University of Stuttgart
Institute for Structural Mechanics

Application of optimization on manifolds to nonlinear shell theory

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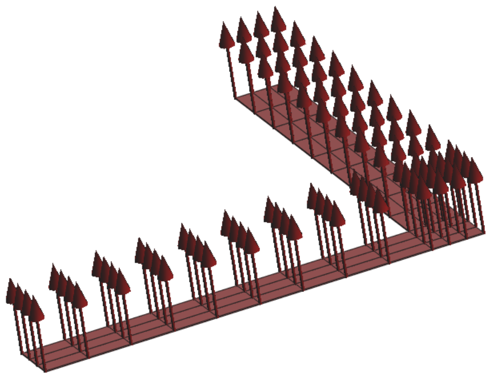
Workshop on
Nonlinear Bending,
University of Freiburg

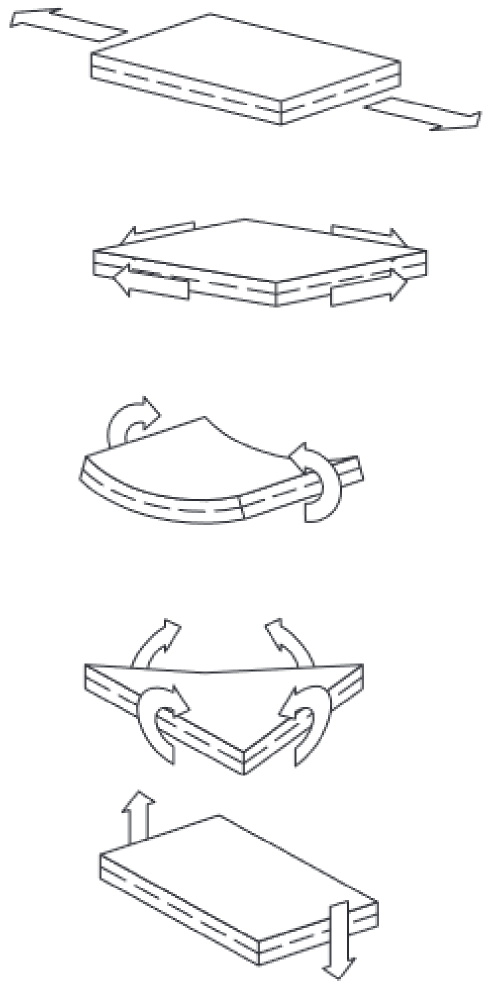
24.05.2022



Baustatik und Baudynamik

Kinematics of a nonlinear Reissner-Mindlin shell model

Energy contributions



BISCHOFF (1999)

- Membrane strains
- In-plane shear
- Bending
- Twisting
- Transverse shear

Membranes

Kirchhoff-Love shell

Reissner-Mindlin Shell (Simo-Fox shell)

Outline

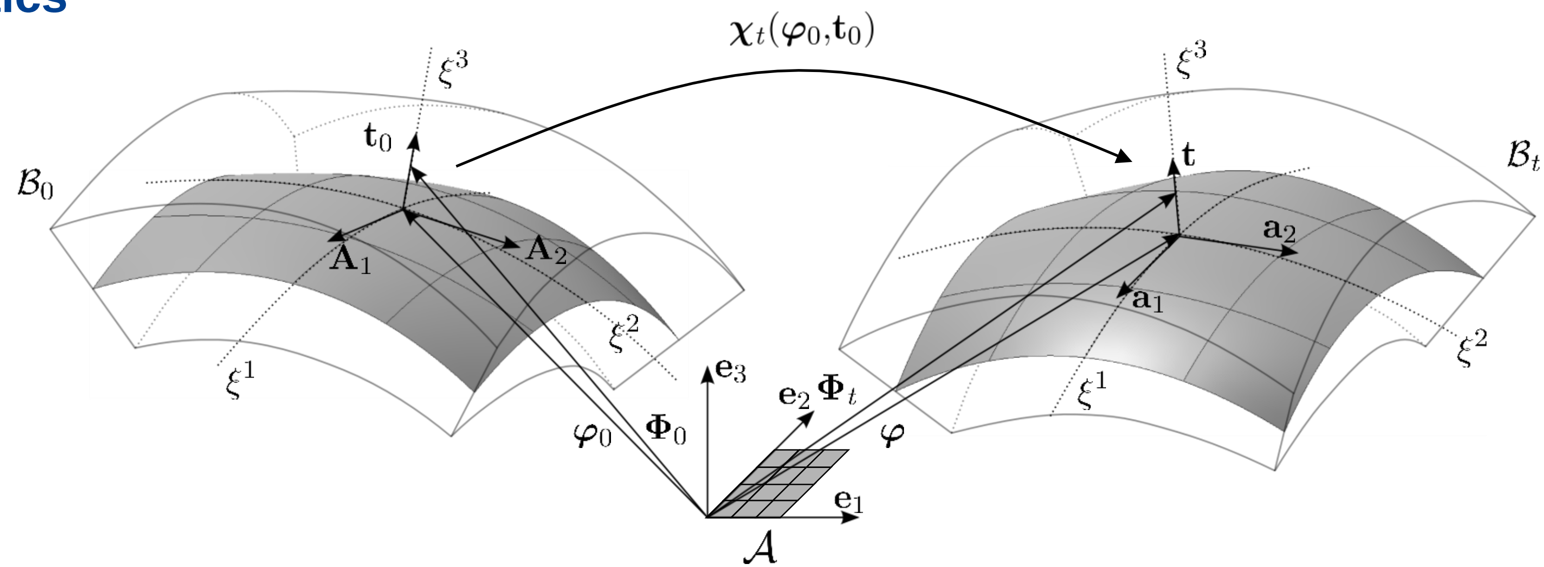
Brief review of the kinematics of a nonlinear Reissner-Mindlin shell model

Challenges for a consistent formulation

Overcoming these challenges with optimization on manifolds

Kinematics of a nonlinear Reissner-Mindlin shell model

Kinematics



$$\boldsymbol{\xi} = [\xi^1, \xi^2, \xi^3]^T \in \mathcal{A}$$

$$\mathbf{X} = \mathbf{\Phi}_0(\xi^1, \xi^2, \xi^3) = \boldsymbol{\varphi}_0(\xi^1, \xi^2) + \xi^3 \mathbf{t}_0(\xi^1, \xi^2)$$
$$\mathbf{x} = \mathbf{\Phi}_t(\xi^1, \xi^2, \xi^3) = \boldsymbol{\varphi}(\xi^1, \xi^2) + \xi^3 \mathbf{t}(\xi^1, \xi^2)$$

Mappings:

$$\mathbf{\Phi}_0 : \begin{cases} \mathcal{A} \rightarrow \mathcal{B}_0 \subset \mathbb{R}^3 \\ \boldsymbol{\xi} \mapsto \mathbf{X} = \mathbf{\Phi}_0(\boldsymbol{\xi}) \end{cases}$$

$$\mathbf{\Phi}_t : \begin{cases} \mathcal{A} \rightarrow \mathcal{B}_t \subset \mathbb{R}^3 \\ \boldsymbol{\xi} \mapsto \mathbf{x} = \mathbf{\Phi}_t(\boldsymbol{\xi}) \end{cases}$$

$$\chi_t = \mathbf{\Phi}_t \circ \mathbf{\Phi}_0^{-1}, \quad \chi_t : \begin{cases} \mathcal{B}_0 \rightarrow \mathcal{B}_t \subset \mathbb{R}^3 \\ \boldsymbol{\xi} \mapsto \mathbf{x} = \chi_t(\mathbf{X}) \end{cases}$$

Kinematics of a nonlinear Reissner-Mindlin shell model

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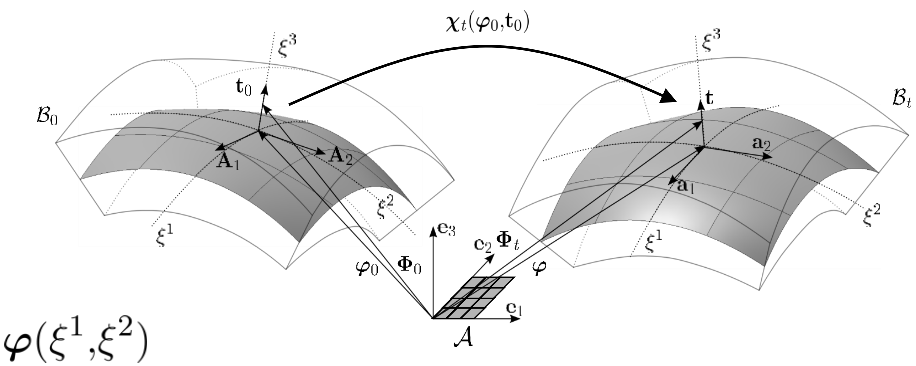
Kinematic assumptions



- Geometry approximation:

$$\mathbf{x} = \mathbf{\Phi}_t(\xi^1, \xi^2, \xi^3) = \boldsymbol{\varphi}(\xi^1, \xi^2) + \xi^3 \mathbf{t}(\xi^1, \xi^2)$$

- First order transverse shear effects are taken into account:
  - The director field $\mathbf{t}(\xi^1, \xi^2)$ is independent of the midsurface field $\boldsymbol{\varphi}(\xi^1, \xi^2)$ (in contrast to Kirchhoff-Love)
- Thickness change is not contained in kinematic description:
  - The director is a unit vector, i.e. $\mathbf{t} : \mathcal{A} \rightarrow \mathcal{S}^2 \subset \mathbb{R}^3$ $\quad \mathcal{S}^2 = \{\mathbf{x} \in \mathbb{R}^3 \,||\, \mathbf{x} \cdot \mathbf{x} = 1\}$

Discretization

- Discretization of the midsurface field $\boldsymbol{\varphi} : \mathcal{A} \rightarrow \mathbb{R}^3$ trivial since it maps onto a vector space $\mathbb{R}^3$
- Discretization and parametrization of the director field $\mathbf{t} : \mathcal{A} \rightarrow \mathcal{S}^2$ difficult due to the nonlinear space $\mathcal{S}^2$

Challenges

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Interpolation on the unit sphere

(Algebraic) optimization on manifolds

Update of nodal values

Interpolation: Review of historic approaches

(for non-linear Reissner-Mindlin shell formulations)

Interpolation: Review of existing approaches

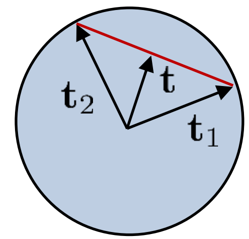
Angles

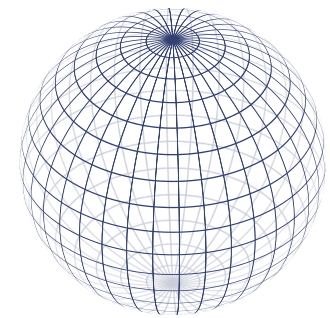
- The unit sphere can be parameterized with an angle pair $(\alpha,\beta) \rightarrow \quad \mathbf{t} = \mathbf{R}(\alpha,\beta)\mathbf{t}_0, \;\; \mathbf{R}(\alpha,\beta) \in \mathcal{SO}(3)$

RAMM (1976), ARGYRIS(1982), BAŞAR ET AL(1992), WRIGGERS & GRUTTMANN (1993)

