Published in final edited form as:

IEEE Trans Ultrason Ferroelectr Freq Control. 2018 January ; 65(1): 50–59. doi:10.1109/TUFFC.

2017.3772331

A hybrid boundary element model for simulation and optimization of large piezoelectric micromachined ultrasonic transducer arrays

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A hybrid boundary element model is proposed for the simulation of large piezoelectric micromachined ultrasonic transducer (PMUT) arrays in immersion. Multi-physics finite element method (FEM) simulation of a single membrane structure is used to determine stiffness and piezoelectrically-induced actuation loading of the membranes. To simulate arrays of membranes in immersion, a boundary element method (BEM) is employed wherein membrane structures are modeled by a surface mesh which is coupled mechanically by mass, stiffness, and damping matrices, and acoustically by a mutual impedance matrix. A multi-level fast multipole algorithm (ML-FMA) speeds up computation time and reduces memory usage, enabling the simulation of thousands of membranes in a reasonable time. The model is validated with FEM for a small 3 by 3 matrix array for both square and circular membrane geometries. Two practical optimization examples of large PMUT arrays are demonstrated: membrane spacing of a 7 by 7 matrix array with circular membranes, and material choice and top electrode coverage of a 32-element linear array with 640 circular membranes. In addition, a simple analytical approach to electrode optimization based on normal mode theory is verified.

I. Introduction

MICROMACHINED ultrasonic transducer arrays based on flexible membrane structures have gained traction in the last decade as a viable alternative to traditional bulk piezoelectrics which have been the dominant transducer technology for non-destructive evaluation [1], medical imaging [2], medical therapeutics [3], and many other applications. These membrane transducers may be actuated electrostatically in the case of capacitive micromachined ultrasonic transducers (CMUTs) or by induced bending moment in the case of piezoelectric micromachined ultrasonic transducers (PMUTs). In both cases, the primary advantage is a closely-matched impedance with water without the complex matching layers associated with bulk piezoelectrics. Furthermore, membrane-based designs are suitable for wafer-level microfabrication for applications where small size and high element density are critical. Benefits of micromachining include improved manufacturing control, per device cost reduction with batch processing, and the potential for direct integration with CMOS electronics [4], [5].

Recently, considerable focus has been placed on design and manufacturing of PMUT arrays. Unlike their capacitive counterpart, PMUTs do not require bias voltages and have a higher capacitance and lower electrical impedance suitable for integration with low voltage electronics. Looking at just the past few years, PMUT arrays have been demonstrated in

devices for applications such as wireless energy transfer [6], ultrasonic fingerprint sensing [7], and intracardiac imaging [8]. With expanding interest in large PMUT arrays, there exists a need for practical and accurate simulation tools to aid in the design process.

To date, many authors have contributed to the growing literature on PMUT modeling and optimization. Perhaps the most fundamental approach is to consider analytical solutions based on boundary-fixed thin circular disks. For instance, in [9], differential equations were derived to describe the static deformation of a piezoelectric unimorph actuator with full electrode coverage. Solutions were obtained by considering axisymmetric deflection of the PMUT with simple support boundary conditions under a uniform load or concentrated load. In [10], general solutions in the form of Bessel (and modified Bessel) functions were obtained for the case of harmonic excitation of a unimorph PMUT with partial piezoelectric and electrode layers. The addition of partial layers introduces extra boundary conditions which must be satisfied in conjunction with the condition for the perimeter. Analytical solutions for other PMUT geometries have also been explored, including curved PMUTs with spherical diaphragms [11] and bimorph PMUTs actuated with opposite phase [12].

Another effective approach, particularly suitable for geometries with multiple electrodes, is to consider normal mode solutions to the governing equation of motion. For example, in [13], a lumped electromechanical model was obtained by consideration of the first mode shape only of a rectangular clamped membrane. In [14], [15], the problem of multiple layer, multi-electrode PMUTs was explored, wherein a Green's function solution was proposed and solved by projection onto the normal modes of a clamped circular disk. A similar approach was used by Sammoura et. al. to develop an equivalent circuit model, with the addition of residual stress and consideration only of the first two axisymmetric modes [16]. Finally, a numerical approach was proposed based on a build-test finite element model, where parameters such as coupling coefficient, acoustic impedance, and resonance frequency are extracted from the model for the purpose of optimization [17].

In all the preceding contributions, the focus has been on accurate modeling of single PMUTs in vacuum and air, or in fluid by first-order approximation of the PMUT as a circular piston radiator. However, when placed in the context of an array, it is well known that membrane-based transducers in immersion will be affected by fluid-born and potentially substrate-born mechanical waves which couples the dynamics of the individual membranes together. In CMUT arrays, the phenomena of acoustic cross-talk has been characterized extensively in simulation and in experiment [18]–[20]. It has been found that these coupled waves can drastically change the dynamic response of CMUTs and create interference in the primary band that degrades the bandwidth and directionality performance of the transducer. Accurate simulation of these physics is therefore critical to the design and optimization of membrane-type transducer arrays.

