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Using FreeFEM open software for modelling the vibrations of piezoelectric devices

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Abstract Modelling vibrations of piezoelectric transducers has been a topic discussed in the literature for many decades. The first models - so-called one-dimensional - describe the vibrations only near operating frequency and near its harmonics. Attempts to introduce two-dimensional models were related to the possibility of one transducer working at several frequencies, including both thickness vibrations and those resulting from the transducer horizontal dimensions. In recent decades, thanks to the use of the finite element method and its derivatives, and the progress related to the increase in processor speed and memory availability, the implementation of models based on three-dimensional modelling is possible using software on personal computers. As the implementation of finite element method algorithms is characterized by high complexity, several professional software packages have been created on the commercial market, among which only a few implement the piezoelectric equations. In this context, this article presents how to use open source software along with developed programming language for intuitive definition of piezoelectric equations and its solution.

Keywords: Finite element methods, piezoelectric devices models, FreeFEM

1. Introduction

The problem of modelling vibration of piezoelectric transducers is well recognized in the literature. The number of authors have proposed different modifications of the equivalent circuit model of piezoelectric ceramic element vibrating in thickness mode as proposed by Mason in his early works in 1948 (i.e. [1-5]) . They include additional elements in the form of complex coefficients that allow modelling some effects observed in measurements, that maybe interpreted as dielectric, electro-mechanical and mechanical losses. Recently, due to numerical implementations of partial differential equations solvers it is relatively easy to model vibrations of transducer composed from any number of piezoelectric elements by finite element methods. Finite element analysis helps predict the behaviour of products affected by many physical effects, including: mechanical stress, mechanical vibration, fatigue, motion, heat transfer, fluid flow, electrostatics, plastic injection moulding etc.

FEM-based commercial modelling software is a result of last two decades of development in software engineering. They implement internally variety of PDE allowing for solution of multiphysics problems (i.e. COMSOL Multiphysics® - [6], ANSYS® - [7]). As not all FEM software implements piezoelectric problem due to its complexity several also research oriented solutions (i.e. Atila® [8], FEMP® [9]) has been developed. Additionally, especially in last decade, due to popularity of open software idea, several solutions appeared like OpenFoam® or FreeFEM® that allows for user-defined scripting. As they require special knowledge of programming, in the following section FreeFEM language is introduced and examined from perspective of application in modelling of vibration of piezoelectric devices.

2. FreeFEM and its language

FreeFEM is a popular 2D and 3D partial differential equations (PDE) solver used by thousands of researchers across the world [10]. It runs on macOS, Linux, Windows operating systems and have also distribution on Docker virtualized platform. It allows easily implement user-defined physics modules using the provided FreeFEM language and offers a large list of finite elements, like the Lagrange, Taylor-Hood, etc., usable in the continuous and discontinuous Galerkin method framework. FreeFEM has it own internal mesher that is compatible with the best open-source mesh and visualization software like Tetgen, Gmsh, Mmg and ParaView. It is written in C++ to optimize for speed, FreeFEM is interfaced with the other popular solvers like mumps, PETSc and HPDDM. With Qarnot's HPC platform, 7 lines of python code is all you need to run a FreeFEM simulation in the cloud. It is also available on Rescale's ScaleX® Pro. Rescale offers academic users up to 500 core hours on their HPC cloud.

The FreeFEM language is typed, polymorphic and re-entrant with macro generation. It is a C++ idiom with something that is more akin to LaTeX and rarely generates an internal finite element array. This was adopted for speed and consequently FreeFEM could be hard to beat in terms of execution speed, except for the time lost in the interpretation of the language. The development cycle includes the following steps: modelling, programming and code running. In modelling phase from strong forms of PDE to weak forms, one must know the variational formulation and should also have an eye on the reusability of the variational formulation so as to keep the same internal matrices. Programming in FreeFEM language is simply done using any text editor. Finally the code in terminal mode or by integrated environment or even online in a webpage. The extremely versatile plot function inserted directly in code allows for displaying while FreeFEM is running. FreeFEM has internal pre-built physics for several PDE problems including incompressible Navier-Stokes, Lamé equations (linear elasticity), Neo-Hookean, Mooney-Rivlin (nonlinear elasticity), thermal diffusion, thermal convection, thermal radiation, magnetostatics, electrostatics and fluid-structure interaction. As it does not contain pre-build support for piezoelectric equations the paper verifies its usefulness for defining and solving theoretical equations for vibration of piezoelectric circular transducer.

