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# Thermal Effects on the Frequency Response of Piezoelectric Crystals\*

Thomas R. Canfield, Mark T. Jones, Paul E. Plassmann,  
Argonne National Laboratory  
Argonne, Illinois 60439  
and  
Michael S. H. Tang  
Motorola, Inc.  
Schaumburg, Illinois 60196

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## Abstract

In this paper we describe a solution strategy to determine the natural frequencies of piezoelectric crystals subject to moderate changes in temperature and a variety of boundary constraints. The finite element equations governing piezoelectricity are derived based upon a Galerkin formulation of the problem. Suitable assumptions are made to linearize the steady-state (static) problem leading to an iteration scheme that can be used to refine the solution and include non-linear geometric effects caused by deformation. The eigenvalue problem is cast in this perturbed state to allow more accurate prediction of resonant frequencies.

## Introduction

Finite element formulations of the three dimensional piezoelectric crystal vibration problem employ the principle of virtual work to derive a coupled system of linear equations involving nodal displacements and nodal values of the electric field potential. Allik and Hughes' (1970) formulation is based upon assumptions of infinitesimal strain for the deformation of anisotropic crystals and the existence of an electric field potential. Because the electric field is assumed to be time independent, they were able to remove this extra field variable by using static condensation. They illustrated their implementation using linear tetrahedral finite elements.

The paper of Ostergaard and Pawlak (1986) present an adaptation of the formulation Allik and Hughes (1970) to two multi-field elements in the ANSYS (1990) finite element code. They illustrated the use of these elements in static analysis, mode-frequency analysis, and standing wave response to harmonic driving forces. In this implementation the symmetric ( $6 \times 6$ ) anisotropic elasticity tensor was stored in compact form that allows all 21 independent terms to be specified, a full ( $3 \times 6$ ) piezoelectric tensor was stored in full form and the ( $3 \times 3$ ) dielectric tensor was limited to diagonal terms only. In the static formulation the global stiffness matrix was assembled into a form that is partitioned into four sections. Two symmetric parts along the diagonal form the mechanical stiffness and dielectric stiffness that are block diagonal in form. The off diagonal blocks are filled with a coupling matrix and its transpose. Several examples were given in which the vibrational characteristics of crystals were determined using the full system and a reduced matrix analysis using the Guyan reduction procedure.

Yong (1987) extended the formulation given in Allik and Hughes (1970) and Ostergaard and Pawlak (1986) to include temperature effects in the analysis of free vibrations of piezoelectric crystals using the finite-element method. He incorporated three important effects of temperature in these problems: approximation of the elasticity tensor as cubic function of the change in temperature, approximation of the thermal expansion of the crystal as cubic function of the change in temperature, and a nonlinear geometric effect produced by thermal expansion. The present analysis incorporates these three important effects in a more rigorous formulation that permits the analysis to include the effect of mounting fixtures as fixed boundary constraints or attached structures.

### Deformation and Electric Field Potential

Rectangular cartesian coordinates are employed for the present analysis. Bold symbols are used to represent vector and tensor quantities in coordinate free notation, e.g.,  $\mathbf{v}$  is a vector and  $\mathbf{T}$  is a tensor. The components of vectors and tensors employ Latin subscripts ranging over the values 1 to 3 to indicate the corresponding coordinate direction. Vectors (tensors of rank 1) have a single subscript, e.g.,  $v_i$ , and tensor of rank 2 or more have the number of subscripts equal to the rank, e.g.,  $T_{ij}$  are the components of a second order tensor.

The cartesian coordinates,  $x_k$ , are the components of a position vector,  $\mathbf{r}$ , directed from the origin to the coordinate point. Therefore,

$$\mathbf{r} = x_k \mathbf{i}_k \quad (1)$$

where  $\mathbf{i}_k$  are the unit base vectors directed in the three coordinate directions. Summation is assumed on repeated indices.

