COMPUTATIONAL MODELING OF SHAPE MEMORY MATERIALS

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based on joint works with Martin Kružík and Miroslav Frost

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1. Introduction to shape memory materials

2. Mathematical models
   - Nonlinear elasticity
   - Sharp interface
   - Dissipation
   - Energetic solutions

3. Numerical implementation (main contribution)
   - Simplified model with 2 variants of martensite
   - Integer minimization problems
   - Computational benchmarks

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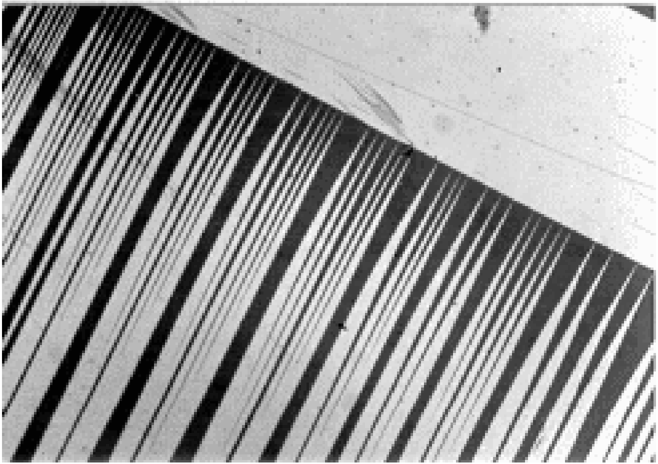
Motivation: martensitic patterns

Source: `http://www.lassp.cornell.edu/sethna/Tweed/What_Are_Martensites.html`



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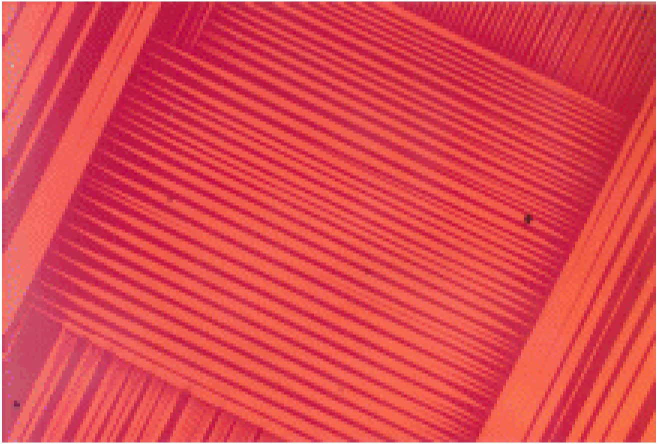

Shape memory alloys

Principle of shape memory:

- high temperature: atomic grid with high symmetry (usually cubic): the so-called austenite, higher heat capacity

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Our model - two variants of martensite only!

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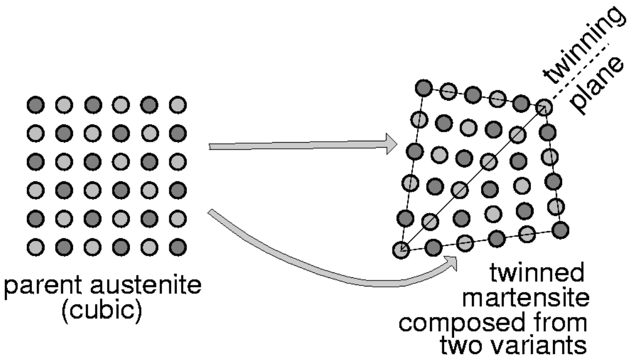

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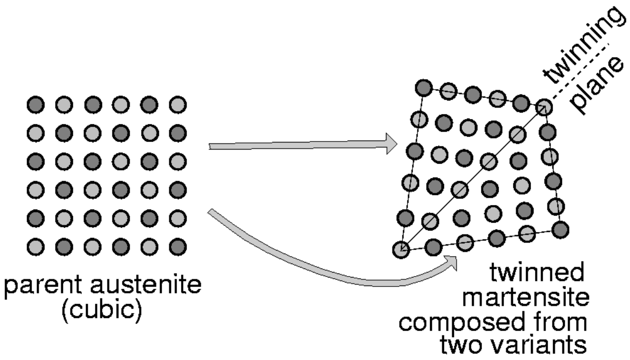

More details later.

