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TUNING OF THE EQUILIBRATED RESIDUAL METHOD FOR APPLICATIONS IN GENERAL, DIRECT AND INVERSE PIEZOELECTRICITY[1]

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This paper presents application and tuning of the equilibrated residual method (ERM) of a posteriori error estimation for coupled electromechanical problems of direct, inverse and general piezoelectricity. In these three cases, either electric potential is induced by strains or strains appear due to the applied electric potential or both phenomena occur simultaneously. The mentioned ERM is assigned for the assessment of modeling and approximation errors of the numerical finite element solution. Such error values usually serve as indication for adaptive hierarchical modeling and adaptive mesh changes within thin and/or solid piezoelectric members so as to obtain the solution of assumed accuracy.

Keywords: coupled problems, piezoelectricity, finite element method, a posteriori error estimation, equilibrated residual method

1. Introduction

The origins and development of the residual equilibrated approach to a posteriori error estimation can be attributed to Ladeveze and Leguillon (1983), Kelly (1984), Bank and Weisser (1985), and Ainsworth and Oden (1993c). Implementation of the equilibrated residual method (ERM) to error estimation of finite element solutions was presented by Ainsworth and Oden (1992). The method was applied to elliptic problems by the same authors in (1993a,b). In 1994, they used the method for analysis of elasticity problems. Application of the method to thin- or thick-walled elastic structures was performed by Oden and Cho (1996), and Zboiński (2013) as well. The recent works on the method concern: stability analysis (Ainsworth *et al.*, 2007), generalizations to singularly perturbed reaction-diffusion problems (Ainsworth and Babuska, 1999), and application to conforming, non-conforming and discontinuous Galerkin finite element methods (Ainsworth, 2005). Application of the method to dielectricity (elliptic) and piezoelectricity (coupled) problems was suggested in (Zboiński, 2018). Recently (Zboiński, 2020), tuning of the method was performed in the case of thin elastic structures and suggested for dielectric and piezoelectric domains. It results from the above works that effective application of ERM may need its tuning by a modified definition of ERM local problems. Particularly, thin-walled elastic and piezoelectric domains need such procedures. In this context, the novelty and scope of the paper include: presentation of ERM for coupled problems as exemplified by piezoelectricity, and introduction of the tuning procedure to thick- or thin-walled piezoelectric domains.

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2. Model problems

Let us start with the functional of electromechanical potential energy defined within volume V which may represent any bounded three-dimensional piezoelectric domain. In this paper, we limit it to symmetric-thickness, thin- or thick-walled domains defined in a standard way (Zboiński, 2010, 2019) with the use of mid-surface and thickness concepts as this is a typical geometry of piezoelectric transducers (actuators or sensors). After taking the first variation of this functional, one can obtain

$$\begin{aligned}&\int\limits_V (-D^{ijkl}\varepsilon_{kl}\delta\varepsilon_{ij} + C^{ijk}E_k\delta\varepsilon_{ij} + f^i\delta u_i)\,dV + \int\limits_P p^i\delta u_i\,dS\\ &\quad + \int\limits_V (\gamma^{ij}E_j\delta E_i + C^{ikl}\varepsilon_{kl}\delta E_i)\,dV - \int\limits_Q c\delta\phi\,dS = 0\end{aligned} \tag{2.1}$$

With the strain and electric field definitions, weak formulation (2.1) becomes a functional of $\mathbf{u} = \{u_i\}$, $i = 1, 2, 3$ and ϕ, where $\mathbf{u}$ and $\delta\mathbf{u}$ denote the solution and virtual (or admissible) displacements, while ϕ and $\delta\phi$ denote the solution and virtual (or admissible) electric potential. Note that $\delta\mathbf{u} \in \mathbf{w}+U$, with $\mathbf{w}$ being the lift (given displacements) of Dirichlet data (Demkowicz, 2007), and $U = \{\delta\mathbf{u} \in (H^1(V))^3 : \ \delta\mathbf{u} = \mathbf{0} \text{ on } W\}$ representing the space of kinematically admissible displacements within the domain V. Also, $\delta\phi \in \chi + \Phi$, with χ being the lift (given potential) of Dirichlet data, and $\Phi = \{\delta\phi \in H^1(V) : \ \delta\phi = \mathbf{0} \text{ on } F\}$ representing the space of electrically admissible potentials in V. The searched coupled solution belongs to $(\mathbf{u}, \phi) \in U \times \Phi$, i.e.

