BILAYER PLATES: MODEL REDUCTION, Γ-CONVERGENT FINITE ELEMENT APPROXIMATION AND DISCRETE GRADIENT FLOW

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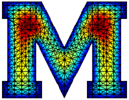

joint with

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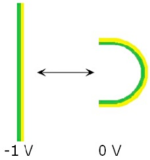
Outline

OUTLINE

Bilayer Bending

Applications: thermostats, nanotubes, microrobots



General setting:

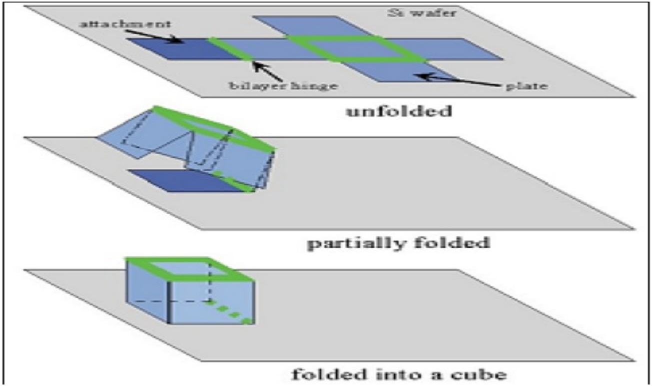
- two thin sheets attached to each other
- thermal or electrical stimuli
- one material compresses, one expands
- small forces, large deformations
- bending: small energies

Goals:

- effective mathematical description
- convergent discretization
- reliable (and efficient) solution technique
- applications

Laboratory Experiments of E. Smela (Mechanical Engineering, UMD)

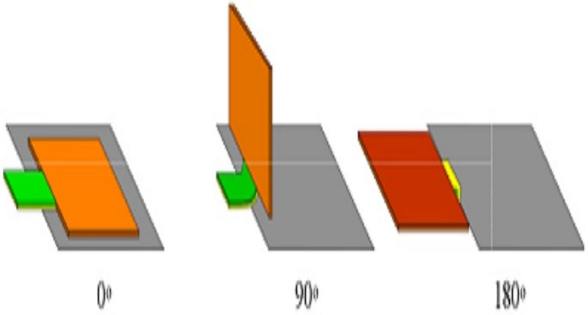
Experiment 1: Selfassembling Microcube. Conducting layers of polypyrrole (polymer) and gold (Au) were used as hinges to connect ridig plates to each other and to a Si substrate. The bending of the hinges was electrically controlled.



E. W. H. JAGER, E. SMELA, AND O. INGANÄS, *Microfabricating conjugated polymer actuators*, Science, 290 (2000), 1540–1545.

Experiment 2: Bilayers Moving Rigid Plates

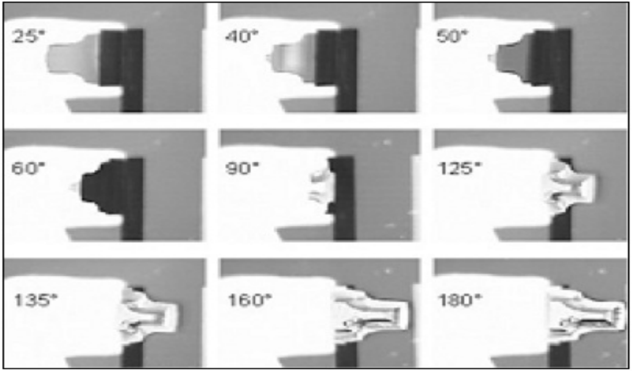
The plates are 150 μm on each side, and the hinges are 30 x 30 μm. Hinges of that size were also able to rotate plates that were 1 mm on a side - these bilayers are strong.



E. Smela, M. Kallenbach, and J. Holdenried, *Electrochemically driven polypyrrole bilayers for moving and positioning bulk micromachined silicon plates*, J. Microelectromechanical Systems, 8 (4) (1999), 373–383.

Experiment 3: Moving Silicon Plates with Bilayer Hinges

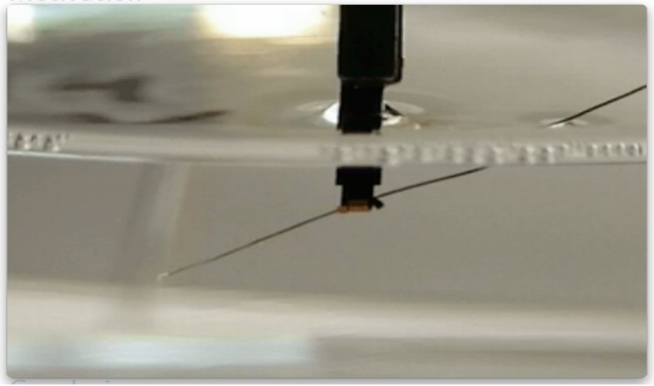
The actuator holds a couple of fixed positions and is robust: it operates even when it comes into contact with macro-scale obstacles.



E. Smela, M. Kallenbach, and J. Holdenried, *Electrochemically Driven Polypyrrole Bilayers for Moving and Positioning Bulk Micromachined Silicon Plates*, J. Microelectromechanical Systems, 8(4), (1999), 373–383.

Experiment 4: Polypyrrole (PPy)/Gold (Au) Micro-Bilayers on a Silicon Substrate

The actuators move from completely flat to fully curled and back (to/from fully oxidized to/from fully reduced) in about 1 second (the PPy is $0.5\ \mu m$ thick).



E. Smela, O. Inganäs, and I. Lundström, *Controlled folding of micrometer-size structures*, Science, 268 (1995), 1735–1738.

Simulation: Partially Clampled Plate

- **Domain:** $\Omega = (-2, 2) \times (0, 10)$
- **Boundary Condition:** $\partial_D \Omega = (-1, 1) \times \{0\}$.