A material point in the body in the unstrained, unstressed, initial configuration is given by the coordinates  $X_k$ . The position vector of this point can be denoted by

$$\mathbf{R} = X_k \mathbf{i}_k . \quad (2)$$

After deformation this material point is displaced to a new position,  $\mathbf{r}$ , whose coordinates are given by  $x_k$ . The displacement of the material point is a vector that can be computed by the difference in the coordinate positions,

$$\mathbf{u} = \mathbf{r} - \mathbf{R} \quad (3)$$

or expressed in component form

$$u_k = x_k - X_k . \quad (4)$$

The deformation gradient,  $F_{ij}$ , is defined as

$$F_{ij} = \frac{\partial x_i}{\partial X_j} = x_{i,j} \quad (5)$$

where the ‘,j’ denotes partial differentiation with respect to the variable  $X_j$  and the Lagrangian strain tensor is given by

$$\gamma_{ij} = \frac{1}{2}(F_{ki}F_{kj} - \delta_{ij}) \quad (6)$$

where  $\delta_{ij}$  is the identity tensor.

It is assumed that the electric field vector has components,  $E_k^R$ , that are derivable from a scalar field,  $\phi(X_k)$ . This scalar field,  $\phi$ , is called the electric field potential. The components of the electric field are given by first partial derivatives of the electric field potential,

$$E_k^R = -\phi_{,k} . \quad (7)$$

The electric field is a vector with the dimensions of force per unit charge.

### Field Equations

The two partial differential equations that govern the behavior of piezo-electric crystals are the balance of linear momentum,

$$\frac{\partial T_{ij}}{\partial x_j} + b_i = \rho \ddot{u}_i , \quad (8)$$

and Gauss’ Law in the absence of magnetic fields,

$$\frac{\partial D_i}{\partial x_i} = \sigma , \quad (9)$$

where the  $\dot{\cdot}$  denotes partial differentiation with respect to time, and  $\ddot{\cdot}$  denotes second partial differentiation with respect to time. In the first equation  $T_{ij}$  is the Cauchy Stress tensor,  $\rho$  is the mass density,  $b_i$  is the body force vector and  $u_i$  is the displacement. In the second  $D_i$  is the electric displacement and  $\sigma$  is the charge density.

The field equations in the preceding section are subjected to the boundary conditions

$$T_{ij}\nu_j = t_i \text{ on } S_T , \quad (10)$$

$$u_i = U_i \text{ on } S_U , \quad (11)$$

and

$$D_i\nu_i = \sigma_S \text{ on } S , \quad (12)$$

where  $\nu_i$  is the unit vector normal to the surface,  $S$ , of a body,  $S_T$  is the portion of the surface  $S$  subjected to traction forces,  $t_i$  are the surface tractions on  $S_T$ .  $S_U$  is the portion of the surface  $S$  with prescribed displacements,  $U_i$  are the prescribed displacements on  $S_U$ . Finally,  $\sigma_S$  is the surface charge density on  $S$ . Note that  $S = S_T \cup S_U$ , and  $S_T \cap S_U = \emptyset$ .

The Cauchy stress,  $T_{ij}$ , are the true physical components of stress, with dimensions of force per unit area with respect to the deformed configuration. It is related to the Piola stress,  $T_{ij}^R$ , with dimensions of force per unit area with respect to the reference configuration, by the following relationship

$$T_{ij} = J^{-1} F_{ik} T_{kl}^R F_{jl} , \quad (13)$$

where  $J$  is the Jacobian of the transformation from the undeformed to the deformed configuration. The physical meaning of  $J$  in this context is given by

$$\begin{aligned} J &= \frac{\rho^R}{\rho} \\ &= \frac{1}{6} \varepsilon_{ijk} \varepsilon_{lmn} F_{il} F_{jm} F_{kn} , \end{aligned} \quad (14)$$

where  $\varepsilon_{ijk}$  is the alternating tensor.

Similarly, the electric displacement,  $D_i$ , gives true physical components with dimensions of charge per unit area with respect to the deformed configuration. It is related to a "Piola" electric displacement,  $D_i^R$ , with the same physical dimensions with respect to the reference configuration, by the analogous relationship,

$$D_i = J^{-1} F_{ij} D_j^R . \quad (15)$$

The general form of the constitutive laws that govern piezoelectric crystals are given by

$$T_{ij}^R = C_{ijkl} \gamma_{kl} - e_{kij} E_k^R \quad (16)$$

and

$$D_i^R = e_{ijk} \gamma_{jk} + \epsilon_{ij} E_j^R \quad (17)$$

where  $C_{ijkl}$  is the elasticity tensor,  $e_{ijk}$  is the piezoelectric tensor and  $\epsilon_{ij}$  is the dielectric tensor.

