Computational challenges in the simulation of nonlinear electroelasticity

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Abstract

Nonlinear electroelasticity is not a new problem, its theory involving nonlinear deformation and nonlinear material behavior has been well established. However, the numerical simulation of nonlinear electroelasticity is until now still far from satisfactory, especially when the interaction between electric fields and matter cannot be considered as confined in the finite space occupied by matter. It is understood that under the application of an electric field, the deformation of an elastic body is governed not always by what happens inside the material body but in many cases also by the environment surrounding it. This is notably true in the case of electronic electroactive polymers, the kind of materials that emerges today as a leading candidate in developing artificial muscles. In this text, we present the simulation of nonlinear electroelasticity by assuming large deformation, nonlinear polarization and by paying attention to the contribution of the space surrounding the bodies of interest.

Keywords: nonlinear electricity, nonlinear elasticity, nonlinear coupling, coupled BEM-FEM analysis.

1. Introduction

In nonlinear electroelasticity we study the interaction between polarizable material bodies and electric fields. This coupled phenomenon can be viewed in a simple way as follows: when being immersed in an electric field a polarizable body deforms because of the electric forces acting on electric dipoles that appear inside the body. The polarization and the deformation of the body lead to changes in the electric field and correspondingly the electric forces, whose changes in turn effect the polarization and the deformation. The process continues to take place until a stable state is established. When the body of interest and the electric field can be considered as a close system and the total energy is considered as stored inside the space occupied by the body, a stored energy function can be assumed to be a function of the electric field and the deformation at every point, which helps to construct a virtual work equation for the coupled problem. This virtual work equation can be discretized by using the finite element method and the system of nonlinear equations obtained from the discretization can be linearized and solved numerically. In the case the energy is stored not only inside the body of interest but also in the space surrounding it (normally air or, as we can in this context consider equivalently, vacuum), the simulation becomes more cumbersome. In this case, as it is well known in the numerical simulation of electric fields, a large finite element mesh can be used to simulate a sufficiently large part of the surrounding space or the boundary element method can be employed. When dealing with large deformation, the difficulty in using a large finite element mesh does not lie entirely in the amount of effort that needs to be spent on the computation of the electric field inside this mesh, but also in the effort to remesh the surrounding space after every few iterations. Besides, the construction of such finite element mesh is not user friendly since tests must be realized to determine a suitable shape and size for the part of the surrounding space that needs to be taken into account. In using the boundary element method, the electric field in vacuum can be simulated in a very efficient manner. However, this is only true for the case of small deformation and small displacement since no linearization of the boundary surface is required. More work needs to be done to find an efficient approach in using the boundary element method in the case of large deformation. In what follows, we present a virtual work equation for nonlinear electroelasticity, in which the effect of the surrounding space is taken into account with the help of the electric traction and electric charge at the boundary of the material body. These traction and charge will be computed with the help of some boundary integration equations. In order to solve the problem, the finite element method will be used to discretize the virtual work equation and the boundary element method will be used to discretize the boundary integral equations. We restrict ourself in the case of static electric loading with no body charge, no current and no magnetic field. No dynamic effect is considered here.

2. Virtual work and boundary integral equations for nonlinear electroelasticity

Let us consider a body made of elastic material. The undeformed configuration of the body is denoted by $\mathcal{B}_0$. In this configuration the position of each point is denoted by $\boldsymbol{X}$. Corresponding to $\mathcal{B}_0$, the deformed configuration is denoted by $\mathcal{B}_t$. The position of each point in the deformed configuration $\mathcal{B}_t$ is denoted by $\boldsymbol{x}$: $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X})$. The deformation of the body at every point inside the body is characterized by the deformation gradient $\boldsymbol{F}$. The virtual work equation of the problem can be written as