3. Case study: vibrations of circular piezoelectric disc

When a time-harmonic solution is considered, the piezoelectric equations governing displacement u, stress tensor T, electric displacement field D, strain tensor S and electrical field E components are given (using Einstein's compact notation, that implies summation and with comma denoting derivation operator) as:

$$\begin{aligned} -\omega^2\rho_p u_i &= T_{ij,j} \\ D_{i,i} &= 0 \\ T_{ij} &= c^E_{ijkl}S_{kl}(u) - e_{kij}E_k(\phi) \\ D_i &= e_{ikl}S_{kl}(u) + \epsilon^S_{ik}E_k(\phi) \end{aligned} \tag{1}$$

where ρ_p is the density of piezoelectric material, c^E_{ijkl} represents 3x3x3x3 elastic tensor, e_{kij} represents 3x3x3 piezoelectric tensor, ϵ^S_{ij} – 3x3 dielectric matrix, $S_{kl}(u) = (u_{k,l} + u_{l,k})/2$ and $E_k(\phi) = -\phi_{,i}$. Indices i, j, k, l =1,2,3 passes through three axes of arbitrary coordinate system. Unknown variables in such formulated boundary-value problem are displacement vector u and scalar potential ϕ. Eq (1) represents strong formulation of the problem. The weak formulation usually used for obtaining numerical solution may be obtained by multiplying the differential equations governing the problem with weight functions, and integrating over the solution domain. In case of piezoelectric PDE expressed by first two equations of Eq. (1) it leads to [11]:

$$\begin{aligned} -\omega^2\rho_p \int_{\Omega_p} v_i u_i \, d\Omega &= \int_{\Omega_p} v_i T_{ij,j}\, d\Omega \quad \left(= \int_{\Gamma_p} v_i T_{ij} n_j \, d\Gamma - \int_{\Omega_p} S_{ij}(v_i) T_{ij}\, d\Omega\right) \\ \left(\int_{\Gamma_p} w\, D_i n_i d\Gamma + \int_{\Omega_p} E_i(w)\, D_i d\Omega =\right) \int_{\Omega_p} w D_{i,i}\, d\Omega &= 0 \end{aligned} \tag{2}$$

where Ω_p represents a volume of piezoelectric disc, n_i - normal vector, whereas v_i for i=1,2,3 - weight functions for displacement components and w - for potential. The weight functions are arbitrary except boundary where they needs to be equal to zero. The expressions in parentheses are obtained using integration by parts and allows including conditions on the boundary Γ_p. Furthermore, for axisymmetric problem as illustrated in Fig.1 the analysis could be reduced to two dimensions with radial and axial coordinates. Additionally, when piezoelectric material have hexagonal structure (10 independent linearizing coefficients) the last two equations of Eq. (1) can be expressed in circular coordinate system in matrix form (with relabeling tensor coefficients into two indices) as follows:

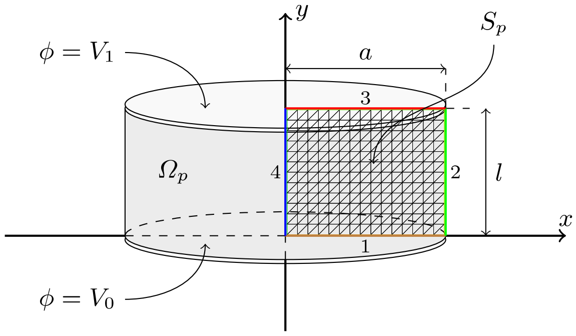

Fig. 1. Domain of calculation S_p as the half of a cross-section of whole domain Ω_p for axisymmetric problem as used for sample piezoelectric disc (a – disc radius, l – its thickness, V_0, V_1 – electrode potentials, 1,2,3,4 – labels of boundary Γ_p).

