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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, at least one of which is a piezoelectric transducer. Piezoelectric structures have mainly been numerically modeled using the finite element method. An alternative approach based on the finite volume method offers the following advantages: 1) the ordinary differential equations resulting from the discretization process can be interpreted directly as corresponding circuits; and 2) phenomena occurring at boundaries can be treated exactly. This paper presents a method for implementing the boundary conditions between the bonded materials in composite piezoelectric structures modeled with the finite volume method. The paper concludes with a modeling example of a unimorph structure.

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 is the piezoelectric effect. Alternatively, if the material is exposed to an electric field, the material undergoes a mechanical deformation. This is 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]–[11]. The converse piezoelectric effect is used to generate force or mechanical displacement. Therefore, these materials are also used in the design and construction of piezoelectric traveling-wave rotary ultrasonic motors [12]–[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]–[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]–[21] or coupled with other metallic or nonmetallic materials as complex piezoelectric devices such as piezoelectric motors [12]–[14].

Systematic numerical modeling of a piezoelectric plate has been performed in the past with the finite element method (FEM) in [14], [22]–[27], 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 regard, this paper shows that the internal boundary conditions are handled in an intuitive manner when using the FVM.

The FVM model for a simple piezoelectric plate is presented in [28]. To model a composite piezoelectric structure which consists of two or more materials, one must 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; therefore, dynamic simulations of initial value problems could be performed, but are not presented here. Simulations performed in the FEM software package COMSOL (COMSOL AB, Stockholm, Sweden) are used as a benchmark for the validation of the results obtained with the FVM model. COMSOL is used as a benchmark because the displacement of a simple piezoelectric plate calculated using COMSOL is the same as the displacement calculated using a known exact solution [28]. There are also benchmark examples in the COMSOL literature [30] and [31] showing a very good agreement between the results obtained in COMSOL simulations and theoretical and experimental values.

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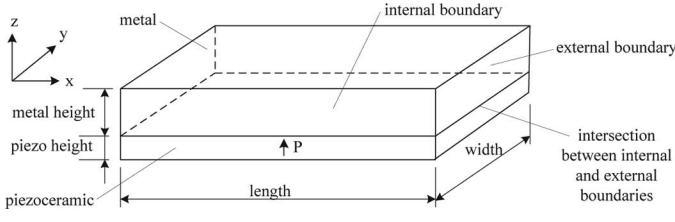


Fig. 1. Unimorph structure.

II. THE PARTIAL DIFFERENTIAL EQUATION MODEL

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

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \rho \mathbf{u}_{tt} = \nabla \cdot \mathbf{T}, \quad (1)$$

the absence of sources or sinks of charge

$$\nabla \cdot (\mathbf{eS} + \epsilon^S \mathbf{E}) = 0, \quad (2)$$

and appropriate boundary conditions. In (1), ρ is the mass density of the piezoelectric material and

$$\mathbf{u}(x, y, z, t) = \begin{pmatrix} u(x, y, z, t) \\ v(x, y, z, t) \\ w(x, y, z, t) \end{pmatrix}, \quad (3)$$

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, $\mathbf{S}(x, y, z, t)$ is the strain, and $\mathbf{E}(x, y, z, t)$ is the electric field at each point in the material, at each moment in time. The actuator equation

$$\mathbf{T} = \mathbf{c}^E \mathbf{S} - \mathbf{e}^t \mathbf{E}, \quad (4)$$

gives the stress in terms of the strain and the electric field; the superscript t denotes the transpose, $\mathbf{c}^E$ is the stiffness or elasticity matrix, and $\mathbf{e}$ is the electromechanical coupling matrix.

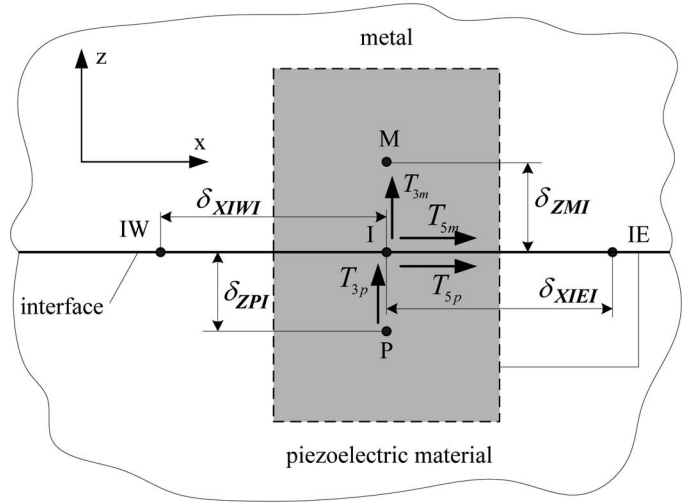
In this article, the piezoelectric material is assumed to be thin in the z -direction (see Fig. 1) and so the electric field $\mathbf{E}$ is assumed to be constant and in the z -direction only

$$\mathbf{E}(x, y, z, t) = (0, 0, E_3)^t. \quad (5)$$

With this assumption, one only needs to solve (1) and (4) for $\mathbf{u}$.

