Discretization of Manifold-Valued Partial Differential Equations

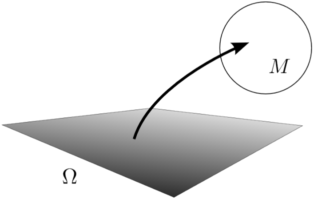
Oliver Sander, RWTH Aachen

Université catholique de Louvain, 17. 3. 2015

Partial differential equations for functions

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

M a Riemannian manifold.



Applications:

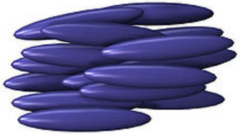
- Liquid crystals: S^2, $\mathbb{PR}^2$, SO(3)
- Cosserat shells and continua: S^2, SO(3)
- σ-models: SU(2), SO(3)
- Image processing: S^2, Sym$^+(3)$
- Positivity-preserving systems: $\mathbb{R}^+$, Sym$^+(3)$
- [...]

The challenge: Nonlinear function spaces

Example: Liquid Crystals

Molecules with an orientation:

$$\phi : \mathbb{R}^d \supset \Omega \to S^2 \qquad \text{(alt.: } \mathbb{RP}^2, \text{SO}(3))$$

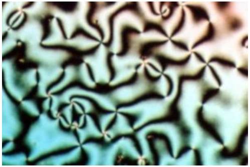


Properties: (nematic phase)

- Positional disorder
- Orientational order

Examples:

- Para-Azoxyanisole
- Soap, detergents
- Biomembranes



Source: Wikipedia

Modelling:

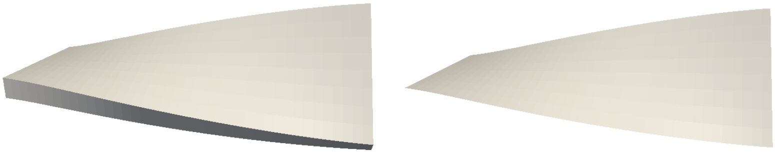
- Various elliptic and parabolic models

Director model for finite-strain shells:

- Configurations:

$$\mathbb{R}^2 \supset \Omega \to \mathbb{R}^3 \times \mathrm{SO}(3)$$

- Elastic, viscoelastic, and plastic materials
- Allows for size effects and microstructure
- Fully nonlinear, geometrically exact theory



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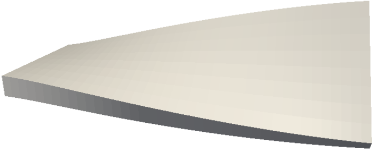

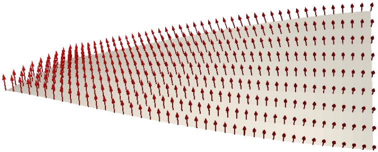

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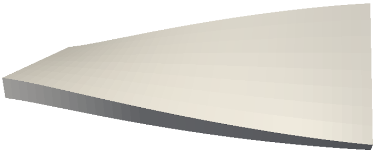

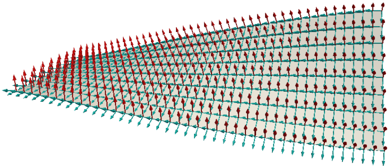

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Finite Elements (on one slide)

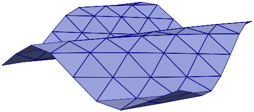
Partial differential equation (PDE)

Find $u : \Omega \to \mathbb{R}$ such that $-\Delta u = f$ (mit $\nabla u := \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} u$)

Minimization formulation

Solutions u are minimizers of

$$\mathcal{J}(v) := \frac{1}{2} \int_\Omega \|\nabla v\|^2 \, dx - \int_\Omega f v \, dx$$



in the Sobolev space $H^1(\Omega)$.

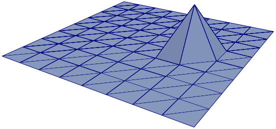
Finite elements

Look for minimizers u_h in the finite-dimensional subspace

$$V_h := \{v_h \in C(\Omega) \; : \; v_h \text{ is linear on each triangle of a fixed triangulation}\}$$

Pick nodal basis in V_h

V_h is isomorphic to $\mathbb{R}^N$.



Algebraic formulation

Minimize $J(x) = \frac{1}{2} x^T A x - b^T x$ in $\mathbb{R}^N$.

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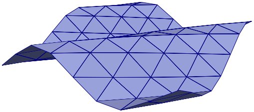

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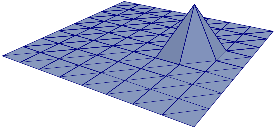

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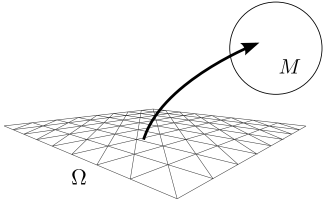
Partial differential equations for functions

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



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 $\mathbb{R}^m$
- Project back onto M

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

Optimal discretization error bounds.