$$\begin{bmatrix} T_{rr} \\ T_{\theta\theta} \\ T_{zz} \\ T_{rz} \\ D_r \\ D_z \end{bmatrix} = [C] \begin{bmatrix} S_{rr} \\ S_{\theta\theta} \\ S_{zz} \\ S_{rz} \\ E_r \\ E_z \end{bmatrix} \text{ where } [C] = \begin{bmatrix} c_{11}^E & c_{12}^E & c_{13}^E & 0 & 0 & -e_{31} \\ c_{12}^E & c_{11}^E & c_{13}^E & 0 & 0 & -e_{31} \\ c_{13}^E & c_{13}^E & c_{33}^E & 0 & 0 & -e_{33} \\ 0 & 0 & 0 & c_{44}^E & -e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & \epsilon_{11}^S & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & \epsilon_{33}^S \end{bmatrix} \text{ and } \begin{bmatrix} S_{rr} \\ S_{\theta\theta} \\ S_{zz} \\ S_{rz} \\ E_r \\ E_z \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial r} u_r \\ \frac{1}{r} u_r \\ \frac{\partial}{\partial z} u_z \\ \frac{\partial}{\partial r} u_r + \frac{\partial}{\partial z} u_z \\ -\frac{\partial}{\partial r} \phi \\ -\frac{\partial}{\partial z} \phi \end{bmatrix} = L\left(\begin{bmatrix} u_r \\ u_z \\ \phi \end{bmatrix} \right) \quad (3)$$

[C] matrix introduced in Eq. (3) represents generalized stiffness matrix for the piezoelectric problem. Combining unknown variables u_r, u_z, ϕ to form a vector and assuming the case of free vibration (without external load on boundaries) Eq. (2) may be expressed as:

$$\int_{S_p} \omega^2 \rho_p \begin{bmatrix} v_r \\ v_z \end{bmatrix}^T \begin{bmatrix} u_r \\ u_z \end{bmatrix} dS_p - \int_{S_p} L\left(\begin{bmatrix} v_r \\ v_z \\ w \end{bmatrix} \right)^T [C] \; L\left(\begin{bmatrix} u_r \\ u_z \\ \phi \end{bmatrix} \right) dS_p = 0 \quad (4)$$

where S_p represents now cross-section surface of a disc and $L(\,)$ operator defined in Eq. (3) could be interpreted as a derivative operator of the piezoelectric problem expressed in cylindrical coordinates.

4. Software implementation

FreeFEM language implementing finite element solver - beside typical numerical types - contains definitions of special types like `mesh` for definition of surfaces and/or volumes of a problem, `vespace` for a definitions of variational variables and `solve` for solution of a problem. It introduces functions like `int1d`, `int2d` and `int3d` that implements numerical integration that allows for natural definition of integral equation and `on` function - for the definition of Dirichlet boundary conditions.

The example code modelling the free vibrations of circular piezoelectric disk with diameter of 2.5cm and thickness of 1cm (D/T=2.5) is presented in Fig. 2. The code implements Eq. (4) with definitions from Eq. (3) nearly in a straightforward way. The variational equation (4) is defined in lines 38-43 using derivative operator $L(.)$ which is earlier defined in the form of macro (lines 28-29) and coefficient matrix $[C]$ defined in the form of `func` type (lines 20-25). Note that there is also natural way of defining derivatives using `dx()` and `dy()` functions (line 29). The boundary conditions corresponds to exciting one electrode with a voltage of 500V (lines 41-42). One additional condition is related to axisymmetry, which enforces lack of radial displacement on axis of symmetry (line 43). The matrix elements (lines 16-18) represents coefficient values without losses for PZT5A material, what makes the problem to be real valued. The volume of integration for axisymmetric case is reduced to surface and for disk shape could be defined as a `mesh` containing the output result of `square` function with its horizontal dimension equal to the half of diameter in first (r) coordinate and its thickness in second (z) coordinate. Two other parameters of this function defines the size of the mesh. In the example the size is rather coarse having only 15x12 grid points. This could be easily changed for more accurate analysis as the accuracy of solution depends mainly on mesh density. Precise calculation with larger domain and larger grids are more time-consuming and may require parallel supercomputer environments as a computing platform. The results of executed code are presented in Fig. 3. The `plot` function makes the visualisation of mesh grid representing the displacement amplitude overlaid with false coloured values of potential in disc cross-section. The analysis was performed in ten frequencies below thickness mode (defined in line 5) which were selected on purpose to illustrate the change of potential field inside material near five different modes: two first radial modes R1 and R2 (Figs. 3a, 3b and Fig. 3c, 3d), edge mode E (Figs. 3e, 3f), thickness shear mode TS1 (Figs. 3g, 3h) and first thickness extension mode TE1 (Figs. 3i, 3j). The solution contained in u_r, u_z and ϕ variables allows for further calculations of all values of interest according to Eq. (3). The aperture vibration are accessible by taking u_z values on border labelled 3. It is worth to mention, that for coarse grids the modal frequencies are not precisely determined and increasing the grid size will gradually allow assigning its proper values. These frequencies obtained by 15x12 grid may vary from those obtained by fine grids by 3kHz for presented case study.