OUTLINE

Notation

- **Domain:** $\Omega_t = \Omega \times (-t/2, t/2) \subset \mathbb{R}^3$ with thickness t and midplane $\Omega \subset \mathbb{R}^2$;
- **Plate deformation:** $u : \Omega_t \to \mathbb{R}^3$;
- **Scaled hyperelastic energy:** $I_t[u] = t^{-3} \int_{\Omega_t} \big(W(\nabla u, x) - f_t \cdot u\big) dx$;
- **Energy density:** $W : \mathbb{R}^{3\times 3} \times \Omega_t \to \mathbb{R}$ is taken to be

  $$W(F, x) = \mathrm{dist}^2\Big(F, [I_3 \pm \delta N(x')]SO(3)\Big), \quad \pm x_3 > 0,$$

  where $x = (x', x_3) \in \mathbb{R}^3$, $\delta > 0$, and $N = N(x') : \Omega \to \mathbb{R}^{3\times 3}$ is a symmetric matrix ($N = I_3$ for homogeneous isotropic materials)

  $$N = \begin{bmatrix} N_{11} & m \\ m^T & n \end{bmatrix},$$

  where $N_{11} = N_{11}(x') \in \mathbb{R}^{2\times 2}, m = m(x') \in \mathbb{R}^2$ and $n \in \mathbb{R}$ is a constant.
- **Bilayers:** $\{x \in \Omega_t : \pm x_3 > 0\}$ are composed of two different materials.

Goal 1: Characterizing the asymptotic bending behavior of the plate Ω_t as $t \to 0$ upon assuming that the energy remains bounded in this limit.

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Approximations and Surface Representation

- **Energy density:** For small values of $W(\nabla u, x)$ we have

$$W(F,x) \approx \frac{1}{4}\left|F^T F - (I_3 \pm \delta N)^T (I_3 \pm \delta N)\right|^2 = \frac{1}{4}\left|F^T F - (I_3 \pm 2\delta N + \delta^2 N^2)\right|^2;$$

- **Surface parametrization:**

$$y : \Omega \to \mathbb{R}^3, \quad \Gamma = y(\Omega);$$

- **Unit normal to Γ:**

$$\nu : \Omega \to \mathbb{R}^3, \quad b = \beta\nu \quad (\beta > 0);$$

- **Deformation:**

$$u(x', x_3) = y(x') + x_3 b(x');$$

- **Deformation gradient:** $\nabla u = [\partial_i u]_{i=1}^3 \in R^{3\times 3}$ can be written as

$$\nabla u = [\nabla' y, b] + x_3 [\nabla' b, 0]$$

Approximate Energy

- **Auxiliary matrix $M \in \mathbb{R}^{3\times3}$:**

$$M = I_3 \pm 2\delta N + \delta^2 N^2 = \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^T & M_{22} \end{bmatrix}$$

- **Approximate energy (with load $f_t = 0$):**

$$I_t[u] \approx \frac{1}{4t^3} \int_{\Omega_t} \left| (\nabla u)^T \nabla u - M \right|^2$$

- **Role of y and b in the approximate energy:**

$$I_t[u] = \frac{1}{4t^3} \int_{\Omega_t} \Bigg| \begin{bmatrix} (\nabla' y)^T (\nabla' y) - M_{11} & -M_{12} \\ -M_{12}^T & |b|^2 - M_{22} \end{bmatrix}$$

$$+ x_3 \begin{bmatrix} 2(\nabla' b)^T \nabla' y & (\nabla' b)^T b \\ b^T (\nabla' b) & 0 \end{bmatrix} + x_3^2 \begin{bmatrix} (\nabla' b)^T \nabla' b & 0 \\ 0 & 0 \end{bmatrix} \Bigg|^2 dx$$

Asymptotics as $t \to 0$

- **Relation between δ and t:** We expect $\delta \approx t$;
- **Vector b:** $|b|^2 - M_{22}$ should be at least order t^2

$$|b|^2 - M_{22} = |b|^2 - (1 \pm \delta n)^2 - \delta^2 |m|^2 = -\delta^2 |m|^2 \quad \Leftarrow \quad |b| = 1 \pm \delta n, \quad \pm x_3 > 0;$$

- **Relation between b and ν:** $b = (1 \pm \delta n)\nu$ is independent of x', whence

$$\nabla' b = (1 \pm \delta n) \nabla' \nu \quad \Rightarrow \quad (\nabla' b)^T b = 0;$$

- $(1-2)$ **Term of energy:**

$$\frac{1}{4t^3} \int_{\Omega_t} |M_{12}|^2 \approx \frac{1}{t^3} \int_{\Omega_t} \delta^2 |m|^2 = \frac{\delta^2}{t^2} \int_{\Omega} |m|^2 \quad \Rightarrow \quad \delta \approx t$$

Asymptotics as $t \to 0$ (continued)

- **First fundamental form:** For $I_t[u]$ to remain bounded, we must impose

$$g = (\nabla' y)^T \nabla' y = I_2 \quad \Rightarrow \quad \partial_i y \cdot \partial_j y = \delta_{ij}.$$

This implies that the parametrization y of surface Γ is an isometry.

- **Second fundamental form:** $h = -(\nabla' \nu)^T \nabla' y$

- **Approximate energy:** Let $\lambda := \delta/t$ and drop terms that are order t or higher

$$I_t[u] \approx \frac{1}{12} \int_\Omega \Big(|h|^2 + 6\lambda N_{11} : h \Big) dx' + \lambda^2 \int_\Omega \Big(|N_{11}|^2 + 2|m|^2 \Big) dx'$$

- **Rearrange and take limit $t \to 0$:**

$$\lim_{t\to 0} I_t[u] = \frac{1}{12} \int_\Omega \big| h + 3\lambda N_{11} \big|^2 dx' + \lambda^2 \int_\Omega \Big(\frac{1}{4} |N_{11}|^2 + 2|m|^2 \Big) dx'.$$

Reduced Model

- **Reduced energy:** Dropping constant terms and rescaling

$$E[y] = \frac{1}{2}\int_\Omega \left|h + Z\right|^2 dx' - \int_\Omega f \cdot y \, dx'$$

with load f and

$$Z = 3\lambda N_{11}$$

subject to the *isometry* constraint

$$[\nabla' y]^T [\nabla' y] = I_2.$$

- **Spontaneous curvature tensor:** The quantity Z acts as a *spontaneous curvature* for the bending energy $E[y]$ and encodes properties of the bilayer material. If the material is homogeneous and isotropic, then $Z = \alpha I_2$ with $\alpha \in \mathbb{R}$. On the other hand, the material could possess inhomogeneities and anisotropies which are x'-dependent and are encoded in N_{11}. We observe that both n and m play no role in the reduced energy.

