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APPLICATION OF THE FINITE ELEMENT METHOD TO MODEL THE PROBLEM OF ELECTROMECHANICAL COUPLING IN MICROSYSTEMS

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Abstract. *For understanding and simulating the behavior of microsystems it is necessary to analize several physical domains. Analytical solutions for coupled-field problems are hard to be obtained and numerical modeling tools are needed. The coupling between domains can be caused by imposed boundary conditions or when there is a superposition of different domains. These coupling mechanisms are identified as coupling by surface and by volume, respectively. In this work, attention is given to electromechanical devices where the existing coupling is by surface and occurs by the interaction between a structure and the electrostatic forces generated on it by the existence of an electric field. The solution methodology involves a sequential strategy where the two domains are modeled separately and the interaction is done by inserting the results of one domain analysis into the other. The process is executed iteratively until convergence. The Finite Element Method is used for the numerical modeling and its implementation is done in an object oriented code written in C++. The equations governing the mechanical and electrical domains are presented and the coupling mechanism is explained. The case study of a silicon microbeam subjected to an electric potential difference is done. Results for static analysis are shown, and mesh managing strategies are tested and discussed.*

Keywords*. Coupled-field problems, microsystems, finite element method.*

1. Introduction

The study of microsystems is related to the engineering area known as microengineering. Microengineering refers to the development of technologies to design and fabricate structures and devices with dimensions in the order of micrometers. One of its main goals is to integrate microelectronics together with microstructures to produce completely integrated systems. Because of the possibility of batch manufacturing and reduction of mass and size, the miniaturization of components and devices enables a very low cost of production. The number of applications involving microsystems is already large and tends to increase in the following years. Current examples are: components for rigid disks drives for data storage (Temesvary, 1995), inkjet print heads (Lee et all, 1999), micro pumps (Saif et all, 1999), sensors for endoscopes and medical equipment used in minimally invasive surgery (Dargahi et all, 2000 and Peirs et all, 2001), drug delivery systems (Cao et all, 2001), microrockets (Rossi et all, 2002), and sensors and actuators in general (Bhailís et all, 2000 and Johnson and Warne, 1995).

The design of microsystems is based on multi-physics simulation, i.e., it is necessary to deal with several physical domains. Usual domains appearing are electrical, mechanical, fluidic and thermal. The focus of this work is the analysis and simulation of microsystems with electrostatic actuation. Although the electrostatic actuation is not generally used for traditional applications (e.g. motors) (Trimmer,1988), at the micrometer level it is advantageously employed. In microscale the electrostatic surface forces are dominant (high surface to volume ratio) (Fujita and Omodaka, 1987) and large enough to move or deform parts of a system. In addition, the actuation is simply driven by voltage application. For the design of microsystems with electrostatic actuation it is necessary to analyze and simulate two domains: the mechanical (structural) and the electrical. Analytical solutions for coupled-field problems are hard to be obtained and then numerical modeling tools are needed. Common numerical methods used for simulating the behavior of microelectromechanical systems are the Finite Element Method (FEM) (Malkus, 1989 and Silvester, 1990) and the Boundary Element Method (BEM) (Kane, 1994).

The coupling between domains can be caused by imposed boundary conditions or when there is a superposition of different domains (Zienkiewicz, 1984). These coupling mechanisms are identified as coupling *by surface* and coupling *by volume*, respectively. In this work attention is given to electromechanical devices where the existing coupling is by surface and occurs by the interaction between a structure and the electrostatic pressures generated on it by the existence of an electric field. Such coupling can be found in electromechanical filters, resonant sensors, oscillators and in general microsensors and microactuators. The solution methodology implemented involves a sequential strategy where the two domains are modeled separately and the interaction between them is done by inserting the results of one domain analysis into the other until convergence is reached. The electromechanical analysis is difficult because the electrostatic pressures are non-uniform and change as the structure deforms.

This work concerns to our first efforts towards the construction of a FEM-based numerical tool to solve and optimize the coupled-field problem encountered in microelectromechanical systems. The numerical method together with the coupled-field solution algorithm is being programmed in our own software Meflab++. The Meflab++ is an oriented object code written in C++ where numerical modeling methods and strategies for solving engineering problems are inserted.