  - The resulting interpolation is, e.g. RAMM (1976)

$$\mathbf{t} = \sum_{A=1}^{n} N^A(\xi)\mathbf{R}_A(\alpha^A,\beta^A)\mathbf{t}_0^A, \quad \mathbf{t}_A = \mathbf{R}_A\mathbf{t}_0^A$$





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  - Singularities, violates objectivity, unit length constraint violated

Interpolation: Review of existing approaches

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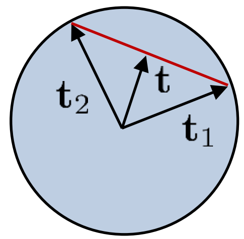
Direct interpolation of the current nodal directors in the embedding space

- Standard interpolation formula for finite elements in vector spaces
  - Simple straightforward interpolation

    HUGHES & LIU (1981), BATHE & BOLOURCHI (1980), BETSCH & STEINMANN (2002), BENSON ET AL (2010)

$$\mathbf{t} = \sum_{A=1}^{n} N^A(\xi)\mathbf{t}_A$$



$\mathbf{t} \notin \mathcal{S}^2$

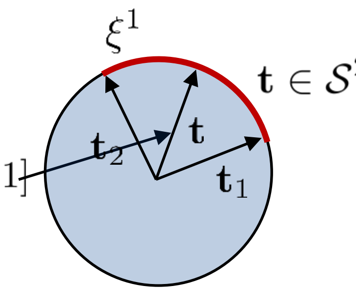
  - Interpolated value does not lie on the unit sphere
  - Objective

Interpolation: Review of existing approaches

Generalized Spherical Linear interpolation (SLERP)

- SLERP: Interpolation between two unit vectors $\mathbf{t}_1, \mathbf{t}_2$

$$\mathbf{t} = \mathrm{SLERP}(\mathbf{t}_1, \mathbf{t}_2, \xi^1) = \frac{\sin((1-\xi^1)\arccos(\mathbf{t}_1 \cdot \mathbf{t}_2))}{\sin(\arccos(\mathbf{t}_1 \cdot \mathbf{t}_2))}\mathbf{t}_1 + \frac{\sin(\xi^1 \arccos(\mathbf{t}_1 \cdot \mathbf{t}_2))}{\sin(\arccos(\mathbf{t}_1 \cdot \mathbf{t}_2))}\mathbf{t}_2, \quad \xi^1 = [0,1]$$



Directors have unit length

- Generalization for four vectors in 2D

$$\mathbf{t} = \mathrm{SLERP}[\mathrm{SLERP}(\mathbf{t}_1, \mathbf{t}_2, \xi^1), \mathrm{SLERP}(\mathbf{t}_3, \mathbf{t}_4, \xi^1), \xi^2]$$ AREIAS (2013)

  - Complicated interpolation
  - Objective

Interpolation: Desired Properties

- **Objective**
- **Singularity-free**
- **Useable for arbitrary polynomial order**
- **Invariant to node numbering**
- **Unit length** in the domain

Suitable interpolation schemes for the director field

Suitable interpolation schemes for the director field

Geodesic Finite Elements SANDER (2012)

- GFE define a class of finite elements to interpolate on manifold

  - Consider the following interpolation scheme

$$\mathbf{x}^*(\boldsymbol{\xi}, \mathbf{x}_i) = \arg \min_{\mathbf{x} \in \boxed{\mathbb{R}^n}} f(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}_i) \qquad f(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}_i) = \sum_{i=1}^{n} N^i(\boldsymbol{\xi}) ||\mathbf{x}_i - \mathbf{x}||^2$$

Identical to standard interpolation!

  - Since: $\dfrac{\partial f(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}_i)}{\partial \mathbf{x}} \overset{!}{=} \mathbf{0} = \sum_{i=1}^{n} N^i(\boldsymbol{\xi})(\mathbf{x}_i - \mathbf{x}) = \sum_{i=1}^{n} N^i(\boldsymbol{\xi})\mathbf{x}_i - \underbrace{\sum_{i=1}^{n} N^i}_{=1} \mathbf{x} \Rightarrow \mathbf{x}^* = \sum_{i=1}^{n} N^i(\boldsymbol{\xi})\mathbf{x}_i$

  - Euclidean distance can be generalized for the manifold $\mathcal{M}$

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \in \boxed{\mathcal{M}}} \sum_{i=1}^{n} N^i(\boldsymbol{\xi}) \operatorname{dist}(\mathbf{x}_i, \mathbf{x})^2_{\mathcal{M}} = \mathbf{x}_{GP}$$

  - objective since distances are a priori rotational invariant
  - Directors have unit length
  - Implicit interpolation by minimization problem → Nonlinear minimization problem at each integration point

Suitable interpolation schemes for the director field

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Projection-Based Finite Elements GROHS ET AL (2019)

- Projection-based interpolation is a special kind of geodesic finite elements
  - In contrast to the GFE definition

$$\mathbf{x}^* = \arg\min_{\mathbf{x}\in\mathcal{M}} \sum_{i=1}^{n} N^i(\boldsymbol{\xi})\,\mathrm{dist}(\mathbf{x}_i,\mathbf{x})^2_{\boxed{\mathcal{M}}} = \mathbf{x}_{GP}$$

  - PB finite elements use the distance of the embedding space

$$\mathbf{x}^* = \arg\min_{\mathbf{x}\in\mathcal{M}} \sum_{i=1}^{n} N^i(\boldsymbol{\xi})\,\mathrm{dist}(\mathbf{x}_i,\mathbf{x})^2_{\boxed{\mathbb{R}^n}} = \mathbf{x}_{GP}$$

  - objective since distances are a priori rotational invariant
  - Directors have unit length
  - Implicit interpolation by minimization problem

Suitable interpolation schemes for the director field

What does all that mean for the unit sphere?

Example with two directors:

- **NFE**/Standard interpolation:

$$N^1(\xi) = 1 - \xi, \quad N^2(\xi) = \xi$$

$$\mathbf{t}_{\mathrm{GP}} = \sum_{i=1}^{n} N^i(\xi)\mathbf{t}_i \ = \arg\min_{\mathbf{t}\in\mathbb{R}^n} \sum_{i=1}^{n} N^i(\xi)||\mathbf{t}_i - \mathbf{t}||^2$$

- Projection-Based (**PBFE**): GROHS ET AL (2019)

$\mathbf{t}_1$ $\mathbf{t}_2$

$$\begin{aligned}\mathbf{t}_{\mathrm{GP}} &= \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\xi)\,\mathrm{dist}(\mathbf{t}_i, \mathbf{t})^2_{\mathbb{R}^n} \\ &= \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\xi)||\mathbf{t}_i - \mathbf{t}||^2 = \frac{\sum_{i=1}^{n} N^i(\xi)\mathbf{t}_i}{||\sum_{i=1}^{n} N^i(\xi)\mathbf{t}_i||}\end{aligned}$$

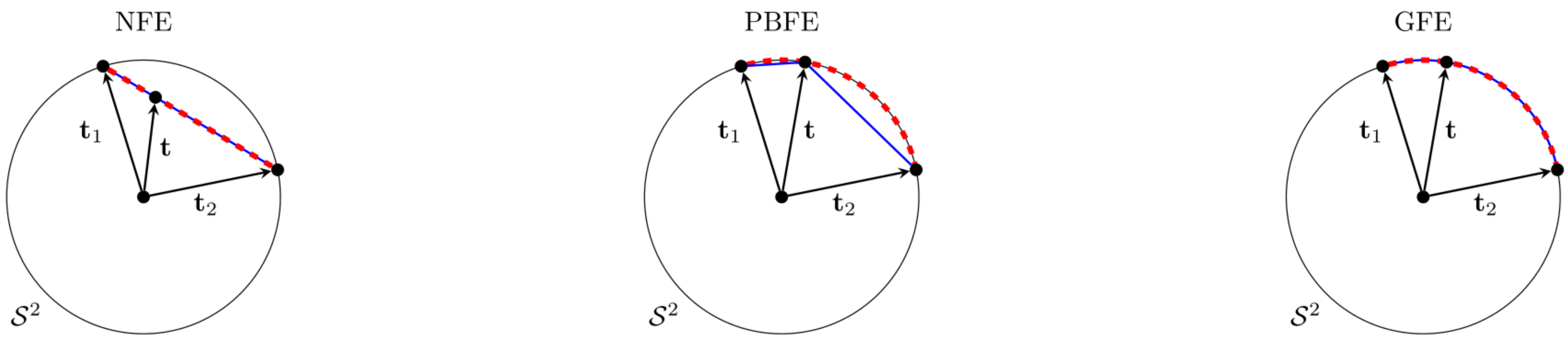
- Geodesic Finite Elements (**GFE**): SANDER (2012)

$$\begin{aligned}\mathbf{t}_{\mathrm{GP}} &= \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\xi)\,\mathrm{dist}(\mathbf{t}_i, \mathbf{t})^2_{\mathcal{S}^2} \\ &= \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\xi)\arccos(\mathbf{t}_i \cdot \mathbf{t})^2\end{aligned}$$

Suitable interpolation schemes for the director field

What does all that mean for the unit sphere?

Example with two directors:



$$\mathbf{t}_{\mathrm{GP}} = \arg\min_{\mathbf{t}\in\mathbb{R}^n} \sum_{i=1}^{n} N^i(\boldsymbol{\xi})||\mathbf{t}_i - \mathbf{t}||^2 = \sum_{i=1}^{n} N^i(\boldsymbol{\xi})\mathbf{t}_i$$

$$\mathbf{t}_{\mathrm{GP}} = \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\boldsymbol{\xi})||\mathbf{t}_i - \mathbf{t}||^2 = \frac{\sum_{i=1}^{n} N^i(\boldsymbol{\xi})\mathbf{t}_i}{||\sum_{i=1}^{n} N^i(\boldsymbol{\xi})\mathbf{t}_i||}$$

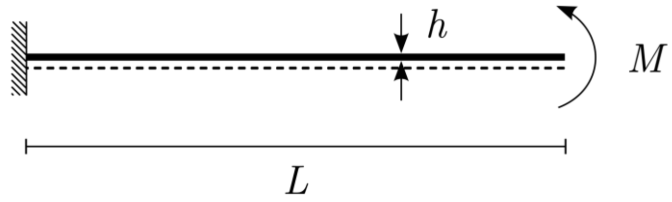
$$\mathbf{t}_{\mathrm{GP}} = \arg\min_{\mathbf{t}\in\mathcal{S}^2} \sum_{i=1}^{n} N^i(\boldsymbol{\xi}) \arccos(\mathbf{t}_i \cdot \mathbf{t})^2$$

