Solving piezoelectric inverse problems using Algorithmic Differentiation

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Motivation and objective

As a consequence of high prototyping costs and increasing computing power, design processes in general are getting more and more simulation driven. The result of these simulation processes heavily depends on the quality of the applied material parameters describing the behaviour of the involved components. In the case of piezoceramics, the standard material characterisation technique needs four specimens of different geometry to excite different fundamental modes used for an analytic material parameter calculation [1]. A problem that arises from the usage of several specimens is the incompatibility and inconsistency of the obtained material parameters. Only subsets of the material parameters can be derived from each specimen and are combined to form a single set of parameters. Varying processing and poling conditions thus distort the composed full set of parameters. Furthermore, material parameters can only be estimated for a certain material, but not for a unique specimen.

Emerging from the increasing use of simulation tools in design, several numerical identification methods have been developed applying an inverse approach, i.e. optimising a set of model parameters to fit the model output with a measured quantity [2, 3]. These techniques allow the application of more complex set-ups that are not computable analytically.

Therefore, a material characterisation method is developed to use a single disc-shaped specimen to determine all relevant parameters in a consistent way. A simple piezoelectric disc with electrodes covering both base surfaces is chosen for its common application in single-element transducers. The geometry is considered fixed to a radius of $r_\mathrm{o} = 5\,\mathrm{mm}$ and a thickness of $t = 1\,\mathrm{mm}$. Since such a simple and symmetric configuration does not yield sufficient sensitivity to all parameters, a custom triple-ring electrode set-up is applied [4, 5]. Thereby, two optimisation problems arise in the context of characterising a piezoceramic material using a single disc-shaped sample:

1. The determination of an electrode set-up that maximises the sensitivity to all material parameters.
2. The determination of the material parameters itself from measurements conducted on a specimen with the optimised electrode set-up.

These two optimisation problems are used to illustrate the possible advantages and disadvantages of using Algorithmic Differentiation (AD) [6] in comparison to well-known Finite Differences (FD) techniques. Algorithmic Differentiation is a tool for calculating derivatives of a given computer program up to machine precision by successively applying the chain rule to each of the program's calculations whereas Finite Differences approximates derivatives by a difference quotient implying numerical errors.

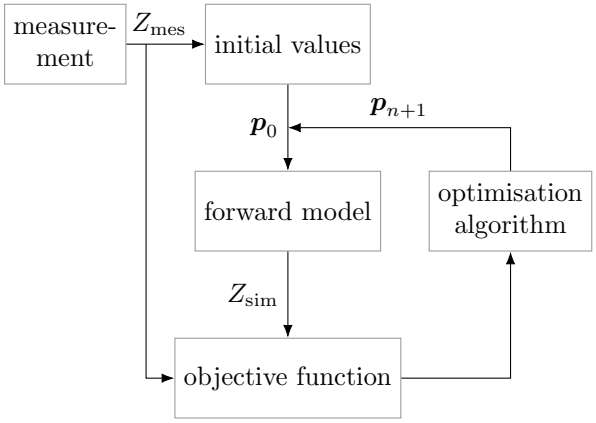

Figure 1: Inverse measurement procedure for piezoelectric material characterisation.

Inverse measurement procedure

Generally, a complex measurement task can be performed by an inverse problem approach. When a quantity is not measurable directly, a parametrisable model can be build to represent a real measurement set-up which output depends on the required quantity. For an iterative solution, the model parameters then have to be adjusted until the model behaves just like the real system. In order to account for inaccuracies and uncertainties of the two systems, a model outcome that minimises an objective function assigning a value to the model's deviation from the measurements is called the inverse problem's solution (see figure 1). Thus, solving an inverse problem iteratively is mostly an optimisation task. In order to get meaningful results with sufficiently small uncertainties, the model as well as the measurement set-up have to be sensitive to the required parameters.