Unfortunately, for large arrays composed of hundreds of individual membranes, simulation with finite element method (FEM) is computationally prohibitive. In some restrictive cases, assumptions can be made about the periodicity and symmetry of the problem to reduce the total mesh size [18], [21], [22]. Other authors have developed electromechanical mesh network models where membrane-to-membrane interactions are calculated from analytical

expressions for fixed-boundary circular disks [23]–[25]. Specifically, the mutual radiation impedance of two fixed-boundary vibrating disks is derived by assuming axisymmetric deflection profiles represented by finite power series which satisfy the boundary condition at the disk perimeter. This modeling approach is also employed by Akhbari et. al. in a notable recent work on PMUT arrays [26].

In this paper, we develop a practical simulation tool for large PMUT arrays with a focus on the accurate capture of acoustic cross-talk. A boundary element method (BEM) simulation is employed where membrane motion is represented by a surface mesh. Membrane dynamics such as stiffness and piezoelectrically-induced actuation loading are extracted from finite element method (FEM) simulation of a single membrane structure. Acoustic interactions are calculated using a multi-level fast multipole algorithm (ML-FMA), which we have reported on previously [27]. This approach has a number of distinct advantages when compared with previous models. First, because acoustic interactions are calculated on a node-to-node basis, membranes are not restricted to simple axisymmetric deflection. In fact, we have shown previously that high-order modes and anti-symmetric modes may contribute to cross-talk, even within the first frequency band of the transducer [27]. Second, by utilizing FEM simulation, the BEM model is generalized to cover more complicated membrane structures. Here, the only restrictions on the membrane structure is that it is approximately flat, it operates linearly about its static position, and that it can be simulated feasibly with FEM. Although we do not demonstrate all these cases here, the method applies equally to PMUT geometries featuring small curvature (domed), pre-stressed layers, mass-loading, multiple layers, low aspect ratio (thick), and complex boundary terminations. Finally, through the application of a multi-level fast algorithm, arrays with thousands of membranes can be simulated with reasonable computational resources.

The structure of the paper is as follows. In Section II, the methods of the proposed hybrid boundary element model are described. In Section III, the model is validated by comparison with FEM simulation for a 3 by 3 array for both circular and square membrane geometries. In Section IV, two simulation and optimization examples of large PMUT arrays are demonstrated: (1) a matrix array with 49 membranes, and (2) a 32-element linear array with 640 membranes. Finally, discussion and concluding remarks are given in Section V.

II. Methodology

A. Boundary element method simulation for membrane-type transducers

Micromachined piezoelectric transducers based on a membrane-type design (sometimes referred to as flextensional) are composed of alternating layers of active (in the piezoelectric sense) and passive materials suspended over a vacuum or air-filled gap. When the active layers are driven by an electric field, uneven expansion and contraction between the layers results in deflection of the membrane. A standard PMUT design is depicted in Fig. 1. We consider here, without loss of generality, a simplifying case of this design: a single elastic layer of thickness h_m bonded to a piezoelectric layer of thickness h_p .

A numerical model of membrane motion based on the boundary element method strikes a good balance between complexity and efficiency, achieved by leveraging boundary integral

equations for acoustics. Such a model has been demonstrated extensively in previous works for the simulation of CMUTs [28]–[32]. In BEM, the problem is compressed from three dimensions (x, y, z) to two (x, y) . A surface mesh is defined, where equilibrium for the mesh nodes are described in terms of lumped mass, damping, stiffness, and radiation impedance. This is expressed by the following complex linear system of angular frequency ω , vertical displacement $\vec{w}$, and actuating load $\vec{p}_{act}$

$$(-\omega^2 \mathbf{M} + i\omega \mathbf{C} + \mathbf{K} + i\omega \mathbf{Z}_{rad}) \vec{w} = \vec{p}_{act} \quad (1)$$

Here, $\mathbf{M}$ is a mass matrix with diagonal entries representing the mass per unit area of each node, i.e. $M_{ii} = \rho_m h_m + \rho_p h_p$ in the case of a composite plate, where ρ_m is the density of the elastic material and ρ_p is the density of the piezoelectric material. $\mathbf{C}$ is a damping matrix, where we have chosen to employ a simple nodal damping model such that the diagonal entries are $C_{ii} = \beta$ for some damping coefficient β .

