Computation of geometric flows

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- Working fields: Numerical methods for geometric PDEs, PDEs on surfaces, including moving surfaces, applications.
- Group: C. Eilks, H. Fritz, P. Pozzi, Ph. Reiter, J. Steinhilber.
- Collaborations: K. Deckelnick (Magdeburg), C. M. Elliott (Warwick), D. Kröner (Freiburg), Chr. Lubich (Tübingen).
- DFG Research Center SFB TR 71 "Geometric partial differential equations" (Freiburg, Tübingen, Zürich).
- Survey article: "Computation of geometric PDEs and mean curvature flow." (Deckelnick, Dziuk, Elliott), Acta Numerica (2005) 14, 139–232.

Outline of this talk

- Applications of geometric flows.
- Discretization techniques for geometric flows.
  - Piecewise polynomial surfaces.
  - Discrete spaces on discrete surfaces.
  - Approximation of curvature and the second fundamental form.
  - Consistent approximation of geometric functionals.
- Computational Willmore flow.
  - An adequate form of the first variation of the Willmore functional.
  - Willmore flow.
  - Stability and convergence results.
  - Numerical tests.
- Approximation of Ricci curvature.

The standard geometric functionals

Area functional $$A(\Gamma) = \int_\Gamma 1$$

The classical bending energy of Γ:

Willmore functional $$W(\Gamma) = \frac{1}{2}\int_\Gamma H^2$$

Area in Finsler geometry:

Anisotropic area $$A_\gamma(\Gamma) = \int_\Gamma \gamma(\nu)$$

$\gamma : S^n \to (0,\infty)$ is a given function. ν is the normal to Γ.

Crystal growth (Anisotropic mean curvature flow):

Kinetic PDE on the free boundary - forced anistropic mean curvature flow.

Forced strongly anisotropic mean curvature flow

The mathematical model contains the Gibbs-Thomson law on the phase boundary. The underlying geometric functional is anisotropic area. γ is a given function which models the anisotropic structure of the material.

Dealloying (Mean curvature flow)

Production of a nanoporous gold sponge from a binary Ag-Au alloy. Dealloying by surface dissolution. The gold atoms diffuse on the surface, agglomerate in clusters and expose the next layer of silver atoms for dissolution. The bulk introduces new gold atoms into the system. Etching: Inhomogeneous mean curvature flow.

$$v = R(u)(1 - \delta H)\nu$$

Conservation and diffusion on the surface: Cahn-Hilliard equation on the moving surface. [Eilks, Elliott 2008]

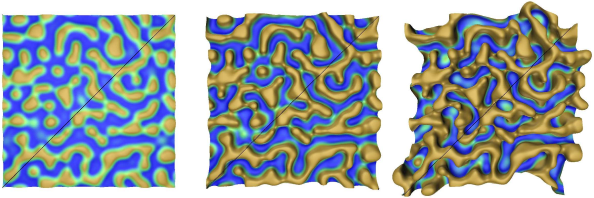
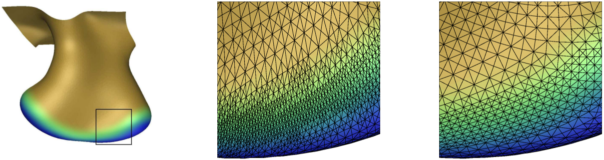


Image processing (Willmore flow): Reconstruction of surfaces.

[Clarenz, Diewald, D., Rumpf, Rusu: 2004]

Numerical tools, remeshing: A harmonic map $\varphi : \Gamma \to \mathbb{R}^2$ was computed. The inverse (conformal) map was used to transfer a good grid onto the surface.



[Eilks, 2009]

Modelling of cell membranes (Willmore functional)

The main part of the energy for a cell membrane Γ is modelled by the Helfrich energy.

$$W_0(\Gamma) = \frac{1}{2}\int_\Gamma \alpha(H - H_0)^2 + \int_\Gamma \beta K$$

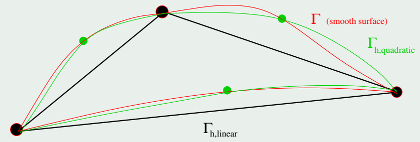
with mean curvature H and Gaussian curvature K of Γ. H_0 is a given "spontaneous curvature".

