Modeling of Composite Piezoelectric Structures with the Finite Volume Method

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Abstract

Piezoelectric devices, such as piezoelectric traveling wave rotary ultrasonic motors, have composite piezoelectric structures. A composite piezoelectric structure consists of a combination of two or more bonded materials, where at least one of them is a piezoelectric transducer. Numerical modeling of piezoelectric structures has been done in the past mainly with the finite element method. Alternatively, a finite volume based approach offers the following advantages: (a) the ordinary differential equations resulting from the discretization process can be interpreted directly as corresponding circuits and (b) phenomena occurring at boundaries can be treated exactly. This paper extends the work of IEEE Transactions on UFFC 57(2010)7:1673-1691 by presenting a method for implementing the boundary conditions between the bonded materials in composite piezoelectric structures. The paper concludes with one modeling example of a unimorph structure.

Index Terms

composite piezoelectric structure, finite volume method, finite element method, control volume, displacement, boundary, unimorph.

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I. INTRODUCTION

Piezoelectric materials generate a dipole surface charge distribution on surfaces of the material, normal to the direction of the polarization, when the material is subjected to mechanical stress. This represents the piezoelectric effect. Alternatively, if the material is exposed to an electric field, the material suffers a mechanical deformation. This represents the converse piezoelectric effect. Therefore, these materials are used in the design and construction of sensors which sense and measure vibrations ([1], [2]), pressure ([3], [4]), force ([5], [6]), acceleration ([7], [8]) or as energy harvesting devices ([9], [10], [11]). The converse piezoelectric effect is used in generating forces and/or mechanical displacements. Therefore, these materials are also used in the design and construction of piezoelectric traveling wave rotary ultrasonic motors ([12], [13], [14]), bending actuators [15], V-stack actuators [16], biomorph actuators [17], and torsional actuators [18]. The piezoelectric effect and converse piezoelectric effect are also used together in electrical energy conversion in the design and construction of piezoelectric transformers ([19], [20], [21]).

Piezoelectric materials are constructed in different shapes such as plates, discs, tubes and rings and can be used on their own as simple piezoelectric devices such as piezoelectric transformers ([19], [20], [21]) or coupled with other metallic or nonmetallic materials as complex piezoelectric devices such as piezoelectric motors ([12], [13], [14]).

Systematic numerical modeling of a piezoelectric plate has been performed in the past with the Finite Element Method (FEM) in [22], [23], [24], [25], [26], [27], [14], and more recently with the Finite Volume Method (FVM) in [28]. It was shown in [28] that the FVM has the following strengths:

- The FVM ordinary differential equations (ODE) can be interpreted intuitively in terms of coupled circuits that represent the piezoelectric system [29]. These circuits can then be implemented using schematic capture packages. This makes it easier to interface the FVM model of the piezoelectric system with control circuits.
- The FVM works easily with surface integrals making it easier to deal with phenomena that occur at the boundary between two different materials. Therefore, this method may be more suitable to model an ultrasonic motor because the operating principle of the motor is based on the friction mechanism that takes place at the common contact boundary between the stator and the rotor. In this direction, this paper shows that the internal boundary conditions
are handled in an intuitive manner when using the FVM.

The FVM model presented in [28] is for a simple piezoelectric plate. In order to model a composite piezoelectric structure, which consists of two or more materials, one has to model the boundaries between the materials, in addition to modeling each material and the external boundaries. The objective of this paper is to present the FVM as applied to a unimorph structure and to compare the resulting FVM model to FEM simulations. Specifically, static deformations are computed as are eigenfrequencies. The model presented results in a system of ordinary differential equations and so dynamic simulations of initial value problems could be performed but are not presented here. Simulations performed in the FEM software package COMSOL are used as a benchmark for the validation of the results obtained with the FVM model. COMSOL is used as a benchmark because when using a simple piezoelectric plate the displacement of the plate calculated using a known exact solution is the same as the displacement calculated using COMSOL [28]. There are also benchmark examples in the COMSOL literature ([30] and [31]) that show a very good agreement of the results obtained in COMSOL simulations with theoretical and experimental values.

