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Sensitivity Analysis of Piezoelectric Material Parameters Using Sobol Indices

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Abstract
The applicability of the method of Sobol to the non-smooth, resonant behavior of a vibrational eigenmode of a piezoelectric element is examined. The goal is to quantify the sensitivity of the system upon variation of the piezoelectric material parameters. The randomly distributed piezoelectric material parameters needed for this statistical approach are taken from a Latin hypercube sampling (LHS). For each such sampling point a frequency-domain study is performed, from which the resonance frequency of the considered eigenmode is extracted. The Sobol indices are computed from the statistical distribution of these resonance positions. A hybrid computational approach by means of the MATLAB® LiveLink™ feature is chosen. The LHS process, the COMSOL® model creation, the extraction of the resonance frequencies, and the calculation of the Sobol indices is performed in MATLAB®. COMSOL® is used for the computation of the electrical impedance of the considered block-shaped piezoceramic test specimen. To this end, a frequency-domain study is set up, combined with a parametric sweep with the LHS parameter combinations as input. A batch sweep is employed to speed up the computation by parallel model execution.

Keywords: Sensitivity Analysis, Sobol, Piezoelectricity, MATLAB LiveLink

Introduction

One way to extract piezoelectric material data from measurements is to utilize vibrational eigenmodes of block-shaped test specimens [1]. Within a simulation-aided approach this results in optimizing the values of the material data parameters to fit the experimental result, namely, the frequency-dependent resonant behavior of the electrical impedance of the test sample. As this is a high-dimensional inverse problem, the question of a sensitivity analysis quickly arises. The latter provides information about the sensitivity of a model (here: resonance position) to fluctuations in the model parameters (here: piezoelectric material parameters). Knowing the most relevant parameters leads potentially to a reduced and more manageable dimension of the optimization problem. One established way of expressing sensitivity quantitatively in the form of a measure is to calculate Sobol indices [2]. Their applicability to the non-smooth, resonant behavior of above mentioned eigenmodes upon variation of the piezoelectric material parameters is examined in this contribution.

The calculation of Sobol indices is a statistical method, which means that many randomly generated model values are required for a meaningful calculation. These are taken from a Latin hypercube sampling (LHS) of independently varied piezoelectric material parameters. For each such sampling point a frequency-domain study is performed, resulting in an electrical impedance curve rather than a single data point. From this curve the resonance frequency is extracted, by means of which the Sobol indices of the selected piezoelectric material parameters are finally calculated.

Theoretical Aspects

This section provides a brief overview on piezoelectricity and the method of Sobol, which are both essential for this contribution.

Piezoelectric Materials

In piezoelectric materials the direct and inverse piezoelectric effect occurs. The material exhibits a crystal structure and consists of positively and negatively charged ions with overlapping charge centers in the absence of external influences. When a force is applied to the structure, the crystal structure deforms, the charge centers shift, and dipoles form (direct piezoelectric effect), resulting in a measurable voltage difference across the deformed geometry. Similarly, an applied voltage results in a deformation of the material (inverse piezoelectric effect).

The quantitative relationship between the magnitude of the displacement and the magnitude of the voltage difference can, in the linear case, be described by two coupled state equations for the dielectric displacement (D_m) and the mechanical stress (T_{ij}) (stress-charge form),

$$D_m = e_{mkl} S_{kl} + \epsilon_{mn}^S E_n,$$
$$T_{ij} = c_{ijkl}^E S_{kl} - e_{ijn} E_n,$$

where E_n is the electric field and S_{kl} the mechanical strain [1]. The material specific parameters are ϵ_{mn}^S (electric permittivity at constant strain), c_{ijkl}^E (elastic stiffness at constant electric field), and e_{ijn} (the piezoelectric stress tensor); they describe the electrical and mechanical properties as well as their coupling.