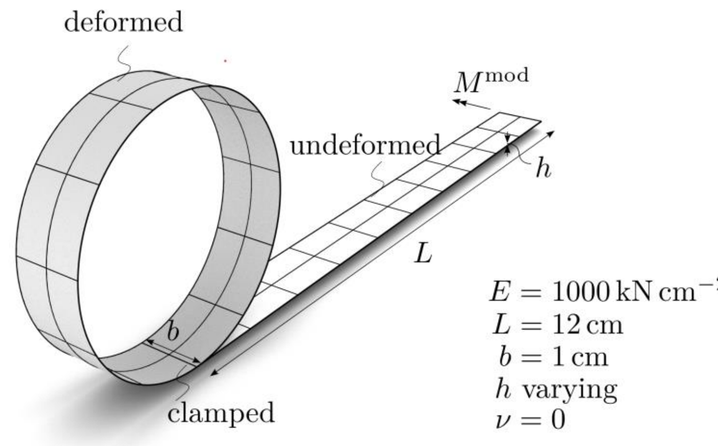
Comparison of interpolation schemes

Interpolation: Numerical experiments

Roll-up of clamped beam

- 16 Iterations of Newton's method to reach equilibrium





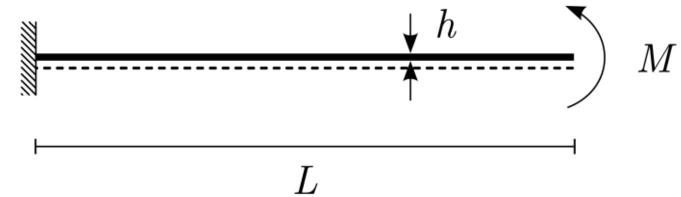
$$\Pi(\boldsymbol{\varphi}, \mathbf{t}) = \int_{\mathcal{B}} \psi_{\mathrm{strain}}(\boldsymbol{\varphi}, \mathbf{t})\, \mathrm{d}V + \Pi_{\mathrm{ext}}(\boldsymbol{\varphi}, \mathbf{t})$$

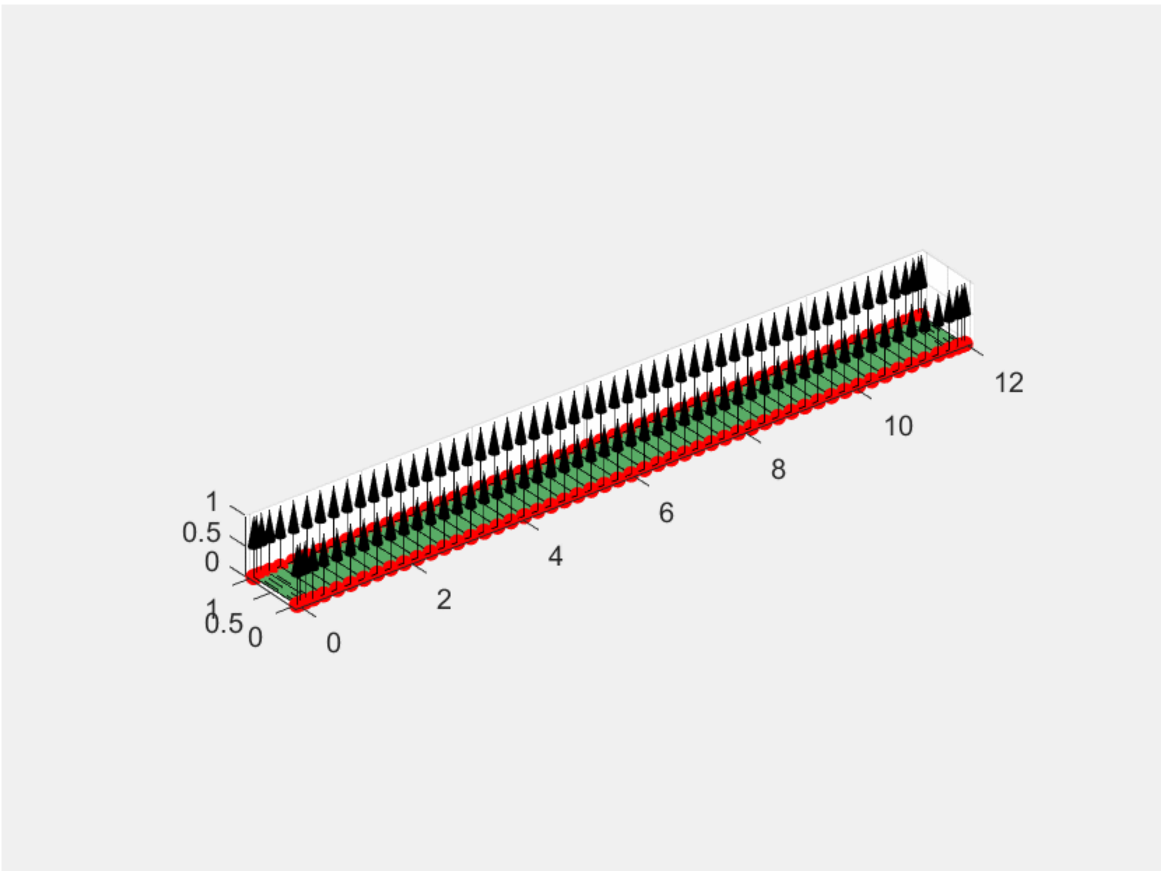
$$\{\boldsymbol{\varphi}^*, \mathbf{t}^*\} = \arg\left\{ \min_{\boldsymbol{\varphi}\in\mathbb{R}^d} \min_{\mathbf{t}\in\mathcal{S}^{d-1}} \Pi(\boldsymbol{\varphi}, \mathbf{t}) \right\}.$$

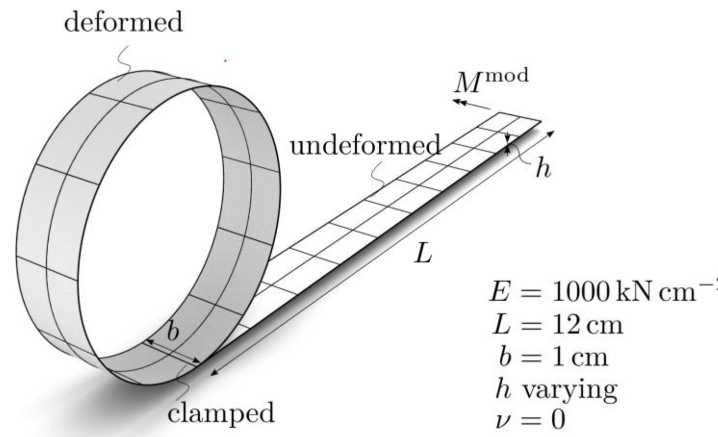
Interpolation: Numerical experiments

Roll-up of clamped beam

- 16 Iterations of Newton's method to reach equilibrium







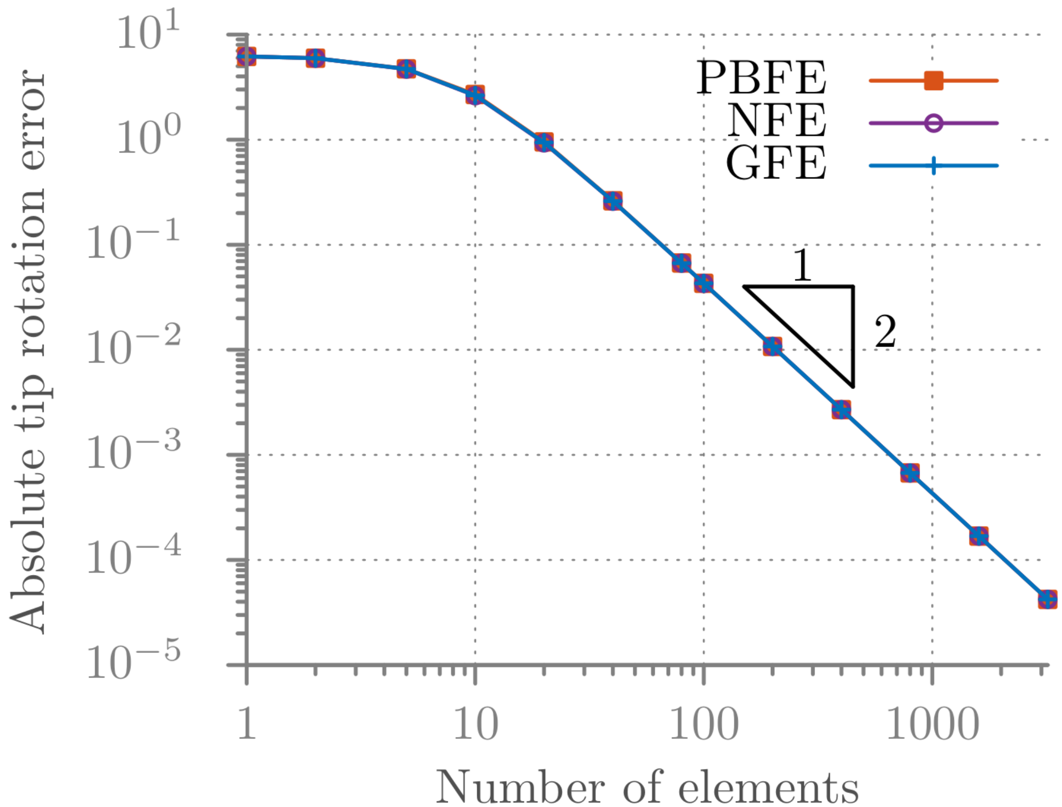
$$\Pi(\boldsymbol{\varphi}, \mathbf{t}) = \int_{\mathcal{B}} \psi_{\text{strain}}(\boldsymbol{\varphi}, \mathbf{t})\, \mathrm{d}V + \Pi_{\text{ext}}(\boldsymbol{\varphi}, \mathbf{t})$$

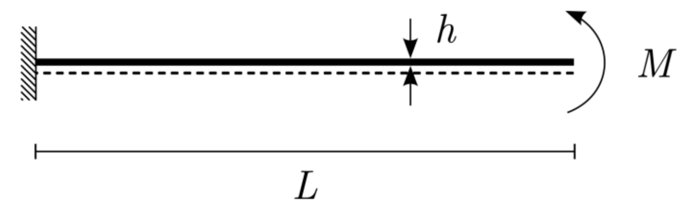
$$\{\boldsymbol{\varphi}^*, \mathbf{t}^*\} = \arg\left\{ \min_{\boldsymbol{\varphi}\in\mathbb{R}^d} \min_{\mathbf{t}\in\mathcal{S}^{d-1}} \Pi(\boldsymbol{\varphi}, \mathbf{t}) \right\}.$$

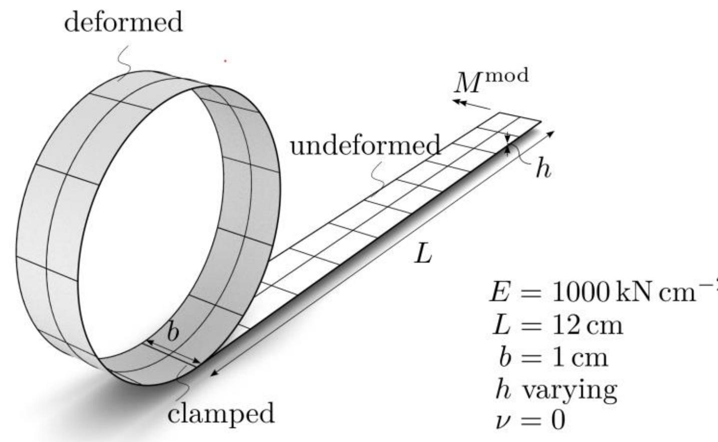
Interpolation: Numerical experiments

Roll-up of clamped beam

- Reference plane → Reference interpolation identical
- Q1 shell elements, C^0-continuity between elements
- Moderate initial slenderness $L/h = 12$ → Moderate locking



