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A primal/dual approach for the accurate evaluation of the electromechanical coupling in MEMS

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ABSTRACT

This paper presents a primal/dual approach to solve the coupled electromechanical problem arising in the modelling of electrostatically actuated micro-electromechanical systems (MEMS). After a derivation of complementary energy functionals for both the mechanical and the electrical problems, an original coupling strategy using a displacement-based (primal) mechanical formulation and an electric vector potential-based (dual) electrostatic formulation are elaborated. A derivation of the electric force and the tangent stiffness matrix of the coupled problem is obtained, based on the virtual work principle. The new formulation has interesting properties with respect to error estimation and pull-in voltage calculation, which is highlighted on the finite element solution of a micro-resonator structure.

1. Introduction

Micro-electromechanical systems (MEMS) are microscopic devices often used as sensors and actuators. They are composed of mechanical elements such as beams or plates that move thanks to some actuation mean. The simplest and most efficient type of actuation is electrostatic actuation. Indeed, the electrostatic force appears at the surface of the mechanical structure and at the scale of microsystems surface forces are predominant compared to volume forces [1]. To accurately model the behaviour of MEMS, it is thus necessary to accurately compute the coupling between mechanical and electrostatic fields, and in particular it is crucial to accurately compute the electrostatic force.

Following the early work by Synge [2], it has been known for a long time that complementarity can provide bilateral bounds on energy in numerical approximations of electrostatic problems [3]. Bilateral bounds on other quantities of interest like capacitances can also be obtained [4], and although such bounds do not exist in general for forces (being derivatives of the energy), useful bounds can nevertheless be obtained on averages over some range of variation of the configuration parameter [5]. When using numerical techniques like the finite element method, such bounds can be used for accurate error estimation. Optimal mesh adaptation can then greatly reduce the overall computational cost, which can quickly become prohibitive in MEMS modelling due to the huge aspect ratios of the electromechanical structures.

In this paper we investigate one way to obtain complementary solutions for electrostatically actuated MEMS, based on the resolution of the electrostatic problem in terms of an electric vector potential. This vector potential formulation is the dual of the scalar potential approach commonly used in the literature [6,7].

The paper is structured as follows. After a derivation of complementary energy functionals for both the mechanical and the electrical problems in Section 2, we present in Section 3 an original coupling strategy using a displacement-based (primal) mechanical formulation and the electric vector potential-based (dual) electrostatic formulation. An analytic derivation of the electric force and the tangent stiffness of the coupled problem is obtained on a simple reference problem. A finite element formulation of the coupled problem is then derived in Section 4 using the virtual work principle and some interesting properties of this formulation with respect to error estimation and pull-in voltage calculation are highlighted on the finite element solution of a micro-resonator structure in Section 5.

2. Uncoupled mechanical and electrical problems

2.1. Basic equations

We start by considering the mechanical and electrical problems separately, defined, respectively, over domains Ω_m and Ω_e. The boundaries of Ω_m and Ω_e are $\partial\Omega_m = \Gamma_s \cup \Gamma_t$ and $\partial\Omega_e = \Gamma_e \cup \Gamma_d$, respectively (cf. Fig. 1). Denoting the mechanical strain tensor by **S**,

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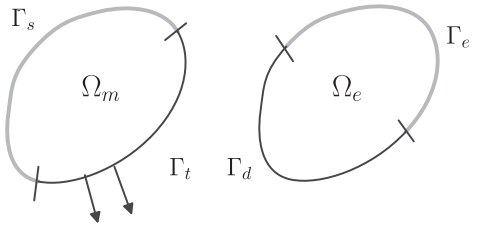

Fig. 1. Domains for the mechanical and the electrostatic problems.

the mechanical stress tensor by **T**, the electric field by **E** and the electric displacement by **D**, the following equations govern the behaviour of an electrostatically actuated microsystem.