Principles for a good discretization

- The discretization must be valid for all dimensions and all codimensions.
- Approximation of surfaces by piecewise polynomial surfaces.
- Consistent approximation of the geometric functionals.
- Computability of the first variation of the functional for discrete surfaces. The linear systems to be solved in each time step after time discretization should be sparse, symmetric and positive definite.
- We should have - if possible - an n-dimensional algorithm for an n-dimensional surface.

Discrete surfaces

The given smooth surface Γ is approximated by a piecewise polynomial surface Γ_h interpolating points on the smooth surface.



The discrete surface Γ_h then consists of curved n-simplices T_h,

$$\Gamma_h = \bigcup_{T_h \in \mathcal{T}_h} T_h,$$

which form an admissible triangulation $\mathcal{T}_h$ with maximal grid size h.

Lemma (Approximation of the surface)

Assume that Γ_h is the interpolation of Γ by polynomials of degree s. Then

$$\|d\|_{L^\infty(\Gamma_h)} \le ch^{s+1},$$
$$\|\nu - \nu_h\|_{L^\infty(\Gamma_h)} \le ch^s,$$
$$|1 - \delta_h| \le ch^{s+1}, \quad dA = \delta_h \, dA_h.$$

$d(x)$ is the oriented distance from x to Γ and $\nu(x) = \nabla d(x)$.

Note, that the discrete surface Γ_h is only Lipschitz – also for higher order polynomial approximation! The normal vectors are discontinuous.

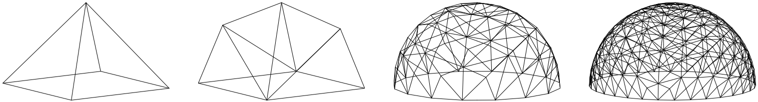
The most important case is the piecewise linear approximation $s = 1$.

There is a *theoretical* equivalence between

Γ_h as an n−dimensional triangulation sitting in some $\mathbb{R}^m$	Γ_h as given by piecewise polynomial discrete charts
Γ_h is given by the vertices of the triangulation plus topology	Γ_h is given by maps
Use function spaces on Γ_h	Use function spaces given in local coordinates
Direct implementation in existing software is possible	Write an overhead for the discrete geometry

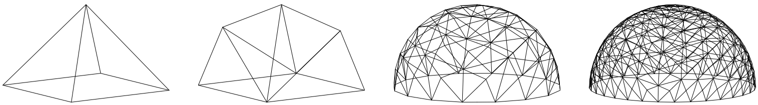
But *practically* there is a difference.

What is the mean curvature of a polyhedral surface?

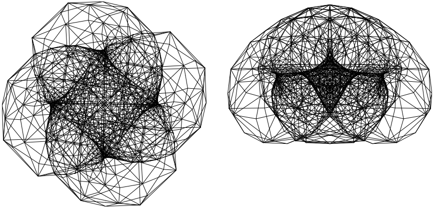


Successively refined grids approximating a half sphere.

What is the mean curvature of a polyhedral surface?



Successively refined grids approximating a half sphere.



Polyhedral approximation to a Willmore sphere.

Piecewise linear finite elements

We introduce useful finite dimensional function spaces on the discrete (polygonal) surface Γ_h, which consists of n-simplices T_h,

$$\Gamma_h = \bigcup_{T_h \in \mathcal{T}_h} T_h,$$

forming an admissible triangulation $\mathcal{T}_h$ with maximal grid size h. The most simple finite element space is:

$$S_h = \left\{ \eta \in C^0(\Gamma_h) \middle| \, \eta\big|_{T_h} \in \mathbb{P}_1(T_h), T_h \in \mathcal{T}_h \right\}.$$

A basis of S_h is given by the common nodal basis functions

$$\phi_j : \Gamma_h \to \mathbb{R}, \quad \phi_j \in S_h, \quad \phi_j(a_i) = \delta_{ij}$$

with the vertices (nodes) a_i of Γ_h.

