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PDE based determination of piezoelectric material tensors

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The exact numerical simulation of piezoelectric transducers requires the knowledge of all material tensors that occur in the piezoelectric constitutive relations. To account for mechanical, dielectric and piezoelectric losses, the material parameters are assumed to be complex. The issue of material tensor identification is formulated as an inverse problem: As input measured impedance values for different frequency points are used, the searched-for output is the complete set of material parameters. Hence, the forward operator F mapping from the set of parameters to the set of measurements, involves solutions of the system of partial differential equations arising from application of Newton's and Gauss' law to the piezoelectric constitutive relations. This, via two or three dimensional finite element discretisation, leads to an indefinite system of equations for solving the forward problem. Well-posedness of the infinite dimensional forward problem is proven and efficient solution strategies for its discretized version are presented. Since unique solvability of the inverse problem may hardly be verified, the system of equations we have to solve for recovering the material tensor entries can be rank deficient and therefore requires application of appropriate regularisation strategies. Consequently, inversion of the (nonlinear) parameter-to-measurement map F is performed using regularised versions of Newton's method. Numerical results for different piezoelectric specimens conclude this paper.

1 Introduction

Piezoelectric materials are widely used in electromechanical sensors and actuators, e.g. ultrasound transducers in medical imaging and therapy, force and acceleration sensors, positioning sensors, surface acoustic wave (SAW) filters, with a permanently growing range of applications. Their mode of action is based on the piezoelectric effect, that couples the electrical and the mechanical behaviour of such materials. For the optimal design of piezoelectric devices, efficient numerical simulation tools have been developed, that avoid expensive and time-consuming experiments by numerically solving the mathematical formulation of the underlying physical model, i.e. a system of partial differential equations with appropriate boundary conditions (e.g. cf. [23, 25, 29], and § 2.1 below). These equations contain as essential information a set of about ten material parameters steering the interplay of mechanical and electrical quantities. A priori knowledge of the exact values of these parameters is for obvious reasons indispensable for obtaining useful

results in computational system simulations. So far, these quantities have been estimated by experiments with test samples, whose special shapes were supposed to allow for simplifications in the model and hence lead to explicit formulas for their computation from the resonance frequencies [13, 23].

However, the results of these estimation formulas do not seem to provide sufficiently precise information on the material coefficients [30], showing deviations of up to 10–20%, which gave rise to inaccurate results in the computational simulations. Moreover, the handling of such test samples is complicated and their production costly. Therefore it was our aim to propose and implement a computational scheme that enables a precise and automatic reconstruction of the whole material parameter set from relatively simple measurements by iterative adjustment based on simulations of the full two or three dimensional piezoelectric equations. The proposed methodology extends to material tensors with complex valued entries. This is important in view of the fact that in general, piezoelectric transducers are lossy, i.e. there is a dissipation of power. As Holland showed [21] these losses are represented by the imaginary parts of the elastic, dielectric and piezoelectric coefficients. In the introductory part of Du *et al.* [9], a detailed comparison of existing strategies to determine complex valued material parameters can be found. All these methods rely on model simplifications according to the common resonator geometries [13, 23].

This paper is organised as follows. §2 is devoted to the forward problem, i.e. the solution of the piezoelectric PDEs. Here, we provide results on well-posedness in the infinite-dimensional time-harmonic setting, which are new, to our knowledge. Moreover, we address the issue of efficient numerical solution of the linear system arising from discretisation by finite elements. In the subsequent §3, we commit ourselves to the inverse problem of parameter identification, considering the question of identifiability and discussing the aspect of ill-posedness. Most of this section is concerned with stable numerical reconstruction schemes based on Newton's method. Moreover, results of various numerical experiments are presented in §4. The final §5 provides conclusions and an outlook to possible future research tasks related to the subject of this paper.

2 The forward problem

2.1 The piezoelectric equations

The material law describing the piezoelectric effect in the linearised case of small mechanical deformations and electric fields reads as

$$\vec{\sigma} = \mathbf{c}^E \vec{S} - \mathbf{e}^T \vec{E} \quad (2.1a)$$

$$\vec{D} = \mathbf{e} \vec{S} + \boldsymbol{\epsilon}^S \vec{E}, \quad (2.1b)$$

relating the mechanical stress $\vec{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{zx}, \sigma_{xy})^T$ and the electrical displacement $\vec{D} = (D_x, D_y, D_z)^T$, respectively, to the mechanical strain $\vec{S} = (S_{xx}, S_{yy}, S_{zz}, S_{yz}, S_{zx}, S_{xy})^T$ and the electric field $\vec{E} = (E_x, E_y, E_z)^T$. An equivalent formulation that we will make use of in the next subsection is

$$\vec{S} = \mathbf{s}^E \vec{\sigma} + \mathbf{d}^T \vec{E} \quad (2.2a)$$

$$\vec{D} = \mathbf{d} \vec{\sigma} + \boldsymbol{\epsilon}^\sigma \vec{E}. \quad (2.2b)$$

Since the temporal change of the magnetic field is negligible – note that the sound velocity of piezoelectric waves is by a factor of at least one thousand smaller than the electromagnetic wave speed – the electric field can be considered as irrotational. For details we refer to Ikeda [24]. Hence, we can rewrite $\vec{E}$ as the negative gradient of an electric potential $\vec{E} = -\text{grad } \phi$, and $\vec{S}$ in terms of the mechanical displacements $\vec{d} = (d_x, d_y, d_z)^T$ as $\vec{S} = \mathcal{B}\vec{d}$, where the first order differential operator $\mathcal{B}$ is

$$\mathcal{B} = \begin{pmatrix} \frac{\partial}{\partial x} & \cdot & \cdot & \cdot & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \cdot & \frac{\partial}{\partial y} & \cdot & \frac{\partial}{\partial z} & \cdot & \frac{\partial}{\partial x} \\ \cdot & \cdot & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & \cdot \end{pmatrix}^T,$$

i.e. the transposed of the divergence of a dyadic. The material tensors $\mathbf{c}^E$, $\mathbf{\epsilon}^S$ and $\mathbf{e}$, appearing in (2.1) are the elasticity coefficients, the dielectric coefficients, and the piezoelectric coupling coefficients, respectively. Since we concentrate on the small signal behaviour of piezoelectric materials here, we assume these coefficients to be constants. Due to the crystal structure and the polarisation of the piezoelectric material, these matrices show a certain symmetry and sparsity pattern [23]. In the 6mm crystal class, e.g. on which we will concentrate on in the further expositions, this is given by

$$\mathbf{c}^E = \begin{pmatrix} c_{11}^E & c_{12}^E & c_{13}^E & \cdot & \cdot & \cdot \\ c_{12}^E & c_{11}^E & c_{13}^E & \cdot & \cdot & \cdot \\ c_{13}^E & c_{13}^E & c_{33}^E & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & c_{44}^E & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & c_{44}^E & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & c_{66}^E \end{pmatrix}, \quad (2.3)$$

$$\mathbf{e} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & e_{15} & \cdot \\ \cdot & \cdot & \cdot & e_{15} & \cdot & \cdot \\ e_{31} & e_{31} & e_{33} & \cdot & \cdot & \cdot \end{pmatrix}, \quad \mathbf{\epsilon}^S = \begin{pmatrix} \epsilon_{11}^S & \cdot & \cdot \\ \cdot & \epsilon_{11}^S & \cdot \\ \cdot & \cdot & \epsilon_{33}^S \end{pmatrix}.$$

with $c_{66}^E = \frac{1}{2}(c_{11}^E - c_{12}^E)$. Note, however, that our approach will of course be directly applicable to material tensors of any type satisfying

$$\mathbf{c}^E, \mathbf{\epsilon}^S \text{ symmetric, } \text{Re}(\mathbf{c}^E), \text{Re}(\mathbf{\epsilon}^S) \text{ positive definite.} \quad (2.4)$$

Now, by Newton's law for the mechanical behaviour

$$\mathcal{B}^T \vec{\sigma} = \rho \frac{\partial^2 \vec{d}}{\partial t^2},$$

where ρ is the density, and Gauss' law, together with the fact that piezoelectric materials are insulating, i.e., do not contain free volume charges

$$\text{div} \vec{D} = 0,$$

we arrive at a system of four partial differential equations for $\vec{d}$ and ϕ , inside a piezoelectric body Ω

$$\rho \frac{\partial^2 \vec{d}}{\partial t^2} - \mathcal{B}^T (\mathbf{c}^E \mathcal{B} \vec{d} + \mathbf{e}^T \text{grad } \phi) = 0 \quad \text{in } \Omega \quad (2.5a)$$

$$-\text{div}(\mathbf{e} \mathcal{B} \vec{d} - \boldsymbol{\varepsilon}^S \text{grad } \phi) = 0 \quad \text{in } \Omega. \quad (2.5b)$$

Note that $\mathcal{B}^T \mathbf{c}^E \mathcal{B}$ with $\mathbf{c}^E$ replaced by $\begin{pmatrix} 2I_3 & 0 \\ 0 & I_3 \end{pmatrix}$ is the well known $\vec{\Delta} + \nabla \nabla \cdot$ operator appearing, for example, in elasticity. In fact, the differential operator $\mathcal{B}^T \mathbf{c}^E \mathcal{B}$ in (2.5) is used to describe the elastic behaviour of the material. By the structure of $\mathbf{c}^E$ in (2.3) we here deal with a mechanically anisotropic material.

Considering the experimental setting of vanishing normal stress at the boundary, and two electrodes being applied at opposite positions Γ_g and Γ_e of Ω , one of them loaded with a prescribed voltage ϕ^e and the other one grounded, we arrive at the boundary conditions

$$\begin{aligned} \mathbf{N}^T \boldsymbol{\sigma} &= 0 & \text{on } \partial\Omega \\ \phi &= 0 & \text{on } \Gamma_g \\ \phi &= \phi^e & \text{on } \Gamma_e \\ \vec{n}^T \vec{D} &= 0 & \text{on } \partial\Omega \setminus (\Gamma_g \cup \Gamma_e), \end{aligned} \quad (2.6)$$

where $\vec{n} = (n_x, n_y, n_z)$ is the outer unit normal vector and

$$\mathbf{N} = \begin{pmatrix} n_x & . & . & . & n_z & n_y \\ . & n_y & . & n_z & . & n_x \\ . & . & n_z & n_y & n_x & . \end{pmatrix}^T.$$

Note that we model the electrodes as equipotential surfaces, i.e., $\phi^e = \phi^e(t)$ is independent of the space variable.

We assume sufficient decay as $|t| \rightarrow \infty$, so that for each $x \in \Omega$, the field quantities $\vec{d}, \phi$ and their derivatives as appearing in (2.5) are L^2 -functions of time. This is no restriction, since in practice they will have compact support. Thus, we can apply the Fourier transform with respect to the time variable to (2.5) and obtain the harmonic version of the piezoelectric PDEs

$$-\rho \omega^2 \vec{d} - \mathcal{B}^T (\mathbf{c}^E \mathcal{B} \vec{d} + \mathbf{e}^T \text{grad } \hat{\phi}) = 0 \quad \text{in } \Omega \quad (2.7a)$$

$$-\text{div}(\mathbf{e} \mathcal{B} \vec{d} - \boldsymbol{\varepsilon}^S \text{grad } \hat{\phi}) = 0 \quad \text{in } \Omega, \quad (2.7b)$$

where ω is the angular frequency, as well as the same boundary conditions as (2.6) for the Fourier transformed displacement $\vec{d}$ and potential $\hat{\phi}$.