$$\begin{aligned}&B(\delta\mathbf{u}, \mathbf{u}) - C(\delta\mathbf{u}, \phi) = L(\delta\mathbf{u})\\ &- C(\delta\phi, \mathbf{u}) - b(\delta\phi, \phi) = -l(\delta\phi)\end{aligned} \tag{2.2}$$

where the bilinear, coupling and linear forms are

$$\begin{aligned}B(\delta\mathbf{u}, \mathbf{u}) &= \int\limits_V D^{ijkl}\varepsilon_{kl}\delta\varepsilon_{ij}\,dV = \int\limits_V D^{ijkl}u_{k,l}\delta u_{i,j}\,dV\\ C(\delta\mathbf{u}, \phi) &= \int\limits_V C^{ijk}E_k\delta\varepsilon_{ij}\,dV = \int\limits_V C^{ijk}E_k\delta u_{i,j}\,dV\\ L(\delta\mathbf{u}) &= \int\limits_V f^i\delta u_i dV + \int\limits_P p^i\delta u_i\,dS\\ b(\delta\phi, \phi) &= \int\limits_V \gamma^{ij}E_j\delta E_i\,dV = \int\limits_V \gamma^{ij}\phi_{,j}\delta\phi_{,i}\,dV\\ C(\delta\phi, \mathbf{u}) &= \int\limits_V C^{ikl}\varepsilon_{kl}\delta E_i\,dV = \int\limits_V C^{ikl}\varepsilon_{kl}\delta\phi_{,i}\,dV\\ l(\delta\phi) &= \int\limits_Q c\delta\phi\,dS = 0\end{aligned} \tag{2.3}$$

and represent the first variations of (or virtual) strain, electric field and coupling energies, respectively, B, b and C, and the first variations of (or virtual) works, L and l, of the external forces and charges, respectively. With the reciprocity theorem (Ieşan, 1990), one can convert the above functional into the corresponding local (strong) formulation (Zboiński, 2016). Existence and uniqueness of the solution to problem (2.2) and (2.3) is based on the Lax-Milgram theorem (cf. Cimatti, 2004).

In Eqs. (2.3), ε_{kl} and D^{ijkl}, $i,j,k,l=1,2,3$ stand for the strain and elastic constant tensors, while f^i represent components of the mass load vector $\mathbf{f}$. Additionally, d^i, E_j, $i,j=1,2,3$ are the electric displacement and electric field vectors. The tensors γ^{ij}, C^{kij} and C^{ikl}, $i,j,k,l=1,2,3$ represent dielectric and piezoelectric constants under constant strain. Additionally, p^i are components of the surface load $\mathbf{p}$, while $-c$ stands for the surface charge. Finally, P, W, Q and F denote the loaded, supported, charged and grounded parts of the boundary $S \equiv \partial V$ of the body domain. We assume $S \equiv P \cup W = Q \cup F$.

After finite element hpq- and $h\pi\rho$-approximation (Zboiński, 2016, 2018), where h, p, q and π, ρ are the element size, and longitudinal and transverse approximation orders within the displacement and electric potential fields, respectively, above relations (2.2) and (2.3) can be defined with the aproximation of the solution quantities and spaces, i.e. $(\mathbf{u}^{hpq}, \phi^{h\pi\rho}) \in U^{hpq} \times \Phi^{h\pi\rho}$.

In the case of direct piezoelectricity (sensing), the external, mechanical (volume and/or surface) loadings produce strains which in turn induce electric potential within the piezoelectric member. No external electric charges are present in this case. As a result, the assumption of $c=0$ has to be substituted into the second line of (2.1). In the case of inverse piezoelectricity (actuation), the mechanical loadings are not present – $\mathbf{f}=\{f^i\}=\mathbf{0}$ and $\mathbf{p}=\{p^i\}=\mathbf{0}$ in the first line of (2.1).