The identity trick

We use the identity map on the surface Γ:

$$u = id_\Gamma, \quad u(x) = x \text{ for } x \in \Gamma$$

and write $A(\Gamma) = A(u) = \int_\Gamma 1$

Lemma

The first variation of the area functional at u in direction φ is given by

$$\langle A'(u), \varphi \rangle = \int_\Gamma \nabla_\Gamma \cdot \varphi = \int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \varphi$$

Here $\varphi : \Gamma \to \mathbb{R}^{n+1}$ is an arbitrary function.

$$\langle A'(u), \varphi \rangle = -\int_\Gamma \Delta_\Gamma u \cdot \varphi = \int_\Gamma H\nu \cdot \varphi$$

The approximation of mean curvature

So, for all test functions φ we have for the mean curvature vector $v = -H\nu$:

$$\int_\Gamma v \cdot \varphi = -\int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \varphi = -\sum_{i,k=1}^{n+1} \int_\Gamma (\nabla_\Gamma)_i \, u_k \, (\nabla_\Gamma)_i \, \varphi_k$$

For a discrete surface Γ_h we define the discrete curvature vector $v_h \in S_h^{n+1}$ by that equation:

$$\int_{\Gamma_h} v_h \cdot \varphi_h = -\int_{\Gamma_h} \nabla_{\Gamma_h} u_h : \nabla_{\Gamma_h} \varphi_h \quad \text{for all } \varphi_h$$

Formally we have written $u_h(x) = x$ for $x \in \Gamma_h$.

The bad news

Question: Does the discrete curvature vector v_h approximate the continuous curvature vector v? Answer: Yes, ...

Lemma

For a polygonal surface and for piecewise linear finite elements we have the estimate

$$\|v - v_h^l\|_{H^{-1,\infty}(\Gamma)} \leq ch.$$

$H^{-1,\infty}(\Gamma)$ *is the dual space of* $H^{1,1}(\Gamma)$.

... but only in a very weak norm.

For $n \geq 2$ the mean curvature vector is not approximated pointwise or in $L^1(\Gamma)$.

Similarly we can approximate the Weingarten map $\mathcal{H} = \nabla_\Gamma \nu$ on Γ. For this we use

$$\int_\Gamma \eta \mathcal{H}_{ik} = \int_\Gamma \eta \left(\nabla_\Gamma\right)_i \nu_k = -\int_\Gamma \nu_k \left(\nabla_\Gamma\right)_i \eta + \int_\Gamma \eta H \nu_i \nu_k$$

for every test function η. The right hand side of this equation is well defined for Lipschitz surfaces too, so that we define the discrete Weingarten map $\mathcal{H}_h \in S_h^{(n+1)\times(n+1)}$ by

$$\int_{\Gamma_h} \eta_h \mathcal{H}_{h,ik} = -\int_{\Gamma_h} \nu_{h,k} \left(\nabla_{\Gamma_h}\right)_i \eta_h + \int_{\Gamma_h} v_{h,i} \nu_{h,k} \eta_h \quad \forall \eta_h \in S_h$$

where we used the discrete mean curvature vector v_h.

Consistency test

The sphere $\Gamma = S^2$ has Willmore energy

$$W(u) = 8\pi \approx 25.1327$$

Approximate the smooth sphere by a discrete sphere Γ_h and calculate its Willmore energy according to

$$W(u_h) = \frac{1}{2}\int_{\Gamma_h} |v_h|^2,$$

where

$$\int_{\Gamma_h} v_h \cdot \psi_h = -\int_{\Gamma_h} \nabla_{\Gamma_h} u_h : \nabla_{\Gamma_h} \psi_h \quad \forall \psi_h \in S_h^3$$

N	h	$W(u_h)$	$W(u) - W(u_h)$
34	0.707106	21.064188	0.161882
130	0.513578	25.022492	0.00438645
514	0.280935	26.140487	-0.0400971
2050	0.143613	26.428208	-0.0515452
8194	0.0722037	26.501071	-0.0544443
32770	0.0361516	26.519625	-1.386889

No Consistency! The Willmore functional is not approximated.

