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A variational and computational framework for large strain electromechanics based on convex multi-variable energies

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Micro Abstract
This paper presents a variational and computational framework for nonlinear electromechanics based on a new convex multi-variable definition of the internal energy. This ensures: a) the material stability of the governing equations (ellipticity) and b) allows to introduce new multi-field variational principles which open up interesting possibilities in terms of using various interpolation spaces for the different fields, leading to enhanced type formulations.

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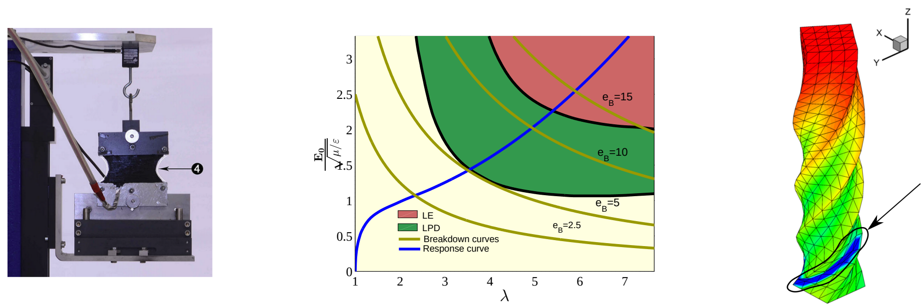
Introduction

Electro Active Polymers (EAPs) have been identified as ideal candidates for the fabrication of soft robots due to their ability to undergo highly complex stretching, bending and twisting actuation when subjected to electric stimuli. As an example, Dielectric Elastomer EAPs have shown impressive nonlinear electrically-induced strains of around 100%. Moreover, recent research on Dielectric Elastomer VHB4910 [2] has reported unprecedented area expansions of 1962%, opening up a wealth of new design possibilities in a previously unthinkable giant actuation range. The tremendous potential of EAPs has attracted the interest of eminent scientists in the field of computational mechanics (Steinmann [7], Castañeda [6], and many others). Robustness, reliability, efficiency and accuracy are the four crucial characteristics sought in a computer program. Unfortunately, even state-of-the-art computer models fail to realistically. The reason for this pitfall is not necessarily the algorithm per se. It is far more fundamental: it is due to the constitutive model upon which the algorithm is based.

A prototypical example, widely available in the literature [6], will be used to illustrate this. A standard set up used for the material characterisation of isotropic EAP films via laboratory experiments (see Figure 1_a) is that where an imposed out-of-plane (to the film) electric field actuates an in-plane uniform expansion and an out-of-plane thinning of the film. Laboratory data is then used to calibrate the constitutive model response curve. The blue curve in Figure 1_b displays this response for a constitutive model widely used in the literature. A careful analysis (requiring computing the acoustic wave speeds of the model), illustrated in Figure 1_b, identifies in red the regions in which the model fails. Specifically, for any combination of electric field ($\mathbf{E}_0$) and electrically induced stretch (λ) located inside the red region, the model becomes ill-posed or non-elliptic [6], leading inevitably to catastrophic consequences from the numerical standpoint, characterised by mesh-biased results and areas of unphysical zero thickness (see Figure 1_c). This is the reason why, in the context of EAPs, computer models cannot be reliably [6] used beyond moderate actuation scenarios without risking physically impossible results. A new methodological approach for the development of constitutive models which are well-posed *ab initio* for the entire range of deformations and electric fields is presented in this paper.



(a) (b) (c)

Figure 1. (a) Material characterisation of EAP VHB4910; (b) Response curve (in blue) and stability analysis of widely used constitutive model for the standard experimental set up described; (c) Development of localised deformations in unrealistic zero thickness shear bands in the simulation of a piezoelectric EAP material.

1 Nonlinear continuum electromechanics: multi-variable convexity

The set of equations governing the physics of EAPs, namely conservation of linear momentum and the Gauss's law [7], can be mathematically stated as,

$$\mathrm{DIV}\mathbf{P} + \mathbf{f}_0 = \mathbf{0}; \qquad \mathrm{DIV}\mathbf{D}_0 - \rho_0 = 0, \tag{1}$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, $\mathbf{f}_0$, the Lagrangian body force vector, $\mathbf{D}_0$, the Lagrangian electric displacement field and ρ_0, the electric charge per unit volume. Rotational equilibrium dictates that $\mathbf{F}^T\mathbf{P} = \mathbf{P}\mathbf{F}^T$, where $\mathbf{F}$ represents the deformation gradient tensor, and the Faraday's law can be written as $\mathbf{E}_0 = -\nabla_0\phi$, with $\mathbf{E}_0$ the Lagrangian electric field and ϕ the electric potential. The internal energy density e, encapsulating the constitutive information necessary to close the system of governing equations in (1), is defined as $e = e(\mathbf{F}, \mathbf{D}_0)$. Recently, the concept of multi-variable convexity has been introduced in References [1,3–5], postulated as