Nonlinear Kirchhoff Models: References

Theory:

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Applications:

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- M. Wardetzky, M. Bergou, D. Harmon, D. Zorin, and E. Grinspun, *A Quadratic Bending Model for Inextensible Surfaces*, Eurographics Symposium on Geometry Processing (2006), K. Polthier, A. Sheffer (eds).
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OUTLINE

Geometric Identities

The following geometric identities are valid for isometries y:

$$\partial_i y \cdot \partial_j y = \delta_{ij} \quad i, j = 1, 2.$$

- **Second fundamental form:**

$$\partial_i \partial_j y = h_{ij} \nu,$$

- **Gauss Curvature (developable surfaces):**

$$\kappa = 0;$$

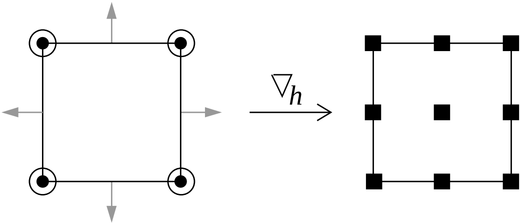
- **Hessian of parametrization and second fundamental form:**

$$|D^2 y|^2 = |h|^2 = |\Delta y|^2 = H^2.$$

OUTLINE

Choice of Finite Element Space

- **Notation: Derivatives in Ω:** $\nabla' = \nabla$, $\partial_i' = \partial_i$;
- **4-th Order:** $y \in [H^2(\Omega)]^3 \quad \Rightarrow \quad y_h \in W_h$ nonconforming space;
- **Unit normal:** $\nu = \partial_1 y \times \partial_2 y \quad \Rightarrow \quad y_h \in W_h$ subspace of $H^1(\Omega)$;
- **Isometry constraint:** $[\nabla y]^T[\nabla y] = I_2 \quad \Rightarrow \quad \Phi_h = \nabla_h y_h \approx \nabla y_h$ must satisfied nodal constraints.
- **Gradient space:** $\Phi_h \in \Theta_h \quad \Rightarrow \quad \Theta_h$ subspace of $H^1(\Omega)$
- **Kirchhoff quadrilaterals:** W_h continuous $\mathbb{Q}_3$, Θ_h continuous $[\mathbb{Q}_2]^2$



Definition of Degrees of Freedom (on Quadrilateral T)

- **Deformation Space W_h:** $w_h \in W_h \subset C(\overline{\Omega})$
  - Function values of w_h at vertices of T
  - Gradients ∇w_h at vertices of T
  - Normal derivatives at midpoint of edges E of T (z_E^i vertices of E): $\nabla w_h(z_E) \cdot \mathbf{n}_E = \frac{1}{2}\big(\nabla w_h(z_E^1) + \nabla w_h(z_E^2)\big) \cdot \mathbf{n}_E$.
- **Gradient Space Θ_h:** $\theta_h \in \Theta_h \subset C(\overline{\Omega}; \mathbb{R}^2)$
  - Nodal values of vector θ_h.

The Reduced Gradient $\nabla_h : W_h \to \Theta_h$: Definition

The operator $\nabla_h : W_h + H^2(\Omega)^3 \to \Theta_h$ is uniquely defined by the degrees of freedom:

- **Vertices $z \in \mathcal{N}_h$:**

$$\nabla_h w_h(z) = \nabla w_h(z);$$

- **Barycenter x_T of $T \in \mathcal{T}_h$:**

$$\nabla_h w_h(z_T) = \frac{1}{4} \sum_{z \in \mathcal{N}_h \cap T} \nabla w_h(z);$$

- **Midpoint x_E of Edges $E \in \mathcal{E}_h$:**

$$\nabla_h w_h(z_E) = \nabla w_h(z_E).$$

Properties of the Reduced Gradient ∇_h

There exist constants $c_1, c_2, c_3, c_4 > 0$ depending on shape regularity but not on h such that

- H^1**-Stability:** The operator ∇_h is well defined and for all $w_h \in W_h$ we have
$$c_1^{-1} \|\nabla w_h\| \le \|\nabla_h w_h\| \le c_1 \|\nabla w_h\|;$$
- H^2**-Stability:** For all $w_h \in W_h$ and $T \in \mathcal{T}_h$ we have
$$c_2^{-1} \|D^2 w_h\|_{L^2(T)} \le \|\nabla \nabla_h w_h\|_{L^2(T)} \le c_2 \|D^2 w_h\|_{L^2(T)};$$
- **Approximation in** $H^3(\Omega)$**:** For all $w \in H^3(\Omega)$ and $T \in \mathcal{T}_h$ we have
$$\|\nabla w - \nabla_h w\|_{L^2(T)} + h_T \|D^2 w - \nabla \nabla_h w\|_{L^2(T)} \le c_3 h_T^2 \|D^3 w\|_{L^2(T)};$$
- **Approximation in** W_h**:** For all $w_h \in W_h$ and $T \in \mathcal{T}_h$ we have
$$\|\nabla w_h - \nabla_h w_h\|_{L^2(T)} \le c_4 h_T \|D^2 w_h\|_{L^2(T)}.$$

OUTLINE

Energy Reformulation

- **Reduced energy:**

$$E[y] = \frac{1}{2}\int_\Omega |h + Z|^2 dx - \int_\Omega f \cdot y dx$$

- **Unit normal vector:** $\nu = \partial_1 y \times \partial_2 y / |\partial_1 y \times \partial_2 y|$ for isometries also reads

$$\nu = \partial_1 y \times \partial_2 y = \frac{\partial_1 y}{|\partial_1 y|} \times \frac{\partial_2 y}{|\partial_2 y|}$$

