University of Stuttgart
Institute for Structural Mechanics

Optimization On Manifolds For The Advanced Discretization Of Director Fields

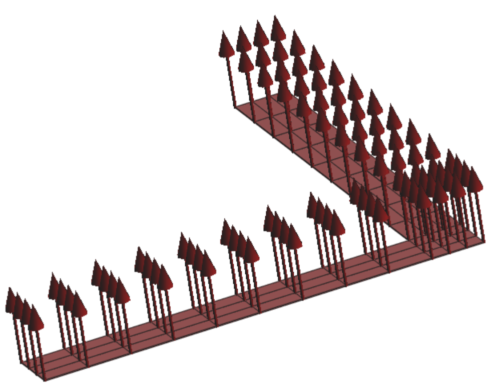
Alexander Müller, Manfred Bischoff

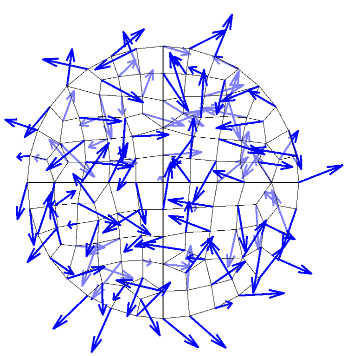
GACM

9th Colloquium on Computational Mechanics

21.9.22–23.9.22

MS 30

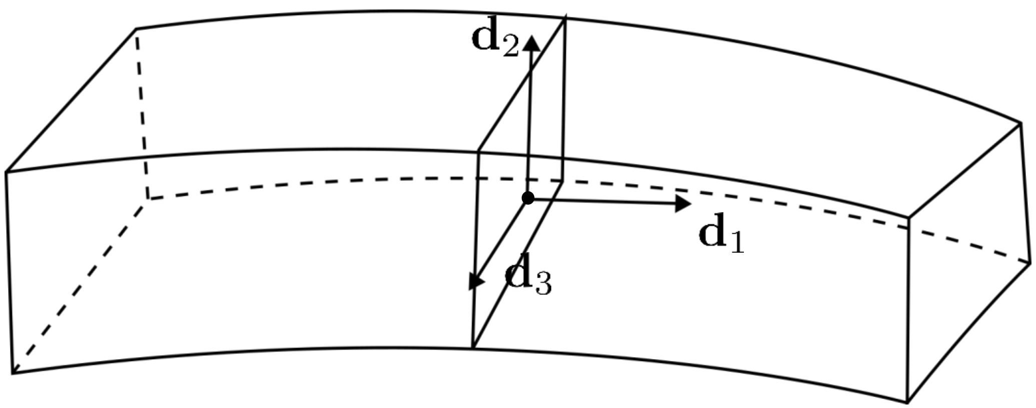




Baustatik und Baudynamik

Director fields

Example 1: geometrically non-linear beam



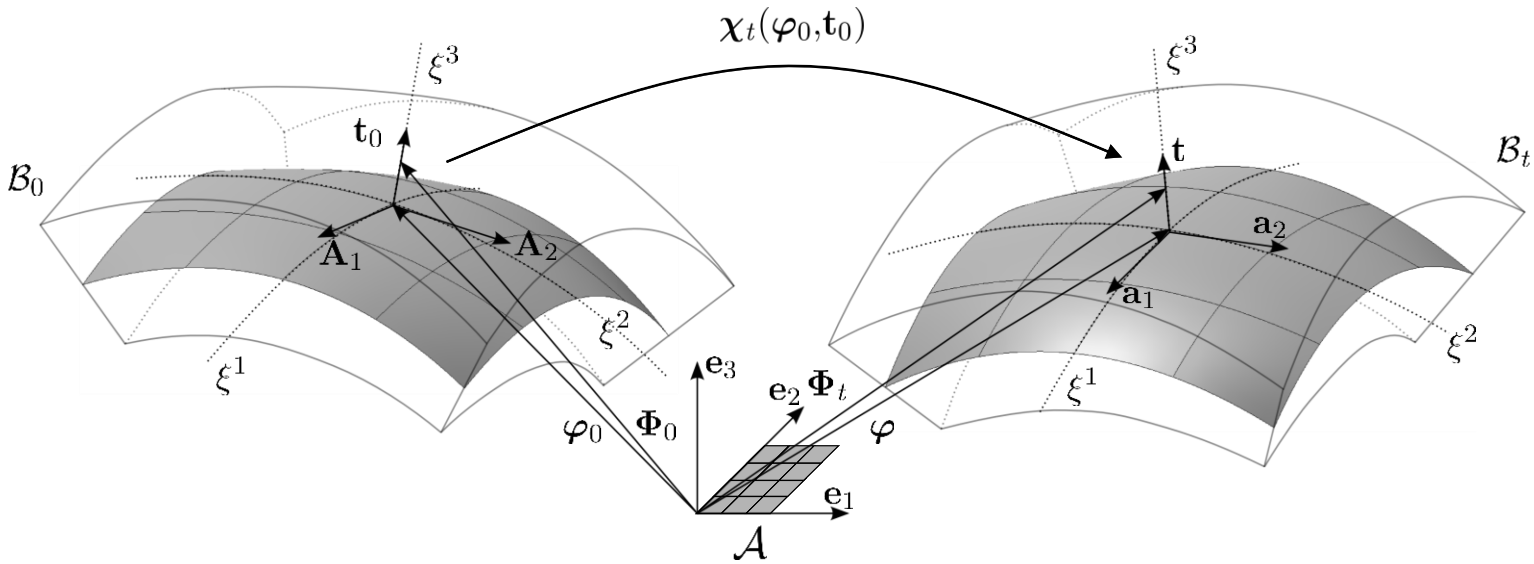
$$\mathbf{R} = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3] \quad \mathbf{d}_i \cdot \mathbf{d}_j = \delta_{ij}$$

$$\Downarrow$$

$$\mathbf{R} \in \mathcal{SO}(3)$$

Director fields

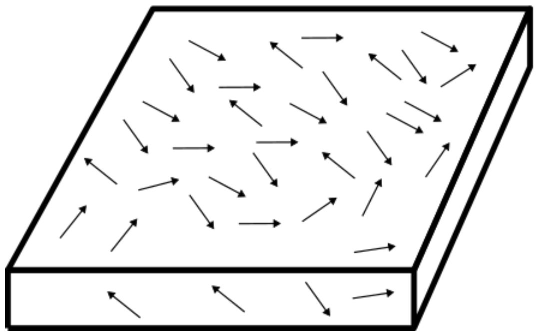
Example 2: geometrically non-linear Reissner-Mindlin shell



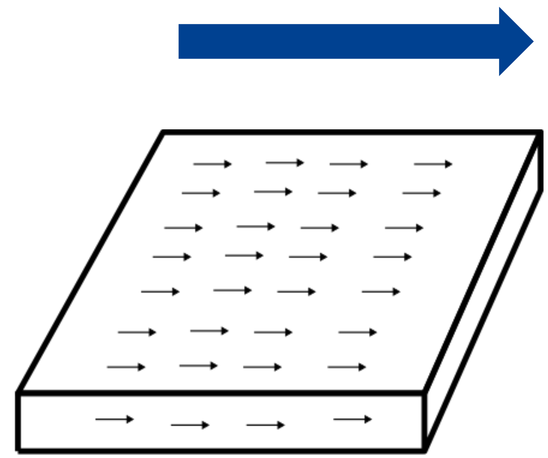
$\mathbf{t}(\xi^1,\xi^2)$ $\qquad$ $\mathbf{t} : \mathcal{A} \rightarrow \mathcal{S}^2 \subset \mathbb{R}^3$

