Finite element methods for surface PDEs

Gerd Dziuk [1] Charlie Elliott[2]

[1]Angewandte Mathematik
University of Freiburg

[2]Mathematics Institute
University of Warwick

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Applications

Partial differential equations on surfaces occur in many applications.

- Transport and diffusion of surfactants on fluid interfaces
- Diffusion within phase boundaries DIGM
- Conservation and diffusion on bio-membranes
- Formation of nanoporosity via surface spinodal decomposition
- Imaging
  - Texture synthesis via reaction diffusion equations
  - Flow vizualization via anisotropic diffusion
  - Segmentation

Surface Derivatives

Tangential gradient on the surface Γ with normal ν:

$$\nabla_\Gamma f = \nabla f - \nabla f \cdot \nu \, \nu$$

The tangential gradient only depends on the values of f on the surface.

Laplace-Beltrami-Operator on Γ:

$$\Delta_\Gamma f = \nabla_\Gamma \cdot \nabla_\Gamma f.$$

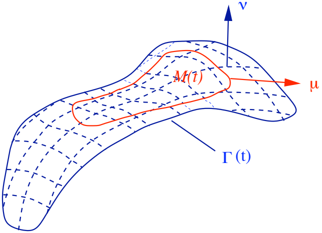
Integration by parts on a surface:

$$\int_\Gamma \nabla_\Gamma f = - \int_\Gamma f H \nu + \int_{\partial\Gamma} f \mu$$

with mean curvature H of Γ and conormal vector μ on $\partial\Gamma$.

Conservation

$$\frac{d}{dt}\int_{M(t)} u = -\int_{\partial M(t)} q \cdot \mu$$



u is a scalar quantity on $\Gamma(t)$, e. g. a density.
q is a flux on the surface, a tangent vector to $\Gamma(t)$. Integration by parts on Γ gives

$$\int_{\partial M(t)} q \cdot \mu = \int_{M(t)} \nabla_\Gamma \cdot q + \int_{M(t)} q \cdot \nu H = \int_{M(t)} \nabla_\Gamma \cdot q$$

Leibniz rule

Let the surface $\Gamma(t)$ move with velocity $v = v(x,t)$, $x \in \Gamma(t)$. Then one has:

$$\frac{d}{dt}\int_\Gamma f \quad = \quad \int_\Gamma \dot{f} + f\,\nabla_\Gamma \cdot v$$

where a dot denotes the material derivative

$$\dot{f} = \frac{\partial f}{\partial t} + v \cdot \nabla f.$$

Application:

$$\frac{d}{dt}\int_{M(t)} u = \int_{M(t)} \dot{u} + u\,\nabla_\Gamma \cdot v$$

Conservation equation

Conservation holds if and only if

$$\int_{M(t)} \dot{u} + u\,\nabla_\Gamma \cdot v = -\int_{M(t)} \nabla_\Gamma \cdot q$$

and since $M(t)$ is an arbitrary portion of $\Gamma(t)$, one obtains the partial differential equation

$$\dot{u} + u\,\nabla_\Gamma \cdot v + \nabla_\Gamma \cdot q = 0 \quad \text{on } \Gamma$$

Here v is the velocity of Γ.

Diffusion equation

The constitutive law

$$q = -D_0 \nabla_\Gamma u$$

leads to an initital value problem for a parabolic PDE on an evolving surface.

For given data $\Gamma(t)$, $t \in [0, T]$ und $u_0 : \Gamma_0 \to \mathbb{R}$ determine a solution $u(\cdot, t) : \Gamma(t) \to \mathbb{R}$ of

$$\begin{aligned} \dot{u} + u \nabla_\Gamma \cdot v - D_0 \Delta_\Gamma u &= 0, \quad \text{on } \Gamma(t), \\ u(\cdot, 0) &= u_0 \quad \text{on } \Gamma_0 \end{aligned}$$

If the surface Γ has a boundary, then one additionally has to impose suitable boundary conditions.

