CONVERGENCE AND DISCRETIZATION CHARACTERISTICS OF A STAGGERED ALGORITHM FOR MICROELECTROMECHANICAL SYSTEMS SIMULATION

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Abstract. *Microelectromechanical systems have their working principles based in the interaction between two or more physical fields. To design them multi-physics simulation tools are needed. For surface type electromechanical coupling, a staggered procedure can be used to treat the problem. The involved domains are solved separately and the coupling is taken into account by inserting electrostatic pressures coming from an electrical analysis into the structure, and updating the electrical mesh with the deformations originated from a mechanical analysis. The staggered procedure is iterative and the convergence criteria is based in the displacement variation between successive iterations. In this paper, a study about the convergence properties of the staggered algorithm for coupled problems implemented in our finite element code, MefLab, is done. A 0.5% variation in the displacement prooved to be sufficient to reach convergence in the simulation. A second analysis is related to the use of the Finite Element Method to model the electrical domain. A study about mesh dimension and proper boundary conditions to get good results saving computational time is carried out. Although not representing exactly the behavior of an unbounded field, the imposition of a null electric potential gradient on the external limit of the electrical mesh has shown to produce good results in the case of microelectromechanical systems simulation.*

Keywords*: microelectromechanical systems, numerical simulation, finite elements, convergence criteria, electrical mesh analysis*

1. Introduction

Applications related to Microsystems technology have grown up very quickly in the last years. Micro devices and sensors are present not only in scientific equipments and laboratories but also in the daily life of any human being. Mobiles phones, computers and compact disc players are common products where microsystems technology is present. Miniaturization also turns possible a series of applications that could not be developed with devices at macro scale. For example, research activities related to biomedical engineering leaded to the appearance of the minimally invasive surgery. This refers to medical procedures where micro instruments are used to execute interventions in the patient. The instruments are inserted in the human body through small incisions and all the needed actions are done by remote operation, with as little aggression as possible to the patient's organism. Advantages when compared to the traditional surgery are reduction of trauma, lower risk of inflammation, reduced postoperative complications and fast recovery (Dargahi *et al.*, 2000). Others examples of microsystems technology are scanners for laser printers and bar code readers (Ferreira and Moehlecke, 1999; Yan *et al.*, 2004), microelectromechanical relays and switchers (Grettilat *et al.*, 1999; McCarthy *et al.*, 2002), and micro grippers used for safe transport of small objects as electronic components or even cells in biological manipulations (Millet *et al.*, 2004).

Microsystems usually have their working principles based in the interaction between two or more physical domains. To design them multi-physics simulation tools are needed. Microsystems typical domains are mechanical, fluidic, chemical, thermal, electrical and electromagnetic. This work deals specifically with electromechanical micro devices, i.e., devices with electrostatic actuation and where coupling between an electrical field and a mechanical structure must be treated.

Coupling mechanisms can be divided into volume and surface type (Wachutka, 1999). In the first, the different fields occupy the same physical space. An example is the piezoelectricity, where the mechanical and electrical domains are overlapped. In the surface type coupling the interaction between the domains occurs through the interfaces. A dam under pressure caused by water contact is a problem of this class. The two domains, structural and fluidic, are separated and the interaction occurs through the common interface, which in this case lies on the wall. The electromechanical problems addressed in this work belong to the surface type coupling class. The electrical field and mechanical structure are detached and they influence each other only through their surfaces. Numerical methodologies to solve such problems can be elaborated by means of staggered algorithms.

In staggered algorithms the fields are treated as isolated entities that are separately analyzed, at each time step in the transient case, or for each equilibrium condition in a static analysis. The solution of one domain is transferred somehow as load for the other. The process is iterative and continues until convergence is reached. Depending on the involved domains different criteria can be used to indicate that results converged. In this work one possibility for electromechanical coupling is indicated and evaluated. It refers to the one adopted in our code MefLab for coupled field and optimization solution of engineering problems. The MefLab is a finite element software written in C++.