Director fields

Example 3: micromagnetics (Magnetic Maxwell equations in matter)

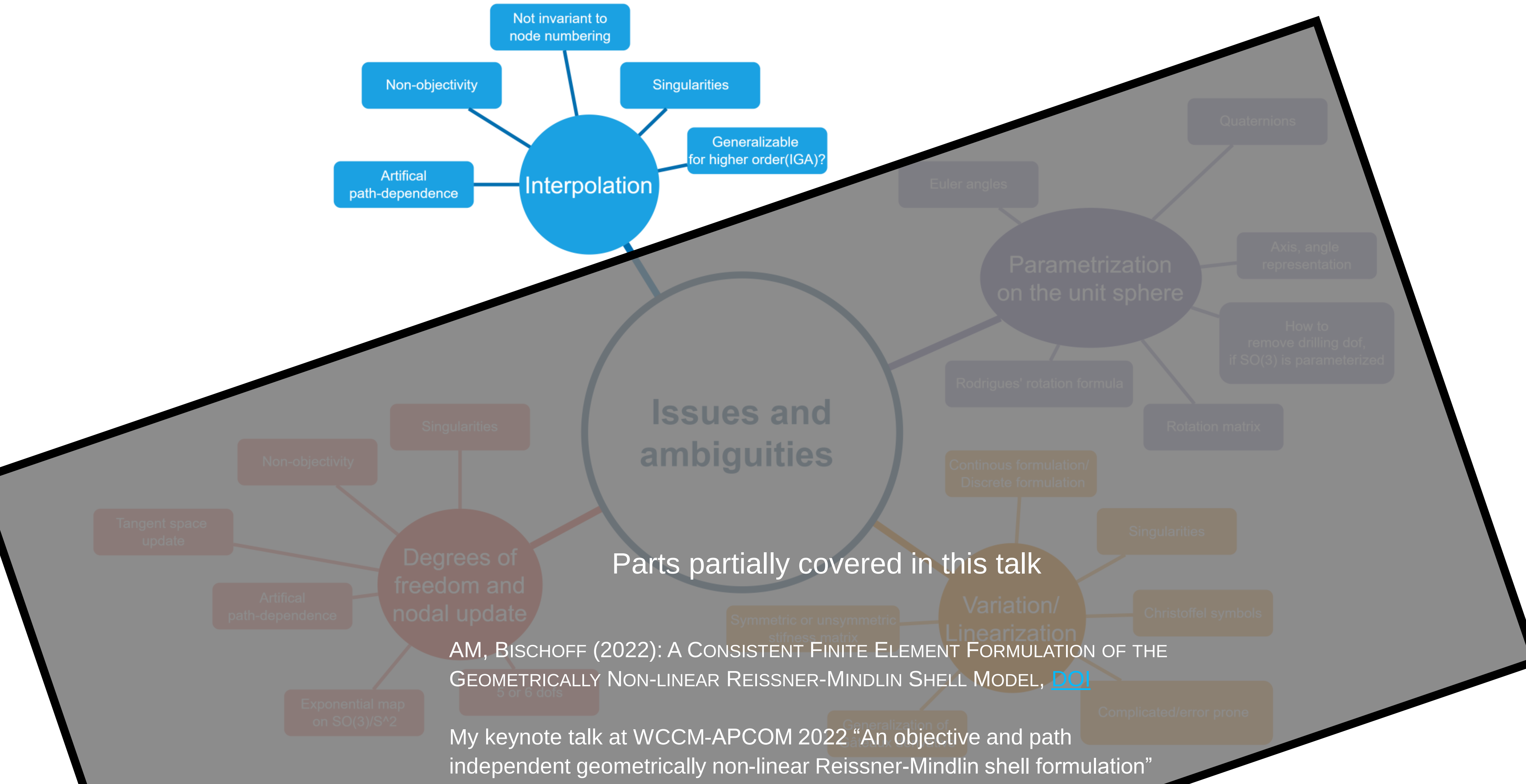


$$\mathbf{m}(\xi^1,\xi^2,\xi^3)$$



$$\mathbf{m} : \mathcal{A} \rightarrow \mathcal{S}^2 \subset \mathbb{R}^3$$

Director fields



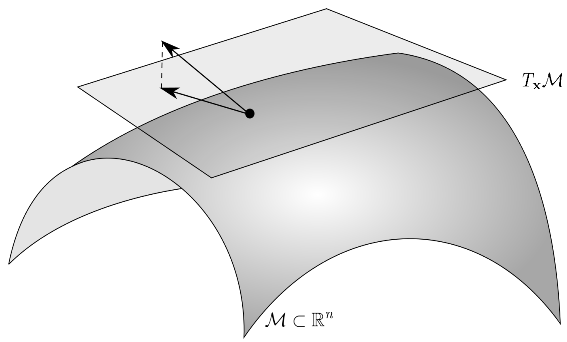
Parts partially covered in this talk

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

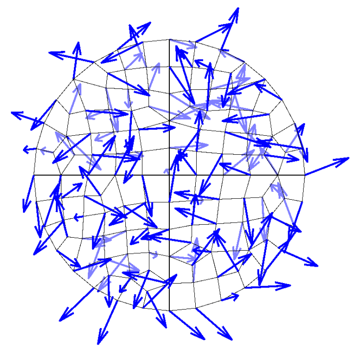
My keynote talk at WCCM-APCOM 2022 “An objective and path independent geometrically non-linear Reissner-Mindlin shell formulation”

Outline

Optimization on manifolds



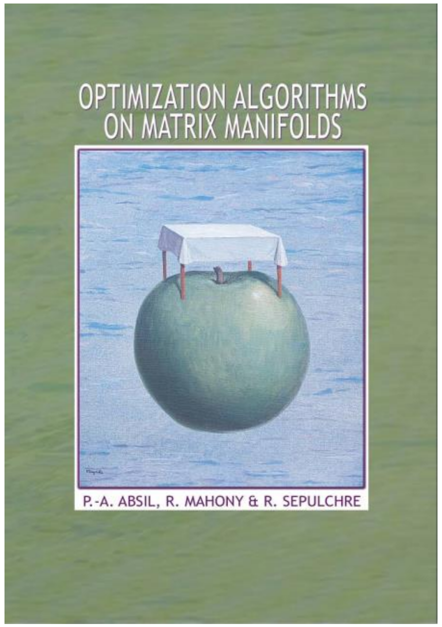
Numerical examples



Optimization on manifolds

Optimization on manifolds

Literature



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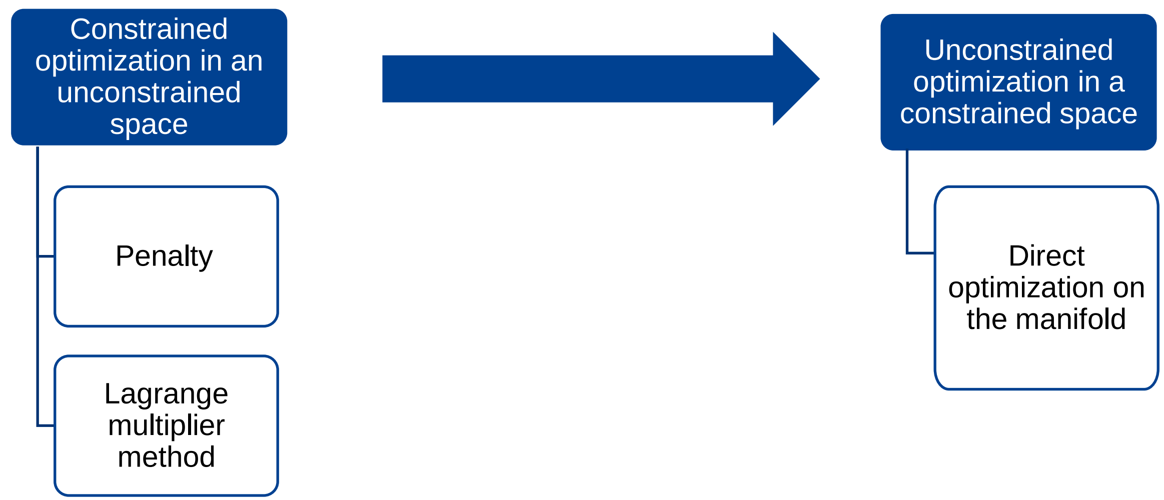
Boumal N (2020) An introduction to optimization on smooth manifolds. Available online, Link



