Density-based Topology Optimisation considering nonlinear electromechanics[1]

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Introduction

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Topology optimization of smart materials opens up for the possibility of exploiting the unconventional properties of these materials by conceiving new designs beyond human intuition

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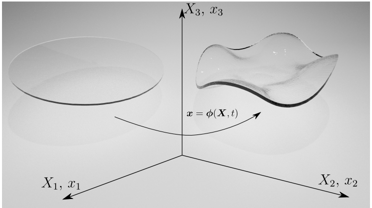
- We consider both a dielectric elastomer and a piezoelectric polymer model
- Large electrically induced deformations may occur, so finite elasticity modeling is required
- Multiphysics problem: equilibrium is obtained as the solution of a couple system of nonlinear PDE's

Nonlinear continuum electromechanics

The solid occupies the reference configuration $\mathcal{B}_0$, and after being deformed, the deformed configuration, $\mathcal{B}$.

ϕ is the deformation and $\mathbf{F} = \nabla_0 \phi(\mathbf{X})$ the deformation gradient.

$\mathbf{H}$ and J are the cofactor and determinant of $\mathbf{F}$ respectively.



Elastic equilibrium

The elastic equilibrium comes as the solution of

$$\begin{aligned} \operatorname{div}\mathbf{P} + \mathbf{f}_0 = \mathbf{0}; &\qquad \text{in } \mathcal{B}_0; \\ \mathbf{Pn} = \mathbf{t}_0; &\qquad \text{on } \partial_{\boldsymbol{t}}\mathcal{B}_0; \\ \phi = \bar{\phi}; &\qquad \text{on } \partial_{\phi}\mathcal{B}_0, \end{aligned}$$

where $\mathbf{f}_0$ a distributed external force and $\mathbf{t}_0$ a boundary force. $\bar{\phi}$ Dirichlet boundary condition.

$\mathbf{P}$ the first Piola-Kirchhoff stress tensor.

Gauss and Faraday' laws

- Gauss's law:

$$\begin{aligned} \operatorname{div} \mathbf{D}_0 - \rho_0 = 0; \qquad & \text{in } \mathcal{B}_0; \\ \mathbf{D}_0 \cdot \mathbf{N} = -\omega_0; \qquad & \text{on } \partial_\omega \mathcal{B}_0, \end{aligned}$$

where $\mathbf{D}_0$ the electric displacement, ρ_0 the electric volumetric charge and ω_0 the boundary charge.

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- Faraday's law:

$$\begin{aligned} \mathbf{E}_0 = -\nabla_0 \varphi; &\qquad \text{in } \mathcal{B}_0; \\ \varphi = \bar{\varphi}; &\qquad \text{on } \partial_\varphi \mathcal{B}_0, \end{aligned}$$

where $\mathbf{E}_0$ the electric field and φ the scalar potential.

Constitutive equations

In order to close the equilibrium state equations we use the **Helmhotz functional**:

$$\Psi = \Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0),$$

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$$\begin{cases} \mathbf{P} = \partial_{\mathbf{F}} \Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0), \\ \mathbf{D}_0 = -\partial_{\mathbf{E}_0} \Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0) \end{cases}$$

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FE numerical approximation of the continuum will be approximated by a a Newton-Raphson algorithm.

Dielectric elastomer

Example of a constitutive model for isotropic dielectric elastomers in finite strain electromechanics:

$$\Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0) = \Psi_m(\mathbf{X}, \mathbf{F}) + \Psi_{em}(\mathbf{X}, \mathbf{F}, \mathbf{E}_0).$$

with,

- Mechanical (*Mooney-Rivlin*):

$$\Psi_m(\mathbf{F}) = \Psi_m^{MR}(\mathbf{F}) := \frac{\mu_1}{2} II_{\mathbf{F}} + \frac{\mu_2}{2} II_{\mathbf{H}} + f(J);$$
$$f(J) = -(\mu_1 + 2\mu_2)\ln(J) + \frac{\lambda}{2}(J-1)^2, \quad II_{\mathbf{A}} = \mathbf{A} \cdot \mathbf{A}$$

- Electricalmechanical (*isotropic ideal dielectric*):

$$\Psi_{em}(\mathbf{F}, \mathbf{E}_0) = -\frac{\varepsilon_r \varepsilon_0}{2J} II_{\mathbf{HE}_0} = -\frac{\varepsilon_r \varepsilon_0}{2J}(\mathbf{HE}_0 \cdot \mathbf{HE}_0),$$