$$\delta \int_{\mathcal{B}_t} \hat{W}_{t\boldsymbol{F}} dv - \int_{\mathcal{B}_t} \boldsymbol{b}_t \cdot \delta\boldsymbol{\varphi} dv - \int_{\partial\mathcal{B}_t} \bar{\boldsymbol{t}}_t \cdot \delta\boldsymbol{\varphi} ds + \int_{\partial\mathcal{B}_t} \delta\psi \cdot \bar{q}_t ds = 0 \quad (1)$$

in reference to $\mathcal{B}_t$ and

$$\delta \int_{\mathcal{B}_0} \hat{W}_{0\boldsymbol{F}} dV - \int_{\mathcal{B}_0} \boldsymbol{b}_0 \cdot \delta\boldsymbol{\varphi} dV - \int_{\partial\mathcal{B}_0} \bar{\boldsymbol{t}}_0 \cdot \delta\boldsymbol{\varphi} dS + \int_{\partial\mathcal{B}_0} \delta\phi \cdot \bar{q}_0 dS = 0 \quad (2)$$

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in reference to $\mathcal{B}_0$. In the above formulation, $\hat{W}_{0\boldsymbol{F}}$ is some energy density function per unit volume of the undeformed configuration: $\hat{W}_{0\boldsymbol{F}} = \hat{W}_{0\boldsymbol{F}}(\boldsymbol{F}, \mathbb{E})$, $\hat{W}_{t\boldsymbol{F}} = J^{-1}\hat{W}_{0\boldsymbol{F}}$, $J = \det\boldsymbol{F}$, $\mathbb{E}$ is the electric field vector in $\mathcal{B}_0$, ψ and ϕ are the electric potentials, $\boldsymbol{b}_t$ and $\boldsymbol{b}_0$ are body forces, $\bar{\boldsymbol{t}}_t$ and $\bar{\boldsymbol{t}}_0$ are surface tractions, $\bar{q}_t$ and $\bar{q}_0$ are surface charges. The surface tractions and surface charges are computed with the help of the following boundary integral equations, which describe the electric field in the free space surrounding the body under consideration

$$\psi(\boldsymbol{\xi}) - \psi_\infty - \int_{\partial\mathcal{B}_t} [\psi(\boldsymbol{x}) - \psi(\boldsymbol{\xi})] \frac{\partial G(\boldsymbol{\xi}, \boldsymbol{x})}{\partial n} ds + \int_{\partial\mathcal{B}_t} \frac{\partial\psi(\boldsymbol{x})}{\partial n} G(\boldsymbol{\xi}, \boldsymbol{x}) ds = 0 \qquad (3)$$

and
$$\int_{\partial\mathcal{B}_t} q ds = 0 \qquad (4)$$

where ψ_∞ is the electric potential at infinity, $\boldsymbol{x}$ is called the field point, $\boldsymbol{\xi}$ is the source point, $\frac{\partial[\bullet]}{\partial n}$ is the directional derivative along the unit normal vector $\boldsymbol{n}$ of the boundary, $G(\boldsymbol{\xi}, \boldsymbol{x})$ is the so-called fundamental solution, $q = -\frac{\partial\psi(\boldsymbol{x})}{\partial n}$ and the total free charge of the system is assumed to be zero.

3. Numerical simulation

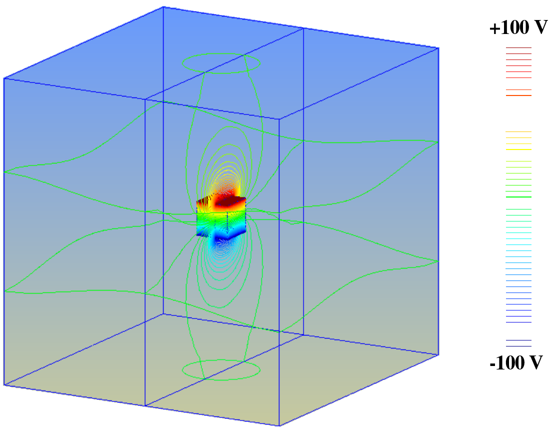

Figure 1: Electric potential.