- **Second fundamental form:** $h = -[\nabla \nu]^T \nabla y$ for isometries also reads

$$h_{ij} = \partial_i \partial_j y \cdot (\partial_1 y \times \partial_2 y) = \partial_i \partial_j y \cdot \frac{\partial_1 y}{|\partial_1 y|} \times \frac{\partial_2 y}{|\partial_2 y|}$$

- **Equivalent reduced energy:**

$$\begin{aligned}\widetilde{E}[y] = {} & \frac{1}{2}\int_\Omega |D^2 y|^2 dx \\ & + \sum_{i,j=1}^{2} \int_\Omega \partial_i \partial_j y \cdot \Big(\frac{\partial_1 y}{|\partial_1 y|} \times \frac{\partial_2 y}{|\partial_2 y|} \Big) Z_{ij} dx \\ & + \frac{1}{2}\int_\Omega |Z|^2 dx - \int_\Omega f \cdot y dx,\end{aligned}$$

Discrete Minimizers

- **Discrete energy**

$$\widetilde{E}_h[y_h] = \frac{1}{2}\int_\Omega |\nabla \Phi_h|^2 dx + \sum_{i,j=1}^{2} \left(\partial_i \mathcal{I}_h^1[\Phi_{h,j}] \cdot \left(\frac{\Phi_{h,1}}{|\Phi_{h,1}|} \times \frac{\Phi_{h,2}}{|\Phi_{h,2}|}\right), Z_{ij}\right)_h + \frac{1}{2}\int_\Omega |Z|^2 dx - \int_\Omega f \cdot y_h dx.$$

- **Almost discrete minimizers:** Let $y_h \in W_h$ be a minimizer of $\widetilde{E}_h[y_h]$ with $\Phi_h = \nabla_h y_h \in \Theta_h$ satisfying the inexact isometry constraint

$$\left|[\Phi_h(z)]^T \Phi_h(z) - I_2\right| \leq Ch \quad \forall z \in \mathcal{N}_h;$$

pairs (y_h, Φ_h) are limits of k-th iterates (y_h^k, Φ_h^k) of the discrete H^2 gradient flow with $\tau \approx h$ to be discussed later.

- **Boundary data:** $y_h = y_{D,h} \to y_D$ and $\Phi_h = \Phi_{D,h} \to \Phi_D$ in $L^2(\Gamma_D)$ as $h \to 0$.

Γ-Convergence

- **Attainment:** Given any $y \in H^2(\Omega;\mathbb{R}^3)$ with $[\nabla y]^T \nabla y = \mathrm{Id}_2$ and $y|_{\Gamma_D} = y_D$, $\nabla y|_{\Gamma_D} = \Phi_D$ there exists a sequence $\{y_h\}_{h>0}$ such that $y_h \in W_h$, $\Phi_h = \nabla_h y_h \in \Theta_h$ with $y_h|_{\Gamma_D} = y_{D,h}, \Phi_h|_{\Gamma_D} = \Phi_{D,h}$ and

$$[\Phi_h(z)]^T [\Phi_h(z)] = \mathrm{Id}_2 \quad \forall z \in \mathcal{N}_h$$

  for all $h > 0$ and

$$y_h \to y \text{ in } H^1(\Omega;\mathbb{R}^3), \quad \Phi_h \to \Phi = \nabla y \text{ in } H^1(\Omega;\mathbb{R}^{3\times 2}), \quad \widetilde{E}_h[y_h] \to E[y]$$

  as $h \to 0$.

- **Lower bound property:** If $\{y_h\}_{h>0}$ is a sequence with $y_h \in W_h$, $\widetilde{E}_h[y_h] \le C$, and $\left|[\nabla_h y_h(z)]^T \nabla_h y_h(z) - \mathrm{Id}_2\right| \le Ch$ for all $z \in \mathcal{N}_h$ and all $h > 0$, then there exist $y \in H^2(\Omega;\mathbb{R}^3)$ and $\Phi = \nabla y \in H^1(\Omega;\mathbb{R}^{3\times 2})$ such that $[\Phi]^T \Phi = \mathrm{Id}_2$, $y|_{\Gamma_D} = y_D$ and $\Phi|_{\Gamma_D} = \Phi_D$ and

$$y_h \to y \text{ in } H^1(\Omega;\mathbb{R}^3), \quad \Phi_h \rightharpoonup \Phi \text{ in } H^1(\Omega;\mathbb{R}^{3\times 2}),$$

  as well as

$$E[y] \le \liminf_{h\to 0} \widetilde{E}_h[y_h].$$

Convergence of Almost Global Minimizers

Let $C > 0$ be a constant independent of h and $\{y_h\}_h$ be a sequence of almost global discrete minimizers of $\widetilde{E}_h$, namely

$$\widetilde{E}_h[y_h] \le \inf_{w_h \in \mathcal{A}_h} \widetilde{E}_h[w_h] + \epsilon_h \le C, \tag{1}$$

where $\epsilon_h \to 0$ as $h \to 0$. Then $\{y_h\}_h$ is precompact in $H^1(\Omega)^3$ and every cluster point y of y_h is a global minimizer of E, namely

$$E[y] = \inf_{w \in \mathcal{A}} E[w]. \tag{2}$$

Moreover, there exists a subsequence of $\{y_h\}_h$ (not relabeled) such that

$$\lim_{h\to 0} \|y - y_h\|_{H^1(\Omega)} = 0 \qquad \text{and} \qquad \lim_{h\to 0} \widetilde{E}_h[y_h] = E[y]. \tag{3}$$

OUTLINE

Semi-Discrete H^2 Gradient Flow

Algorithm 1 (H^2 gradient flow): Let $\tau, \varepsilon_{\text{stop}} > 0$ and set $k = 0$. Choose $y^0 \in H^2(\Omega; \mathbb{R}^3)$ such that $y^0|_{\Gamma_D} = y_D, \nabla y^0|_{\Gamma_D} = \Phi_D$ and

$$[\nabla y^0]^T [\nabla y^0] = \mathrm{Id}_2.$$

(1) Compute $y^{k+1} \in H^2(\Omega; \mathbb{R}^3)$ which is minimal for

$$y \mapsto F_\tau^k[y] = \frac{1}{2\tau} \|D^2(y - y^k)\|^2 + \widetilde{E}[y]$$

subject to $y|_{\Gamma_D} = y_D, \nabla y|_{\Gamma_D} = \Phi_D$ and the linearized isometry constraint

$$[\nabla(y - y^k)]^T [\nabla y^k] + [\nabla y^k]^T [\nabla(y - y^k)] = 0.$$

(2) Stop if $\|D^2(y^{k+1} - y^k)\| \leq \varepsilon_{\text{stop}}$; otherwise increase $k \to k + 1$ and go to (1).