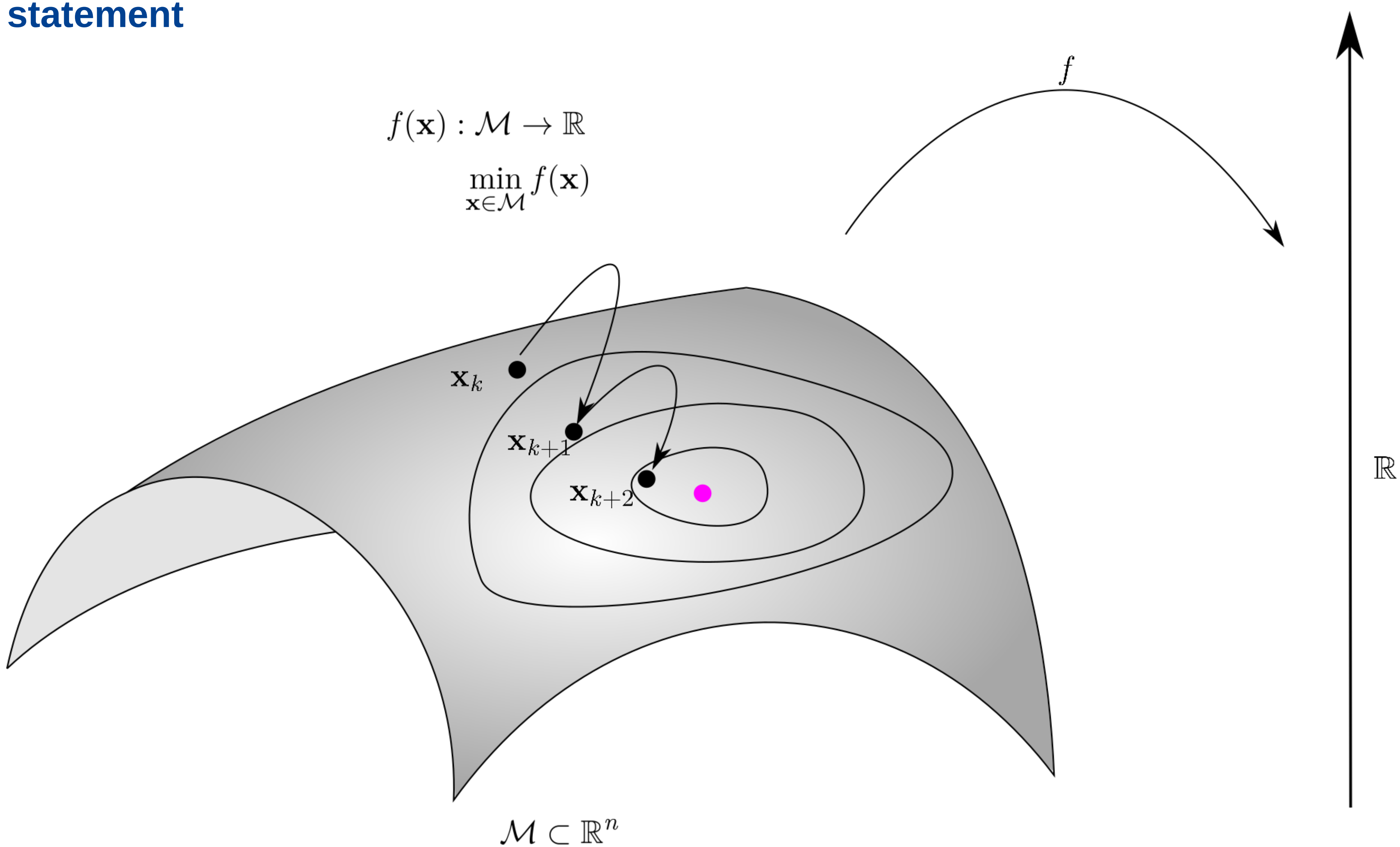
Optimization on manifolds

Baustatik und Baudynamik

Problem statement

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

$$\min_{\mathbf{x} \in \mathcal{M}} f(\mathbf{x})$$



Riemannian gradient

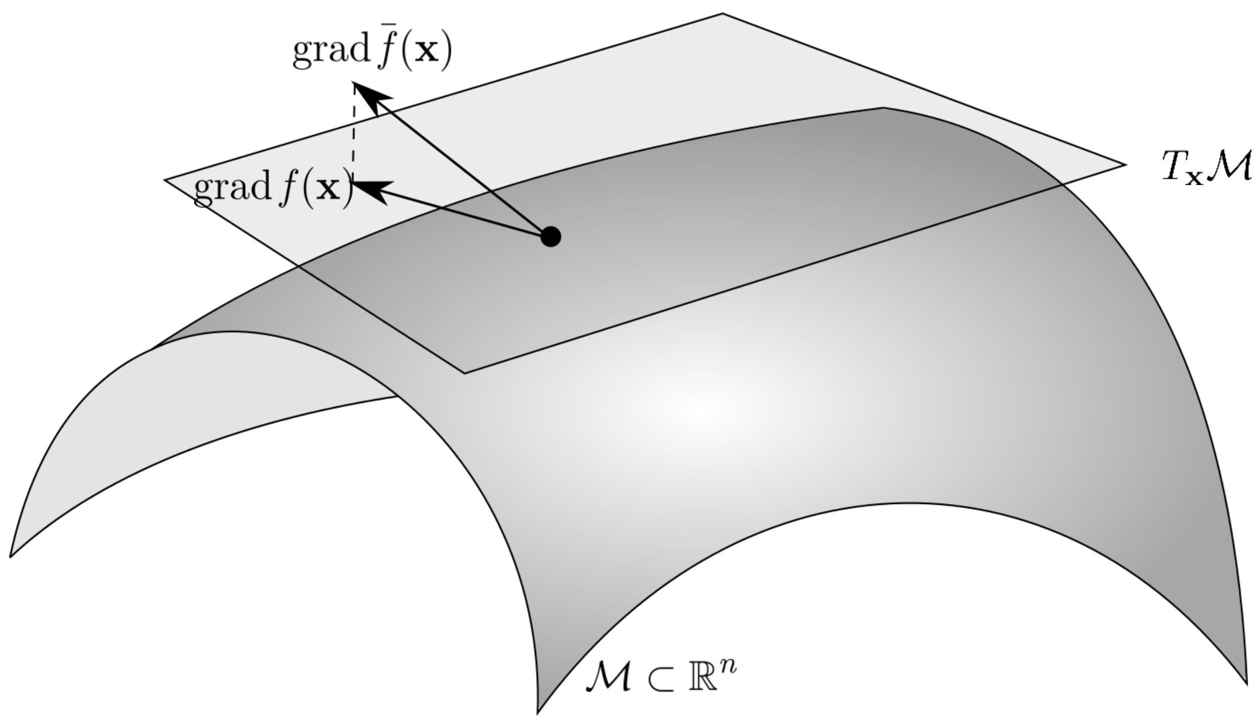
Riemannian gradient: submanifolds

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

"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.