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$\operatorname{div} T = 0$ equilibrium equations
$y = y_0$ on $\Gamma_0 \subset \partial\Omega$, g=Tn on $\Gamma_1 \subset \partial\Omega$ boundary conditions

Hyperelasticity

Assumption: 1st Piola-Kirchhoff stress tensor T has a potential:

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$W : \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{+\infty\}$ stored energy density

$$J(y) := \int_\Omega W(\nabla y(x))\,\mathrm{d}x - \int_{\Gamma_1} f \cdot y\,\mathrm{d}S\ .$$

Minimizers of J satisfy equilibrium equations.

Properties of W

(i) $W : \mathbb{R}^{3\times 3}_{+} \to \mathbb{R}$ is continuous

(ii) $W(F) = W(RF)$ for all $R \in \mathrm{SO}(3)$ and all $F \in \mathbb{R}^{3\times 3}$

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!!! (iii) **excludes convexity** of W !!!

A sharp interface model

- only the first gradient of y
- non-diffuse boundary between phases (phase indicator z)

$$\mathcal{Y} = \Big\{ y \in W^{1,p}(\Omega, \mathbb{R}^3) : \ \det \nabla y > 0 \text{ a.e. } , \int_\Omega \det \nabla y(x) \, \mathrm{d}x \le \mathcal{L}^3(y(\Omega)) \Big\},$$

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$$\mathcal{Z} := \Big\{ z \in \mathrm{BV}(\Omega, \{0,1\}^{M+1}) : z_i z_j = 0 \text{ for } i \neq j, \ \sum_{i=0}^{M} z_i = 1 \text{ a.e. in } \Omega \Big\}.$$

Loading

We assume that the body is exposed to possible body and surface loads, and that it is elastically supported on a part Γ_0 of its boundary. The part of the energy related to this loading is given by a functional $L \in C^1([0, T]; W^{1,p}(\Omega; \mathbb{R}^3))$ in the form

$$L(t, y) := \int_\Omega b(t) \cdot y \,\mathrm{d}x + \int_{\Gamma_1} s(t) \cdot y \;\mathrm{d}S + \frac{K}{2} \int_{\Gamma_0} |y - y_D(t)|^2 \,\mathrm{d}S.$$

Here, $b(t, \cdot) : \Omega \to \mathbb{R}^3$ represents the volume density of some given external body forces and $s(t, \cdot) : \Gamma_1 \subset \partial\Omega \to \mathbb{R}^3$ describes the density of surface forces applied on a part Γ_1 of the boundary. The last term in with $y_D(t, \cdot) \in W^{1,p}(\Omega; \mathbb{R}^3)$ represents energy of a spring with a spring stiffness constant $K > 0$.

Dissipation

$$D(z^1, z^2) := |z^1 - z^2|_{M+1} \ .$$

The total dissipation reads

$$\mathcal{D}(z^1, z^2) := \int_\Omega D(z^1(x), z^2(x))\, \mathrm{d}x \ .$$

The dissipation of a curve $z : [0, T] \to \mathrm{BV}(\Omega, \{0, 1\})$ with $[s, t] \subset [0, T]$ is correspondingly given by

$$\mathrm{Diss}_{\mathcal{D}}(z, [s, t]) := \sup \Big\{ \sum_{j=1}^{N} \mathcal{D}(z(t_{i-1}), z(t_i)) \\ : N \in \mathbb{N}, s = t_0 \leq \ldots \leq t_N = t \Big\}.$$

Total energy

$$\mathcal{E}(t, y, z) := E_{\mathrm{b}}(y, z) + E_{\mathrm{int}}(y, z) - L(t, y).$$

Energetic solution (Mielke & Theil)

We say that $(y,z) \in \mathcal{Y} \times \mathcal{Z}$ is an energetic solution to $(\mathcal{E},\mathcal{D})$ on the time interval $[0,T]$ if $t \mapsto \partial_t E(y(t),z(t)) \in L^1((0,T))$ and if for all $t \in [0,T]$, the stability condition

$$\mathcal{E}(t,y(t),z(t)) \le \mathcal{E}(t,\tilde{y},\tilde{z}) + \mathcal{D}(z(t),\tilde{z}) \quad \forall (\tilde{y},\tilde{z}) \in \mathcal{Q}.$$

and the condition of energy balance

$$\mathcal{E}(t,y(t),z(t)) + \mathrm{Diss}_{\mathcal{D}}(z;[0,t]) = \mathcal{E}_0 + \int_0^t \frac{\partial \mathcal{E}}{\partial t}(s,y(s),z(s))\,\mathrm{d}s$$

where $\mathcal{E}_0 = \mathcal{E}(0,y(0),z(0))$, are satisfied.

