SEQUENTIAL SOLUTIONS OF FIELD EQUATIONS USING A SINGLE BEM MODEL

Per B. Ljung

Berkeley Sensor & Actuator Center
497 Cory Hall
University of California Berkeley
Berkeley, CA 94720

ABSTRACT

A new portable CAD tool is introduced allowing a single boundary element model to solve coupled nonlinear Laplace, Poisson and Navier field equations. The compact formulation of the model and discretized differential equations allows the software to be implemented on standard personal computers in vectorized Matlab code. Several 2D and 3D examples are given using common micromachined structures.

INTRODUCTION

Designers of microelectromechanical systems need to be able to analyze 3D coupled multi-energy domains within a single integrated CAD environment. Currently separate analysis tools [1]-[7] are used for thermal, electrostatic, elastostatic, thermoelastic, and magnetostatic field solutions, iterating between tools until results converge. This requires redundant data preparation since the domains must be modeled appropriately for each individual CAD tool. Further, this results in inefficient operation due to the overhead of translating intermediate results between different CAD tools. Nontrivial models become unwieldy requiring up to 1 month processing time [5] to solve coupled electrostatic and elastostatic problems using iteration between separate CAD packages. These large coupled FEM problems have also been solved with parallel computation [8] of linked workstations.

DUAL RECIPROCITY BEM

In contrast to earlier work, this paper presents an integrated CAD tool capable of solving coupled field equations using a single boundary element method (BEM) mesh. Since only the boundaries of the system are modeled, this results in simple data preparation as well as small data structures and fast simulation. Further, the single BEM mesh is used for each desired field analysis resulting in efficient numerical interaction for large nontrivial coupled problems as depicted schematically in Figure 1.

Figure 1. A single BEM model suffices to solve an arbitrary sequence of coupled field equations.

Compared to FEM which only solves for the desired state variable, BEM simultaneously solves for both the state variable and flux. While traditional BEM programs can solve static 2D and 3D

Laplace and Navier field equations, the dual reciprocity boundary element method (DR-BEM) [9] used here can solve:
Laplace

$$\nabla^2 u = 0; \quad (1)$$

time-dependent Poisson

$$\nabla^2 u = b(x, y, z, u, t); \quad (2)$$

and time-dependent Navier

$$Gu_{j,kk} + \frac{G}{1-2\nu} u_{k,kj} + b_j = \rho \ddot{u}_k \quad (3)$$

field equations. The DR-BEM is implemented in portable vectorized Matlab [10] code using isoparametric surface elements to solve Poisson and Navier equations [11] enabling the calculation of distributed LCR-networks, electrostatics, elastostatics, thermoelastics, magnetostatics and modal analysis. Figure 2 shows a diagram where the field equation, valid in the domain Ω , is evaluated on the discretized boundary elements and internal nodes.

Figure 2. DR-BEM boundary discretization using linear elements consisting of N external nodes and L internal nodes.

Problems with nonhomogeneous time-varying forcing functions and material nonlinearities are fully supported by DR-BEM while problems with geometric nonlinearities are solved using iteration. Coupled systems such as electrostatic-elastostatic problems are solved by iteration between the DR-BEM field solutions, whereas coupled systems such as thermoelastic-modal analysis problems are solved directly using the first field solution.

PORTABLE MATLAB IMPLEMENTATION

Solving a discretized boundary element problem requires matrix manipulation, numerical integration and solving linear systems. For this reason, it was expedient to use Matlab as the platform for the boundary element software. Consider

$$\nabla^2 u = b \quad (4)$$

which allows the modelling of:

- (i) Laplace problems, where $b = 0$;
- (ii) diffusion problems, where $b = b(\partial u / \partial t)$;
- (iii) convection problems, where $b = b(\partial u / \partial x)$;
- (iv) nonlinear material problems; and
- (v) modal analysis problems, where $b = -u$.