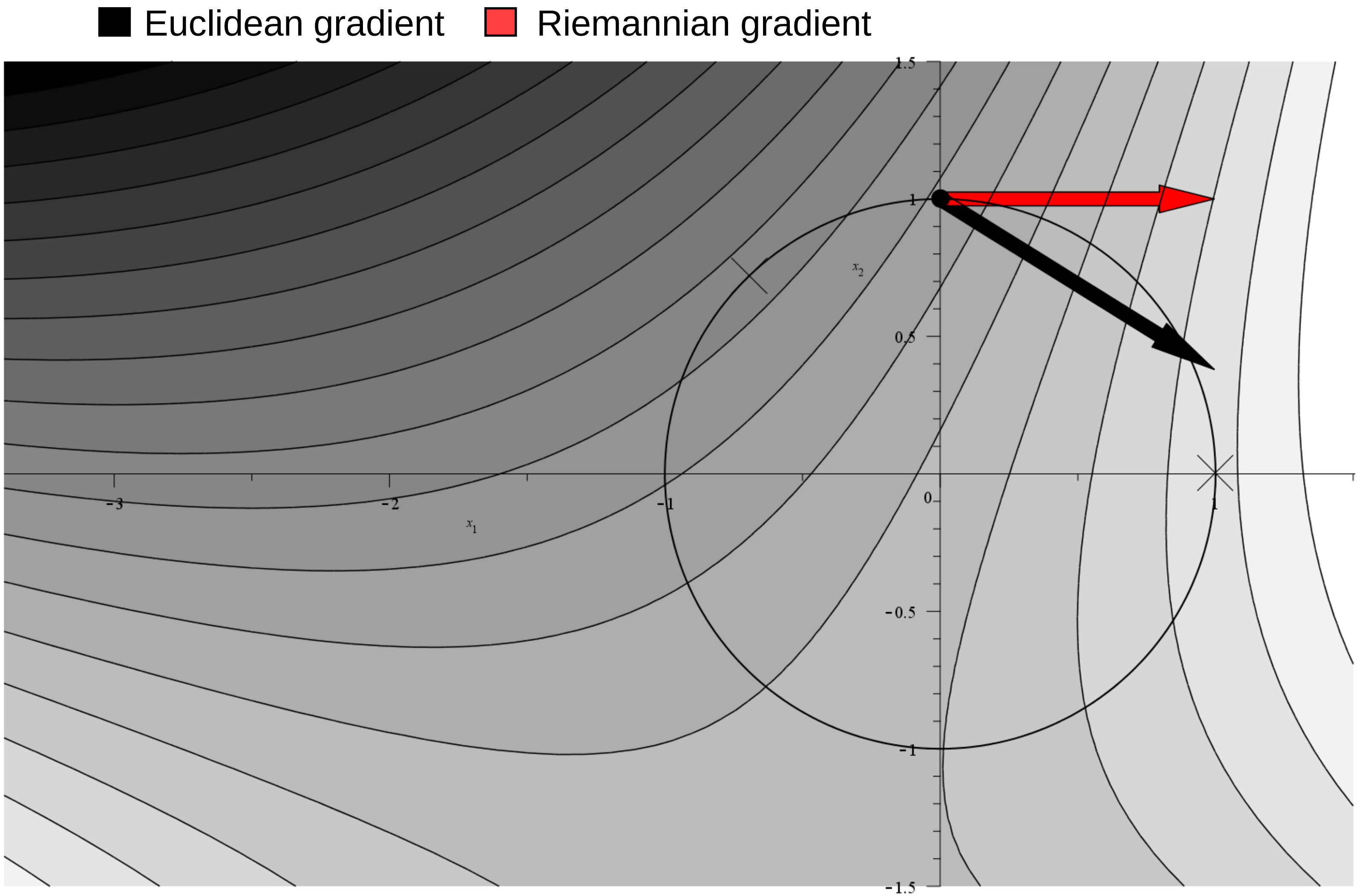
$$\operatorname{grad} f(\mathbf{x}) = P_{\mathbf{x}} \operatorname{grad} \bar{f}(\mathbf{x})$$



- No parametrization
- No artificial singularities
- Simple linearization

Optimization on manifolds

Toy problem, gradient and Riemannian gradient



Riemannian Hessian

Optimization on Manifolds

Riemannian Hessian: submanifolds

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

Levi-Civita connection: $\nabla_{\boldsymbol{\eta}_{\mathbf{x}}} \boldsymbol{\xi} = P_{\mathbf{x}} \mathrm{D}_{\boldsymbol{\eta}_{\mathbf{x}}} \boldsymbol{\xi} \qquad \boldsymbol{\xi}, \boldsymbol{\eta} \in T_{\mathbf{x}} \mathcal{M}$

$$\operatorname{Hess} f(\mathbf{x}) \boldsymbol{\eta} = P_{\mathbf{x}} \operatorname{Hess} \bar{f}(\mathbf{x}) P_{\mathbf{x}} \boldsymbol{\eta} + W_{\mathbf{x}}(\boldsymbol{\eta}, P_{\mathbf{x}}^{\perp} \operatorname{grad} \bar{f}(\mathbf{x}))$$

ABSIL PA, MAHONY R, TRUMPF J (2013) AN EXTRINSIC LOOK AT THE RIEMANNIAN HESSIAN

"[…] This shows that, for Riemannian submanifolds of Euclidean spaces, the Riemannian Hessian is the projected Euclidean Hessian plus a correction term which depends only on the normal part of the Euclidean gradient."

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

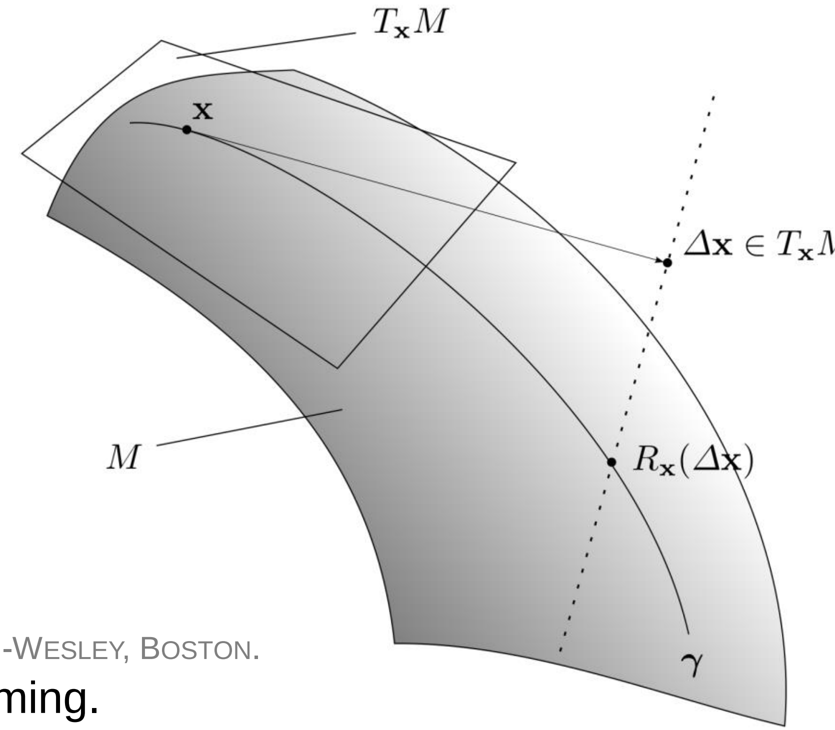
Update of nodal values

Optimization on manifolds

Baustatik und Baudynamik

Update of nodal values

$\mathbf{x}_k + \Delta\mathbf{x}_k \notin \mathcal{M}$ $\boldsymbol{\gamma}(t) = \exp_{\mathbf{x}_k}(t\Delta\mathbf{x}_k)$



ABSIL PA , "OPTIMIZATION ON MANIFOLDS: METHODS AND APPLICATIONS", LEUVEN, 18 SEP 2009.
LUENBERGER, D.G. (1973) INTRODUCTION TO LINEAR AND NONLINEAR PROGRAMMING. ADDISON-WESLEY, BOSTON.