Existence

A standard way how to prove the existence of an energetic solution is to construct time-discrete minimization problems and then to pass to the limit. For given $N \in \mathbb{N}$ and for $0 \le k \le N$, we define the time increments $t_k := kT/N$. Furthermore, we use the abbreviation $q := (y, z) \in \mathcal{Q}$. Assume that at $t = 0$ there is given an initial distribution of phases $z^0 \in \mathcal{Z}$ and $y^0 \in \mathcal{Y}$ such that $q^0 = (y^0, z^0) \in \mathcal{S}(0)$. For $k = 1, \ldots, N$, we define a sequence of minimization problems

$$\text{minimize } \mathcal{E}(t_k, y, z) + \mathcal{D}(z, z^{k-1}) \ , \ (y, z) \in \mathcal{Q} \ .$$

We denote a minimizer for a given k as $(y^k, z^k) \in \mathcal{Q}$.

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Model: a FEM mesh

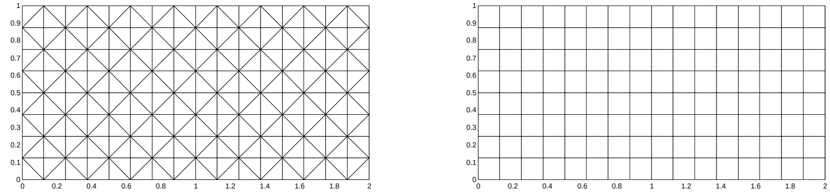


Figure: A FEM triangular mesh (left) and the corresponding rectangular mesh (right) for visualization.

The FEM mesh consists of triangles $T \in \mathcal{T}$ and edges $E \in \mathcal{E}$. The subset $\mathcal{E}_{\mathcal{I}} \subset \mathcal{E}$ denotes the set of internal edges.

Bulk energy with two variants of martensite

The bulk energy $E_{\rm b}$ is considered in the form

$$E_{\rm b}(y,z) := \int_\Omega \Big(z(x)\hat{W}_1(F(y(x))) + (1-z(x))\hat{W}_2(F(y(x))) \Big)\,{\rm d}x,$$

where $\hat{W}_1, \hat{W}_2$ are densities in the form

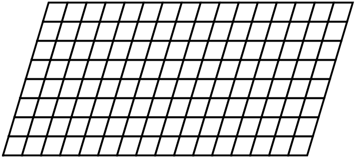
$$\hat{W}_1(F) := \underline{W}(FF_1^{-1}), \quad \hat{W}_2(F) := \underline{W}(FF_2^{-1}).$$

Bulk energy with two variants of martensite

Here, F_1, F_2 are given stretching matrices

$$F_1 := \begin{pmatrix} 1 & \epsilon \\ 0 & 1 \end{pmatrix}, \qquad F_2 := \begin{pmatrix} 1 & -\epsilon \\ 0 & 1 \end{pmatrix}$$

defined by a parameter $\epsilon > 0$.



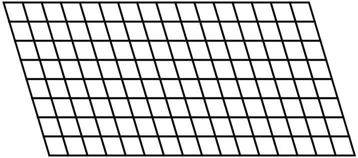


Figure: Examples of mesh deformations corresponding to stretching matrices F_1 (left), F_2 (right) for $\epsilon = 0.3$.

Two-dimensional compressible Mooney-Rivlin material model

The form of $\underline{W}$ is given by

$$\underline{W}(F) := \alpha \operatorname{tr}(F^T F) + \delta_1 (\det F)^2 - \delta_2 \ln(\det F).$$

Parameters $\alpha, \delta_1, \delta_2 > 0$ satisfy the relation

$$\delta_2 = 2\alpha + 2\delta_1$$

and it holds $\underline{W}(F) \to \infty$ for $\det F \to 0+$ and

$$I = \operatorname{argmin}_F \underline{W}(F).$$

Interfacial energy

We consider the interfacial energy E_i in the form

$$E_\mathrm{i}(z) := \int_{E \in \mathcal{E}_\mathcal{I}} \alpha_\mathrm{i} |z^+(s) - z^-(s)| \,\mathrm{d}s,$$

where z^+ and z^- denote restrictions of z to triangles T^+ and T^- and $\alpha_\mathrm{i} \geq 0$ is a parameter.

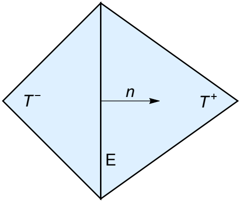


Figure: An internal edge $E \in \mathcal{E}_\mathcal{I}$ shared by two elements $T^+, T^- \in \mathcal{T}$ and its normal vector n.