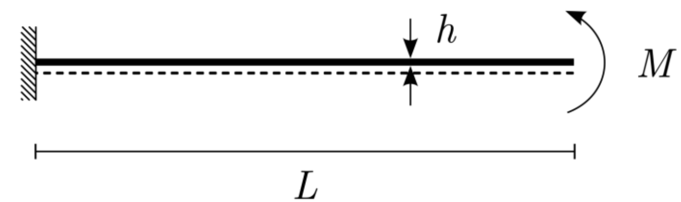


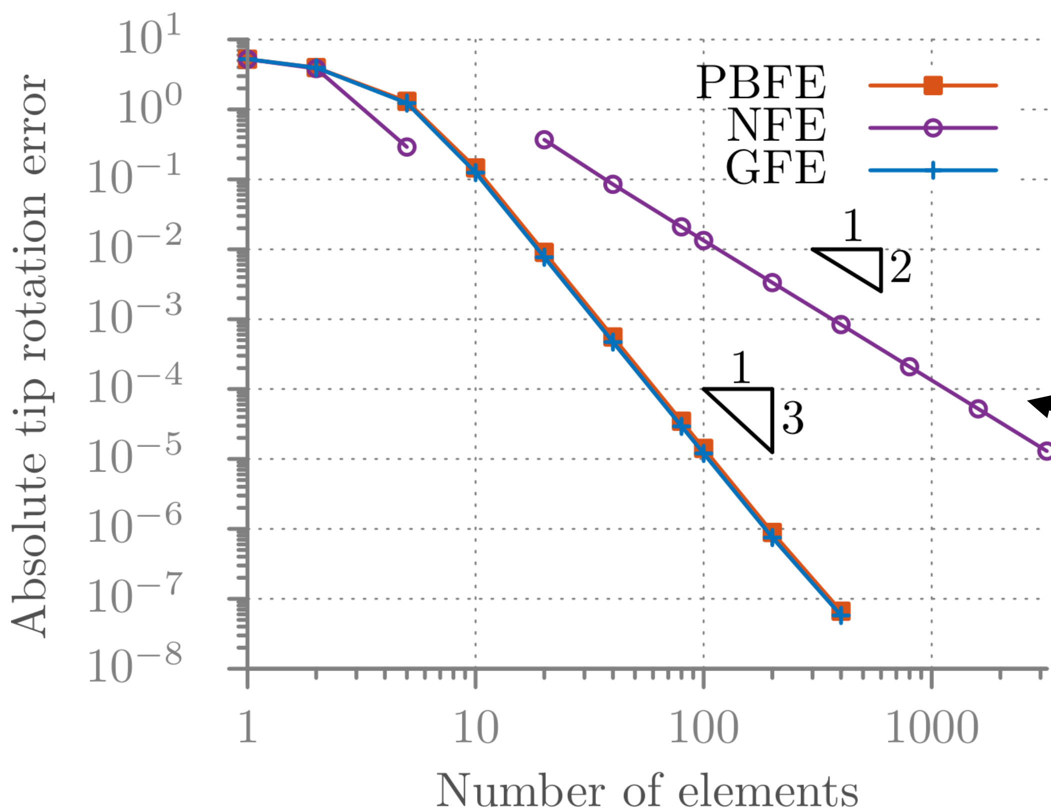


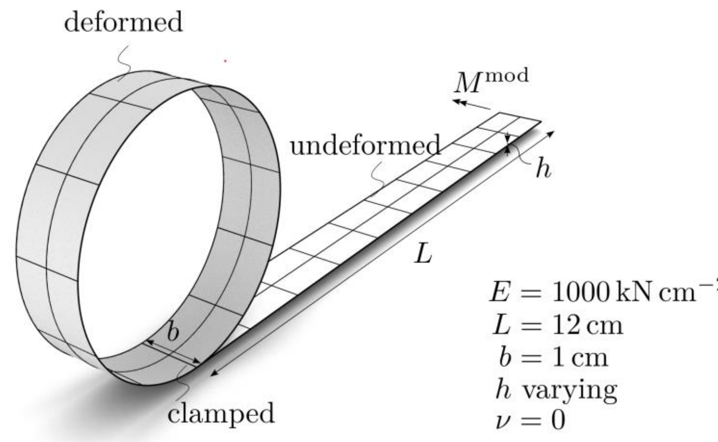
Interpolation: Numerical experiments

Roll-up of clamped beam

- Reference plane → Reference interpolation identical
- Quadratic $p = 2$ B-spline shell elements, C^1-continuity between elements
- Moderate initial slenderness $L/h = 12$ → Moderate locking





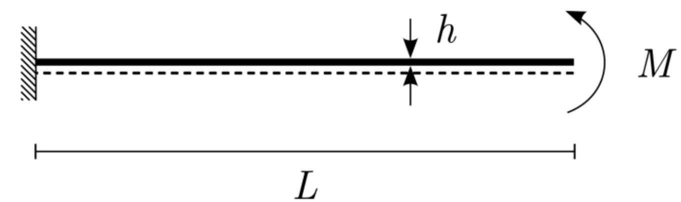


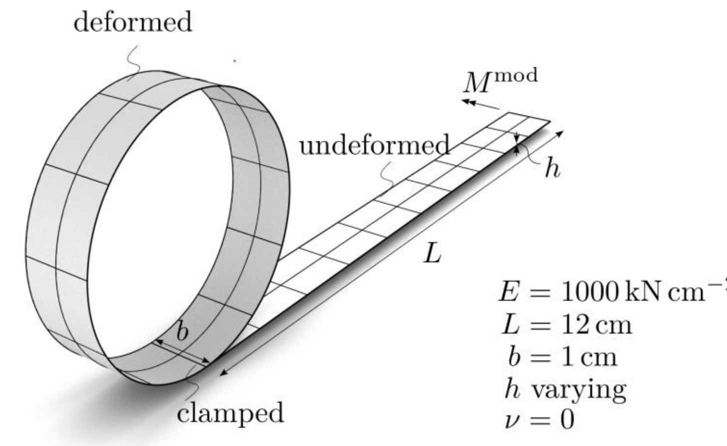
Convergence order degenerates!

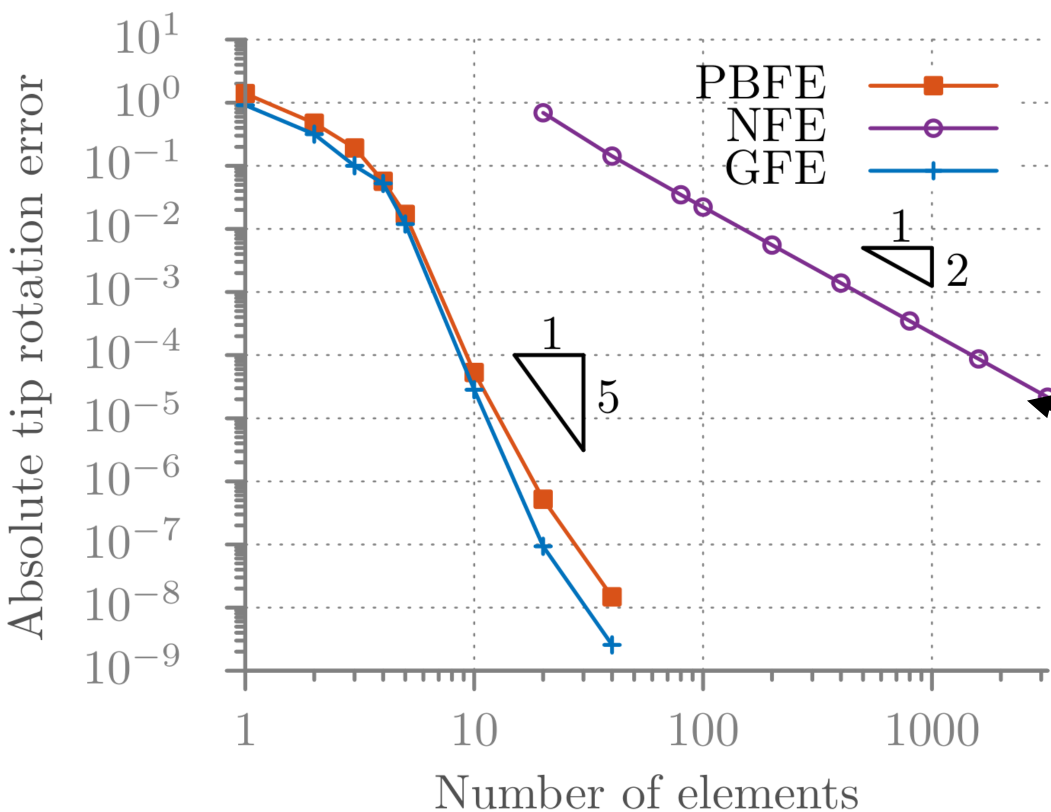
Interpolation: Numerical experiments

Roll-up of clamped beam

- Reference plane → Reference Interpolation identical
- Quartic $p = 4$ B-spline shell elements, C^3-continuity between elements
- Moderate initial slenderness $L/h = 12$ → Moderate locking







Convergence order degenerates!

Challenges

Baustatik und Baudynamik

Interpolation on the unit sphere

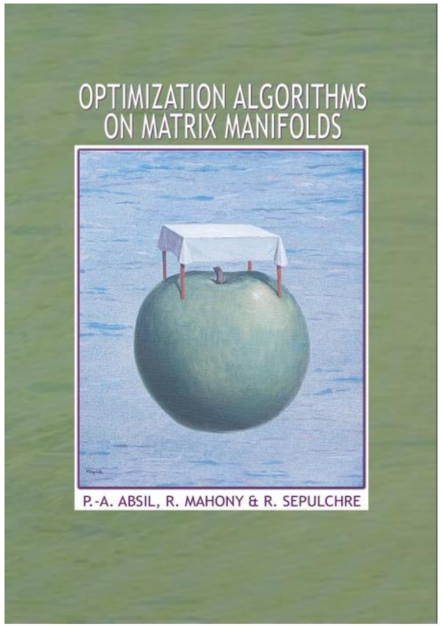
(Algebraic) optimization on manifolds

Update of nodal values

Algebraic optimization on manifolds

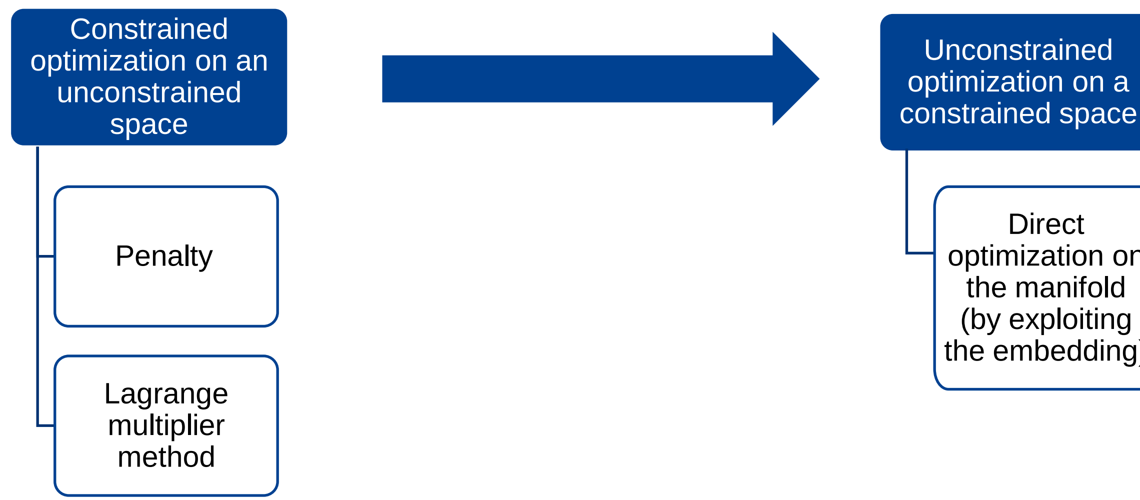
Algebraic optimization on manifolds

Literature



Absil PA, Mahony R, Sepulchre R (2008) Optimization Algorithms on Matrix Manifolds. Princeton University Press, doi:10.1515/9781400830244