In general, piezoelectric materials are anisotropic, hence the tensor formulation above. Symmetries of the crystalline structure reduce the number of independent tensor components. For transversely isotropic behavior this leaves the parameters c_{11}^E, c_{12}^E, c_{13}^E, c_{33}^E, c_{44}^E, e_{31}, e_{33}, e_{15}, ϵ_{11}^S, and ϵ_{33}^S [1]; note that the indices are given in the Voigt notation [3]. That is, these ten material parameters characterize the behavior of a given piezoelectric material. Which of them are truly relevant and which only play a minor role (and thus do not need to be known with the same accuracy) can be evaluated by means of a sensitivity analysis.

The Method of Sobol

A sensitivity analysis provides information about the sensitivity of a model to variations in the model parameters. It helps to distinguish between influential and insignificant parameters. This can be useful, for example, to identify the critical control variables of the model.

In this work, Sobol indices are employed to perform a sensitivity analysis. The variance of the model output $y[\boldsymbol{x}]$ is calculated upon variation of the n model parameters $\boldsymbol{x} = \{x_1, \dots, x_n\}$ (here: piezoelectric material parameters) and then decomposed into the contributions attributable to the individual input parameters x_i. The first-order Sobol index (the so-called main effect) of parameter x_i is defined as

$$S_i = \frac{\mathcal{V}_{x_i}\left[E_{x_{\sim i}}[y|x_i]\right]}{\mathcal{V}_x[y]} \in [0,1],$$

where $\mathcal{V}_{x_i}[y]$ is the total variance of the model $y[\boldsymbol{x}]$ over all input parameters and $E_{x_{\sim i}}[y|x_i]$ is the mean value of y with given parameter x_i [5]; the indices x_i and $\boldsymbol{x}_{\sim i}$ denote which parameters ought to be varied, the latter meaning all but the ith one. The total Sobol sensitivity index, another popular variance-based measure, is defined as

$$S_i^T = \frac{E_{x_{\sim i}}\left[\mathcal{V}_{x_{\sim i}}[y|\boldsymbol{x}_{\sim i}]\right]}{\mathcal{V}_x[y]} = 1 - \frac{\mathcal{V}_{x_{\sim i}}\left[E_{x_i}[y|x_{\sim i}]\right]}{\mathcal{V}_x[y]},$$

again being normalized [5]. S_i describes the contribution of the uncertainty of x_i to the total variance while S_i^T gives the mean variance remaining when all parameters but x_i are fixed [4].

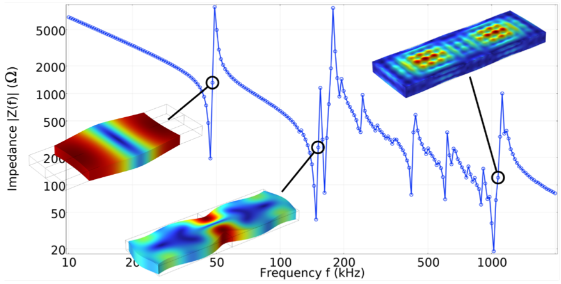

Figure 1. Electrical impedance magnitude of the block-shaped sample geometry of this study. Three different eigenmodes are highlighted, from which the leftmost at about 50kHz is used.

Direct calculation of above Sobol indices by means of solving the variance integrals is not feasible. Instead, a statistical method based on quasi-Monte Carlo sampling is used, needing only $m \cdot (n+2)$ model evaluations [6]; n denotes the number of parameters to be investigated and m the desired sample size. Within this method, two $n \times m$ matrices A and B are generated using LHS. Each column of these matrices represents a parameter set for the simulation. These matrices with independent samples are rearranged into cross matrices AB_i, which represent the dependencies among individual variables. For this purpose, the ith row of matrix B is inserted at the position of the ith row of matrix A. In this way, exactly one parameter x_i in the parameter set is changed in matrix A.