- The *constitutive equations* are

$$\mathbf{T}=\mathbf{H}\mathbf{S} \quad \text{and} \quad \mathbf{D}=\boldsymbol{\varepsilon}\mathbf{E}, \tag{1}$$

  where **H** is Hooke's matrix and $\boldsymbol{\varepsilon}$ is the permittivity matrix.
- The *compatibility equations* are

$$\begin{cases} \mathbf{S}=\nabla_s\mathbf{u} & \text{in } \Omega_m \\ \mathbf{u}=\overline{\mathbf{u}} & \text{on } \Gamma_s \end{cases} \quad \text{and} \quad \begin{cases} \mathbf{E}=-\nabla\phi & \text{in } \Omega_e \\ \phi=\overline{\phi} & \text{on } \Gamma_e \end{cases}, \tag{2}$$

  where **u** and ϕ are, respectively, the mechanical displacement vector and the electric scalar potential (the overlined quantities denoting imposed values). The operator ∇ denotes the gradient operator and ∇_s is the matrix operator for mechanics, i.e., for three-dimensional problems in cartesian coordinates (x,y,z):

$$\nabla_s=\begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \end{pmatrix}.$$

  The term "compatibility" is used for electrostatics by analogy; the second system in (2) comes from Faraday's law for electrostatics, i.e., $\nabla\times\mathbf{E}=0$ in Ω_e.
- The *equilibrium equations* are

$$\begin{cases} \nabla_s\cdot\mathbf{T}=\overline{\mathbf{f}} & \text{in } \Omega_m \\ \mathbf{n}_s\cdot\mathbf{T}=\overline{\mathbf{t}} & \text{on } \Gamma_t \end{cases} \quad \text{and} \quad \begin{cases} \nabla\cdot\mathbf{D}=\overline{\rho} & \text{in } \Omega_e \\ \mathbf{n}\cdot\mathbf{D}=\overline{d} & \text{on } \Gamma_d \end{cases}, \tag{3}$$

  where $\overline{\mathbf{f}}$ and $\overline{\rho}$ are imposed force and charge densities, $\overline{\mathbf{t}}$ and $\overline{d}$ are imposed surface tensions and normal electric displacements, **n** denotes the normal to the boundary, and $\mathbf{n}_s$ is defined (in cartesian coordinates) as

$$\mathbf{n}_s=\begin{pmatrix} n_x & 0 & 0 \\ 0 & n_y & 0 \\ 0 & 0 & n_z \\ n_z & 0 & n_x \\ n_y & n_x & 0 \\ 0 & n_z & n_y \end{pmatrix}.$$

  Again, the term "equilibrium" is used for electrostatics by analogy; the equation for the electric displacement in (3) is Gauss's law.

2.2. Complementary energy functionals

In order to derive the energy functional for both the mechanical and the electrostatic problems in complementary ways, we start from the 3-field functional of Fraeiis de Veubeke [8,9], impose the constitutive equations strongly, then either impose the compatibility equations strongly (which leads to the primal formulation), or the equilibrium equation strongly (which leads to the dual formulation).

2.2.1. Mechanical energy functionals

For the mechanical problem, the 3-field functional reads

$$\mathcal{F}_m^{\mathrm{FHW}}(\mathbf{u},\mathbf{T},\mathbf{S})=\int_{\Omega_m}\{w_m(\mathbf{S})-\mathbf{T}\cdot(\mathbf{S}-\nabla_s\mathbf{u})-\overline{\mathbf{f}}\cdot\mathbf{u}\}\,d\Omega - \int_{\Gamma_s}(\mathbf{u}-\overline{\mathbf{u}})\cdot\mathbf{n}_s\cdot\mathbf{T}\,d\Gamma-\int_{\Gamma_t}\overline{\mathbf{t}}\cdot\mathbf{u}\,d\Gamma \tag{4}$$

with

$$w_m(\mathbf{S})=\tfrac{1}{2}\mathbf{S}\cdot\mathbf{H}\mathbf{S}.$$

Following the work of Hellinger–Reissner by imposing the constitutive relation (1) as essential conditions (i.e., strongly) in (4) we obtain the 2-field functional