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

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

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

Motivation

Baustatik und Baudynamik

Riemannian Newton

	Classic Newton	Riemannian Newton
Update	$\mathbf{x}_{k+1} = \mathbf{x}_k + \Delta\mathbf{x}_k$	$\mathbf{x}_{k+1} = R_{\mathbf{x}_k}(\Delta\mathbf{x}_k)$
Gradient	$\operatorname{grad} f(\mathbf{x})$	$\operatorname{grad} f(\mathbf{x}) = P_{\mathbf{x}} \operatorname{grad} \bar{f}(\mathbf{x})$
Hessian	$\operatorname{Hess} f(\mathbf{x})$	$\operatorname{Hess} f(\mathbf{x})\boldsymbol{\eta} = P_{\mathbf{x}} \operatorname{Hess} \bar{f}(\mathbf{x}) P_{\mathbf{x}}\boldsymbol{\eta} + W_{\mathbf{x}}(\boldsymbol{\eta}, P_{\mathbf{x}}^{\perp} \operatorname{grad} \bar{f}(\mathbf{x}))$

Ingredients:

$R_{\mathbf{x}} : T_{\mathbf{x}}\mathcal{M} \to \mathcal{M}$

$\mathbf{P}_{\mathbf{x}} : \mathbb{R}^n \to T_{\mathbf{x}}\mathcal{M}$

$W_{\mathbf{x}} : T_{\mathbf{x}}\mathcal{M} \times T_{\mathbf{x}}^{\perp}\mathcal{M} \to T_{\mathbf{x}}\mathcal{M}$

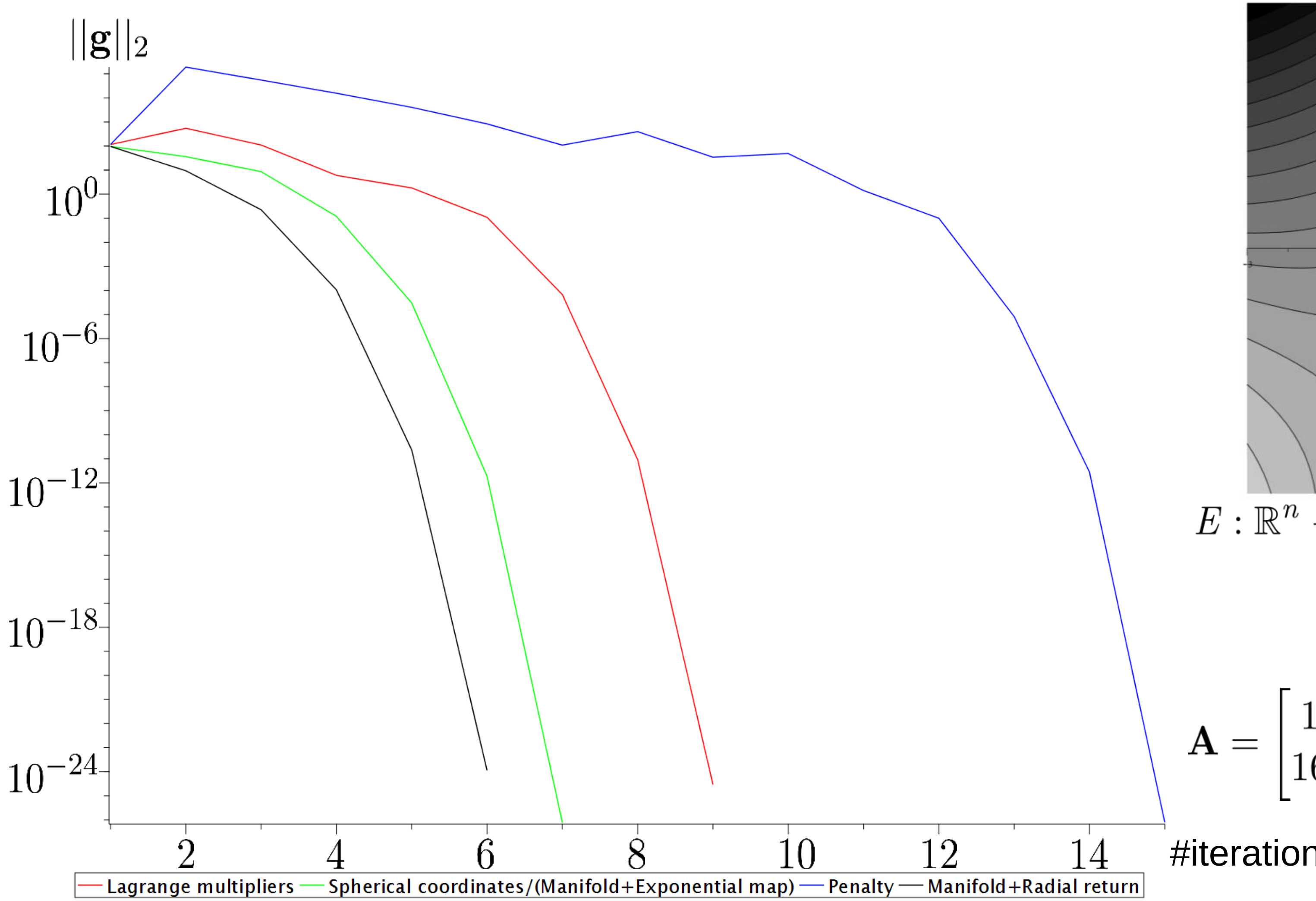
$\operatorname{Hess} \bar{E}(\mathbf{x})$

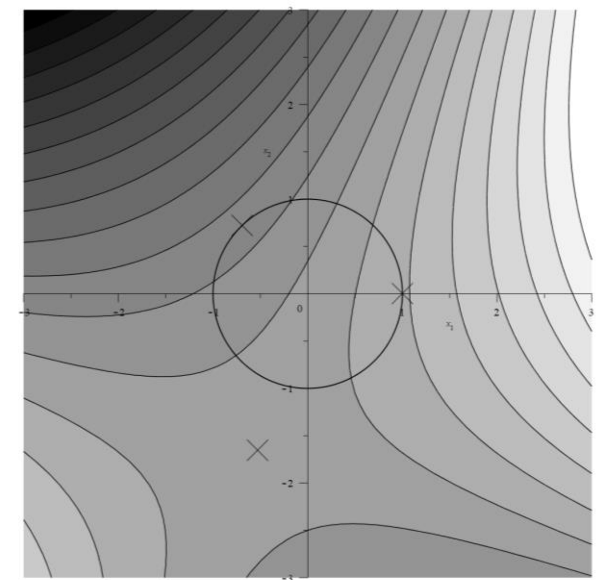
$\operatorname{grad} \bar{E}(\mathbf{x})$