When numerically simulating an electrical field an extra difficulty arises because the domain is unbounded. Some are the options to treat this problem (Mesquita and Pavanello, 2005). We highlight three of the most popular. The first is the Finite Element Method (FEM) with its particular elements called infinite elements. When using this methodology the domain is truncated and at its limits a layer with these infinite elements is constructed. The second is the Dirichlet-to-Neumann (DtN) method (Givoli, 1992; Zavala, 1999), used together with the FEM. The domain is truncated but instead of a layer with infinite elements, an artificial boundary condition representing the decaying behavior of the field is imposed. The last method is the Boundary Element Method (BEM) (Kane, 1994), which treats the unbounded field in a more natural way, although not always advantageous. In this work, a simple boundary condition will be used, and the limits of this approach will be tested. It requires no special procedures in the implementation.

This paper is organized as follows. In Section 2, a succinct description of the electromechanical coupled problem, including its governing equations, is done. In Section 3, the convergence criteria of the algorithms is explained and results obtained from a microbeam simulation are shown. In Section 4, the methods for electrical field modeling already cited are briefly analyzed and the one implemented in MefLab is presented. Conclusions are given in Section 5.

2. Surface type electromechanical coupling

In this section the governing equations for the electrical and mechanical domains are presented. Then, the way the coupling between the fields occurs and the implemented staggered algorithm for its solution are explained.

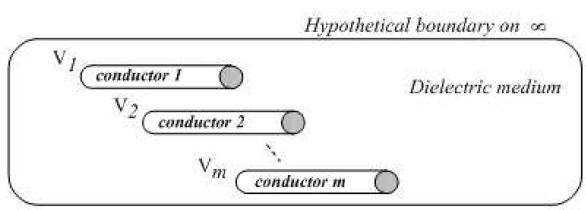


Figure 1. Lossless dielectric medium with conductors.

Consider a lossless dielectric medium with *m* embedded conductors, each one having a different electric potential, as shown in Fig. 1. The external boundary is artificial once the electrical field in unbounded. The distribution of electric potential in the dielectric medium is given by the Laplace equation:

$$\nabla^2 V = 0 \tag{1}$$

where V is the electric potential.

The electrostatic surface force (pressure) acting on a conductor is:

$$f_i = \frac{1}{2}\varepsilon_e \left(\frac{\partial V}{\partial n}\right)^2 n_i \tag{2}$$

where ε_e is the dielectric constant, $\partial V/\partial n$ is the electric potential derivative in the normal direction, n_i are the components of an unit normal vector, and the index i is 1, 2 or 3, indicating, respectively, the x, y or z direction.

For the structural counterpart, consider a body subjected to tractions, body forces and Dirichlet boundary conditions, as shown in Fig. 2.

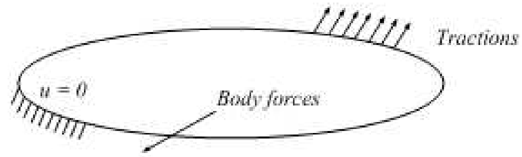


Figure 2. Deformable body under external loadings.

The mechanical behavior of the structural domain in Fig. 2 is described by the equilibrium equation:

$$\sigma_{ij,j} + \rho \ddot{u}_i = F_i \tag{3}$$

where σ_{ij} is the stress tensor, ρ is the specific mass, F_i is the body force and u_i is the displacement. The indexes i and j goes from 1 to 3.

The electromechanical coupling can be explained as follows. The electrostatic solution obtained through Eq. (1) gives the distribution of electric potential in the dielectric medium. Equation (2) allows the determination of the electrostatic pressures acting on the embedded conductors or structures. With these loads the structure deforms, defines new boundaries for the electrical field and the pressures have to be re-computed. The process goes on until equilibrium.

