A Relaxation/Multipole-Accelerated Scheme for Self-Consistent Electromechanical Analysis of Complex 3-D Microelectromechanical Structures *

X. Cai, H. Yie, P. Osterberg, J. Gilbert, S. Senturia and J. White
Res. Lab. of Elec. and the Microsystems Tech. Lab.
Depart. of Elec. Eng. and Comp. Sci., Mass. Inst. of Tech.,
Cambridge, MA 02139 U.S.A.

Abstract

In this paper, two approaches to self-consistent electromechanical analysis of three-dimensional micro-electro-mechanical structures are described. Both approaches combine finite-element mechanical analysis with multipole-accelerated electrostatic analysis, the first using a relaxation algorithm and the second using a surface/Newton generalized conjugate-residual scheme. Examples are given to demonstrate the relative merits of the two approaches.

1 Introduction

Electrostatic microactuators, such as the suspended polysilicon comb drive [2] and the electrostatatic micropump [1], are typically controlled by applied voltages that create electrostatic forces which then deform the structure. As the structure deforms, the electrostatic forces change, making the final structure's shape difficult to predict. For this reason, designers of microelectromechanical systems (MEMS) are interested in using computer simulation tools to perform this self-consistent analysis. In theory, the finite-element method (FEM) commonly used for mechanical analysis can be used to perform self-consistent electromechanical analysis, but three-dimensional meshing problems make using FEM impractical. Specifically, an FEM mesh is needed in the interior of structure to determine mechanical forces, and an FEM mesh is needed in the exterior of the structure to determine electric fields. Resolving fields quantities on, and maintaining the alignment of, a large three-dimensional exterior mesh is extremely computationally expensive.

Another approach is to exploit the fact that electrostatic forces can be determined using only the normal electric fields at the structure surfaces. This implies that electrostatic forces can be computed using boundary-element methods (BEM), in which only structure surfaces are discretized and only surface quantities computed [4]. Though standard BEM methods generate dense matrix problems which are expensive to solve, recently developed multipole-accelerated iterative methods reduce the cost of solving BEM matrices associated with electrostatic analysis to order N operations, where N is the number of elements in the surface discretization [6].

In this paper, we describe two efficient approaches to combining finite-element mechanical analysis with multipole-accelerated electrostatic analysis. The first method is the obvious relaxation algorithm and the second method is a more sophisticated surface/Newton generalized conjugate-residual scheme. We start, in the next section, by describing self-consistent analysis, and give these two methods. Then in Section 3, examples are given to demonstrate that the methods are accurate, and that the Surface/Newton-GCR algorithm converges more reliably than the relaxation algorithm. Conclusions and acknowledgements are given in Section 4.

2 Self-Consistent Electromechanical Analysis

Elastic deformation analysis performed by finite-element programs like ABAQUS [5] involves solving a

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system of equations of the form

$$x, S(x) = F_M(x_i, S(x_i), P) \quad (1)$$

where $x \in \Re^N$ is the vector unknown of discretization mesh node positions associated with a force-balanced state, $S(x) \in \Re^M$ is a vector of element stresses associated with the position x, $x_i \in \Re^N$ is a vector of given initial node positions, $S(x_i) \in \Re^M$ is a vector of element stresses associated with the given initial position x_i, and $P \in \Re^L$ is the vector of applied pressure forces. Here, N is the number of nodes, L is the number of surface faces, and M is the number of degrees of freedom associated with the elements.

The electrostatic pressure, P, acts in the direction of the structure surface normal and is given by $P = \frac{1}{2}E_n * \sigma$, where σ is the surface charge density and E_n is the normal electric field at the surface. Given the applied potential, V, P can be determined from an equation of the form

$$P = F_E(x, V), \quad (2)$$

where $P \in \Re^L$ is the unknown vector of surface pressures, $x \in \Re^N$ is the vector of given discretization mesh node positions, and V is the applied voltage. The multipole-accelerated boundary-element based electrostatic analysis program, FASTCAP [6], can be used to efficiency solve (2) even for complicated three-dimensional structures.