A weighted residual formulation of Eq. 4 produces

$$\int_{\Omega} (\nabla^2 u - b) \underline{u} d\Omega = \int_{\Gamma_2} (q - \bar{q}) \underline{u} d\Gamma - \int_{\Gamma_1} (u - \bar{u}) \underline{q} d\Gamma \quad (5)$$

where Ω is the solution domain, $\underline{u}$ is the fundamental solution [11] such that $\nabla^2 \underline{u} = -\Delta$, and where Δ is the Dirac delta function. The specified boundary conditions are u_1 on Γ_1 and $q_2 = \partial u / \partial n$ on Γ_2 where $\Gamma = \Gamma_1 + \Gamma_2$ is the total boundary and n is the normal to the boundary. Eq. 5 is integrated twice by parts and grouping all the boundary terms together, one obtains for a point source i

$$c_i u_i + \int_{\Gamma} u \underline{q} d\Gamma - \int_{\Gamma} q \underline{u} d\Gamma = \int_{\Omega} b \underline{u} d\Omega. \quad (6)$$

Standard BEM schemes [11] cannot evaluate the domain integral on the right-hand side of Eq. 6. However, using the dual reciprocity approximation [9], the domain term is approximated as

$$b \equiv \sum_{j=1}^{N+L} \alpha_j f_j \quad (7)$$

where N are the number of boundary nodes, L are the number of internal nodes, α_j are a series of unknown coefficients and f_j are a set of approximating functions, which for the case of the Laplace operator satisfy

$$\nabla^2 \hat{u}_j = f_j. \quad (8)$$

Substituting Eq. 8 into Eq. 7 results in

$$\nabla^2 u = b \equiv \sum_{j=1}^{N+L} \alpha_j (\nabla^2 \hat{u}_j). \quad (9)$$

Multiplying by the fundamental solution $\underline{u}$ and integrating over the domain gives

$$\int_{\Omega} b \underline{u} d\Omega = \sum_{j=1}^{N+L} \alpha_j \int_{\Omega} (\nabla^2 \hat{u}_j) \underline{u} d\Omega. \quad (10)$$

Integrating twice by parts for each source point i leads to

$$c_i u_i + \int_{\Gamma} u \underline{q} d\Gamma - \int_{\Gamma} q \underline{u} d\Gamma = \sum_{j=1}^{N+L} \alpha_j \left(c_i \hat{u}_{ij} + \int_{\Gamma} \hat{u}_j \underline{q} d\Gamma - \int_{\Gamma} q \hat{u}_{ij} d\Gamma \right). \quad (11)$$

Discretizing over N boundary elements and evaluating the integrals using gaussian numerical integration produces

$$c_i u_i + \sum_{k=1}^N H_{ik} u_k - \sum_{k=1}^N G_{ik} q_k = \sum_{j=1}^{N+L} \alpha_j \left(c_i \hat{u}_{ij} + \sum_{k=1}^N H_{ik} \hat{u}_{kj} - \sum_{k=1}^N G_{ik} \hat{q}_{kj} \right). \quad (12)$$

After evaluation at all boundary nodes i , the following matrix equation results

$$Hu - Gq = \sum_{j=1}^{N+L} \alpha_j (H\hat{u}_j - G\hat{q}_j). \quad (13)$$

Collecting the vectors $\hat{u}_j$ and $\hat{q}_j$, the nonhomogeneous terms form the vector

$$C = (H\hat{U} - G\hat{Q}) F^{-1} b \quad (14)$$

This can be rearranged to reflect that either the state variable u_1 or flux q_2 is known at each node

$$\begin{bmatrix} H_{u_1} & H_{u_2} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} - \begin{bmatrix} G_{q_1} & G_{q_2} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = C. \quad (15)$$

Rearranging so that all the unknowns are on the left-hand side results in

$$\begin{bmatrix} -G_{q_1} & H_{u_2} \end{bmatrix} \begin{bmatrix} q_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} -H_{u_1} & G_{q_2} \end{bmatrix} \begin{bmatrix} u_1 \\ q_2 \end{bmatrix} + C. \quad (16)$$

which is in the form of $Ax = B$ which can be solved using the Matlab linear system solver. Note that the matrices G and H are fully populated and nonsymmetric. Typically 95% of the simulation time is spent forming the matrices G and H and the remaining 5% in solving the linear system of Eq. 16.

Note that only boundary elements are required for homogeneous equations, and that no approximations were made other than the discretization of the boundary and numerical integration. Internal nodes are required for nonhomogeneous equations using DR-BEM which introduces an approximation in the evaluation of the volume integral. In contrast, the FEM introduces approximations in the solution over each element as well as discretization and numerical integration approximations. Even with a coarse boundary mesh and few internal nodes, the DR-BEM is extremely accurate compared with a much finer volume mesh used in FEM. Using DR-BEM allows the problem to be easily discretized with coarse meshes leading to low memory requirements allowing its implementation on standard personal computers.