Applying the finite element method to the electrical and mechanical governing differential equations, the discrete equilibrium system representing the coupled field problem can be written as (v.d. Poel Filho, 2005):

$$\begin{bmatrix} [K_M] & 0 \\ 0 & [K_E(V,u)] \end{bmatrix} \begin{Bmatrix} \{u\} \\ \{V\} \end{Bmatrix} = \begin{Bmatrix} \{F_M\} + \{P_M\} + \{P_E(V(u))\} \\ \{Q_E\} \end{Bmatrix} \tag{4}$$

where $[K_M]$ is the mechanical stiffness, $[K_E]$ is the "electrical stiffness", $\{u\}$ is the nodal displacement, $\{V\}$ is the nodal electric potential, $\{F_M\}$ is the equivalent body force, $\{P_M\}$ is the equivalent mechanical traction, $\{P_E\}$ is the equivalent electrostatic traction, and $\{Q_E\}$ is the equivalent electric load vector caused by the volume charge density in the dielectric medium.

The first line in Eq. (4) refers to the mechanical domain while the second refers to the electrical. The coupling is evidenced by the dependence of $[K_E]$ not only on the electric potential V but also on the mechanical displacement u, and by the occurrence of the term $\{P_E\}$ on the mechanical equation. In microsystems, usually $\{F_M\}$ and $\{P_M\}$ are null. For electrostatic problems, i.e., the case addressed here, the volume charge density is zero and the vector $\{Q_E\}$ is also null.

The vector $\{Q_E\}$ being null may lead to the false idea of solving the system $[K_E]\{V\}=\{0\}$. As there are imposed Dirichlet boundary conditions, i.e., voltages applied in part of the nodes, some values in $\{V\}$ are known. When arranging the final linear system, these values are transferred to the right side of the equation and the nodal solution can be straightforwardly found.

For more insight on the governing equations of both domains and details about the electromechanical coupling problem itself, see v.d. Poel Filho and Pavanello (2003), v.d. Poel Filho (2005) and v.d. Poel Filho *et al.*(2005).

3. Convergence criteria for surface type electromechanical coupling

The algorithm for simulating the electromechanical coupled problem is iterative. The pressures coming from the electrical analysis are inserted in the mechanical model and this simulation is carried on. The computed displacements are then considered in the electric model, i.e., the electrical field geometry is updated (the mesh is modified), and another electrical simulation takes place. New pressures are computed and again transferred to the mechanical model. The program must end at a point and to accomplish this, a stop condition has to be chosen. When this stop condition is reached the simulation is considered to be converged. Hereafter it will be referred as the convergence criteria of the algorithm.

The better way to write the convergence criteria, naturally, is by using the physical parameters involved in the solution algorithm (and avoiding extra computations). In MefLab, the electrical analysis gives the electric potential distribution and the electrostatic pressures, and the mechanical analysis gives the structure displacement. Then, immediate possibilities for variables used in evaluating the convergence are the electrostatic energy computed from the potential distribution, the pressures and the displacements.

The adopted stop condition is based on the displacement variation between an iteration and the subsequent one. When this variation is lesser than a pre-defined value the program ends. The preference for this parameter instead of the electric ones is explained as follows. Firstly, the use of the electrostatic energy would need an extra computation to be done by the code. At the same time, once the mechanical displacement has stopped changing, the electrical mesh geometry does not suffer further modifications and the electric potential distribution is not affected anymore, what leads to convergence of the electrostatic energy value. This can be seen through the equation for the energy in an electrical field with embedded conductors (Silvester and Ferrari, 1990):

$$W = \frac{1}{2}\varepsilon_e \int_{\Omega_{elec}} \mathbf{E}^2 d\Omega \tag{5}$$

where **E** is the electrical field and the integration domain extends over all regions where there is an electrical field. The following relation relates the electrical field to the electric potential:

$$\mathbf{E} = -\nabla V \tag{6}$$

According to the electrical equation in Eq. (4), $[K_E]\{V\}=\{0\}$, with Dirichlet conditions applied always to the same nodes, the potential distribution is only changed when modifications take place in the electrical mesh geometry. Guaranteeing a converged displacement, the gradient of the potential stops varying and consequently, by Eq. (6), the electrical field **E** too. Then, analyzing Eq. (5), the conclusion is that the electrostatic energy has also to converge.