Complex-valued material tensors

By using not necessarily real but complex entries in the material tensors, one can model mechanical relaxation, dielectric dissipation and also imperfect piezoelectric energy conversion. For a proper description of the behaviour of piezoelectric transducers all of these

three phenomena have to be taken into account [31]. An analysis of the power dissipation density in the material (cf. Holland [21]) shows that the imaginary parts of the tensors have to be such that the composed 9×9 matrix

$$MM := -\text{Im} \begin{pmatrix} \mathbf{s}^E & \mathbf{d}^T \\ \mathbf{d} & \boldsymbol{\varepsilon}^\sigma \end{pmatrix} = -\text{Im} \begin{pmatrix} (\mathbf{c}^E)^{-1} & (\mathbf{c}^E)^{-1} \mathbf{e}^T \\ \mathbf{e}(\mathbf{c}^E)^{-1} & \boldsymbol{\varepsilon}^S + \mathbf{e}(\mathbf{c}^E)^{-1} \mathbf{e}^T \end{pmatrix} \quad (2.8)$$

is nonnegative definite. Since the tensors $\mathbf{s}^E$, $\mathbf{d}$, and $\boldsymbol{\varepsilon}^\sigma$ have the same pattern as $\mathbf{c}^E$, $\mathbf{e}$, and $\boldsymbol{\varepsilon}^S$ [23], the condition of nonnegative definiteness of M can be written as

$$\begin{aligned} & \text{Im} \begin{pmatrix} s_{11}^E & s_{12}^E & s_{13}^E \\ s_{12}^E & s_{11}^E & s_{13}^E \\ s_{13}^E & s_{13}^E & s_{33}^E \end{pmatrix} \text{ nonpositive definite} \\ & \text{Im}(s_{ii}^E) \leq 0 \quad i \in \{1, 3, 4, 6\} \\ & \text{Im}(\varepsilon_{ii}^\sigma) \leq 0 \quad i \in \{1, 3\} \\ & \text{Im}(d_{15})^2 \leq \text{Im}(s_{44}^E) \text{Im}(\varepsilon_{11}^\sigma) \\ & \text{Im}(d_{31})^2 \leq \text{Im}(s_{11}^E) \text{Im}(\varepsilon_{33}^\sigma) \\ & \text{Im}(d_{33})^2 \leq \text{Im}(s_{33}^E) \text{Im}(\varepsilon_{33}^\sigma). \end{aligned}$$

Remark 1 The usual Rayleigh damping model for (2.7) [22, 27] is given by

$$-\rho \omega^2 \vec{\hat{d}} + i\omega \left(\alpha(\omega) \rho \vec{\hat{d}} - \beta(\omega) \mathcal{B}^T \mathbf{c}^E \mathcal{B} \vec{\hat{d}} \right) - \mathcal{B}^T \left(\mathbf{c}^E \mathcal{B} \vec{\hat{d}} + \mathbf{e}^T \text{grad } \hat{\phi} \right) = 0 \quad \text{in } \Omega \quad (2.9a)$$

$$-\text{div} \left(\mathbf{e} \mathcal{B} \vec{\hat{d}} - \boldsymbol{\varepsilon}^S \text{grad } \hat{\phi} \right) = 0 \quad \text{in } \Omega \quad (2.9b)$$

with real non-negative damping parameters α , β coupled to the frequency via

$$\alpha(\omega) = \alpha_0 \omega, \quad \beta(\omega) = \frac{\beta_0}{\omega}.$$

This damping model can be interpreted as a special case of complex valued material tensors, which can be seen by multiplying both lines in (2.9) with $\frac{1}{1-i\alpha_0}$ and setting $\tilde{\mathbf{c}}^E := \frac{1+i\beta_0}{1-i\alpha_0} \mathbf{c}^E$, $\tilde{\mathbf{e}} := \frac{1}{1-i\alpha_0} \mathbf{e}$, $\tilde{\boldsymbol{\varepsilon}}^S := \frac{1}{1-i\alpha_0} \boldsymbol{\varepsilon}^S$ to arrive at a system of PDEs of the form (2.7).

The rotationally symmetric case

Test samples are often rotationally symmetric and obviously the computational effort for solving the piezoelectric PDEs is reduced considerably when using the corresponding two dimensional model if appropriate. Therefore, if possible, we consider this special case, i.e. we assume that

$$d_\theta = 0, \quad \partial/\partial\theta = 0$$

so that we obtain for the mechanical displacements (cf. [34])

$$\begin{aligned} S_{rr} &= \frac{\partial d_r}{\partial r}, \quad S_{\theta\theta} = \frac{d_r}{r}, \quad S_{zz} = \frac{\partial d_z}{\partial z}, \\ S_{r\theta} &= S_{z\theta} = 0, \quad S_{rz} = \frac{\partial d_r}{\partial z} + \frac{\partial d_z}{\partial r}. \end{aligned}$$

Therefore, the vectors of mechanical displacement, strain and stress change to

$$\vec{\tilde{d}} := (d_r, d_z)^T, \quad (S_{rr}, S_{zz}, S_{rz}, S_{\theta\theta})^T, \quad (\sigma_{rr}, \sigma_{zz}, \sigma_{rz}, \sigma_{\theta\theta})^T \quad (2.10)$$

(with components depending on r and z only) and the material tensors to

$$\begin{aligned} \check{\mathbf{c}}^E &= \begin{pmatrix} c_{11}^E & c_{13}^E & \cdot & c_{12}^E \\ c_{13}^E & c_{33}^E & \cdot & c_{13}^E \\ \cdot & \cdot & c_{44}^E & \cdot \\ c_{12}^E & c_{13}^E & \cdot & c_{11}^E \end{pmatrix}, \\ \check{\mathbf{e}} &= \begin{pmatrix} \cdot & \cdot & e_{15} & \cdot \\ e_{31} & e_{33} & \cdot & e_{31} \end{pmatrix}, \quad \check{\mathbf{e}}^S = \begin{pmatrix} \varepsilon_{11}^S & \cdot \\ \cdot & \varepsilon_{33}^S \end{pmatrix}. \end{aligned} \quad (2.11)$$

With the corresponding differential operator

$$\check{\mathcal{B}} = \begin{pmatrix} \frac{\partial}{\partial r} & \cdot & \frac{\partial}{\partial z} & \frac{1}{r} \\ \cdot & \frac{\partial}{\partial z} & \frac{\partial}{\partial r} & \cdot \end{pmatrix}^T \quad (2.12)$$

the harmonic piezoelectric equations become

$$-\rho\omega^2 \vec{\tilde{d}} - \check{\mathcal{B}}^T (\check{\mathbf{c}}^E \check{\mathcal{B}} \vec{\tilde{d}} + \check{\mathbf{e}}^T \text{grad } \hat{\phi}) = 0 \quad \text{in } D \quad (2.13a)$$

$$-\text{div} (\check{\mathbf{e}} \check{\mathcal{B}} \vec{\tilde{d}} - \check{\mathbf{e}}^S \text{grad } \hat{\phi}) = 0 \quad \text{in } D. \quad (2.13b)$$

where D denotes the cross-sectional area of the rotationally symmetric domain Ω .

Comparing (2.11) to (2.3), it is important to note that in the computationally less expensive rotationally symmetric case still the whole parameter set is involved. By this fact we conjecture that it might suffice to use measurements of rotationally symmetric test samples in the parameter identification procedure and hence do with two-dimensional forward computations for identifying all tensor entries except for c_{12}^E . For the latter, the sensitivity in the rotationally symmetric case is too weak, as is obvious from physical considerations and also from the fact that, by inspection of (2.12), in (2.13) c_{12}^E goes with an only first order differential operator while all other coefficients are multiplied with second order differential operators.

2.2 Well-posedness and discretisation

For well-posedness results for the piezoelectric equations we refer, for example, to Geis et al. [14] in the quasistatic case and Akamatsu & Nakamura [1] and Miara [32] in the transient case. However, for the harmonic case considered here, no analysis exists yet, to the best of the authors' knowledge. Therefore, we here provide some well-posedness results for the boundary value problem (2.6), (2.7).

A weak formulation of the (2.6), (2.7) (with $\vec{d}, \phi$ replaced by $\vec{\tilde{d}}, \hat{\phi}$ in (2.6)), can be obtained by testing (2.7a) with vector-valued C^∞ -functions $\vec{b} = (b_x, b_y, b_z) : \Omega \rightarrow \mathbb{C}^3$, and

(2.7 a) with scalar C^∞ -functions vanishing at the electrodes Γ_g, Γ_e . Integrating by parts

$$\int_{\Omega} (\mathcal{B}^T \vec{\sigma})^T \bar{b} d\Omega = - \int_{\Omega} \vec{\sigma}^T \overline{\mathcal{B} b} d\Omega + \int_{\partial\Omega} (\mathbf{N}^T \vec{\sigma})^T \bar{b} d\Gamma, \quad (2.14)$$

we arrive at

$$\begin{aligned} \hat{\phi}_0(\cdot, \omega) &:= \hat{\phi}(\cdot, \omega) - \hat{\phi}^e(\omega) \chi(\cdot) \in H_{0,\Gamma}^1(\Omega) \\ \hat{d}(\cdot, \omega) &\in H_{\mathcal{B}}^1(\Omega) \end{aligned}$$

$$\begin{aligned} \forall \vec{b} \in H_{\mathcal{B}}^1(\Omega) \quad w \in H_{0,\Gamma}^1(\Omega) : \\ \int_{\Omega} \left(-\rho \omega^2 \vec{d}(\omega)^T \bar{b} + (\mathbf{c}^E \mathcal{B} \vec{d}(\omega))^T \overline{\mathcal{B} b} + (\mathbf{e}^T \text{grad } \hat{\phi}_0(\omega))^T \overline{\mathcal{B} b} \right. \\ \left. + (\mathbf{e} \mathcal{B} \vec{d}(\omega))^T \overline{\text{grad } w} - (\mathbf{e}^S \text{grad } \hat{\phi}_0(\omega))^T \overline{\text{grad } w} \right) d\Omega \\ = \hat{\phi}^e(\omega) \int_{\Omega} \left(-(\mathbf{e}^T \text{grad } \chi)^T \overline{\mathcal{B} b} + (\mathbf{e}^S \text{grad } \chi)^T \overline{\text{grad } w} \right) d\Omega. \end{aligned} \quad (2.15)$$

Here, $\bar{z}$ denotes the complex conjugate of some $z \in \mathbb{C}$ and the function $\chi \in H^1(\Omega)$ is supposed to be constructed such that

$$\chi|_{\Gamma_g} \equiv 0 \quad \chi|_{\Gamma_e} \equiv 1;$$

such a χ exists if

$$\Omega \text{ is a Lipschitz domain and } \Gamma_e \cap \Gamma_g = \emptyset. \quad (2.16)$$

The function spaces

$$\begin{aligned} H_{0,\Gamma}^1 &:= \overline{\{w \in C^\infty(\Omega) : w|_{\Gamma_g} = w|_{\Gamma_e} = 0\}}^{H^1}, \\ H_{\mathcal{B}}^1 &:= \overline{(C^\infty(\Omega))^3}^{H_{\mathcal{B}}^1}, \quad \|\vec{b}\|_{H_{\mathcal{B}}^1} := \|\vec{b}\|_{L^2} + \|\mathcal{B} \vec{b}\|_{L^2}, \end{aligned}$$

are the closures of the above-mentioned test function spaces with respect to appropriate topologies, and to be understood as spaces of complex valued functions. Note that in our situation of imposing Neumann boundary conditions on the mechanical part, Korn's inequality [5] does not apply so that $H^1(\Omega)^3$ is a strict subset of $H_{\mathcal{B}}^1$.

Regarding (2.15) for fixed frequency ω as a weakly formulated differential equation with respect to the space variables, one immediately obtains some assertions on its well-posedness by using well-known results on eigenvalues of self-adjoint coercive operators. In doing so, we first of all consider the case of real valued material parameters.

Proposition 1 *Let $\mathbf{c}^E \in \mathbb{R}_6^6$, $\mathbf{e} \in \mathbb{R}_3^6$, $\mathbf{e}^S \in \mathbb{R}_3^3$ with (2.4) and (2.16) hold. Then there exists a sequence $(\lambda_n)_{n \in \mathbb{N}}$ accumulating only at ∞ such that for all $\omega \in \mathbb{R} \setminus \{\lambda_1, \lambda_2, \dots\}$, the system of PDEs (2.7) with boundary condition 2.6) has a unique weak solution $\vec{\hat{d}}, \hat{\phi}$ satisfying (2.15).*

Proof The part of (2.15) belonging to (2.7 b) (i.e. setting $\vec{b} \equiv 0$ in (2.15)) induces a second order equation that is elliptic (since $\mathbf{e}^S$ is real positive definite) and therefore can be

resolved (in the weak sense) with respect to $\hat{\phi}_0$:

$$\hat{\phi}_0(\omega) = (-\Delta_\varepsilon)^{-1} \operatorname{div}_0 \left(-\mathbf{e} \mathcal{B} \vec{d}(\omega) + \hat{\phi}^e(\omega) \varepsilon^S \operatorname{grad} \chi \right). \quad (2.17)$$

Here

$$\begin{aligned} -\Delta_\varepsilon &: H_{0,\Gamma}^1 \rightarrow (H_{0,\Gamma}^1)^* \\ v &\mapsto \begin{cases} -\Delta_\varepsilon v & : H_{0,\Gamma}^1 \rightarrow \mathbb{C} \\ w & \mapsto \int_\Omega (\varepsilon^S \operatorname{grad} v)^T \overline{\operatorname{grad} w} d\Omega \end{cases} \end{aligned}$$

and div_0 denotes the weak divergence operator

$$\begin{aligned} \operatorname{div}_0 &: (L^2(\Omega))^3 \rightarrow (H_{0,\Gamma}^1)^* \\ \vec{f} &\mapsto \begin{cases} \operatorname{div}_0 \vec{f} & : H_{0,\Gamma}^1 \rightarrow \mathbb{C} \\ w & \mapsto -\int_\Omega \vec{f}^T \overline{\operatorname{grad} w} d\Omega \end{cases} \end{aligned}$$

Inserting this into the first part ($w \equiv 0$) of (2.15) corresponding to (2.7a), we get that $\vec{d}$ satisfies

$$\begin{aligned} \forall \vec{b} \in H_{\mathcal{B}}^1(\Omega) : \\ \int_\Omega \left(-\rho \omega^2 \vec{d}(\omega)^T \vec{b} + (\mathbf{c}^E \mathcal{B} \vec{d}(\omega))^T \overline{\mathcal{B} \vec{b}} + ((-\Delta_\varepsilon)^{-1} \operatorname{div}_0 \mathbf{e} \mathcal{B} \vec{d}(\omega))^T \operatorname{div}_0 \mathbf{e} \overline{\mathcal{B} \vec{b}} \right) d\Omega \\ = \hat{\phi}^e(\omega) \int_\Omega \left(-(\mathbf{e}^T \operatorname{grad} \chi)^T \overline{\mathcal{B} \vec{b}} + ((-\Delta_\varepsilon)^{-1} \operatorname{div}_0 \varepsilon^S \operatorname{grad} \chi)^T \operatorname{div}_0 \mathbf{e} \overline{\mathcal{B} \vec{b}} \right) d\Omega. \end{aligned} \quad (2.18)$$

Hence, we obtain equivalence of (2.15) to a problem of the form

$$(L - \rho \omega^2 \operatorname{Id}) \vec{d}(\omega) = U f(\omega) \quad (2.19)$$

(and $\hat{\phi}$ being given by (2.17)) where

$$U : (H_{\mathcal{B}}^1(\Omega))^* \rightarrow H_{\mathcal{B}}^1(\Omega)$$

is the isometric isomorphism according to the Riesz Representation Theorem, and $f(\omega)$ is the bounded linear functional on $H_{\mathcal{B}}^1(\Omega)$ given by the right hand side in (2.18). The self-adjoint operator L is given by the left hand side in (2.18) and induces a coercive bilinear form on $H_{\mathcal{B}}^1$, so that, e.g., by Theorem 17.11 in Wloka [43], it has countably many eigenvalues, that accumulate only at infinity. $\square$

In case of complex-valued material tensors satisfying (2.4), the damping properties induced by the negative-definite imaginary parts of $\mathbf{c}^E$ and ε^S even imply wellposedness for all frequency values.