With the use of decoupling assumptions of $C^{ijk}=0$, $C^{ikl}=0$, $i,j,k=1,2,3$, functional (2.1) is replaced with two independent mechanical and electric potential energy functionals.

3. ERM a posteriori error estimation

In this Section, we present our original results of implementetion of the equilibrated residual method (ERM) of a posteriori error estimation to the coupled problems of piezoelectricity. The global η and element $\overset{e}{\eta}$ error estimators are defined by us as

$$\begin{aligned}\eta = \sum_e \overset{e}{\eta} = \sum_e \Bigg[&- \overset{e}{\Pi}(\mathbf{u},\phi) - \int\limits_{S_e \setminus S} \mathbf{u}^{\mathrm{T}} \langle \overset{e}{\mathbf{r}}(\mathbf{u}^{hpq}) \rangle \, d\overset{e}{S} + \int\limits_{S_e \setminus S} \phi \langle \overset{e}{h}(\phi^{h\pi\rho}) \rangle \, d\overset{e}{S} \\ &- \frac{1}{2}\overset{e}{B}(\mathbf{u}^{hpq},\mathbf{u}^{hpq}) + \frac{1}{2}\overset{e}{C}(\mathbf{u}^{hpq},\phi^{h\pi\rho}) + \frac{1}{2}\overset{e}{C}(\phi^{h\pi\rho},\mathbf{u}^{hpq}) + \frac{1}{2}\overset{e}{b}(\phi^{h\pi\rho},\phi^{h\pi\rho}) \Bigg]\end{aligned} \tag{3.1}$$

Note that in (3.1), the sum (over elements e) of terms of the first line represents electromechanical potential energy $\mathit{\Pi}(\mathbf{u},\phi)$ of the exact solution $(\mathbf{u},\phi)$, while the sum of terms of the second line the analogous energy $\mathit{\Pi}(\mathbf{u}^{hpq},\phi^{h\pi\rho})$ of the numerical solution $(\mathbf{u}^{hpq},\phi^{h\pi\rho})$, the error of which is a posteriori estimated. In the first line, the potential energy is defined as a sum of the strain, electric field and coupling energies deminished by the work of external forces and charges, i.e. $\mathit{\Pi}=0.5B-C-0.5b-L+l$. After the partitioning of the domain V into finite elements of volumes $\overset{e}{V}$, $\partial\overset{e}{V}=\overset{e}{S}$, this energy has to be completed by the work of the internal (interelement) forces and charges represented by the last two components of the first line. The terms $\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle$ and $\langle\overset{e}{h}(\phi^{h\pi\rho})\rangle$ represent the equilibrated interelement stress reaction vectors and the equilibrated interelement equivalent electric charge, respectively, typical for the equilibrated residual method.

In the second line of (3.1), the equivalent definition, $\mathit{\Pi}=-0.5B+C+0.5b$, of the electromechanical potential energy is applied. It needs introduction of stationarity results (2.2), with $\delta\mathbf{u}$ and $\delta\phi$ replaced by $\mathbf{u}$ and ϕ, i.e. $L=B-C$ and $-l=-b-C$ into the former definition so as to eliminate the external work from the modified potential energy definition before the partitioning.