Surface energy

The surface energy E_{s} is given as

$$E_{\mathrm{s}}(F) := \int_{E \in \mathcal{E}_{\mathcal{I}}} \alpha_{\mathrm{s}} |\mathrm{cof}\, \mathbb{F}(s) n| |z^{+}(s) - z^{-}(s)| \; \mathrm{d}s.$$

It is based on the cofactor of the surface deformation gradient

$$\mathbb{F} := F(I - n \otimes n),$$

where I represents an identity matrix. A parameter $\alpha_{\mathrm{s}} \geq 0$ is given.

Model: a dissipation

The dissipation is assumed in the form

$$\mathcal{D}(z, z^{k-1}) := \int_\Omega \beta |z - z_{k-1}| \,\mathrm{d}x,$$

where $\beta \geq 0$ is a given parameter.

Discrete minimization problem

The time sequence of incremental minimizations rewrites as:

minimize

$$\sum_{T \in \mathcal{T}} \left(z\hat{W}_1(F) + (1-z)\hat{W}_2(F) + \beta|z - z_{k-1}| \right) |T| \\ + \sum_{E \in \mathcal{E}_\mathcal{I}} \left(|z^+ - z^-| (\alpha_\mathrm{i} + \alpha_\mathrm{s} |\mathrm{cof}\, \mathbb{F} n|) \right) |E| \tag{1}$$

over $y \in [P^1(\mathcal{T})]^2, z \in P^0_{\{0,1\}}(\mathcal{T})$.

All terms are either constant on each triangle $T \in \mathcal{T}$ or constant on each edge $E \in \mathcal{E}_\mathcal{I}$.

Discrete minimization problem in z only for given $F(y)$

We introduce an incremental variable

$$\tilde{z} := z - z_{k-1} \in P^0_{\{-z_{k-1}, 1-z_{k-1}\}}(\mathcal{T}),$$

(z-independent terms are dropped):

$$\begin{aligned}
&\text{minimize} \\
&\sum_{T \in \mathcal{T}} \left(\tilde{z}[\hat{W}_1(F) - \hat{W}_2(F)] + \beta|\tilde{z}| \right) |T| \\
&+ \sum_{E \in \mathcal{E}_{\mathcal{I}}} \left(\alpha|\tilde{z}^+ - \tilde{z}^- + z^+_{k-1} - z^-_{k-1}| \right) |E| \\
&\text{over } \tilde{z} \in P^0_{\{-z_{k-1}, 1-z_{k-1}\}}(\mathcal{T}).
\end{aligned} \tag{2}$$

Further transformations lead to zero-one integer programming problem.

Discrete minimization problem in z only for given $F(y)$

minimize

$$\sum_{T\in\mathcal{T}} \left(\tilde{z}\hat{W}_{1,2} + \beta\tilde{\lambda}\right)|T| + \sum_{E\in\mathcal{E}_\mathcal{I}} \alpha\tilde{\sigma}|E|$$

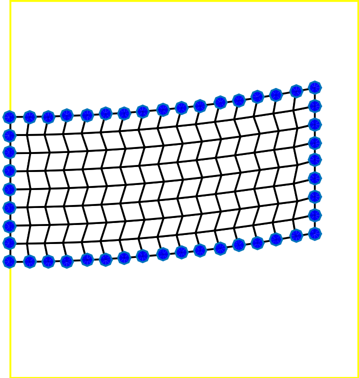
over $\tilde{z} \in P^0_{[-z_{k-1},1-z_{k-1}]}, \tilde{\lambda} \in P^0_{[-1,1]}(\mathcal{T}), \tilde{\sigma} \in P^0_{[-1,1]}(\mathcal{E}_\mathcal{I})$

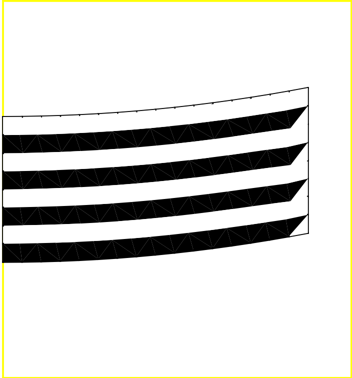
subject to constraints:

$$\begin{aligned} \tilde{z} - \tilde{\lambda} &\leq 0 \\ -\tilde{z} - \tilde{\lambda} &\leq 0 \end{aligned} \qquad \text{on all triangles } T \in \mathcal{T},$$

$$\begin{aligned} \tilde{z}^+ - \tilde{z}^- - \tilde{\sigma} &\leq -(\tilde{z}^+_{k-1} - \tilde{z}^-_{k-1}) \\ -(\tilde{z}^+ - \tilde{z}^-) - \tilde{\sigma} &\leq \tilde{z}^+_{k-1} - \tilde{z}^-_{k-1} \end{aligned} \qquad \text{on all edges } E \in \mathcal{E}_\mathcal{I}.$$

