Geometric finite element methods for oriented materials

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joint work with

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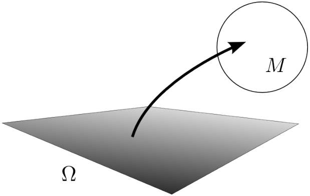
TECHNISCHE UNIVERSITÄT DRESDEN

Partial differential equations for functions

$$\phi : \Omega \to M, \qquad \Omega \subset \mathbb{R}^d,\ d \geq 1,$$

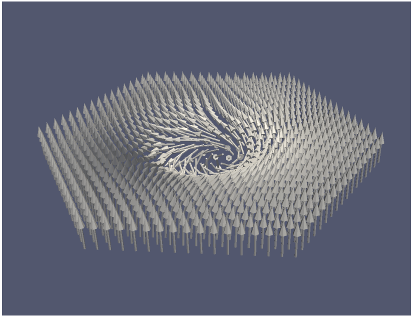
M a Riemannian manifold.



Applications:

- Cosserat shells and continua: S^2, SO(3)
- Liquid crystals: S^2, $\mathbb{PR}^2$, SO(3)
- σ-models: SU(2), SO(3)
- Image processing: S^2, Sym$^+(3)$
- Positivity-preserving systems: $\mathbb{R}^+$, Sym$^+(3)$
- [...]

The challenge: Nonlinear function spaces



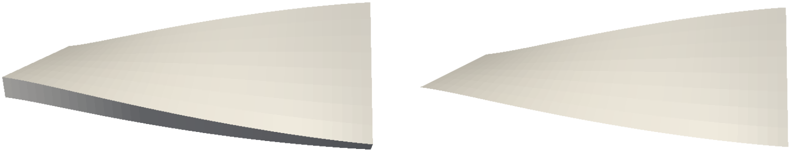
Quasi-particle in a magnetic material

- Maps $\mathbf{m} : \mathbb{R}^2 \to S^2$
- Minimizers of

$$E(\mathbf{m}) = \int_{\mathbb{R}^2} \left(\frac{1}{2} |\nabla \mathbf{m}|^2 + \kappa \, \mathbf{m} \cdot (\nabla \times \mathbf{m}) + \frac{h}{2} |\mathbf{m} - \mathbf{e}_3|^2 \right) dx$$

Dimensional reduction

- Model thin solid object by 2d equation

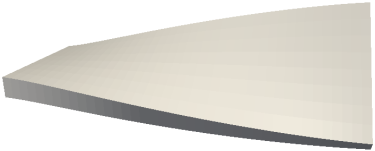


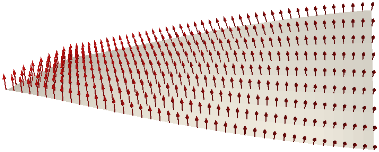
Kinematics:

- $\Omega \subset \mathbb{R}^2$
- Midsurface deformation: $m : \Omega \to \mathbb{R}^3$

Dimensional reduction

- Model thin solid object by 2d equation



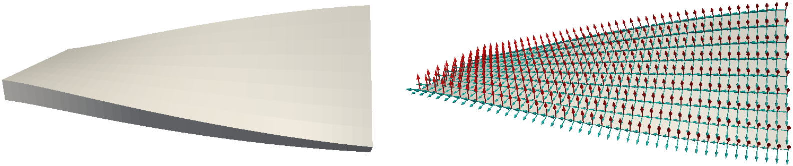


Kinematics:

- $\Omega \subset \mathbb{R}^2$
- Midsurface deformation: $m : \Omega \to \mathbb{R}^3$
- Direction field: $R : \Omega \to S^2$

Dimensional reduction

- Model thin solid object by 2d equation

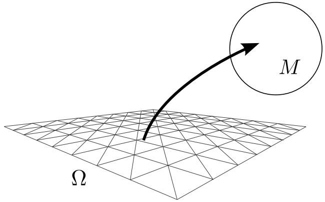


Kinematics:

- $\Omega \subset \mathbb{R}^2$
- Midsurface deformation: $m : \Omega \to \mathbb{R}^3$
- Microrotation field: $R : \Omega \to \mathrm{SO}(3)$

Partial differential equations for functions

$$\phi : \Omega \to M, \qquad \Omega \subset \mathbb{R}^d,\ d \geq 1, \qquad M \text{ a Riemannian manifold.}$$



Problem: Discretization

- Finite elements presuppose vector space structure
- But codomain M is nonlinear

Find a discretization that:

- works for any Riemannian manifold M
- is conforming
- is frame-invariant (i.e., equivariant under isometries of M)

Theorem ([Nash])

For each manifold M there exists a smooth, isometric embedding into a Euclidean space $\mathbb{R}^N$.