Proposition 2 *Let $\mathbf{c}^E \in \mathbb{C}_6^6$, $\mathbf{e} \in \mathbb{C}_3^6$, $\varepsilon^S \in \mathbb{C}_3^3$ with (2.4) as well as (2.16) and*

$$\begin{aligned} &-\operatorname{Im}(\mathbf{c}^E), -\operatorname{Im}(\varepsilon^S) \text{ positive definite,} \\ &\lambda_{\min}(-\operatorname{Im}(\mathbf{c}^E)) \cdot \lambda_{\min}(-\operatorname{Im}(\varepsilon^S)) > \lambda_{\max}(\operatorname{Re}(\mathbf{e})^T \operatorname{Re}(\mathbf{e})) \end{aligned} \quad (2.20)$$

hold. Then for all $\omega \in \mathbb{R}$, the system of PDEs (2.7) with boundary condition (2.6) has a unique weak solution $\vec{d}, \phi$ satisfying (2.15).

Proof Similarly to the proof of Proposition 1, we reformulate (2.15) as an equation for $\hat{d}(\omega)$ only, by eliminating $\hat{\phi}(\omega)$ by means of the second equation in (2.13). To see that $-\Delta_\varepsilon$ is boundedly invertible, consider the decomposition

$$-\Delta_\varepsilon = V^{-1}(A - iB)$$

with

$$V : (H_{0,\Gamma}^1(\Omega))^* \rightarrow H_{0,\Gamma}^1(\Omega)$$

the Riesz isomorphism, and

$$\langle Av, w \rangle_{H_{0,\Gamma}^1} = \int_{\Omega} (\operatorname{Re}(\varepsilon^S) \operatorname{grad} v)^T \overline{\operatorname{grad} w} d\Omega, \quad \langle Bv, w \rangle = - \int_{\Omega} (\operatorname{Im}(\varepsilon^S) \operatorname{grad} v)^T \overline{\operatorname{grad} w} d\Omega$$

for all $v, w \in H_{0,\Gamma}^1(\Omega)$ where both A and B , mapping $H_{0,\Gamma}^1(\Omega)$ into itself are bounded and self-adjoint, and B is positive definite, with

$$\|B^{-1}\| \leq \frac{1}{\lambda_{\min}(-\operatorname{Im}(\varepsilon^S))}. \quad (2.21)$$

We now assume that the operator

$$-\Delta_\varepsilon = V^{-1}B^{\frac{1}{2}}(B^{-\frac{1}{2}}AB^{-\frac{1}{2}} - iI)B^{\frac{1}{2}}$$

is not boundedly invertible. Hence, since B is positive definite, i has to be contained in the spectrum of the operator $B^{-\frac{1}{2}}AB^{-\frac{1}{2}}$, which yields a contradiction to the fact that this operator is self-adjoint and therefore has a real valued spectrum.

For the inverse of $-\Delta_\varepsilon$ one again obtains a representation via two self-adjoint operators $A^\varepsilon, B^\varepsilon$, namely

$$(-\Delta_\varepsilon)^{-1} = (A^\varepsilon + iB^\varepsilon)V$$

with

$$A^\varepsilon = B^{-\frac{1}{2}}T(I + T^2)^{-1}B^{-\frac{1}{2}} = B^{-\frac{1}{2}}T^{\frac{1}{2}}(I + T^2)^{-1}T^{\frac{1}{2}}B^{-\frac{1}{2}},$$

$$B^\varepsilon = B^{-\frac{1}{2}}(I + T^2)^{-1}B^{-\frac{1}{2}},$$

where

$$T := B^{-\frac{1}{2}}AB^{-\frac{1}{2}}.$$

To show that the operator

$$T^2 + I = (T + iI)(T - iI) = B^{-\frac{1}{2}}(A + iB)B^{-1}(A - iB)B^{-\frac{1}{2}}$$

is boundedly invertible, we can proceed analogously to the above to prove that not only $A - iB$ but also $A + iB$ is boundedly invertible. Note that

$$BB^\varepsilon + A^\varepsilon(B^\varepsilon)^{-1}A^\varepsilon = B^{-1}. \quad (2.22)$$

Inserting this into (2.18), we obtain that the operator L in (2.19) takes the form

$$L = \tilde{A} - i\tilde{B}$$

with

$$\begin{aligned}
\langle \tilde{A}\vec{d}, \vec{b} \rangle_{H^1_{\mathcal{B}}} &= \int_{\Omega} \left((\operatorname{Re}(\mathbf{c}^E) \mathcal{B} \vec{d})^T \overline{\mathcal{B} \vec{b}} \right. \\
&\quad + (A^\varepsilon V \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad - (A^\varepsilon V \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad - (B^\varepsilon V \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad \left. - (B^\varepsilon V \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \right) d\Omega \\
\langle \tilde{B}\vec{d}, \vec{b} \rangle_{H^1_{\mathcal{B}}} &= \int_{\Omega} \left(-(\operatorname{Im}(\mathbf{c}^E) \mathcal{B} \vec{d})^T \overline{\mathcal{B} \vec{b}} \right. \\
&\quad - (B^\varepsilon V \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad + (B^\varepsilon V \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad - (A^\varepsilon V \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \\
&\quad \left. - (A^\varepsilon V \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \mathcal{B} \vec{d})^T \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \overline{\mathcal{B} \vec{b}} \right) d\Omega
\end{aligned}$$

for all $\vec{d}, \vec{b} \in H^1_{\mathcal{B}}(\Omega)$. Obviously, under assumption (2.20), both $\tilde{A}$ and $\tilde{B}$ are self-adjoint and $\tilde{B}$ is positive definite on the orthogonal complement of its nullspace $\mathcal{N}(\mathcal{B})$. The latter can be seen as follows: For any $\vec{b} \in H^1_{\mathcal{B}}$ we have with $\vec{u} := V \operatorname{div}_0 \operatorname{Re}(\mathbf{e}) \mathcal{B} \vec{b}$, $\vec{v} := V \operatorname{div}_0 \operatorname{Im}(\mathbf{e}) \mathcal{B} \vec{b}$, that

$$\begin{aligned}
&\langle \tilde{B}\vec{b}, \vec{b} \rangle_{H^1_{\mathcal{B}}} \\
&= \int_{\Omega} -(\operatorname{Im}(\mathbf{c}^E) \mathcal{B} \vec{b})^T \overline{\mathcal{B} \vec{b}} d\Omega - \langle B^\varepsilon \vec{u}, \vec{u} \rangle_{H^1_{\mathcal{B}}} + \langle B^\varepsilon \vec{v}, \vec{v} \rangle_{H^1_{\mathcal{B}}} - \langle A^\varepsilon \vec{v}, \vec{u} \rangle_{H^1_{\mathcal{B}}} - \langle A^\varepsilon \vec{u}, \vec{v} \rangle_{H^1_{\mathcal{B}}} \\
&= \int_{\Omega} -(\operatorname{Im}(\mathbf{c}^E) \mathcal{B} \vec{b})^T \overline{\mathcal{B} \vec{b}} d\Omega - \langle B^\varepsilon \vec{u}, \vec{u} \rangle_{H^1_{\mathcal{B}}} + \|(B^\varepsilon)^{\frac{1}{2}} \vec{v} - (B^\varepsilon)^{-\frac{1}{2}} A^\varepsilon \vec{u}\|_{H^1_{\mathcal{B}}}^2 - \|(B^\varepsilon)^{-\frac{1}{2}} A^\varepsilon \vec{u}\|_{H^1_{\mathcal{B}}}^2 \\
&\geq \int_{\Omega} \left(-(\operatorname{Im}(\mathbf{c}^E) \mathcal{B} \vec{b})^T \overline{\mathcal{B} \vec{b}} d\Omega - \langle (B^\varepsilon + A^\varepsilon (B^\varepsilon)^{-1} A^\varepsilon) \vec{u}, \vec{u} \rangle_{H^1_{\mathcal{B}}} \right) \\
&\geq \left(\lambda_{\min}(-\operatorname{Im}(\mathbf{c}^E)) - \frac{\lambda_{\max}(\operatorname{Re}(\mathbf{e})^T \operatorname{Re}(\mathbf{e}))}{\lambda_{\min}(-\operatorname{Im}(\mathbf{e}^S))} \right) \|\mathcal{B} \vec{b}\|_{L^2},
\end{aligned}$$

where we have used (2.21), (2.22) and

$$\|\vec{u}\|_{H^1_{\mathcal{B}}} \leq \|\operatorname{Re}(\mathbf{e})\|_{\mathbb{R}^6 \rightarrow \mathbb{R}^3} \|\mathcal{B} \vec{b}\|_{L^2} = \sqrt{\lambda_{\max}(\operatorname{Re}(\mathbf{e})^T \operatorname{Re}(\mathbf{e}))} \|\mathcal{B} \vec{b}\|_{L^2}$$

in the last inequality. Denoting by P the orthogonal projection onto $\mathcal{N}(\mathcal{B})$ in $H^1_{\mathcal{B}}(\Omega)$, we obtain equivalence of (2.19) to

$$\begin{aligned}
(I - P)(L - \rho\omega^2 \operatorname{Id})(I - P)\vec{d}(\omega) &= (I - P)Uf(\omega) \\
-\rho\omega^2 P\vec{d}(\omega) &= P Uf(\omega) = 0
\end{aligned}$$

where we have used the fact that $PL = 0$ and for $f(\omega)$ in (2.19) according to (2.18), we have $P Uf(\omega) = 0$ since for all $\vec{b} \in \mathcal{N}(\mathcal{B})$, there holds $\langle Uf(\omega), \vec{b} \rangle = f(\omega) \vec{b} = 0$. Now we

can apply the same argument as for $-\Delta_\varepsilon$ to the operator

$$(I - P) (-\rho\omega^2 + \tilde{A} - i\tilde{B}) (I - P).$$

If this operator were not continuously invertible, then by the fact that the operator $\tilde{\tilde{B}} := (I - P)\tilde{B}(I - P)$ is positive definite, this would imply that i is an element of the spectrum of the self-adjoint operator

$$\tilde{\tilde{B}}^{-\frac{1}{2}} (I - P) (-\rho\omega^2 + \tilde{A}) (I - P) \tilde{\tilde{B}}^{-\frac{1}{2}}.$$

□

Remark 2 Note that condition (2.20) is sufficient for negativity of $\text{Im}(\mathbf{s}^E) = \text{Im}((\mathbf{c}^E)^{-1})$ and $\text{Im}(\varepsilon^\sigma) = \text{Im}(\varepsilon^S + \mathbf{e}(\mathbf{c}^E)^{-1}\mathbf{e}^T)$ as it is necessary for defining physically admissible damping terms (cf. (2.8) in § 2.1). Namely, analogously to the decomposition of $(-\Delta_\varepsilon)^{-1}$ in the proof of Proposition 2, but this time for real valued symmetric matrices in place of self-adjoint operators, it can be seen that

$$(\mathbf{c}^E)^{-1} = \mathbf{a}^c + i\mathbf{b}^c$$

with

$$\mathbf{a}^c = (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}} \mathbf{t} (I + \mathbf{t}^2)^{-1} (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}},$$

$$\mathbf{b}^c = (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}} (I + \mathbf{t}^2)^{-1} (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}},$$

where

$$\mathbf{t} := (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}} \text{Re}(\mathbf{c}^E) (-\text{Im}(\mathbf{c}^E))^{-\frac{1}{2}},$$

and where we have

$$\mathbf{b}^c + \mathbf{a}^c (\mathbf{b}^c)^{-1} \mathbf{a}^c = (-\text{Im}(\mathbf{c}^E))^{-1}.$$

Hence, it is readily checked that

$$-\text{Im}(\varepsilon^\sigma) = -\text{Im}(\varepsilon^S) - \text{Re}(\mathbf{e}) (-\text{Im}(\mathbf{c}^E))^{-1} \text{Re}(\mathbf{e})^T + \mathbf{r} \mathbf{r}^T$$

where

$$\mathbf{r} = (\mathbf{b}^c)^{\frac{1}{2}} \text{Im}(\mathbf{e}) - (\mathbf{b}^c)^{-\frac{1}{2}} \mathbf{a}^c \text{Re}(\mathbf{e})$$

so that (2.20) implies that $-\text{Im}(\varepsilon^\sigma)$ is positive definite. In this sense, (2.20) can be seen as a natural assumption.