The problem of self-consistent electromechanical analysis is then to find the node displacements, x^*, and the associated electrostatic pressures, P^*, such that

$$\begin{aligned} x^*, S(x^*) &= F_M(x^*, S(x^*), P^*) \quad (3)\\ P^* &= F_E(x^*, V). \end{aligned}$$

2.1 Solution Algorithms

Given a program like ABAQUS to solve (1), and a program like FASTCAP to solve (2), the nonlinear Gauss-Seidel relaxation algorithm below can be used to combine the two programs into a procedure for solving (3).

Algorithm 1: Relaxation Procedure for Solving (3).
$k = 1, x^k = 0$.
Repeat
$P^{k+1} = F_E(x^k, V)$.
$x^{k+1}, S(x^{k+1}) = F_M(x^k, S(x^k), P^{k+1})$.
k = k + 1;
until $||x^k - x^{k+1}|| < \epsilon$.

As will be shown subsequently, Algorithm 1 does not always terminate because the Gauss-Seidel relaxation often fails to converge. To derive an algorithm with superior convergence properties, consider reorganizing (3) by eliminating P^*, and then expressing the problem as

$$F(x) = x - F_M(x, S(x), F_E(x, V)) \quad (4)$$

where $F(x^*) = 0$.

Now consider that x is a vector of discretization mesh node positions throughout the volume of the structure being analyzed. However, once the node positions on the structure surface are known, both the surface pressure and the interior node positions can be determined by decoupled electrostatic and mechanical analysis. This suggests that to reduce the dimensionality of the coupled problem, (4) can be rewritten as

$$\begin{aligned} &F_s(x_s) = \\ &-Surf\,[F_M(F_M(x_s), S(F_M(x_s)), F_E(x_s, V))] \quad (5) \end{aligned}$$

where $x_s \in \Re^s$ is the vector of surface node positions, the function $Surf$ extracts x_s from x, and $F_M(x_s)$ is used to denote the fact that mechanical analysis alone is sufficient to determine all the node positions given the surface node positions.

A Newton method combined with the generalized-conjugate-residual method (GCR) can be used to solve (5), as given below.

Algorithm 2: Surface/Newton procedure
$k = 1, x_s^k = 0$.
Repeat
Solve $J(x_s^k)\delta_k = -F_s(x_s^k)$ using GCR.
Set $x_s^{k+1} = x_s^k + \delta_k$
k = k + 1;
until $||x_s^k - x_s^{k+1}|| < \epsilon$.

Here, $J(x_s) = F_s'(x_s)$ is the system Jacobian.

Since GCR is used to solve $J(x_s^k)\delta_k = -F_s(x_s^k)$, the Jacobian is never needed explicitly. That is, only matrix-vector products, $J * r_k$, are needed, and they can be approximated by

$$J(x) * r \approx \frac{F(x + \theta * r) - F(x)}{\theta} \quad (6)$$

where

$$\theta = sign(x * r) * min(1, \tfrac{a||x||}{||r||}, \tfrac{b||F(x)||}{||r||})$$
$$a \in (0.01, 0.5) \qquad b \in (0.1, 1)$$