Euler-Lagrange Equations

Every step of the semi-discrete gradient flow requires computing the solution $y^{k+1} \in H^2(\Omega; \mathbb{R}^3)$ of the nonlinear system of equations

$$
\begin{aligned}
&\frac{1}{\tau}(D^2[y^{k+1} - y^k], D^2 w) + (D^2 y^{k+1}, D^2 w) \\
&\qquad + \sum_{i,j=1}^{k} \int_\Omega \Big\{ \partial_i \partial_j w \cdot \Big(\frac{\partial_1 y^{k+1}}{|\partial_1 y^{k+1}|} \times \frac{\partial_2 y^{k+1}}{|\partial_2 y^{k+1}|} \Big) \\
&\qquad + \partial_i \partial_j y^{k+1} \cdot \Big[\frac{\partial_1 w}{|\partial_1 y^{k+1}|} - \frac{\partial_1 y^{k+1} (\partial_1 y^{k+1} \cdot \partial_1 w)}{|\partial_1 y^{k+1}|^3} \Big] \times \frac{\partial_2 y^{k+1}}{|\partial_2 y^{k+1}|} \\
&\qquad + \partial_i \partial_j y^{k+1} \cdot \frac{\partial_1 y^{k+1}}{|\partial_1 y^{k+1}|} \times \Big[\frac{\partial_2 w}{|\partial_2 y^{k+1}|} - \frac{\partial_2 y^{k+1} (\partial_2 y^{k+1} \cdot \partial_2 w)}{|\partial_2 y^{k+1}|^3} \Big] \Big\} Z_{ij} \, dx = (f, w)
\end{aligned}
$$

for all $w \in H^2(\Omega; \mathbb{R}^3)$ with $w|_{\Gamma_D} = 0, \nabla w|_{\Gamma_D} = 0$ and

$$
[\nabla w]^T [\nabla y^k] + [\nabla y^k]^T [\nabla w] = 0,
$$

subject to $y^{k+1}|_{\Gamma_D} = y_D, \nabla y^{k+1}|_{\Gamma_D} = \Phi_D$ and

$$
[\nabla (y^{k+1} - y^k)]^T [\nabla y^k] + [\nabla y^k]^T [\nabla (y^{k+1} - y^k)] = 0.
$$

Euler-Lagrange Equations: Reformulation

- **Deformation gradient:** $\Phi^k = \nabla y^k \in H^1(\Omega, \mathbb{R}^{3\times 2})$, $\Phi^k_j = \partial_j y^k$;
- **Projection matrix:** Given $a \in \mathbb{R}^3$ with $|a| \geq 1$ let $P_a \in \mathbb{R}^{3\times 3}$ be
$$P_a := \frac{1}{|a|}\Big(I_3 - \frac{a^T}{|a|}\frac{a}{|a|}\Big);$$
- **Linearized isometry constraint:**
$$L[\Phi;\Phi^k] := \Phi^T\Phi^k + [\Phi^k]^T\Phi = 0;$$
- **Euler-Lagrange equation:** Seek $\Phi = \Phi^{k+1} \in H^1(\Omega)$ with $\Phi_{\Gamma_D} = \Phi_D$ and
$$\frac{1}{\tau}(\nabla[\Phi - \Phi^k], \nabla\Psi) + (\nabla\Phi, \nabla\Psi)$$
$$+ \sum_{i,j=1}^{2}\Big(\partial_i\Psi_j \cdot \Big(\frac{\Phi_1}{|\Phi_1|} \times \frac{\Phi_2}{|\Phi_2|}\Big), Z_{ij}\Big)$$
$$+ \sum_{i,j=1}^{2}\Big(\partial_i\Phi_j \cdot \Big([P_{\Phi_1}\Psi_1] \times \frac{\Phi_2}{|\Phi_2|} + \frac{\Phi_1}{|\Phi_1|} \times [P_{\Phi_2}\Psi_2]\Big), Z_{ij}\Big) = (f, w)$$
for $\Psi = \nabla w \in H^1(\Omega)$ with $w|_{\Gamma_D} = 0, \Psi_{\Gamma_D} = 0$ and $L(\Psi;\Phi^k) = 0$, subject to
$$L(\Phi - \Phi^k;\Phi^k) = 0.$$

Key Property of Linearized Isometry Constraint

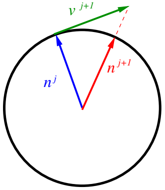
- If $\Phi \in H^1(\Omega, \mathbb{R}^{3\times 2})$ satisfies $L(\Phi - \Phi^k; \Phi^k) = 0$, then

$$\begin{aligned}\Phi^T\Phi - I_2 &= [\Phi^k + \Phi - \Phi^k]^T[\Phi^k + \Phi - \Phi^k] - I_2 \\ &= [\Phi^k]^T\Phi^k - I_2 + [\Phi - \Phi^k]^T[\Phi - \Phi^k] \geq [\Phi^k]^T\Phi^k - I_2;\end{aligned}$$

- Induction starting from $[\Phi^0]^T\Phi^0 = I_2$ yields

$$[\Phi^k]^T\Phi^k \geq I_2 \quad \Rightarrow \quad |\Phi_i| \geq 1 \quad i = 1, 2;$$

This extends similar property for director fields $|n_j| = 1$.