As the exact solution $(\mathbf{u},\phi)$ of (3.1) can hardly be found, we approximate this functional with the finite element method and search for the approximation $(\mathbf{u}^{HPQ},\phi^{H\Pi P})$ of the exact solution. Here, H, P, Q and Π, P stand for the element size, and longitudinal and transverse approximation orders within the displacement and electric potential fields, respectively. After taking the first variation of approximated functional (3.1) with respect to $\delta\mathbf{u}^{HPQ}$ and $\delta\phi^{H\Pi P}$ and equating it to zero, one obtains the following global stationarity condition

$$0=\sum_e\left[-\delta\overset{e}{\Pi}(\mathbf{u}^{HPQ},\phi^{H\Pi P})-\int\limits_{S_e\setminus S}(\delta\mathbf{u}^{HPQ})^{\mathrm{T}}\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle\,d\overset{e}{S}+\int\limits_{S_e\setminus S}\delta\phi^{H\Pi P}\langle\overset{e}{h}(\phi^{h\pi\rho})\rangle\,d\overset{e}{S}\right] \tag{3.2}$$

equivalent to the following element (or local) sets of two coupled conditions (cf. Zboiński, 2016)

$$\begin{aligned}&\overset{e}{B}(\delta\mathbf{u}^{HPQ},\mathbf{u}^{HPQ})-\overset{e}{C}(\delta\mathbf{u}^{HPQ},\phi^{H\Pi P})=\overset{e}{L}(\delta\mathbf{u}^{HPQ})+\int\limits_{\overset{e}{S}\setminus S}(\delta\mathbf{u}^{HPQ})^{\mathrm{T}}\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle\,d\overset{e}{S}\\&\overset{e}{C}(\delta\phi^{H\Pi P},\mathbf{u}^{HPQ})+\overset{e}{b}(\delta\phi^{H\Pi P},\phi^{H\Pi P})=\overset{e}{l}(\delta\phi^{H\Pi P})+\int\limits_{\overset{e}{S}\setminus S}\delta\phi^{H\Pi P}\langle\overset{e}{h}(\phi^{h\pi\rho})\rangle\,d\overset{e}{S}\end{aligned} \tag{3.3}$$

where the first definition of the potential energy was utilized on the element level. The searched coupled solution belongs to $(\mathbf{u}^{HPQ},\phi^{H\Pi P})\in U^{HPQ}\times\Phi^{H\Pi P}$, where $\delta\mathbf{u}^{HPQ}\in\mathbf{w}^{HPQ}+U^{HPQ}$, with $\mathbf{w}^{HPQ}$ being the approximated lift of Dirichlet data, and $U^{HPQ}=\{\delta\mathbf{u}^{HPQ}\in(H^1(\overset{e}{V}))^3:\ \delta\mathbf{u}^{HPQ}=\mathbf{0}\text{ on }W\cap d\overset{e}{S}\}$ representing the local (element) space of kinematically admissible displacements within the domain $\overset{e}{V}$. Also, $\delta\phi^{H\Pi P}\in\chi^{H\Pi P}+\Phi^{H\Pi P}$, with $\chi^{H\Pi P}$ being the lift of Dirichlet data, and $\Phi^{H\Pi P}=\{\delta\phi^{H\Pi P}\in H^1(\overset{e}{V}):\ \delta\phi^{H\Pi P}=\mathbf{0}\text{ on }F\cap d\overset{e}{S}\}$ representing the element space of electrically admissible potentials. The above set (3.3) can also be written in the finite element language (Zboiński, 2016, 2018).

The above set (3.3) corresponds to the general piezoelectricity case. The cases of direct or inverse piezoelectricity need neglecting the works of external forces $\overset{e}{l}$ or $\overset{e}{L}$, respectively. For the decoupled problems of elasticity and dielectricity, one needs to neglect coupling energies $\overset{e}{C}$ in both equations (3.3) so as to obtain two independent equations for these cases.

4. ERM local problems determination

It can be demonstrated that above coupled local problems (3.3) can be either Dirichlet ($\overset{e}{S}\cap W\neq\emptyset$ and $\overset{e}{S}\cap F\neq\emptyset$) or Neumann ($\overset{e}{S}\cap W=\emptyset$ and $\overset{e}{S}\cap F=\emptyset$ or mixed (Dirichlet--Neumann of two-types: $\overset{e}{S}\cap W=\emptyset$ and $\overset{e}{S}\cap F\neq\emptyset$ or $\overset{e}{S}\cap W\neq\emptyset$ and $\overset{e}{S}\cap F=\emptyset$). The Dirichlet local problems are well-posed (they are solvable by their definition).