More generally, consider for

$$\vec{f}_1(\omega) \in (H^1_{\mathcal{B}}(\Omega))^* \text{ with } \mathcal{N}(\mathcal{B}) \subseteq \mathcal{N}(\vec{f}_1(0)),$$

$$\hat{f}_2(\omega) \in (H^1_{0,\Gamma}(\Omega))^*,$$

$$\vec{g}_1(\omega) \in tr^{(1)}_{\partial\Omega}(H^1_{\mathcal{B}}(\Omega)),$$

$$\hat{\phi}^e(\omega) \in \mathbb{C},$$

$$\hat{g}_2(\omega) \in tr^{(1)}_{\partial\Omega \setminus (\Gamma_g \cup \Gamma_e)}(H^1_{0,\Gamma}(\Omega)),$$

where $tr_{\Gamma}^{(1)}$ is the trace operator $v \mapsto \frac{\partial v}{\partial \vec{n}}|_{\Gamma}$, to be understood component wise for vector valued v , the boundary value problem

$$\begin{aligned} -\rho\omega^2\vec{d} - \mathcal{B}^T(\mathbf{c}^E\mathcal{B}\vec{d} + \mathbf{e}^T \text{grad } \hat{\phi}) &= \vec{f}_1(\omega) & \text{in } \Omega \\ -\text{div}(\mathbf{e}\mathcal{B}\vec{d} - \boldsymbol{\varepsilon}^S \text{grad } \hat{\phi}) &= \hat{f}_2(\omega) & \text{in } \Omega \\ \mathbf{N}^T(\mathbf{c}^E\mathcal{B}\vec{d} + \mathbf{e}^T \text{grad } \hat{\phi}) &= \vec{g}_1(\omega) & \text{on } \partial\Omega \\ \hat{\phi} &= 0 & \text{on } \Gamma_g \\ \hat{\phi} &= \hat{\phi}^e(\omega) & \text{on } \Gamma_e \\ \vec{n}^T(\mathbf{e}\mathcal{B}\vec{d} - \boldsymbol{\varepsilon}^S \text{grad } \hat{\phi}) &= \hat{g}_2(\omega) & \text{on } \partial\Omega \setminus (\Gamma_g \cup \Gamma_e). \end{aligned} \quad (2.23)$$

Analogously to Propositions 1, 2, one sees that for all ω (up to countably many in case of real valued tensors), there exists a unique stable weak solution $(\vec{d}(\omega), \hat{\phi}(\omega))$.

In our parameter identification approach, we will repeatedly have to solve forward problems of the form (2.23) for several values of ω and for different right-hand sides $\vec{f}_1, \hat{f}_2, \hat{\phi}^e, \vec{g}_1, \hat{g}_2$, which we do by using piezoelectric finite elements (see Kaltenbacher[27] and Lerch [29] and the following subsection).

Space discretisation with finite elements

With the finite element ansatz

$$\begin{aligned} \hat{d}_x^h(x, y, z; \omega) &= \sum_{i=1}^{n_{eq}} N_i^d(x, y, z) \hat{d}_{ix} \\ \hat{d}_y^h(x, y, z; \omega) &= \sum_{i=1}^{n_{eq}} N_i^d(x, y, z) \hat{d}_{iy} \\ \hat{d}_z^h(x, y, z; \omega) &= \sum_{i=1}^{n_{eq}} N_i^d(x, y, z) \hat{d}_{iz} \\ \hat{\phi}^h(x, y, z; \omega) &= \sum_{i=1}^{n_{eq}} N_i^\phi(x, y, z) \hat{\phi}_i \end{aligned} \quad (2.24)$$

with n_{eq} nodes, coefficients $\hat{d}_{ix}, \hat{d}_{iy}, \hat{d}_{iz}, \hat{\phi}_i \in \mathbb{C}$ and interpolation functions N_i^d, N_i^ϕ , for the field quantities $\vec{d}^h(\omega), \hat{\phi}^h(\omega)$, and analogously for the test functions $\vec{b}, w$, we arrive at a finite dimensional system of linear equations

$$\begin{pmatrix} -\omega^2 \mathbf{M}_{dd} + \mathbf{K}_{dd} & \mathbf{K}_{d\phi} \\ \mathbf{K}_{d\phi}^T & -\mathbf{K}_{\phi\phi} \end{pmatrix} \begin{pmatrix} \{\vec{d}\} \\ \{\hat{\phi}\} \end{pmatrix} = \begin{pmatrix} \{\vec{F}\} \\ \{\hat{Q}\} \end{pmatrix}, \quad (2.25)$$

where the matrices $\mathbf{M}_{dd}, \mathbf{K}_{dd}, \mathbf{K}_{d\phi}, \mathbf{K}_{\phi\phi}$ consist of

$$\begin{aligned} (m_{dd})_{ij} &= \int_{\Omega} \rho N_i^{dT} N_j^d d\Omega \quad (\text{mass matrix}) \\ (k_{dd})_{ij} &= \int_{\Omega} (\mathcal{B} N_i^d)^T \mathbf{c}^E (\mathcal{B} N_j^d) d\Omega \quad (\text{stiffness matrix}) \\ (k_{d\phi})_{ij} &= \int_{\Omega} (\mathcal{B} N_i^d)^T \mathbf{e} (\text{grad } N_j^\phi) d\Omega \quad (\text{piezoelectric coupling matrix}) \\ (k_{\phi\phi})_{ij} &= \int_{\Omega} (\text{grad } N_i^\phi)^T \boldsymbol{\varepsilon}^S (\text{grad } N_j^\phi) d\Omega \quad (\text{permittivity matrix}) \end{aligned} \quad (2.26)$$

with $N_i^d = \text{diag}(N_i^d, N_i^d, N_i^d)$ and

$$\begin{aligned} \hat{F}_{ix} &= \int_{\Omega} \hat{f}_{1x}(\omega) N_i^d d\Omega + \int_{\partial\Omega} \hat{g}_{1x}(\omega) N_i^d d\Gamma \\ \hat{F}_{iy} &= \int_{\Omega} \hat{f}_{1y}(\omega) N_i^d d\Omega + \int_{\partial\Omega} \hat{g}_{1y}(\omega) N_i^d d\Gamma \\ \hat{F}_{iz} &= \int_{\Omega} \hat{f}_{1z}(\omega) N_i^d d\Omega + \int_{\partial\Omega} \hat{g}_{1z}(\omega) N_i^d d\Gamma \\ \hat{Q}_i &= \int_{\Omega} \hat{f}_2(\omega) N_i^\phi d\Omega + \int_{\partial\Omega \setminus (\Gamma_g \cup \Gamma_e)} \hat{g}_2(\omega) N_i^\phi d\Gamma. \end{aligned}$$

The inhomogeneous Dirichlet boundary conditions for $\hat{\phi}$ at Γ_e can either be eliminated or enforced by penalisation [22].

2.3 Efficient solution of the discretised piezoelectric PDEs

For the efficient solution of a linear system $Ax = b$ the properties of the system matrix A play a crucial role. The most important criteria when choosing a solution approach are typically the size and sparsity of A , and whether it is non-singular, definite and/or symmetric resp. hermitian.

Using the FEM discretisation of the piezoelectric forward problem as briefly described in §2.2 the system matrix in (2.25) will be a square non-singular $n \times n$ matrix (assuming appropriate boundary conditions). The dimension n is $\leq 4n_{eq}$ with its precise value depending on the way inhomogeneous boundary conditions are treated. Equation (2.25) in combination with (2.26) also shows that the system matrix A will be symmetric, but not hermitian. Concerning the other properties one must distinguish the case of real-valued and complex-valued material parameters (resp. the case with or without Rayleigh damping, see Remark 1).

In the real-valued case the symmetry of A leads to a set of n real eigenvalues. The spectrum, however, is indefinite. This can most intuitively be understood when we, instead of (2.25), consider the linear system arising from the discretisation of a static problem (or of the spatial part of the transient problem (2.5)). In this case the system matrix is given by

$$A = \begin{pmatrix} \mathbf{K}_{dd} & \mathbf{K}_{d\phi} \\ \mathbf{K}_{d\phi}^T & -\mathbf{K}_{\phi\phi} \end{pmatrix}. \quad (2.27)$$

Since $\mathbf{K}_{dd}$ and $\mathbf{K}_{\phi\phi}$ stem from a standard FEM discretisation of coercive, self-adjoint operators, both matrices are symmetric and positive definite (for appropriate boundary conditions). The indefiniteness then enters via the sign change of $\mathbf{K}_{\phi\phi}$ in (2.27). This is a typical saddle point problem and the number of positive eigenvalues equals $\dim(\mathbf{K}_{dd})$ while that of negative ones equals $\dim(\mathbf{K}_{\phi\phi})$ [4].

The $-\omega^2 \mathbf{M}_{dd}$ term in (2.25) contains only negative entries. Thus, depending on the size of the frequency ω it will reduce the number of positive eigenvalues. In fact, for very large frequencies the spectrum will consist mostly of negative eigenvalues. However, for frequencies typically considered in piezoelectric simulations the problem will remain indefinite. Figure 1 gives as an example the spectrum $\sigma = \{\lambda_k \mid k = 1, \dots, n\}$ of the system matrix for a rotationally symmetric 2D model of a thickness resonator, see also Sect. 4, consisting of a typical lead zirconate titanate material (PZT4) with real-valued parameters. The left part of the figure shows the spectrum for the static case (equivalent to $\omega = 0$) while the right part shows the spectrum in the harmonic case for a selected frequency. As mentioned above, in the case of complex material parameters the system matrix will still be symmetric, but not hermitian, which leads to eigenvalues with non-vanishing imaginary part. The latter is demonstrated in Figure 2 for the same configuration but a complex-valued material (Motorola 3203 HD PZT – see §2.1). Here we plot the spectrum for the case of *equilibration* of the material parameters, too. In this approach we scale the mechanical parameters by 10^{-10} and the electrical ones by 10^{10} to get their

magnitudes and also that of the piezoelectric coupling terms into comparable ranges – see also § 3.6 in this respect. This scaling can easily be removed again from the computed results.

The size of the linear systems arising in parameter identification is usually not very large, seldom exceeding $n = 4000$. The reason for this is that the test specimens which must be simulated, in general, have a very simple geometry and can thus quite accurately be represented by a moderate number of Finite Elements and reduction to a 2D problem by employing symmetry is often an alternative. From this perspective a direct solution approach will be well suited for solving the linear system. This can be done by means of an $A = LDL^T$ factorisation. In the case that pivoting is required to ensure existence of an LDL decomposition and/or numerical stability the state-of-the-art is considered to be the use of the Bunch–Kaufmann algorithm. The latter is a pivoting strategy working with 1×1 and 2×2 blocks which retains the symmetry of the problem – see elsewhere [3, 4, 7] for details and further references. Note, however, that for the real version of (2.27) pivoting is not required to ensure existence, since the matrix is quasidefinite [4, 42]. Depending on the size of n either a dense or sparse implementation of the LDL decomposition should be employed and several efficient program codes are available [2, 33].

When the material parameters identified by the inverse solution process are to be used in a simulation the situation is quite different. Here the computational domains can exhibit quite complicated geometries and a precise result is desired. Depending on the number of Finite Elements (and the resulting degrees of freedom n) even a sparse direct solution approach may run into difficulties with respect to run-time and storage requirements. This is mainly due to the effect of fill-in occurring during the factorisation process. While sophisticated re-ordering strategies, such as nested dissection, exist that try to minimise fill-in, its occurrence cannot be completely avoided. Thus, for problems that require a fine resolution iterative solution approaches are indispensable.

The field of iterative algorithms for the solution of linear systems with square matrices, however, is quite diverse and numerous different approaches exist. While the conjugate gradient algorithm is often considered to be the method of choice for symmetric/hermitian, positive definite systems, there is no approach that is equally applicable as well as superior for the remaining kinds of classes like for instance symmetric, indefinite problems. A comparison of several different solution schemes, consisting of a solver – preconditioner combination, is beyond the scope of this paper. Instead we want to briefly consider in the following a possible solution strategy that we employ for large-scale piezoelectric simulations. For a general overview on iterative methods we point the reader elsewhere [15, 16, 38]. An overview for the special case of saddle point problems can be found in Benzi *et al.* [4].