Similar DR-BEM expansions for the Navier fundamental solution [11] are readily generated such that

$$Ad - Bt = C \quad (17)$$

where d_i is the displacement and t_i is the traction at node i .

Thermoelastic problems can be written as two matrix equations

$$\begin{aligned} Hu - Gq &= C_1 \\ Ad - Bt + Eu - Fq &= C_2 \end{aligned} \quad (18)$$

where the temperature u and flux q are solved from the thermal Laplace equation and d and t are the resulting elastostatic deflection and traction, respectively. If the thermal variables u, q do not rely on the elastostatic deflection t , then the thermal and thermoelastic equations can be solved simultaneously.

Coupled electrostatic and elastostatic field equations can be written as two matrix equations

$$\begin{aligned} Hu - Gq &= C_1 \\ Ad - Bt - Fq &= C_2 \end{aligned} \quad (19)$$

where the electrostatic force is calculated in the F matrix. Due to the strong coupling between the Laplace solution the elastostatic deflection, these coupled equations must be solved using iteration.

For modal analysis, the problem to be solved is

$$\nabla^2 u + \omega^2 u = 0 \quad (20)$$

which is of the form Eq. 4 where $b = -\omega^2 u$. In this case Eq. 14 can be rewritten as

$$C = \omega^2 (H\hat{U} - G\hat{Q}) F^{-1} u \quad (21)$$

which can be repartitioned [12] to form a generalized eigenvalue problem

$$Ku = \omega^2 Mu \quad (22)$$

where Matlab can solve for the eigenvalues and eigenvectors. Note that since the matrices are full and nonsymmetric, complex eigenvalues may result due to numerical discretization.

ELECTROSTATIC EXAMPLES

3D electrostatic fields must be addressed even for nominally planar geometries such as parallel-plate capacitors. While the BEM program FASTCAP [6] can solve Laplace's equation with constant dielectrics, it has several disadvantages including the use of constant elements, no provision for symmetry planes to simplify modeling, and no provision for groundplanes. The present program can solve the more general Poisson's equation allowing for continuously varying dielectrics. Further, it fully supports the use of symmetry planes and groundplanes. Finally, it uses isoparametric elements allowing linear or quadratic interpolation of the potential and flux over the element resulting in much higher accuracy with fewer elements.

Simple parallel-plate example

The potential and flux are calculated for the 3D parallel-plate over a groundplane as shown in Figure 3. The model consists of the surfaces of the plate (width=4, thickness=2) and an underlying groundplane (gap=2) forming a capacitor. The arrows indicate the flux direction and magnitude. Note the flux concentration along the bottom surface edges. This concentration leads to a higher capacitance than the ideal parallel-plate model indicates.

Figure 3. Cross-section of 3D parallel-plate over a groundplane showing equipotential lines and flux. Note the flux concentration along the corners.

The fringing field capacitance associated with each surface is calculated and shown in Figure 4 for the 2D case and in Figure 5 for the 3D case.

Figure 4. Capacitance of 2D parallel plate showing the fringing field contributions from the bottom, side and top surfaces.

The 2D BEM simulations show that the capacitance is about 2x larger than the ideal 2D parallel-plate capacitor. As shown in Table 1, the 2D BEM shows relative errors >1% compared to the exact 2D conformal mapping capacitance. While no analytical solution for the 3D parallel-plate capacitance exists, simulations show that the converged 3D BEM capacitance is about 6x larger than the ideal 3D parallel-plate.

Figure 5. Capacitance of 3D parallel plate showing the fringing field contributions from the bottom, side and top surfaces.

For large plate thicknesses, the total sidewall area rapidly becomes larger than the bottom surface area. The flux concentration along the bottom and side edges increases the capacitance of the plate, accounting for the large capacitance difference between the calculated 2D and 3D models. The simulation times on a Macintosh PowerPC portable computer is also shown in Table 1.