Finite element space

- For each t we have a finite element space

$$S_h(t) = \left\{\phi \in C^0(\Gamma_h(t)) : \phi|_e \text{ is linear affine for each } e \in \mathcal{T}_h(t)\right\}$$

- Transport Property of Basis Functions
  On $\Gamma_h(t)$, for each $j = 1, \ldots, N$,

$$\dot{\phi}_j = 0$$

and for each $\phi = \sum_{j=1}^{N} \gamma_j(t)\phi_j \in S_h(t)$

$$\dot{\phi} = \sum_{j=1}^{N} \dot{\gamma}_j(t)\phi_j.$$

Evolving Surface Finite Element Method: ESFEM

Our ESFEM is based on the evolving finite element spaces introduced in this section and the variational form of the diffusion equation:-
Find $U(\cdot,t) \in S_h(t)$ such that

$$\frac{d}{dt}\int_{\Gamma_h(t)} U\phi + \int_{\Gamma_h(t)} \nabla_{\Gamma_h} U \cdot \nabla_{\Gamma_h}\phi = \int_{\Gamma_h(t)} U\dot{\phi} \quad \forall \phi \in S_h(t).$$

Setting

$$U(\cdot,t) = \sum_{j=1}^{N} \alpha_j(t)\phi_j(\cdot,t)$$

and using the transport property of the basis functions we find that

$$\frac{d}{dt}\left(\mathcal{M}(t)\alpha\right) + \mathcal{S}(t)\alpha = 0.$$

$\mathcal{M}(t)$ is the evolving mass matrix

$$\mathcal{M}(t)_{jk} = \int_{\Gamma_h(t)} \phi_j \phi_k,$$

$\mathcal{N}(t)$ is a mass matrix weighted by the surface divergence of the velocity,

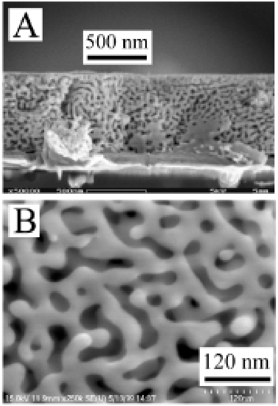
$$\mathcal{N}(t)_{jk} = \int_{\Gamma_h(t)} \phi_j \phi_k \nabla_{\Gamma_h(t)} \cdot v_h$$

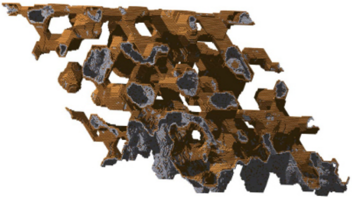
and $\mathcal{S}(t)$ is the evolving stiffness matrix

$$\mathcal{S}(t)_{jk} = \int_{\Gamma_h(t)} \mathcal{D}_0^{-l} \nabla_{\Gamma_h} \phi_j \nabla_{\Gamma_h} \phi_k.$$

Dealloying by selective dissolution

- Dealloying of a binary alloy by the selective removal of one component via electrochemical dissolution in an electrolyte such that there is surface phase separation of the other component.
- A protypical example is that of the etching of silver in an Ag-Au alloy whose surface is immersed in an electrolyte.
- The dissolution of silver atoms occurs at the surface whilst the surface gold atoms agglomerate in clusters and expose the next layer of silver atoms for dissolution.
- The result is the growth of porosity into the bulk.





J. Erlebacher, M.J. Aziz, A. Karma, N. Dimitrov and K. Sieradzki *Evolution of nanoporosity in dealloying* Nature **410**(2001)

Mathematical model

Find a periodic evolving surface $\Gamma(t), \;\; t \in (0,T)$ and a surface periodic function $c : \bigcup_{t\in[0,T]} \Gamma(t) \rightarrow \mathbb{R}$, such that the surface moves in normal direction with the velocity