Our approach consists in using the so called Generalised Minimal Residual (GMRES) approach [38]. This method works by constructing in each iteration step an approximate solution $x_i = x_0 + v$ with $v \in \mathbb{K}_i$ such that

$$\|b - Ax_i\|_2 \leq \|b - A(x_0 + u)\|_2, \text{ for all } u \in \mathbb{K}_i. \quad (2.28)$$

Thus, the new approximate x_i minimises the Euclidean norm of the residual with respect

FIGURE 1. Spectrum of the system matrix A for an example 2D problem. The ordinate shows $|\log_{10}(\lambda_k)|$ with $\circ$ marking negative λ_k and $\bullet$ positive ones.

to the Krylov subspace given by

$$\mathbb{K}_i(r_0, A) = \text{span}\{r_0, Ar_0, A^2r_0, \dots, A^{i-1}r_0\}. \quad (2.29)$$

The advantage of GMRES is its universality. It can be used for all types of system matrices and (at least theoretically) cannot fail as other methods, e.g. Bi-Conjugate Gradients. This stability of GMRES comes at the price of computing, via an Arnoldi process, and storing a complete orthonormal/unitary basis of $\mathbb{K}_i$. An alternative that bounds the costs per iteration step from above is to employ GMRES(m), i.e. a version that re-starts building up the Krylov subspace once it has reached its maximal allowed dimension $m + 1$ using x_m as new initial guess. Unfortunately the convergence speed of GMRES(m) may depend critically on the re-start parameter m .

In a piezoelectric simulation the system matrix is typically not very well conditioned, as can be seen from the example in Figure 1. Thus, preconditioning is indicated in order to improve the spectral properties of the matrix and obtain a better convergence speed. We employ the well-known ILU(k) approach, i.e. we compute as preconditioner an incomplete LDL^T decomposition where entries l_{ij} of L are dropped, if their fill-level exceeds the threshold k . The fill-level can be imagined as a measure of the distance of nodes i and j in the graph corresponding to the matrix A . For more details on incomplete LU preconditioners and the (graph theoretical) motivation of the dropping strategy see e.g. [38]. In order to improve the performance and stability of the method we reorder the matrix using the Sloan algorithm, see e.g. [41], before applying the preconditioner. This turned out to be superior to a minimum degree re-ordering.

Note that due to the symmetry of the matrix A also the MINRES or SYMMLQ method [40] could be employed. These replace the Arnoldi method of GMRES by a three-term Lanczos recurrence, which can save considerably on storage and computational costs. We have refrained from using these approaches for the following reasons. Finding good preconditioners that retain the symmetry of the problem is not an easy task. Also the methods would only be applicable in the case of real-valued material parameters, since A will not be hermitian in the complex-valued setting. Finally, it was shown [40] that the use

FIGURE 2. Spectrum of the system matrix A for an example 2D problem and complex-valued material parameters. Plotted are the polar co-ordinates of the eigenvalues λ_k ; 'standard' denotes the spectrum for original parameters and 'equilibrated' that for a scaling of the mechanical and electrical parts.

FIGURE 3. Electric potential distribution [in V] and mechanical deformation of a 5-layer stack actuator model.

of three-term recurrences in both methods may lead to severe problems with respect to convergence (MINRES) or convergence speed (SYMMLQ) in the case of ill-conditioned system matrices.

We test the algorithm on a simplified model of a stack actuator. The latter are layers of piezoelectric ceramics with electrodes in between that are used to amplify the displacement that can be attained. Figure 3 shows the respective model together with simulation results for the PZT4 material.

We first consider the static problem (2.27) with real-valued parameters and discretise the model using hexahedral Finite-Elements with tri-linear Ansatz functions. The resulting linear system is solved with GMRES(30). The convergence rate for different levels k of the ILDL(k) preconditioner is given in Figure 4 for a system with 36,519 unknowns. We see that the unsatisfactory convergence rate of plain GMRES is significantly improved by the preconditioner. Also quite typical for an ILU(k) approach is the decrease in improvement for growing levels of k .

FIGURE 4. Convergence rate of GMRES(30) with ILDL(k) preconditioning and real-valued material.

FIGURE 5. Number of iterations to satisfy stopping criterion $\|r_i\|_2 < 10^{-6}$ for different re-start parameters of GMRES(m), $n = 77,679$ and real-valued material.

Besides the pure iteration count the number of arithmetic operations to solve the problem is of interest. Here the higher costs of the preconditioner for larger k compete with the reduced number of iterations. In our test example the solution of the system, up to $\|r_i\|_2 < 10^{-6}$, required 633 MFLOP ($k = 1$), 639 MFLOP ($k = 2$), 608 MFLOP ($k = 3$), 662 MFLOP ($k = 4$), and 675 MFLOP ($k = 5$). Thus, taking also into account the costs for the setup of the preconditioner, which increases with k , a level of $k = 1$ or 2 seems the best choice. Concerning the sensitivity with respect to the restart parameter Figure 5 demonstrates that this appears not to be very crucial especially for the $k = 2$ case. As a last point let us consider the scaling behaviour of the approach. Figure 6 shows the influence of the problem dimension n , resulting from increasingly fine discretisations, on the number of iterations. Here we have altered the stopping criterion to $\|r_i\|_2 / \|b\|_2 < 10^{-6}$. We see that while the iteration count is not constant, which would lead to an $\mathcal{O}(n)$ method, it still behaves quite well.

We also want to point out that tests with the system for equilibrated material parameters as mentioned above did not yield significantly different results in the real-valued setting. The situation is completely different, however, when we consider the complex-valued Motorola 3203 HD PZT material. In this case the very unsatisfactory convergence speed

FIGURE 6. Iteration count of GMRES(30) for different problem sizes n : $A = 36,519$, $B = 77,679$, $C = 300,243$ and $D = 618,403$ and real-valued material.

FIGURE 7. Convergence rate of GMRES(30) with ILDL(k) preconditioning and equilibrated complex-valued material ($n = 36,519$).

FIGURE 8. Iteration count of GMRES(30) for different problem sizes n : $A = 36,519$, $B = 77,679$, $C = 300,243$ and $D = 618,403$ and equilibrated complex-valued material.

of GMRES is not improved by the suggested preconditioning approach and the method becomes quite unstable. However, if we use equilibration on the material parameters, the new system is very amenable to ILDL(k) preconditioning and we obtain good convergence speeds as demonstrated in Figures 7 and 8.

3 The inverse problem

Our aim is to identify the $n_{par} = 10$ parameters

$$\begin{aligned} p &= (p_1, p_2, p_3, p_4, p_5, p_6, p_7, p_8, p_9, p_{10})^T \\ &= (c_{11}^E, c_{33}^E, c_{12}^E, c_{13}^E, c_{44}^E, e_{15}, e_{31}, e_{33}, e_{11}^S, e_{33}^S)^T, \end{aligned} \quad (3.1)$$

i.e. the non vanishing entries of $\mathbf{c}^E$, $\mathbf{e}$, $\mathbf{e}^S$. For this purpose, we use phase and amplitude measurements of the impedance curve

$$Z(\omega) = \frac{U(\omega)}{I(\omega)} = \frac{\hat{\phi}^e(\omega)}{i\omega \hat{q}^e(\omega)} \quad (3.2)$$

for prescribed voltage $\hat{\phi}^e = \hat{\phi}^e(\omega)$ at the electrode Γ_e and several (non-eigen-)frequencies ω_l , $l = 1, \dots, n_{mp}$. Multiplication of $\hat{\phi}^e(\omega)$ with $(i\omega Z(\omega))^{-1}$ yields the data

$$(\hat{y}_1, \dots, \hat{y}_{n_{mp}}) = (\hat{q}^e(\omega_1), \dots, \hat{q}^e(\omega_{n_{mp}})) \in \mathbb{C}_{n_{mp}},$$

where $\hat{q}^e$ is the surface charge at the loaded electrode

$$\hat{q}^e = \int_{\Gamma_e} \hat{n}^T \vec{D} d\Gamma = \int_{\Gamma_e} \hat{n}^T \left(-\mathbf{e} \mathcal{B}^T \vec{\hat{d}}(\omega) + \mathbf{e}^S \text{grad } \hat{\phi}(\omega) \right) d\Gamma. \quad (3.3)$$

In addition, one can, for these frequencies or part of them, measure the mechanical deformation in a boundary point, or rather, its mean value $\frac{1}{|\tilde{\Gamma}|} \int_{\tilde{\Gamma}} \vec{\hat{d}}(\omega) d\Gamma$ (possibly only in one space direction) over a small region $\tilde{\Gamma}$ of the boundary:

$$(\hat{y}_{n_{mp}+1}, \dots, \hat{y}_{n_{mp}+n_{mp}^d}) = (\hat{u}(\omega_1), \dots, \hat{u}(\omega_{n_{mp}^d})) \in \mathbb{C}_{n_{mp}^d},$$

where

$$\hat{u}(\omega) = \frac{1}{|\tilde{\Gamma}|} \int_{\tilde{\Gamma}} W \vec{\hat{d}}(\omega) d\Gamma, \quad (3.4)$$

and n_{mp}^d is the number of these mechanical measurements. Here, $|\tilde{\Gamma}|$ is the measure of the surface area $\tilde{\Gamma}$ and the matrix W serves as a weight for scaling the mechanical measurements, since these are usually several orders of magnitude smaller in absolute value than the electrical ones. In sum we therefore have $n_{mp} + n_{mp}^d$ data values by measurements of electrical and mechanical quantities at n_{mp} different frequency points. We denote by $\hat{\mathbf{F}}$ the forward operator mapping the set of parameters to the measurements

$$\begin{aligned} \hat{\mathbf{F}} : \mathbb{C}_{n_{par}} &\rightarrow \mathbb{C}_{n_{mp} + n_{mp}^d} \\ p &\mapsto \left(\hat{q}_1^e, \dots, \hat{q}_{n_{mp}}^e, \hat{u}_1, \dots, \hat{u}_{n_{mp}^d} \right)^T, \end{aligned} \quad (3.5)$$

where $(\vec{\hat{d}}^l, \hat{\phi}^l)$ solves (2.15) with $\omega := \omega_l$ and $\hat{q}_l^e$, $\hat{u}_l$ are derived from $(\vec{\hat{d}}^l, \hat{\phi}^l)$ according to (3.3), (3.4). Therewith, we can rewrite the inverse problem under consideration as a nonlinear operator equation

$$\hat{\mathbf{F}}(p) = \hat{y}. \quad (3.6)$$

This is a finite system of equations for finitely many unknowns. Note, however, that the evaluation of the forward operator involves an infinite dimensional subproblem, namely the solution of (2.15).

3.1 Identifiability and ill-posedness

The one-dimensional case

An important question in this context is of course whether the searched-for quantities are uniquely determined by the given data. While the European norm [13] as well as the IEEE standard [23] prescribe measurements of resonance and antiresonance for identifying the material parameters, we here aim at identifying them from measurements at non-eigenfrequencies in order to deal with well-posed forward problems. In this subsection we argue that also with our approach uniqueness can be achieved by appropriately choosing the non-eigenfrequencies for which the measurements are made. This holds at least for the one-dimensional case, that by the way also the European norm and the IEEE-standard are based on.