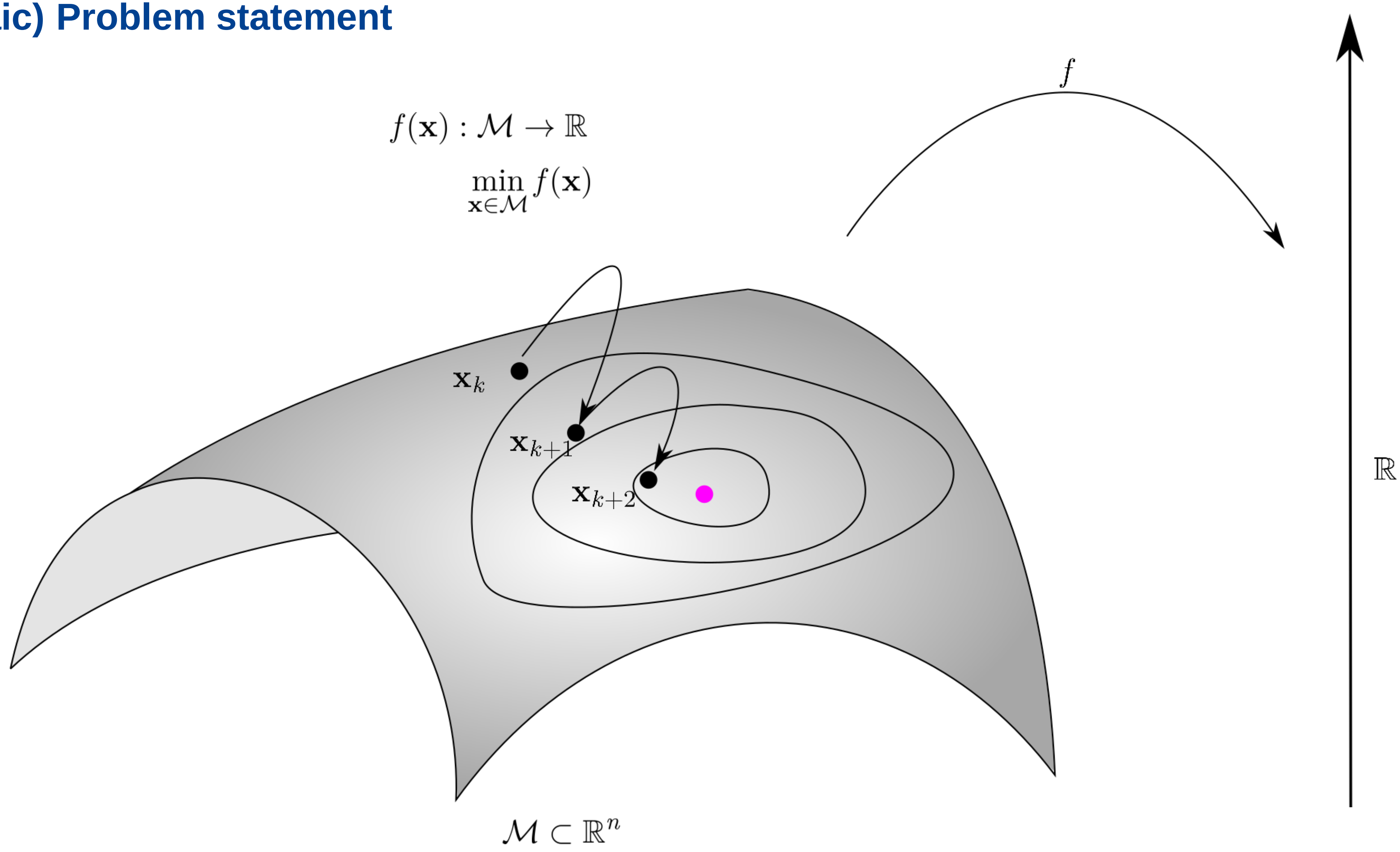
Boumal N (2020) An introduction to optimization on smooth manifolds. Available online, Link



Algebraic optimization on manifolds

Baustatik und Baudynamik

(Algebraic) Problem statement

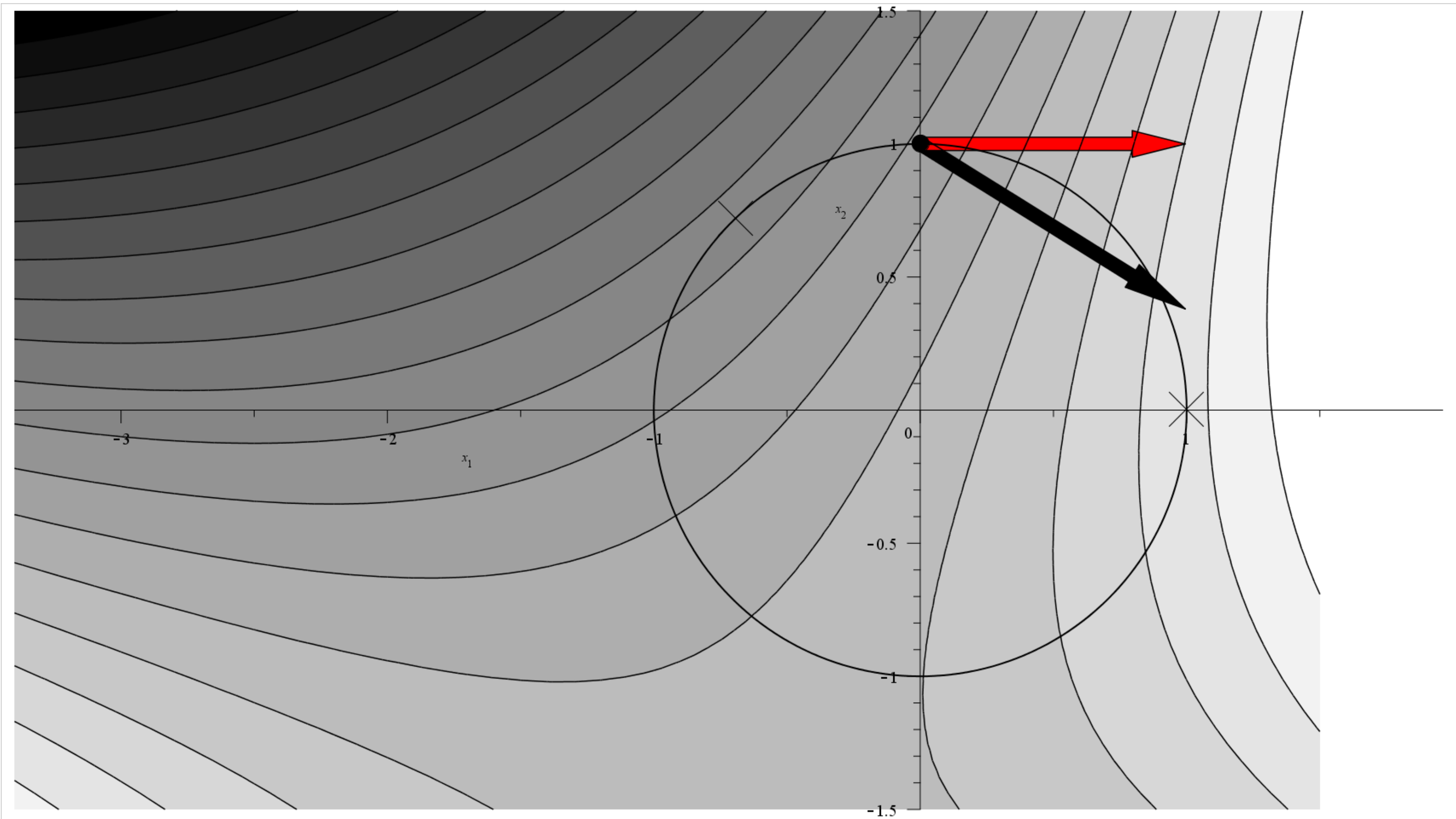


Riemannian gradient

(exploiting embedding information)

Algebraic optimization on manifolds

Toy problem, gradient and Riemannian gradient



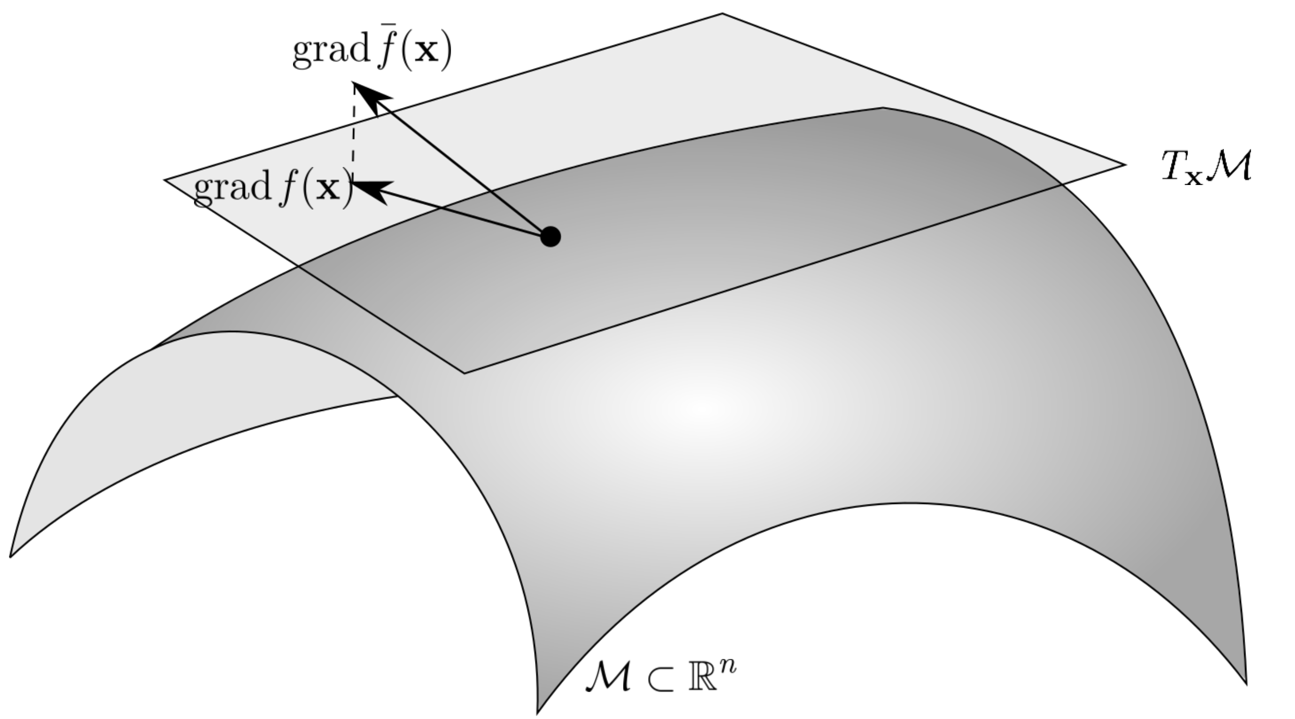
Riemannian Gradient: submanifolds

$f(\mathbf{x}) : \mathcal{M} \to \mathbb{R}$ $\bar{f}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$

“For Riemannian submanifolds, the Riemannian gradient is the orthogonal projection of the “classical” gradient to the tangent spaces.”