### Displacement Decomposition

The deformation of a body subjected to a combination of thermal and piezoelectric time varying loads has the following form,

$$x_i = \chi_i(X_j, \theta, \phi, t) , \quad (18)$$

where  $x_i$  are the current coordinates of a material point,  $X_i$ , are the coordinates of the same material point in the undeformed reference configuration,  $\theta$  is the scalar change in temperature,  $\phi$  is the scalar electric field potential, and  $t$  is time. Without loss of generality the right hand side of the above expression can be written as

$$x_i = u_i(X_j, \theta, \phi, t) + X_i , \quad (19)$$

where  $u_i$  is the total time varying displacement of the material point.

For the purpose of the present analysis, it is convenient to partition this displacement into three components. Let

$$u_i(X_j, \theta, \phi, t) = u_i^*(X_j, \phi^*, t) + \bar{u}_i(X_j, \bar{\phi}) + \alpha_{ij}(\theta) X_j . \quad (20)$$

The first term,  $u_i^*$ , is the time varying component of the displacement. It is driven by external excitations and coupling to time varying components of the electric field,  $\phi^*$ . In the case of free vibration, the  $u_i^*$ 's and the  $\phi^*$  are the eigenvectors corresponding to the eigenvalues determined in the deformed state,  $\bar{u}_i(X_j, \bar{\phi}) + \alpha_{ij}(\theta)X_j$ .

The second term,  $\bar{u}_i$ , are the mechanical displacements due to static loads, body forces, static electric field, and external boundary conditions. The overline is used to indicate the static quantities. In the case of a crystal, these displacements are produced by the direct interaction of mounting fixtures and adjacent structures.

Finally, the last term is the unconstrained response of the crystal to thermal load,  $\theta = T - T_0$ . The thermal expansion of anisotropic crystals is governed by  $\alpha_{ij}$ 's which can be approximated to a high degree of accuracy as cubic functions of  $\theta$  for quartz as in Yong (1987)

$$\alpha_{ij}(\theta) = \alpha_{ij}^{(1)}\theta + \alpha_{ij}^{(2)}\theta^2 + \alpha_{ij}^{(3)}\theta^3. \quad (21)$$

Similarly, the temperature variation in the components of the elasticity tensor  $C_{ijkl}$ , are also approximated by cubic functions as well,

$$C_{ijkl}(\theta) = C_{ijkl}^{(0)} + C_{ijkl}^{(1)}\theta + C_{ijkl}^{(2)}\theta^2 + C_{ijkl}^{(3)}\theta^3. \quad (22)$$

In the present analysis, only uniform temperature distributions will be considered. Under these conditions, the  $\alpha_{ij}$ 's as well as the  $C_{ijkl}$ 's are independent of position and the thermal expansion if unobstructed will also be uniform. This only occurs when the boundaries are free of external tractions, the body forces are zero and the displacements are not constrained. In this state the body is *stress free* and its deformation is characterized by

$$x_i = X_i + \alpha_{ij}(\theta)X_j, \quad (23)$$

when the origins of the deformed and undeformed coordinate systems coincide. If we let

$$\beta_{ij} = \delta_{ij} + \alpha_{ij} \quad (24)$$

the differential element of arc length is given by  $dx_i = \beta_{ij}dX_j$ .

When the body is subject to a combination of time independent external loads, surface tractions, body forces, and boundary constraints, stresses do develop. In these circumstances the deformation is given by

$$\bar{x}_i = \bar{u}_i(X_i, \bar{\phi}) + \beta_{ij}(\theta)X_j, \quad (25)$$

with the additional  $\bar{u}_i$  term. From the preceding equation, the deformation gradient is computed to be

$$\bar{F}_{ij} = \bar{u}_{i,j} + \beta_{ij}. \quad (26)$$

A measure of the strain computed relative to the unconstrained state of thermal expansion can be deduced by taking the difference between the Lagrangian strains in these two states. Hence,

$$\begin{aligned} \bar{\gamma}_{ij} &= \frac{1}{2}(\bar{F}_{ki}\bar{F}_{kj} - \beta_{ki}\beta_{kj}) \\ &= \frac{1}{2}(\bar{u}_{k,i}\beta_{kj} + \beta_{ki}\bar{u}_{k,j} + \bar{u}_{k,i}\bar{u}_{k,j}) \end{aligned} \quad (27)$$

will be used in place of  $\gamma_{ij}$  in equation 16.