Choose for u_h a Ritz type projection of u.

$$\int_{\Gamma_h} \nabla_{\Gamma_h} u_h : \nabla_{\Gamma_h} \psi_h = \int_{\Gamma_h} \nabla_{\Gamma_h} u^{-l} : \nabla_{\Gamma_h} \psi_h, \quad \forall \psi_h \in S_h^3$$

$$\int_{\Gamma_h} u_h = \int_{\Gamma_h} u^{-l}.$$

Here for $x \in \Gamma_h$

$$u^{-l}(x) = u(a(x)) = a(x)$$

with $a(x)$ being the orthogonal projection of the point x onto the smooth surface Γ.

N	h	$W(u_h)$	$W(u) - W(u_h)$	eoc
34	0.707106	14.685165	10.447570	–
130	0.513578	21.843107	3.289628	3.6
514	0.280935	24.248481	0.884255	2.2
2050	0.143613	24.906125	0.226610	2.0
8194	0.0722037	25.075551	0.0571843	2.0
32770	0.0361516	25.118388	0.0143478	2.0

Consistency!

Theorem

Assume that Γ is sufficiently smooth. Let u_h be the "Ritz" projection of u and calculcate the discrete curvature vector v_h as

$$\int_{\Gamma_h} v_h \cdot \psi_h = -\int_{\Gamma_h} \nabla_{\Gamma_h} u_h : \nabla_{\Gamma_h} \psi_h \quad \forall \psi_h \in S_h^{n+1}.$$

Then the curvature vector $v = -H\nu$ is approximated,

$$\|v - v_h^l\|_{L^2(\Gamma)} \leq ch,$$

and the Willmore functional is approximated,

$$|W(u) - W(u_h)| \leq ch^2.$$

The constants c depend on $\|v\|_{H^2(\Gamma)}$ and thus on the fourth derivatives of the parametrization of the surface Γ.

Mean curvature flow: the good news

For given initial surface Γ_0 and $u_0 = id_{\Gamma_0}$ determine $u : G_T \to \mathbb{R}^{n+1}$ so that $u(\cdot, t) = id_{\Gamma(t)}$, $u = u_0$ on $\Gamma_0 \times \{0\}$ and

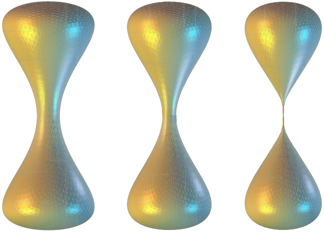
$$\int_\Gamma \dot{u} \cdot \varphi = -\langle A'(u), \varphi \rangle \quad \forall \varphi$$

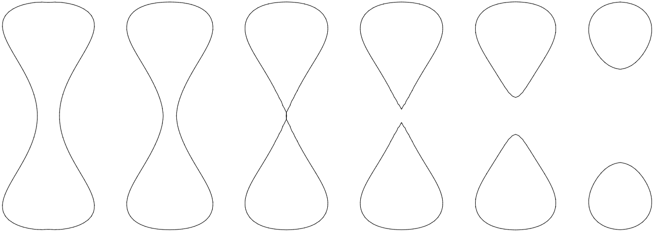
on G_T. Or equivalently

Mean curvature flow

$$\int_\Gamma \dot{u} \cdot \varphi + \int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \varphi = 0 \quad \forall \varphi$$

This is an equation in a dual space! Therefore the mean curvature vector has only to be approximated in a dual space.





Calculation of the first variation of the Willmore functional

Again use the mean curvature vector $v = -H\nu$ in weak form,

$$\int_\Gamma v \cdot \psi + \int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \psi = 0 \qquad \forall \psi.$$

Note that this equation can be understood as defining v as the L^2-projection of the functional $\Delta_\Gamma u$. Or as

$$(v, \psi)_{L^2(\Gamma)} = -\langle A'(u), \psi \rangle \qquad \forall \psi$$

with the area functional $A = |\Gamma|$.