II. THE PDE MODEL

The dynamics of the piezoelectric material are determined [32] from Newton’s second law

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \rho \mathbf{u}_{tt} = \nabla \cdot \mathbf{T},$$

the absence of sources or sinks of charge

$$\nabla \cdot \left( \varepsilon \mathbf{S} + \varepsilon \mathbf{S} \mathbf{E} \right) = 0,$$

and appropriate boundary conditions. Above, $\rho$ is the mass density of the piezoelectric material and

$$\mathbf{u}(x, y, z, t) = \begin{pmatrix} u(x, y, z, t) \\ v(x, y, z, t) \\ w(x, y, z, t) \end{pmatrix},$$

where $u$, $v$, and $w$ are the local displacements from rest in the x, y, and z directions respectively. $\mathbf{T}(x, y, z, t)$ is the stress, $\mathbf{S}(x, y, z, t)$ the strain, and $\mathbf{E}(x, y, z, t)$ the electric field at each point in the material, at each moment in time. The actuator equation

$$\mathbf{T} = c^E \mathbf{S} - c' \mathbf{E}$$
gives the stress in terms of the strain and the electric field; the superscript $t$ denotes the transpose, $C^E$ is the stiffness or elasticity matrix, and $e$ is the electromechanical coupling matrix.

In this article, the piezoelectric material is assumed to be thin in the $z$ direction (see Fig. 1) and so the electric field $E$ is assumed to be constant and in the $z$ direction only

$$E(x, y, z, t) = (0, 0, E_3)^t.$$  \hspace{1cm} (5)

With this assumption, one only needs to solve equations (1) and (4) for $u$.

### III. Modeling of a Piezoelectric-Metal Structure

In [28], a thin piezoelectric plate was studied using the FVM to discretize equations (1) and (4). To model a composite piezoelectric device using a similar approach, it is first useful to model a unimorph structure made of two rectangular plates (one metal, the other piezoelectric) bonded together, see Figure 1. The two plates have the same length and width but they differ in thickness. The piezoelectric plate has the polarization $P$ oriented along its thickness.

When using the FVM to discretize the PDE, one starts by dividing the domain into “control volumes” and averaging the PDE over each one. The averaging yields a system of ODE for each volume. The structure of the (system of) ODE is different for internal volumes (all six faces are internal to the metal or to the piezoelectric), face volumes (one face is at an external boundary or at the metal/piezo interface), edge volumes (two faces are at an external boundary or at the metal/piezo interface), and corner volumes (three faces are at an external boundary or at the metal/piezo interface).

In [28], the ODE for internal volumes (see (37)–(39) therein) and for volumes with faces at external boundaries (ODE (37)–(39) with constraints (49)–(51) and (162)–(200) therein) are presented. In this article, the discretization for volumes at the metal/piezo interface is discussed.
Fig. 2 shows two control volumes; one in the metal (centered at M) and one in the piezoelectric material (centered at P). Their common face has the point I at its center. The ODE for the displacements at M and P ($u_M$ and $u_P$) will have terms involving the displacements at I and hence mechanical boundary conditions are needed at I.

1) **Displacement Boundary Conditions:** The displacement $u(x, y, z, t)$ must be continuous at the metal/piezo interface: there is no jump. Hence one can, without ambiguity denote the displacement at I by $u_I$.

2) **Stress Boundary Conditions:** The normal and tangential stresses must be continuous at the metal/piezo interface. For example, continuity of the tangential stress in the $x$ direction at the point I in Fig. 2 states

$$c_{55m} \left( \frac{\partial u_m}{\partial z} \bigg|_I + \frac{\partial w_m}{\partial x} \bigg|_I \right) = c_{55p} \left( \frac{\partial u_p}{\partial z} \bigg|_I + \frac{\partial w_p}{\partial x} \bigg|_I \right)$$ (6)

where $c_{55p}$ and $c_{55m}$ are entries from the stiffness matrices of the metal and the piezoelectric material and the derivatives “at I” are the limiting values of the derivatives taken from within the respective materials (see Figure 2). The partial derivatives of the displacements in equation (6) are then approximated using the displacements at the points M, P, I, IE and IW, yielding

$$c_{55m} \left( \frac{u_M - u_I}{\delta_{ZMI}} + \frac{w_{IE} - w_{IW}}{\delta_{XIEI} + \delta_{XIW}} \right) = c_{55p} \left( \frac{u_I - u_P}{\delta_{ZPI}} + \frac{w_{IE} - w_{IW}}{\delta_{XIEI} + \delta_{XIW}} \right)$$ (7)

Equation (7) then yields the displacement $u_I$ as a linear combination of other displacements. In a similar way, the continuity of the normal stress and the tangential stress in the $y$ direction
yields the displacements $v_I$ and $w_I$ as linear combinations of other displacements [33]. The forcing terms generated by the electric field appear in the normal stress equation and hence in the equation for $w_I$.