Dielectric elastomer

- E Young's modulus and ν Poisson's ratio:

$$\mu_1 + \mu_2 = \frac{E}{2(1+\nu)}; \qquad \lambda - 2\mu_2 = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

- $\varepsilon_0 = 8.854 \times 10^{-}12\,\mathrm{Fm}^{-1}$ electric permitivity of vaccum
- ε_r relative electric permitivity

Piezoelectric polymer

- Mechanical:

$$\Psi_m(\mathbf{F}) = \Psi_m^{MR}(\mathbf{F}) + \frac{\mu_3}{2}\left(II_{\mathbf{FV}} + II_{\mathbf{HV}}\right) + \frac{\mu_4}{4}\left(II_{\mathbf{FV}}^2 + II_{\mathbf{HV}}^2\right) + g(J);$$

$$g(J) = -\left(\mu_3 + \mu_4\right)\ln(J) + \frac{\lambda}{2}\left(J-1\right)^2,$$

with $\mathbf{V}$ the polarization direction;

- Electromechanical:

$$\Psi_{em}(\mathbf{X}, \mathbf{F}, \mathbf{E}_0) = -\frac{\varepsilon_1}{2} II_{\mathbf{HE}_0} - \frac{\varepsilon_2}{2}\left(\mathbf{E}_0 \cdot \mathbf{V}\right)^2 - e_1 \mathbf{V} \cdot \widetilde{\mathbf{E}}\mathbf{E}_0 - e_2\left(\mathbf{E}_0 \cdot \mathbf{V}\right)\operatorname{tr}(\widetilde{\mathbf{E}}) - e_3\left(\mathbf{E}_0 \cdot \mathbf{V}\right)\left(\mathbf{N} \cdot \widetilde{\mathbf{E}}\mathbf{V}\right),$$

Problem

Minimize $\mathcal{J}(\Phi_\chi) = -\int_{\partial\mathcal{B}_0} \mathbf{l}_0 \cdot \Phi_\chi \, dA$,

subject to:

- The displacement Φ is obtain from the solution of the nonlinear electromechanics system with constitutive law given by the Helmholtz energy functional

$$\Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0) = \Psi^\chi(\chi(\mathbf{X}), \mathbf{F}, \mathbf{E}_0),$$

  where $\chi(\mathbf{X}) \in \{0, 1\}$ is the *discrete design* differentiating solid from void regions;
- Volumen constraint: $\int_{\Omega_0} \chi(\mathbf{X}) \, dV \leq c|\Omega_0|$.

$\mathbf{l}_0$ unitary fixed vector in the direction where the displacement is maximized and defined on $\partial\mathcal{B}_0$.

SIMP approach

- From discrete (*binary*) to density approach: $\chi \to \rho,\ \rho \in \{0, 1\}$

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$$\tilde{\rho}(\mathbf{X}) = (\rho * \Delta)(\mathbf{X}) = \int_{\mathcal{B}_0} \rho(\mathbf{X}')\Delta(\|\mathbf{X} - \mathbf{X}')\, dV,$$

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- Density projection: we define the *physical density field*

$$\hat{\rho}(\mathbf{X}) = \frac{\tanh(\beta\eta) + \tanh(\beta(\tilde{\rho}(\mathbf{X}) - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))},$$

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- **Interpolated strain energy density**:
  $\Psi(\mathbf{X}, \mathbf{F}, \mathbf{E}_0) = \Psi^{SIMP}(\hat{\rho}(\mathbf{X}), \mathbf{F}, \mathbf{E}_0)$

Energy interpolation scheme

Homogenized Helmholtz functional

$$\Psi = \Psi^{\text{SIMP}}(\hat{\rho}(\mathbf{X}), \mathbf{F}, \mathbf{E}_0)$$
$$:= \underbrace{(\hat{\rho}(\mathbf{X}))^{p_m}\, \Psi_m^{\text{solid}}(\mathbf{F}) + [1 - (\hat{\rho}(\mathbf{X}))^{p_m}]\Psi_m^{\text{void}}(\mathbf{F})}_{\text{Homogenised mechanical component}}$$
$$+ \underbrace{(\hat{\rho}(\mathbf{X}))^{p_e}\, \Psi_{em}^{\text{solid}}(\mathbf{F}, \mathbf{E}_0) + [1 - (\hat{\rho}(\mathbf{X}))^{p_e}]\Psi_{em}^{\text{void}}(\mathbf{E}_0)}_{\text{Homogenised electromechanical component}},$$

p_m and p_e are, respectively, the mechanical and electromechanical penalisation exponents