With

$$u_\epsilon = u + \epsilon\varphi, \qquad u_\epsilon = id_{\Gamma_\epsilon}$$

and v_ϵ defined by

$$\int_{\Gamma_\epsilon} v_\epsilon \cdot \psi + \int_{\Gamma_\epsilon} \nabla_{\Gamma_\epsilon} u_\epsilon : \nabla_{\Gamma_\epsilon} \psi = 0 \quad \forall \psi$$

we get

$$\begin{aligned} \langle W'(u), \varphi \rangle &= \frac{d}{d\epsilon} W(u_\epsilon)\Big|_{\epsilon=0} = \frac{1}{2} \frac{d}{d\epsilon} \int_{\Gamma_\epsilon} |v_\epsilon|^2 \Big|_{\epsilon=0} \\ &= \int_\Gamma v \cdot \frac{d}{d\epsilon} v\Big|_{\epsilon=0} + \frac{1}{2} \int_\Gamma |v|^2 \nabla_\Gamma \cdot \varphi \end{aligned}$$

Differentiate

$$\int_{\Gamma_\epsilon} v_\epsilon \cdot \psi + \int_{\Gamma_\epsilon} \nabla_{\Gamma_\epsilon} u_\epsilon : \nabla_{\Gamma_\epsilon} \psi = 0$$

with respect to ϵ and get

$$\int_\Gamma \frac{d}{d\epsilon} v\Big|_{\epsilon=0} \cdot \psi + v \cdot \psi \nabla_\Gamma \cdot \varphi + \int_\Gamma \nabla_\Gamma \varphi : \nabla_\Gamma \psi + \nabla_\Gamma \cdot \psi \nabla_\Gamma \cdot \varphi - D(\varphi) \nabla_\Gamma u : \nabla \psi = 0$$

with the symmetric tensor

$$D(\varphi)_{ij} = (\nabla_\Gamma)_i \varphi_j + (\nabla_\Gamma)_j \varphi_i$$

Then finally choose $\psi = v$.

Lemma (D. 2007)

Let v *be given by* ↙ $v = -\Delta_\Gamma u$

$$\int_\Gamma v \cdot \psi + \int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \psi = 0 \qquad \forall \psi.$$

Then the first variation of the Willmore functional is given as

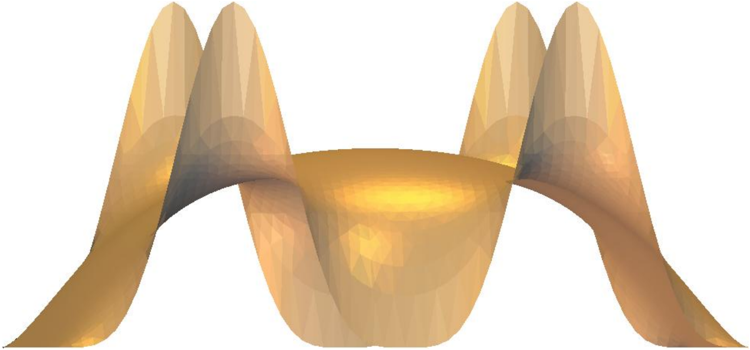
$$\langle W'(u), \varphi \rangle = -\frac{1}{2} \int_\Gamma |v|^2 \nabla_\Gamma \cdot \varphi - \int_\Gamma \nabla_\Gamma v : \nabla_\Gamma \varphi - \int_\Gamma \nabla_\Gamma \cdot v \nabla_\Gamma \cdot \varphi + \int_\Gamma D(\varphi) \nabla_\Gamma u : \nabla_\Gamma v$$

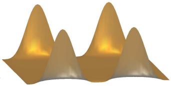
Here, $\varphi : \Gamma \to \mathbb{R}^{n+1}$ is an arbitrary variation in space and

$$D(\varphi)_{ij} = (\nabla_\Gamma)_i \varphi_j + (\nabla_\Gamma)_j \varphi_i$$

. No second derivatives appear in this formula!

A Willmore surface with prescribed boundary and mean curvature zero on the boundary.