- Algorithm 1, which contains $\Phi_i/|\Phi_i|$, is well defined.

Discrete Gradient Flow: Ingredients

- **Reduced gradient:** $\nabla_h : W_h \to \Theta_h$;
- **Interpolation operator:** $\mathcal{I}_h^1 : [L^2(\Omega)]^3 \to [V_h]^3 \subset H^1(\Omega)$, the space of piecewise bilinear finite elements;
- **Quadrature:** If $\mathcal{I}_h : C(\bar{\Omega}) \to \mathbb{V}_h$ is the Lagrange interpolation operator, then

$$(\phi, \psi)_h = \int_\Omega \mathcal{I}_h[\phi\psi] dx;$$

- **Discrete energy:** Let $\Phi_h := \nabla_h y_h$ and

$$\begin{aligned} \widetilde{E}_h[y_h] &= \frac{1}{2} \int_\Omega |\nabla \Phi_h|^2 dx \\ &\quad + \sum_{i,j=1}^{2} \left(\partial_i \mathcal{I}_h^1 [\Phi_j] \cdot \left(\frac{\Phi_{h,1}}{|\Phi_{h,1}|} \times \frac{\Phi_{h,2}}{|\Phi_{h,2}|} \right), Z_{ij} \right)_h \\ &\quad + \frac{1}{2} \int_\Omega |Z|^2 dx - \int_\Omega f \cdot y_h dx; \end{aligned}$$

- **Discrete linearized isometry constraint:** $L(\Phi_h; \Phi_h^k) = 0$ enforced at vertices

$$L_h(\Phi_h; \Phi_h^k) := \mathcal{I}_h \Big(\Psi_h^T \Phi_h^k + [\Phi_h^k]^T \Psi_h \Big).$$

Discrete Gradient Flow: Algorithm 2

Let $\tau, \varepsilon_{\text{stop}} > 0$ and set $k = 0$. Choose $y_h^0 \in W_h$ and $\Phi_h^0 = \nabla_h y_h^0$ with $y_h^0|_{\Gamma_D} = y_{D,h}, \Phi_h^0|_{\Gamma_D} = \Phi_{D,h}$ and

$$[\Phi_h^0(z)]^T[\Phi_h^0(z)] = \mathrm{Id}_2 \quad \forall\, z \in \mathcal{N}_h;$$

(1) Compute $y_h^{k+1} \in W_h$ which is minimal for

$$y_h \mapsto F_{h,\tau}^k[y_h] = \frac{1}{2\tau}\|\nabla(\Phi_h - \Phi_h^k)\|^2 + \widetilde{E}_h[y_h]$$

subject to $y_h|_{\Gamma_D} = y_D, \Phi_h|_{\Gamma_D} = \Phi_{D,h}$ and

$$L_h(\Phi_h - \Phi_h^k; \Phi_h^k) = 0;$$

(2) Stop if $\|\nabla\Phi_h^{k+1} - \Phi_h^k)\| \le \varepsilon_{\text{stop}}$; otherwise increase $k \to k+1$ and go to (1).

Discrete Euler-Lagrange Equation

Let $\widetilde{\Phi}_h := \Phi_h^k$ for $k \geq 0$. Seek $y_h \in W_h, \Phi_h = \nabla_h y_h \in \Theta_h$ such that $y_h|_{\Gamma_D} = y_D, \Phi_h|_{\Gamma_D} = \Phi_{D,h}$ and

$$
\begin{aligned}
\frac{1}{\tau}(\nabla[\Phi_h - \widetilde{\Phi}_h], \nabla\Psi_h) + (\nabla\Phi_h, \nabla\Psi_h)& \\
+ \sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i \Psi_{h,j}] \cdot \Big(\frac{\Phi_{h,1}}{|\Phi_{h,1}|} \times \frac{\Phi_{h,2}}{|\Phi_{h,2}|}\Big), Z_{ij}\Big)_h& \\
+ \sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i \Phi_{h,j}] \cdot \Big([P_{\Phi_{h,1}} \Psi_{h,1}] \times \frac{\Phi_{h,2}}{|\Phi_{h,2}|}\Big), Z_{ij}\Big)_h& \\
+ \sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i \Phi_{h,j}] \cdot \Big(\frac{\Phi_{h,1}}{|\Phi_{h,1}|} \times [P_{\Phi_{h,2}} \Psi_{h,2}]\Big), Z_{ij}\Big)_h& = (f, w_h)
\end{aligned}
$$

for all $\Psi_h = \nabla_h w_h \in \mathbb{V}_{0,h}$ with $L_h(\Psi_h; \widetilde{\Phi}_h) = 0$, and subject to the condition

$$L_h(\Phi_h - \widetilde{\Phi}_h; \widetilde{\Phi}_h) = 0.$$

Constructive Existence: Fixed Point Iteration

Algorithm 3: Let $\delta_{\text{stop}} > 0$, define $\Phi_h^0 = \widetilde{\Phi}_h \in \mathbb{V}_a$, and set $\ell = 0$.

(1) Compute $\Phi_h^{\ell+1} \in \mathbb{V}_a$ with $L_h(\Phi_h^{\ell+1} - \widetilde{\Phi}_h; \widetilde{\Phi}_h) = 0$ such that

$$
\begin{aligned}
\frac{1}{\tau}&(\nabla[\Phi_h^{\ell+1} - \widetilde{\Phi}_h], \nabla\Psi_h) + (\nabla\Phi_h^{\ell+1}, \nabla\Psi_h) \\
&= -\sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i\Psi_{h,j}] \cdot \Big(\frac{\Phi_{h,1}^{\ell}}{|\Phi_{h,1}^{\ell}|} \times \frac{\Phi_{h,2}^{\ell}}{|\Phi_{h,2}^{\ell}|}\Big), Z_{ij}\Big)_h \\
&\quad - \sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i\Phi_{h,j}^{\ell}] \cdot \big[P_{\Phi_{h,1}^{\ell}}\Psi_{h,1}\big] \times \frac{\Phi_{h,2}^{\ell}}{|\Phi_{h,2}^{\ell}|}, Z_{ij}\Big)_h \\
&\quad - \sum_{i,j=1}^{2} \Big(\mathcal{A}_h[\partial_i\Phi_{h,j}^{\ell}] \cdot \frac{\Phi_{h,1}^{\ell}}{|\Phi_{h,1}^{\ell}|} \times \big[P_{\Phi_{h,2}^{\ell}}\Psi_{h,2}\big], Z_{ij}\Big)_h + (f, w_h)
\end{aligned}
$$

for all $\Psi_h = \nabla_h w_h \in \mathbb{V}_{0,h}$ with $L_h(\Psi_h; \widetilde{\Phi}_h) = 0$.