This paper is organized as follows. In Section 2, the mathematical formulation for the electromechanical coupled problem is presented. The mathematical models are shown separately for each domain and the way the coupling happens is explained. In Section 3, discussions about different approaches to treat coupled-field problems and the use of the FEM or BEM as numerical modeling tools for microsystems are done. The solution algorithm is also described. In section 4, the case study of a microbeam with an applied voltage is done and details of the implemented algorithm are provided. Conclusions are given in Section 5.

2. Mathematical formulation

The governing equations for the mechanical and electrical domains are presented in this section. The coupling mechanism between the domains is also explained.

2.1. Electric domain

Consider a number m of conductors within a lossless dielectric medium, Fig. (1). The electrostatic potential in the exterior region satisfies the Laplace Equation (Eq. (2.1.1)). On the conductors an electric potential ϕ_k is applied. In Fig. (1), Γ_1, Γ_2, ..., Γ_m are the boundaries of the conductors and Γ_∞ is a far-field boundary or reference plane. Ω_{el} is the electrical domain.

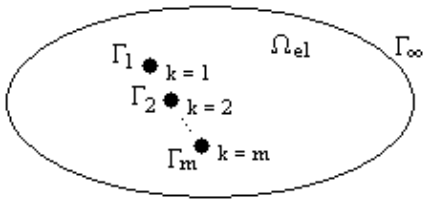


Figure 1. Electrostatic system with conductors embedded in a uniform lossless dielectric medium.

The electrostatic problem for the system in Fig. (1) can be written as:

$$\nabla^2\phi = 0 \quad \text{in } \Omega_{el} \tag{2.1.1}$$

$$\phi = \phi_k \quad \text{on } \Gamma_1, \Gamma_2, ..., \Gamma_m \tag{2.1.2}$$

$$\left.\begin{array}{l}\phi = \phi_\infty \\ \text{or} \\ \phi_{,n}\end{array}\right\} \quad \text{on } \Gamma_\infty \tag{2.1.3}$$

where n represents the outward normal direction.

After the application of a voltage, electric charges are induced on the surface of each conductor. The charge density γ on a conductor surface satisfies (Griffiths, 1998)

$$\gamma_k = -\varepsilon_e \phi_{,n} \tag{2.1.4}$$

where ε_e is the dielectric constant of the medium.

The potential in the normal direction is

$$\phi_{,n} = \phi_{,i}\, n_i \tag{2.1.5}$$

where n_i are the components of the unit normal vector. The index i goes from 1 to 3 and represents the x, y and z directions.

Once the charge density is know, it is possible to determinate the electrostatic surface force (pressure) acting on a conductor through the equation

$$f_i = -\frac{1}{2}\frac{\gamma^2}{\varepsilon_e} n_i \tag{2.1.6}$$

2.2. Mechanical domain

Consider a mechanical (structural) domain Ω_{mec} with boundaries Γ_{mec1} and Γ_{mec2}. There are body forces, Dirichlet boundary conditions in Γ_{mec1} and traction in Γ_{mec2}. This problem is described by the following equations (Gould, 1983):

$$\sigma_{ij,j} - \rho_s \ddot{u}_i = F_i \qquad \text{in } \Omega_{mec} \qquad (2.2.1)$$

$$u = u_o \qquad \text{on } \Gamma_{mec1} \qquad (2.2.2)$$

$$\sigma_{ij} n_j = f_i \qquad \text{on } \Gamma_{mec2} \qquad (2.2.3)$$

where σ_{ij} is the stress tensor, ρ_s the specific mass, F_i the body forces, f_i the traction vector acting on the surface and u_i is the displacement. The indexes i and j are 1,2 and 3.