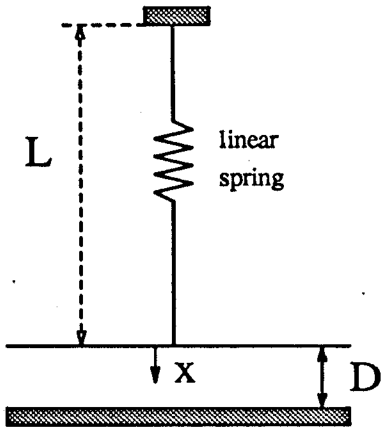

Figure 1: The beam structure

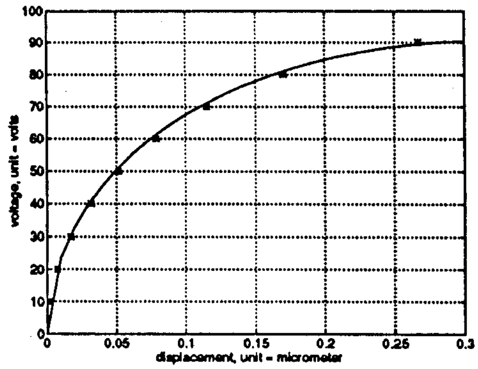

Figure 2: Beam structure displacement versus applied voltage

3 Demonstration Examples

To begin, consider a structure whose behavior can be determined analytically, so that the simulation results can be verified. The structure consists of an elastic beam attached to the top plate of a parallel plate capacitor, as shown in Figure 1. The top of the beam is held fixed, as is the bottom plate of the capacitor. When a voltage is applied to the parallel plate capacitor, the induced electrostatic pressure will pull the top plate down and stretch the attached beam. The plate will be displaced to the point where the electrical and mechanical forces are in balance, and this point can be approximately determined analytically. Ignoring fringing fields, the electrostatic force is given by

$$f_e = \frac{\epsilon_0 A_p V^2}{2(D-x)^2}, \tag{7}$$

where ϵ_0 is the permitivity, A_p is the plate area, V is the applied voltage, D is the "at rest" plate separation (with $V = 0$), and x the displacement of the top capacitor plate. The mechanical restoring force due to stretching the beam also has a simple form,

$$f_m = kx = \frac{Y A_b}{L+x} x, \tag{8}$$

where Y is the Young's Modulus of the beam, A_b is the beam cross sectional area, and L is the beam's length.

For the case $V = 70$ volts, $Y = 1GPa$, $A_b = 2um^2$, $D = 1um$, $A_p = 100um^2$, the analytical and the simulation results are plotted in Figure 2. As is clear from the plot, the analytical results (the solid line) is in good agreement with the simulation results (the stars).

The example in Fig. (3) is of two silicon bars whose potentials differ by 1000 V. Here, each bar is $0.5\mu m \times 0.5\mu m \times 10\mu m$, the minimum distance between the two bars is $0.5\mu m$, the Young's modulus of silicon is $162.7GPa$, the density of silicon is $2.328 \times 10^3 Kg/m^3$, and the Poisson ratio is 0.223. In Fig. (4), the convergence characteristics of relaxation and surface-Newton-GCR are compared, and as the graphs show, the relaxation fails to converge but the surface-Newton-GCR algorithm converges rapidly.

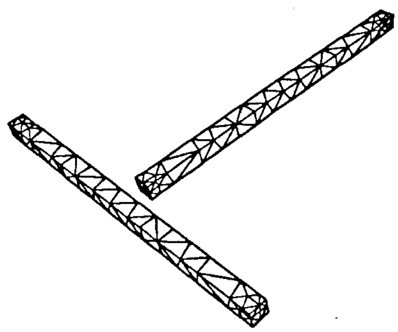

Figure 3: Silicon bars at different potentials.

Comb drive resonantors often fail to function properly because the ground plane induces a levitation force. For example, we consider a comb structure over a ground plane, shown slightly levitated in Fig. (5). For this experiment, the dimension of the structure is $20\mu m \times 8\mu m \times 3.5\mu m$, and the distance between fingers is $1\mu m$. The ground plane and the two fingers structure are assumed to be fixed, and a voltage is applied on the two fingers structure. The one finger structure is fixed at one side and aluminium material properties are assumed (the Young's modulus is $77.4GPa$, the density is $2.7 \times 10^3 Kg/m^3$ and the Poisson ratio is 0.346). When a positive potential is appled to the two-fingered structure, there will be a repulsive electrostatic force between the one-fingered structure and the ground plane, even if both are at zero potential. This repulsive force is due to the induced negative charge on both the one-fingered structure and the ground plane. In Fig. (6) the convergence versus CPU time for the relaxation method and the surface/Newton-GCR method are compared, and as can be seen from the convergence cutve, the surface/Newton-GCR method is more than two orders of magnitude faster than the relaxation method.