III. MODELING OF A PIEZOELECTRIC-METAL STRUCTURE

In [28], a thin piezoelectric plate was studied using the FVM to discretize (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

Fig. 2. The metal-piezoelectric material interface in the xz plane.

together, see Fig. 1. The two plates have the same length and width but they differ in thickness. The piezoelectric plate has the polarization $\mathbf{P}$ oriented along its thickness.

When using the FVM to discretize the partial differential equation (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 [28, Eqs. (37)–(39)] and for volumes with faces at external boundaries (ODE [28, Eqs. (37)–(39)] with constraints [28, Eqs. (49)–(51) and (162)–(200)]) 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 ($\mathbf{u}_M$ and $\mathbf{u}_P$) will have terms involving the displacements at I , and, hence, mechanical boundary conditions are needed at I .

A. Displacement Boundary Conditions

The displacement $\mathbf{u}(x, y, z, t)$ must be continuous at the metal/piezo interface: there is no jump. Hence, one can, without ambiguity, denote the displacement at I by $\mathbf{u}_I$.

B. 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 point I in Fig. 2 requires

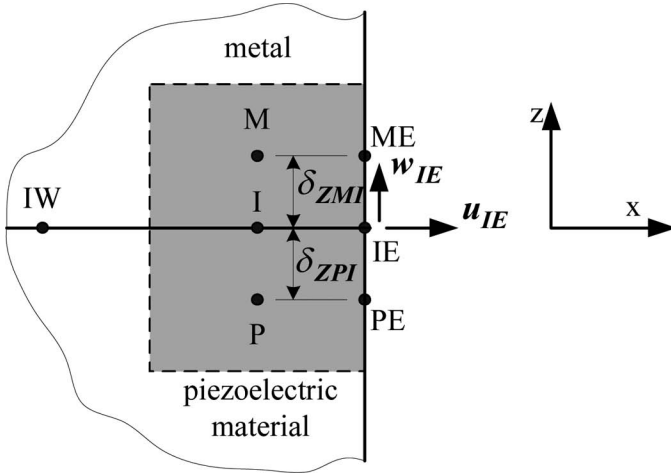


Fig. 3. The IE point at the East boundary.

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

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 Fig. 2). The partial derivatives of the displacements in (6) are then approximated using the displacements at the points M, P, I, IE, and IW, yielding

$$\begin{aligned} c_{55m} \left(\frac{u_M - u_I}{\delta_{ZMI}} + \frac{w_{IE} - w_{IW}}{\delta_{XIEI} + \delta_{XIWI}} \right) \\ = c_{55p} \left(\frac{u_I - u_P}{\delta_{ZPI}} + \frac{w_{IE} - w_{IW}}{\delta_{XIEI} + \delta_{XIWI}} \right). \end{aligned} \quad (7)$$

Eq. (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 (see supplemental technical report [64]). The forcing terms generated by the electric field appear in the normal stress equation and hence in the equation for w_I .

Fig. 2 shows control volumes that are away from external boundaries. Fig. 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

$$u_{IE} = u_I + \frac{\delta_{XIEI}}{\delta_{XIWI}} (u_I - u_{IW}) \quad (8)$$

$$w_{IE} = w_I + \frac{\delta_{XIEI}}{\delta_{XIWI}} (w_I - w_{IW}). \quad (9)$$

The displacements at similar points where the interface meets an external boundary are presented in the technical

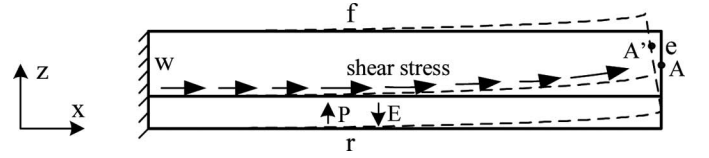


Fig. 4. Bending of the unimorph piezoelectric-metal plate.

report [64], 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 Fig. 1 consists of the ODE [28, Eqs. (37)–(39)] with constraints [28, Eqs. (49)–(51) and (162)–(200)], as well as the constraints (7)–(9) in the previous section and similar constraints in the technical report [64]. This results in a system of ODE of the form

$$\frac{d}{dt} X = \mathbf{A}_1 X + \mathbf{B}_1, \quad (10)$$

where $\mathbf{A}_1$ is the system matrix and the vector $\mathbf{B}_1$ includes the forces from the electric field and boundary conditions (see [28, Eq. (59)]). The system of equations (10) can then be processed as shown in [28] and solved in a program such as Matlab (The MathWorks Inc., Natick, MA).