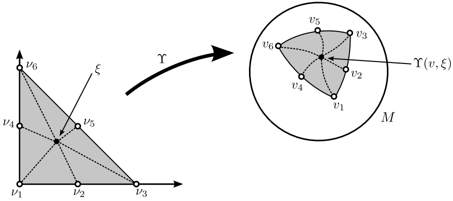
Properties

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

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 ξ
- Lagrange nodes ν_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

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

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

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])

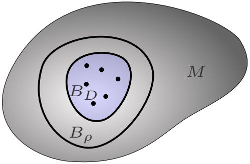
Let $v_i \in M$, $i = 1, \dots, m$ be coefficients and ξ coordinates on T_{ref}. Then

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

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 $v_1, \ldots, v_m$ 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* ξ *and the* v_i.

Objectivity: Equivariance under an isometric group action

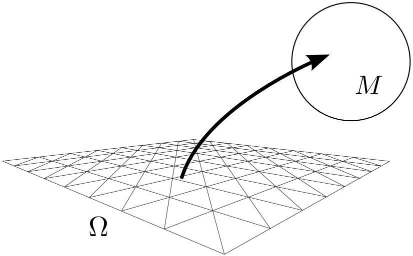
Lemma (Objectivity, [S '10, S '13])

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.

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.,

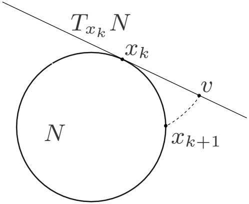
$$V_h^M \subset H^1(\Omega, M).$$

Proof:

- Geodesic FE functions are piecewise C^1 in M
- Geodesic FE functions are piecewise C^1 in $\mathbb{R}^m$ (smooth embedding)
- A function $v : \Omega \to \mathbb{R}^m$ that is piecewise C^1 is in $H^1(\Omega, \mathbb{R}^m)$ if and only if $v \in C(\Omega, \mathbb{R}^m)$.

Riemannian Trust-Region Methods

[Absil, Baker, Gallivan '06, S '08]



Algebraic minimization problem:

- On product manifold $N = M^n$, (n large)

Riemannian Trust-Region Method

- $x_k \in N$ the current iterate
- Instead of $J : N \to \mathbb{R}$ consider

$$\hat{J}_k : T_{x_k}N \to \mathbb{R}, \qquad \hat{J}_k = J \circ \exp_{x_k}$$

- Get correction $v \in T_{x_k}N$ by a trust-region step for $\hat{J}_k$ with quadratic model m_k
- If step was successful set

$$x_{k+1} = \exp_{x_k} v$$

Inner quadratic problem:

- m_k quadratic approximation of $\hat{J}_k$
- Sparse hessian
- Choice of trust-region norm $\rightarrow$ pick ∞-norm
- Trust region

$$K_{k,\rho} = \{v \in T_{x_k}N \mid \|v\|_\infty \leq \rho\}$$

  is described by box constraints in $T_{x_k}N$.

Monotone multigrid method: [Kornhuber '94]

- Multigrid method for quadratic problems with box constraints
- Linear multigrid speed
- Provable convergence for convex problems
- Also works for nonconvex quadratic models

Definition:

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

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

$$\frac{\partial F(\xi,q)}{\partial q} \cdot \frac{\partial \Upsilon}{\partial \xi} = -\frac{\partial F(\xi,q)}{\partial \xi}$$

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

Gradient and Hessian of an Energy Functional

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...

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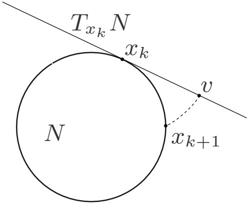
Hessian of the energy functional J: Even worse.

Use automatic differentiation!

(less pain)

Riemannian Trust-Region Methods

[Absil, Baker, Gallivan '06, S '08]



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Minimize harmonic energy:

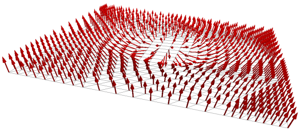
$$\phi : \Omega \to S^2, \qquad E(\phi) = \int_\Omega \|\nabla \phi\|^2 \, dx$$

Lemma

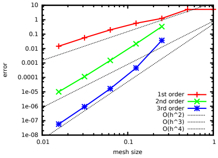
The inverse stereographic map minimizes E in its homotopy class.

Setup

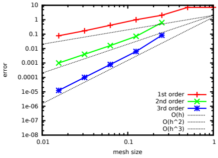
- Domain $\Omega = [-5, 5]^2$
- Dirichlet boundary conditions
- Discretization error for $d = 2$, $p = 1, 2, 3$:



solution field



L^2-error over mesh size



H^1-error over mesh size

Optimal A priori Discretization Error Bounds

[with P. Grohs and H. Hardering]

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?