In the 1-d case, the Fourier transformed piezoelectric equations with boundary conditions become

$$\begin{aligned} -\rho\omega^2\hat{d} - c^E\hat{d}_{xx} - e\hat{\phi}_{xx} &= 0 & \text{in } (0, L) \\ -e\hat{d}_{xx} + \varepsilon^S\hat{\phi}_{xx} &= 0 & \text{in } (0, L) \\ (c^E\hat{d}_x + e\hat{\phi}_x)(0) &= 0, & \hat{\phi}(0) = 0 \\ (c^E\hat{d}_x + e\hat{\phi}_x)(L) &= 0, & \hat{\phi}(L) = \hat{\phi}^e(\omega) \end{aligned}$$

and therefore can be solved explicitly:

$$\begin{aligned} \hat{d}(x, \omega) &= -\frac{e\hat{\phi}^e(\omega)\left(\exp(i\sqrt{\frac{\rho}{c^E}}\omega x) - \exp(i\sqrt{\frac{\rho}{c^E}}\omega(L-x))\right)}{2(\bar{c} - c^E)\left(1 - \exp(i\sqrt{\frac{\rho}{c^E}}\omega L)\right) + \bar{c}i\sqrt{\frac{\rho}{c^E}}\omega L\left(1 + \exp(i\sqrt{\frac{\rho}{c^E}}\omega L)\right)} \\ \hat{\phi}(x, \omega) &= \frac{e}{\varepsilon^S}\left(\hat{d}(x, \omega) - \hat{d}(0, \omega) - (\hat{d}(L, \omega) - \hat{d}(0, \omega))\frac{x}{L}\right) + \hat{\phi}^e(\omega)\frac{x}{L} \end{aligned}$$

for all non-eigenfrequencies $\omega \notin \Sigma := \{\frac{2\pi}{L}\sqrt{\frac{\bar{c}}{\rho}}n | n \in \mathbb{N}\}$, where $\bar{c} := c^E + \frac{e^2}{\varepsilon^S}$. Hence, the computed measurements can be written as

$$\hat{q}(\omega; c^E, \varepsilon^S, e) = \frac{\varepsilon^S\hat{\phi}^e(\omega)}{L(\tilde{e}f(\tilde{c}\omega) + 1)}$$

with $\tilde{c} = \sqrt{\frac{\rho}{c^E}}L$, $\tilde{e} := \frac{\bar{c} - c^E}{\bar{c}} = \frac{e^2}{\bar{c}\varepsilon^S}$ and $f(\alpha) = \frac{2(1 - \exp(i\alpha))}{i\alpha(1 + \exp(i\alpha))}$, so that using auxiliary parameters $\tilde{c}$, $\tilde{e}$, and $\tilde{e} := \frac{1}{\varepsilon^S}$, we can write our parameter identification problem $\hat{q}^{meas}(\omega_l) = \hat{q}(\omega_l; c^E, \varepsilon^S, e)$, $l \in \{1, 2, 3\}$ where $\hat{q}^{meas}$ is the measured data (see (3.2)), as

$$i\tilde{e}(\tilde{e}f(\tilde{c}\omega_l) + 1) = \frac{\hat{\phi}^e(\omega_l)}{L\hat{q}^{meas}(\omega_l)} =: r(\omega_l), \quad l \in \{1, 2, 3\} \quad (3.7)$$

Note that r vanishes nowhere since we assume a nontrivial excitation $\hat{\phi}^e$ at each frequency point. Dividing (3.7) with $l = 1, 3$ by (3.7) with $l = 2$ and extracting $\tilde{e}$ gives

$$\left(\frac{f(\tilde{e}\omega_1)}{r(\omega_1)} - \frac{f(\tilde{e}\omega_2)}{r(\omega_2)} \right) = \frac{1}{r(\omega_2)} - \frac{1}{r(\omega_1)}, \quad l \in \{1, 3\}. \quad (3.8)$$

Now we can divide (3.8) with $l = 3$ by (3.8) with $l = 1$ to arrive at

$$\underbrace{\frac{f(\tilde{e}\omega_3)r(\omega_2) - f(\tilde{e}\omega_2)r(\omega_3)}{f(\tilde{e}\omega_1)r(\omega_2) - f(\tilde{e}\omega_2)r(\omega_1)} - \frac{r(\omega_1)(r(\omega_3) - r(\omega_2))}{r(\omega_3)(r(\omega_1) - r(\omega_2))}}_{=:g(\tilde{e}, \omega_3)} = 0 \quad (3.9)$$

Fix $\omega_1 \neq \omega_2$, $\omega_1, \omega_2 > 0$ such that $r(\omega_1) \neq r(\omega_2)$, and consider the left hand side in (3.9) as a function g of $\tilde{e}$ and ω_3 . Both denominators in (3.9) are nonzero, since else (3.8) with $l = 1$ would give a contradiction to our assumption $r(\omega_1) \neq r(\omega_2)$. Moreover, the derivative $\frac{\partial g}{\partial \tilde{e}}$ is piecewise continuous and for any fixed $\tilde{e} > 0$, $\frac{\partial g}{\partial \tilde{e}}(\tilde{e}, \cdot)$ considered as a function of ω_3 , obviously does not vanish identically. Hence there exists an $\omega_3 > 0$ such that $\tilde{e}$ can be locally uniquely determined from $g(\tilde{e}, \omega_3) = 0$.

Once we have determined $\tilde{e}$, we can insert it into (3.8) with $l = 1$ and then into (3.7) with $l = 1$ (where the factor going with $\tilde{e}$ cannot vanish due to our assumption $r(\omega_1) \neq 0$) to uniquely determine $\tilde{\epsilon}$ and $\tilde{\epsilon}$, respectively.

This unique identifiability of $\tilde{e}, \tilde{\epsilon}, \tilde{\epsilon}$ implies identifiability of the original parameters $c^E = (1 - \tilde{e}) \left(\frac{L}{\tilde{e}}\right)^2 \rho$, $e = \pm \sqrt{\frac{\tilde{e}}{\rho \tilde{\epsilon}}} \frac{\tilde{e}}{L}$, $\epsilon^S = \frac{1}{\tilde{\epsilon}}$, as long as the sign of e is known, which is usually the case.

Ill-posedness by rank deficiency

The results of the previous subsection imply that if we used measurements of all test samples prescribed in the IEEE Standard or the European Norm, respectively, at appropriate non-eigenfrequencies we would be able to uniquely determine all tensor entries. However, since our intention is to provide a method using measurements of only one or a few test samples that can be arbitrarily shaped, we have no guarantee of uniqueness. Hence, the nonlinear system of equations (3.6) is rank deficient in the sense that the system matrix of its linearisation does not have numerical full rank at the solution.

Systems of equations with a matrix whose rank is unknown and not full tend to be unstable if the matrix entries are given only approximately, as it is the case in our situation [11, 20]. Instability here occurs in the sense that the generalised inverses of a sequence of matrices converging norm wise to a rank deficient matrix not necessarily converge to the generalised inverse of this matrix.

Moreover, certain parameters have a very small influence on the measured data. This leads to numerical rank deficiency, i.e. to small singular values of the system matrices that have to be inverted during the reconstruction process.

FIGURE 9. Singular values of $\hat{\mathbf{F}}'(p)$ at the solution p .

In Figure 9 we plot the singular values of the sensitivity matrix $\hat{\mathbf{F}}'(p)$ at the solution p . It can be seen that some very small singular values occur, which reflects the mentioned ill-posedness. Therefore, we apply regularisation methods, that provide a stable way of treating rank deficient and unstable problems.

3.2 Regularisation by Newton type Methods

Newton's method for the iterative solution of the nonlinear equation (3.6) formally reads as

$$p^{k+1} = p^k + s^k \quad \text{with} \quad \hat{\mathbf{F}}'(p^k)[s^k] = \hat{y} - \hat{\mathbf{F}}(p^k). \quad (3.10)$$

To implement Newton's method and related regularisation strategies we have to evaluate

- $\hat{\mathbf{F}}(p^k) \in \mathbb{C}^{(n_{mp} + n_{mp}^d)}$,
- $\hat{\mathbf{F}}'(p^k) : \mathbb{C}^{n_{par}} \rightarrow \mathbb{C}^{(n_{mp} + n_{mp}^d)}$,

In particular, for the computation of the right hand side $\hat{y} - \hat{\mathbf{F}}(p^k)$ one needs the solution $(\tilde{d}_k, \hat{\phi}_k)(\omega)$ of the Fourier transformed piezoelectric equations (2.15) with the tensor entries of $\mathbf{c}^E$, $\mathbf{e}$, and $\mathbf{e}^S$ being given by the respective values in the vector p^k , for $\omega = \omega_1, \dots, \omega_{n_{mp}}$, which, as we will see below, also enters into the evaluation of $\hat{\mathbf{F}}'(p^k)$. It is computed approximately via a finite element ansatz (cf. § 2.2); we denote the respective coefficients by $(\{\tilde{d}_k^l\}, \{\hat{\phi}_k^l\})$. The electric charge $q(\omega_l) = -\int_{\Gamma_e} \hat{n}^T \vec{D} d\Gamma$ is then obtained by numerical integration.

The Jacobian $\hat{\mathbf{F}}'(p^k)$ is given implicitly, via the piezoelectric equations. The local linearisation of $\hat{\mathbf{F}}$ at p^k in direction $\underline{dp}$ is given by

$$\hat{\mathbf{F}}'(p^k)[\underline{dp}] = \left(\underline{dq}_1, \dots, \underline{dq}_{n_{mp}}, \underline{d\hat{u}}_1, \dots, \underline{d\hat{u}}_{n_{mp}^d} \right). \quad (3.11)$$

Here, $\underline{dq}_l$, $\underline{d\hat{u}}_l$ are determined by (3.3), (3.4) from $(\underline{d\hat{d}}^l, \underline{d\hat{\phi}}^l)$, where $(\underline{d\hat{d}}^l, \underline{d\hat{\phi}}^l)$ weakly solves (2.23) with

$$\begin{aligned}\vec{f}_1 &= \mathcal{B}^T(\underline{d\mathbf{c}}^E \mathcal{B} \vec{\hat{d}} + \underline{d\mathbf{e}}^T \text{grad } \hat{\phi}) \\ \vec{f}_2 &= \text{div}(\underline{d\mathbf{e}} \mathcal{B} \vec{\hat{d}} - \underline{d\mathbf{e}}^S \text{grad } \hat{\phi}) \\ \vec{g}_1 &= -\mathbf{N}^T(\underline{d\mathbf{c}}^E \mathcal{B} \vec{\hat{d}} + \underline{d\mathbf{e}}^T \text{grad } \hat{\phi})|_{\partial\Omega} \\ \hat{\phi}^e &= 0 \\ \vec{g}_2 &= -\vec{n}^T(\underline{d\mathbf{e}} \mathcal{B} \vec{\hat{d}} - \underline{d\mathbf{e}}^S \text{grad } \hat{\phi})|_{\Omega \setminus (\Gamma_g \cup \Gamma_e)},\end{aligned}\tag{3.12}$$

and $\underline{d\mathbf{c}}^E$, $\underline{d\mathbf{e}}$, $\underline{d\mathbf{e}}^S$ are the tensors formed from the respective entries in $\underline{dp}$. Via a weak formulation, we can compute FE approximations to $(\underline{d\hat{d}}^l, \underline{d\hat{\phi}}^l)$ from the following system for their coefficients $(\underline{d\hat{d}}^l, \underline{d\hat{\phi}}^l)$:

$$\begin{pmatrix} -\omega_l^2 \mathbf{M}_{dd} + \mathbf{K}_{dd} & \mathbf{K}_{d\phi} \\ \mathbf{K}_{d\phi}^T & -\mathbf{K}_{\phi\phi} \end{pmatrix} \begin{pmatrix} \{\underline{d\hat{d}}^l\} \\ \{\underline{d\hat{\phi}}^l\} \end{pmatrix} = \begin{pmatrix} \{\vec{F}^l\} \\ \{\hat{Q}^l\} \end{pmatrix},\tag{3.13}$$

with

$$\begin{pmatrix} \{\vec{F}^l\} \\ \{\hat{Q}^l\} \end{pmatrix} = - \begin{pmatrix} \underline{d\mathbf{K}}_{dd} & \underline{d\mathbf{K}}_{d\phi} \\ \underline{d\mathbf{K}}_{d\phi}^T & -\underline{d\mathbf{K}}_{\phi\phi} \end{pmatrix} \begin{pmatrix} \{\hat{d}_k^l\} \\ \{\hat{\phi}_k^l\} \end{pmatrix}.$$

The matrices $\underline{d\mathbf{K}}_{dd}$, $\underline{d\mathbf{K}}_{d\phi}$, $\underline{d\mathbf{K}}_{\phi\phi}$ are defined analogously to $\mathbf{K}_{dd}$, $\mathbf{K}_{d\phi}$, $\mathbf{K}_{\phi\phi}$ with the material parameters p replaced by the material parameter increments $\underline{dp}$. The coefficients $(\{\hat{d}_k^l\}, \{\hat{\phi}_k^l\})$ are known from the (approximate) computation of $\hat{\mathbf{F}}(p^k)$.

To obtain from this implicit representation of the Jacobi matrix a search direction s^k according to (3.10), i.e. the solution of a linear system with the Jacobi matrix as system matrix and in order to obtain a symmetric system matrix we consider the normal equation

$$\hat{\mathbf{F}}'(p^k)^* \hat{\mathbf{F}}'(p^k)[s^k] = \hat{\mathbf{F}}'(p^k)^*(\hat{y} - \hat{\mathbf{F}}(p^k)).\tag{3.14}$$

This general form of (3.10) also enables us to incorporate overdetermined data, i.e. $n_{mp} + n_{mp}^d > n_{par}$. Therefore, and for the following iterative solution methods of (3.14) we need the adjoint operator $\hat{\mathbf{F}}'(p^k)^* = \hat{\mathbf{F}}'(p_k)^H$ of $\hat{\mathbf{F}}'(p^k)$.

Note that according to our remarks in §3.1, the condition number of the Jacobi matrix is large and the one of the normal equation is even its square. However, in the common regularization methods as used here for computing the Newton step (especially in the conjugate gradient method), self-adjoint operators are required. On the other hand, these regularization method are just designed to cope with the large condition number of the system, so that no numerical problems arise from the bad condition of (3.14).

3.3 Inexact Newton iterations

Due to the need for regularisation mentioned above, we replace the direct solution of the Newton step equation by a so-called inexact approach [10]. The regularising effect of such methods has been studied by Hanke [19] and Rieder [36, 37]. When applying an iterative regularisation method to (3.14) the inexact Newton method for solving (3.6) can be written as follows.