Figure 2 concerns control volumes that are away from external boundaries. Figure 3 presents volumes that also have a face on an external boundary; the point IE is on both an external boundary and on the metal/piezo interface. In this case, the displacements at IE can be found via either interpolation or extrapolation. For example, if $u_{IE}$ is expressed as a linear extrapolation of $u_I$ and $u_{IW}$, and $w_{IE}$ is expressed as a linear extrapolation of $w_I$ and $w_{IW}$ then

$$u_{IE} = u_I + \frac{\delta_{XIEI}}{\delta_{XIW}} (u_I - u_{IW})$$  
$$w_{IE} = w_I + \frac{\delta_{XIEI}}{\delta_{XIW}} (w_I - w_{IW})$$

The displacements at similar points where the interface meets an external boundary are presented in [33], as are the displacements when interpolation is used.

IV. THE SYSTEM OF EQUATIONS

The system of equations necessary to solve the unimorph structure shown in Figure 1 consists of the ODE (37)-(39) with constraints (49)-(51), and (162)-(200) from [28] as well as the constraints (7)-(9) above and their brethren (see [33]). This results in a system of ODE of the form

$$\frac{d}{dt} X = A_1 X + B_1$$
where $A_1$ is the system matrix and the vector $B_1$ includes the forces due the electric field and boundary conditions (see equation (59) in [28]). The system of equations (10) can then be processed as shown in [28] and solved in a program such as Matlab.

V. EXAMPLE - UNIMORPH STRUCTURE

In this section, the FVM discretization is compared to the FEM discretization of COMSOL. For the simulation, the unimorph structure shown in Figure 1 is held fixed at one end and is otherwise free to move. An electric field is applied along polarization direction of the piezoelectric material, resulting in a deformation. The resulting stresses at the metal/piezoelectric interface will then cause the metal to deform. It is a fully three-dimensional deformation with bending in both the $xz$ plane (see Figure 4) and in the $yz$ plane. To sample the bending, the position of a point A is tracked; this point is the midpoint of the metal portion of the face furthest from the fixed end. The dimensions of the unimorph structure are: length = 0.021m, width = 0.003m, piezoelectric material height = 0.0005m, and metal height = 0.001m. The metal used is copper and the piezoelectric material used is the PIC151 piezo-ceramic material manufactured by Physic Instrumente. See [33] for the material properties.

A. Static Analysis

For the static analysis, a 100V voltage is applied to the piezoelectric plate. The FVM model is then used to compute an (approximate) solution to the PDE (1) and (4) under the assumption (5). The $z$-component of the resulting displacement $u_A$ is tabulated in Table I for an increasing number of control volumes. These results are to be compared to those from the FEM discretization of the PDE (1), (2), and (4) as implemented by COMSOL shown in Table II. Note that COMSOL is simulating solutions of the full system while the FVM model is simulating solutions of the approximate system (for which the electric field is assumed to be constant and unidirectional).
The displacements in the z direction at point A calculated with the proposed FVM model for different numbers of control volumes, the corresponding degrees of freedom (DoF), and the deviation from the best available approximation of the displacement (7.044µm).

<table>
<thead>
<tr>
<th>Volumes</th>
<th>DoF</th>
<th>Displ. (µm)</th>
<th>Approx. Rel. error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>105</td>
<td>1.334</td>
<td>-81.06</td>
</tr>
<tr>
<td>315</td>
<td>945</td>
<td>4.617</td>
<td>-34.45</td>
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<tr>
<td>875</td>
<td>2625</td>
<td>6.034</td>
<td>-14.34</td>
</tr>
<tr>
<td>1715</td>
<td>5145</td>
<td>6.581</td>
<td>-6.57</td>
</tr>
<tr>
<td>2835</td>
<td>8505</td>
<td>6.835</td>
<td>-2.97</td>
</tr>
<tr>
<td>4235</td>
<td>12705</td>
<td>6.972</td>
<td>-1.02</td>
</tr>
<tr>
<td>5915</td>
<td>17745</td>
<td>7.054</td>
<td>0.14</td>
</tr>
<tr>
<td>7875</td>
<td>23625</td>
<td>7.107</td>
<td>0.89</td>
</tr>
<tr>
<td>10115</td>
<td>30345</td>
<td>7.143</td>
<td>1.41</td>
</tr>
</tbody>
</table>