Tangent space basis $\boldsymbol{\Lambda}$

Algebraic optimization on manifolds

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





$$E : \mathbb{R}^n \to \mathbb{R}, \quad E(\mathbf{x}) = (\mathbf{x}+\mathbf{b})^T \mathbf{A}(\mathbf{x}+\mathbf{b})$$

$$\min_{\mathbf{x}\in\mathcal{S}^1} E(\mathbf{x})$$

$$\mathbf{A} = \begin{bmatrix} 12.6 & 16.23 \\ 16.23 & -14.92 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0.53 \\ 1.65 \end{bmatrix}$$

Optimization on manifolds

Summary

	LAM	Penalty	Coordinates	Manifold optimization
Linearization	☺	☺	☹	☺
Singularities	☺	☺	☹	☺
Search space dimensions	3	2	1	1
Minimization	☹	☺	☺	☺
Iterations	☹	☹	☺	☺

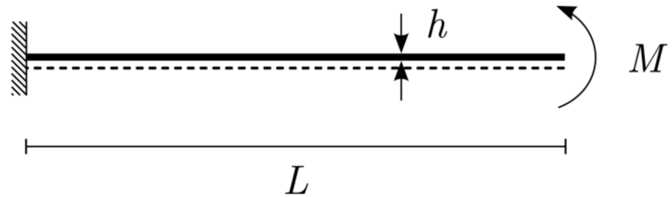
2D example from before

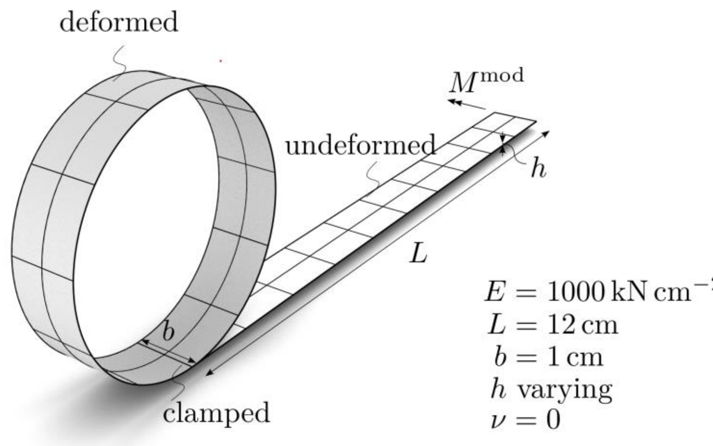
Numerical examples

Numerical examples

Reissner-Mindlin: roll-up of clamped beam

- 1 loadstep
- 16 iterations of Newton's method to reach equilibrium using MIP





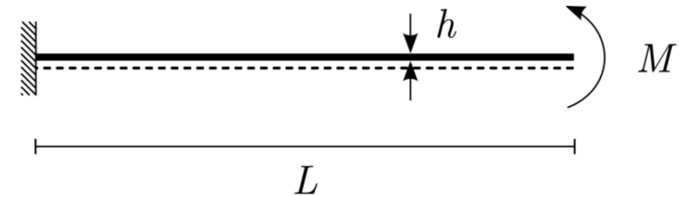
$$\Pi(\boldsymbol{\varphi}, \mathbf{t}) = \int_{\mathcal{B}} \psi_{\mathrm{strain}}(\boldsymbol{\varphi}, \mathbf{t})\, \mathrm{d}V + \Pi_{\mathrm{ext}}(\boldsymbol{\varphi}, \mathbf{t})$$

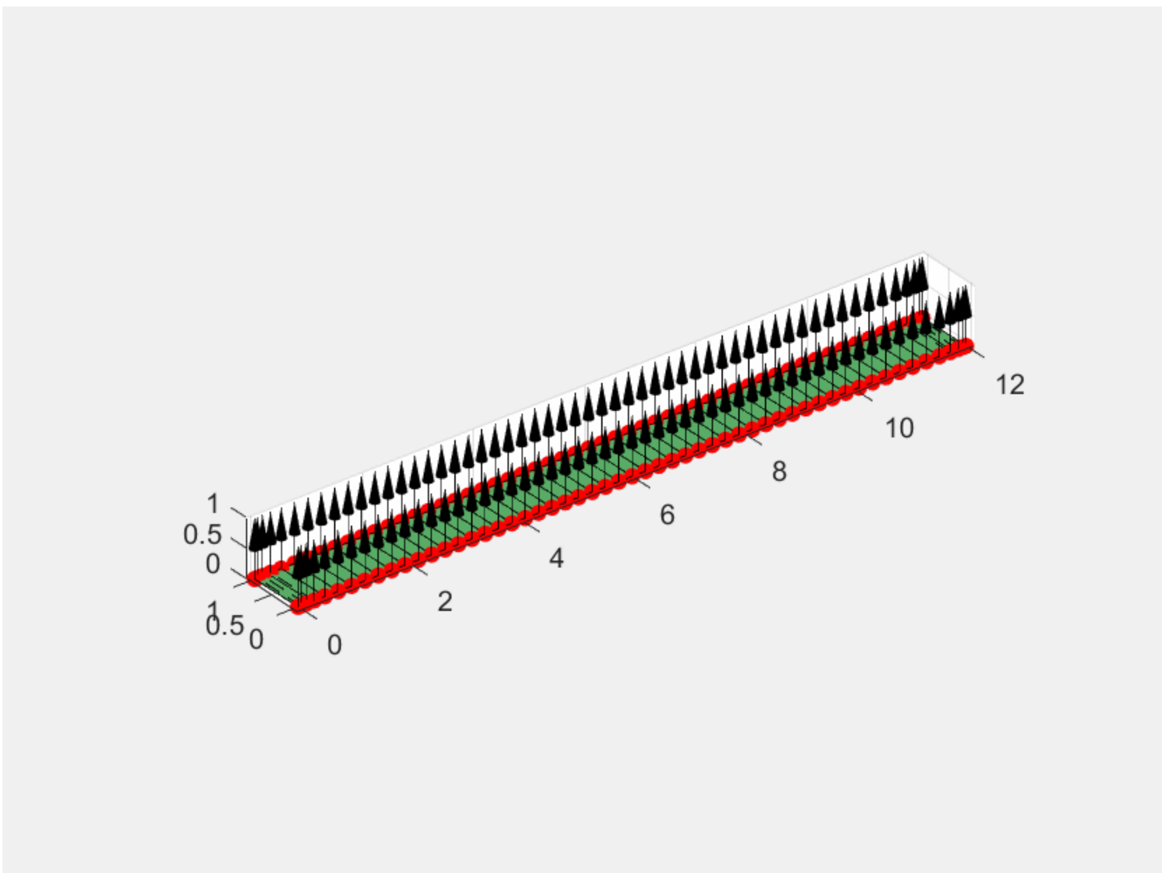
$$\{\boldsymbol{\varphi}^*, \mathbf{t}^*\} = \arg\left\{ \min_{\boldsymbol{\varphi}\in\mathbb{R}^d} \min_{\mathbf{t}\in\mathcal{S}^{d-1}} \Pi(\boldsymbol{\varphi}, \mathbf{t}) \right\}.$$

