# On Wrinkles

# $\label{eq:one-state} \begin{array}{l} \mbox{Oliver Sander,} \\ \mbox{RWTH Aachen} \Rightarrow \mbox{TU Dresden} \end{array}$

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#### Wong, Pellegrino 2006:



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

#### Tension field theory

- Scalar "wrinkling density field"
- Partial differential equation / relaxed energies
- ► No details, but averaged effect of the wrinkles on stress distribution

#### Semi-analytical models

- Semianalytical solutions of plate/shell equations
- Power laws for wrinkle amplitude/wavelength
- Only in specific situations

#### Full continuum mechanics

- Detailed local wrinkling behavior
- Very expensive
- Let's see...



- ► Geometrically linear
- St. Venant–Kirchhoff material
- ►  $E = 71240 \text{ N/mm}^2$ ,  $\nu = 0.31$



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#### Kinematics

- Deformation  $\varphi:\Omega\to\mathbb{R}^3$
- Deformation gradient  $F = \nabla \varphi$
- Strain  $C = F^T F$

#### Mooney-Rivlin material (for example)

Energy density

$$W(F) = a ||F||^2 + b ||Cof F||^2 + \Gamma(\det F), \qquad a, b > 0$$

Volumetric term

$$\Gamma(s) := s^2 - \log s$$

is  ${\ensuremath{C}}^2$  and convex













#### Why doesn't the solver converge?

Energy volumetric term

$$W(F) = \dots + \Gamma(\det F)$$
 with  $\Gamma(s) := s^2 - \log s$ 

prevents local inversion / flipping of elements

- Object/elements very thin
- Very difficult to find admissible correction steps

#### Dimensional reduction

• Object is virtually 2-dimensional  $\Rightarrow$  model it by 2d equation



#### Zoo of models

- Shells vs. plates vs. membranes
- Kirchhoff type (schubstarr) vs. director theories
- ▶ 4th order vs. 2nd order
- ▶ 1 director vs. 3 directors



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#### Kinematics:

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

#### 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)

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

Membrane energy:

#### Bending energy:

$$W_{\text{bend}}(\mathfrak{K}_{\mathfrak{b}}) = \mu \|\text{sym}(\mathfrak{K}_{b})\|^{2} + \mu_{c} \|\text{skew}(\mathfrak{K}_{b})\|^{2} + \frac{\mu\lambda}{2\mu + \lambda} \operatorname{tr}[\text{sym}(\mathfrak{K}_{b})]^{2}$$

Curvature energy:

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

## Theorem ([Neff])

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



Partial differential equations for functions

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

M a Riemannian manifold.

#### Applications:

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

#### The challenge: Nonlinear function spaces



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:

- $\blacktriangleright$  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

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#### But

- What if such an embedding is not available?
- Not elegant, because relies on embedding.

# Generalizing Lagrangian Interpolation

#### Reference element $T_{ref}$ :

- Arbitrary type
- Coordinates  $\xi$
- Lagrange nodes  $\nu_i$ ,  $i = 1, \ldots, m$
- Shape functions  $\{\varphi_i\}$  of p-th order

#### Lagrange interpolation:

Assume values  $v_1, \ldots, v_m \in M$  given at the Lagrange nodes. If M is a vector space, interpolation between the  $v_i$  can be written as

$$\sum_{i=1}^{m} v_i \varphi_i(\xi) = \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{m} \varphi_i(\xi) \|v_i - q\|^2.$$

Indeed, if 
$$M = \mathbb{R}$$
: gradient is  $2\sum_{i=1}^{m} \varphi_i(\xi)(v_i - q)$ 



#### Geodesic Interpolation

Idea: Generalize

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

to

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

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

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

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

$$\Upsilon^{p}(v,\xi) = \operatorname*{arg\,min}_{q \in M} \sum_{i=1}^{m} \varphi_{i}(\xi) \operatorname{dist}(v_{i},q)^{2}$$

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:

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



- ▶ 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  $D, \rho$  with  $0 < D < \rho$ , depending on the curvature of M and the total variation of the weights  $\varphi_i$ , such that if the values  $v_1, \ldots, v_m$  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  $\xi$  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.