Tab 1. The values of PZT5A material constants as used in the case study.

ρ_p	c_{11}^E	c_{12}^E	c_{13}^E	c_{33}^E	c_{44}^E	e_{31}	e_{33}	e_{15}	ϵ_{11}^S	ϵ_{33}^S
$7750\frac{kg}{m^3}$	$120\frac{GN}{m^2}$	$75.2\frac{GN}{m^2}$	$75.1\frac{GN}{m^2}$	$110\frac{GN}{m^2}$	$21.1\frac{GN}{m^2}$	$-5.4\,\frac{C}{m^2}$	$15.8\,\frac{C}{m^2}$	$12.3\,\frac{C}{m^2}$	$8.1\,\frac{nF}{m}$	$7.3\,\frac{nF}{m}$

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```
// Free vibrations of 2.5cm x 1cm PZT5A cylindrical disc
// Marek Moszynski 30.03.2020

// ------ Variables ------
real[int] ff=[72e3, 73e3, 128e3, 129e3, 156e3, 157e3, 164e3, 165e3, 189
    e3, 190e3];  // the table of selected frequencies

// ------ Geometry -------
real a=0.025/2, l=0.01;                       // disc dimensions
int MM=15, NN=12;                             // grid resolution
mesh Sp = square(MM, NN, [a*x, l*y]);         // grid generation
plot(Sp, ps="ff_mesh.eps");                   // plot and save mesh

// ------ Consts -------
real V0=0, V1=500;                            // electrode potentials
real rho = 7750;                              // material density
real e31 = -5.4,  e33 = 15.8,  e15 = 12.3,    // piezoelectric consts
     eps11S = 8.1e-9 , eps33S = 7.3e-9,       // dielectric consts
     c11 = 120e9, c12 = 75.2e9, c13 = 75.1e9, c33 = 110e9, c44 = 21.1e9;
                                              // elastic consts
func C =  [[c11, c12, c13, 0  ,   0   , -e31 ],  // "stiffness" matrix
           [c12, c11, c13, 0  ,   0   , -e31 ],
           [c13, c13, c33, 0  ,   0   , -e33 ],
           [0  , 0  , 0  , c44, -e15,     0  ],
           [0  , 0  , 0  , e15, eps11S,   0  ],
           [e31, e31, e33, 0  ,   0   ,eps33S]];

// ------ Macros --------
macro L(ur,uz,phi) [
 dx(ur), ur/x, dy(uz), dy(ur)+dx(uz), -dx(phi),-dy(phi)] // diff op

for(int ii=0; ii<ff.n; ii++) {                // for all frequencies
  real f0 = ff[ii], w0 = 2*pi*f0; cout << f0/1e3 << "kHz" << endl;

  // ------ Problem -------
  fespace Vh3(Sp,[P1,P1,P1]);                 // piecewise linear FE
  Vh3 [ur,uz,phi], [vr,vz,w];                 // variational variables

  solve Piezo2D([ur,uz,phi],[vr,vz,w])        // variational equation!
   = int2d(Sp)( x * rho*w0^2*[vr,vz]'*[ur,uz] ) // "mass" part
   - int2d(Sp)( x * L(vr,vz,w)'*C*L(ur,uz,phi)) // "stiffness" part
   + on(1, phi=V0)                            // BC: bottom side
   + on(3, phi=V1)                            // BC: top side
   + on(4, ur=0);                             // BC: axis of symmetry