Simulation model

An inverse problem always needs a parametrised model of the actual measurement set-up. For the piezoelectric material characterisation a Finite-Element (FE) model is used to solve the discretised piezoelectric equations

numerically. The material description applies a coupling between mechanical and electrical quantities [7]:

$$\boldsymbol{T} = -\boldsymbol{e}^{\mathrm{t}}\boldsymbol{E} + \boldsymbol{c}^{E}\boldsymbol{S} \tag{1}$$

$$\boldsymbol{D} = \boldsymbol{\varepsilon}^{S}\boldsymbol{E} + \boldsymbol{e}\boldsymbol{S} \tag{2}$$

with the mechanical stress $\boldsymbol{T}$ and strain $\boldsymbol{S}$ and the electric field $\boldsymbol{E}$ and displacement $\boldsymbol{D}$. $\boldsymbol{c}^{\boldsymbol{E}}$, $\boldsymbol{\varepsilon}^{\boldsymbol{S}}$ and $\boldsymbol{e}$ denote the the mechanical stiffness, the permittivity and the coupling matrices, respectively. The underlying differential equations are based on Newton's equations of motion and the electrostatic Gauss law:

$$\rho\ddot{\boldsymbol{u}} = \mathcal{B}^{\mathrm{t}}(\boldsymbol{c}^{\boldsymbol{E}}\,\mathcal{B}\,\boldsymbol{u} + \boldsymbol{e}^{\mathrm{t}}\nabla\phi) \tag{3}$$

$$q = \nabla(\boldsymbol{e}\,\mathcal{B}\,\boldsymbol{u} - \boldsymbol{\varepsilon}^{\boldsymbol{S}}\nabla\phi) \tag{4}$$

where $\boldsymbol{u}$, ϕ, q are the mechanical displacement, the electric potential and the charge and ρ denotes the density. $\mathcal{B}$ and ∇ are the operator of spacial derivatives and the nabla/del operator, respectively. The material parameters to be determined are the entries of the matrices $\boldsymbol{c}^{\boldsymbol{E}}$, $\boldsymbol{\varepsilon}^{\boldsymbol{S}}$ and $\boldsymbol{e}$, when the density is considered to be known. Because of the transverse isotropy of piezoceramic materials certain entries have to be zero or are dependant leaving only ten independent parameters. For adding Rayleigh damping [8], additional two parameters have to be considered resulting in the parameter vector

$$\boldsymbol{p}_{\mathrm{mat}} = \big[c^{E}_{11}, c^{E}_{12}, c^{E}_{13}, c^{E}_{33}, c^{E}_{44}, \varepsilon^{S}_{11}, \varepsilon^{S}_{33}, e_{15}, e_{31}, e_{33}, \alpha_{\mathrm{M}}, \alpha_{\mathrm{K}}\big]\,. \tag{5}$$

The measured quantity is chosen to be the electrical impedance since it is easy to obtain. Applying a given charge pulse $q(t)$ with an appropriate broadband spectrum the resulting potential $\phi(t)$ can be calculated using e.g. the Finite Element software CFS++. The frequency dependant electrical impedance then is given by

$$Z_{\mathrm{sim}}(f) = \frac{\mathcal{F}\{\phi(t)\}}{\mathrm{j}2\pi f\,\mathcal{F}\{q(t)\}}, \tag{6}$$

where j describes the imaginary unit, f is the frequency and $\mathcal{F}\{\cdot\}$ denotes the Fourier transform.

The chosen triple-ring set-up for increased sensitivities can be parametrised using four parameters being the ring radii when the disc radius $r_{\mathrm{o}} = 5\,\mathrm{mm}$ and the thickness $t = 1\,\mathrm{mm}$ are given (see figure 2):

$$\boldsymbol{r} = [r_1, r_2, r_3, r_4]. \tag{7}$$

Caused by the multiple electrodes, several impedances have to be measured and computed by considering the impedance between two shortened electrodes and the remaining electrodes.

- Z_1: el_2 and el_3 to el_1
- Z_2: el_1 and el_3 to el_2
- Z_3: el_1 and el_2 to el_3

This leads to a total of three impedances whose absolute values are shown for an exemplary realistic material in figure 3. For the optimisation process these impedances can be combined by simple addition.