$$Vel = v_0(c)\,(1 - \delta H)\,\nu,$$

c satisfies

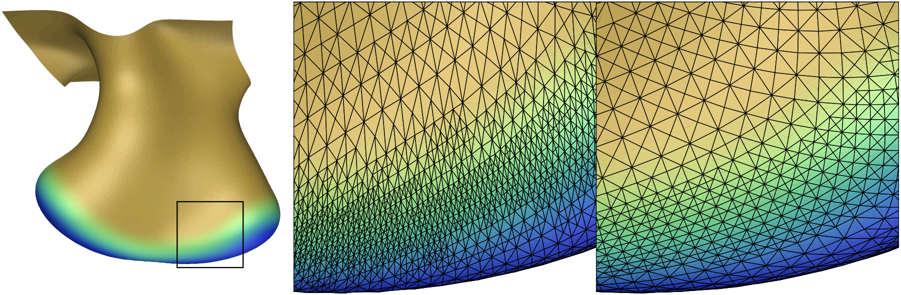
$$\dot{c} = -\nabla_\Gamma \cdot \left(b(c)\nabla_\Gamma \left(\gamma\Delta_\Gamma c - \Psi' c\right)\right) - c\nabla_\Gamma \cdot Vel + c_0 Vel \cdot \nu,$$

and the initial values

$$c(\cdot,0) = c_i(\cdot) \;\text{ and }\; \Gamma(0) = \Gamma_0$$

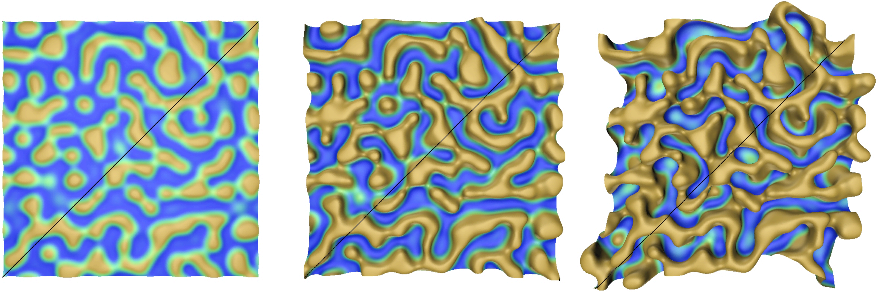
are prescribed.

- Computations based on E.S.F.E.M.
- Discretization of curvature flow uses approach of Dziuk
- Discretization of Cahn-Hilliard uses approach of Elliott, Copetti,Blowey
- Computations by Carsten Eilks
- Analysis of Cahn-Hilliard on evolving surfaces Eilks in preparation.



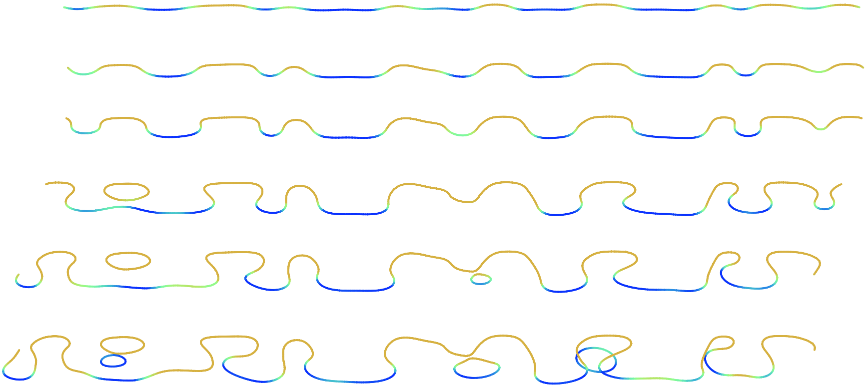
Remeshed surface, closeup before and after remeshing

Computational Experiment:- Early stages of etching



Simulation on a large square, t=0.04 , t=0.1 and t=0.2; $v_{max} = 1.6$

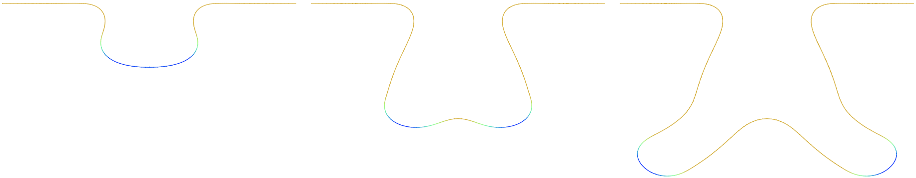
Computational Experiment:- Early stages of etching