### Variational Formulation

The Galerkin formulation is employed to approximate the solution to equations 8 and 9. For the momentum equation

$$\Pi_1 = \int_V \delta \hat{u}_i \left( \frac{\partial T_{ij}}{\partial x_j} + b_i - \rho \ddot{u}_i \right) dV, \quad (28)$$

and for Gauss' Law

$$\Pi_2 = \int_V \delta \hat{\phi} \left( \frac{\partial D_i}{\partial x_i} - \sigma \right) dV, \quad (29)$$

where  $\Pi_1$  and  $\Pi_2$  are functionals to be minimized, and  $\delta \hat{u}_i$  and  $\delta \hat{\phi}$  are virtual displacements and electric field potentials, respectively.

We note that both the displacements,  $u_i$ , and the electric field potential,  $\phi$ , will be approximated by interpolation over the element subdomains. Let  $N_a$  be the set of piecewise continuous shape functions such that  $N_a = 1$  at the node  $a$  and zero at all other nodes in the domain. Over an element subdomain

$$u_i \simeq u_{ia} N_a(\xi_j) \quad (\text{sum on } a) \quad (30)$$

and



$$\phi \simeq \phi_a N_a(\xi_j) \quad (\text{sum on } a) \quad , \quad (31)$$

where  $\xi_j$  are the local element coordinates,  $u_{ia}$  and  $\phi_a$  are the nodal displacements and the nodal electric field potentials, respectively.

After differentiation and application of Gauss' theorem the following equations are obtained:

$$\int_V N_a \rho \ddot{u}_i dV + \int_V \frac{\partial N_a}{\partial x_j} T_{ij} dV = \int_{S_T} N_a t_i dS + \int_V N_a b_i dV \quad , \quad (32)$$

and

$$\int_V \frac{\partial N_a}{\partial x_i} D_i dV = \int_S N_a D_i \nu_i dS - \int_V N_a \sigma dV \quad . \quad (33)$$

If we introduce equations 13 through 17 and noting that  $dV = JdV^R$  the above equations can be rewritten as

$$\int_{V^R} N_a \rho^R \ddot{u}_i dV^R + \int_{V^R} N_{a,j} F_{ik} T_{kj}^R dV^R = \int_{S^R} N_a F_{ij} t_j^R dS^R + \int_{V^R} N_a F_{ij} b_j^R dV^R \quad , \quad (34)$$

and

$$\int_{V^R} N_{a,i} D_i^R dV^R = \int_{S^R} N_a \sigma_S^R dS^R - \int_{V^R} N_a \sigma^R dV^R \quad . \quad (35)$$

### Solution Strategy

The equations in the preceding section can be re-written in matrix form when the appropriate substitutions are made for accelerations, stress, deformation gradient, electric field, and electric displacement. For the steady state solution of equations 34 and 35 one obtains the coupled set of non-linear equilibrium equations

$$\begin{aligned} \mathbf{K}_{iajb}(\bar{\mathbf{u}}) \bar{u}_{jb} + \mathbf{N}_{bia}(\bar{\mathbf{u}}) \bar{\phi}_b &= \mathbf{f}_{ia}(\bar{\mathbf{u}}) \\ \mathbf{N}_{ajb}(\bar{\mathbf{u}}) \bar{u}_{jb} - \mathbf{P}_{ab} \bar{\phi}_b &= \sigma_a(\bar{\mathbf{u}}) \end{aligned} \quad (36)$$

where  $\mathbf{K}_{iajb}$ ,  $\mathbf{N}_{cia}$ , and  $\mathbf{P}_{ab}$  are the global stiffness, global piezoelectric coupling, and the global dielectric matrices respectively. The quantities  $\bar{u}_{ia}$  and  $\bar{\phi}_d$  are the mechanical degrees of freedom and the electrical degrees of freedom. Finally,  $\mathbf{f}_{ia}$  and  $\sigma_a$  are the mechanical and electrical forcing terms.

The above system of equations is ill conditioned because the values of  $\mathbf{K}_{iajb}$  are many orders of magnitude larger than the values of  $\mathbf{P}_{ab}$ . However, this ill conditioning can be removed with diagonal scaling. In addition, the combined system of equations can also be quite large in order to resolve the frequencies of interest. For this reason iterative techniques such as the pre-conditioned conjugate gradient method (Manteuffel, 1980) may be employed to obtain good approximate solutions for the system.