(2) Stop if $\|\nabla(\Phi_h^{\ell+1} - \Phi_h^{\ell})\| \le \delta_{\text{stop}}$; otherwise increase $\ell \to \ell + 1$ and go to (1).

Contraction Property of Algorithm 3

If the previous iterate $\widetilde{\Phi}_h$ satisfies

$$\|\nabla\widetilde{\Phi}_h\| \leq C_1,$$
$$|\widetilde{\Phi}_{h,j}(z)| \geq 1 \quad \forall z \in \mathcal{N}_h, j = 1, 2,$$

then

- the iterates Φ_h^ℓ satisfy $|\Phi_h^\ell(z)| \geq 1$ for all $z \in \mathcal{N}_h, \ell \geq 0$ and Algorithm 3 is well defined;
- there is a unique solution $\Phi_h^{\ell+1}$ which is uniformly in $H^1(\Omega)$ in the sense

  $$\|\nabla\Phi_h^{\ell+1}\| \leq (1+\sqrt{\tau})\|\nabla\widetilde{\Phi}_h\|$$

  provided $\tau \leq C_0$ depending on $\|\nabla\tilde{\Phi}_h\|_{L^2(\Omega)}$, the Poincaré constant of Ω, $\|f\|_{L^\infty(\Omega)}$ and $\|Z\|_{L^\infty(\Omega)}$.
- Algorithm 3 is a contraction with constant $C_5\tau$.

Energy Decay and Violation of Isometry Constraint

Let $(y_h^k)_{k=0}^\infty$ be the iterates of Algorithm 2 (discrete H^2 gradient flow) and $\Phi_h^k = \nabla_h y_h^k$. We then have for all $k \geq 0$

- **Energy decay:**

$$\widetilde{E}_h[y_h^{k+1}] + \frac{1}{2\tau} \sum_{\ell=0}^{k} \|\nabla(\Phi_h^{\ell+1} - \Phi_h^{\ell})\|^2 \leq \widetilde{E}_h[y_h^0];$$

- **Lower energy bound:** $\|\nabla \Phi_h^k\| \leq C_1$ and

$$\widetilde{E}_h[y_h^k] \geq \frac{1}{4}\|\nabla \Phi_h^k\|^2 - C_2\Big(\|Z\|^2 + \|f\|^2\Big);$$

- **Violation of isometry constraint:** there is $C_3 > 0$ depending on y_h^0, f, and Z such that

$$\|[\Phi_h^k]^T[\Phi_h^k] - \mathrm{Id}_2\|_{L_h^1(\Omega)} \leq C_3\tau,$$

  where $\|v\|_{L_h^1(\Omega)} = \int_\Omega \mathcal{I}_h|v|$.

OUTLINE

Experiment 1: Aspect Ratio and Homogeneous Spontaneous Curvature

- From Right to Left: aspect ratio (length/clamped side) = 0.5, 1.0, 7/4, 10/4
- From Bottom to Top: spontaneous curvature $Z = aI, a = 1, 2, 5$

Rectangular Plates

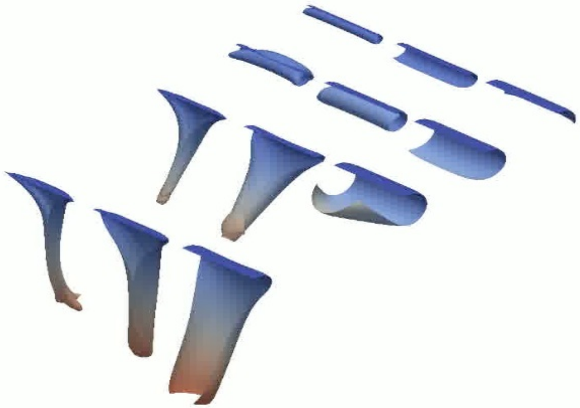
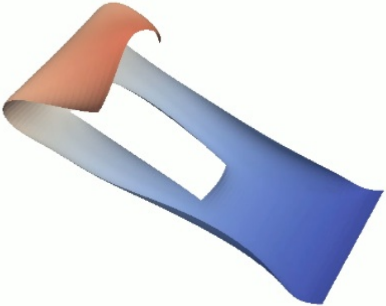


Plate with a Hole

- aspect ratio $= 10/4$, spontaneous curvature $Z = 2I$

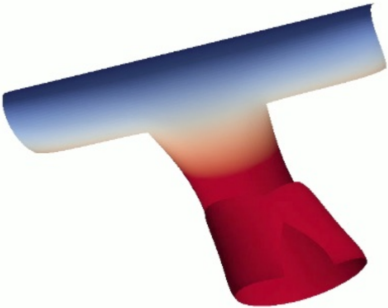
Plate with a hole



I-Shaped Plate

- aspect ratio $= 1$, spontaneous curvature $Z = I$

I-shaped plate



Partially Clampled Plate

- **Domain:** $\Omega = (-2, 2) \times (0, 10)$
- **Boundary Condition:** $\partial_D \Omega = (-1, 1) \times \{0\}$.
- **Spontaneous Curvature:** $Z = I_2$.