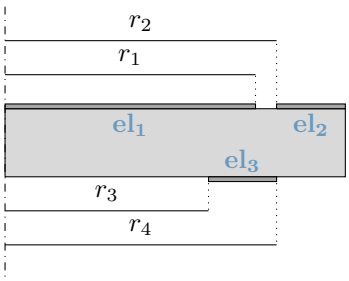

Figure 2: Triple-ring electrode set-up

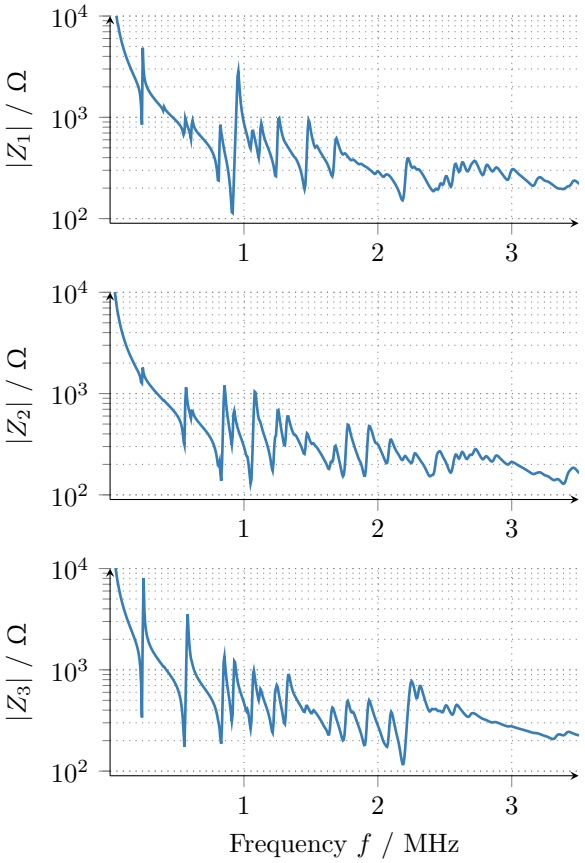

Figure 3: Electric impedances for an exemplary material.

Sensitivity calculation

For the solution of an inverse problem a change in the input parameters has to be visible in the impedance. This property can be described by a measure of sensitivity, e.g. the derivative of the impedance with respect to the material parameters:

$$\Upsilon(p_j, \boldsymbol{r}) = \sum_{n=1}^{3} \left\| \partial_{p_j} |Z_n(f_i, \boldsymbol{p}, \boldsymbol{r})| \right\|_{f_i}, \tag{8}$$

with the discrete frequencies f_i and $\|\cdot\|_x$ denoting the L_2-norm regarding x. The overall sensitivity can be calculated by

$$\bar{\Upsilon}(\boldsymbol{r}) = \left\| w_j \Upsilon(p_j, \boldsymbol{r}) \right\|_{p_j}, \tag{9}$$

where w_j is a weighting factor compensating the different magnitudes and units of the material parameters.

Optimisation problems

The determination of piezoelectric material parameters with a triple-ring electrode set-up involves two consecutive optimisation problems. First the ring radii are optimised (assuming an initial set of material parameters) in order to increase the overall sensitivity $\bar{\Upsilon}$. When a sufficient sensitivity is obtained, the set-up is used for the fitting of the material parameters to a measured impedance. During these optimisation processes derivatives play a crucial role for the sensitivity calculation and for the trust-region-based optimisation algorithms [9, 10]. Typically, these derivatives are approximated using Finite Difference approaches. In the following, it is to be evaluated in how far an Algorithmic Differentiation approach yields advantages in the described optimisation problems.

Optimising the ring radii

The first optimisation problem can mathematically be stated by

$$\min_{\boldsymbol{r}} -\bar{\Upsilon}(\boldsymbol{r}). \tag{10}$$

For practical purposes, electrodes have to be at least 1 mm for electrical contacting and the distance between electrodes at least 0.3 mm. In this case, two different derivatives have to be calculated:

1. The derivative of the impedance with respect to the material parameters being the sensitivities for the calculation of the objective function.