The individual terms in equation 36 are computed by making the following iterative approximations

$${}^{(n)}\bar{F}_{ij} = \beta_{ij} + {}^{(n-1)}\bar{u}_{i,j} \quad (37)$$

and

$${}^{(n)}\bar{\gamma}_{ij} = \frac{1}{2}(\beta_{ik} {}^{(n)}\bar{u}_{k,j} + {}^{(n)}\bar{u}_{k,i}\beta_{jk} + {}^{(n-1)}\bar{u}_{k,i} {}^{(n-1)}\bar{u}_{k,j}), \quad (38)$$

where the superscript  ${}^{(n)}$  before the variable denotes the  $n$ th approximation to that variable. When these expressions are incorporated into equations 32 and 35 and terms are rearranged, the individual matrices in equation 36 are given by

$${}^{(n)}\mathbf{K}_{iajb} = \int_{VR} N_{a,l}[\beta_{ik} + {}^{(n)}\bar{u}_{i,k}]C_{klmn}[\beta_{jm} + {}^{(n)}\bar{u}_{j,m}]N_{b,n}dV^R \quad (39)$$

$$- \frac{1}{2} \int_{VR} N_{a,l} {}^{(n)}\bar{u}_{i,k}C_{klmn} {}^{(n)}\bar{u}_{j,m}N_{b,n}dV^R$$

$${}^{(n)}\mathbf{N}_{ajb} = \int_{VR} N_{a,k}[\beta_{jl} + {}^{(n)}\bar{u}_{j,l}]e_{klm}N_{b,m}dV^R \quad (40)$$

and

$$\mathbf{P}_{ab} = \int_{VR} N_{a,j}\epsilon_{jk}N_{b,k}dV^R \quad (41)$$

and the vectors in equation 36 are given by

$$\begin{aligned}
{}^{(n)}\mathbf{f}_{ia} = & \\
& \int_{S_T} N_a F_{ij} t_j^R dS^R + \int_{V^R} N_a F_{ij} b_j^R dV^R \\
& + \frac{1}{2} \int_{V^R} N_{a,l} \beta_{ik} C_{klmn} {}^{(n)}\bar{u}_{j,m} {}^{(n)}\bar{u}_{j,n} dV^R
\end{aligned} \tag{42}$$

and

$$\begin{aligned}
{}^{(n)}\sigma_a = & \\
& \int_{S^R} N_a \sigma_S^R dS^R - \int_{V^R} N_a \sigma^R dV^R \\
& + \frac{1}{2} \int_{V^R} N_{a,l} e_{ljk} {}^{(n)}\bar{u}_{m,j} {}^{(n)}\bar{u}_{m,k} dV^R .
\end{aligned} \tag{43}$$

The following steps are executed to obtain the nonlinear solution and determine the frequencies of the crystal:

1. Calculate the unconstrained thermal expansion of the crystal due to a uniform temperature load of  $\theta = T - T_0$ .

$$\begin{aligned}
\beta_{ij} &= \delta_{ij} + \alpha_{ij}(\theta) \\
{}^{(0)}\bar{u}_{ia} &= -\alpha_{ij}(\theta) X_{ja} \\
{}^{(0)}\bar{\phi}_a &= 0
\end{aligned} \tag{44}$$

2. Solve the static problem (equation 36) to determine  ${}^{(1)}\bar{\phi}_a$  and  ${}^{(1)}\bar{u}_{ia}$ .
3. Iterate the solution to refine the estimate of  ${}^{(n)}\bar{\phi}_a$  and  ${}^{(n)}\bar{u}_{ia}$ .
4. Solve the eigenvalue problem in this perturbed state:

$$\left| \begin{pmatrix} \mathbf{K}_{iajb}^{(n)}(\bar{\mathbf{u}}) & \mathbf{N}_{bia}^{(n)}(\bar{\mathbf{u}}) \\ \mathbf{N}_{ajb}^{(n)}(\bar{\mathbf{u}}) & -\mathbf{P}_{ab} \end{pmatrix} - \lambda^2 \begin{pmatrix} \mathbf{M}_{iajb} & 0 \\ 0 & 0 \end{pmatrix} \right| = 0 \tag{45}$$

with expression for the consistent mass matrix  $\mathbf{M}_{iajb}$  given by

$$\mathbf{M}_{iajb} = \int_{V^R} \rho^R \delta_{ij} N_a N_b dV^R . \tag{46}$$

We note that  $\mathbf{K}_{i_a j_b}$  is a weak quadratic function of  $\bar{\phi}_a$  and  $\bar{u}_{i_a}$ , and the suggested iteration could fail to converge at large values.