Time evolution: a full Dirichlet BC





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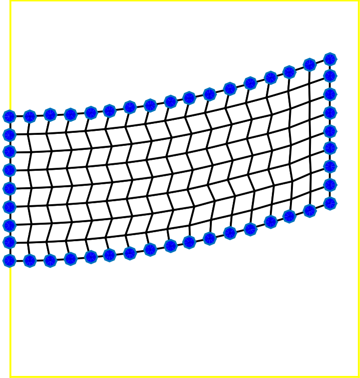

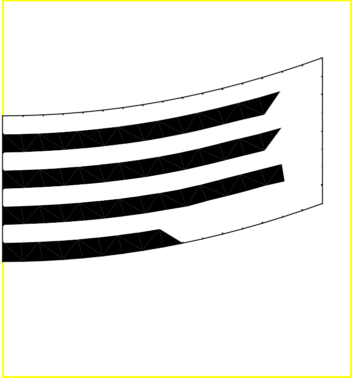

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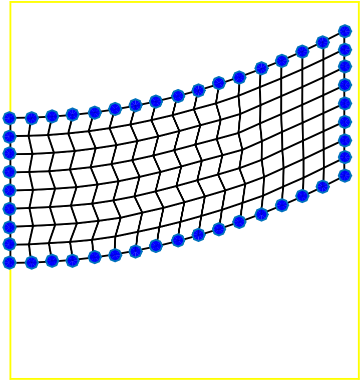

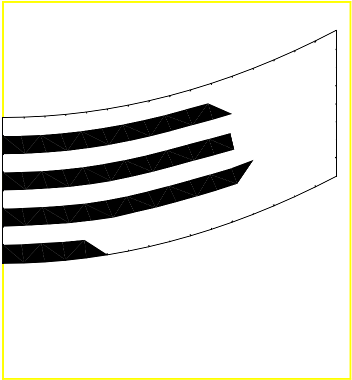

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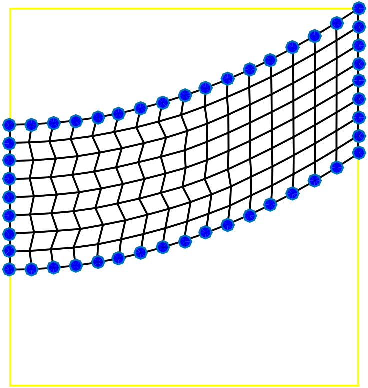

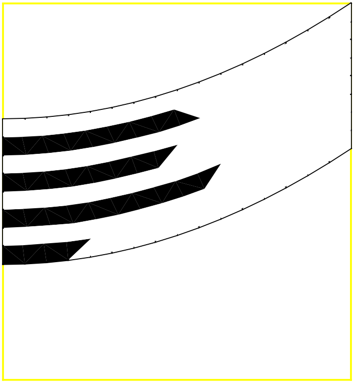

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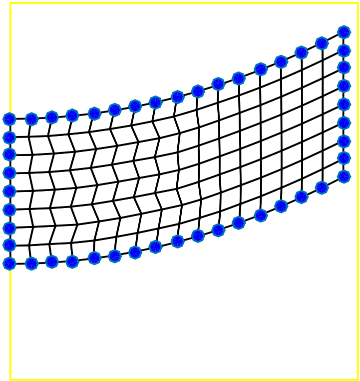

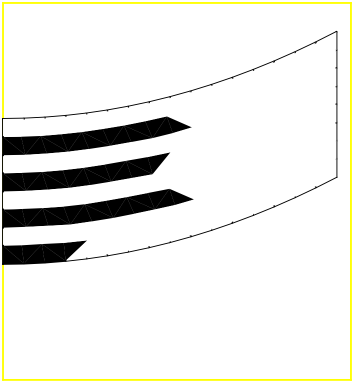

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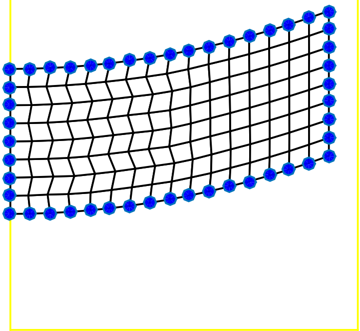