Coupled behavior of the nodes arises from the two remaining matrices. The $\mathbf{K}$ matrix captures the mutual stiffness between nodes of the membrane. For a thin plate, $\mathbf{K}$ can be derived by finite difference approximation of the equation of motion (see Appendix A). For example, the fourth derivative at a node x_n can be approximated by the following second-order finite difference

$$\frac{\partial^4 f_n}{\partial x^4} \approx \frac{1}{\Delta x^4} \begin{bmatrix} -1/12 \\ 4/3 \\ -5/2 \\ 4/3 \\ -1/12 \end{bmatrix}^T \begin{bmatrix} f_{n-2} \\ f_{n-1} \\ f_n \\ f_{n+1} \\ f_{n+2} \end{bmatrix} + O(\Delta x^4) \quad (2)$$

where Δx is the node spacing and the shorthand notation $f_n = f(x_n)$ is used. Decomposition of ∇^4 into finite differences will yield a stencil relating the displacement of a node with the displacement of its neighbors. However, it will be shown that $\mathbf{K}$ can be derived more accurately and for a wider range of membrane geometries from FEM simulation.

The mutual radiation impedance matrix $\mathbf{Z}_{rad}$ captures the acoustic cross-coupling between nodes. The nodes are modeled as simple sources of surface area a_j which radiate according to the three-dimensional free space Green's function. The nodes' self impedances are approximated by that for piston radiators. In both cases, it is assumed that the sources radiate in an infinite rigid baffle. The entries of $\mathbf{Z}_{rad}$ are

$$Z_{rad}^{ij} = \begin{cases} i\omega \rho a_j \frac{e^{-ik|\vec{r}_i - \vec{r}_j|}}{2\pi|\vec{r}_i - \vec{r}_j|}, & \text{for } i \neq j \\ \rho c \left[\frac{1}{2\pi} k^2 a_j + i \frac{8}{3\pi} k \left(\frac{a_j}{\pi} \right)^{1/2} \right] & \text{for } i=j \end{cases} \quad (3)$$

where ρ is the fluid density, c is the fluid sound speed, k is the wavenumber, and $\vec{r}_i$ and $\vec{r}_j$ are the vectors pointing to the i -th and j -th node, respectively.

Finally, the vector $\vec{p}_{act}$ is a placeholder for the normal load applied by the actuating mechanism. In the case of PMUTs, $\vec{p}_{act} = \vec{p}_{piezo}$ is a result of the application of an electric potential which introduces a strain mismatch between the piezoelectric and elastic layer via the inverse piezoelectric effect. For thin membranes, this effect can be expressed analytically by a bending moment function which depends on the size and shape of the top electrode (see Appendix A). An equivalent normal load representation (i.e., the piezoelectrically-induced actuation loading) of this bending moment will necessarily contain step and spatial derivatives of delta functions. For example, for a rectangular top electrode geometry bounded by $x = \pm x_e$ and $y = \pm y_e$, the equivalent normal load for a voltage V_0 is given by

$$p_{piezo} = \frac{d_{31} Y_p V_0 (z_2 + z_1)}{2(1 - \nu_p)} \left[(\delta'(x + x_e) - \delta'(x - x_e)) \times (H(y + y_e) - H(y - y_e)) + (\delta'(y + y_e) - \delta'(y - y_e)) \times (H(x + x_e) - H(x - x_e)) \right] \quad (4)$$

where $\delta(\cdot)$ is the Dirac delta function, $H(\cdot)$ is the Heaviside step function, and the prime specifies the derivative with respect to the argument. The prefactor depends on the piezoelectric material constants, namely the Young's modulus Y_p , Poisson's ratio ν_p , piezoelectric strain coefficient d_{31} , and geometrical constants $z_1 = h_m - c$ and $z_2 = h_m + h_p - c$ which are related to the coordinate of the neutral plane c .

The equivalent normal load representation can be understood as the application of a pair of opposing normal loads at the boundaries of the top electrode, creating a bending moment with magnitude in proportion to the applied voltage. Upon inspection of (4), the appearance of step functions and delta function derivatives makes numerical implementation difficult, if not impossible. A natural idea is to smooth the discontinuities of this function by filtering or perhaps by employing sigmoid functions. However, to achieve reasonable accuracy, such an approach would necessitate very fine spatial sampling around sharp features that would greatly increase mesh size to the point of impracticality for large simulation. Rather than attempt to find a suitable analytical approximation of (4), we seek a numerical equivalent obtained by utilizing FEM simulation of a single membrane structure. This procedure is detailed in the following section.