### Computational Results

A specialized finite element program has been developed to solve the non-linear static thermal stress problem and the associated eigenvalue problem. The program employs scalable algorithms to evaluate the element matrices and solve the sparse linear algebraic systems (Jones and Plassmann, 1991).

An efficient 27-node brick element was developed using second order Lagrangian polynomials to interpolate the displacements and the electric field potential. It has 8 corner nodes, 12 mid-edge nodes, 6 mid-side nodes and a center node. The element matrices were computed with  $3 \times 3 \times 3$  Gauss quadrature. It was necessary to use second order interpolation to more accurately model the thickness-shear modes of vibration.

The solution of the non-linear static thermal stress problem requires a series of linear systems of the form of equation 36. Because of these systems are very large and sparse, iterative solutions were preferred. The iterative solver uses an incomplete matrix factorization as a preconditioner for the conjugate gradient algorithm (Manteuffel, 1980). The linear vibration problem requires the solution of a generalized eigenvalue problem given in equation 45. A shifted, inverted variant of the Lanczos algorithm was used to solve for the eigenvalue problem (Nour-Omid, et. al., 1987).

The piezoelectric crystals analyzed in this study are used in strip resonators. These are thin strips of quartz that vibrate at a fixed frequency when an electric current is applied to surface electrodes. The finite element model of the strip resonator is shown in Figure 1. The dimensions of the crystal are  $8 \text{ mm} \times 1.6 \text{ mm} \times 0.4 \text{ mm}$ , where the long axis of the strip is cut at  $35.15^\circ$  with respect to the x-axis of the quartz. The figure depicts a mesh of  $15 \times 9 \times 3$  of 405 elements used to debug the model. A  $47 \times 27 \times 9$  mesh of 5,589 elements was used to model the resonator. This results in a system of 45,684 equations which must be solved many times to order to obtain the static solution and determine eigenvalues. The crystal is mounted on an aluminum substrate by epoxy joints at each end. For simplicity, nodes were fixed to simulate the epoxy joints.

A set of five calculations were performed simultaneously on the 520 processor Intel DELTA to determine frequency shifts as a function of temper-

ature for four modes clustered near 668 KHz. Each calculation required 56 processors. About 54% of the machine was used in the process and took less than 2 hours of wallclock time to complete. Results are shown in Table 1 and in Figure 2 as where they have plotted to show the relative variation in frequency normalized to the frequency at 25°C.

Temperature (°C)	Mode 1 (KHz)	Mode 2 (KHz)	Mode 3 (KHz)	Mode 4 (KHz)
15	647.70	662.80	684.19	708.65
20	647.68	662.77	684.13	708.59
25	647.65	662.74	684.06	708.54
30	647.62	662.71	683.98	708.48
35	647.57	662.67	683.92	708.41

**Table 1.** Cluster of frequencies near 668 KHz as a function of temperature in °C.

### Conclusions

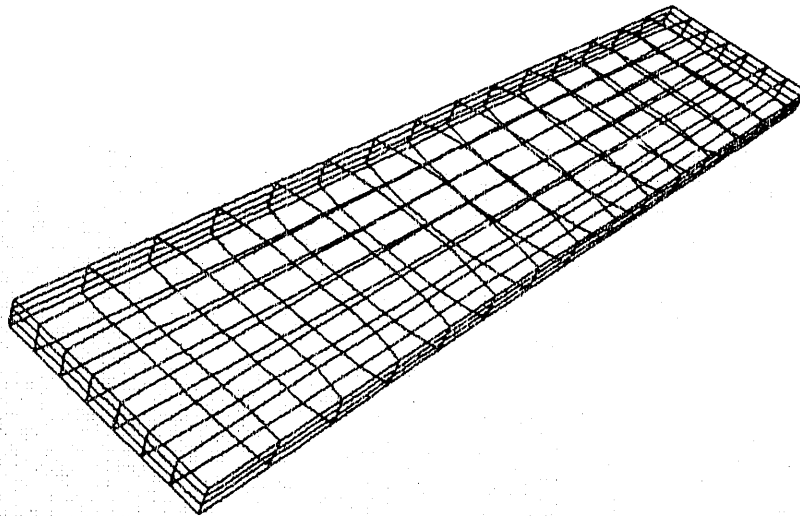
The current method extends the current capability to model piezoelectric devices subjected thermal strains and including mechanical restraints. It has been implemented to run efficiently on a massively parallel supercomputer and can solve complex eigenvalue problems involving coupling between mechanical and electrical modes of vibration in a reasonable time frame.