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.,

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



#### Definition:

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

#### Values: Minimize

 $f_{\xi}(q) := \sum_{i=1}^{m} \varphi_i(\xi) \operatorname{dist}(v_i, q)^2$ 

by a Newton-type method in  $\dim M$  variables. [Absil et al.]

Gradients: i.e.,  $\partial \Upsilon / \partial \xi$ Total derivative of  $F(\xi, q) := \frac{\partial f_{\xi}}{\partial q} = 0$  yields  $\partial F(\xi, q) \quad \partial \Upsilon \qquad \partial F(\xi, q)$ 

$$\frac{\partial q}{\partial q} \cdot \frac{\partial q}{\partial \xi} = -\frac{\partial q}{\partial \xi}$$

- Evaluate  $q := \Upsilon(v; \xi)$
- Solve a small linear system

Assume PDE has minimization formulation for functional

$$J(v) := \int_{\Omega} W(\nabla v(x), v(x), x) \, dx \qquad \text{on } H^1(\Omega_1).$$

Conformity: functional is well-defined on geodesic FE space

Gradient of J:

- Derivatives of geodesic FE function values wrt. to coefficients
- Derivatives of geodesic FE gradients wrt. to coefficients

Total derivative again:

 $\frac{\partial F}{\partial q} \cdot \frac{\partial^2 \Upsilon}{\partial v_i \, \partial \xi} = -\frac{\partial^2 F}{\partial v \, \partial q} \cdot \frac{\partial q}{\partial \xi} - \frac{\partial^2 F}{\partial q^2} \cdot \frac{\partial q}{\partial v} \cdot \frac{\partial q}{\partial \xi} - \frac{\partial^2 F}{\partial v_i \, \partial \xi} - \frac{\partial^2 F}{\partial q \, \partial \xi} \cdot \frac{\partial q}{\partial v_i}.$ 

Hessian of the energy functional J: Even worse...

# Gradient and Hessian of an Energy Functional

 $J(v) := \int_{\Omega} W(\nabla v(x), v(x), x) \, dx \quad \text{ on } H^1(\Omega_1)$ Assume PDE has minimization formulation for functional Conformity: functional is well-defined on geodesic FE spectrum Gradient of J: Derivatives of geodesic FE function vells wrt. to coefficients Derivatives of geodesic FE gradien Ovrt. to coefficients Total derivative again: al derivative again:  $\frac{\partial F}{\partial q} \cdot \frac{\partial^2 \Upsilon}{\partial v_i \, \partial \xi} = \underbrace{\partial^2 f}_{\partial v} \frac{\partial q}{\partial \xi} \cdot \frac{\partial q}{\partial \xi} - \frac{\partial^2 F}{\partial q^2} \cdot \frac{\partial q}{\partial v} \cdot \frac{\partial q}{\partial \xi} - \frac{\partial^2 F}{\partial v_i \, \xi} \cdot \frac{\partial q}{\partial q \, \xi} \cdot \frac{\partial q}{\partial v_i}$ Hessian of the energy functional J: Even worse.

#### 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:







#### 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

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

#### 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?

#### And:

- Do we get optimal orders?
- Do we need more regularity than in the linear case?

#### Distance

$$D_{1,2}(u,v)^{2} := \int_{D} \left| \log(u(x), v(x)) \right|_{u(x)}^{2} dx + \sum_{\alpha=1}^{d} \int_{D} \left| \frac{D}{dx^{\alpha}} \log(u(x), v(x)) \right|_{u(x)}^{2} dx.$$

- Not a distance metric
- ▶ But: dist<sub>H1</sub>(u, v) < CD<sub>1,2</sub>(u, v) and  $||i(v) i(u)||_{H^1} < CD_{1,2}(u, v)$

#### Convexity

# Definition (Convexity along paths)

Let H be a set of functions from  $\Omega$  into M. Let

 $J:H\to \mathbb{R}$ 

be a  $C^2$  energy functional. We say that J is elliptic along a curve  $\Gamma:I\to H$  if there exist constants  $\lambda,\Lambda$  such that

$$\lambda |\dot{\Gamma}|_G^2 \le \frac{d^2}{dt^2} J(\Gamma(t)) \le \Lambda |\dot{\Gamma}|_G^2.$$