In a static case, Eq. (2.2.1) becomes

$$\sigma_{ij,j} = F_i \qquad \text{in } \Omega_{mec} \qquad (2.2.4)$$

To solve the elastic problem two other sets of equations are needed. Relating displacements and deformations (Gould, 1983),

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \qquad (2.2.5)$$

where ε_{ij} is the deformation tensor. The constitutive law for a linear elastic solid is (Gould, 1983)

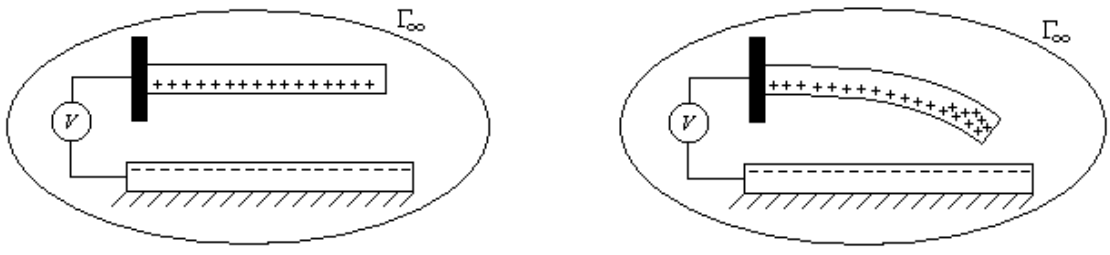
$$\varepsilon_{ij} = \frac{1}{E}[(1+\nu)\sigma_{ij} - \nu\delta_{ij}\sigma_{kk})] \qquad (2.2.6)$$

where ν is the coefficient of Poisson and E is the elasticity or Young modulus.

Equations (2.2.1) to (2.2.6), plus the compatibility relations, form the basis of the Theory of Elasticity.

2.3. Coupling between the electrical and mechanical domain

The coupling mechanism involving the electrical and mechanical domains can be better understood looking at the system in Fig. (2). When a voltage is applied between the cantilever beam and ground, electrostatic charges are induced on the surfaces of the conductors, Fig. (2a). These electrostatic charges are responsible for the appearance of electrostatic pressures acting in a direction normal (outward) to the surface. The electrostatic pressures deform the beam and then a redistribution of the charges, Fig. (2b), takes place. The charge redistribution results in a change in the electrostatic pressures and consequently new deformations occur. The process goes on until the equilibrium state is reached. The equilibrium happens when the electrostatic forces are balanced by the elastic restoring forces of the structure. The dependence of the electrostatic pressures on the charge distribution can be seen in the Eq. (2.1.6).



(a) (b)

Figure 2. Electromechanical system: (a) applied voltage causing charge distribution and (b) deformed structure with redistributed charges.

3. Numerical modeling and solution algorithm

The need for numerical modeling tools comes from the fact that analytical solutions for coupled-field problems are difficult to be obtained. The most used numerical methods for microsystem simulation are the FEM and BEM. Usually, the mechanical domain is modeled by the FEM because many structural members in microsystems have long aspect ratios that make the BEM inefficient (Shi et all, 1995). For the exterior problem, i.e., the electrical domain, both the FEM and BEM can be used, existing advantages and disadvantages for each one. The application of the FEM requires the construction of a mesh for the whole exterior domain. However, in the electromechanical simulation the electrical domain is constantly changed and it is necessary to modify the mesh for each solution step. This modification makes the simulation computationally expensive and it is a drawback of the FEM. The BEM avoids constructing a mesh for the

domain and consequently reduces the computational effort (Senturia et all, 1997). The disadvantage of the BEM are the dense matrices generated by the method (Funk et all, 1997 and Senturia et all, 1997). Efficiency is only achieved when sparsification algorithms are inserted within the implementation (Senturia et all, 1997 and Cai et all, 1993). The FEM, in turn, generates sparsely populated matrices that are easy to be solved.

In this work the FEM is used for both the electrical and mechanical domain. The chosen formulation is the weighted residual with the Galerkin Method and isoparametric elements. Electrostatic and mechanical quadrilaterals with four nodes and triangles with three nodes are implemented. The degree of freedom (dof) on the nodes of the electrostatic elements is the electric potential. The mechanical nodes have displacements in the x and y directions. Body and surface forces and Dirichlet boundary conditions are supported. Through post-processing of the electrical domain, flux values and electrostatic pressures can be computed. The electrostatic pressures are fundamental because they serve as input for the simulation of the structural behavior. The post-processing of the mechanical simulation allows attainment of strain and stress results.