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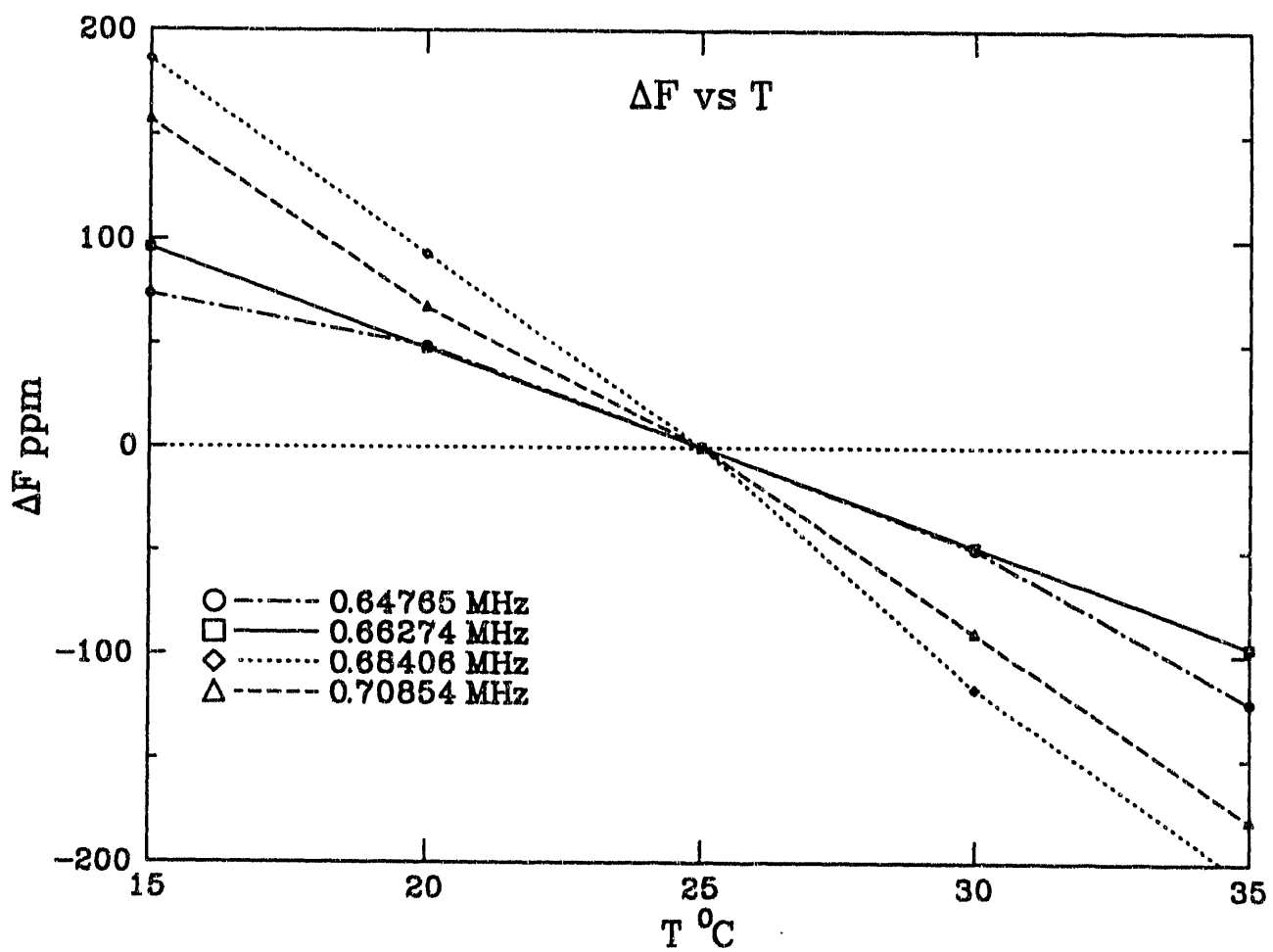
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**Figure 1.** Finite element model of a strip resonator.



**Figure 2.** Change in frequency (PPM) of modes near 668 KHz as a function of temperature in °C.





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