Simulation on a large square, cross-sections along the diagonal for $t = 0.04$ to $t = 0.24$

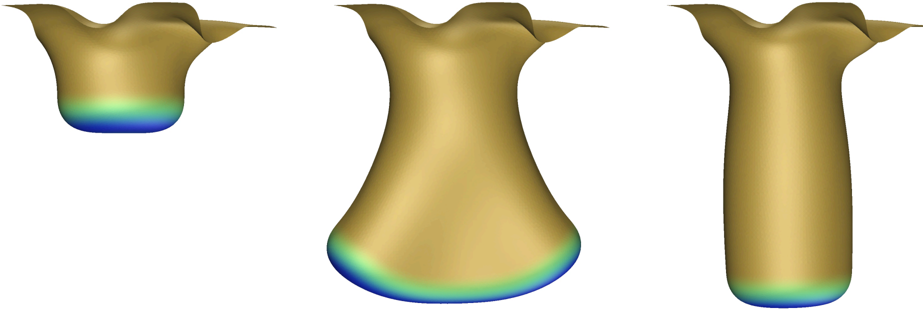
$v_{max} = 0.8, v_{max} = 1.6$ and $v_{max} = 3.2$

Computational Experiment 2:- Etching in a circular pit



Crosssections for etching into circular pit.
$v_{\max} = 1.0$,$t = 0.25$,$t = 0.5$ and $t = 0.75$

Computational Experiment 3:- Etching in a non symmetrical pit



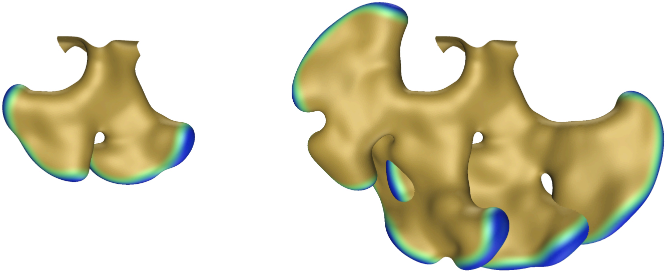
Constant bulk concentration

$t = 0.25$ and $t = 0.75$ for $v_{\max} = 1.0$ $\qquad$ $t = 1.5$ for $v_{\max} = 0.5$

Computational Experiment 4:- Fluctuations in the bulk and etching into single pit

Etching for a single pit, random bulk concentration, $t = 1.2$ and $t = 2.0$ for $v_{\max} = 0.4$

Computational Experiment 4:- Fluctuations in the bulk and etching into single pit, increasing dissolution rate



Etching for a single pit, random bulk concentration, $t = 0.3$ and $t = 0.5$ for $v_{\max} = 1.6$

ESFEM: Assorted Issues

- Remeshing
- Adaptivity
- Topological Change
- PDES in the Bulk coupled with PDEs on Surface

ESFEM Summary

- Formulation of Conservation on Evolving Surface
- Variational formulation of Advection-Diffusion
- Evolving Surface Finite Element Method (E.S.F.E.M.)
- Transport Property of Basis Functions

Level set tangential gradients

- Extension of ν to all of Ω by the normal vector field

$$\nu(x) = \frac{\nabla\Phi(x)}{|\nabla\Phi(x)|},\ x \text{ in } \overline{\Omega}.$$

- We define the projection

$$\mathcal{P}_\Phi := I - \nu \otimes \nu\ ,\ (\mathcal{P}_\Phi)_{ij} = \delta_{ij} - \nu_i\nu_j,\ \ i,j = 1, ...n+1.$$

- Thus $\mathcal{P}(x)$ is the projection onto the tangent space of the surface

$$\Gamma_r := \{y \in \mathbb{R}^{n+1} | \Phi(y) = r\}, r = \Phi(x),$$

so that

$$\mathcal{P}_\Phi \nu = 0.$$

Level set tangential gradients

- Eulerian surface gradient

$$\nabla_\Phi \eta := \mathcal{P}_\Phi \nabla \eta$$

- $$\nabla_\Phi \eta = \nabla \eta - \nabla \eta \cdot \nu \, \nu$$

  where $\nabla \eta$ denotes the usual gradient on $\mathbb{R}^{n+1}$.