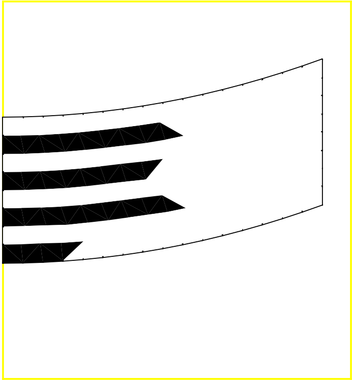

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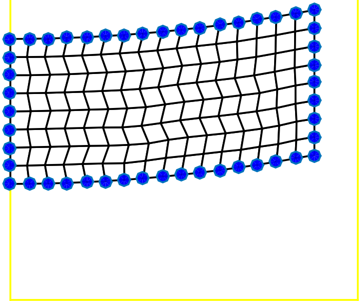

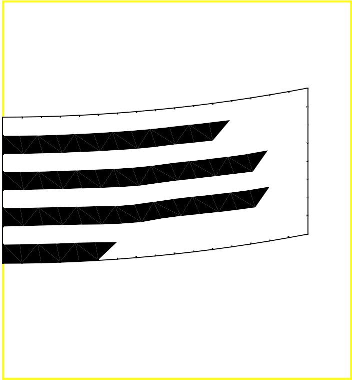

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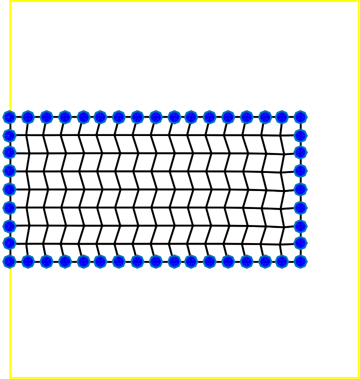

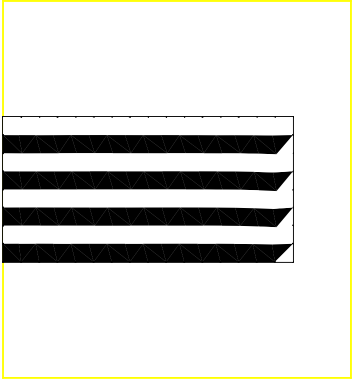

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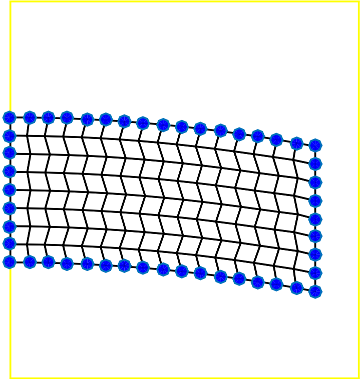

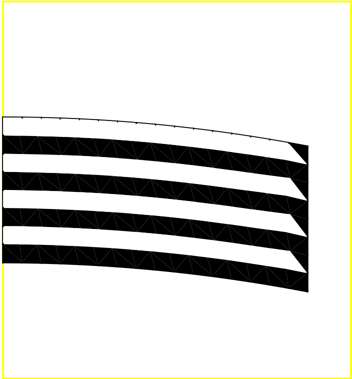

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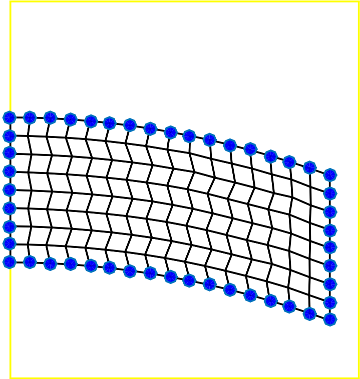