Algorithm

- Interpolate in $\mathbb{R}^N$
- Project back onto M

Theorem ([Grohs, Sprecher, S, in prep.])

Optimal discretization error bounds.

Properties

- Simple and fast, if an "easy" embedding/projection is given

The unit sphere S^m

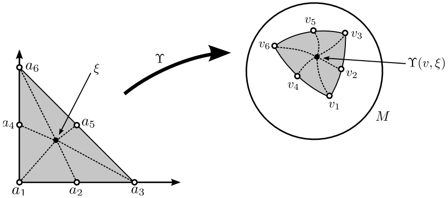
- $\mathbf{v} \mapsto \frac{\mathbf{v}}{|\mathbf{v}|}$

The special orthogonal group SO(3)

- Polar decomposition
  - Minimization property
  - Closed-form expression available, but unwieldy
  - Better: evaluate iteratively
- Gram–Schmidt orthogonalization
- Embed into quaternions – interpolate there

Symmetric positive definite matrices

- Open set in $\mathbb{R}^{m \times m}$
- Projection?



Reference element T_{ref}:

- Arbitrary type
- Coordinates ξ
- Lagrange nodes a_i, $i = 1, \dots, m$
- Shape functions $\{\varphi_i\}$ of p-th order

Lagrange interpolation:

Assume values $v_1, \dots, v_m \in M$ given at the Lagrange nodes.

If M is a vector space, interpolation between the v_i can be written as

$$\sum_{i=1}^{m} v_i \varphi_i(\xi) = \arg\min_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi) \|v_i - q\|^2.$$

Idea: Generalize

$$\arg\min_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi) \|v_i - q\|^2.$$

to

$$\arg\min_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi) \operatorname{dist}(v_i, q)^2$$

($\operatorname{dist}(\cdot, \cdot)$ being the Riemannian distance on M)

Definition (Geodesic interpolation [S '11, S '13, Grohs '12])

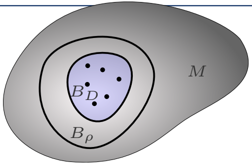
Let $v_i \in M$, $i = 1, \dots, m$ be coefficients and ξ coordinates on T_{ref}. Then

$$\Upsilon^p(v, \xi) = \arg\min_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi) \operatorname{dist}(v_i, q)^2$$

is the p-th order geodesic interpolation between the v_i.

Properties:

- Reduces to standard Lagrange interpolation if $M = \mathbb{R}^m$
- Reduces to geodesics if $d = 1$, $p = 1$ (hence the name)



Existence of minimizers of:

$$\arg\min_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi)\, \mathrm{dist}(v_i, q)^2$$

- $p = 1$: all weights $\varphi_i(\xi)$ are nonnegative $\longrightarrow$ [Karcher(1977)]
- $p > 1$: weights may become negative.

Idea:
There is a minimizer if the v_i are "close enough" to each other on M.

Theorem ([S '12, Hardering '15])

Denote by $B_r(p_0)$ the geodesic ball of radius r around $p_0 \in M$. There are constants D, ρ with $0 < D < \rho$, depending on the curvature of M and the total variation of the weights φ_i, such that if the values $v_1, \dots, v_m$ are contained in $B_D(p_0)$ for some $p_0 \in M$, then the minimization problem has a unique local minimizer in $B_\rho(p_0)$.

Differentiability:

Lemma ([S '11])

Under the assumptions of the previous theorem, the function $\Upsilon^p(v;\xi)$ is infinitely differentiable with respect to ξ and the v_i.