And:

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

Distance

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

- Not a distance metric
- But: $\operatorname{dist}_{H^1}(u,v) < C D_{1,2}(u,v)$ and $\|i(v) - i(u)\|_{H^1} < C D_{1,2}(u,v)$

Convexity

Definition (Convexity along paths)

Let H be a set of functions from Ω 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 λ, Λ such that

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

Theorem

Assume that J is elliptic along geodesic homotopies. Denote

$$u = \arg\min_{w \in H_K} J(w) \qquad \text{(“continuous solution”)}$$

and

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

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

$$v = \arg\min_{w \in V} J(w). \qquad \text{(“discrete solution”)}$$

Then we have that

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

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

Definition (k-th order smoothness descriptor)

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

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

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

Lemma

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

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

with

$$C(u, \Delta) = \Bigg(\sup_{1 \leq l \leq k} \sup_{(p,q) \in \mathbb{I}_\Delta u(\Delta) \times u(\Delta)} \left\| \nabla_2^l \log(p, q) \right\|^2 + \sup_{1 \leq l \leq k} \sup_{(p,q) \in \mathbb{I}_\Delta u(\Delta) \times \in u(\Delta)} \left\| \nabla_2^l \nabla_1 \log(p, q) \right\|^2 \Bigg).$$

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

$$u = \operatorname*{arg\,min}_{v \in W^{1,2},\ v|_{\partial\Omega} = \Phi} J(u), \qquad \text{("continuous solution")}$$

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

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

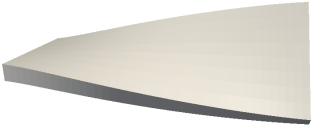
Then, whenever $p \geq k - 1$, we have the a-priori error estimate

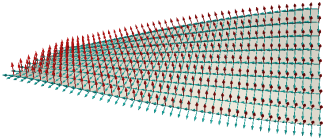
$$D_{1,2}(u, v^h) \lesssim h^{k-1}.$$

Executive Summary / tl;dr:

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

Optimal orders under mild additional smoothness assumptions.





Kinematics:

- $\Omega \subset \mathbb{R}^2$
- 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: (h = shell thickness)

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

Membrane energy:

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

Bending energy:

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

Curvature energy:

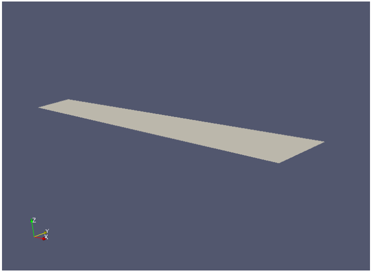
$$W_{\text{curv}}(\mathfrak{K}) = \mu L_c^{1+p} \|\mathfrak{K}\|^{1+p}$$

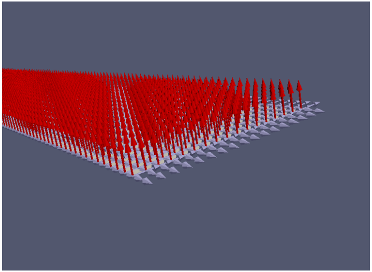
Theorem ([Neff])

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

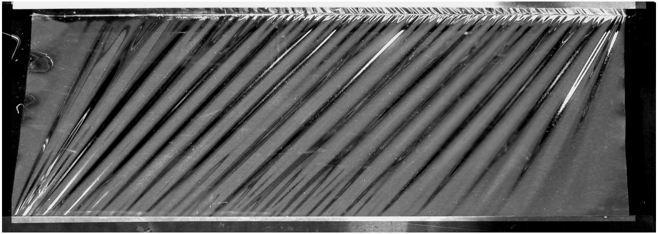
Twisting of a strip:

- 10×1 strip clamped at one short end
- Time-dependent Dirichlet boundary conditions
- Free end twisted by 8π
- Challenge for a discretization: very large rotations



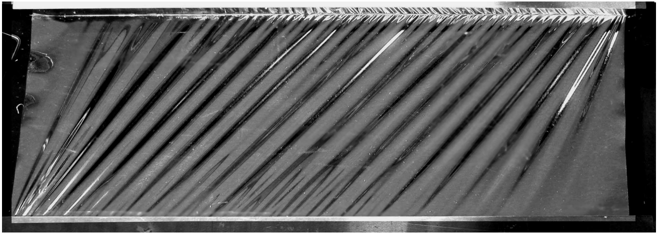


Wrinkling in experiments:



Wrinkling of Plastic Sheets [With Patrizio Neff]

Wrinkling in experiments:



Simulation: