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A Multi-level Newton Method for Static and Fundamental Frequency Analysis of Electromechanical Systems

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Abstract— **A matrix-implicit multi-level Newton method for black-box self-consistent analysis of 3-D microelectromechanical systems (MEMS) is described. The approach is shown to converge very rapidly and is much faster than relaxation algorithm for tightly coupled problems. In addition, the matrix-implicit approach is used to derive a computationally efficient technique to extract the fundamental frequency as a function of applied voltage for a microstructure. While this paper focusses on coupled electromechanical analysis, the proposed algorithm can be extended to include several coupled domains encountered in MEMS.**

I. Introduction

Microelectromechanical devices such as microvalues, acceleration sensors, gyroscopes, or display micromirrors, use electrostatic forces to move micromachined aluminium and single- or poly-crystalline silicon. Since most of the structures of interest are geometrically complicated, electromechanically coupled, and inherently three-dimensional, microelectromechanical CAD (MEMCAD) tool developers have been focussed on improving the usability, efficiency and robustness of coupled 3-D electromechanical analysis [14], [7], [5], [3], [1]. However, in the last few years micromachine design techniques and applications have been expanding rapidly, creating interest in coupled-domain simulation which not only allows for elastic parts and electrostatic forces, but also includes magnetic and fluidic forces, heat transfer, and piezoelectric effects. This large number of possibly coupled domains, combined with the existence of commercially-available single domain simulation software, makes approaches to coupled-domain simulation which require no modification of the single domain simulators extremely attractive. Nonlinear relaxation is the simplest of these *black-box* approaches, and it has well-known convergence problems [11].

In this paper we describe a matrix-implicit multilevel-Newton method for black-box coupled-domain analysis, and give particulars for the case of self-consistent electromechanical analysis. We begin in the next section by briefly describing electromechnical analysis, and the standard black-box approaches. In Section III we describe a multi-level Newton approach as a black-box technique for electromechanical analysis and a computationally efficient approach to extract fundamental frequencies is presented in Section IV. Numerical results are presented in Section V and conclusions are given in Section VI.

II. Background

A. Electromechanical Analysis

The elastic deformation of the structure can be predicted by studying nonlinear elastostatics (or elastodynamics, as the case may be). Commercial simulators such as ABAQUS [9] typically use finite element methods to solve nonlinear force-balance equations. Somewhat more specifically, the elastostatic force-balance equations can be written as

$$F_s(u) + F_p(q) = 0, \tag{1}$$

where u is the vector of discretized structural displacements, F_s relates structural displacements to forces due to strain, and $F_p(q)$ relates the surface charge to the surface electrostatic forces. From an input-output perspective, elastostatic analysis can be written as

$$u = R_M(q) \tag{2}$$

where $R_M(q)$ is a black-box elastostatic solver which computes deformation as a function of the surface charges, q. Note that the elastostatic equations are nonlinear and typically a Newton method is employed to compute the displacement, u.

Given conductor potentials, the surface charge can be computed by solving the electrostatic equations in the conductor exterior. Commercial simulators often use boundary-element methods, typically combined with accelerated iterative methods [10], [12]. Mathematically, the solution of the electrostatic equations can be represented as

$$q = R_E(u) \tag{3}$$

where $R_E(u)$ denotes a black-box electrostatic solve to compute the surface charges, q, given the conductor geometry, u, and applied potentials. The dependence of the electrostatic solve on u is explained by the change in the conductor geometry as it undergoes deformation due to electrostatic forces.

Coupled electromechanical analysis requires the self-consistent solution of equations (2) and (3). With the availability of black-box solvers such as ABAQUS for mechanical analysis and FASTCAP for electrical analysis, coupled electromechanical analysis has been implemented with the black-box algorithms discussed in the next section.

B. Nonlinear Relaxation

A simple black-box approach to coupled electromechanical analysis is the nonlinear Gauss-Seidel relaxation algorithm. In this approach the data is passed back and forth between black-box electrostatic and elastostatic analysis programs until a converged solution is obtained. The relaxation procedure is summarized below:

Algorithm 1: Relaxation Technique
$k = 1, u^k = 0.$
Repeat
Compute $q^k = R_E(u^k)$.
Compute $u^{(k+1)} = R_M(q^k)$.
k = k + 1;
until $\|u^k - u^{k+1}\| < \epsilon$.

As is evident from the above procedure, black-box approaches based on relaxation are easily implemented for coupled electrome-

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chanics, and the extension to coupling other domains is straightforward. Sufficient conditions for relaxation convergence [11] is that

$$\|\frac{\partial R_E}{\partial u}\frac{\partial R_M}{\partial q}\| < 1, \tag{4}$$

which will be satisfied if the structure is sufficiently mechanically pliant and the applied potentials are sufficiently small [15]. More precise conditions for relaxation convergence can be given for classes of geometries, as in [16]. Nonlinear relaxation converges sufficiently frequently to be quite useful for electromechanical analysis, but as will be shown in the results section, the relaxation algorithm can fail for micromachined structures.

III. The Multi-Level Newton Algorithm

One approach to curing the relaxation convergence problem for electromechanical analysis is to switch to a fully-coupled Newton method [3], [1], [2]. The main difficulty with such methods is that they require more access to the Jacobian and to coupling terms than is usually available from black-box simulators. Instead, for domains which interact only at surfaces (this excludes magnetic fields for example), it is possible to use a matrix-free surface-Newton method [15]. The main difficulty with surface-Newton methods is that their performance is much too sensitive to one of the perturbation parameters to be of practical use. In this section we describe a matrix-implicit multi-level Newton technique for black-box analysis of coupled electromechanical equations. The multi-level Newton technique converges rapidly even when relaxation fails, and is not sensitive to its associated perturbation parameters.

In the multi-level Newton technique, the coupled electromechanical equations are solved by employing a nested Newton-Raphson method. The outer-Newton iteration solves the following residual equation

$$R(u,q) = \left\{ \begin{array}{c} q - R_E(u) \\ u - R_M(q) \end{array} \right\}. \tag{5}$$

In equation (5), $R_E(u)$ is the charge on the conductors for the conductor geometry displaced by u, $R_M(q)$ is the structural displacement due to the electrostatic forces generated by q, and if both $q - R_E(u)$ and $u - R_M(q)$ are zero or approximately zero, then the charge q and the displacement u are a self-consistent solution to the electromechanical system. Note that because the residual R is defined in a certain way it can be computed using black-boxes. The Jacobian for the residual given in equation (5) is given as

$$J(u,q) = \left[\begin{array}{cc} I & -\partial R_E/\partial u \\ -\partial R_M/\partial q & I \end{array} \right] \tag{6}$$

With the definition of the residual and the Jacobian in (5) and (6) respectively, the multi-level Newton technique for solving the coupled electromechanical equations can be summarized as follows:

Algorithm 3: Multi-level Newton Technique

$k = 1, u^k = 0, q^k = 0.$

Repeat

Solve $J(u^k, q^k) \left\{ \begin{array}{c} \delta_q \\ \delta_u \end{array} \right\} = -R(u^k, q^k)$ for δ_q, δ_u.

Set $u^{k+1} = u^k + \delta_u$.

Set $q^{k+1} = q^k + \delta_q$.

k = k + 1;

until $\|u^k - u^{k+1}\| < \epsilon$.

The Newton-update linear system in Algorithm 3 can be solved with Krylov-subspace based iterative methods like GMRES [13]. In that case, only matrix-vector products are needed, but not the explicit Jacobian.

The matrix-vector product required in the Krylov-subspace based iterative solver can be computed approximately using only black-box elastostatic and electrostatic solves, as in

$$J \left\{ \begin{array}{c} \delta_q \\ \delta_u \end{array} \right\} \approx \left\{ \begin{array}{c} \delta_q - \frac{1}{\theta}(R_E(u + \theta\delta_u) - R_E(u)) \\ \delta_u - \frac{1}{\theta}(R_M(q + \theta\delta_q) - R_M(q)) \end{array} \right\} \tag{7}$$

where θ is a perturbation parameter whose value is selected so as to insure an accurate approximation. In particular, θ is selected from the range given by

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

when a matrix-vector product $\partial R/\partial x \cdot r$ is to be performed.

To summarize, the coupled nonlinear system (5) can be solved using Newton's method. Each Newton iteration requires the solution of the Newton-update linear system, and this linear system can be solved with a Krylov-subspace algorithm. Each iteration of a Krylov-subspace algorithm requires a matrix-vector product which can be computed using black-box elastostatic and electrostatic solvers. Since elastostatic solvers typically use Newton's method, we describe the combined approach as a multi-level Newton method.

IV. Fundamental Frequency Computation

Once the equilibrium position has been computed for a given bias, the structure's resonant frequency can be estimated as the square root of the dominant eigenvalue of the product of mass matrix and the inverse of the linearized electromechanical system. This relation follows from the low damping assumption and from the fact that the quasistatic forces are directly proportional to the product of the mass matrix and the second time derivative of the displacements. A matrix-free Power method is employed to compute the dominant eigenvector. Denoting $\tilde{M}$ and $\tilde{K}$ to be the mass and effective stiffness matrices of the linearized system, respectively, the fundamental mode and frequency are computed as

$$X_1^{(i+1)} = \tilde{K}^{-1}\tilde{M}X_1^{(i)} / \max(\tilde{K}^{-1}\tilde{M}X_1^{(i)}) \tag{8}$$