In this context, the discrete finite element equilibrium equations for the coupled problem could be written as follows:

$$[K(u)]\{u\} = \{F_{str}\} + \{F_{elec}(\phi_n)\} \tag{3.1}$$

$$[H(\phi, u)]\{\phi\} = \{F\} \tag{3.2}$$

where $[K(u)]$ is the structural stiffness matrix, $\{u\}$ is the nodal displacement vector, $\{F_{str}\}$ is the mechanical load vector, $\{F_{elec}(\phi,_n)\}$ is the electrostatic load vector, $[H(\phi,u)]$ is the electrical stiffness matrix, $\{\phi\}$ is the nodal electric potential vector, and $\{F\}$ is the electrical load vector. Equation (3.1) is for the mechanical problem and Eq. (3.2) for the electrical. The terms $\{F_{elec}(\phi,_n)\}$ and $[H(\phi,u)]$ show their mutual dependence.

Once the domains are being separately modeled by a numerical method, in this case the FEM, a strategy to deal with the coupling between them must be chosen. Several authors (Korvink et all, 1994, Schroth et all, 1996, Gerlach and Klein, 1998, König et all, 1999, Wachutka, 1999 and Felippa et all, 2001) indicate approaches to treat coupled-field problems. In a general sense, three are the methodologies (Felippa et all, 2001): *field elimination*, *monolithic treatment* (*simultaneous or direct)* and *partitioned treatment* (*sequential*). In the field elimination one or more components are eliminated by techniques such as integral transforms and the remaining components treated by a simultaneous time-integration scheme. This approach is restricted to special linear problems that permit efficient decoupling and often it leads to higher order differential systems in time, or to temporal convolutions (Felippa et all, 2001). These problems can be source of numerical difficulties and then the monolithic and partitioned treatments are more frequently used. In the simultaneous treatment the whole problem is treated as a monolithic entity and all the components are analyzed simultaneously. In the partitioned treatment, the domain models are treated as isolated entities that are separately analyzed for each time step in the transient case or for each equilibrium condition in the static case. The problem is solved iteratively and the coupling is done by taking the results from one analysis and inserting them as loads in the other(s).

For problems with coupling by surface, the most common methodology is the partitioned treatment. This approach is often used with commercially available tools specific for each domain. In Senturia et all (1992) and Gilbert et all (1995), the ABAQUS finite element code is used for the mechanical analysis and other software based on boundary elements, FASTCAP, is used for the electrical analysis. Through an iterative algorithm, the solution of one program is applied in the other, and vice-versa, until the convergence of the results. In a similar way, Schroth et all (1996) employed ANSYS for the analysis of the mechanical domain and Pspice for the simulation of the electrical domain. The Pspice program works through macro models. Funk et all (1997) presented a numerical tool for static analysis of microsystems of possible different actuating mechanisms (thermomechanics, surface electrostatic forces and piezoelectric effects). Their solution algorithm employs a sequential strategy and applies the FEM for all the involved domains. Iterations schemes like Gauss-Seidel, Newton-Raphson and relaxation were used. Hybrid methods with both FEM and BEM are often used (Shi et all, 1995, Shi et all, 1996 and Aluru and White, 1997).

The main advantage of the sequential treatment is the modularity. Additional coupling effects can always be added to the computational code without having to change significantly what is already working.

Our implementation uses no commercial tools and is done in our own software Meflab++. The Meflab++ is a simulation environment where numerical methods and strategies for solving engineering problems are inserted. The software is based on object oriented programming and is written in C++. The software has a general central core from which the specific tasks are developed.

Figure (3) shows a flow chart with the sequential strategy implemented in the Meflab++. The analysis is static. The simulation starts with the analysis of the electrical domain. The nodal electric potentials are obtained and with these results a post-processing is realized. The electrostatic pressures are computed. These pressures are input loads for the mechanical analysis. As a pre-processing step in the structural simulation, the nodal load vector is computed from the electrostatic pressures on the conductor's surfaces. The mechanical problem is then solved. The mesh in the electrical domain, if altered in a previous iteration, is reset to its original configuration. With the mechanical displacements the electrical mesh is morphed. Convergence check is performed and when the displacement variations are below 0,5% the program stops.