Variational form of Willmore flow

For given initial value u_0 determine u and v such that $u = id_\Gamma$ and

$$\int_\Gamma \dot{u} \cdot \varphi - \int_\Gamma \nabla_\Gamma v : \nabla_\Gamma \varphi + \int_\Gamma \nabla_\Gamma v : D(\varphi) \nabla_\Gamma u - \int_\Gamma \nabla_\Gamma \cdot v \nabla_\Gamma \cdot \varphi - \frac{1}{2} \int_\Gamma |v|^2 \nabla_\Gamma \cdot \varphi = 0$$

$$\int_\Gamma v \cdot \psi + \int_\Gamma \nabla_\Gamma u : \nabla_\Gamma \psi = 0$$

for all φ, ψ.

Stability

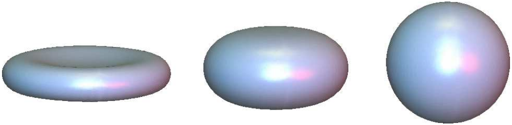
Theorem

Assume that u_h, v_h is a solution of the discrete Willmore flow. Then the energy relation

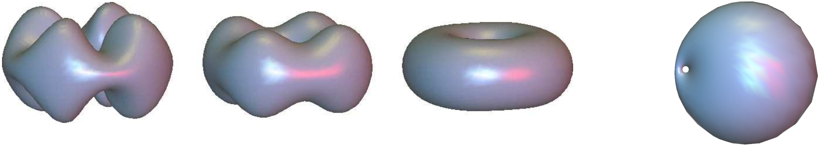
$$\int_{\Gamma_h} |\dot{u}_h|^2 + \frac{1}{2}\frac{d}{dt}\int_{\Gamma_h} |v_h|^2 = 0$$

holds. Thus we have stability of the spatially discrete scheme in adequate norms.

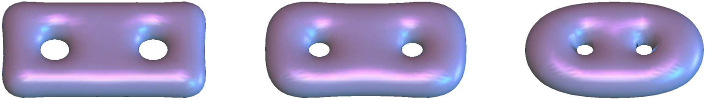
The proof follows directly from the consistent derivation of the algorithm (for Lipschitz surfaces!).



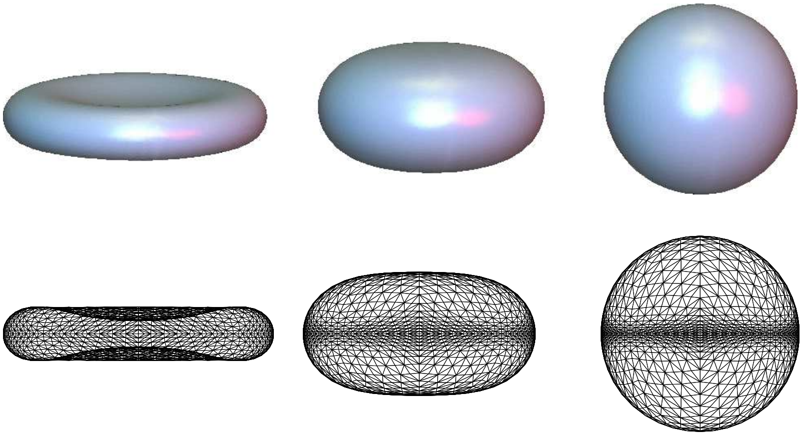
Willmore flow towards a sphere.



Willmore flow towards a Clifford torus



Evolution of a double torus under Willmore flow



Willmore flow towards a sphere. Surface at times $t = 0.001755$, $t = 0.01053$ and $t = 0.04387$.