V. EXAMPLE—UNIMORPH STRUCTURE

In this section, the FVM discretization is compared with the FEM discretization of COMSOL. For the simulation, the unimorph structure shown in Fig. 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 Fig. 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 = 0.021 m, width = 0.003 m, piezoelectric material height = 0.0005 m, and metal height = 0.001 m. The metal used is copper and the piezoelectric material used is the PIC151 piezo-ceramic material manufactured by Physik Instrumente (Karlsruhe, Germany). See the technical report for the material properties [64].

A. Static Analysis

For the static analysis, a 100-V voltage is applied to the piezoelectric plate. The FVM model is then used to compute an (approximate) solution to the PDE (1) and

TABLE I. 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 ($7.044 \mu\text{m}$).

Volume	DoF	Displacement (μm)	Approximate relative error (%)
35	105	1.334	-81.06
315	945	4.617	-34.45
875	2625	6.034	-14.34
1715	5145	6.581	-6.57
2835	8505	6.835	-2.97
4235	12705	6.972	-1.02
5915	17745	7.054	0.14
7875	23625	7.107	0.89
10115	30345	7.143	1.41

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 ($7.044 \mu\text{m}$).

Number of tetrahedra	DoF	Displacement (μm)	Relative error (%)
84	137	0.541	-92.32
222	318	2.346	-66.70
1076	1247	3.839	-45.50
1458	1596	4.369	-37.98
4146	3716	5.593	-20.60
23852	16833	6.549	-7.03
84899	59977	6.821	-3.17
264969	173495	6.935	-1.55
833552	532897	7.001	-0.61
2561662	1603052	7.029	-0.21
7966923	4894756	7.044	

(4) under the assumption (5). The z -component of the resulting displacement $\mathbf{u}_A$ is tabulated in Table I for an increasing number of control volumes.

These results are to be compared with those from the FEM discretization of the PDE (1), (2), and (4), as implemented by COMSOL, shown in Table II. Note that COMSOL simulates solutions of the full system, whereas the FVM model simulates solutions of the approximate system (for which the electric field is assumed to be constant and unidirectional).

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 the restriction 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 V .

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 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 ($7.044 \mu\text{m}$) 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 because 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 Fig. 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 10600 degrees of freedom, the FVM model is within 2% of the highly resolved FEM model; the FEM model needs about 142000 degrees of freedom to get that close.

¹Indeed, the electric field that COMSOL computes is nearly constant and unidirectional.