In our implementation, the program stops when the displacement variation Δu between two iterations varies less than *0.5%*. It has been chosen because tests indicated almost no alterations in the results adopting $\Delta u<0.5\%$. As example, consider the microbeam in Fig. 3. The geometric parameters and material properties are: $L=150\mu m$, $t=2\mu m$, $g=6\mu m$, $E=150GPa$ (modulus of elasticity) and $\varepsilon_e=8.854x10^{-6}pF/\mu m$. Figure 4 shows a graphic plotting the microbeam tip displacement against the Δu used in the simulation, with electric potentials of 60V and 80V. The results remain practically the same reducing Δu from *0.5%* to values close to zero. The difference in the structural displacement using $\Delta u=0.5\%$ and $\Delta u=1x10^{-6}\%$ is insignificant and does not exceed *0.03%*. Also, no oscillations around the equilibrium position were evidenced after reaching the stop condition. Convergence was achieved after four iterations. The deformed beam (15 times amplified) in the equilibrium position is drawn in Fig. 5.

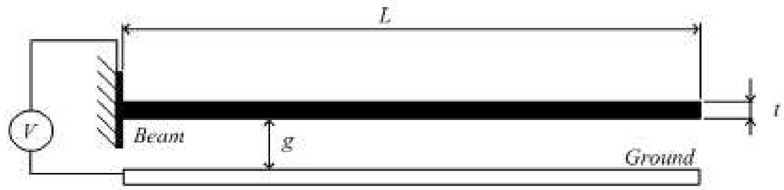


Figure 3. Microbeam under electrostatic load.

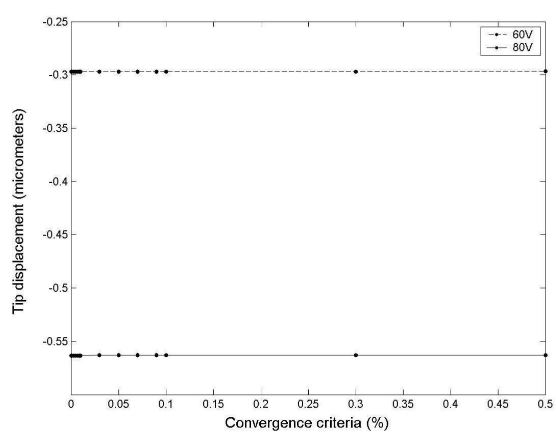


Figure 4. Microbeam tip displacement versus convergence criteria.

4. Electrical field analysis

The electrical field simulation needs special care by the fact that the domain is unbounded. A few methodologies are used to treat this particular characteristic. Three are emphasized in this section and our solution is exposed.

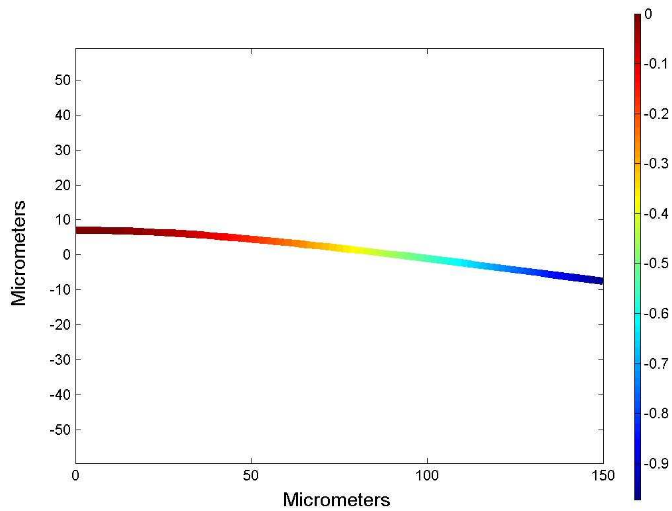


Figure 5. Deformed microbeam in equilibrium position. *V=100V*.

The first possibility is the use of the FEM with its special elements called infinite elements (Cook, 1989). These kinds of elements have simple implementation and are often found in commercial codes (e.g., ANSYS®). Their formulation contains shape functions that attempt to represent the far field behavior of the solution. In the numerical model of the unbounded field the domain is truncated and meshed with "normal" finite elements while in the limits a layer of infinite elements is constructed. This method normally permits satisfactory results even though according to Givoli (1992), the numerical solution of such elements still contains errors due to the fact that the infinite domain is not accounted for exactly. To guarantee accurate results the infinite elements would have to be inserted highly deep in the far field (Givoli, 1992), which means the truncated domain should be large and consequently filled with a large mesh.