BOUMAL N (2020) AN INTRODUCTION TO OPTIMIZATION ON SMOOTH MANIFOLDS.

$$\operatorname{grad} f(\mathbf{x}) = P_{\mathbf{x}} \operatorname{grad} \bar{f}(\mathbf{x})$$



- No charts
- No artificial singularities
- Simple linearization

Challenges

Interpolation on the unit sphere

(Algebraic) optimization on manifolds

Update of nodal values

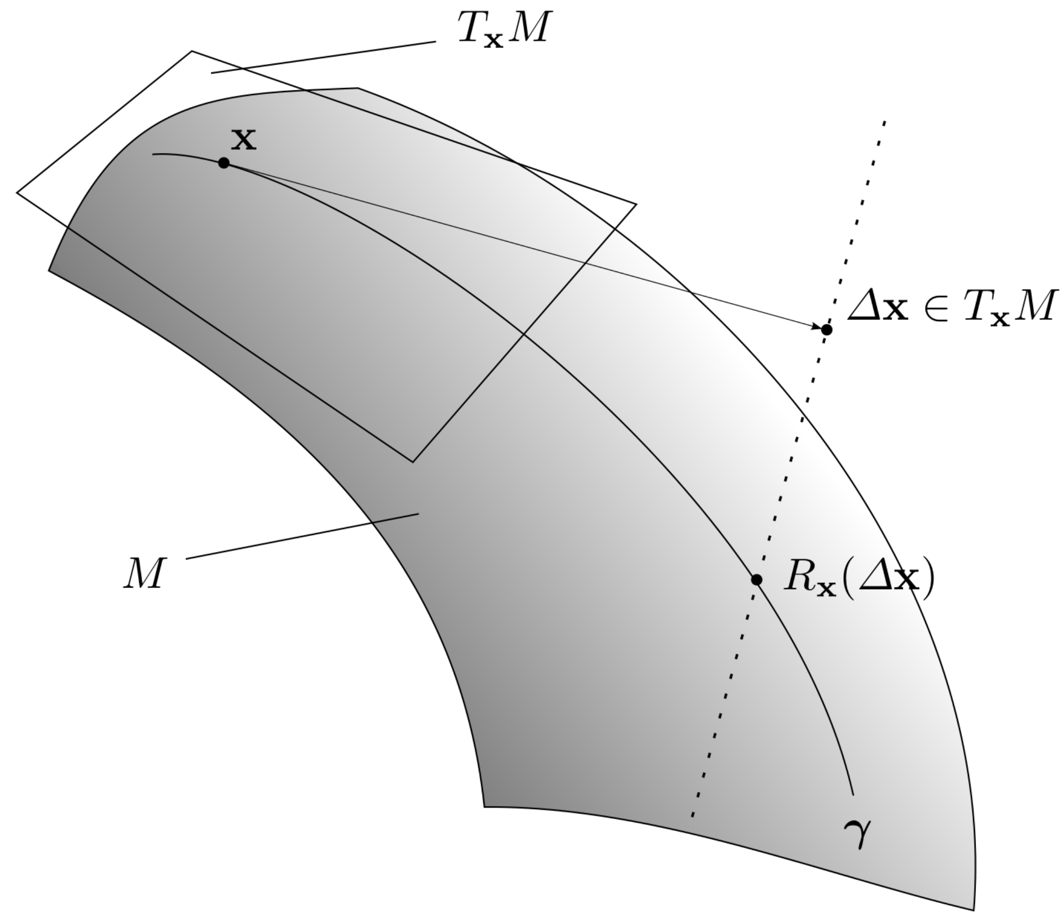
Update of nodal values

Algebraic optimization on manifolds

Update of nodal values

$\mathbf{x}_k + \Delta\mathbf{x}_k \notin \mathcal{M}$

Geodesics generalize the concept of straight lines



The exponential map creates the *unique* geodesic curve starting at $\mathbf{x}_k$ in direction $\Delta\mathbf{x}_k$ with constant speed

$$\boldsymbol{\gamma}(t) = \exp_{\mathbf{x}_k}(t\Delta\mathbf{x}_k) \quad \Rightarrow \quad \mathbf{x}_{k+1} = \exp_{\mathbf{x}_k}(\Delta\mathbf{x}_k)$$

Along these geodesics one could perform e.g. line search

Algebraic optimization on manifolds

Update of nodal values

Absil PA , "Optimization on manifolds: methods and applications", Leuven, 18 Sep 2009.

Luenberger (1973), Introduction to linear and nonlinear programming.
Luenberger mentions the idea of performing line search along geodesics, "*which we would use if it were computationally feasible (which it definitely is not)*".

Generalize the concept of the exponential map → Retractions

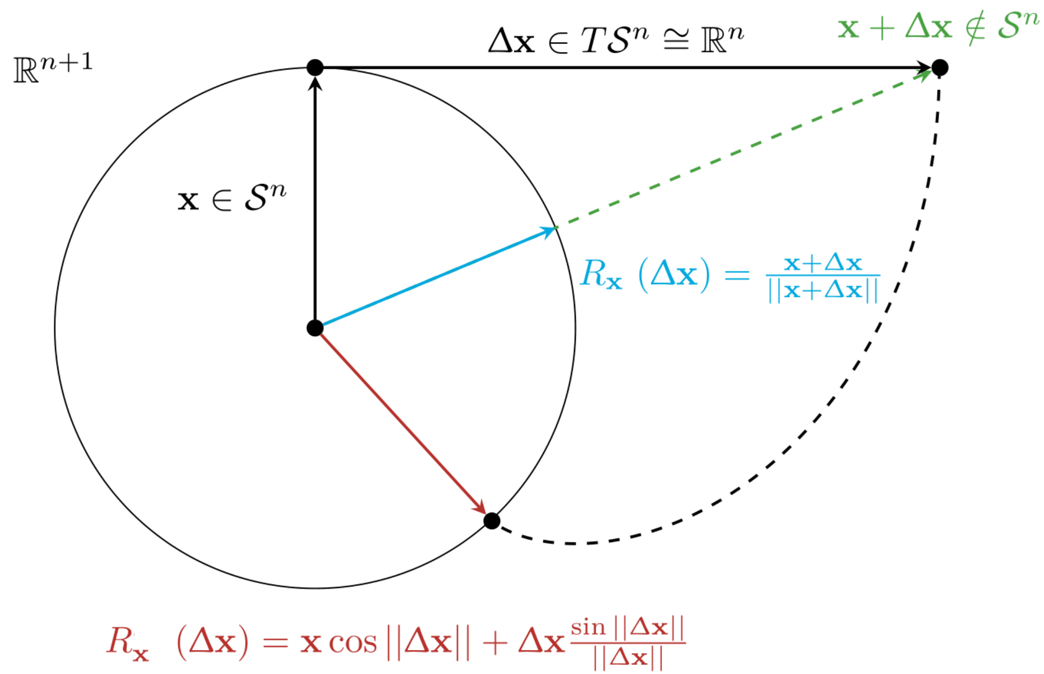
Algebraic optimization on manifolds

Update of nodal values

Retractions for the unit sphere

$$R_{\mathbf{x}}^{\exp}(\Delta\mathbf{x}) = \exp_{\mathbf{x}}(\Delta\mathbf{x}) = \cos(||\Delta\mathbf{x}||)\mathbf{x} + \frac{\sin(||\Delta\mathbf{x}||)}{||\Delta\mathbf{x}||}\Delta\mathbf{x}$$

$$R_{\mathbf{x}}^{\mathrm{rrn}}(\Delta\mathbf{x}) = \frac{\mathbf{x}+\Delta\mathbf{x}}{||\mathbf{x}+\Delta\mathbf{x}||}$$