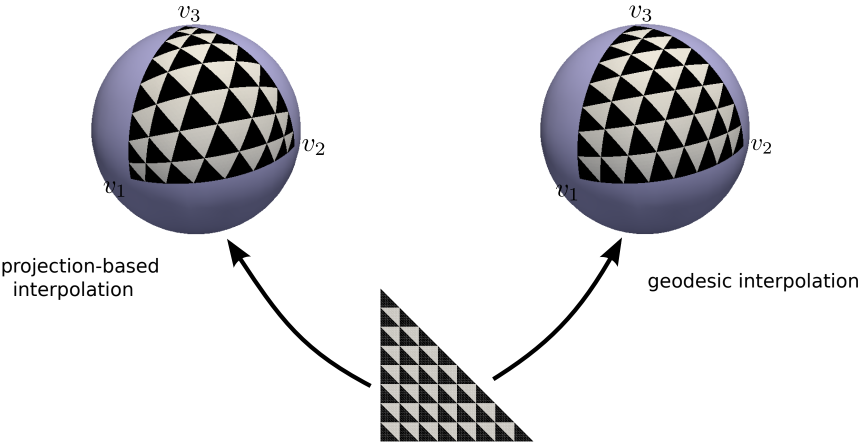
Objectivity: Equivariance under an isometric group action

Lemma (Objectivity, [S '10, S '13])

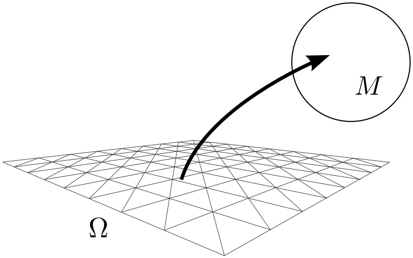
For any isometry Q acting on M and any $\xi \in T_{ref}$ we have

$$Q\Upsilon(v;\xi) = \Upsilon(Qv;\xi).$$

Consequence: Discretizations of frame-invariant models are frame-invariant.


v_3
v_2
v_1
v_3
v_2
v_1
projection-based interpolation
geodesic interpolation

Construct global finite element spaces:



Definition (Geodesic finite elements)

Let M be a Riemannian manifold and G a grid for a d-dimensional domain, $d \geq 1$. A geodesic finite element function is a continuous function $v_h : G \to M$ such that for each element T of G, $v_h|_T$ is given by geodesic interpolation on T.

Denote by V_h^M the space of all such functions.

Nonlinear Sobolev space:
Let M be smoothly embedded into $\mathbb{R}^m$. Define

$$H^1(\Omega, M) := \{v \in H^1(\Omega, \mathbb{R}^m) \mid v(s) \in M \text{ a.e.}\}$$

Conforming discretization:

Lemma ([S '11])

Geodesic finite elements are conforming, i.e.,

$$V_h^M \subset H^1(\Omega, M).$$

Minimize harmonic energy:

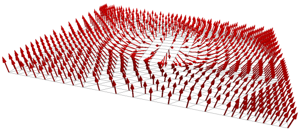
$$\phi : \Omega \to S^2, \qquad E(\phi) = \int_\Omega \|\nabla\phi\|^2 \, dx$$

Lemma

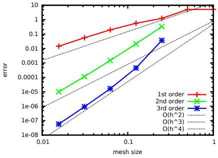
The inverse stereographic map minimizes E in its homotopy class.

Setup

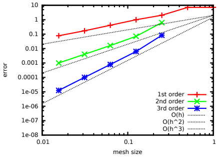
- Domain $\Omega = [-5, 5]^2$
- Dirichlet boundary conditions
- Discretization error for $d = 2$, $p = 1, 2, 3$:



solution field



L^2-error over mesh size



H^1-error over mesh size

Linear result:

Theorem

Let J be a quadratic coercive functional on $H_0^1(\Omega)$. Let u be the minimizer of J in $H_0^1(\Omega)$, and u_h the minimizer in a p-th order Lagrangian finite element space contained in H_0^1. Then

$$\|u - u_h\|_{H^1} \leq Ch^p|u|.$$

Questions for a proof in nonlinear spaces:

- What replaces the error $\|u - u_h\|_{H^1}$?
- Appropriate measure of solution regularity $|u|$?
- Ellipticity/coercivity in a nonlinear function space?