$$w_1^2 = 1 / \max(\tilde{K}^{-1}\tilde{M}X_1^{(i)}) \tag{9}$$

where $X_1^{(i)}$ is the ith approximation to the fundamental mode shape and w_1^2 is the fundamental frequency. Note here that multiplication by $\tilde{K}^{-1}$ is peformed by solving the linearized static equations using a matrix-free GCR or GMRES. To multiply a vector v by $\tilde{K}^{-1}$ we solve

$$[\frac{\partial F_s}{\partial u} + \frac{\partial F_p}{\partial q}\frac{\partial R_E}{\partial u}]y = v \tag{10}$$

using a matrix-implicit method similar to that in Section III.

For the examples examined in this paper, no more than four power iterations were needed to accurately determine the fundamental mode shape and frequency. For more general examples, and to determine higher order modes, it is likely that a more general Arnoldi-based matrix-free approach will be necessary.

V. Results

Numerical results are presented for two examples: a beam over a ground plane and a comb drive structure. The performance of the multi-level Newton and relaxation algorithms is examined for both the examples. In particular, the convergence characteristics and the simulation times are compared.

The beam example considered here is 500 μm long, 50 μm wide, 14.35 μm thick and is positioned 1 μm above the ground plane. The beam is discretized into 50 parabolic elements and the ground plane is discretized into 250 4-node elements. When a positive potential with reference to the ground plane is applied on the beam, the beam deflects towards the ground plane because of the electrostatic force. As the potential difference increases, the tip of the beam approaches the ground plane, and touches the ground plane for a certain bias defined as the pull-in voltage. The pull-in voltage for the beam considered here is 17.24 volts.

TABLE I
COMPARISON OF RELAXATION AND MULTI-LEVEL NEWTON ALGORITHMS FOR A BEAM OVER A GROUND PLANE EXAMPLE

Bias	# Iterations		CPU(sec)	
	Relaxation	ML Newton	Relaxation	ML Newton
2.0	4	2	283.5	698.7
4.0	5	3	381.0	967.0
6.0	6	3	507.7	1244.9
8.0	7	3	608.4	1079.6
10.0	8	3	710.2	1086.8
12.0	10	3	909.5	1086.7
14.0	13	4	1244.4	1530.7
16.0	20	4	2015.8	1499.0
17.0	41	5	4248.1	1957.0
17.20	94	5	9713.83	2145.7
17.23	200	7	20910.5	2823.5

The performance of the relaxation and multi-level Newton algorithms for the beam example is summarized in Table I. Observe that the multi-level Newton algorithm takes fewer iterations and is much faster compared to the relaxation algorithm for tightly coupled cases. Figure 1 compares the convergence of the relaxation and multi-level Newton algorithms for the beam and ground plane example. Note that closer to pull-in the relaxation algorithm converges slowly, but the multi-level Newton algorithm converges rapidly. The slow convergence of the relaxation algorithm, near pull-in, is due to the increased coupling between elastostatic and electrostatic systems. As the multi-level Newton algorithm accurately accounts for all the coupling it exhibits rapid convergence behavior.

The resonant frequency as a function of the applied bias for the beam structure is shown in Figure 2. As the bias increases, the frequency decreases and when the bias reaches the pull-in voltage, the frequency goes to zero. Noting that the frequency is proportional to the effective stiffness of the structure, the frequency decreases as the effective stiffness decreases for increasing bias.

The comb example consists of a deformable comb structure, a drive structure and a ground plane (see [2] for a description of the device). The comb is discretized into 172 parabolic elements, the drive is discretized into 144 linear bricks and the ground plane is discretized into 2688 4-node elements. When a positive potential is applied on the drive structure, and zero potential on the comb and the ground plane, the comb structure deforms out of plane.

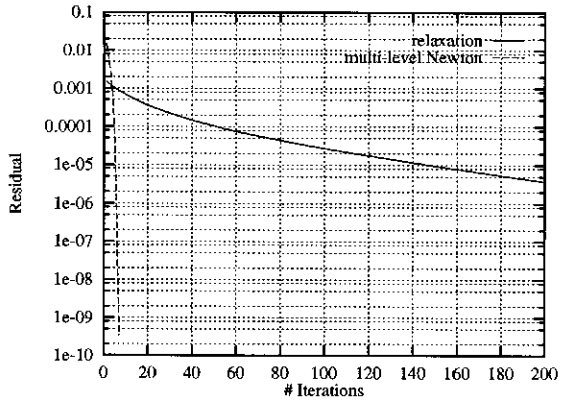

Fig. 1. Convergence of relaxation and multi-level Newton algorithms for a beam and ground plane structure for a bias of 17.23V