B. Extracting parameters from finite element method simulation of a single membrane

The piezoelectrically-induced actuation loading $\vec{p}_{piezo}$ is determined by matching BEM simulation and FEM simulation of a single membrane structure. Consider the linear system for a single membrane with mass, stiffness and radiation impedance denoted by $\mathbf{M}_1$, $\mathbf{K}_1$, and $\mathbf{Z}_{1rad}$ respectively.

$$(\omega^2 \mathbf{M}_1 + \mathbf{K}_1 + i\omega \mathbf{Z}_{1rad}) \vec{w} = \vec{p}_{piezo} \quad (5)$$

We build, as closely as possible, a multi-physics model of the membrane in FEM software and solve for the case of 1 V harmonic excitation. We have chosen to omit mechanical damping in both BEM and FEM, although damping from radiation has been retained in order to avoid sharp resonance peaks. The displacement of the membrane $\vec{w}_{fem}$ is extracted from FEM at grid points corresponding to the BEM surface mesh. With this solution in hand, (5) is solved for $\vec{p}_{piezo}$, obtaining a numerical approximation which can be considered exact for the given boundary element model and surface mesh.

$$\vec{p}_{piezo} \approx (-\omega^2 \mathbf{M}_1 + \mathbf{K}_1 + i\omega \mathbf{Z}_{1rad}) \vec{w}_{fem} \quad (6)$$

In this way, at each frequency, it is ensured that the displacement $\vec{w}_{fem}$ for a single membrane is enforced in the boundary element model. It is important to note that this model assumes linear PMUT operation which may not be true for cases of large excitation voltage and for specific piezoelectric materials (for example, see [33]). This simple but effective procedure results in an efficient framework which combines the general power of FEM with the numerical efficiency of BEM. Here, FEM handles the complex electromechanical coupling which determines the single membrane behavior, while BEM handles the large-scale fluid-structure radiation which determines the overall behavior of the array. An example of the piezoelectrically-induced actuation loading obtained using this method is shown in Fig. 2. Naturally, the accuracy of this approach will depend on the ability to correctly match the relevant physics in both BEM and FEM.

FEM simulation can also be used to determine the stiffness matrix $\mathbf{K}$ for membrane geometries that are not described accurately by thin-plate theory. Note that $\mathbf{K}$ is block-diagonal with blocks $\mathbf{K}_1$. The following procedure was first proposed by Zahorian et. al. [5]. Static deformation of the membrane is calculated under a 1 Pa load applied individually to each node of the membrane. Care is taken to ensure that the boundary element and finite element nodes correspond to the same locations. For each applied load, the displacements calculated on the node grid of N total nodes are used to form the columns of the compliance matrix $\mathbf{K}^{-1}$. That is,

$$\mathbf{K}_1 = [\vec{w}_1 \ \vec{w}_2 \ \dots \ \vec{w}_N]^{-1} \quad (7)$$

where $\vec{w}_n$ is the displacement for loading of the n -th node. By obtaining stiffness $\mathbf{K}_1$ and piezoelectrically-induced actuation loading $\vec{p}_{piezo}$ from FEM, simulation of common PMUT designs, such as those with stepped layers (e.g. mass-loaded), low aspect ratios, and multiple layers, is possible.

C. Implementation details

Practical implementation of these procedures was carried out using a combination of commercial, open source, and in-house tools. Single membrane behavior, defined by the piezoelectrically-induced actuation loading and membrane stiffness matrix, was determined from models built and simulated using finite element software (COMSOL multiphysics, COMSOL Group, Burlington, MA).

To obtain the piezoelectrically-induced actuation loading of (6), membrane displacement under 1 V harmonic actuation was solved using a quarter symmetric multi-physics model of a single membrane in a fluid (water) half-space. The membrane geometry consisted of boundary-clamped piezoelectric and elastic layers, wherein full material anisotropy were considered. Electrode layers (typically on the order of 100 nm), were omitted to avoid the meshing of very thin domains. Electric potential was applied across the surfaces of the piezoelectric layer in accordance with the desired electrode coverage. The displacement solution of the model was extracted at points corresponding to the nodes of a surface BEM mesh of the same membrane.

This model was meshed in accordance with standard meshing procedures for fluid-structure interaction. Auto-generated free tetrahedral meshes were used for the structural and fluid domains, with a maximum element size enforced to ensure that the mesh contained at least 5 elements per wavelength. For the absorption of radiating and evanescent waves, the fluid domain was surrounded by a hemi-spherical polynomial perfectly matched layer (PML) with a swept mesh containing 5 elements along the radial direction. Note that this meshing strategy is fairly conservative, with considerable room for further optimizations (e.g. swept meshes for structural domains and frequency-adaptive element sizing).

To determine the membrane stiffness matrix $\mathbf{K}$, a purely structural model—without fluid, piezoelectric, or electrostatic physics—was built of the membrane using COMSOL. A static pressure load with area $\Delta x \Delta y$, where Δx and Δy are the node spacing of a corresponding surface BEM mesh, was applied to the mid-plane at the location of a specified node. This model was solved iteratively for different locations of the pressure load using a MATLAB (MathWorks, Natick, MA) script which automatically builds, meshes, and solves the corresponding geometry.