Linear result:

Theorem

Let J be a quadratic coercive functional on $H^1_0(\Omega)$. Let u be the minimizer of J in $H^1_0(\Omega)$, and u_h the minimizer in a p-th order Lagrangian finite element space contained in H^1_0. Then

$$\|u - u_h\|_{H^1} \leq C h^p |u|.$$

Questions for a proof in nonlinear spaces:

- What replaces the error $\|u - u_h\|_{H^1}$?
- Appropriate measure of solution regularity $|u|$?
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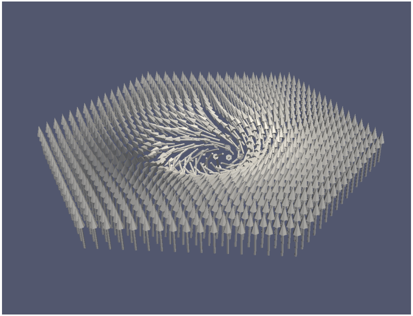
Theorem ([Grohs, Hardering, S (2014), Hardering (2016)])

Optimal H^1 and L^2 discretization error bounds.



Magnetic skyrmion

- Quasi-particle in a magnetic material
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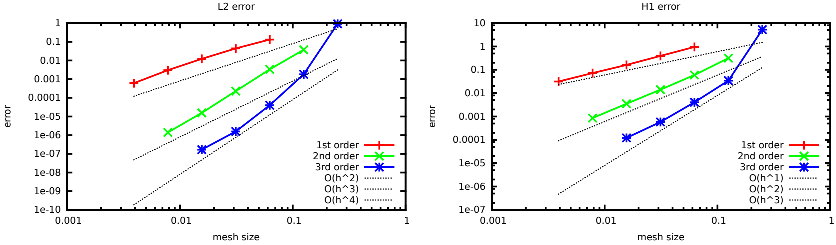
Magnetic skyrmions

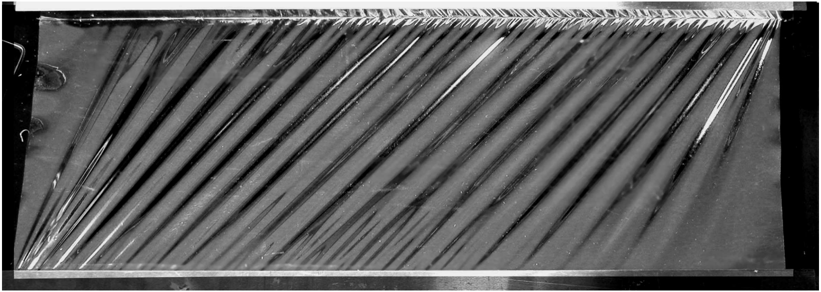
Problem settings

- Hexagonal domain
- Unstructured triangle grid
- Dirichlet boundary conditions
- Projection-based finite elements of orders $1, 2, 3$

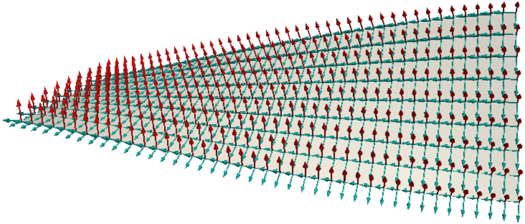
Discretization errors:



Wong, Pellegrino 2006:



- Shearing of a rectangular plastic sheet
- 380 mm x 128 mm x 25 μm
- $E = 71240$ N/mm^2, $\nu = 0.31$
- Prescribed displacement at horizontal edges
- 3 mm shear



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- Midsurface deformation: $m : \Omega \to \mathbb{R}^3$
- Microrotation field: $R : \Omega \to \mathrm{SO}(3)$

Strain measures:

- Deformation gradient: $F := (\nabla m | R_3) \in \mathbb{M}^{3\times 3}$
- Translational strain: $U := R^T F$
- Rotational strain: $\mathfrak{K} := R^T \nabla R$

Hyperelastic material law: [Neff] ($h =$ shell thickness)

$$J(m,R) = \int_\Omega \Big[hW_{\text{memb}}(U) + \frac{h^3}{12} W_{\text{bend}}(\mathfrak{K}) + hW_{\text{curv}}(\mathfrak{K}) \Big]\, dx$$

Membrane energy:

$$W_{\text{memb}}(U) = \mu \|\text{sym}(U-I)\|^2 + \mu_c \|\text{skew}(U-I)\|^2 + \frac{\mu\lambda}{2\mu+\lambda} \frac{1}{2} \Big((\det U - 1)^2 + (\frac{1}{\det U} - 1)^2$$