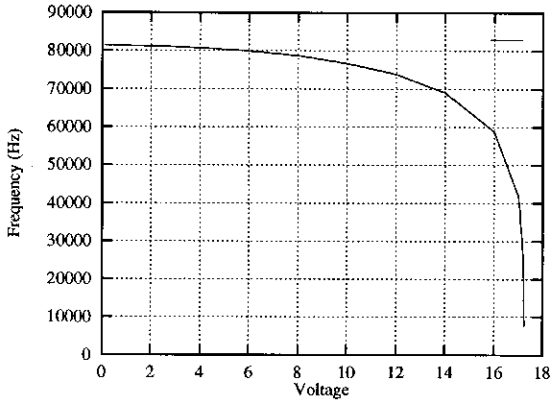

Fig. 2. Resonant frequency vs. bias for the beam structure

A comparison of the relaxation and multi-level Newton algorithms for the comb example is summarized in Table II. At low voltages, the deflection of the comb is small, the coupling between the electrical and mechanical systems is weak and the relaxation algorithm works very well. At low voltages, the multi-level Newton algorithm takes fewer iterations compared to the relaxation algorithm but the simulation time for the multi-level Newton algorithm is a little longer. For higher voltages, the multi-level Newton algorithm converges much faster compared to the relaxation algorithm. For a bias of 80 volts, the multi-level Newton algorithm is about 7.7 times faster. For an application of 85 V on the drive, the relaxation algorithm fails to converge and the multi-level Newton algorithm converges very rapidly and takes only 3 iterations. This is illustrated in Figure 3.

The frequency for the comb-drive structure as a function of the applied bias is shown in Figure 4. As the applied bias on the drive increases, the frequency increases. The increase in the frequency can be explained by the effective increase in the stiffness of the structure.

VI. Conclusion and Acknowledgements

In this paper, we presented a matrix-free based, multi-level Newton algorithm for 3-D electromechanical analysis. Similar to the relaxation algorithm, the multi-level Newton algorithm employs repeated black-box calls to elastostatic and electrostatic analysis. While the relaxation algorithm fails to converge for tight coupling between mechanical

TABLE II

COMPARISON OF RELAXATION AND MULTI-LEVEL NEWTON ALGORITHMS FOR A COMB DRIVE EXAMPLE (A * INDICATES THAT THE ALGORITHM FAILS TO CONVERGE FOR THE BIAS)

Bias	# Iterations		CPU(sec)	
	Relaxation	ML Newton	Relaxation	ML Newton
25.0	7	3	3595.4	5802.2
50.0	16	4	9138.0	10195.1
75.0	70	4	42160.3	12053.2
80.0	142	3	81827.0	10660.4
85.0	*	3	*	10767.8

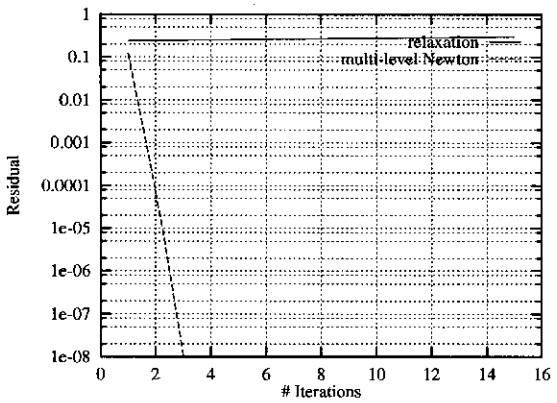

Fig. 3. Comparison of convergence of relaxation and multi-level Newton algorithms for a comb example at an applied bias of 85 V.

and electrical domains, the multi-level Newton algorithm is shown to converge very rapidly. Numerical results indicate that the multi-level Newton technique is much faster compared to the relaxation technique. The multi-level Newton technique described in this paper can be extended for other coupled domains in MEMS, but the choice of the matrix-free parameter may need more investigation.

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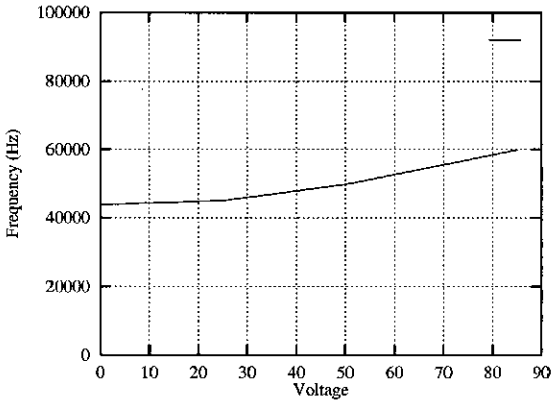

Fig. 4. Resonant frequency vs. bias for the comb drive structure

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