2. The derivative of the objective function with respect to the radii for the optimisation process (i.e. mixed second derivatives).

Here, the focus lies on the first kind of derivatives, since the use for the optimisation process is analysed in the second case. Calculating the optimal radii using AD leads to an electrode configuration resulting in higher sensitivities (e.g. for the parameter ε_{11} FD yields an increase in sensitivity by 1.37 whereas AD increases the sensitivity by 2.57 in comparison to an initial set-up [11]). This can easily be explained when the objective function is calculated for a fixed $[r_2, r_3, r_4] = [3.5, 3, 4]$ mm and a varying r_1 in figure 4. It is obvious that the vast number of local minima in the FD case lead to a very tedious optimisation, whereas the quite smooth AD case seems much more viable, what is exactly what the optimisation results show. For the higher dimensional case with four radii, the problem only increases. Thus, when the objective function itself includes derivatives like in the case of maximising sensitivities, using AD is inevitable. The resulting radii that are used in the following are

$$\boldsymbol{r}_{\text{opt}} = [3.68, 4, 4, 5] \text{ mm}. \tag{11}$$

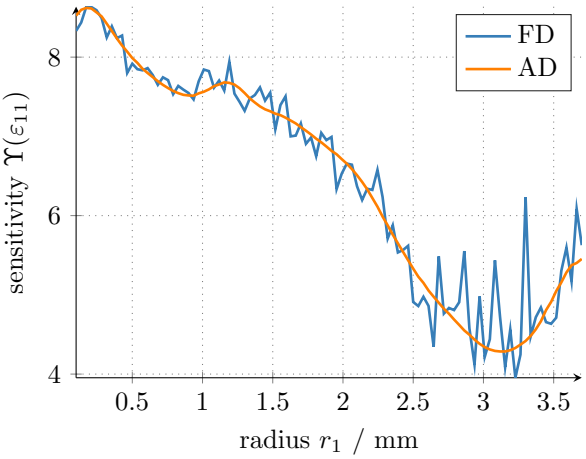

Figure 4: Sensitivity regarding ε_{11} for different radii r_1 [11].

Optimising the material parameters

The second optimisation problem can mathematically be described by

$$\min_{\boldsymbol{p}} \| \log_{10} |Z_{\text{meas}}(f_i)| - \log_{10} |Z_{\text{sim}}(f_i, \boldsymbol{p}, \boldsymbol{r}_{\text{opt}})| \|^2_{f_i}, \tag{12}$$

where Z_{meas} is an objective impedance, Z_{sim} is the simulated impedance and $\boldsymbol{r}_{\text{opt}}$ are the optimal radii calculated beforehand. Normally, the objective impedance would be a measured one, but here, a simulated one is used to enable the possibility to explicitly evaluate the optimisation outcome. For the optimisation, a step-by-step strategy is applied (see [12]), where a preceding sensitivity analysis identifies certain frequency ranges best suited for optimising each parameter. Derivatives for the gradient-based algorithm are calculated using FD or AD (where possible, i.e. unfortunately not for damping parameters). The optimisation using FD leads to a reconstruction of the material parameters in a relatively short time. Using AD does in this case not yield any relevant advantages and might possibly even introduce certain disadvantages. On the one hand, the FD optimisation is more robust for certain cases. E.g. when the sampling frequency for the excitation and resulting signals is chosen too small, this effect is much stronger in the AD derivatives than in those calculated via FD. For a realistic material parameter set $\boldsymbol{p}_{\text{ideal}}$ and a sampling frequency of 50 MHz the optimisation does not recover the material parameters $\boldsymbol{p}_{\text{ideal}}$ and the objective function does not converge to zero. When the sampling frequency is doubled or a harmonic simulation is used, this phenomenon disappears. On the other hand, the calculation time for the given FE-implementation increases when AD is used (despite the reduced number of function evaluations). This is mainly due to the application of the forward mode of AD implemented in CFS which needs a whole simulation for each material parameters. Using reverse mode would drastically reduce the computation time, but was not implementable in the simulation software CFS++ (see [11] for further explanations).