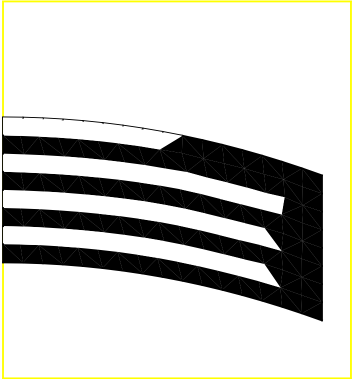

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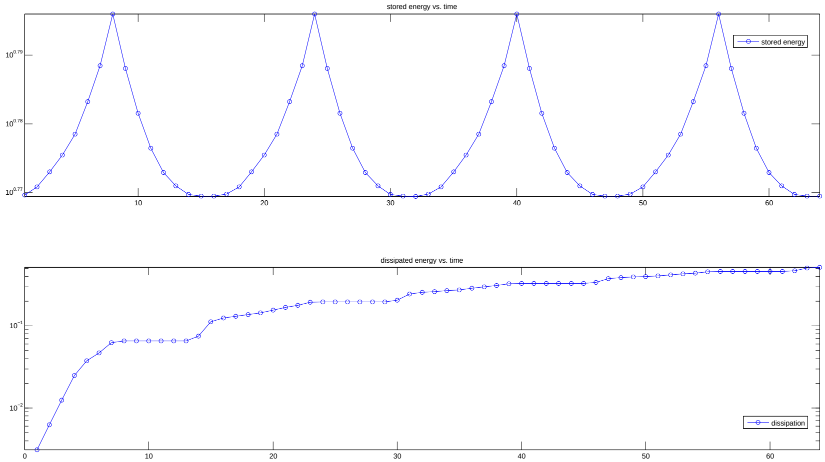

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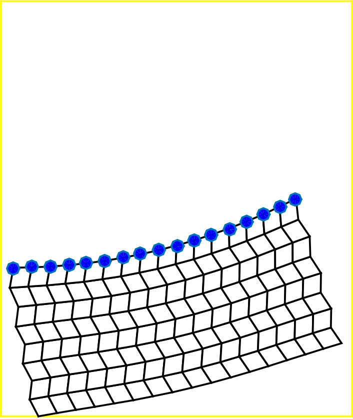

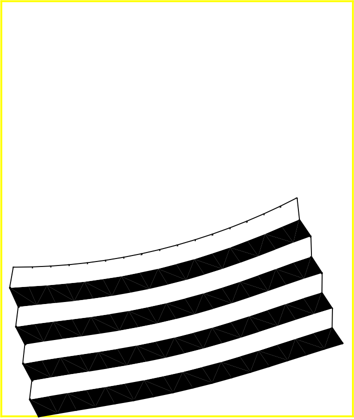

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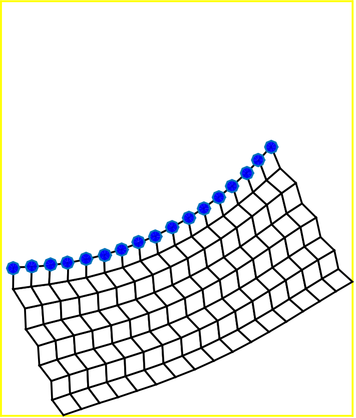
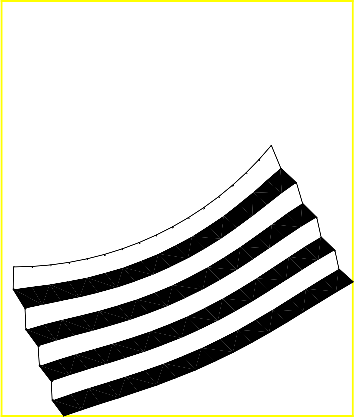
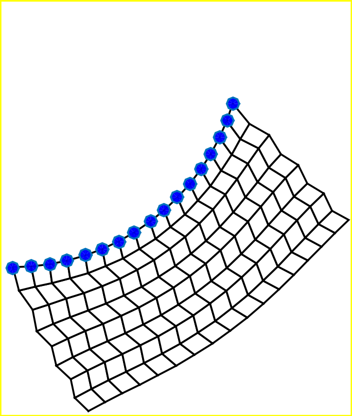
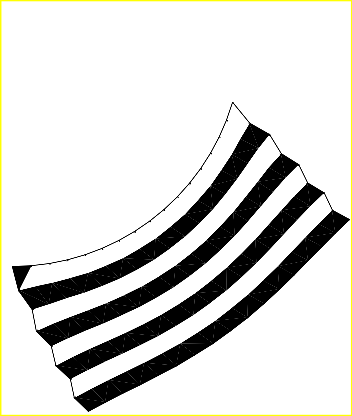