With both harmonic membrane displacement and membrane stiffness information, the piezoelectrically-induced actuation loading was determined from the single membrane BEM model of (6). Finally, large array behavior was simulated by using the piezoelectrically-induced actuation loading as an input to an in-house BEM fast multipole solver. This code is built on several open source tools: Python (Python Software Foundation), Cython (optimising compiler), NumPy (multi-dimensional arrays), and SciPy (scientific programming). For implementation details of our solver, please refer to [27].

III. Validation with finite element method software

For validation purposes, a 3 by 3 matrix array was simulated using both the proposed hybrid method and exclusively in COMSOL. The simulated membranes consisted of a 1 μm thick

lead zirconate titanate (PZT) layer deposited on a 2.2 μm silicon oxide layer, both extending across the entire membrane. For simplicity, the default material properties from COMSOL were used (specifically, bulk PZT-5H and isotropic SiO_2 with $\rho_m = 2200 \text{ kg/m}^3$, $Y_m = 80 \text{ GPa}$ and $\nu_m = 0.17$); simulation of realistic piezoelectric thin films are explored in Section IV. To avoid the meshing of very thin layers in FEM, the electrode layers (typically on the order of $\sim 100 \text{ nm}$) were omitted from this analysis. The array pitch was 55 μm in both x and y dimensions. Both square membranes (45 by 45 μm) and circular membranes (45 μm diameter) were simulated, with 50% top electrode coverage with respect to the lateral dimension. All membranes were excited in phase with a 1 V harmonic potential for frequencies over a wide range from 0 to 50 MHz. Due to the extensive computation time required, a coarse 500 kHz step was used in COMSOL simulation, with extra refinement (50 KHz step) around significant features. A fine 50 kHz step was used for all simulations with hybrid BEM.

First, mesh convergence behavior of hybrid BEM was investigated by varying the number of nodes from 5 to 29 nodes per membrane dimension (see Fig. 3) Pressure was calculated from displacement via the Rayleigh integral at a distance of 1 mm above the array. Convergence behavior was quantified by observing the change in the solution as the node density is increased. Specifically, a normalized root mean squared difference (NRMSD) pressure magnitude and a root mean squared difference (RMSD) phase are defined as

$$\text{NRMSD} = \frac{\sqrt{\sum_{w,f} (|p_n| - |p_{n-1}|)^2}}{|p_n|_{\max}} \quad (8)$$

$$\text{RMSD} = \sqrt{\sum_{w,f} (\phi_n - \phi_{n-1})^2} \quad (9)$$

where $|p|$ is the pressure magnitude, ϕ is the pressure phase, the subscripts n and $n-1$ denote the current and previous node densities, respectively, and the sum is taken over all nodes and all frequencies. The pressure magnitude is normalized to the maximum observed value $|p_n|_{\max}$ to counter the effect of geometric spreading. At a mesh density of 13 nodes per membrane dimension, the magnitude change is observed to be less than 2% and the phase change less than 0.4 radians.

Next, the simulated displacements from hybrid BEM (square membranes) are compared with the reference results from COMSOL simulation. The mean displacement of the center membrane is plotted as a function of frequency for both cases (see Fig. 4). The comparison indicates that hybrid BEM accurately captures the displacement behavior of the array, predicting the resonance features in the 6 – 9 MHz band, and also around 32 MHz. However, small discrepancies (less than 300 kHz) are observed in the predicted frequency at which these features occur. These discrepancies are attributed to approximation error resulting from the point source model employed in BEM.

Finally, the pressure response calculated at a distance of 1 mm from the center of the array is shown in Fig. 5. For both square and circular membranes, the pressure response shows good agreement between hybrid BEM and COMSOL simulation. Here, the small discrepancies in the displacement response are mostly reduced by the integration over the surface of the array.

IV. Large array simulation and optimization examples

With the efficiency of hybrid BEM, optimization of large PMUT arrays can be performed in a reasonable time. Two examples of large array simulation are demonstrated here.

A. Investigating cross-talk phenomena with a 7 by 7 matrix array

A 7 by 7 matrix array with circular membranes was simulated (material properties and geometry remain the same). Top electrode coverage was set to 70% of the membrane diameter. This membrane was found to have a first resonance in water at $f_o = 8.75$ MHz. Array pitch was $55 \mu\text{m}$, corresponding to an area fill-factor of 53%.

The response of the array was investigated for the cases of excitation of the center membrane only and excitation of all membranes. The mean displacement response of the center membrane in each case is plotted as a function of frequency in Fig. 6. It is apparent that significant array modes (dispersive-guided modes) are excited in the 8 – 9 MHz range due to cross-coupling of the first membrane mode. For an array pitch of $55 \mu\text{m} < \lambda_o/2$, where $\lambda_o = 171 \mu\text{m}$ is the wavelength associated with the first membrane resonance f_o , both subsonic trapped modes (with associated phase speed below c) and leaky supersonic modes (with associated phase speed above c) are supported by the array [20]. Broadening of the bandwidth associated with increased aperture size is also observed when comparing center and full excitation cases. A secondary array mode is excited around 19 MHz corresponding to coupling of a higher-order mode.