COMSOL is set to use linear tetrahedral elements and no losses. COMSOL uses both the structural mechanics module (for the metal plate) and the MEMS module Piezo Solid 3 (for the piezoelectric plate). COMSOL automatically imposes that the internal boundary is bonded to the materials on each side — there can be no relative motion; the displacements are continuous across the internal boundary. Both modules require that the type of load is specified at the internal boundary; the type of load is taken to be “distributed load” with zero loads. Also, both modules require a constraint condition at the internal boundary; it is taken to be “free”. The mechanical boundary conditions at the external boundaries were taken to be free at five faces and fixed at the sixth. In addition, the Piezo Solid 3 module requires electrical boundary conditions; the internal boundary was set to “ground” and the bottom of the piezoelectric plate is taken to be a constant potential of −100 Volts.

The simulations show that as the number of degrees of freedom increase, the two solutions appear to be converging to similar, but slightly different, limits — this shows that the constant
TABLE II
The displacements in the z direction at point A simulated in COMSOL for different numbers of elements in the mesh, the corresponding degrees of freedom (DoF), and the deviation from the best available approximation of the displacement (7.044 µm).

<table>
<thead>
<tr>
<th>Number of tetrahedra</th>
<th>DoF</th>
<th>Displ. (µm)</th>
<th>Rel. error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>84</td>
<td>137</td>
<td>0.541</td>
<td>-92.32</td>
</tr>
<tr>
<td>222</td>
<td>318</td>
<td>2.346</td>
<td>-66.70</td>
</tr>
<tr>
<td>1076</td>
<td>1247</td>
<td>3.839</td>
<td>-45.50</td>
</tr>
<tr>
<td>1458</td>
<td>1596</td>
<td>4.369</td>
<td>-37.98</td>
</tr>
<tr>
<td>4146</td>
<td>3716</td>
<td>5.593</td>
<td>-20.60</td>
</tr>
<tr>
<td>23852</td>
<td>16833</td>
<td>6.549</td>
<td>-7.03</td>
</tr>
<tr>
<td>84899</td>
<td>59977</td>
<td>6.821</td>
<td>-3.17</td>
</tr>
<tr>
<td>264969</td>
<td>173495</td>
<td>6.935</td>
<td>-1.55</td>
</tr>
<tr>
<td>833552</td>
<td>532897</td>
<td>7.001</td>
<td>-0.61</td>
</tr>
<tr>
<td>2561662</td>
<td>1603052</td>
<td>7.029</td>
<td>-0.21</td>
</tr>
<tr>
<td>7966923</td>
<td>4894756</td>
<td>7.044</td>
<td></td>
</tr>
</tbody>
</table>

electric field assumption (5) was not an extreme one\(^1\). For the purposes of computing a relative error for the FVM model, the displacement provided by the best–resolved COMSOL run (7.044 µm) is taken as the “true” value of the displacement. In a given period of time COMSOL was able to compute a solution with many more degrees of freedom than the FVM model run on Matlab could — this is to be expected since COMSOL is a well-developed commercial product which has been optimized in a variety of ways.

The results are shown in Tables I and II and plotted in Figure 5. The FEM and FVM models are discretizations of related, but different, systems of PDE and so their solutions will not be exactly the same, however with only about 10,600 degrees of freedom the FVM model is within 2% of the highly resolved FEM model while the FEM model needs around 142,000 degrees of

\(^1\)Indeed, the electric field that COMSOL computes is nearly constant and unidirectional.
The number of degrees of freedom for Table I is taken to be three times the number of volumes because to find the displacements a linear system $AX = B$ has to be solved where $A$ is $3N \times 3N$ and $N$ is the number of volumes (see equation (57) in [28]). Rather than solving for six unknowns per node in the piezoelectric region (the displacements $u, v, w$, and the electric field $E$), COMSOL solves for four unknowns per node: the displacements $u, v, w$, and the voltage $V$. In the metal region, there are three unknowns per node: the displacements $u, v$, and $w$. Hence COMSOL’s number of degrees of freedom is $3a + 4b - 3c$ where $a$ is the number of nodes in the metal region, $b$ is the number of nodes in the piezoelectric material, and $c$ is the number of nodes that are in both regions (i.e. are in the internal boundary). The $3c$ term is subtracted prevent overcounting.

In [33] the effect of choosing different approximations of the displacements at points like IE in Figure 3 are considered; no large effects were found.