A second way to deal with the unbounded characteristic of the electrical field is the Dirichlet-to-Neumann (DtN) method (Givoli, 1992; Zavala, 1999). The domain is truncated and then an artificial boundary condition is imposed to the forced limits. The name of the method comes from the fact that it maps a Dirichlet data that extends itself to the far field into a Neumann data in the perimeter appeared with the truncation. The computed solution is exact. The mapping procedure is based in an analytical solution of the residual domain, i.e., the removed part where no mesh is constructed. It is not always easy to realize this mapping but once is has been done for one differential equation, it will be the same whenever this equation is to be solved. The DtN is usually applied together with the FEM.

The third alternative remarked here is the BEM (Kane, 1994). With the BEM the decaying behavior of the field is accounted for exactly. Another advantage of the BEM is that it does not require the whole domain to be meshed but only the boundary lying in the surfaces where the electric potentials are applied. Although modeling the unbounded field more naturally than FEM, the BEM has also some drawbacks. Firstly, the final linear system of algebraic equations is full. If results are needed in a few locations the method is efficient but when many degrees of freedom (*dofs*) are involved it can become computationally very expensive. Also, when modeling structures with parts characterized by high aspect ratios, often happening in microsystems, and with irregularities on the geometry, the BEM might not be effective.

The three solutions above are all able to model accurately the electrical field domain. The use of infinite elements, BEM and DtN method, however, requires extra formulations to be implemented

In a far distance from the charge sources, strictly saying, at infinite, the electrical field is null, i.e., $\mathbf{E}=0$. According to Eq. (6), if a condition $\partial V/\partial n=0$ is imposed to a surface, physically this point has also $\mathbf{E}=0$. The idea is to truncate the electrical domain, construct a relatively small mesh with finite elements, and impose the boundary condition $\partial V/\partial n=0$ on the perimeter of the model/mesh. Naturally this is an approximation because the situation where $\mathbf{E}=0$ happens only at infinite and not close to the charge sources. The error is also minimized in the case of micromechanical systems because normally there are two or more conductors (each with a different voltage) very close one to the other and the electrical field intensity is much higher in these in-between areas than anywhere else. As the pressures are proportional to the electrical field intensity and inversely proportional to the square distance separating the conductors, the attractive behavior of the conductors is dominant in the system. The electrical mesh needs to be larger than the existent gaps but at the same time it does not have to go far in the ambient region (from the structures limits to infinite) of the device.

The imposition of $\partial V/\partial n=0$ to a surface is straightforward in the FEM. The weak form of Eq. (1) is:

$$-\int_{\Omega_{elec}}\left(\frac{\partial\varphi}{\partial x}\frac{\partial V}{\partial x}+\frac{\partial\varphi}{\partial y}\frac{\partial V}{\partial y}+\frac{\partial\varphi}{\partial z}\frac{\partial V}{\partial z}\right)d\Omega+\int_{\Gamma_{elec}}\varphi\frac{\partial V}{\partial n}d\Gamma=0 \tag{7}$$

where φ_i are weight functions, Ω_{elec} is the electrical domain and Γ_{elec} is the boundary. In this configuration $\partial V/\partial n=0$ applied on the contour is a natural boundary condition.

The microbeam in Fig. 3 is again used as example. Four meshes were analyzed. The geometrical parameters are shown in Fig. 6 and Tab. 1. In Fig. 6, the gray color indicates the area filled with the electrical mesh.