It has been shown that cross-talk phenomena is strongly contingent on membrane size and spacing which may be useful parameters for optimization [23], [34], [35]. Additionally, total radiation resistance, which is related to power efficiency [34], can be extracted from the acoustic impedance matrix. Hybrid BEM can be a powerful tool for the comprehensive exploration of these parameter spaces. Simulations were performed to investigate the effect of array pitch in PMUT matrix arrays. A 7 by 7 matrix array with pitches d of 0.3, 0.4, 0.5, 0.6, 0.8 and 1.0 of λ_o was simulated. The corresponding area fill factors were 60%, 34%, 22%, 15%, 8%, and 5%, respectively. In each case, the entire array was excited and the resulting mean displacement response plotted (see Fig. 7).

A number of notable phenomena are observed. For pitches of $0.3\lambda_o$ and $0.4\lambda_o$, both subsonic and supersonic array modes are excited in a small region around the single membrane resonance, resulting in large resonant peaks and dips around f_o . In comparison with the single membrane response, the center frequency shifts upward and the overall bandwidth increases. For imaging applications, it will be typical to operate in this region for the broad bandwidth and fulfillment of the $\lambda/2$ Nyquist criterion. As the array pitch increases, the wavelengths associated with the same array modes lengthen, increasing their

associated phase speeds. When the membrane spacing exceeds $\lambda_o/2$, these phase speeds fall above c , and the array modes no longer appear as resonant peaks and dips in the response. Additionally, an increase in the peak displacement and narrowing of the bandwidth is observed with peak displacement occurring around $d = 0.8\lambda_o$. This suggests that, for narrowband applications, output pressure may be maximized by a sparse arrangement of membranes, as opposed to a tightly-packed arrangement, assuming the moving surface area remains the same in both cases. Eventually, as the membrane spacing tends to infinity, it is expected that the membranes will behave independently and the mean array displacement response will approach that of a single membrane. The asymptotic behavior of the response is verified with a pitch of $10\lambda_o$.

In Fig. 8a, the topography of the array is depicted at 8.75 MHz for harmonic excitation of all membranes. Here, the effect of acoustic cross-talk is shown clearly to enhance and/or suppress the average displacement of certain membranes depending on their geometric relation within the array. Furthermore, deflection profiles at zero phase, obtained along x -directed slices of the membranes, reveals complexity of the deflection beyond vibration of the first membrane mode. The normalized profiles for all 49 membranes, shown in Fig. 8b, indicate contribution from higher-order modes. This shows conclusively that membrane motion, even when excited in an axisymmetric manner, may exhibit non-axisymmetric motion due to the complex acoustic interaction between membranes.

B. Optimization of a 32-element linear PMUT array

As an example of practical optimization of realistic arrays, such as those one may find in diagnostic imaging applications, a very large 32-element linear PMUT array with 640 membranes was simulated. The circular membranes (45 μm diameter) consisted of a 1 μm piezoelectric layer deposited on a 2.2 μm silicon layer. Several common piezoelectric thin-film materials were considered, the properties of which are listed in Table I. Material properties for aluminum nitride (AlN) [36], [37], zinc oxide (ZnO) [36], [38], and textured PZT [39], [40] were obtained from literature. Since mechanical properties of PZT thin-films are not well-characterized, elasticity values of bulk PZT were used instead. Top electrode coverage was set to 70% of the membrane diameter. Each elements of the array consisted of a single column of 20 membranes. Computation time for each simulation was approximately 5 hrs running on 20 CPU threads at 2.3 GHz.

Channel-to-channel cross-talk was characterized by simulating the response of the array for 1 V excitation of the first element (CH0) only. The membranes (AlN/Si) had a resonant frequency of $f_o = 15.10$ MHz. In Fig. 9, the mean displacement response of select elements is plotted as a function of frequency. Here it is observed that the cross-coupling increases sharply as a function of frequency, reaching a peak around 12.8 MHz due to the excitation of strong array modes. The cross-talk between channels is very significant—within 10 to 20 dB below the level of the excited channel—even for channels located at the center (CH16) and at the opposite end (CH31) of the array.

Optimization of top electrode coverage, which can have a significant effect on the total output pressure (for examples, see [15], [16], [41]), is demonstrated. Simulations were performed for electrode coverage from 10% to 90% of the membrane radius (corresponding

to 1% to 81% area coverage, respectively). All membranes (AlN/Si) were excited in phase and the output pressure response was calculated at a distance of 2 mm. The maximum output pressure (normalized) over the first band is plotted as a function of electrode coverage in Fig. 10 for the cases of full array simulation and single membrane simulation. In both cases, maximum output pressure is obtained for approximately 65% electrode coverage which matches reasonably with the 60% figure of [41].