Bilayer Clamped at a Corner

- **Domain:** $\Omega = (-3, 3) \times (-2, 2)$
- **Boundary condition:** $\partial_D \Omega = \{-3\} \times (-2, 0) \cup (-3, 0) \times \{-2\}$
- **Spontaneous curvature:** $N = I_2$

Variable spontaneous curvature

Bilayer Clamped at a Corner

- **Domain:** $\Omega = (-3, 3) \times (-2, 2)$
- **Boundary condition:** $\partial_D \Omega = \{-3\} \times (-2, 0) \cup (-3, 0) \times \{-2\}$
- **Spontaneous curvature:** $N = I_2$

Variable spontaneous curvature

Anisotropic Spontaneous Curvature

- **Spontaneous curvatures:** $Z_1 = \begin{bmatrix} -5 & 0 \\ 0 & -1 \end{bmatrix}; \quad Z_2 = \begin{bmatrix} -3 & 2 \\ 2 & -3 \end{bmatrix}$
- **Principal eigenpairs for Z_2:** $\kappa_1 = 1, \mathbf{e}_1 = [1, -1]^T; \quad \kappa_2 = 5, \mathbf{e}_2 = [1, 1]^T$
- **Domain:** $\Omega = (-2, 2) \times (-3, 3)$

corkscrew-shape

Thermal Actuation: Simplified Mathematical Model

- **Elastic Energy:**

$$I_\delta[u] = \int_{\Omega_\delta} W_\theta(\nabla u(x), x)dx$$

- **Elastic Energy Density:**

$$W_\theta(F, x) = \mu(x)\big|F^T F - (1 + \alpha\theta(x,t))I_3\big|^2$$

with variable rigidity $\mu(x)$ and temperature $\theta(x,t)$.

- **Heat Energy:**

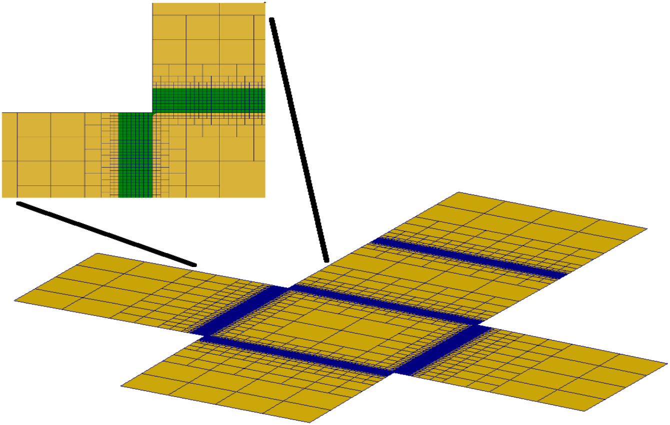
$$D_t\theta - \kappa\Delta\theta = f \quad \text{in } \omega_\delta$$

- **Reduced Elastic Energy:**

$$I[y] = \frac{1}{2}\int_\Omega \mu(x')\big|H - \alpha\theta I_2\big|^2 dx'$$

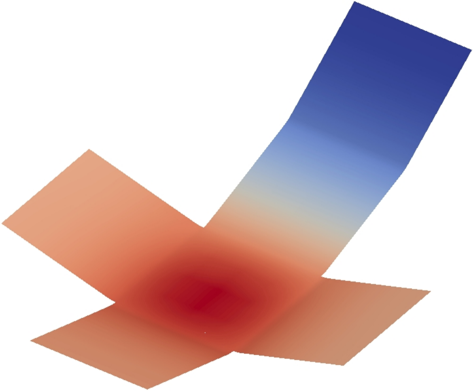
Self-Assembling Composite-Material Box

- **Domain:** 6 squares of size 1x1; **Hinges:** width $\pi/24$
- **Rigidity coefficient:** $\mu = 1$ in the hinges and $\mu = 20$ otherwise
- **Temperature source:** $f = 5$ until $t = 28.2$ then $f = -5$ afterwards
- **Spontaneous curvature:** $= -\theta$ (-temperature)
- **Heat diffusion coefficient:** $\kappa = 5$



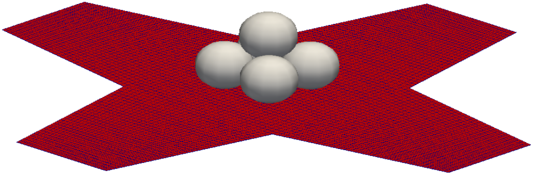
Temperature Distribution

- At iteration 50: Blue: $\theta = 3.98$; Red: $\theta = 4.42$
- At switch of heating: $\theta \approx 23$ everywhere.



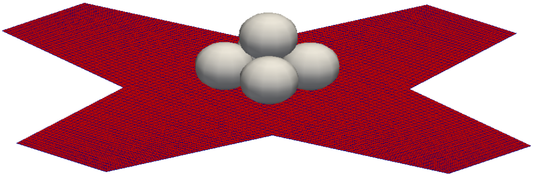
Encapsulation with Self-Folding Microcapsules: Drug Delivery

G. Stoychev, N. Puretskiy, and L. Ionov, *Self-folding all-polymer thermoresponsive microcapsules*, Soft Matter, 7 (2011), 3277–3279.



Encapsulation with Self-Folding Microcapsules: Simulation

- **Domain:** center 1x1 square; sides: trapezoidal base 1 top 3/5 height 1
- **Rigidity coefficient:** $\mu = 1$
- **Spontaneous curvature:** $12I$.



OUTLINE

Conclusions

- **Bilayer model:** Nonlinear Kirchhoff model that allows for bending but not stretching or shearing (isometry constraint). The model allows for a spontaneous curvature tensor and for large deformations.
- **Kirchhoff Quadrilaterals:** Nonconforming FE of $H^2(\Omega)$ and key properties of discrete gradient ∇_h.
- Γ-**convergence:** Convergence of inexact discrete minimizers to mimimizers of the continuous energy $E[y]$.
- **Discrete gradient flow:** H^2 gradient flow for a modified energy $\widetilde{E}[y]$; constructive existence of every iterate; convergence to the discrete problem; control of violation of isometry constraint.
- **Simulations:** Exhibit presence of local minimizers (other than cylinders) and interesting interplay between geometry and bending patterns. Obtained with `deal.II`.
- **Applications:** Microdevices with self-folding mechanisms actuated by temperature (thermal couple), electric current (polymers), hydrogels.