$$e\left(\nabla_0\mathbf{x}, \mathbf{D}_0\right) = W\left(\mathbf{F}, \mathbf{H}, J, \mathbf{D}_0, \mathbf{d}\right); \quad \mathbf{d} = \mathbf{F}\mathbf{D}_0, \tag{2}$$

where W represents a convex multi-variable functional in terms of its extended set of arguments $\mathcal{V} = \{\mathbf{F}, \mathbf{H}, J, \mathbf{D}_0, \mathbf{d}\}$, with $\{\mathbf{H}, J\}$ the co-factor and the Jacobian of $\mathbf{F}$, respectively. The set of work conjugates to $\mathcal{V}$ is defined as $\Sigma_{\mathcal{V}} = \{\boldsymbol{\Sigma}_{\mathbf{F}}, \boldsymbol{\Sigma}_{\mathbf{H}}, \Sigma_J, \boldsymbol{\Sigma}_{\mathbf{D}_0}, \boldsymbol{\Sigma}_{\mathbf{d}}\}$, with $\boldsymbol{\Sigma}_{\mathbf{A}} = \frac{\partial W}{\partial \mathbf{A}}$, for any $\mathbf{A} \in \mathcal{V}$. Both sets $\mathcal{V}$ and $\Sigma_{\mathcal{V}}$ enable a new representation of the first Piola-Kirchhoff stress tensor and the Lagrangian electric field in terms of the elements of both sets as

$$\mathbf{P} = \boldsymbol{\Sigma}_{\mathbf{F}} + \boldsymbol{\Sigma}_{\mathbf{H}} \times \mathbf{F} + \Sigma_J\mathbf{H} + \boldsymbol{\Sigma}_{\mathbf{d}} \otimes \mathbf{D}_0; \qquad \mathbf{E}_0 = \boldsymbol{\Sigma}_{\mathbf{D}_0} + \mathbf{F}^T\boldsymbol{\Sigma}_{\mathbf{d}}. \tag{3}$$

Crucially, the definition of multi-variable convexity in (2) satisfies *ab initio* the ellipticity condition for the entire range of deformations and electric fields.

2 Finite Element implementation and numerical results

Multi-variable convexity guarantees a one-to-one and invertible relationship between the sets $\mathcal{V}$ and $\Sigma_{\mathcal{V}}$ [1]. Therefore, alternative energy functionals established via appropriate Legendre transforms applied to the internal energy $W(\mathcal{V})$ can be defined, including the Gibb's energy $\Upsilon(\Sigma^m_{\mathcal{V}}, \Sigma^e_{\mathcal{V}})$, the Enthalpy $\Psi(\Sigma^m_{\mathcal{V}}, \mathcal{V}^e)$ and the Helmholtz's energy $\Phi(\mathcal{V}^m, \Sigma_{\mathcal{V}^e})$, with $\mathcal{V}^m = \{\mathbf{F}, \mathbf{H}, J\}$, $\mathcal{V}^e = \{\mathbf{D}_0, \mathbf{d}\}$, $\Sigma^m_{\mathcal{V}} = \{\boldsymbol{\Sigma}_{\mathbf{F}}, \boldsymbol{\Sigma}_{\mathbf{H}}, \Sigma_J\}$ and $\Sigma^e_{\mathcal{V}} = \{\boldsymbol{\Sigma}_{\mathbf{D}_0}, \boldsymbol{\Sigma}_{\mathbf{d}}\}$. This opens up the possibility for the definition of new Hu-Wahizu mixed variational principles in terms of the multiple energy functionals mentioned, namely $\{W, \Upsilon, \Psi, \Phi\}$, which can overcome classical drawbacks of traditional Finite Element displacement-potential based formulations, i.e, shear locking, volumetric locking in incompressible scenarios, etc. An example of a Hu-Washizu mixed variational principle presented in $[1, 4, 5]$ in terms of $W(\mathcal{V})$ is