Some references for numerical methods for Willmore flow

L. Hus, R. Kusner, J. Sullivan (1992): Minimization of Willmore energy with Brakke's surface evolver program.
A. Polden (1996): Analysis and numerics for the elastic flow of planar curves.
R. Rusu (2001): Finite element algorithm for Willmore flow.
U. F. Mayer, G. Simonett (2002): Finite differences for axisymmetric surfaces.
G. D., E. Kuwert, R. Schätzle (2002): Elastic flow of curves.
M. Droske, M. Rumpf (2003): Finite element algorithm for Willmore flow of level sets.
A. Bobenko, P. Schroeder (2005): Definition of a discrete Willmore energy, discrete Willmore flow.
K. Deckelnick, G. D. (2006): Convergence and estimates of the error for graphs.
J. W. Barrett, H. Garcke, R. Nürnberg (2007): Discretization of the Weingarten map, automatic redistribution of the surface nodes.
G. D. (2007): Stable algorithm for parametric Willmore flow.

K. Deckelnick, G. D. (2007): convergence and estimates of the error for curves.

Theorem (Deckelnick, G. D., 2007)

Let (u, v) be the solution of Willmore flow for curves on the time interval $(0, T]$. Then the spatially discrete solution (u_h, v_h) exists on the same time interval $(0, T]$ and for the error we have:

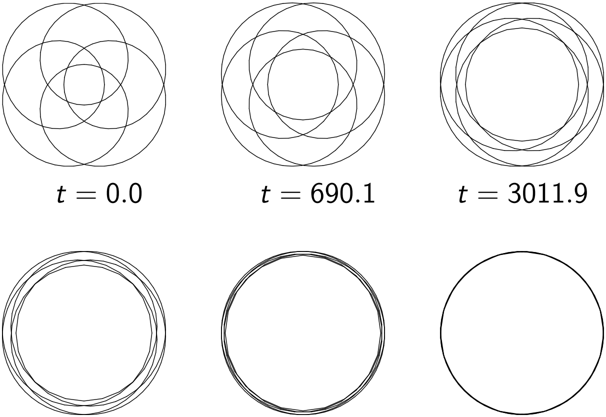
$$\sup_{t\in[0,T]} \|u(\cdot,t) - u_h^l(\cdot,t)\|_{H^1(\Gamma(t))} \leq Ch,$$

$$\sup_{t\in[0,T]} \|v(\cdot,t) - v_h^l(\cdot,t)\|_{L^2(\Gamma(t))} \leq Ch$$

$$\int_0^T \|v(\cdot,t) - v_h^l(\cdot,t)\|^2_{H^1(\Gamma(t))} dt \leq Ch^2$$

for all $0 < h \leq h_0$. The constant C depends on T, $\inf_{(0,2\pi)} |U_{0\theta}|$ and on higher norms of the solution u of the continuous problem.

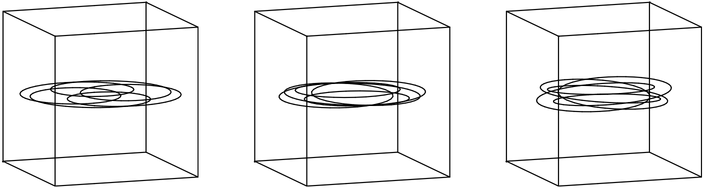
Evolution of a planar hypocycloid.