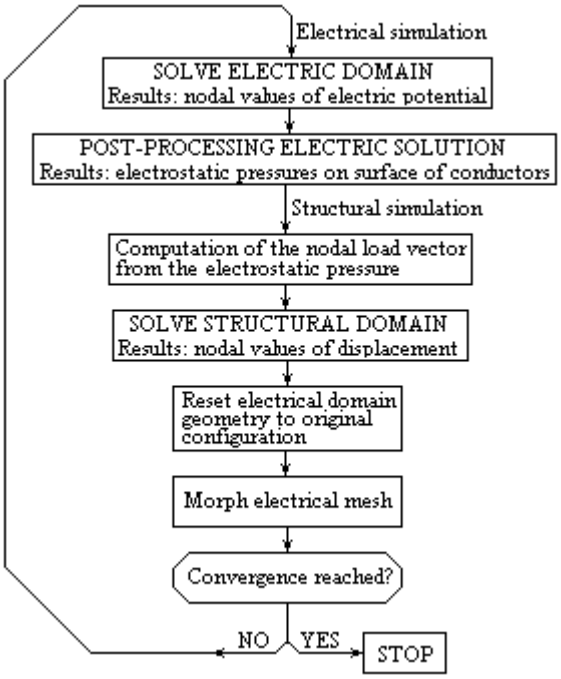


Figure 3. Algorithm for the sequential strategy in Meflab++

Equation (2.1.6) shows the dependence of the electrostatic surface forces on the charge density. Each time the structure deforms there is a redistribution of charges on the conductor's surfaces and consequently an alteration of the electrostatic pressures. These new pressures deform again the structure and naturally other distribution of charges is obtained. This continued action in the two ways couples the two domains. The fact is that mathematically the charge distribution is only altered when the Laplace Equation is solved for each configuration of the exterior domain considering the deformed position of the structure. By this reason, for each solution step it is necessary to modify the electrical mesh. There are two mechanisms for mesh updating: morphing and remeshing. With the morphing there is no reconstruction of the mesh but only an update in the nodes position by summing the displacements of each iteration to the nodes coordinates. The mesh is not reconstructed but just deformed. The remeshing is an action where the whole mesh is removed and another one is built. The advantage of the morphing is that it requires less computational effort than the remeshing. However, when displacements start to get too large this technique becomes ineffective and the remeshing is recommended. The remeshing is computationally expensive because it creates new nodes and elements for each step solution of the coupled-field problem.

4. Case study

In this section the case study of a silicon microbeam with an applied voltage is done. Details of the solution algorithm implemented within the Meflab++ are discussed together with the simulation results.

4.1. Problem description

Figure (4) shows the simulated silicon microbeam. The potential difference between the beam and the ground generates an electric field that induces charges on the surface of the beam. The charges are responsible for the appearance of electrostatic pressures and these make the structure to deform. The parameters in Fig. (4) used in our simulations have the following values: $\boldsymbol{h}_b = 150\mu m$, $\boldsymbol{h}_g = 90\mu m$, $\boldsymbol{b}_b = 2\mu m$, $\boldsymbol{b}_g = 1{,}5\mu m$, $gap = 4.5\mu m$.

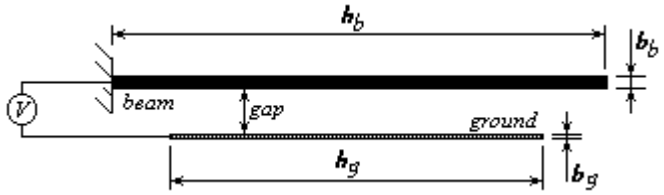
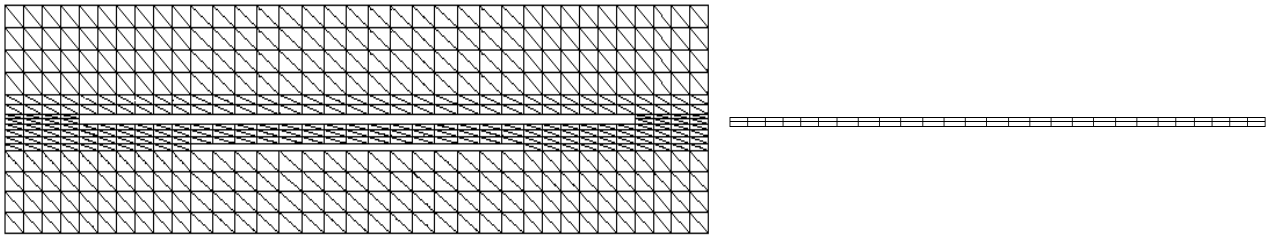