Bending energy:

$$W_{\text{bend}}(\mathfrak{K}_b) = \mu \|\text{sym}(\mathfrak{K}_b)\|^2 + \mu_c \|\text{skew}(\mathfrak{K}_b)\|^2 + \frac{\mu\lambda}{2\mu+\lambda} \text{tr}[\text{sym}(\mathfrak{K}_b)]^2$$

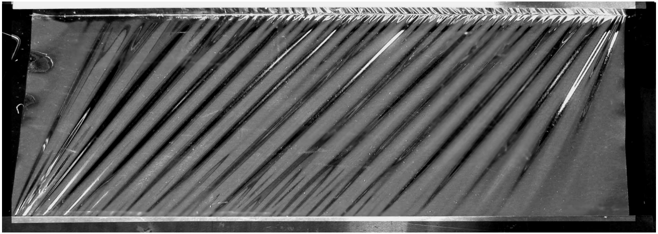
Curvature energy:

$$W_{\text{curv}}(\mathfrak{K}) = \mu L_c^{1+p} \|\mathfrak{K}\|^{1+p}$$

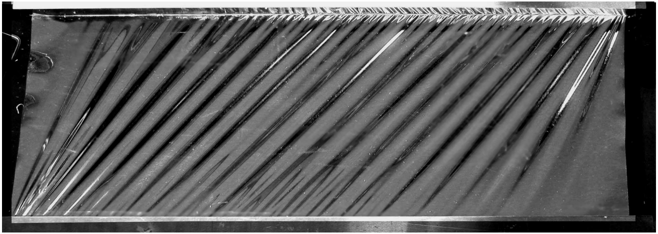
Theorem ([Neff])

Under suitable conditions, the functional J has minimizers in $H^1(\Omega, \mathbb{R}^3) \times W^{1,1+p}(\Omega, SO(3))$.

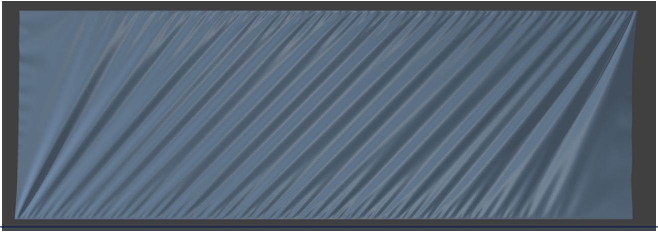
Experiment:



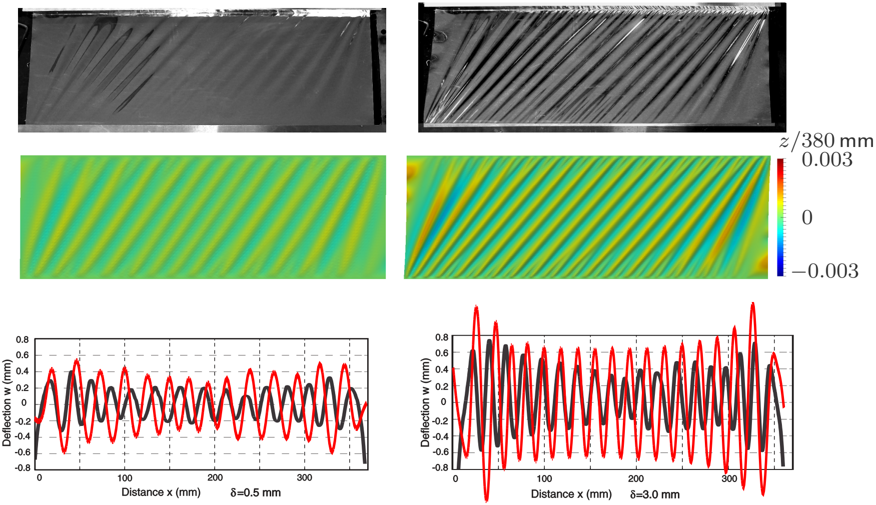
Experiment:



Simulation: [S., Neff, Bîrsan, Comp. Mech.]



Wrinkling



z/380 mm
0.003
0
−0.003
Deflection w (mm)
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
100
200
300
Distance x (mm)
δ=0.5 mm
Deflection w (mm)
Distance x (mm)
δ=3.0 mm


Thank you for your attention!