The computation of the Sobol indices becomes [6]

$$S_i \approx \frac{\frac{1}{m}\sum_{j=1}^m y(B)_j\big(y(AB_i)_j - y(A)_j\big)}{\mathcal{V}_x[y]},$$

$$S_i^T \approx \frac{\frac{1}{2m}\sum_{j=1}^m \big(y(AB_i)_j - y(A)_j\big)^2}{\mathcal{V}_x[y]},$$

$$\mathcal{V}_x[y] \approx \frac{1}{2m}\sum_{j=1}^{2m}\big(y(C)_j\big)^2 - \left(\frac{1}{2m}\sum_{j=1}^{2m} y(C)_j\right)^2,$$

where $y(A)$, $y(B)$ and $y(AB_i)$ are vectors each containing m model outputs for the respective sample matrices. The vector $y(C)$ contains the concatenated vectors of $y(A)$ and $y(B)$ and is thus of size $2m$.

Simulation Model and Methods

This work focuses on vibrational eigenmodes of block-shaped test specimens of piezoelectric materials. The eigenmodes are characterized by an increased vibration at the resonance frequency which can be identified using the electrical impedance $Z(f)$ of a specific test sample, see Figure 1 for an example. Therefore, the computational model needs to provide this resonance position from a frequency sweep study. This is, to our knowledge, not possible within COMSOL Multiphysics. One might try to use an eigenmode study, which would require a method to

Table 1. Material parameters for PIC255 in stress-charge form; material density is taken as $\rho = 7800\ kg/m^3$ [1].

Parameter	Value
c_{11}^E [N/m^2]	$12.46 \cdot 10^{10}$
c_{12}^E[N/m^2]	$7.86 \cdot 10^{10}$
c_{13}^E[N/m^2]	$8.06 \cdot 10^{10}$
c_{33}^E[N/m^2]	$12.06 \cdot 10^{10}$
c_{44}^E[N/m^2]	$2.04 \cdot 10^{10}$
e_{31}[C/m^2]	-6.86
e_{33}[C/m^2]	16.06
e_{15}[C/m^2]	11.90
ϵ_{11}^S[F/m]	$7.31 \cdot 10^{-9}$
ϵ_{33}^S[F/m]	$6.81 \cdot 10^{-9}$

pick the right resonance. Here, we follow another approach, namely, to perform the sample and model creation, post-processing and statistical evaluation in MATLAB®.

COMSOL® Model

To calculate the Sobol indices, a block of length 30mm, width 10mm, and thickness 2mm is used [1]. The block is polarized in the thickness direction (z-direction) and made of the material PIC255, for which optimized material parameters can be found in [1] and are reproduced in Table 1. Furthermore, an isotropic loss factor $\eta_s = 0.0129$ for mechanical damping and an identical dielectric loss factor $\eta_{\epsilon S} = 0.0129$ for the electrical permittivity is assumed.

Piezoelectricity is modelled in COMSOL® via the *Solid Mechanics* and *Electrostatics* physics interfaces which are coupled via the *Piezoelectricity Multiphysics* interface using the *Piezoelectric Material* and *Charge Conservation, Piezoelectric* nodes, respectively. As boundary conditions a *Voltage Terminal* of magnitude 1V is applied to the top surface and *Ground* to the bottom one. Two symmetry planes are implemented to reduce the computational costs; see Figure 2. In the same figure, the mesh is visualized: a cubic mesh consisting of 15 x 5 x 5 elements is chosen.

For the *Frequency Domain* study, frequencies in the range of 35 to 65 kHz with intervals of 500 Hz are selected. The choice of this frequency range is such that the zeroth order transverse mode in the y-direction is excited. As can be seen in Figure 1, this resonance is particularly suitable for this initial study as it is nicely separated from other, overlapping resonances.

From the COMSOL® model an output of the electrical impedances as function of the frequency is needed. The electrical impedance is evaluated as global probe via the expression *abs(1/es.Y11)* and stored in a probe table.