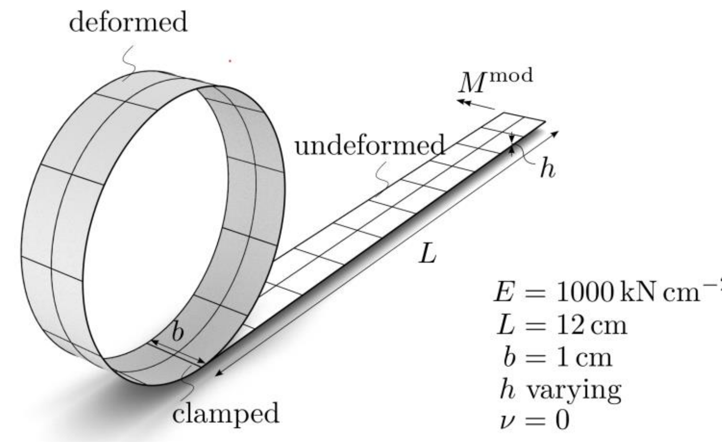
Numerical examples

Reissner-Mindlin: roll-up of clamped beam

- 1 loadstep
- 16 iterations of Newton’s method to reach equilibrium using MIP







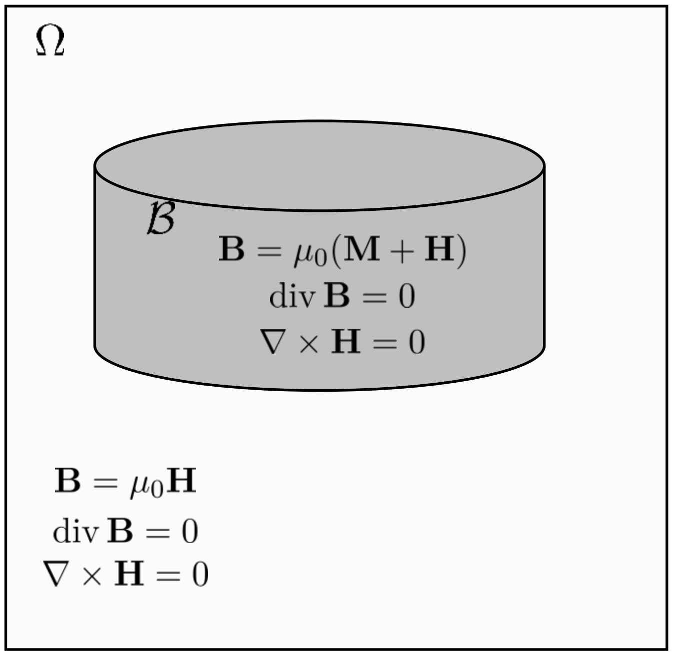
$$\Pi(\boldsymbol{\varphi}, \mathbf{t}) = \int_{\mathcal{B}} \psi_{\mathrm{strain}}(\boldsymbol{\varphi}, \mathbf{t})\,\mathrm{d}V + \Pi_{\mathrm{ext}}(\boldsymbol{\varphi}, \mathbf{t})$$

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

Numerical examples

Simulation of micromagnetics

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



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

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

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

Maxwell's equation in vacuum and matter

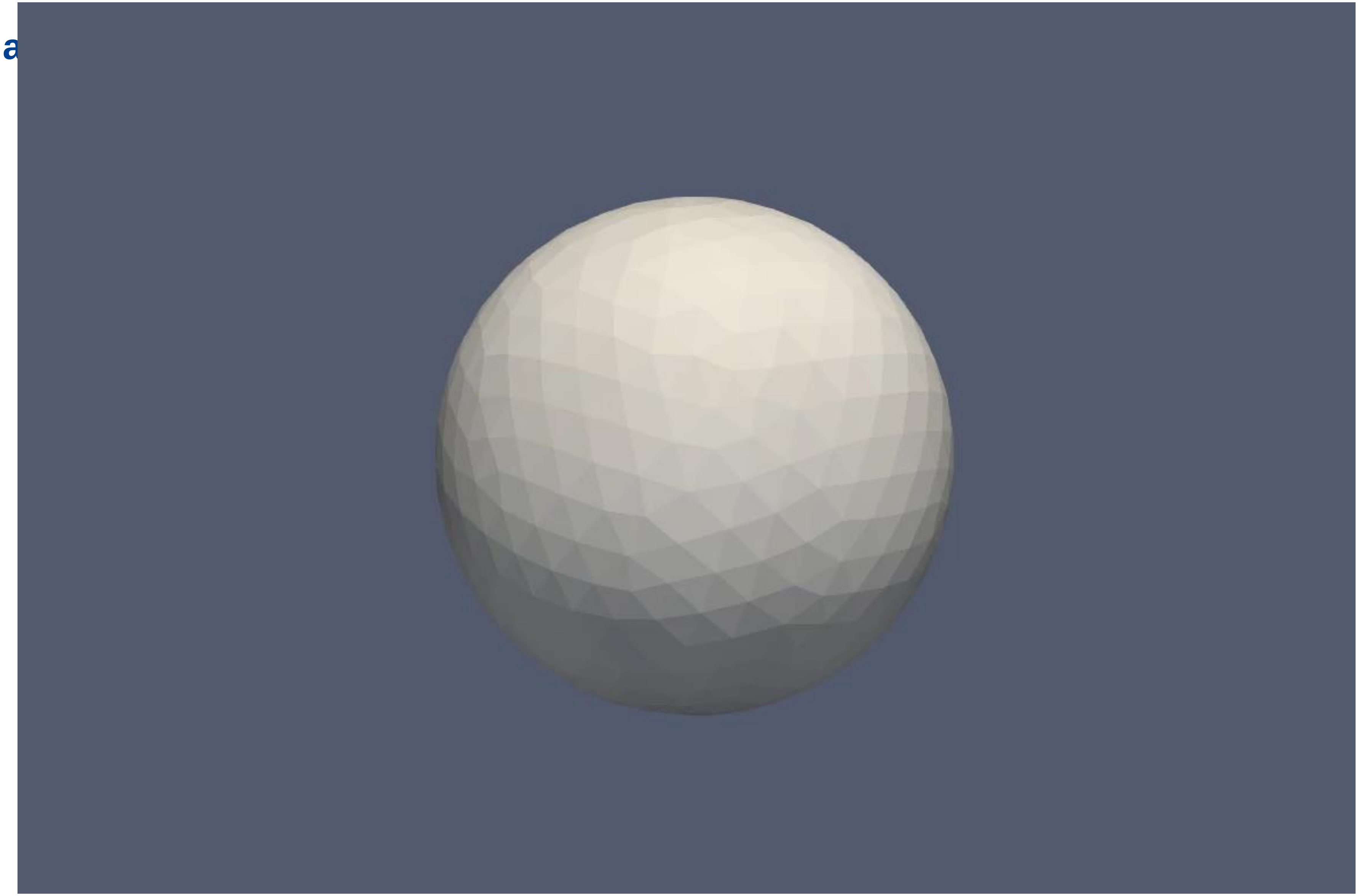
$$\min_{\mathbf{m}\in\mathcal{S}^2}\ \min_{\mathbf{a}\in\mathbb{R}^3} \Pi(\mathbf{m},\mathbf{a})$$