- $$\nabla_\Phi \eta \cdot \nu = 0$$

- For any level surface Γ_r,

$$\nabla_{\Gamma_r} \eta := \nabla_\Phi \eta|_{\Gamma_r}$$

  only depends on the values of η restricted to Γ_r and is the tangential (surface) gradient on Γ_r.

Level set

- PDE formulation Bertalmio, Cheng, Osher and Sapiro
- Eulerian formulation for solving partial differential equations along a moving interface Jian-Ju Xu and Hong-Kai Zhao
- Transport and diffusion of material quantities on propagating interfaces via level set methods D. Adalsteinsson and J. A. Sethian
- Fourth order equations finite differences Greer, Bertozzi and Sapiro
- Interfacial flows with surfactant Xu, Li, Lowengrub, Zhao
- Elliptic finite element method Burger
- Second and fourth order parabolic equations on static surfaces Dziuk and Elliott
- Analysis of elliptic equations Deckelenick, Dziuk and Elliott
- Parabolic equations on evolving surfaces Dziuk and Elliott

Phase field/Diffuse Interface approach

- Diffusion induced grain boundary motion Cahn, Fife, Penrose, Ch. E, Deckelnick, Styles
- Generalised diffuse interface approach Ratz, Voigt

UNFEM (unfitted finite element method) for Surface PDES

Use $n + 1$ dimensional triangulations and compute integrals on n dimensional surfaces Olshanskii, Reusken

Conservation and diffusion on evolving level sets

- Let $v : \Omega_T \to \mathbb{R}^{n+1}$ be a prescribed velocity field which has the decomposition
$$v = V\nu + v_{\mathcal{S}}, \quad V = v \cdot \nu$$
- By a dot we denote the material derivative of a scalar function $\eta = \eta(x,t)$ defined on Ω_T:
$$\dot{\eta} = \frac{\partial \eta}{\partial t} + v \cdot \nabla \eta.$$

Implicit surface Leibniz Formula

Let ϕ be a level set function and η be an arbitrary function defined on $\Omega_T = \Omega \times (0, T)$ such that the following quantities exist.

$$\frac{d}{dt} \int_{\Omega} \eta |\nabla \phi| = \int_{\Omega} \{\dot{\eta} + \eta \nabla_{\phi} \cdot v\} |\nabla \phi| - \int_{\partial\Omega} \eta v \cdot \nu_{\partial\Omega} |\nabla \phi|.$$

Here the level sets of ϕ move with the given velocity $V\nu$, $x \in \Omega$, $t > 0$.

Eulerian variational diffusion on evolving surfaces

- Find a solution $u = u(x, t)$ such that $u(\cdot, 0) = u_0$ for given initial data u_0 and

$$\frac{d}{dt}\int_\Omega u\eta|\nabla\phi| + \int_\Omega D_0\nabla_\phi u \cdot \nabla_\phi\eta|\nabla\phi| = \int_\Omega u\dot{\eta}\,|\nabla\phi|$$

for all $\eta \in H^1_\phi(\Omega)$.

- The co-area formula leads to the classical form of the PDE

$$\dot{u} + u\nabla_\phi \cdot v - \nabla_\phi \cdot (D_0\nabla_\phi u) = 0$$

on $\Omega \times (0, T)$ and the natural boundary condition.

$$(D_0\nabla_\phi u + uv) \cdot \nu_{\partial\Omega} = 0$$

on $\partial\Omega \times (0, T)$.