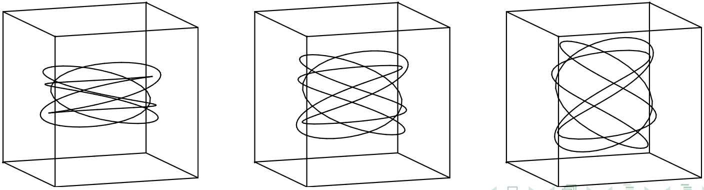
$t = 0.0$ $t = 690.1$ $t = 3011.9$

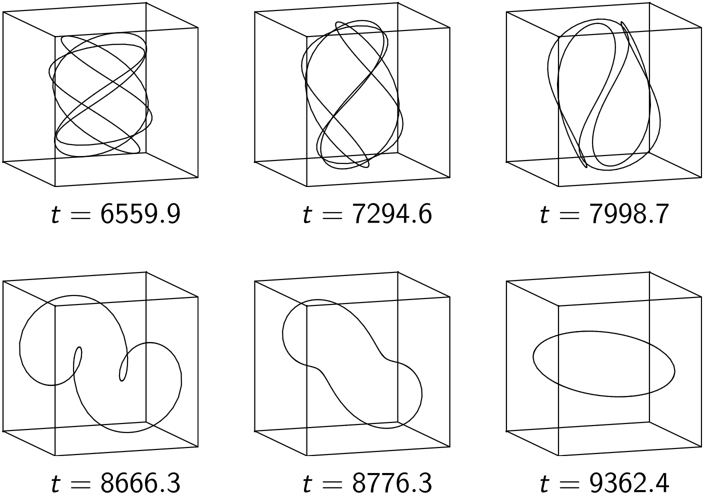
$t = 4930.5$ $t = 7889.5$ $t = 10441.2$

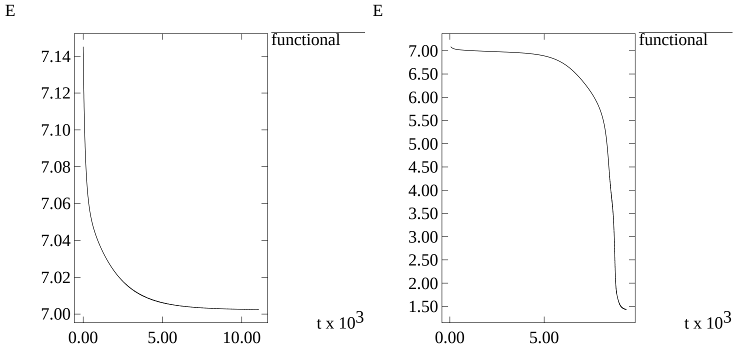
Evolution of a slightly vertically perturbed hypocycloid.



$t = 0.0$ $t = 1723.5$ $t = 3009.5$




$t = 6559.9$
$t = 7294.6$
$t = 7998.7$
$t = 8666.3$
$t = 8776.3$
$t = 9362.4$



Value of the functional during the evolution of a hypocycloid; planar (left) and vertically perturbed (right).

Weak formulation of Ricci curvature on isometrically embedded hypersurfaces

Goal: Definition and computation of a discrete Ricci curvature specially for the higher dimensional case without symmetry assumptions. Our approach is based on an idea of G. Huisken.

Definition

We define $Ric : \Gamma \longrightarrow \mathbb{R}^{(n+1)\times(n+1)}$ by

$$(RicY) \cdot X = ric(PY, PX)$$

for arbitrary vector fields X and Y. P is the projection to the tangent space.

Lemma

For all $X, Y \in H^1(\Gamma)^{n+1}$ *it holds*

$$\int_\Gamma (RicY) \cdot X$$
$$= \int_\Gamma (\nabla_\Gamma)_i (PY)_i (\nabla_\Gamma)_k (PX)_k - (\nabla_\Gamma)_i (PY)_k (\nabla_\Gamma)_k (PX)_i$$

We discretize with our standard methods.

Theorem (H. Fritz 2009)

For quadratically approximated smooth surface Γ *and second order finite elements one has the estimate*

$$\|Ric - Ric_h^l\|_{L^2(\Gamma)} \leq ch$$

with a constant depending only on Γ *but not on the grid size* h.

Numerical tests

DOFS	err_1	eoc_1	err_2	eoc_2	err_4	eoc_4
21 952	6.70e-01	0.42	7.42e-01	0.23	5.08e-01	0.35
174 976	4.89e-01	0.45	3.85e-01	0.94	2.30e-01	1.14
1 398 528	2.15e-01	1.18	1.47e-01	1.39	7.56e-02	1.61
11 185 664	7.76e-02	1.47	5.21e-02	1.50	2.36e-02	1.68
89 480 192	2.63e-02	1.56	1.72e-02	1.60	7.32e-03	1.69

Table: Degrees of freedom (*DOFS*), errors and experimental orders of convergence for the approximation of Ricci curvature (components 1, 2, 4) for the threedimensional surface Γ.

$$\Gamma = \{x \in \mathbb{R}^4 | \, (x_1 - x_2^2)^2 + x_2^2 + x_3^2 + x_4^2 = 1\}$$

We used the finite element program ALBERTA (A. Schmidt, K. G. Siebert).