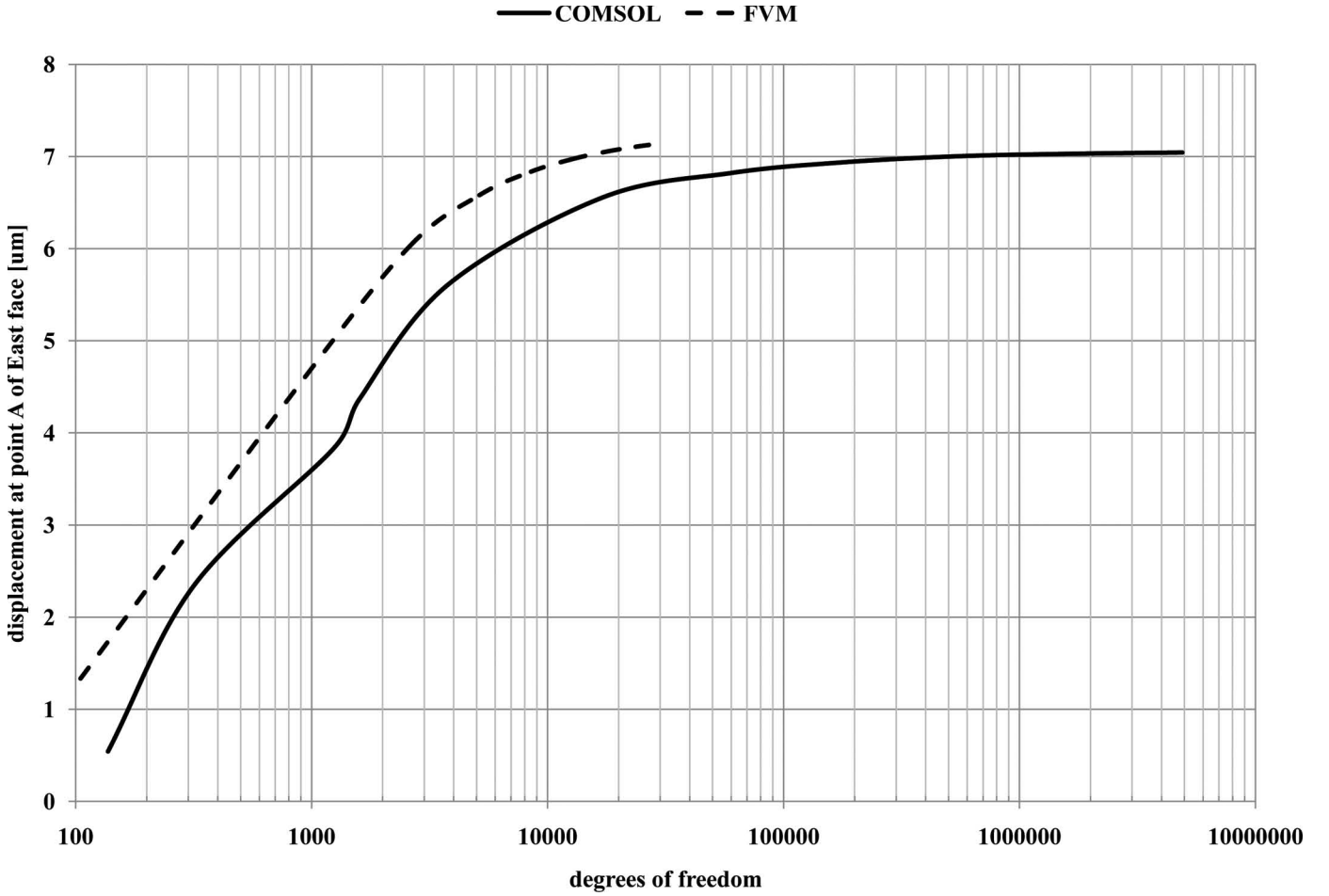


Fig. 5. The displacements in the z -direction at point A on the unimorph piezoelectric-metal structure calculated with the finite volume method (FVM) model and simulated in COMSOL.

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 $AX = B$ must be solved where A is $3N \times 3N$ and N is the number of volumes (see [28, Eq. (57)]). Rather than solving for six unknowns per node in the piezoelectric region (the displacements u , v , w , and the electric field $\mathbf{E}$), 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 to prevent overcounting.

In the technical report ([10]), the effect of choosing different approximations of the displacements at points like IE in Fig. 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 $[\mathbf{A}_1]$ from (7) and finding its eigenvectors and eigenvalues. For a given eigenvector, the displacement $\mathbf{u}$ is reconstructed. Deformations for which all control volumes move simultaneously up or down in the z -direction (see the bending mode in Fig. 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 Section V-A except that the structural mechanics module is used for both the metal and the piezoelectric domains because the electric field does not enter into the system matrix $\mathbf{A}_1$.

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

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 $\mathbf{A}_1$, where $\mathbf{A}_1$ is $6N \times 6N$ and N is the number of volumes [see (7)].

TABLE III. THE EIGENFREQUENCIES FOR THE UNIMORPH STRUCTURE 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 EIGENFREQUENCY (1728 Hz).

Volume	DoF	Frequency (Hz)	Approximate relative error (%)
100	600	2213.3	28.08
900	5400	1805	4.46
2500	15 000	1751.3	1.35
4900	29 400	1734.3	0.36
8100	48 600	1726.9	−0.06

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 (1728 Hz).