$$\mathcal{F}_m^{\mathrm{HR}}(\mathbf{u},\mathbf{T})=\int_{\Omega_m}\{-\tilde{w}_m(\mathbf{T})+\mathbf{T}\cdot\nabla_s\mathbf{u}-\overline{\mathbf{f}}\cdot\mathbf{u}\}\,d\Omega - \int_{\Gamma_s}(\mathbf{u}-\overline{\mathbf{u}})\cdot\mathbf{n}_s\cdot\mathbf{T}\,d\Gamma-\int_{\Gamma_t}\overline{\mathbf{t}}\cdot\mathbf{u}\,d\Gamma \tag{5}$$

with

$$\tilde{w}_m(\mathbf{T})=\mathbf{T}\cdot\mathbf{S}-w_m(\mathbf{S})=\tfrac{1}{2}\mathbf{T}\cdot\mathbf{H}^{-1}\mathbf{T}.$$

To obtain the primal 1-field functional with "Kinematic Admissible" displacement, we impose the compatibility relation (2) strongly in (5), which leads to:

$$\mathcal{F}_m(\mathbf{u})=\underbrace{\int_{\Omega_m}w_m(\nabla_s\mathbf{u})\,d\Omega}_{W_m^{int}}-\underbrace{\left(\int_{\Omega_m}\overline{\mathbf{f}}\cdot\mathbf{u}\,d\Omega+\int_{\Gamma_t}\overline{\mathbf{t}}\cdot\mathbf{u}\,d\Gamma\right)}_{W_m^{ext}}. \tag{6}$$

To obtain the dual 1-field functional with a "Static Admissible" stress field we impose the equilibrium equation (3) strongly in (5), i.e.:

$$\tilde{\mathcal{F}}_m(\mathbf{T})=-\underbrace{\int_{\Omega_m}\tilde{w}_m(\mathbf{T})\,d\Omega}_{\tilde{W}_m^{int}}+\underbrace{\int_{\Gamma_s}\overline{\mathbf{u}}\cdot(\mathbf{n}_s\cdot\mathbf{T})\,d\Gamma}_{\tilde{W}_m^{ext}}. \tag{7}$$

Relations (6) and (7) provide the expressions for the primal and dual energy functionals $\mathcal{F}_m$ and $\tilde{\mathcal{F}}_m$ of the mechanical problem. Each functional can be separated into internal and external energy contributions, respectively, W_m^{int} and W_m^{ext} for the primal functional, and $\tilde{W}_m^{int}$ and $\tilde{W}_m^{ext}$ for the dual.

2.2.2. Electrostatic energy functionals

Following the same methodology as in the previous section, we can write the 3-field energy functional for the electrostatic problem in terms of the electric scalar potential, the electric displacement and the electric field:

$$\mathcal{F}_e^{\mathrm{FHW}}(\phi,\mathbf{D},\mathbf{E})=\int_{\Omega_e}\{w_e(\mathbf{E})-\mathbf{D}\cdot(\mathbf{E}+\nabla\phi)-\overline{\rho}\phi\}\,d\Omega - \int_{\Gamma_e}(\phi-\overline{\phi})\mathbf{n}\cdot\mathbf{D}\,d\Gamma-\int_{\Gamma_d}\overline{d}\phi\,d\Gamma \tag{8}$$

with

$$w_e(\mathbf{E})=\tfrac{1}{2}\mathbf{E}\cdot\boldsymbol{\varepsilon}\mathbf{E}.$$

By imposing the constitutive equation (1) strongly in (8) the 2-field electrostatic functional reads

$$\mathcal{F}_e^{\mathrm{HR}}(\phi,\mathbf{D})=\int_{\Omega_e}\{-\tilde{w}_e(\mathbf{D})-\mathbf{D}\cdot\nabla\phi-\overline{\rho}\phi\}\,d\Omega-\int_{\Gamma_e}(\phi-\overline{\phi})\mathbf{n}\cdot\mathbf{D}\,d\Gamma-\int_{\Gamma_d}\overline{q}\phi\,d\Gamma \tag{9}$$

with

$$\tilde{w}_e(\mathbf{D})=\mathbf{D}\cdot\mathbf{E}-w_e(\mathbf{E})=\tfrac{1}{2}\mathbf{D}\cdot\boldsymbol{\varepsilon}^{-1}\mathbf{D}.$$