Algorithm 1 (SKELETON OF A REGULARISING INEXACT NEWTON METHOD)

```

CHOOSE  $p^0$ ;
SET  $k = 0$ ;
WHILE  $\|\hat{y} - \hat{\mathbf{F}}(p^k)\| \geq \tau\delta$  DO    (*)
    SET  $i = 0$ ;
    SET  $s^{k,0} = 0$ ;
    WHILE  $\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}]\| \geq \eta_k \|\hat{y} - \hat{\mathbf{F}}(p^k)\|$  DO    (**)
         $s^{k,i+1} = \Phi(\hat{\mathbf{F}}'(p^k), \hat{y} - \hat{\mathbf{F}}(p^k), s^{k,i})$ ;
         $i = i + 1$ ;
     $p^{k+1} = p^k + s^{k,i}$ ;
     $k = k + 1$ ;

```

The termination of the outer loop (*) in Algorithm 1 avoids amplification of the data error in the fully nonlinear problem, while the termination of the inner iteration (**) with $0 < \eta_k \leq \bar{\eta} < 1$ suitably chosen (see §3.6) represents the regularising part of this scheme for the linearised subproblems. The operator Φ describes the inner iteration scheme. In the following, we will consider three different choices for Φ , namely Landweber's method, v -methods and the conjugate gradient method.

Since our problem is strongly nonlinear, we do not expect the theoretical convergence conditions of Hanke [18, 19] and Rieder [36] to hold. Therefore, it is essential to carry out a line search within the Newton algorithm (see §3.6).

3.4 Newton – Landweber and v -methods

The idea of Landweber's iteration essentially is to perform a fixed point iteration for the normal equation in (3.14) with an appropriate damping parameter w . The corresponding k -th inexact Newton-step is computed as follows.

Algorithm 2 (LANDWEBER'S ITERATION)

```

SET  $i = 0$ ;
SET  $s^{k,0} = 0$ ;
WHILE  $\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}]\| \geq \eta_k \|\hat{y} - \hat{\mathbf{F}}(p^k)\|$  DO
     $s^{k,i+1} = s^{k,i} - w\hat{\mathbf{F}}'(p^k)^* (\hat{\mathbf{F}}'(p^k)[s^{k,i}] - (\hat{y} - \hat{\mathbf{F}}(p^k)))$ ;
     $i = i + 1$ ;

```

A choice of $w > 0$ such that $w \cdot \|\hat{\mathbf{F}}'(p^k)\|^2 < 1$ guarantees convergence. Our numerical tests (see Figure 12) have shown that one arrives at a very stable but also quite slowly convergent algorithm. To accelerate convergence we consider more advanced iterative, so called, v -methods introduced by Brakhage [6]. Here, the operator Φ in Algorithm 1 is defined via orthogonal polynomials to minimise a weighted residual with a weight $w_v(\lambda) = \frac{\lambda^{2v}}{\sqrt{\lambda(1-\lambda)}}$ [12, 17]. Here, the exponent v accounts for smoothness in the searched-for solution in some function space. In the present finite dimensional situation the choice of v is not crucial, which was also observed in our numerical experiments. The well known three-term recurrence for Jacobi polynomials induces the following two-step iteration:

Algorithm 3 (v – METHOD)

SET $z^0 = 0$; $s^{k,0} = 0$; $z^1 = \frac{4v+2}{4v+1}\hat{y}$; $s^{k,1} = \hat{\mathbf{F}}'(p^k)^* z^1$;
 SET $i = 1$;
 WHILE $\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}]\| \geq \eta_k \|\hat{y} - \hat{\mathbf{F}}(p^k)\|$ DO
 $\quad \zeta_i = \frac{(i-1)(2i-3)(2i+2v-1)}{(i+2v-1)(2i+4v-1)(2i+2v-3)}$;
 $\quad \omega_i = 4 \frac{(2i+2v-1)(i+v-1)}{(i+2v-1)(2i+4v-1)}$;
 $\quad z^{i+1} = z^i + \zeta_i(z^i - z^{i-1}) - \omega_i(\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}])$;
 $\quad s^{k,i+1} = \hat{\mathbf{F}}'(p^k)^* z^{i+1}$;
 $\quad i = i + 1$;

3.5 Newton – CG

As mentioned in §2.3, the conjugate gradient method belongs to the most powerful algorithms for the solution of self-adjoint, positive (semi-)definite well-posed linear equations. Since here it is applied to the normal equation we equivalently abbreviate it with CGNE in the following. In this method, in contrast to Landweber's iteration and the v -methods, Φ is a nonlinear function of the right hand side of (3.14). The iterates $s^{k,i}$ of Algorithm 4 below satisfy

$$\begin{aligned}
 & \|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}]\| \\
 & = \min\{\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s]\| \mid s \in \mathbb{K}_i(\hat{\mathbf{F}}'(p^k)^*(\hat{y} - \hat{\mathbf{F}}(p^k)), \hat{\mathbf{F}}'(p^k)^* \hat{\mathbf{F}}'(p^k))\}
 \end{aligned} \tag{3.15}$$

where $\mathbb{K}_i$ denotes the i -th Krylov subspace (cf. (2.29)), i.e. the iterates $s^{k,i}$ minimise the residual $\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s^{k,i}]\|$ in the i -th Krylov subspace (see Hanke [19] for details).

Algorithm 4 ($\overset{\circ}{\text{CGNE}}$)

SET $s^{k,0} = 0$; $r^0 = \hat{y} - \hat{\mathbf{F}}(p^k)$;
 $z^1 = r^{NE0} = \hat{\mathbf{F}}'(p^k)^*[r^0]$;
 SET $i = 1$;
 WHILE $\|\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[z^i]\| \geq \eta_k \|\hat{y} - \hat{\mathbf{F}}(p^k)\|$ DO
 $\quad q^i = \hat{\mathbf{F}}'(p^k)[z^i]$;
 $\quad \alpha_i = \frac{\|r_{i-1}^{NE}\|^2}{\|q^i\|^2}$;
 $\quad s^{k,i} = s^{k,i-1} + \alpha_i z^i$;
 $\quad r^i = r^{i-1} - \alpha_i q^i$;
 $\quad r^{NEi} = \hat{\mathbf{F}}'(p^k)^*[r^i]$;
 $\quad \beta_i = \frac{\|r^{NEi}\|^2}{\|r^{NEi-1}\|^2}$;
 $\quad z^{i+1} = r^{NEi} + \beta_i z^i$;
 $\quad i = i + 1$;

Due to the residual based stopping criterion (**) in Algorithm 1, and since also the i th Landweber and v -method iterate lie in $\mathbb{K}_i$ [17], CGNE is among the three inner iteration schemes the one requiring the minimal number of steps, by virtue of (3.15).

FIGURE 10. Thickness resonator.

3.6 Further algorithmic details

Scaling

Since the values of the searched-for parameters are of quite different orders of magnitude ($\mathbf{c}^E \sim 10^{11}$, $\mathbf{e} \sim 10$, $\boldsymbol{\varepsilon}^S \sim 10^{-8}$), a proper scaling of the parameter space is necessary, i.e., we apply the previously discussed Newton type methods to $\Psi(\xi) = \hat{\mathbf{y}}$ with $\xi := \text{Scal} \cdot p$, $\Psi(\xi) := \hat{\mathbf{F}}(\text{Scal}^{-1} \cdot \xi)$, where, for example, $\text{Scal} := \text{diag}(1/p_1^k, \dots, 1/p_{n_{par}}^k)$. The measured values are rather different in absolute magnitude (e.g. at resonance and antiresonance, respectively, see Figure 11) too, and have to be appropriately weighted. We do so by multiplying the residual with a diagonal matrix containing the reciprocals of the absolute data values. Since this results in a modified definition of the inner product in data space it affects also the definition of the adjoint $\hat{\mathbf{F}}'(p)^*$.

Newton's method is known to be invariant with respect to affine transformation in pre-image and in image space. Note, however, that the regularised versions of Newton's methods we use here are not scaling invariant.

Linesearch and choice of η_k

Often we can assume that we have quite good starting values for our iterative identification process described in §3.2, using the estimates from the conventional experimental reconstruction methods as described in the introduction, or the material parameters of similar known piezoelectric media. However, if this is not the case or, as it has turned out in our computations, if some of the parameters are extremely sensitive to perturbations in the starting values, the implementation of an additional linesearch strategy seems to be advisable. We here use a simple variant of the linesearch algorithm INB as proposed and analysed in [10]. It is based on a comparison of the predicted and actual reduction of the residual and adapted to inexact Newton methods. The steering parameters of this algorithm were chosen according to Pernice & Walker [35].

4 Numerical results

All of the methods described above were tested on 2D and 3D numerical simulations of piezoelectric transducers. In this section we confine the presentation to results for a rotationally symmetric thickness resonator polarised in thickness direction (see Figure 10) with thickness = 0.5 mm and radius = 10.0 mm. In generating a computational grid,

FIGURE 11. Simulated impedance curves in the frequency range close to resonance, with measurement points indicated by “x”.

we followed the common rule of using at least twenty gridpoints per wavelength, which is in the order of some millimeters here. Detectability and shape dimensions of the piezoelectric transducer are mutually dependent. In particular piezoelectric coefficients relating the impressed electric field to strain perpendicular to the polarisation axis carry more weight if the resonator's thickness is increased. On the other hand decreasing the resonators extension in polarisation direction supports determinability of coefficients acting along this direction.

Our tests were based on synthetically created data. Inverse crimes [8] were avoided by generating the synthetic data using higher order finite elements. Results with measured data can be found in a forthcoming paper [28].

For the identification process we chose up to ten different frequency points around resonance frequency (frequency with minimal impedance value) and let for an impressed voltage of 1V measured phase and amplitude of $Z(\omega_l)$, $l = 1, \dots, 10$ enter via (3.2) as data into our evaluation schemes, see Figure 11. In this figure, the tag “x” denotes the frequency points at which measurements have been taken.

To illustrate the influence of variations of the material parameters on the measured data, we did simulations with variations of 15% of the three essential material parameters which lead to corresponding shifts of the impedance curve, as compared to the one corresponding to the reference parameter set, see solid line in Figure 11.

4.1 Real-valued material parameters

The material under observation is Ferroperm Pz-27 which belongs to the class of soft lead zirconate titanate materials.

We begin the presentation with reconstructions of the real parts of the dominant material parameters, i.e. $\text{Re}(c_{33}^E)$, $\text{Re}(e_{33})$ and $\text{Re}(e_{33}^S)$, where we used five measurement points only. A simultaneous determination was also done for all those nine parameters that can be expected to be obtainable from a rotationally symmetric transducer (cf. the

FIGURE 12. Development of the dominant parameters during their simultaneous reconstruction by Newton's method with Landweber (top left), v -method (top right), and CG (bottom) as inner iteration.

remark at the end of §2.1), see Figure 12. In the case of noise free data considered here first of all, the Newton iteration was stopped as soon as for its weighted residual $\|\hat{\mathbf{F}}(p^k) - \hat{\mathbf{y}}\| < 10^{-4}$ holds. As starting values a 15% variation of all three parameters was chosen when concentrating on the dominant parameters only.

When reconstructing all material parameters simultaneously (see Figure 13), more sophisticated initial guesses were required. Here, we started with a 10% variation for the dominant parameters and a 5% variation for all others. Convergence of the least sensitive parameter e_{31} to within one per cent of its actual value occurred after about 2500 steps.

Moreover, we compared the performance of the proposed methods to a simple least squares fit. The latter only recovered the dominant material parameters while leaving the others unchanged, which is also reflected in a stalling decay of the residual – see Figure 14.

Figure 15 shows results for $\text{Re}(c_{33}^E)$, $\text{Re}(e_{33})$ and $\text{Re}(e_{33}^S)$ where $\hat{\mathbf{y}}$ on the right-hand side of (3.10) was perturbed with uniformly distributed random noise of 2.5% and 5%, respectively.

In all our experiments, average ranges of the inner iteration numbers required by the different methods were 80–100 for Landweber iteration, 6–12 for the v -methods, and 4–8 for CGNE. In the v -methods we chose the parameter $v = 1.5$. For the total computational time these values are hardly relevant, though, since the numerical solution

FIGURE 13. Development of all nine parameters during their simultaneous reconstruction by the Newton-v-method.

FIGURE 14. Comparison of Newton-v-method with least squares gradient method for the simultaneous identification of all nine material parameters.

FIGURE 15. Convergence for perturbed data with 2.5% (left) and 5.0% (right) noise.

Table 1. *Identifiability of different material parameters*

Parameter	exact value	starting value	approximated value	Newton steps
$c_{11}^E [N/m^2]$	1.47e+11	0.98e+11	1.469164068e+11	68
$c_{33}^E [N/m^2]$	1.13e+11	0.88e+11	1.130007046e+11	19
$c_{12}^E [N/m^2]$	1.05e+11	—	—	—
$c_{13}^E [N/m^2]$	9.37e+10	8.37e+10	9.370446315e+10	23
$c_{44}^E [N/m^2]$	2.3e+10	1.533e+10	2.297125406e+10	109
$e_{15} [(C/m)^2]$	11.64	7.76	11.43167959	625
$e_{31} [(C/m)^2]$	−3.09	−2.06	−3.08678653	712
$e_{33} [(C/m)^2]$	16	10.667	15.99979622	5
$\varepsilon_{11}^S [F/m]$	1.00502e-08	0.670e-08	9.765878235e-09	890
$\varepsilon_{33}^S [F/m]$	8.09255e-09	5.395e-09	8.092679236e-09	19

Table 2. *Real and complex material parameters of Motorola 3203 HD PZT [39]*

Material parameter	Real	Imag
$c_{33}^E [N/m^2]$	1.77e+11	0.023e+11
$e_{33} [(C/m)^2]$	19.84	0.066
$\varepsilon_{33}^S [F/m]$	1.06e-8	−0.053e-8

of the piezoelectric equations is by far the most time and memory consuming part: While the regularized computation of the Newton step by one of the three proposed iterative methods took at most half a CPU second on an Intel PIV, 2.8GHz, a forward solve for one frequency point required about 4 seconds in the 2D case (11 seconds in the 3D case).