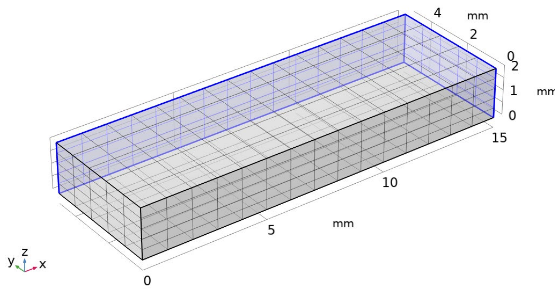

Figure 2. Model geometry and mesh. Highlighted are the symmetry planes used to reduce the model size.

Sensitivity Analysis

The goal of this work is to perform a sensitivity analysis of the selected eigenmode with respect to the piezoelectric material parameters. To this end, the material parameters are sampled in a $\pm 5\%$ interval from the literature values provided in Table 1. However, as it is known from previous studies, the chosen resonance is not sensitive to all material parameters [1]. To reduce the computational effort, a mixture of important and not-so important parameters is selected (c_{11}^E, c_{12}^E, c_{13}^E, c_{33}^E, c_{44}^E). Of course, a sensitivity analysis with respect to all parameters is preferable, but out-of-scope of this particular study due to immense requirements regarding computation time.

The sensitivity analysis is set up in MATLAB®. The LHS parameter sampling is realized using the *lhsdesign()* MATLAB® function. Creating the COMSOL® simulation models is implemented using the COMSOL® LiveLink™ for MATLAB®. This allows to create parameter sweeps for the previously computed parameter combinations programmatically. Setting up the base model with the LiveLink™ is based on the COMSOL® model described in the earlier section exported as *Model File for MATLAB*.

After running the COMSOL® simulations, the probe tables (impedance vs. frequency) are imported from file. For each single parameter set, the resonance frequency of the investigated eigenmode is then extracted by a quadratic fit of the resonance peak. This serves as model output $y[\boldsymbol{x}]$ from which, together with the sample matrices A, B, AB_i, C, the Sobol indices are computed according to the equations presented in the previous section.

Computational Approach

Within this study, sample sizes up to $m = 10\,000$ are realized (see next Section). Therefore, a plain, sequential *Parametric Sweep* is not an ideal choice. Even an optimistically short single simulation duration of one minute would yield a total runtime of about seven weeks. Still, the single model evaluation, a frequency-domain sweep for a fixed set of material parameters, is computationally rather cheap. Therefore, the concept of task parallelism via the batch sweep functionality of COMSOL® is used

[7]. For later analyses, the probe tables of the individual frequency sweeps are automatically stored on file by adding an *Export to File* sub-node to the *Job Configuration* of the *Parametric Sweep*.

The total parameter sweep is distributed between 70 models which can be run in parallel with only one CPU core assigned each. In the case of the present study, these 70 models are distributed once more among four 20-core compute nodes of an HPC cluster at the Erlangen National High Performance Computing Center (NHR@FAU) of the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). This reduces the total runtime of the largest sample size considered in this study to just below 24h.

Simulation Results & Discussion

Table 2 and Table 3 contain the computed first order and total Sobol indices, respectively, for varying sample sizes. Figure 3 and Figure 4 show the evolution of the indices with the sample size. While the first order Sobol indices vary quite substantially, they show some initial trends nevertheless, distinguishing the influential parameters from the remaining ones. The total Sobol indices support the trends seen in the first order index. As they show not much variation upon changing sample size, the total Sobol index can be quite useful to assess the importance of the model parameters more quickly. For example, it could be used in a study with fewer samples but all model parameters included, to rule out the least important ones for following large-sample studies with selected parameters.

For the material parameters investigated in this study, both Sobol indices clearly identify the most influential ones: c_{11}^E and c_{12}^E. This matches the findings of the more qualitative study presented in [1] and is supported by the modal shape of the considered resonance, cf. Figure 1: The deformation mainly occurs in the plane perpendicular to the polarization direction. Hence, this mode is most influenced by material parameters that define the properties in this plane, such as c_{11}^E and c_{12}^E.