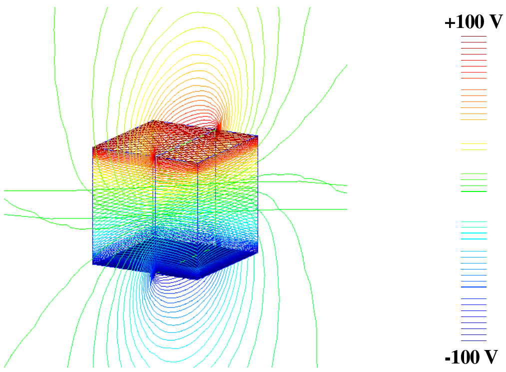

Figure 2: Electric potential near the boundary of the material body (zoom-in of Figure 1).

The above equations can be discretized and solved by using a coupled finite-boundary element procedure. In order to demonstrate the use of these equations, we consider here the simulation of a cube with dimensions $60\mu m \times 60\mu m \times 60\mu m$. The electric potential is given on the lower and upper surfaces of the cube as: $\psi_{lower} = -100\text{V}$ and $\psi_{upper} = +100\text{V}$, respectively. The material's behavior is given through the energy density function $\hat{W}_{0\boldsymbol{F}}$:

$$\hat{W}_{0\boldsymbol{F}} = \frac{\mu}{2}[\boldsymbol{C} : \boldsymbol{I} - 3] - \mu \ln J + \frac{\lambda}{2}[\ln J]^2 + $$
$$+\alpha\boldsymbol{I} : [\mathbb{E} \otimes \mathbb{E}] + \beta\boldsymbol{C} : [\mathbb{E} \otimes \mathbb{E}] - \frac{1}{2}\varepsilon_1 J\boldsymbol{C}^{-1} : [\mathbb{E} \otimes \mathbb{E}] \qquad (5)$$

where $\boldsymbol{C} = \boldsymbol{F}^t \cdot \boldsymbol{F}$, $\mu = 0.05\text{MPa}$, $\lambda = 0.06\text{MPa}$, $\alpha = 0.2\varepsilon_0$, $\beta = 2\varepsilon_0$, $\varepsilon_1 = 5\varepsilon_0$ and the electric permittivity of the outer space is: $\varepsilon_0 = 8.854 \times 10^{-12}\frac{\text{F}}{\text{m}}$. The simulation is carried out here using two approaches. In the first approach, both the cube and the outer space surrounding the cube are modeled by finite elements. Here 1000 solid 4-node hexagonal elements are used for the cube and 26000 solid 4 node hexagonal elements are used for the outer space. In the second approach (coupled BEM-FEM), the cube is also modeled by 1000 solid 4 node hexagonal elements but the outer space is modeled by 600 surface 4-node quadrangular boundary elements. In order to demonstrate the fact that a considerable part of energy is distributed in the outer space, the electric potential computed by using the first approach is plotted in Figure 1. For a better appreciation, the electric potential near the boundary of the cube is plotted in Figure 2. The maximum displacement computed by using the first approach is 0.343 μm and by using the second approach is 0.337 μm. In the second approach, if the outer space is not taken into account, the maximum displacement is 0.212 μm, which is about 30% less than the case when the outer space is taken into account. For higher levels of electric loading, this difference becomes even larger. Under $\psi_{lower} = -500\text{V}$ and $\psi_{upper} = +500\text{V}$, the simulation using the coupled BEM-FEM gives maximum displacement of 10.591 μm whereas the result without the contribution of the outer space is 6.209 μm.

4. Conclusion

The numerical modeling of nonlinear electroelasticity is clearly still a challenge today not only because of the complexity of the nonlinear coupled electro-mechanical characteristics but also because of the dimension of the problem. Evidently it should be noted that the influence of the outer space on the electric field and the deformation field inside a material body depends on the one hand the material properties of the body and on the other hand the geometry of the body as well as the way an electric field is applied on the body. However, in order to build a complete picture of what happens inside a nonlinear electroelastic body, what happens outside it deserves a due attention.

References

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