Figure 4. Silicon microbeam subjected to an electric potential difference.

Linear triangular and linear quadrilateral elements were used for the electrical and mechanical domains, respectively. The initial meshes for solving the coupled-field problem of Fig. (4) are shown in Fig. (5). The mechanical mesh has 84 nodes and 54 elements and the electrical mesh has 586 nodes and 982 elements. Nonzero electric voltages

are applied to the nodes on the biggest interior boundary of the electrical mesh (common boundary of both domains) while for the smallest (relative to the ground) the potentials are zero. The mechanical mesh has the three leftmost nodes with no displacement allowed, and on the exterior surfaces, natural boundary conditions (surface forces) are applied. The domains are solved iteratively as explained in Section 3, Fig. (3).



(a) (b)

Figure 5. (a) electrical domain mesh and (b) mechanical domain mesh.

4.2. Simulation results and discussion

The simulation was done having as convergence test the displacement of the nodes. When the displacements in all nodes change less than 0,5% the program stops running. To validate our methodology, comparisons with simulations in the ANSYS software were done.

Figure (6) shows the maximum displacements at the cantilever beam for a range of applied voltages. Although both curves present a similar behavior, the values of the displacements are not equal. The Meflab++ displacements results were from 3,26% to 5,57% larger than those obtained by ANSYS.

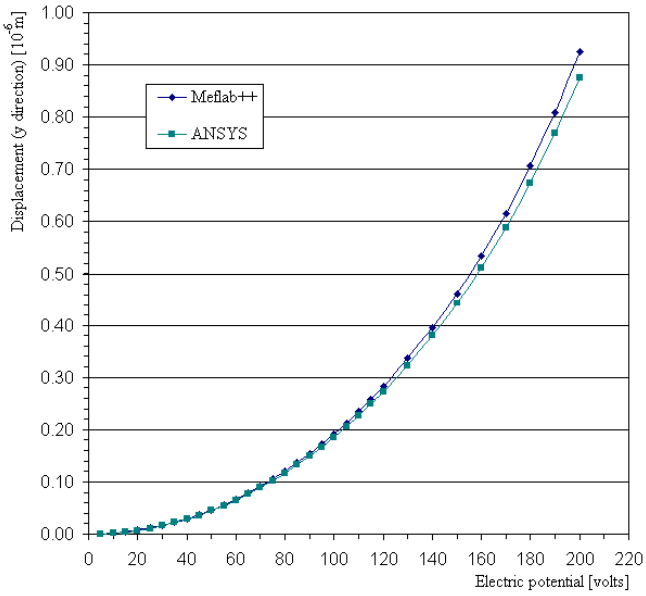


Figure 6. Displacement values versus electric potential

The difference between the Meflab++ and ANSYS results occurs due to simplifications adopted in our code. The first aspect concerns to the transposition of the electrostatic pressures to the mechanical structure. For each displacement of the structure the electrical domain must be modified so that the electrostatic pressures can be recomputed. For the application of these pressures on the surfaces of the beam, the structural mesh must also be altered so that the direction of the forces will be updated. This occurs because by default the pressures are applied on the surfaces following the direction of the normal of the boundary segments. However, care must be taken because a distorted structural mesh would generate another stiffness matrix, what would represent a structure dissimilar from the original one. The stiffness matrix then must be computed for the original beam configuration and used as such for all the subsequent iterations (i.e., the formulation is Lagrangian). For the calculation of the load vector the last deformed position should be taken into account so that the pressures would be applied in the right direction, i.e., normal to the beam surface. The algorithm in the Meflab++ is not updating the structural mesh and as a result the pressures are always being applied following the normals of the boundary segments in the original structure. The consequence of this, in the present case study, is that the load vector computed from the electrostatic pressures has always components only in the y direction. The pressures are being completely transformed into y direction forces when there should be a distribution through the x and y directions. This increases the vertical forces generating bigger displacements in this direction. Initially, the influence is not too large since the forces that should be computed in the x direction are small