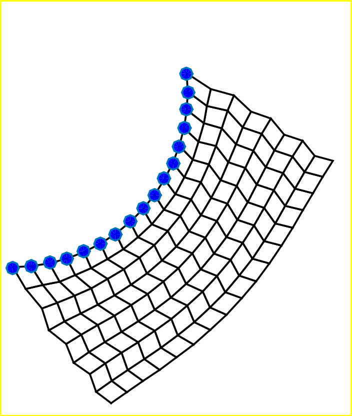


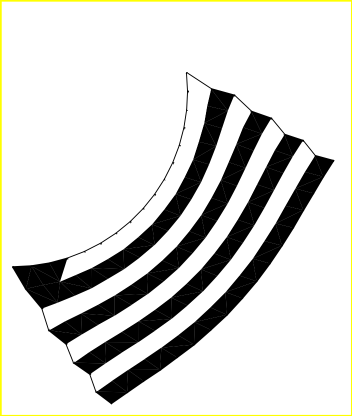
Time evolution: a partial Dirichlet BC



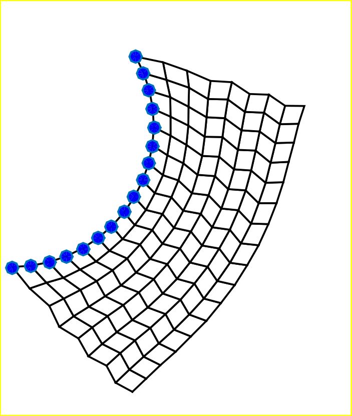


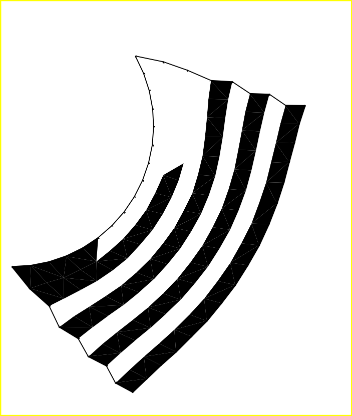
Time evolution: a partial Dirichlet BC



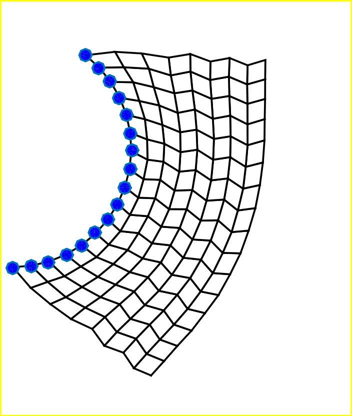


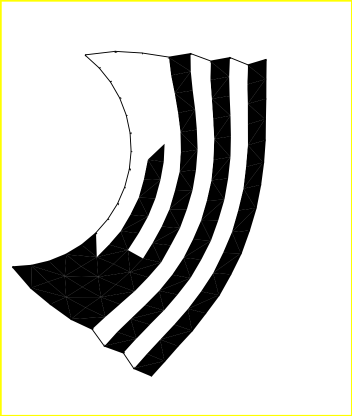
Time evolution: a partial Dirichlet BC



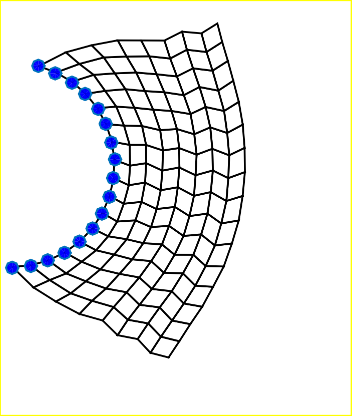


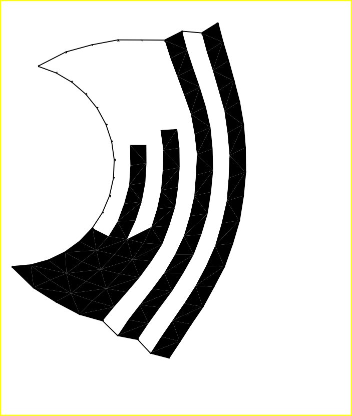
Time evolution: a partial Dirichlet BC



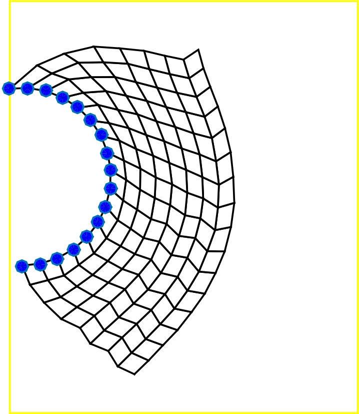


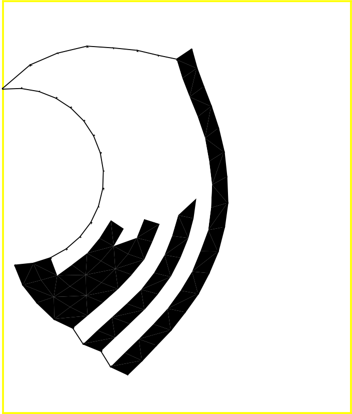
Time evolution: a partial Dirichlet BC





Time evolution: a partial Dirichlet BC





Paper

Miroslav Frost, Martin Kružík and Jan Valdman - Computational modeling of shape memory materials (in preparation)

Thank you for your attention!