4 Conclusions

In this paper it is shown that efficient electromechanical analysis can be performed by combining a standard finite-element based mechanical analysis program with a fast boundary-element based electrostatic solver. Also, we demonstrated that our surface/Newton-GCR algorithm is faster and more robust than the simplier relaxation scheme.

References

[1] M. A. Huff and M. A. Schmidt, "Fabrication, Packaging, and Testing of a Wafer-Bonded Microvalve," Technical Digest, IEEE Solid-State Sensor and Actuator Workshop, Hilton-Head Island, SC, June 1992, pp. 195-197.

[2] W. C. Tang, M. G. Lim, and R. T. Howe, "Electrostatic comb drive levitation and control method," Journal of Microelectromechanical Systems, vol. 1, Number 4, Dec. 1992, pp. 170-178.

[3] K. J. Bathe, *Finite Element Procedures in Engineering Analysis.* Englewood Cliffs, NJ: Prentice-Hall, 1982.

[4] C. A. Brebbia and J. Dominguez, *Boundary Elements: An Introductory Course.* Southampton: Computational Mechanics Publications, 1989. Copublished with McGraw-Hill, New York.

[5] Hibbit, Karlsson, and Sorensen, Inc., Providence, R.I.

[6] K. Nabors and J. White, "FastCap: A multipole-accelerated 3-D capacitance extraction program." *IEEE Transactions on Computer-Aided Design*, vol. 10 no. 10, November 1991, p1447-1459.

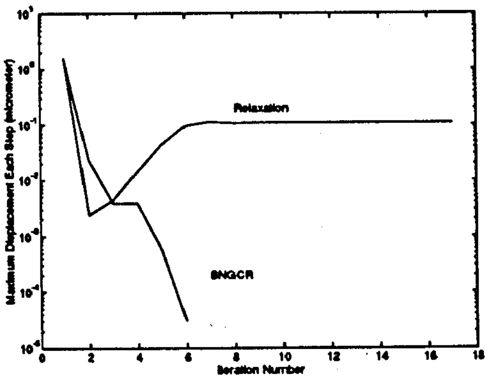

Figure 4: Convergence characteristics of Relaxation and Surface-Newton-GCR.

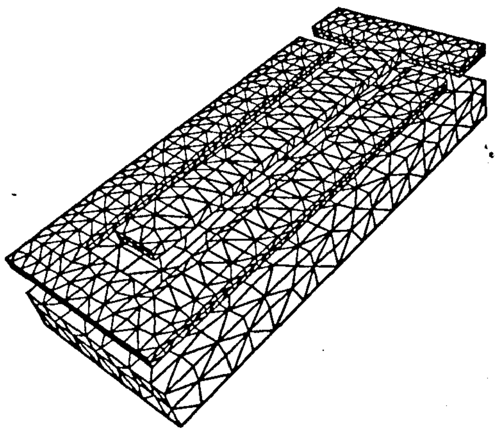

Figure 5: Deformed Comb Drive Resonantor.

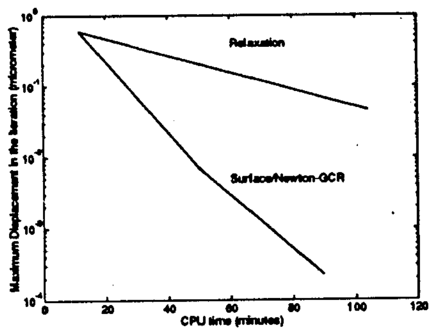

Figure 6: Comparision of CPU times for the relaxation and surface/Newton-GCR methods (The applied potential is 420 volts).