TABLE 1: 2D WIRE CAPACITANCE RATIO C/C_{IDEAL}

thickness gap=2 width=4	2D BEM 26 elements (5 sec)	2D BEM 104 elements (110 sec)	conformal mapping [13]
0.25	2.43 (10.3%)	2.23 (1.2%)	2.21
0.5	2.45 (7.9%)	2.28 (0.4%)	2.27
1	2.52 (6.2%)	2.38 (0.2%)	2.38
2	2.67 (5.5%)	2.53 (0%)	2.53
4	2.90 (5.7%)	2.71 (-1.4%)	2.75
8	3.24 (7.0%)	2.91 (-3.9%)	3.03

Electrostatic comb-finger

Another common structure requiring accurate flux calculation is the electrostatic comb-finger used for forcing and transduction in resonators. The BEM model comprises a rotor finger, a stator finger and a groundplane. Symmetry planes are used such that the model represents a section of an infinite comb-finger array. From the flux results shown in Figure 6, the capacitance and electrostatic forces are directly calculated. Note that no deflection of the rotor is required to calculate the force as is the case with a FEM analysis. The capacitance (Figure 7), lateral electrostatic force (Figure 8) and levitation electrostatic force (Figure 9) are shown for different comb-finger rotor positions. The capacitance and force calculations use the permittivity $\epsilon = 1$.

Note that the drive force does not increase monotonically as the comb-fingers engage due to charge cancellation on the finger sidewalls, an effect which has not previously been reported. The maximum lateral force is obtained when the fingers do not engage: all the flux lines from the sides and tip of the rotor finger then have a component in the x-direction. As the fingers engage, most of the flux on the sides of the rotor no longer has an x-component which reduces the total lateral force. As the rotor tip approaches the sta-

tor anchor, the parallel-plate effect becomes dominant and the attractive force increases.

Also note that the levitation force is 4x larger than the lateral force. If this is undesired, a different shaped groundplane may be used to minimize the levitation force. The capacitance due to the fringing field is about 2x larger than the ideal overlapping plates. A large part of this capacitance can be treated as a constant parasitic capacitance since the lateral drive force is approximately the same as expected for ideal overlapping plates. The levitation force is about 3x larger than expected however due to fringing field components.

Figure 6. Electrostatic flux distribution on a section of an infinite comb-finger assembly.

Figure 7. Comb-finger capacitance as a function of rotor position.

Figure 8. Lateral electrostatic force on comb-finger rotor as a function of rotor position.

Figure 9. Levitation electrostatic force on comb-finger rotor as a function of rotor position.

Electrostatic etch-holes

A 3D BEM model of a plate with etch-holes is shown in Figure 10. Symmetry planes on the vertical surfaces are defined such that the model represents a section of an infinite plate.

Figure 10. BEM model of a section of an infinite parallel plate with etch-holes.

The capacitance matrix consisting of capacitance contributions from the bottom, side and top surfaces is calculated for different size etch-holes. Large etch-holes do not significantly reduce the total capacitance since the flux associated with the edges and side-wall fringing increases. For the same reason, a parallel plate with small etch holes has a larger capacitance than an ideal parallel plate.

Figure 11. Capacitance vs. etch-hole width. The fringing field contributions from the bottom, side and top surfaces are shown.

The flux concentration along the edges of the bottom plate due to the etch-holes result in a bottom plate capacitance contribution

larger than that expected compared to an ideal parallel plate capacitor of the same area. With larger etch-holes, the capacitance contribution from the side walls becomes significant. The capacitance contribution from the top surface is negligible. As Figure 11 shows, an effective capacitance approximation is to ignore the effect of any etch-holes on a parallel-plate.

DIAPHRAGM WITH COUPLED FIELDS

Consider the diaphragm pressure sensor as an example of a common micromachined structure under the influence of several different coupled fields. During the fabrication process, a residual stress and residual stress gradient results in a warping of the diaphragm. During operation, pressure is applied resulting in an elastostatic deformation of the diaphragm. This deformation is capacitively measured by applying a voltage differential between the bottom of the diaphragm and the groundplane. If the resulting electrostatic field is large, the diaphragm will deflect due to the large attractive electrostatic forces. Finally, the natural frequencies of the structure are to be calculated. The effect of each of these applied fields are simulated below using a simple 2D model for clarity.

The diaphragm 2D BEM model consists of two closed regions: the diaphragm and the space between the diaphragm bottom surface and groundplane. The model consists of 30 nodes and 40 linear elements as shown in Figure 12. The appropriate boundary conditions and material properties are defined for each region.

Figure 12. 2D BEM model of diaphragm pressure sensor consisting of 30 linear elements and 19 internal nodes.