$$\begin{aligned}\Pi_W(\mathbf{x}, \mathcal{V}^m, \Sigma^m_{\mathcal{V}}, \varphi, \mathcal{V}^e, \boldsymbol{\Sigma}_{\mathbf{d}}) &= \int_V W(\mathcal{V})\, dV + \int_V \mathbf{D}_0 \cdot \nabla_0\varphi\, dV + \int_V \boldsymbol{\Sigma}_{\mathbf{F}} : (\mathbf{F}_{\mathbf{x}} - \mathbf{F})\, dV \\ &+ \int_V \left[\boldsymbol{\Sigma}_{\mathbf{H}} : (\mathbf{H}_{\mathbf{x}} - \mathbf{H}) + \Sigma_J(J_{\mathbf{x}} - J) + \boldsymbol{\Sigma}_{\mathbf{d}} \cdot (\mathbf{F}_{\mathbf{x}}\mathbf{D}_0 - \mathbf{d})\right] dV - \Pi_{ext}(\mathbf{x}, \varphi),\end{aligned} \tag{4}$$

where $\{\mathbf{F_x}, \mathbf{H_x}, J_\mathbf{x}\}$ denote the geometrically compatible strain measures and Π_{ext} the external work contribution. Figure 2 includes a series of numerical examples which prove the robustness and applicability of the above formulation. Specifically, Figures 2_a-2_c show the electrically induced torsional deformation pattern on an incompressible EAP. Figures 2_d and 2_e show different electrically induced bending actuation patterns of EAPs. Finally, 2_f displays the giant electrically induced deformations on an EAP obtained after the snap-through instability.

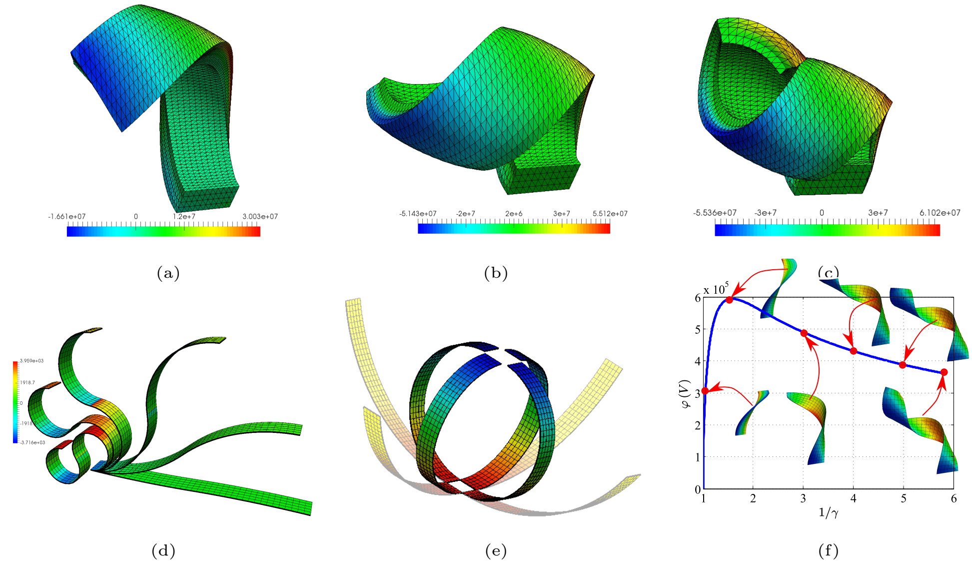


Figure 2. (a)-(c) Electrically induced torsional actuation. (d)-(e) Various electrically induced bending actuation applications. (f) Giant electrically induced deformations on helicoidal actuator.

3 Material characterisation via convex multi-variable constitutive models

For the experimental set up described in Section , a Convex Multi-Variable (CMV) and a non-CMV constitutive models, $W_{el,1}$ and $W_{el,2}$ respectively, defined as

$$
\begin{aligned}
W_{el,1} &= \mu_1 II_\mathbf{F} + \mu_2 II_\mathbf{H} + \frac{1}{2\varepsilon_1} II_\mathbf{d} + \mu_e \left(II_\mathbf{F}^2 + \frac{2}{\mu_e \varepsilon_e} II_\mathbf{F} II_\mathbf{d} + \frac{1}{\mu_e^2 \varepsilon_e^2} II_\mathbf{d} \right) + f(J); \\
W_{el,2} &= \tilde{\mu}_1 II_\mathbf{F} + \tilde{\mu}_2 II_\mathbf{H} + \frac{1}{2\tilde{\varepsilon}_1} II_\mathbf{d} + \frac{2}{\tilde{\varepsilon}_e} II_\mathbf{F} II_\mathbf{d} + \frac{1}{2\tilde{\varepsilon}_2} II_{\mathbf{D}_0} + f(J),
\end{aligned}
\tag{5}
$$