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STUDYING THE INFLUENCE OF THESE PARAMETERS IN THE DESIGN PROCESS IS OF MAJOR IMPORTANCE

Energy interpolation scheme: void modeling

Void energy

- Mechanical:

$$\Psi_m^{\text{void}}(\mathbf{F}) := \frac{\alpha}{2}(\mathbf{F} - \mathbf{I}) : \mathcal{C}|_0 : (\mathbf{F} - \mathbf{I}),$$

with $\mathcal{C}|_0$ solid elasticity tensor at the origin $(\mathbf{F} = \mathbf{I})$

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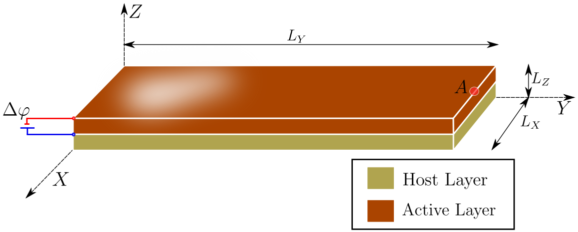
- Electromechanical:

$$\Psi_{em}^{\text{void}}(\mathbf{E}_0) = \left(-\frac{\varepsilon_0}{2J} II_{\mathbf{HE}_0}\right)\Big|_{\mathbf{H}=\mathbf{I},J=1} = -\frac{\varepsilon_0}{2} II_{\mathbf{E}_0}$$

Example 1: dielectric elastomer actuator

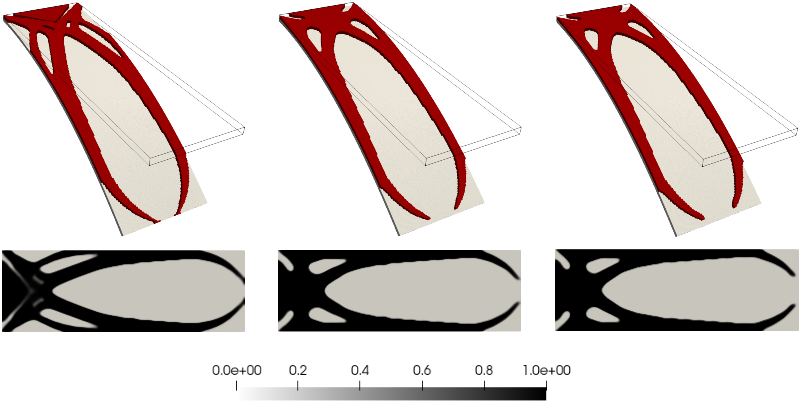


Example 1. Unimorph dielectric elastomer-based device, completely fixed at $Y = 0$, and subjected to $\Delta\varphi = 8 \times 10^3$ V/m. Symmetric boundary conditions have been applied at $X_{med} = (\max(X) + \min(X))/2$, leading to a discretisation of $180 \times 30 \times 2$ $Q2$ (tri-quadratic) Finite Elements, yielding a total of $(180 \times 2 + 1) \times (30 \times 2 + 1) \times (2 \times 2 + 1) \times 3 = 330315$ dofs for ϕ and $(180 \times 2 + 1) \times (30 \times 2 + 1) \times (2 \times 2 + 1) = 110105$ for φ. Objective function aiming at maximising Z direction of displacement at point **A**.