Stress gradient deflection

Surface micromachined structures typically have residual strains σ and residual strain gradients Γ from the fabrication process. The strain gradient Γ results in a warping of the structure which must be modeled. Rather than apply stresses directly to the model, it is possible to calculate an equivalent temperature and temperature gradient which will result in the same stress state. Assuming a stress field varying in the z direction, a temperature field causing the same average stress and deflection is

$$\sigma(z) = E\alpha T(z) = E\alpha \left[T(0) + T'(0)z + \frac{T''(0)z^2}{2!} + \dots \right] \quad (23)$$

By identifying terms one obtains expressions for the average temperature and the linear temperature gradient:

$$\sigma|_{z=0} = E\alpha T|_{z=0} \quad (24)$$

$$\Gamma = \sigma'|_{z=0} = E\alpha T'|_{z=0} \quad (25)$$

The residual stress and stress gradient are modeled by applying a temperature T_1 to the top surface and T_2 to the bottom surface of the diaphragm. The resulting heat problem is readily solved for any unknown node temperatures and element temperature flux. These thermal state variables are then used to calculate the ther-

mal elastostatic stress state. Any externally applied elastostatic deflections and tractions can also be linearly added. In this case, the ends of the diaphragm were specified as fixed $d = 0$ and no external tractions t were applied. The resulting thermoelastic deformation is shown in Figure 13.

Figure 13. Deflection of diaphragm due to residual stress gradient.

Pressure deflection and capacitance

A pressure over the diaphragm is applied by specifying t at each element node on the top surface. Note that because the elements use linear interpolation, a constant t corresponds to a constant evenly applied pressure across the diaphragm. The resulting deflection due to the residual strain gradient and applied pressure is shown in Figure 14. The resulting capacitance can be calculated by applying arbitrary voltages u_1 , u_0 to the bottom of the diaphragm and the groundplane. The resulting electrostatic problem is in the form of Laplace's equation which is readily solved for any unknown node voltage and element electrostatic fluxes.

Figure 14. Deflection of diaphragm due to applied external pressure and residual stress gradient. (The tractions t are defined normal to the diaphragm surface.)

Electrostatic force and deflection

Depending on the diaphragm configuration, the attractive electrostatic forces due to the applied sense voltage can cause significant deflections. This elastostatic deflection in turn changes the electrostatic forces. This coupled problem can be solved by iterating between the elastostatic and electrostatic solvers until the change in deflection is not significant. Figure 15 shows the deflection of the diaphragm due to electrostatic forces, applied pressure and residual stress gradient. Equipotential lines and flux arrows are also shown.

Figure 15. Deflection of diaphragm due to differential sense voltage, applied pressure, and residual stress gradient.

Modal analysis

The DR-BEM can be used to calculate the eigenvalues and mode shapes of the diaphragm. The additional stiffness caused by the applied electrostatic forces, pressure and residual stress gradients has not been included. An additional 19 internal nodes were arranged along the centerline of the diaphragm to form the right-hand side of Eq. 21. Rearranged into effective spring and mass matrices of Eq. 22 allows Matlab to directly calculate the eigenvalues and eigenmodes. Due to discretization approximations, some of these eigenvalues are complex. The first eigenvalues agree closely with those expected for a fixed-fixed diaphragm.

ACCELEROMETER WITH COUPLED FIELDS

Complex 3D structures such as lateral surface micromachined accelerometers can be modelled and simulated in the same manner. Figure 16 shows the exaggerated deflection of the accelerometer due to the same stress gradient. The BE mesh is used to solve for the elastostatic field *inside* the polysilicon structure. The same BE mesh is used to calculate the electrostatic field *outside* the polysilicon structure. In order for the capacitance calculations to converge, many elements are required along the edges of the comb-fingers. Since both FEM and BEM problems scale as $O(N^2)$, this leads to lengthy simulations. Each electrostatic and elastostatic iteration required 0.4 and 6 hours on a Macintosh PowerPC portable computer. The natural frequencies and eigenmodes agree closely with traditional FEM analysis.

Figure 16. Deflection of surface micromachined accelerometer due to residual stress gradients. The ground-plane and stator fingers are not shown for clarity. (Z-axis scaled by 100)

CONCLUSIONS

A new portable BEM tool able to solve arbitrary 2D and 3D Poisson and Navier field equations has been introduced. The modeling effort is minimized since only the boundaries of the field must be described. Further, a single model is sufficient to allow sequences of different field equations to be solved. The compact model and DR-BEM formulation allows the software to be implemented in portable vectorized Matlab code on standard personal computers. Several electrostatic, elastostatic and thermoelastic fields in common micromachined structures are solved using this portable CAD tool.

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