will be considered, with $II_\mathbf{A} = \mathbf{A} : \mathbf{A}$ for second order tensors and $II_\mathbf{A} = \mathbf{A} \cdot \mathbf{A}$ for vectors. Both models can capture intrinsic effects of EAPs such as electristriction, i.e. the dependence of the spatial electric permittivity ε upon the deformation. Careful selection of electrostrictive material parameters $\{f_e, \tilde{f}_e\}$, defined as $\{f_e = \frac{\varepsilon_1}{\varepsilon}, \tilde{f}_e = \frac{\tilde{\varepsilon}_1}{\varepsilon}\}$, can help replicating the electrostrictive behaviour of a simpler model proposed by Zhao et al. [8] (see Figure 3_a). The material parameters for the CMV model have been selected to replicate the response of the non-CMV model (see Figure 3_d). However, a careful analysis, requiring the computation of the minors of the generalised electro-mechanical acoustic tensor (related to the wave speeds in the material), shows that the non-CMV model (Figures 3_b-3_c) becomes non-elliptic. This is represented by the flat regions in Figure 3_c, associated with unphysical imaginary wave speeds. The latter coincides with the loss of ellipticity, represented in Figure 1_b by the red area. On the contrary, the CMV model remains elliptic for the entire range of the experimental set up (Figures 3_e-3_f).

Conclusions

This paper has presented a computational framework for nonlinear electromechanics based on the concept of multi-variable convexity introduced in [1,3–5]. Convex multi-variable definition of the internal energy functional ensures the ellipticity and, hence, the existence of real wave speeds within the material. In addition, from the computational implementation standpoint, multi-variable convexity has enabled the definition of new interesting mixed Hu-Washizu formulations. In forthcoming publications, unexplored energy relaxation techniques based on the computation

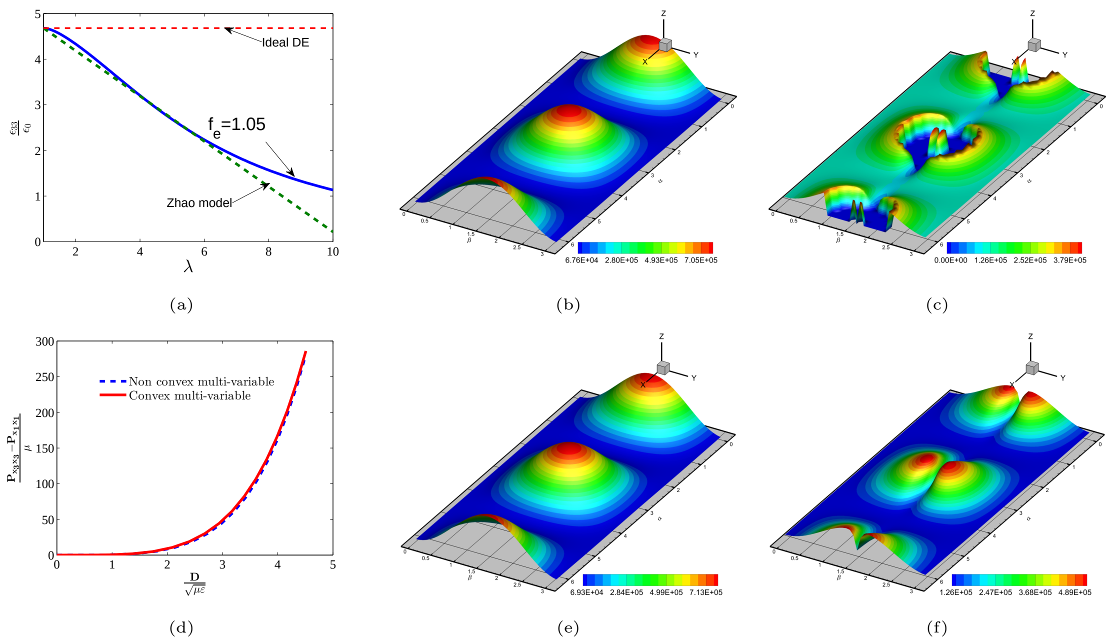


Figure 3. (a) Electrostriction in $W_{el,1}$ and $W_{el,2}$ in (5); (d) response curve for $W_{el,1}$ and $W_{el,2}$; (b)-(c) and (e-f) minors of the acoustic tensor for $W_{el,2}$ and $W_{el,1}$, respectively, for different stages of the experiment.

of CMV envelopes of (widely used) non-CMV energy functionals will be pursued, as a means to regularise the a priori ill-posed response of the latter.

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