### Theorem ([Grohs, Hardering, S])

Assume that  $\boldsymbol{J}$  is elliptic along geodesic homotopies. Denote

$$u = \underset{w \in H_K}{\operatorname{arg\,min}} J(w)$$
 ("continuous solution")

and

 $H^u_{K,L} := H^1 \cap \textit{some extra smoothness}$ 

Let  $V \subset H^u_{K,L}$  and

$$v = \underset{w \in V}{\operatorname{arg\,min}} J(w).$$
 ("discrete solution")

Then we have that

$$D_{1,2}(u,v) \le C_2^2 \sqrt{\frac{\Lambda}{\lambda}} \inf_{w \in V} D_{1,2}(u,w)$$

with a constant  $C_2$  only depending on the product KL and the curvature of M.

#### Definition (k-th order smoothness descriptor, [Grohs])

For a function  $u: U \to M$  defined on a domain  $U \subset \mathbb{R}^d$  define for  $p \in [1, \infty]$  the homogenous k-th order smoothness descriptor

$$\dot{\Theta}_{p,k,U}(u) \coloneqq \sum_{\sum_j |\beta_j|=k} \left( \int_U \prod_j \left| D^{\beta_j} u(x) \right|_{g(u(x))}^p dx \right)^{1/p}$$

Corresponding inhomogenous smoothness descriptor

$$\Theta_{p,k,U}(u) := \sum_{i=1}^{k} \dot{\Theta}_{p,i,U}(u).$$

Slightly weaker than a covariant Sobolev norm.

Let  $\Delta$  be a reference element, and  $\mathbb{I}_{\Delta} u$  the interpolation of u at the Lagrange nodes.

# Lemma ([Grohs, Hardering, S])

For  $k > \frac{d}{2}$  and  $p \ge k - 1$  we have

$$D_{1,2}(\mathbb{I}_{\Delta}U, u)^2 \lesssim C(u, \Delta) \cdot \dot{\Theta}_{k,\Delta}(u)^2$$

with

$$C(u,\Delta) = \left(\sup_{1 \le l \le k} \sup_{(p,q) \in \mathbb{I}_{\Delta}u(\Delta) \times u(\Delta)} \left\| \nabla_{2}^{l} \log\left(p,q\right) \right\|^{2} + \sup_{1 \le l \le k} \sup_{(p,q) \in \mathbb{I}_{\Delta}u(\Delta) \times \in u(\Delta)} \left\| \nabla_{2}^{l} \nabla_{1} \log\left(p,q\right) \right\|^{2} \right).$$

The implicit constants are independent of u and M.

#### Theorem ([Grohs, Hardering, S, FoCM 2014])

Let J be a  $C^2$  energy, elliptic along geodesic homotopies. Denote

$$u = \underset{v \in W^{1,2}, v|_{\partial\Omega = \Phi}}{\arg \min} J(u), \quad (\text{``continuous solution''})$$

and assume that  $u \in W^{k,2}(\Omega, M) \cap W^{1,\infty}(\Omega, M)$  with k > d/2. With  $K \gtrsim \Theta_{\infty,1,\Omega}(u)$ , and L arbitrary, define  $H^u_{K,L}$ . Let

$$V^h = V^M_{p,h} \cap H^u_{K,L}$$

be a Lagrangian GFE space. Further, denote

$$v^h := \underset{w \in V^h}{\operatorname{arg\,min}} J(w).$$
 ("discrete solution")

Then, whenever  $p \ge k - 1$ , we have the a-priori error estimate

$$D_{1,2}(u,v^h) \lesssim h^{k-1}.$$



#### Executive Summary:

# Theorem ([Grohs, Hardering, S, FoCM 2014])

Optimal orders under mild additional smoothness assumptions.



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#### Theorem ([Grohs, Hardering, S, FoCM 2014])

Optimal orders under mild additional smoothness assumptions.

#### Even prettier proofs in:

Hanne Hardering: "Intrinsic Discretization Error Bounds for Geodesic Finite Elements", PhD Thesis, FU Berlin, 2015



#### Experiment:







#### Experiment:



#### Simulation:











# Thank you for your attention!