Elliptic Equation

$$-\Delta_\Phi u + u = f \ , x \in \Omega$$

$$\partial\Omega = \{\Phi = \Phi_m\} \cup \{\Phi = \Phi_M\}$$

Regularity

- $f \in L^2_\Phi(\Omega)$ implies $u \in H^1_\Phi(\Omega)$
- $f_\nu \in L^2_\Phi(\Omega)$ implies $u_\nu \in H^1_\Phi(\Omega)$

Linear diffusion

Setting $w = u$ and $\mathcal{D} = \mathcal{I}$ we find the heat equation on surfaces

$$u_t = \Delta_\Phi u$$

and the variational equation becomes

$$\frac{d}{dt}\int_\Omega u\eta|\nabla\Phi| + \int_\Omega \nabla_\Phi u \cdot \nabla_\Phi \eta|\nabla\Phi| = 0.$$

Simple examples

- $$u_t = u_{xx} + f(x,y)\ ,\ \ (x,y) \in (0,1)^2\ ,\ \ t > 0$$

- $$u_t = \frac{1}{r^2} u_{\theta\theta} + f(r,\theta)\ ,\ \ 0.5 < r < 1\ ,\ \ t > 0$$

Steady solution

$$u_t - \Delta_\Phi u = 0$$

with no flux boundary conditions has the steady solution

$$u_\infty|_{\Gamma_r} = \frac{1}{|\Gamma_r|} \int_{\Gamma_r} u_0$$

so that

$$u_\infty = g(\Phi).$$

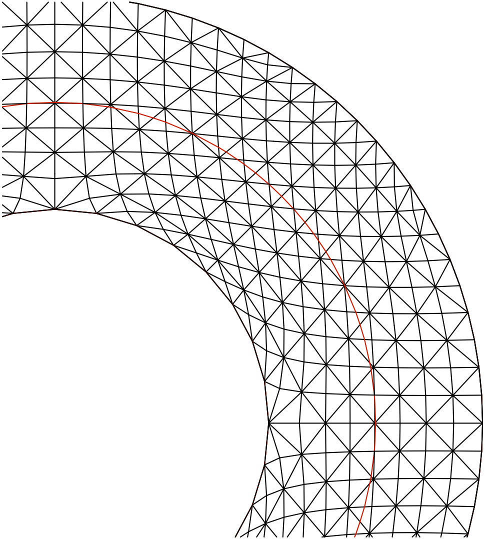
Heat equation on a circle

- $\Omega = \{x \in \mathbb{R}^2 |\, 0.5 < |x| < 1.0\}$
- $\Phi(x) = |x| - 0.75$ so that the boundary $\partial\Omega$ comprises level lines of Φ.
- $u(x,t) = \exp\left(-t/|x|^2\right) x_2/|x|$
- is an exact solution of

  $$u_t - \Delta_\Gamma u = 0$$

  on $\Gamma(t) = \Gamma_0 = \{x \in \mathbb{R}^2 |\, |x| = 0.5\}$
- with initial data $u_0(x) = x_2/|x|$.

Mesh



Heat equation on a circle

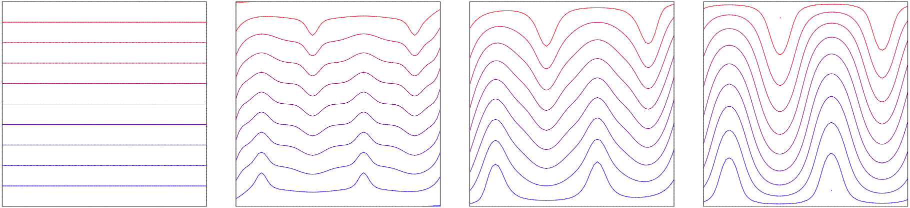
h	$L^\infty(L^2_\Phi(\Omega))$	eoc	$L^2(H^1_\Phi(\Omega))$	eoc	$L^2(H^1(\Omega))$	eoc	$L^\infty(L^\infty(\Omega))$	eoc
0.5176	0.07401	-	0.1090	-	0.09565	-	0.1139	-
0.2831	0.02594	1.74	0.03986	1.67	0.1325	0.93	0.04539	1.52
0.1500	0.007796	1.89	0.01587	1.45	0.07188	0.96	0.01696	1.55
0.07716	0.002192	1.91	0.007147	1.20	0.03879	0.93	0.006144	1.53
0.03912	0.0006067	1.89	0.003438	1.08	0.02042	0.95	0.002333	1.43
0.01969	0.0001694	1.86	0.001699	1.03	0.01061	0.95	0.0009357	1.33