Algebraic optimization on manifolds

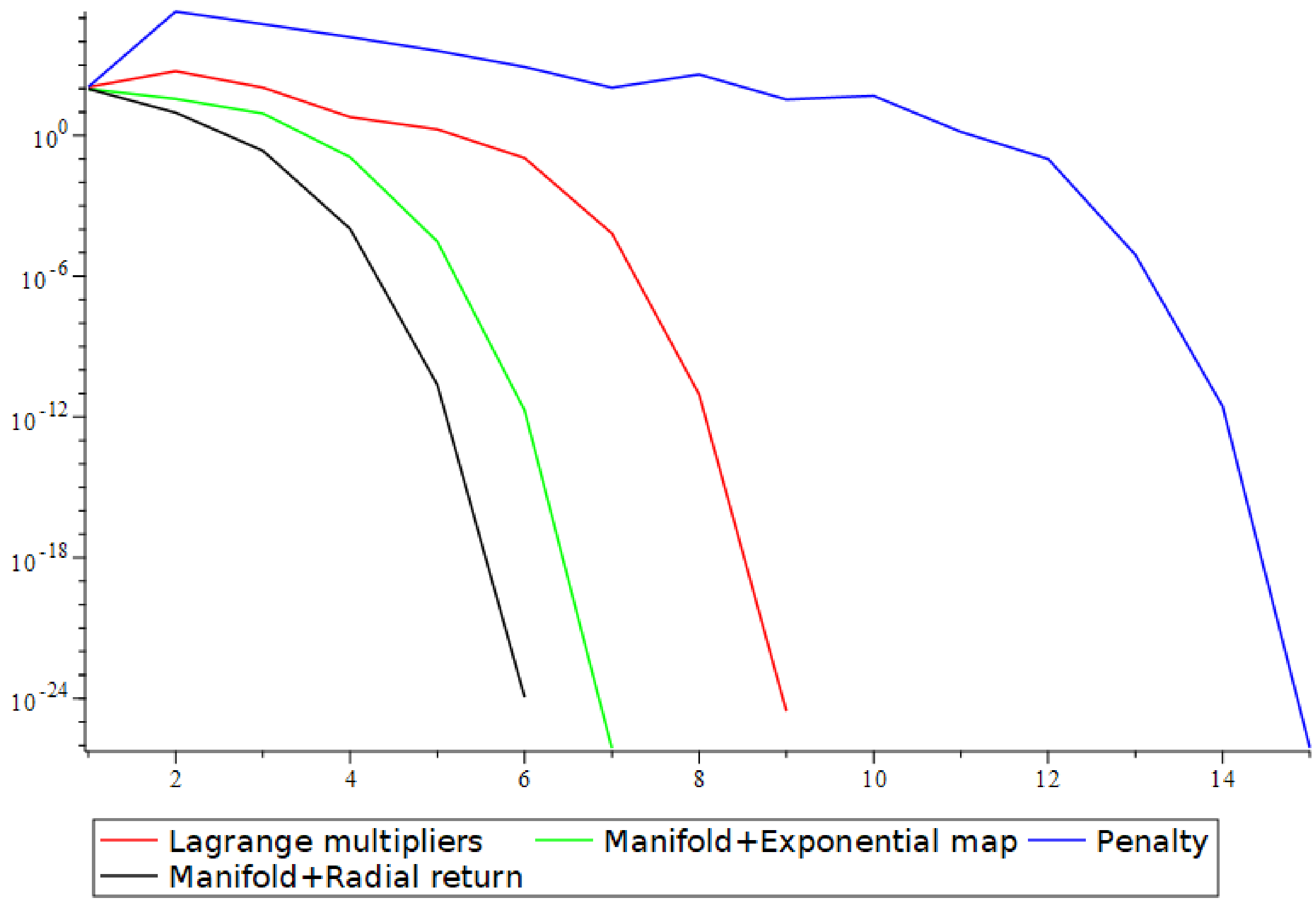
Update of nodal values

Retractions for the unit sphere

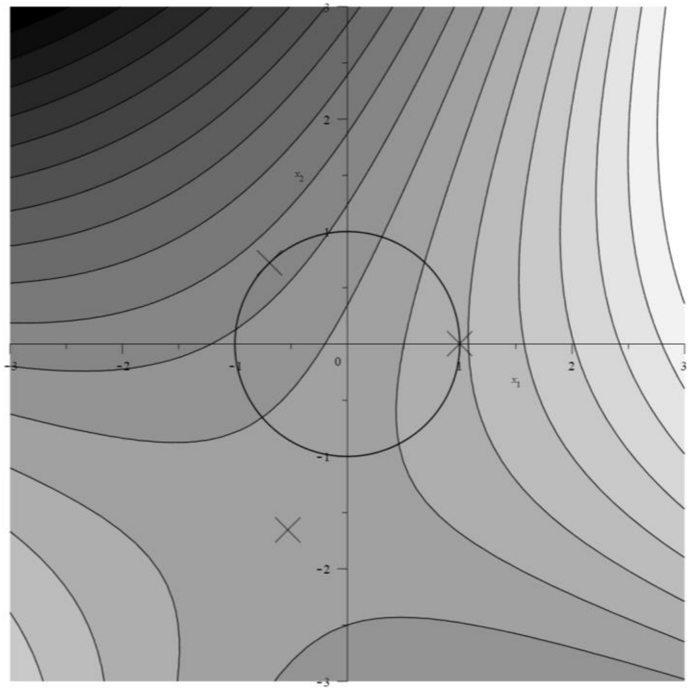
Algebraic optimization on manifolds

Toy problem: Newton's method, iteration count vs. gradient norm

$||\mathbf{g}||_2$



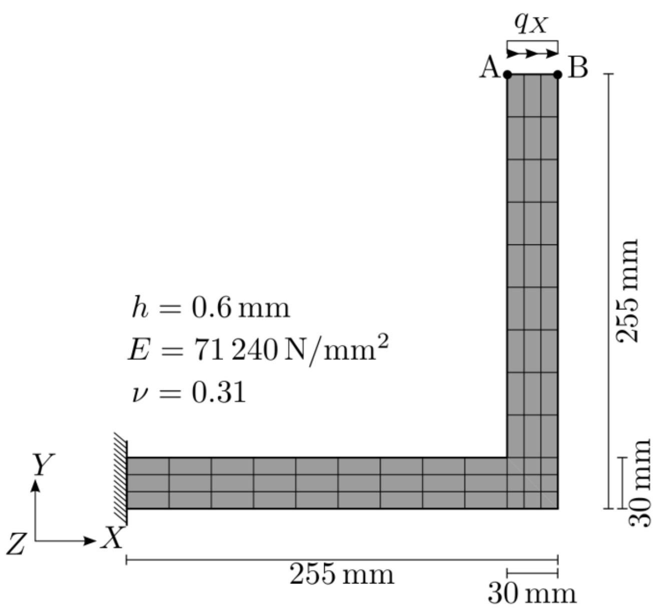
#iteration



Simulations

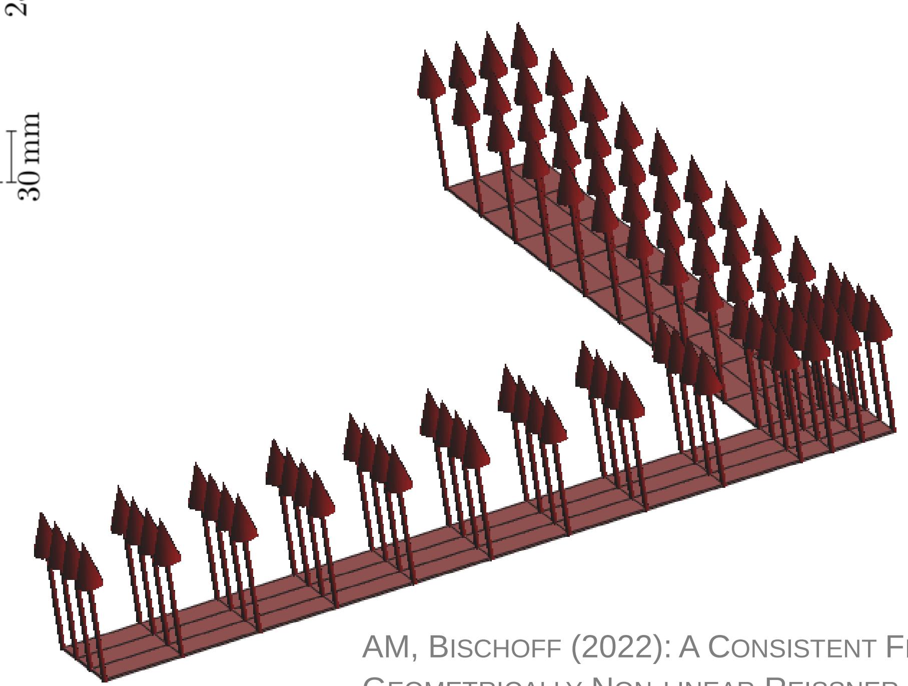
Simulation of magnetic vorticies

Simulation elastic deformation of shells



$$\Pi(\boldsymbol{\varphi}, \mathbf{t}) = \int_{\mathcal{B}} \psi_{\text{strain}}(\boldsymbol{\varphi}, \mathbf{t})\,\mathrm{d}\,V + \Pi_{\text{ext}}(\boldsymbol{\varphi}, \mathbf{t})$$

$$\{\boldsymbol{\varphi}^*, \mathbf{t}^*\} = \arg\left\{\min_{\boldsymbol{\varphi}\in\mathbb{R}^d} \min_{\mathbf{t}\in\mathcal{S}^{d-1}} \Pi(\boldsymbol{\varphi}, \mathbf{t})\right\}.$$

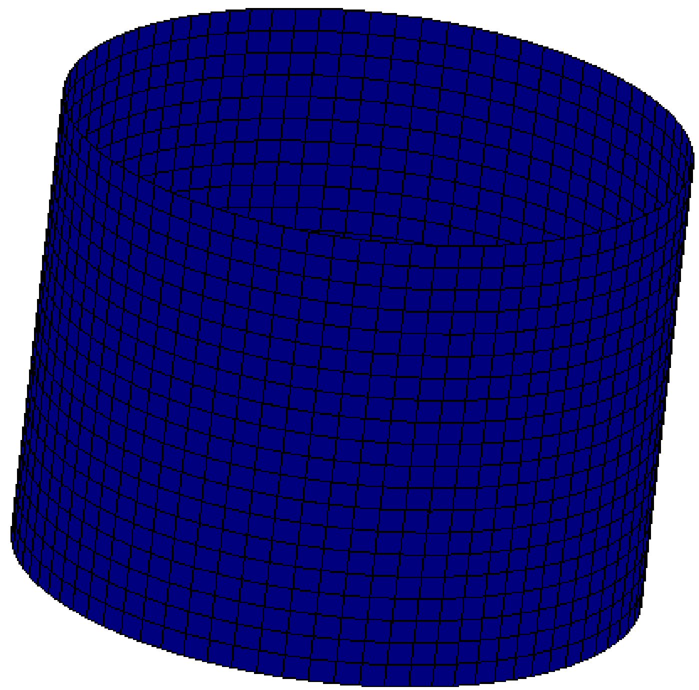


AM, Bischoff (2022): A Consistent Finite Element Formulation of the Geometrically Non-linear Reissner-Mindlin Shell Model, DOI