The simulations suggest that optimal electrode coverage depends primarily on the ability of the electrode shape to couple motion into the first membrane mode. An analytical optimization curve can be derived based on a normal mode solution of the equation of motion for thin membranes (18) in cylindrical coordinates. Consider the piezoelectrically-induced actuation loading function $p_{piezo}(r, \theta)$ in cylindrical coordinates for a top electrode with radius r_e

$$p_{piezo} \propto \nabla^2 (H(r+r_e) - H(r-r_e)) \propto \frac{1}{r} \delta(r+r_e) + \delta'(r+r_e) - \frac{1}{r} \delta(r-r_e) - \delta'(r-r_e) \quad (10)$$

In a normal mode solution, the response is represented by a linear superposition of the mode shapes $\phi_n(r, \theta)$, obtained by solving the homogeneous equation. The contribution of each mode is determined by the projection of the load onto the mode shape. For the first mode, then

$$\langle p_{piezo}, \phi \rangle = \int_0^{2\pi} \int_0^R p_{piezo} \phi_1 r \, dr \, d\theta \quad (11)$$

With the following property

$$\int_{-\infty}^{\infty} \delta^{(n)}(x-y) f(x) dx = (-1)^n f^{(n)}(y) \quad (12)$$

and the fact that ϕ_1 is axisymmetric, it can be concluded that

$$\langle p_{piezo}, \phi \rangle \propto r_e \phi'(r_e) \quad (13)$$

The analytical curve, plotted in Fig. 10, predicts an optimal electrode coverage of about 67%, the difference which can be attributed to violation of the thin membrane condition, neglect of fluid-loading in this analytical approach, and possible contributions from higher-order axisymmetric modes.

A simple design intuition can be gleaned from this result: the electrode boundaries, which dictate the location of the applied bending moment, should be selected to maximize deflection of the desired membrane mode. The analytical curve suggests that the optimal location occurs when the product of the electrode radius and the derivative of the mode shape at that radius is maximized. When generalized to optimization of multiple electrode

designs, the model also suggests that the polarity of neighboring electrodes should alternate to ensure that their associated moments add together. Hybrid BEM can supply additional fine tuning for this type of optimization by accounting for effects not included in the analytical model. Additionally, hybrid BEM provides a method for the numerical calculation and visualization of the piezoelectrically-induced actuation loading function for complex electrode geometries.

Optimization of material choice was investigated by considering the pressure response for phased excitation at 2 mm, shown in Fig. 11. To ensure a fair comparison, membranes with AlN and ZnO layers were thinned while maintaining a constant piezoelectric/elastic thickness ratio (h_p/h_m) of 0.45 in order to match the resonance frequency of PZT/Si. The resulting simulated geometries were: AlN/Si ($f_o = 10.85$ MHz, $h_m = 1.67$ μm , $h_p = 0.76$ μm), ZnO/Si ($f_o = 10.80$ MHz, $h_m = 1.91$ μm , $h_p = 0.87$ μm), and PZT/Si ($f_o = 10.75$ MHz, $h_m = 2.20$ μm , $h_p = 1.00$ μm). Simulation indicates that pressure performance for PZT/Si is over 26 dB better than AlN/Si and over 21 dB better than ZnO/Si. Center frequency and bandwidth are nearly identical in all three cases, with small fractional bandwidth improvements over PZT/Si (29%) for AlN/Si (33%) and ZnO/Si (37%).

V. Conclusion

We have introduced a hybrid boundary element model for the simulation of large PMUT arrays. Model parameters of membrane stiffness and piezoelectrically-induced actuation loading are extracted from finite element method simulation. Simulation of hundreds of membranes is realized through the use of a multi-level fast multipole algorithm. The model was validated against finite element method simulation (COMSOL) for the case of a 3 by 3 matrix array with either square or circular membrane geometries. Through convergence analysis, it was determined that a node density of 13 nodes per membrane dimension was sufficient for a pressure NRMSD below 4% and phase RMSD below 0.4 radians for a wide frequency range of 0 – 50 MHz. Surface displacement indicated good agreement between hybrid BEM and FEM. Cross-talk phenomena and its dependence on array excitation and array pitch was investigated through simulation of a 7 by 7 matrix array with circular membranes. Material and electrode coverage optimization were explored through simulation of a 32-element linear array with 640 membranes.

Acknowledgments

This work was supported in part by the National Institutes of Health under Grant No. U01-HL121838.