h	$L^\infty(L^2_\Phi(\Gamma_0))$	eoc	$L^2(H^1_\Phi(\Gamma_0))$	eoc	$L^\infty(L^\infty(\Gamma_0))$	eoc
0.5176	0.07401	-	0.0874	-	0.06148	-
0.2831	0.03142	1.77	0.04512	1.10	0.02389	1.57
0.1500	0.009560	1.88	0.02653	0.84	0.009116	1.52
0.07716	0.002690	1.91	0.01149	1.26	0.002446	1.98
0.03912	0.0006343	2.13	0.006237	0.90	0.0005447	2.21
0.01969	0.0001484	1.89	0.002943	1.10	0.0001484	1.89

Level sets mapped to level sets

- Homogeneous Neumann boundary conditions: solution is conserved on each level surface
- Solution u evolves to a stationary solution which is constant on each level line of Φ
- In this example $\Phi(x) = x_2 - 2(1 - x_2^2)\sin(0.3)\sin(2\pi x_1)$
- the initital value $u_0(x_1, x_2) = x_2$ on the domain $\Omega = (-1, 1) \times (-1, 1)$
- The function u becomes constant on the level lines of Φ

Level sets mapped to level sets



Level lines of the solution u for the time steps 0, 100, 400 and 5200. The last picture nearly shows the level lines of Φ. Levels between -1 and 1 equally spaced with increment 0.1 are shown.

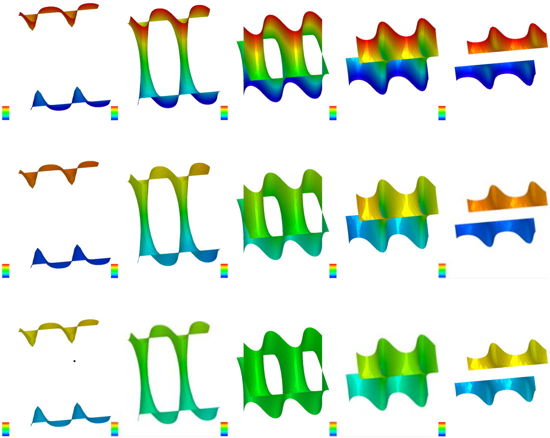
Level sets to level sets in 3-dim

- The computational domain is $\Omega = (-1, 1)^3$, and we use the level set function

$$\Phi(x_1, x_2, x_3) = x_1 x_3 - 2(1 - x_3^2) \sin 0.3 \sin(2\pi x_1).$$

- The initial value is taken to be $u_0(x_1, x_2, x_3) = x_2$.
- In the figures we show various level surfaces of Φ which are coloured according to the values of u_h at three time steps. The continuous solution tends to a constant on the levels of Φ.
- The colour coding is such that blue corresponds to the value -1, red to the value 1 with a linear scale between.

Level sets to level sets in 3-dim

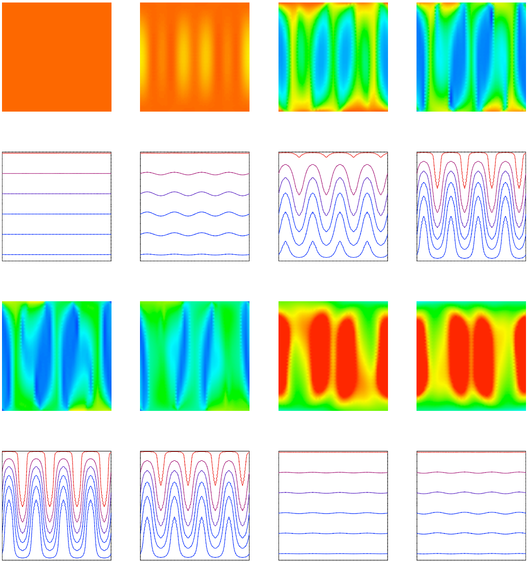


Level surfaces $\Phi = -0.75, -0.5, 0.0, 0.5, 0.75$ with colouring according to the values of u_h: 0 time step,1000-th time step, 3900-th time step.