Number of mesh elements	DoF	Frequency (Hz)	Relative error (%)
80	108	6519	277.26
225	261	3720	115.28
1076	999	2537	46.82
1379	1290	2334	35.07
4154	3171	2043	18.23
23 744	14 670	1836	6.25
84 738	53 070	1767	2.26
264 991	154 602	1746	1.04
784 207	448 593	1733	0.29
2 381 511	1 347 036	1728	

— COMSOL - - FVM

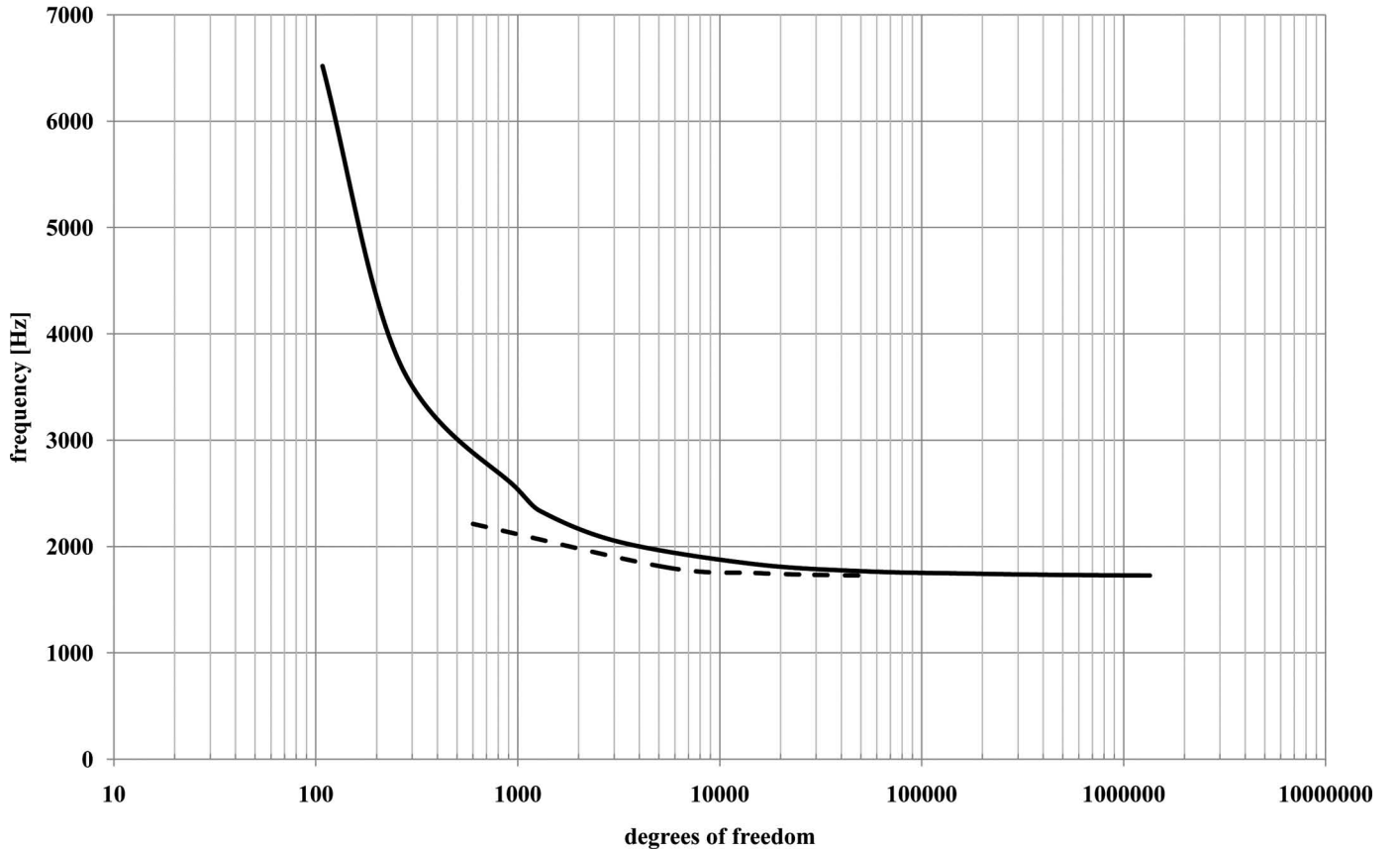


Fig. 6. The eigenfrequencies for the displacements in the z -direction at point A on the unimorph piezoelectric-metal structure calculated with the finite volume method (FVM) model and simulated in COMSOL.

VI. CONCLUSIONS

This paper extends the work of [28] by implementing internal boundary conditions in composite piezoelectric structures using the FVM approach. The FVM approach was used because of its advantages: 1) the ordinary differential equations resulting from the discretization process can be interpreted directly as corresponding circuits; and 2) phenomena occurring at boundaries can 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 with COMSOL's implementation of an FEM discretization. We find that the FVM simulations are able to get within 1 to 2% of the best available limiting value using fewer degrees of freedom.

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