Conclusions

The determination of piezoelectric material parameters using a single specimen implies several challenging optimisation problems. In the context of these optimisation problems derivatives play an important role. Its computation via Finite Differences induces numerical errors that are not present when Algorithmic Differentiation is used. The influence of these two methods for derivative calculation in the context of piezoelectric optimisation problems are analysed. When the derivatives are used for the optimisation algorithm itself, FD does slightly outperform AD especially regarding computation time which might be due to the missing possibility to implement reverse mode for AD. In contrast, when the objective function itself is a derived quantity, using AD is inevitable. The numerical errors using FD leads to a non-smooth objective function showing many local minima and thus preventing a successful optimisation result.

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References

[1] *IEEE Standard on Piezoelectricity*. 1987. DOI: 10.1109/IEEESTD.1988.79638.

[2] J. Smits. "Iterative Method for Accurate Determination of the Real and Imaginary Parts of the Materials Coefficients of Piezoelectric Ceramics". In: *IEEE Transactions on Sonics and Ultrasonics* 23.6 (1976), pp. 393–401. DOI: 10.1109/T-SU.1976.30898.

[3] S. J. Rupitsch and R. Lerch. "Inverse Method to estimate material parameters for piezoceramic disc actuators". In: *Applied Physics A* 97.4 (2009), pp. 735–740. DOI: 10.1007/s00339-009-5438-1.

[4] C. Unverzagt, J. Rautenberg, B. Henning, and K. Kulshreshtha. "Modified electrode shape for the improved determination of piezoelectric material parameters". In: *Proceedings of the 2013 International Congress on Ultrasonics*. Singapore, 2013, pp. 758–763. ISBN: 978-981-07-5938-4.

[5] N. Feldmann, B. Jurgelucks, L. Claes, V. Schulze, B. Henning, and A. Walther. "An inverse approach to the characterisation of material parameters of piezoelectric discs with triple-ring-electrodes". In: *tm - Technisches Messen* 86.2 (2019), pp. 59–65. DOI: 10.1515/teme-2018-0066.

[6] A. Griewank and A. Walther. *Evaluating derivatives: Principles and techniques of algorithmic differentiation*. 2nd ed. Philadelphia, Pa.: Society for Industrial and Applied Mathematics, 2008. ISBN: 0898716594.

[7] T. Lahmer. "Forward and Inverse Problems in Piezoelectricity". doctoral thesis. Erlangen-Nürnberg: University of Erlangen, 2008.

[8] J. W. S. Rayleigh. *The theory of sound: In 2 vol.* New York: Dover Publ, 1945. ISBN: 9780486602929.

[9] M. A. Branch, T. F. Coleman, and Y. Li. "A Subspace, Interior, and Conjugate Gradient Method for Large-Scale Bound-Constrained Minimization Problems". In: *SIAM Journal on Scientific Computing* 21.1 (1999), pp. 1–23. ISSN: 1064-8275. DOI: 10.1137/S1064827595289108.

[10] P. Virtanen et al. *SciPy 1.0–Fundamental Algorithms for Scientific Computing in Python*. 2019. URL: http://arxiv.org/pdf/1907.10121v1.

[11] B. Jurgelucks. "Increased sensitivity in parameter identification problems for piezoelectrics". doctoral thesis. Paderborn: Paderborn University, 2019. DOI: 10.17619/UNIPB/1-654.

[12] N. Feldmann, B. Jurgelucks, L. Claes, and B. Henning. "A sensitivity-based optimisation procedure for the characterisation of piezoelectric discs". In: *2019 International Congress on Ultrasonics*. Proceedings of Meetings on Acoustics. ASA, 2019. DOI: 10.1121/2.0001070.