  // --------Plot ----------
  real c2 = 100;                              // scaling coefficient
  mesh Sp2 = movemesh(Sp,[x+c2*ur, y+c2*uz]); // deformed mesh
  plot(Sp, Sp2, phi, cmm="f0 = " + f0/1e3 + "kHz", fill=true,
    ps="ff_"+(f0/1e3)+"kHz.eps");             // display and save
}
```

Fig. 2. Example of FreeFEM code modelling free vibrations of voltage excited piezoelectric circular disk as a 2D axisymmetric PDE problem.

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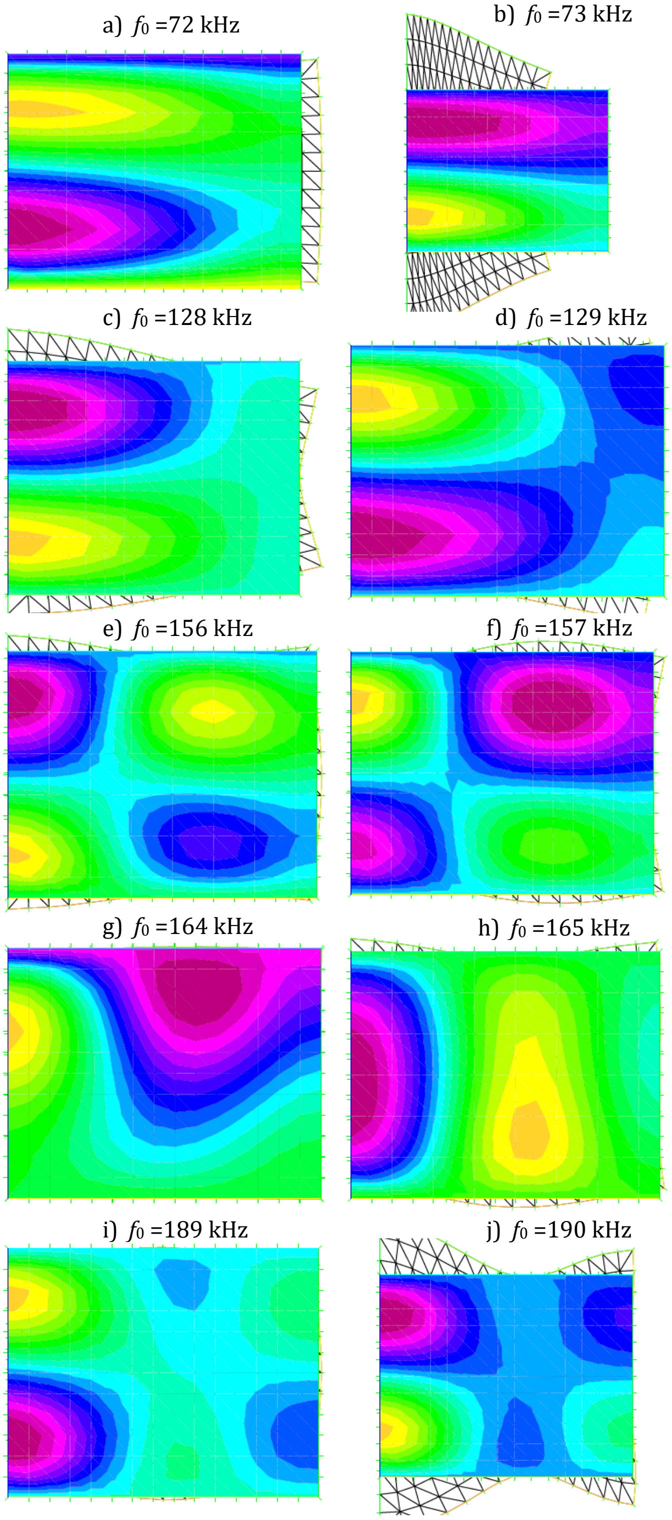

Fig. 3. The result of FreeFEM code execution – the structure vibrations with overlaid potential for selected pair of frequencies: 72kHz and 73kHz, 128 kHz and 129 kHz, 157kHz and 158 kHz, 164 kHz and 165 kHz, 189 kHz and 190 kHz of a PZT5A circular disc with D/T=2.5. The top of rectangular area represents aperture vibration, that is symmetric around disc axis (y-axis). The false colours represents potentials inside the disc that arise between bottom grounded electrode and top electrode excited with 500V.

4. Conclusions

Programmable finite analysis platforms open new opportunities for researchers. The language presented in the paper developed as a scripting language of FreeFEM open software delivers unique possibilities to automate scientific analysis. Due to its implementation based for C++ language it guarantees very fast execution speed allowing at the same time for high level description very similar to mathematical notation used in defining integral formulation of partial differential equations. Its usage in analysis of vibration of piezoelectric devices is nearly straightforward. The sample code presented in the paper could be treated as a starting point for further more realistic models of piezoelectric devices operating in concrete systems. Some of the actual properties of devices require losses of material and specific boundary condition be taken into account, what generate complex valued problems with more integral components. In any case, due to properties of FreeFEM language the details of complicated finite element calculations are not necessary to be considered.

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