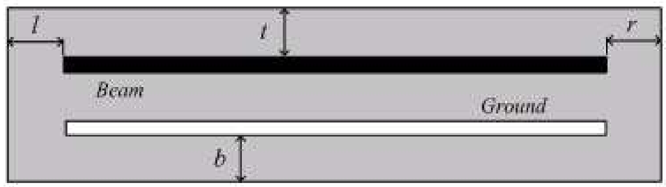


Figure 6. Geometrical parameters of the electrical mesh

Table 1. Electrical mesh configurations

Parameter	*Mesh 1*	*Mesh 2*	*Mesh 3*	*Mesh 4*
t	20	10	40	80
b	8	4	16	32
l=r	14	7	28	56

The color maps for the smaller and larger meshes are shown in Fig. 7 and Fig. 8, respectively. In both cases the electrical field does not change abruptly and is not perturbed with the boundary created by the domain truncation. The curvatures of the contours are soft and not interrupted. Consequently, the electrical field behavior is little influenced by the imposition of the natural boundary condition $\partial V/\partial n=0$ on the external contour.

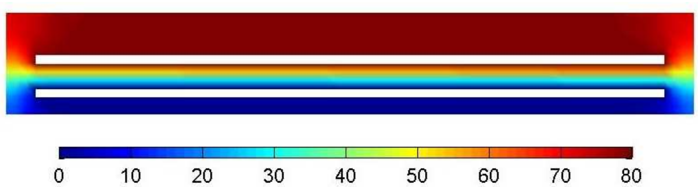


Figure 7. Electrical field distribution with *Mesh 2*. *V=80V*.

The normalized results for the four meshes can be viewed in Fig. 9a. There is a convergence to the same value and the displacements obtained with all the meshes are practically the same. For comparison, results with a different condition in the outer boundary, *V=0*, are plotted in Fig. 9b. In this case, the mesh size has a significant influence and good results come only with *Mesh 4*, the biggest one.

As expected, the imposition of $\partial V/\partial n=0$ on the electrical domain external limit, although it is an approximation, reproduces satisfactorily the hypothesis of large medium. The use of this boundary condition together with small size meshes has proved to be effective for electromechanical microsystems simulation. The size of the mesh is fundamental for saving time in the analysis. *Mesh 1* and *Mesh 2* needed less than 6% of the computational time spent with *Mesh 4*. The number of iterations executed varied from two to four.

An interesting application where the electromechanical analysis scheme pointed here could be used is the static simulation of micromechanical relays. Gretillat *et al.* (1999) presented the device shown in Fig. 10a. The device works by applying a potential difference between the driving electrode and the clamped-clamped beam supporting the contact bar. The electrical connection is established with the beam bending. Bi-dimensional analysis using the meshes with the geometry shown in Fig. 10b could be run to determine the behavior of the device. Other examples of micro devices where electromechanical static analysis is needed are diaphragm based pumps (Teymoori and Abbaspour-Sani, 2002) and micro grippers (Millet *et al.*, 2004). The possibility of using limited size meshes is also useful when transient analysis is required during the design phase of a micro device. Shi *et al.* (1996) and v.d. Poel Filho *et al*. (2005) have applied the implicit direct Newmark method for such simulations. In this method, the displacement solution of the system for a pre-defined period of time is obtained by solving its dynamic equation at several time-steps. At each time-step the electrical mesh must be updated and large meshes could turn the transient analysis impossible to be done. Resonant sensors constitute a typical class where transient analysis is necessary. Samples are dynamic operated pressure sensors (Burns *et al.*, 1995) and accelerometers (Yazdi and Najfi, 2000).