Appendix A: Derivation of the piezoelectrically-induced actuation loading

The application of classical thin-plate theory to PMUTs, described in detail by previous authors [9], [10], is briefly reviewed here. In this limit, the moment resultants are expressed in terms of the plate displacement w and applied electric potential $V(x, y)$ as

$$M_x = -D \left(\frac{\partial^2 w}{\partial x^2} + \nu \frac{\partial^2 w}{\partial y^2} \right) - \frac{d_{31} Y_p (z_2 + z_1)}{2(1 - \nu_p)} V(x, y) \quad (14)$$

$$M_y = -D \left(\nu \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial x^2} \right) - \frac{d_{31} Y_p (z_2 + z_1)}{2(1 - \nu_p)} V(x, y) \quad (15)$$

$$M_{xy} = -D(1 - \nu) \frac{\partial^2 w}{\partial x \partial y} \quad (16)$$

where D is the flexural rigidity of the composite plate, ν is its mean Poisson's ratio, and Y_p , ν_p , and d_{31} are the Young's modulus, Poisson's ratio, and piezoelectric strain coefficient of the piezoelectric material, respectively. The coordinates $z_1 = h_m - c$, $z_2 = h_m + h_p - c$ are related to the coordinate of the neutral plane c . For a rectangular top electrode bounded by $x = \pm x_e$ and $y = \pm y_e$, the potential with amplitude V_0 is prescribed in terms of step functions

$$V(x, y) = V_0 (H(x + x_e) - H(x - x_e)) \times (H(y + y_e) - H(y - y_e)) \quad (17)$$

The equation of motion is

$$\frac{\partial^2 M_x}{\partial x^2} + 2 \frac{\partial^2 M_{xy}}{\partial x \partial y} + \frac{\partial^2 M_y}{\partial y^2} + (\rho_m h_m + \rho_p h_p) \frac{\partial^2 w}{\partial t^2} = -D \nabla^4 w + (\rho_m h_m + \rho_p h_p) \frac{\partial^2 w}{\partial t^2} = p_{piezo} \quad (18)$$

where ∇^4 is the biharmonic operator, ρ_m is the density of the elastic material, ρ_p is the density of the piezoelectric material, and p_{piezo} is the piezoelectrically-induced actuation loading of the plate.

Substituting (14) – (17) into (18), p_{piezo} assumes the following form

$$p_{piezo} = \frac{d_{31} Y_p V_0 (z_2 + z_1)}{2(1 - \nu_p)} \left[(\delta'(x + x_e) - \delta'(x - x_e)) \times (H(y + y_e) - H(y - y_e)) + (\delta'(y + y_e) - \delta'(y - y_e)) \times (H(x + x_e) - H(x - x_e)) \right] \quad (19)$$

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Fig. 1.
Cross-section of a standard PMUT design.

Fig. 2.

Numerical representation of the piezoelectrically-induced actuation loading $\vec{p}_{piezo}$ for a square membrane.

Fig. 3. Normalized root mean square delta (pressure) and root mean square delta (phase) showing convergence behavior of hybrid BEM as a function of increasing node density. The pressure was calculated at a distance of 1 mm for a 3 by 3 array.

Fig. 4. Mean displacement of the center membrane for a 3 by 3 matrix array simulated with hybrid BEM and with COMSOL.

Fig. 5. Comparison between the proposed hybrid BEM and COMSOL simulated pressure response for a 3 by 3 array.

Fig. 6. Mean displacement of the center membrane of a 7 by 7 matrix array when only the center membrane is excited, and when all membranes are excited in phase. Reference case shown is for an isolated membrane (without neighbors).

Fig. 7.
Mean displacement as a function of increasing array pitch.

Fig. 8.

(a) Surface topography of a 7 by 7 matrix array at 8.75 MHz. (b) Displacement slices at the same frequency which indicate contributions from higher-order and non axi-symmetric membrane modes.

Fig. 9. Mean displacement of selected elements of a 32-element linear array for the case of excitation of the first element only.

Fig. 10.

Maximum output pressure (normalized) in the first band as a function of electrode coverage for full array simulation, single membrane simulation, and theoretical optimization from the thin-plate model.

Fig. 11.
Frequency response for AlN/Si, ZnO/Si, and PZT/Si PMUTs.

TABLE I

Thin Film Properties

	Si	AlN [36], [37]	ZnO [36], [38]	PZT [39], [40]
ρ (kg/m^3)	2329	3512	5720	7500
c_{11} (GPa)	166	345	209	114
c_{12} (GPa)	64	125	121	58
c_{13} (GPa)	64	120	105	59
c_{33} (GPa)	166	395	211	98
c_{44} (GPa)	80	118	42	21
c_{66} (GPa)	80	110	44	26
e_{31} (C/m ²)	–	–0.58	–0.57	–8
e_{33} (C/m ²)	–	1.55	1.32	6
e_{15} (C/m ²)	–	–0.48	–0.48	15
ϵ_{33}	–	11	11	1300