In the following we investigated the identifiability of single material parameters. Here we set the tolerance on the residual in the stopping criterion to 10^{-7} . Starting values were constructed by multiplying the exact material parameters with $2/3$. Since the piezoelectric transducer under observation is polarised in z direction, all parameters acting in this direction (those with the double index 33) have a strong impact on the solution of the PDEs. Thus they were easy to determine and their reconstruction required just a few Newton steps. For the other tensor entries a much higher iteration number has to be expected (see Table 1). The parameter c_{12} was not detectable since it has a very small influence on the solution of a radially symmetric problem, see the end of §2.1. Since for c_{13}^E the inversion scheme found an incorrect solution at $7.35 \cdot 10^{10}$, here a closer initial guess was needed.

4.2 Complex-valued material parameters

The determination of the imaginary parts of the different material tensor entries is a much more challenging task since the imaginary parts, due to their smaller order of magnitude, have a much smaller impact on the impedance curve than the corresponding real parts. Here we again concentrate on the dominant coefficients c_{33}^E , e_{33} , ε_{33}^S , see Table 2 for the

FIGURE 16. Development of the normed imaginary parts of the dominant material parameters during their separate reconstruction by the Newton-v-iteration.

FIGURE 17. Development of the normed imaginary parts of the dominant material parameters during their simultaneous reconstruction by the Newton-v-iteration.

parameters of Motorola 3203 HD PZT, which is the material under consideration in this subsection.

The different types of losses in piezoelectricity are usually characterized by the mechanical quality factor $Q_M = \left| \frac{\text{Re}(s_{33}^E)}{\text{Im}(s_{33}^E)} \right|$ as well as the dielectric loss tangent $|\tan \delta| = \left| \frac{\text{Im}(e_{33}^\sigma)}{\text{Re}(e_{33}^\sigma)} \right| = \frac{1}{Q_E}$, where s_{33}^E and e_{33}^σ are tensor entries in the material law (2.2). Since forward simulations are based on version (2.1) of the piezoelectric material law, we rather consider the quotients

$$\tilde{Q}_M = \left| \frac{\text{Re}(c_{33}^E)}{\text{Im}(c_{33}^E)} \right|, \quad \tilde{Q}_P = \left| \frac{\text{Re}(e_{33})}{\text{Im}(e_{33})} \right|, \quad \tilde{Q}_E = \left| \frac{\text{Re}(\epsilon_{33}^S)}{\text{Im}(\epsilon_{33}^S)} \right|.$$

Obviously, it only makes sense to identify imaginary parts of material parameters with low factors $\tilde{Q}_M$, $\tilde{Q}_P$, $\tilde{Q}_E$.

The convergence history of our reconstruction for the imaginary parts of the material parameters of Motorola 3203 HD PZT is displayed in Figures 16 and 17. Here initial guesses were constructed by reducing the exact values by one third. Due to the small influence of the imaginary parts on the solution of the piezoelectric equations, the identification process needs to be run until the norm of the residual falls below a much smaller tolerance. (In our computations $\|\hat{y} - F(p^k)\| \leq 10^{-7}$). Since the material under

consideration has low mechanical and electrical quality factors,

$$\tilde{Q}_M = 77, \quad \tilde{Q}_P = 302, \quad \tilde{Q}_E = 20,$$

the imaginary parts of the elasticity and the dielectric parameters are easier detectable than those of the piezoelectric ones.

5 Conclusions and remarks

In this paper we presented a new approach for identifying piezoelectric material parameters that is based on finite element simulations of the full two or three dimensional piezoelectric system of PDEs, as well as Newton type methods for inverse computations. We discussed solvability of the forward problem, i.e. the piezoelectric PDEs, and considered different efficient numerical strategies for its solution. For the inverse problem of parameter identification, we investigated identifiability and stability and proposed some iterative solution methods based on an inexact Newton approach. Detailed numerical experiments and computational case studies illustrate applicability of the proposed methodology. Note that the latter can in an obvious way also be used to simultaneously take into account measurements of several test samples. Moreover, our approach allows identification of material tensors also for piezoelectric transducers with more complex geometries such as stack actuators (see also the forward computations in §2.3). Besides this, frequency and temperature dependence (in case of external heating, so without conversion of electrical and mechanical energy into heat) can easily be modelled by applying the proposed scheme to measurements in different frequency or temperature ranges, respectively. Note that part of our results immediately extends to the situation of space-dependent parameters. Dependence of the parameters on the field quantities $\vec{d}$ and/or ϕ (as it is relevant for characterising the large signal behaviour) is treated in Kaltenbacher [26] via a generalisation of the approach presented here.

Future research work will be devoted both to the forward and to the inverse problem: In the case of the forward problem we plan to extend our investigations to different preconditioning approaches (especially Schur complement based methods).

Concerning the inverse problem we intend to augment our model to take into account thermal energy conversion as it is relevant in the context of large excitations over longer time intervals. This leads to an additional PDE coupled to the piezoelectric system, and to some further material parameters to be identified. Another challenging task we plan to deal with in the near future is the characterisation of hysteresis in piezoelectric systems by means of inverse methods.

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References

- [1] AKAMATSU, M. & NAKAMURA, G. (2002) Well-posedness of initial-boundary value problems for piezoelectric equations. *Applicable Analysis*, **81**, 129–141.
- [2] ANDERSON, E., BAI, Z., BISCHOF, C., BLACKFORD, S., DEMMEL, J., DONGARRA, J., DU CROZ, J., GREENBAUM, A., HAMMARLING, S., MCKENNEY, A. & SORENSEN, D. (1999) *LAPACK Users' Guide, Third Edition*. Volume 9 of *Software, Environments, and Tools*. SIAM.
- [3] ASHCRAFT, C., GRIMES, R. & LEWIS, J. (1998) Accurate symmetric indefinite linear equation solvers. *SIAM J. Matrix Anal. Applic.* **20**(2), 513–561.
- [4] BENZI, M., GOLUB, G. & LIESSEN, J. (2005) Numerical solution of saddle point problems. *Acta Numerica*, **14**, 1–137.
- [5] BRAESS, D. (1997) *Finite Elemente*. Springer.
- [6] BRAKHAGE, H. (1987) On ill-posed problems and the method of conjugate gradients. In: H.W. Engl and C.W. Groetsch, editors, *Inverse and Ill-Posed Problems*. Academic Press Orlando, FL, pp. 165–175.
- [7] BUNCH, J. R. & KAUFMANN, L. (1977) Some stable methods for calculating inertia and solving symmetric linear systems. *Mathematics of Computation*, **31**(137), 163–179.
- [8] KRESS, R. & COLTON, D. (1992) *Inverse Acoustic and Electromagnetic Scattering Theory*. Applied Mathematical Sciences. Springer-Verlag.
- [9] DU, X.-H., WANG, D.-M. & UCHINO, K. (2004) An accurate method for the determination of complex coefficients of single crystal piezoelectric resonators I: Theory. *IEEE Trans. UFFC*, **51**, 227–235.
- [10] EISENSTAT, S. C. & WALKER, H. F. (1994) Globally convergent inexact Newton methods. *SIAM J. Optimization*, **4**, 393–422.
- [11] ENGL, H. W. (1995) *Inverse Problems*. Sociedad Matematica Mexicana, Mexico.
- [12] ENGL, H. W., HANKE, M. & NEUBAUER, A. (1996) *Regularization of Inverse Problems*. Kluwer.
- [13] European standard prEN 50324-1:1998, 50324-2:1998, 50324-3:2001, 1998-2001.
- [14] GEIS, W., MISHURIS, G. & SÄNDIG, A.-M. (2003) Piezoelectricity in multilayer actuators. Modelling and analysis in two and three dimensions. Technical report, University of Stuttgart.
- [15] GREENBAUM, A. (1997) *Iterative Methods for Solving Linear Systems*. Frontiers in Applied Mathematics. SIAM.
- [16] HACKBUSCH, W. (1994) *Iterative Solution of Large Sparse Systems of Equations*. Volume 95 of *Applied Mathematical Sciences*. Springer-Verlag.
- [17] HANKE, M. (1991) Accelerated Landweber iterations for the solution of ill-posed equations. *Numer. Math.* **60**, 341–373.
- [18] HANKE, M. (1997) A regularization Levenberg–Marquardt scheme, with applications to inverse groundwater filtration problems. *Inverse Problems*, **13**, 79–95.
- [19] HANKE, M. (1997) Regularizing properties of a truncated Newton–CG algorithm for nonlinear inverse problems. *Numer. Funct. Anal. Optim.* **18**, 971–993.
- [20] HANSEN, P. C. (1998) *Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion*. SIAM Monographs on Mathematical Modeling and Computation. SIAM.
- [21] HOLLAND, R. (1967) Representation of dielectric, elastic, and piezoelectric losses by complex coefficients. *IEEE Trans. UFFC*, **14**, 18–20.
- [22] HUGHES, T. J. R. (2000) *Finite Element Method*. Prentice-Hall.
- [23] IEEE Standard on Piezoelectricity (1985) IEEE/ANSI.
- [24] IKEDA, T. (1990) *Fundamentals of Piezoelectricity*. Oxford University Press.
- [25] JAFFE, H. & BELINCOURT, D. A. (1985) Piezoelectric transducer materials. *Proc. IEEE*, **53**, 1372–1386.
- [26] KALTENBACHER, B. (2006) Determination of parameters in nonlinear hyperbolic PDEs via a multiharmonic formulation, applied in piezoelectric material characterization. *Math. Models & Math. Appl. Sci.* (to appear).

- [27] KALTENBACHER, M. (2004) *Numerical Simulation of Mechatronic Sensors and Actuators*. Springer-Verlag.
- [28] KALTENBACHER, M., LAHMER, T., LEDER, E., KALTENBACHER, B. & LERCH, R. (2006) FEM based determination of real and complex elastic, dielectric and piezoelectric moduli in piezoceramic materials. In preparation.
- [29] LERCH, R. (1990) Simulation of piezoelectric devices by two- and three-dimensional finite elements. *IEEE Trans. UFFC*, **37**(3), 33–247.
- [30] LERCH, R. (1996) Verbesserung des Verfahrens zur Bestimmung der elektroelastischen Tensoren von piezokeramischen Materialien. Technical report, University of Linz.
- [31] MARTIN, G. E. (1965) Dielectric, piezoelectric, and elastic losses in longitudinally polarized segmented ceramic tubes. *U.S. Navy J. Underwater Acoustics*, **15**, 329–332.
- [32] MIARA, B. (2001) Controlabilité d'un corps piézoélectrique. *C.R. Acad. Sci. Paris*, **333**, 267–270.
- [33] Pardiso website. <http://www.computational.unibas.ch/cs/scicomp/software/pardiso>.
- [34] PARKUS, H. (1986) *Technische Mechanik*. Springer-Verlag.
- [35] PERNICE, M. & WALKER, H. F. (1998) NITSOL: A Newton iterative solver for nonlinear systems. *SIAM J. Sci. Comput.* **19**, 302–318.
- [36] RIEDER, A. (1999) On the regularization of nonlinear ill-posed problems via inexact Newton iterations. *Inverse Problems*, **82**, 307–327.
- [37] RIEDER, A. (2001) On convergence rates of inexact Newton regularizations. *Numer. Math.* **88**, 347–365.
- [38] SAAD, Y. (2003) *Iterative Methods for Sparse Linear Systems*. SIAM, 2nd edition.
- [39] SHERRIT, S., WIEDERICK, H. D. & MUKHERJEE, B. K. (1997) A complete characterization of the piezoelectric, dielectric, and elastic properties of Motorola PZT 3203 HD, including losses and dispersion. *SPIE Proceedings*.
- [40] SLEIJPEN, G. L. G., VAN DER VORST, H. A. & MODERSITZKI, J. (2000) Differences in the effects of rounding errors in Krylov solvers for symmetric indefinite linear systems. *SIAM J. Matrix Anal. Applic.* **22**(3), 726–751.
- [41] SLOAN, S. W. (1986) An algorithm for profile and wavefront reduction of sparse matrices. *Int. J. Numer. Methods in Eng.* **23**, 239–251.
- [42] VANDERBEI, R. (1995) Symmetric quasidefinite matrices. *SIAM J. Optimization*, **5**(1), 100–113.
- [43] WLOKA, J. (1982) *Partielle Differentialgleichungen*. Teubner.