^{-1}\sqrt{3}$	$1.07999 \cdot 10^{-1}$	—
$2^{-2}\sqrt{3}$	$4.79724 \cdot 10^{-2}$	1.170741
$2^{-3}\sqrt{3}$	$1.37037 \cdot 10^{-2}$	1.807639
$2^{-4}\sqrt{3}$	$4.36489 \cdot 10^{-3}$	1.650548
$2^{-5}\sqrt{3}$	$1.25966 \cdot 10^{-3}$	1.792911
$2^{-6}\sqrt{3}$	$3.25698 \cdot 10^{-4}$	1.951428

Comparison of methods



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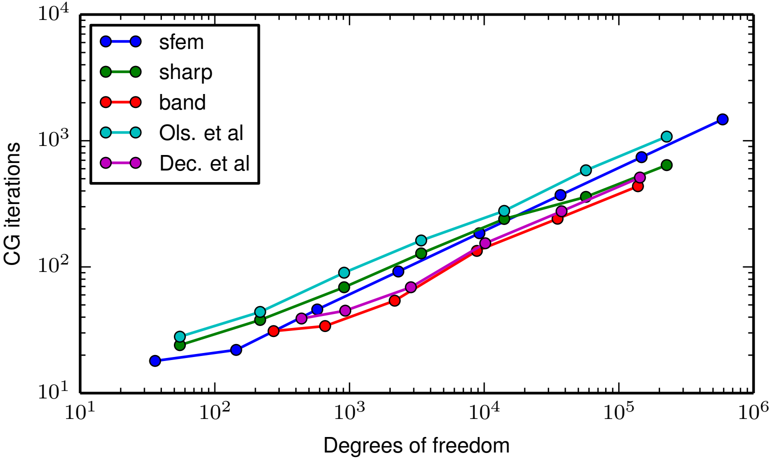

Evolving case?

- Transform to weak form:

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

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- Use sharp interface method for lower order terms and narrow band method for diffusion terms. Use test space $V_h^B(t)$:

$$\frac{d}{dt}\int_{\Gamma_h(t)} u_h\phi_h\, d\sigma_h + \frac{1}{2h}\int_{D_h} \nabla u_h \cdot \nabla \phi_h \left|\nabla I_h d(\cdot,t)\right|\, dx$$

$$= \int_{\Gamma_h(t)} u_h \partial_h^\bullet \phi_h\, d\sigma_h.$$

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$$= \int_{\Gamma_h(t)} u_h \partial_h^\bullet \phi_h \, d\sigma_h.$$

- Discretise in time using semi-Lagrangian formulation:

$$\frac{1}{\tau_m}\left(\int_{\Gamma_h^m} u_h^m \phi_h \, d\sigma_h - \int_{\Gamma_h^{m-1}} u_h^{m-1}\phi_h(\cdot + \tau v) \, d\sigma_h\right)$$
$$+ \frac{1}{2h}\int_{D_h^m} \nabla u^m \cdot \nabla \phi_h \left|\nabla I_h d(\cdot, t^m)\right| \, dx = 0.$$

Evolving case?

Lemma (Conservation of mass)

If $\tau V_{\max} < ch$, *then*

$$\int_{\Gamma_h^m} u_h^m \, d\sigma_h = \int_{\Gamma_h^{m-1}} u_h^{m-1} \, d\sigma_h.$$

Evolving case?

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Extra difficulties:

- Domain, finite element spaces, and matrices must be reconstructed at each time step.
- Semi-Lagrangian formulation implies non-local assemble which is difficult to parallelise.

Evolving unfitted finite element method: 2D solution

[video removed]

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