Finally, Figure 5 shows the distribution of resonance positions for the sample size $m = 10\,000$; remember that for setting up the sample matrices A, B, and AB_i in total $m \cdot (n+2) = 70\,000$ parameter cases are necessary.

Outlook

As it becomes clear from Figure 3, further studies with larger sample sizes for the first order Sobol indices are necessary. In this context, the *Cluster Sweep* functionality of COMSOL® could be a promising approach to utilize more compute nodes in an efficient manner. Alternatively, one could employ a computationally cheaper eigenmode study. In this case the whole sensitivity analysis could potentially be implemented in COMSOL®.

Table 2. First order Sobol indices for different sample sizes.

m	$S_{c_{11}^E}$	$S_{c_{12}^E}$	$S_{c_{13}^E}$	$S_{c_{33}^E}$	$S_{c_{44}^E}$
1000	-0.79	-0.45	-0.04	0.09	0
5000	1.09	0.31	0.10	0.01	0
7500	0.91	0.48	0.07	0.01	0
10000	0.36	0.43	0.02	0	0

Table 3. Total Sobol indices for different sample sizes.

m	$S_{c_{11}^E}^T$	$S_{c_{12}^E}^T$	$S_{c_{13}^E}^T$	$S_{c_{33}^E}^T$	$S_{c_{44}^E}^T$
1000	0.630	0.161	0.0092	0.002	0
5000	0.648	0.176	0.0099	0.002	0
7500	0.635	0.179	0.0097	0.002	0
10000	0.650	0.175	0.0102	0.002	0

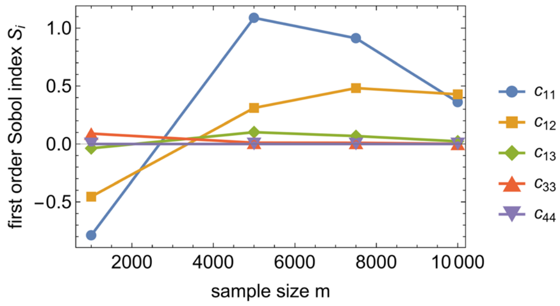

Figure 3. Evolution of the first order Sobol index with the sample size.

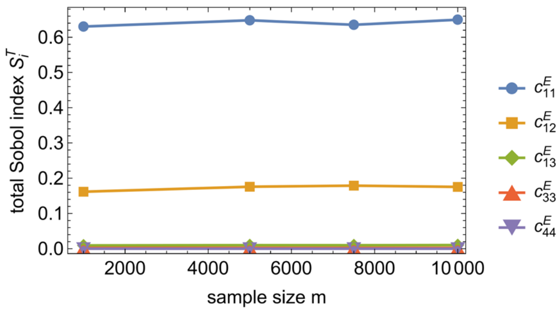

Figure 4. Evolution of the total Sobol index with the sample size.

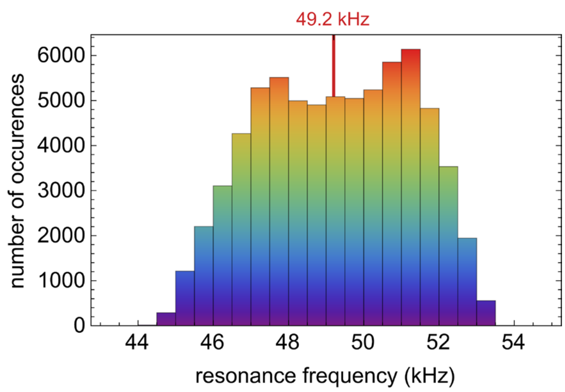

Figure 5. Distribution of resonance positions for the sample size m=10 000. For the reference values of the material parameters, cf. Table 1, the resonance is found at $f_{ref} = 49.2\ kHz$.

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