compared to those in the y direction. The differences are accentuated with greater voltages because the curvature of the beam grows and the x components of the forces would exert more influence. The non updating structural mesh strategy is thus effective and low computational cost, with acceptable precision, for small voltages and displacements configurations.

Considering the same example, the second reason for the distinct simulation results is related to the electrical mesh updating procedure implemented in Meflab++. The mesh morphing is being done only in the nodes on the boundary of the electrical mesh. For a complete updating scheme, the morphing should be applied to all nodes or at least to nodes in several layers of elements surrounding the electrical boundary that follows the deformation of the structure. The difference in the values enlarges with higher electric potentials because the elements start to deform to a great extent. As only the node on the boundary moves, it may considerably approximate to the other nodes of the element and generate a too much distorted element shape.

The morphing procedure programmed in the Meflab++ also affects the convergence of the results. Figure (7) shows the number of iterations executed by the Meflab++ and by the ANSYS to reach convergence. For electric potentials until 160v the Meflab++ needed one or two more iterations than the ANSYS to converge. With values above 160v, the convergence was harder obtained and the Meflab++ needed three or four more iterations than the ANSYS. After 240v our algorithm failed. The failure is reasoned by the accentuated distortion of the elements' shapes with large voltage values. Although the failure occurred at 240v, the distortion of the elements starts to be considerable from 210v and with values above this the results are not trustworthy anymore. The ANSYS fails to converge from 230v, even with the morphing being applied to all the nodes in the electrical mesh.

A last fact to be pointed out is that quadratic triangular elements were used in the ANSYS for the simulation of the electrical domain.

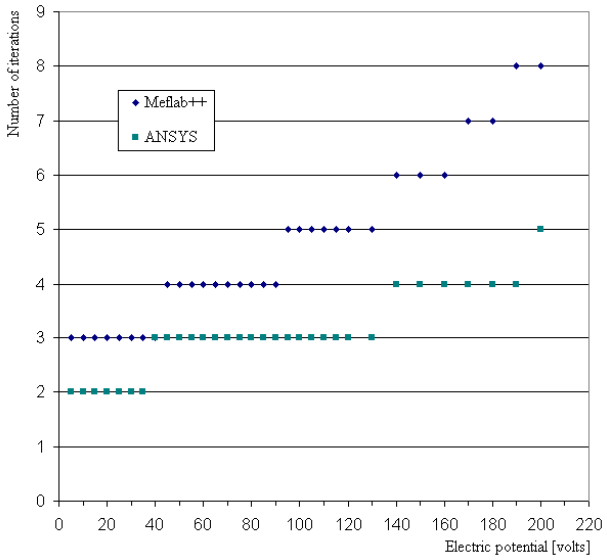


Figure 7. Number of iterations versus electric potential

Considering the presented numerical simulations, the efficiency of the simplified mesh morphing and force transfer approach was shown for configurations where the voltages and displacements are small.

5. Conclusions

This paper has described our first efforts towards the construction of a FEM-based numerical tool for simulating microsystems with electromechanical coupling. A simplified sequential approach was adopted to lead with the coupled-field problem. The algorithm was explained and details of its implementation in the code Meflab++ were given. Discussions about mesh managing and the mechanisms of transition between the electrical and mechanical domains were done. The case study of a silicon microbeam was shown. Although the implementation was done with simplified strategies, the achieved results were satisfactory and indicate good perspectives. The morphing can be enhanced and the transfer of loads from the electrical to the mechanical domain can be refined. These actions can improve the computer code making it capable to generate better results for larger values of electric potential. The simplified low computational cost strategy can be specially effective for future implementation of transient analysis algorithms and topological optimization.

6. Acknowledgement

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