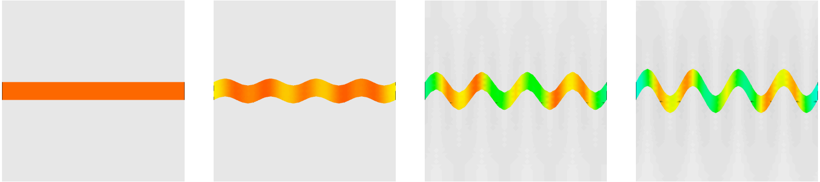
We choose $\Omega = (-1,1)^2$ and constant initial data $u_0(x_1,x_2) = 1$. The level set function is given by

$$\Phi(x_1,x_2,t) = x_2 - (1 - x_2^2)\sin(\pi x_1)\sin(t),$$

and we used $\tau = 0.000390625$ and $h = 0.0625$. We show the solution for times from one period of the level set function Φ. The time dependent levels of Φ are shown in the same Figure. In the second Figure we show the solution on the strip $\Omega_\delta = \{x \in \Omega \,|\, |\Phi(x,t)| < \delta\}$ for $\delta = 0.1$ for some time steps to demonstrate the effect of "heating by motion".

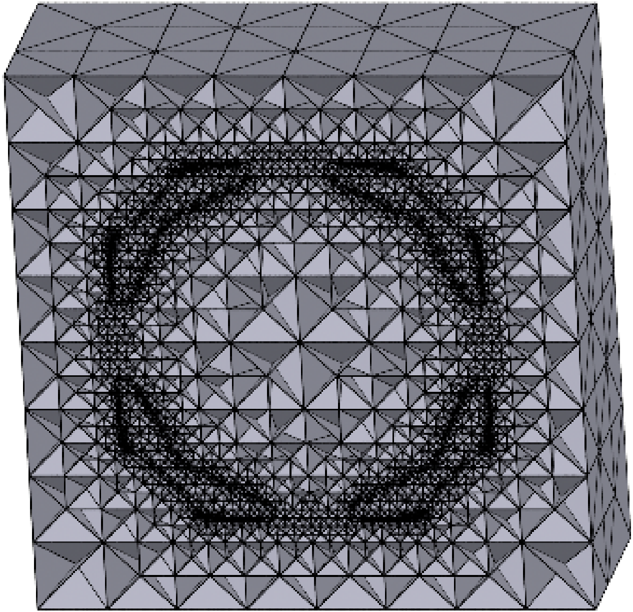


Solution (1st and 3rd row) with levels of Φ (2nd and 4th row) for the times $t = 0.0, 0.039, 0.426, 0.813, 1.59, 2.36, 3.13$ and 6.26. Blue=-0.1, Red =1.1.

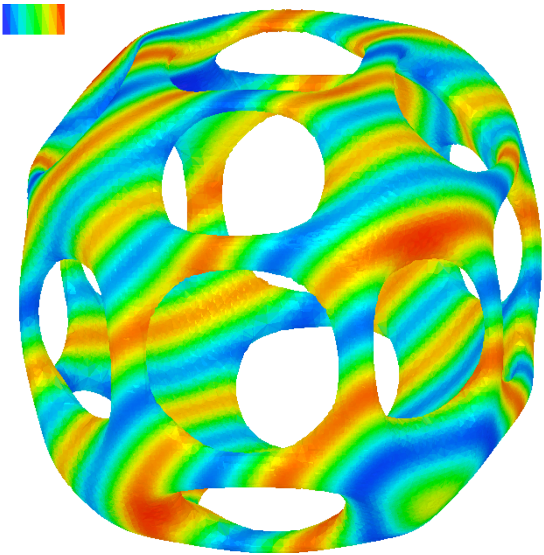


Solution of Example 9 for the times $t = 0.0, 0.039, 0.078, 0.12$ and 0.16 on the strip Ω_δ.

Narrow Band:-Three Dimensional Grid



Narrow Band:-Solution



Conclusion: Implicit surfaces

- Mesh can be independent of geometry
- Data may be given on and as a level surface
- Application may demand a solution on many level surfaces
- Complicated morphology

- Data requires extension off the surface
- One space dimension higher so solve in narrow band–not quite geometry independent mesh
- Discrete solution is not local