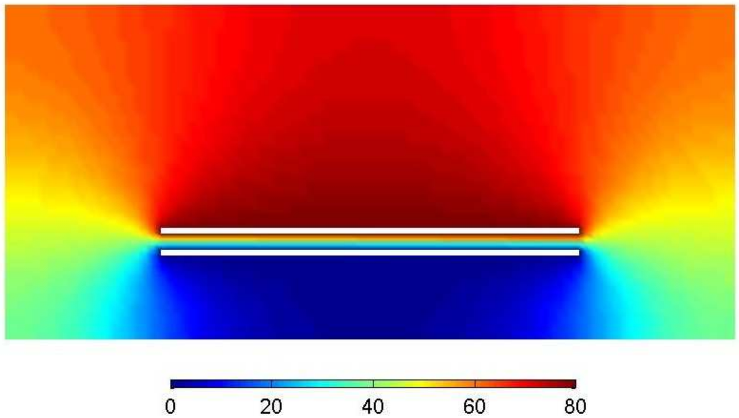
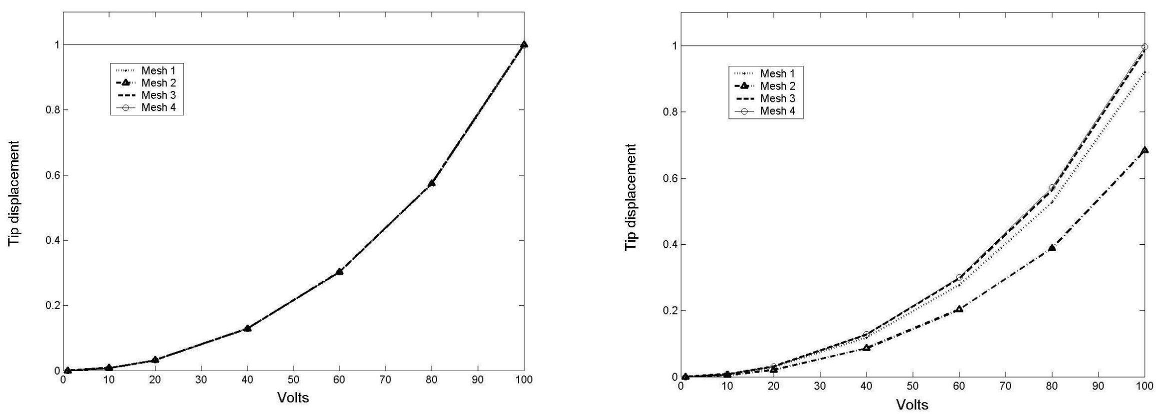
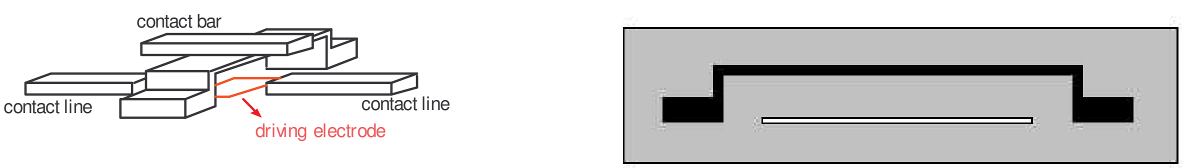


Figure 8. Electrical field distribution with *Mesh 4*. *V=80V*.



(a) (b)

Figure 9. Normalized microbeam tip displacement with (a) $\partial V/\partial n=0$ and (b) $V=0$ in the outer boundary.



(a) (b)

Figure 10. (a) Micromechanical relay and (b) Geometry of 2-D electrical (gray collor) and mechanical (black) meshes.

5. Conclusions

This paper has discussed possible parameters for writing convergence criteria for electromechanical coupled field problems algorithms. The one used in our code, the structural displacement, and the reasons for its choice, were presented. A displacement variation of *0.5%* between two successive iterations proved to be enough to consider the simulation to be converged. Tests indicated that results have insignificant variations when adopting values lesser than *0.5%*. Methodologies to model the electrical field considering the characteristic of being an unbounded domain were briefly explained. These were the use of infinite elements, the DtN method and the BEM. In this work, the application of a simple boundary condition was proposed and evaluated. The idea is to truncate the electrical domain and impose the natural boundary condition $\partial V/\partial n=0$ on the perimeter. This is equivalent to have a null electrical field on the external forced contour. Although the null electrical field takes place rigorously only at infinite, the considered approximation proved to be effective. It does not substitute the other cited methods to treat unbounded problems but, for surface type electromechanical coupling simulation, little influence was verified in the results. The strategy is addressed for systems where the conductors with different electrical potential are close to each other (typically the case of microsystems). No extra procedures have to be done in the implementation and small electrical meshes can be used. Small size meshes allow a great reduction of computational time when modeling the coupled field system with FEM.

6. Acknowledgements

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