Numerically solved using the Riemannian trust region method

COLLABORATION WITH MARC-ANDRÉ KEIP

Numerical examples

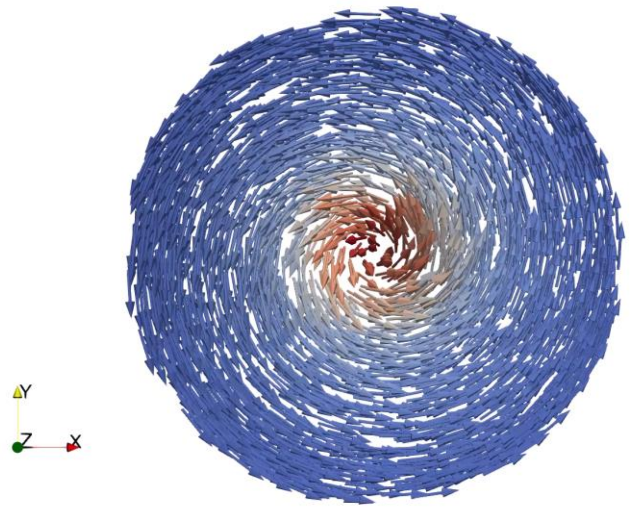
Simula

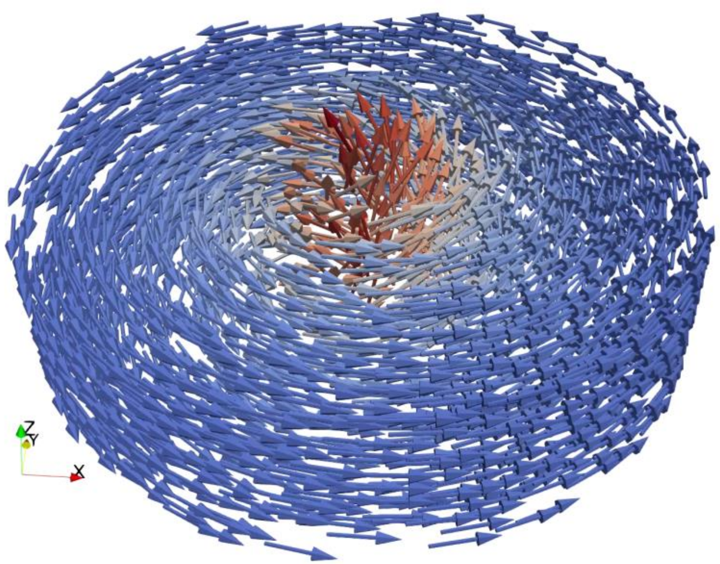


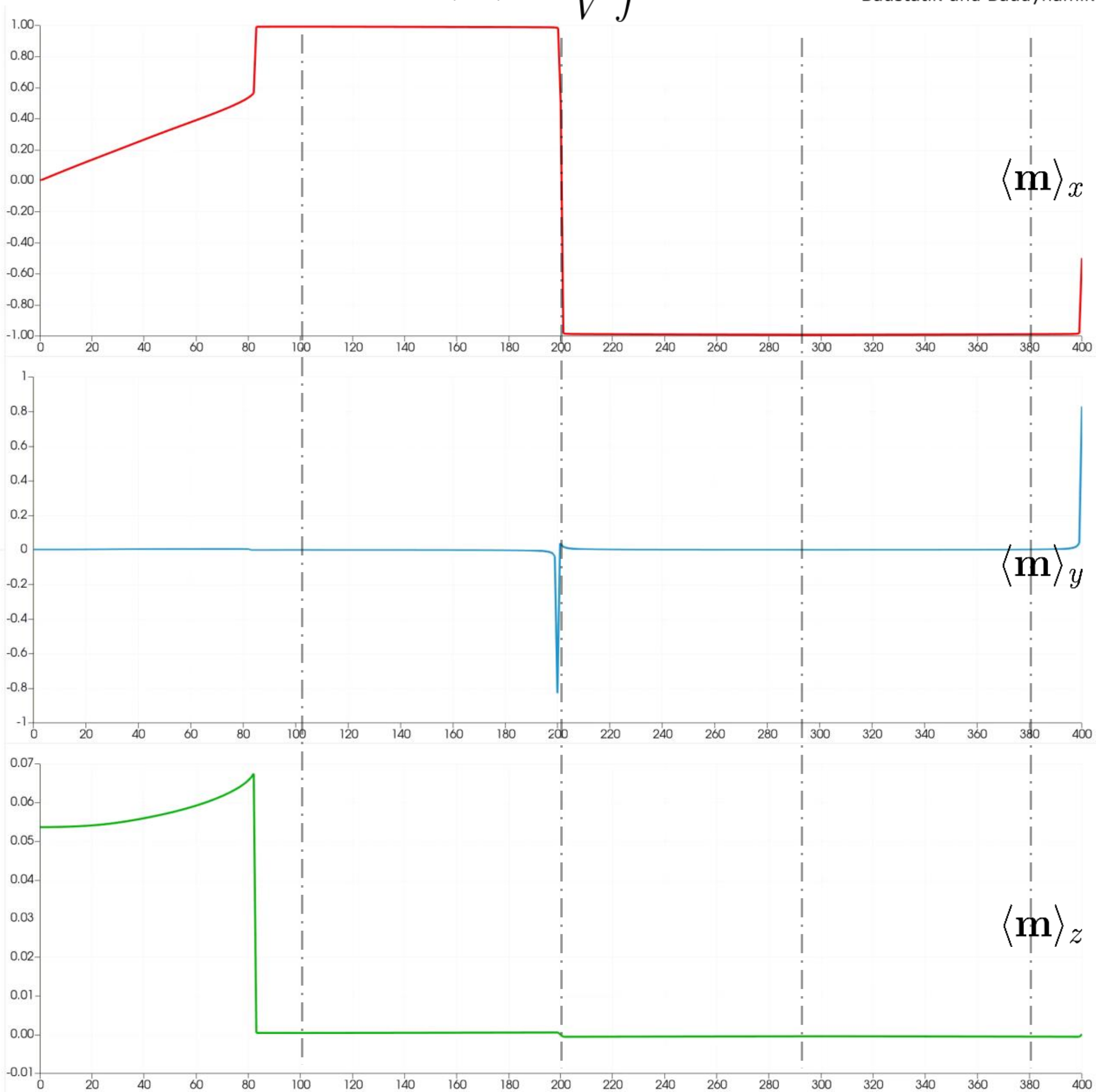
Numerical examples

$$\langle \mathbf{m} \rangle = \frac{1}{V} \int \mathbf{m} \, \mathrm{d}\Omega$$

Baustatik und Baudynamik







Outlook

Baustatik und Baudynamik

Apply results to

- Geometrically non-linear beams $\mathcal{SO}(3)$
- Other manifolds
  - Incompressible Materials/Plasticity $\mathcal{SL}(3)$
  - …

Dynamics on manifolds

- Non-constant mass matrix
- Riemannian Hamiltonian/Lagrangian
- Variational integrators for manifolds
- …

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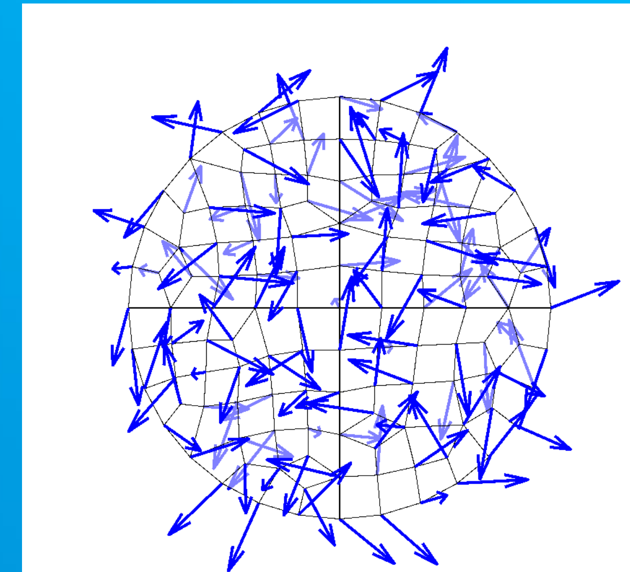

Thank you!

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Slides

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