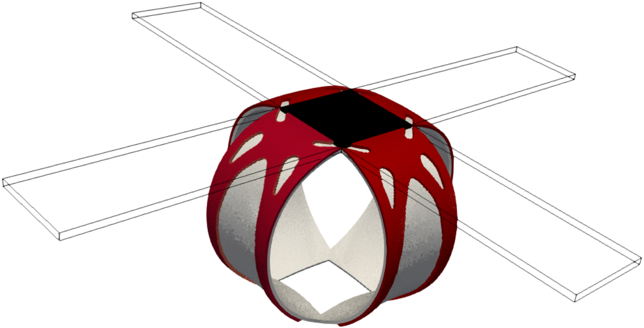
Example 1: dielectric elastomer actuator

$\mathbf{p_m = 3}$

$p_e/p_m = 1$ | $p_e/p_m = 1.5$ | $p_e/p_m = 2$

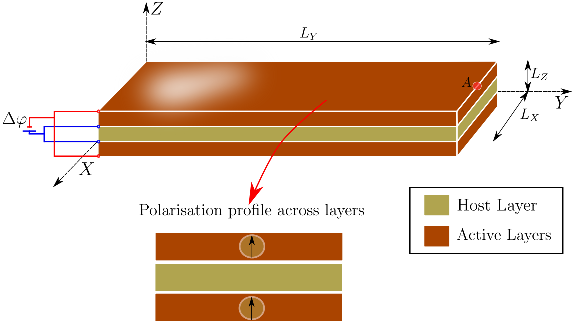


Dielectric-elastomer base gripper



Dielectric elastomer-based gripper. Deformed configuration for voltage gradiens $\Delta\varphi$ of $(\frac{2}{3} \times 10^3) \times \{24\}$ V/m. Results obtained with the optimised design corresponding with $p_m = 3, p_e/p_m = 2$ using **continuation strategy**

Example 2: piezoelectric polymer actuator

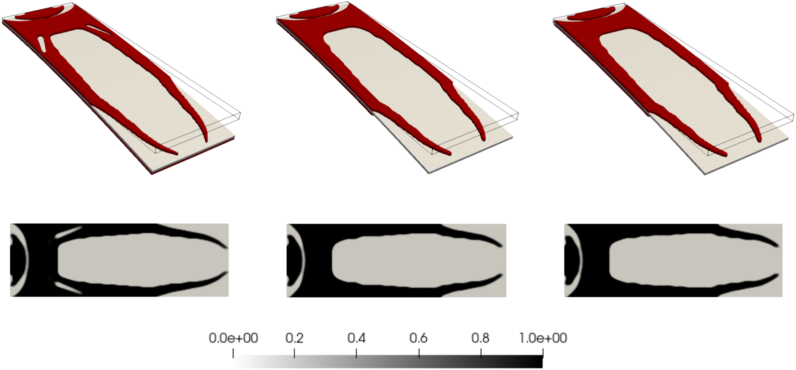


Bimorph piezoelectric polymer-based device, completely fixed at $Y = 0$, and subjected to $\Delta\varphi = 10^4$ V/m. Symmetric boundary conditions have been applied at $X_{med} = (\max(X) + \min(X))/2$. Objective function aiming at maximising Z direction of displacement at point **A**. Polarisation profile across the thickness (vector **V** in equilibrium equations).

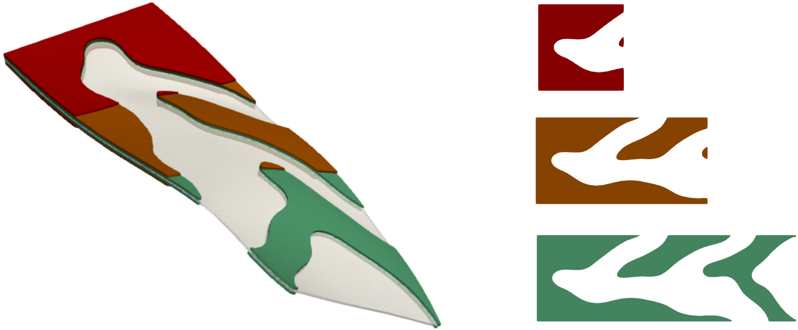
Example 2: piezoelectric polymer actuator

$\mathbf{p_m = 5}$

$p_e/p_m = 1$ | $p_e/p_m = 1.5$ | $p_e/p_m = 2$



Example 3: multilayered torsional piezoelectric actuator



Design of the multilayered torsional piezoelectric actuator for $p_m = 3$ and $p_e = 6$,

Conclusions

- Density-based TO in the context of nonlinear electromechanics, focusing on electro-active materials, capable of undergoing large electrically induced deformations
- Energy interpolation scheme for void and solid regions that works out preventing numerical instabilities associated to low and intermediate densities
- In view of numerical simulations, $p_e > p_m$ is strongly adviced. This is in opposition with linear piezoelectricity, where non-penalisation of electromechanical energy is needed