### B. Eigenfrequency Analysis

The eigenfrequency analysis of the piezoelectric-metal unimorph structure, consists of calculating the system matrix ($A_1$ from equation (10) ) and finding its eigenvectors and eigenvalues. For a given eigenvector the displacement $u$ is reconstructed. Deformations for which all control volumes move simultaneously up or down in the $z$ direction (see the bending mode in Figure
4) are then collected and the one with the lowest eigenvalue is used as a diagnostic. Table III presents the results for the FVM model. Table IV presents the corresponding results for the FEM model. The COMSOL implementation is as discussed in Subsection V-A except that the

**TABLE III**

<table>
<thead>
<tr>
<th>Volumes</th>
<th>DoF</th>
<th>Freq. (Hz)</th>
<th>Approx. Rel. error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>600</td>
<td>2213.3</td>
<td>28.08</td>
</tr>
<tr>
<td>900</td>
<td>5400</td>
<td>1805</td>
<td>4.46</td>
</tr>
<tr>
<td>2500</td>
<td>15000</td>
<td>1751.3</td>
<td>1.35</td>
</tr>
<tr>
<td>4900</td>
<td>29400</td>
<td>1734.3</td>
<td>0.36</td>
</tr>
<tr>
<td>8100</td>
<td>48600</td>
<td>1726.9</td>
<td>-0.06</td>
</tr>
</tbody>
</table>

structural mechanics module is used for both the metal and the piezoelectric domains because the electric field does not enter into the system matrix $A_1$.

As discussed above, the best-resolved FEM run provides an approximate “true” value of 1728Hz to use in defining a relative error. As shown in Tables III and IV and plotted in Figure 6, the FVM model has a relative error less than 1% using around 20,100 degrees of freedom while the FEM model requires around 170,000 degrees of freedom.

The number of degrees of freedom in Table III is taken to be six times the number of volumes because to find the eigenfrequencies one works with the system matrix $A_1$ where $A_1$ is $6N \times 6N$ and $N$ is the number of volumes (see equation (10)).

**VI. CONCLUSIONS**

This paper extends the work of [28], by implementing internal boundary conditions in composite piezoelectric structures using a FVM approach. The FVM approach was used due to its advantages: (a) the ordinary differential equations resulting from the discretization process can be interpreted directly as corresponding circuits and (b) phenomena occurring at boundaries can
TABLE IV

The eigenfrequencies for the unimorph structure simulated in COMSOL for different numbers of elements in the mesh, the corresponding degrees of freedom (DoF), and the deviation from the best available approximation of the eigenfrequency (1728Hz).

<table>
<thead>
<tr>
<th>Number of mesh elements</th>
<th>DoF</th>
<th>Freq. (Hz)</th>
<th>Rel. error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>80</td>
<td>108</td>
<td>6519</td>
<td>277.26</td>
</tr>
<tr>
<td>225</td>
<td>261</td>
<td>3720</td>
<td>115.28</td>
</tr>
<tr>
<td>1076</td>
<td>999</td>
<td>2537</td>
<td>46.82</td>
</tr>
<tr>
<td>1379</td>
<td>1290</td>
<td>2334</td>
<td>35.07</td>
</tr>
<tr>
<td>4154</td>
<td>3171</td>
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<td>18.23</td>
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<tr>
<td>23744</td>
<td>14670</td>
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<td>6.25</td>
</tr>
<tr>
<td>84738</td>
<td>53070</td>
<td>1767</td>
<td>2.26</td>
</tr>
<tr>
<td>264991</td>
<td>154602</td>
<td>1746</td>
<td>1.04</td>
</tr>
<tr>
<td>784207</td>
<td>448593</td>
<td>1733</td>
<td>0.29</td>
</tr>
<tr>
<td>2381511</td>
<td>1347036</td>
<td>1728</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 6. The eigenfrequencies for the displacements in the z direction at point A on the unimorph piezoelectric-metal structure calculated with the FVM model and simulated in COMSOL.
be treated exactly. The boundary conditions at the metal/piezo interface were chosen so that there was no relative motion with respect to one another. However, boundary conditions that allow relative motion could be easily implemented and used in future work, for example, to develop a model for the contact between the rotor and the stator of a piezoelectric traveling wave rotary ultrasonic motor.

The FVM model is then demonstrated for a unimorph piezoelectric structure and its performance is compared to COMSOL's implementation of a FEM discretization. We find that the FVM simulations are able to get within 1-2% of the best available limiting value using fewer degrees of freedom.

REFERENCES