Simulation of magnetic vorticies

Simulation elastic deformation of shells

Riemannian Trust-Region method

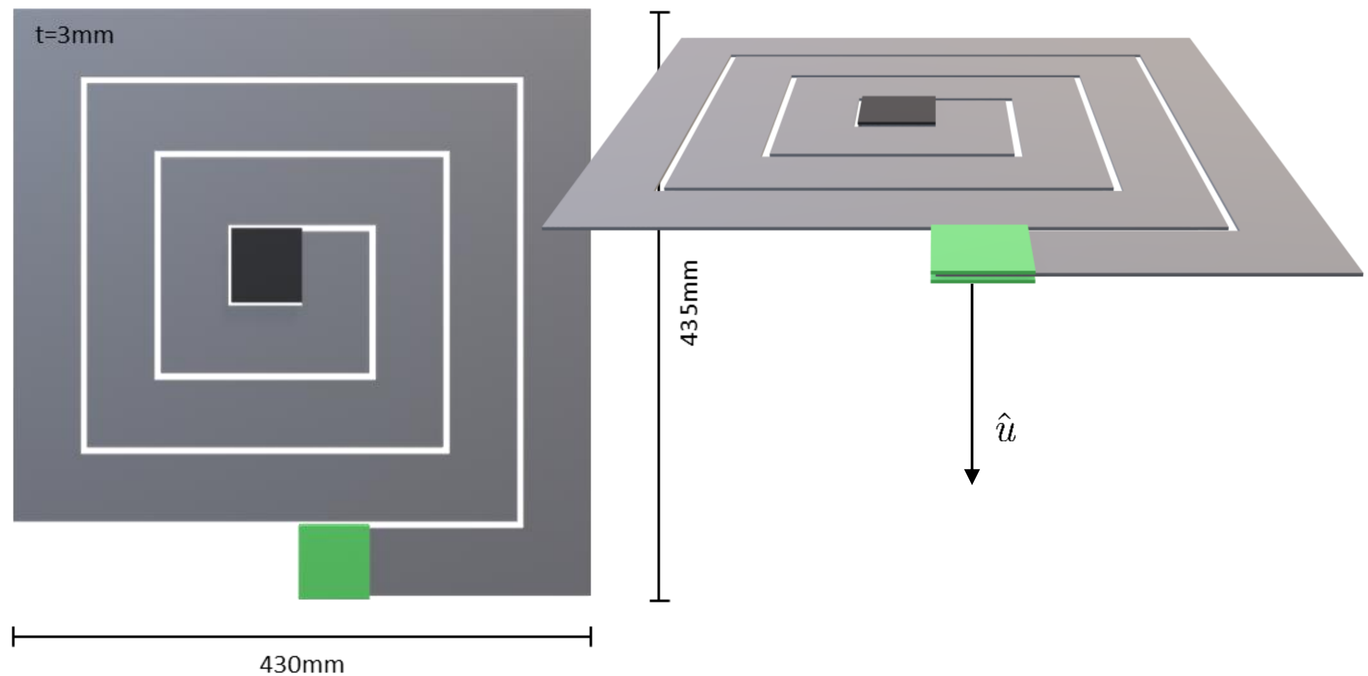


Minimizers for cylinder buckling

Simulation of Reissner-Mindlin shells

Simulation elastic deformation of shells

$$E = 210000$$
$$\nu = 0.3$$



Simulation of Reissner-Mindlin shells

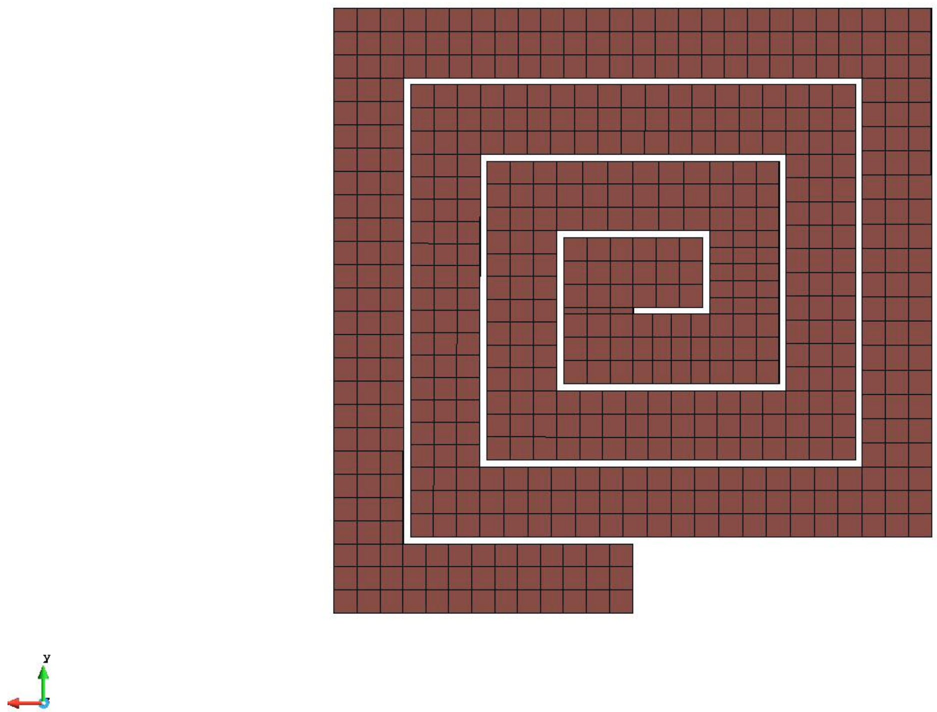
Simulation elastic deformation of shells

50 load steps

Simulation of Reissner-Mindlin shells

Simulation elastic deformation of shells

Several load steps



Deformation (x1): displacement of NumPro, step 0.1.

Other physical problems

Simulation of micromagnetics

Maxwell's equation in vacuum and matter

Ω

$$\mathbf{B} = \mu_0 \mathbf{H}$$

$$\operatorname{div} \mathbf{B} = 0$$

$$\nabla \times \mathbf{H} = 0$$

$\mathcal{B}$

$$\mathbf{B} = \mu_0 (\mathbf{M} + \mathbf{H})$$

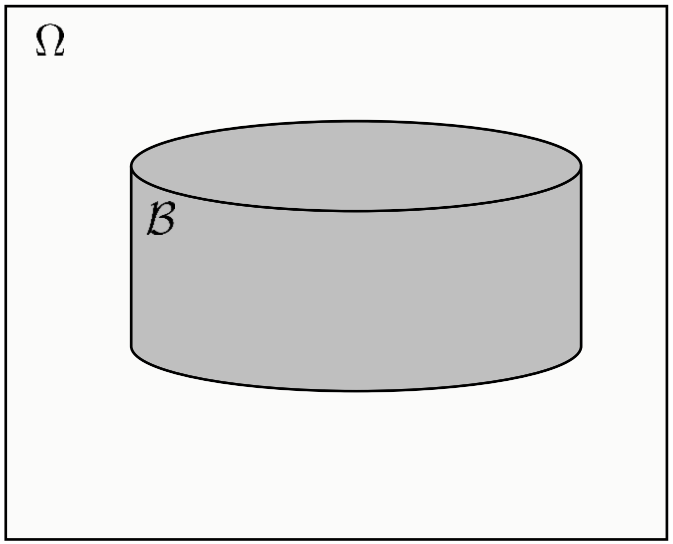
$$\operatorname{div} \mathbf{B} = 0$$

$$\nabla \times \mathbf{H} = 0$$

Other physical problems

Simulation of micromagnetics

$$\Pi(\mathbf{a},\mathbf{m}) = \int_{\Omega\setminus\mathcal{B}} \frac{1}{2}||\,\mathrm{curl}\,\mathbf{a}||^2 \,\mathrm{d}V + \int_{\mathcal{B}} \frac{1}{2}||\,\mathrm{grad}\,\mathbf{m}||^2 + \frac{1}{2}||\,\mathrm{curl}\,\mathbf{a}||^2 - \mathrm{curl}\,\mathbf{a}\cdot\mathbf{m}\,\mathrm{d}V$$

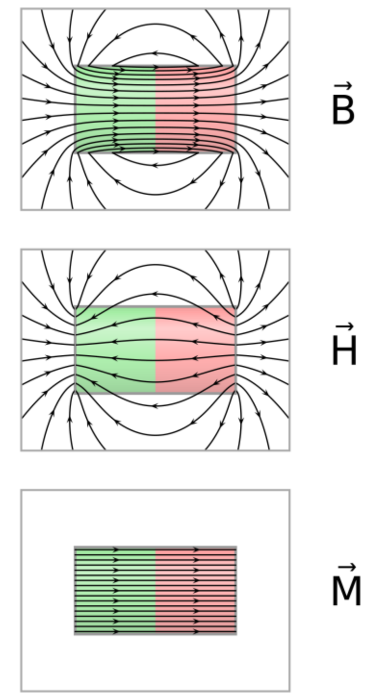


$$\mathbf{m} \in \mathcal{S}^2$$

$$\mathbf{a} \in \mathbb{R}^3$$

$$\mathbf{b} = \nabla \times \mathbf{a}$$

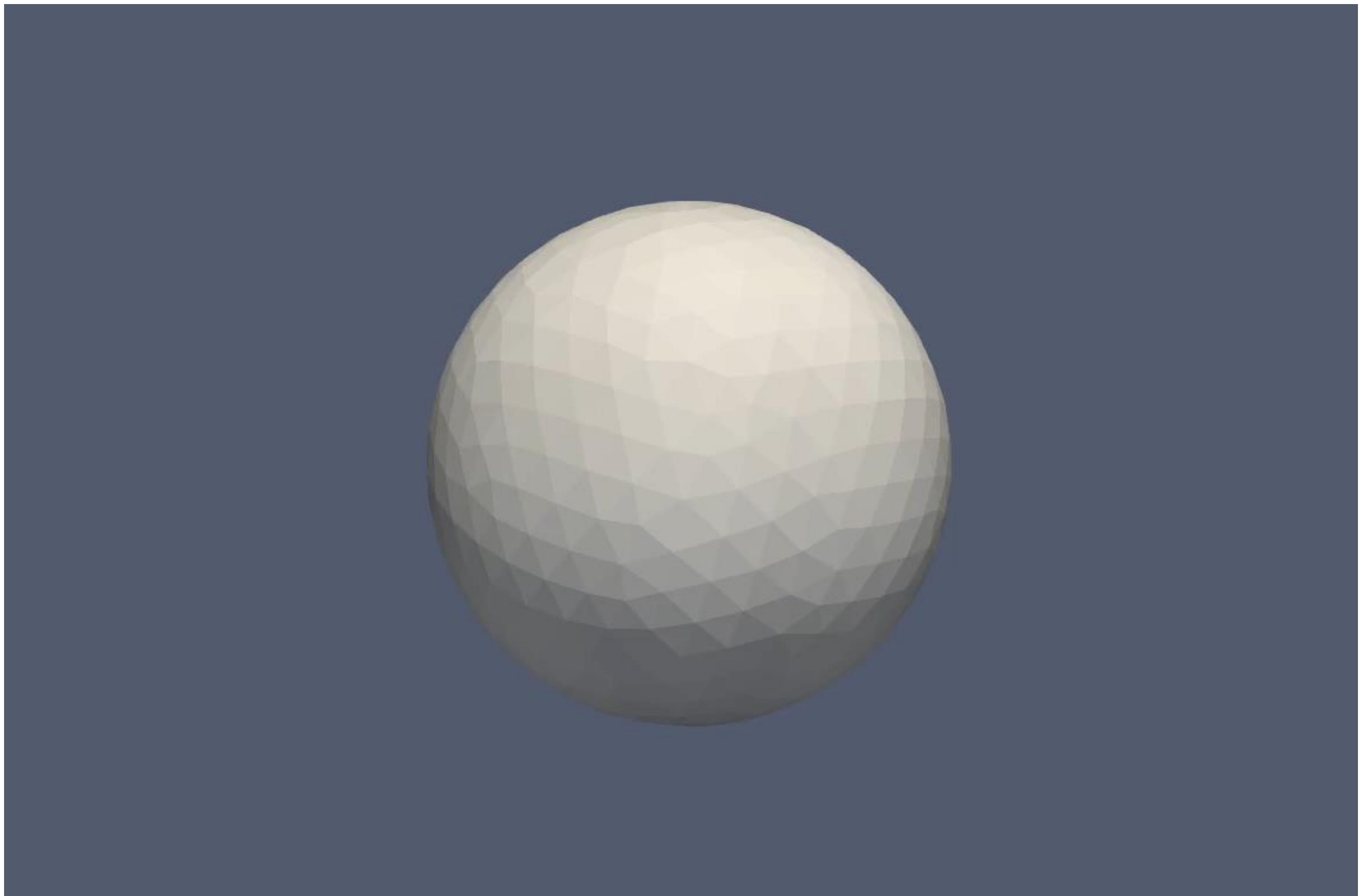
$$\min_{\mathbf{m}\in\mathcal{S}^2}\ \min_{\mathbf{a}\in\mathbb{R}^3} \Pi(\mathbf{m},\mathbf{a})$$



GEEK3, WIKIPEADIA (2022), CC BY-SA 4.0, LINK

Other physical problems

Simulation of micromagnetics



Application of optimization on manifolds to nonlinear shell theory

Summary

- Historical approaches can be outperformed by interpreting the problem as optimization on manifolds
- Interpolation must stay on the manifolds
- Lots of customization points exist, e.g., retractions
- Many other manifolds can be found in literature
- Methods can be used for other physical simulations (micromagnetics)

Not mentioned:

Examples:

The important Sobolev space $W^{1,2}(\Omega, \mathcal{M})$ does not even always possess the structure of a Banach manifold

Geodesics for interpolation are not always unique

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Thank you!

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