In the case of the Neumann displacement boundary conditions, the local piezoelectric problems are solvable provided that the external and internal load compatibility condition is valid (Ainsworth and Oden, 1993c)

$$-\overset{e}{B}(\mathbf{u}^{hpq},\mathbf{1})+\overset{e}{C}(\phi^{hpq},\mathbf{1})+\overset{e}{L}(\mathbf{1})+\int\limits_{\overset{e}{S}\setminus S}\mathbf{1}^{\mathrm{T}}\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle\,d\overset{e}{S}=0 \tag{4.1}$$

where $\mathbf{1} = (1,1,1)^{\mathrm{T}}$. In the case of the Neumann electric potential boundary condition, we suggest that the external and equivalent charge compatibility condition holds, i.e.

$$\overset{e}{b}(\phi^{h\pi\rho},1)+\overset{e}{C}(\mathbf{u}^{hpq},1)-\overset{e}{l}(1)+\int\limits_{\overset{e}{S}\setminus S} 1\langle\overset{e}{h}(\phi^{h\pi\rho})\rangle\, d\overset{e}{S}=0 \tag{4.2}$$

5. Linear and higher-order equilibration

5.1. Equilibrated interelement stress reactions and equivalent charges

Here the linear-equilibration method of Ainsworth and Oden (1993a) and Ainsworth *et al.* (1994) for elliptic (elasticity) problems is utilized. We extend it to the coupled problems (piezoelectricity). In the method, the unknown vectors of the equilibrated interelement stress reactions $\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle$ are defined (Ainsworth and Oden, 1993b; Ainsworth *et al.*, 1994), with the displacements $\mathbf{u}^{hpq}$ from the global problem, i.e.

$$\langle\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})\rangle=\overset{fee}{\boldsymbol{\alpha}}\mathbf{r}(\mathbf{u}^{hpq})+\overset{eff}{\boldsymbol{\alpha}}\mathbf{r}(\mathbf{u}^{hpq}) \tag{5.1}$$

and

$$\overset{e}{\mathbf{r}}(\mathbf{u}^{hpq})=\mathbf{H}(\overset{e}{\boldsymbol{\nu}})\,\overset{e}{\boldsymbol{\sigma}}(\mathbf{u}^{hpq}) \qquad \overset{f}{\mathbf{r}}(\mathbf{u}^{hpq})=\mathbf{H}(\overset{e}{\boldsymbol{\nu}})\,\overset{f}{\boldsymbol{\sigma}}(\mathbf{u}^{hpq}) \tag{5.2}$$

with

$$\mathbf{H}(\overset{e}{\boldsymbol{\nu}})=\begin{bmatrix}\nu_1 & 0 & 0 & \nu_2 & 0 & \nu_3\\ 0 & \nu_2 & 0 & \nu_1 & \nu_3 & 0\\ 0 & 0 & \nu_3 & 0 & \nu_2 & \nu_1\end{bmatrix} \tag{5.3}$$

The vector $\overset{e}{\boldsymbol{\nu}}=[\nu_1,\nu_2,\nu_3]^{\mathrm{T}}$ denotes the normal unit vector, outward to S_e. The terms $\overset{e}{\boldsymbol{\sigma}}$ and $\overset{f}{\boldsymbol{\sigma}}$ represent six-component element stress vectors of the element e and its any neighbour f. The splitting functions are defined with their directional components, i.e. $\overset{fe}{\boldsymbol{\alpha}}=\operatorname{diag}[\alpha_1,\alpha_2,\alpha_3]$, with $\overset{fe}{\boldsymbol{\alpha}}=\mathbf{1}-\overset{ef}{\boldsymbol{\alpha}}$ and $\mathbf{1}=\operatorname{diag}[1,1,1]$. In the case of the first-order equilibration performed within the parametric elements, it is sufficient to define the splitting functions $\overset{fe}{\boldsymbol{\alpha}}$ as linear ones, with the use of the vertex nodes splitting factors $\overset{fe}{\boldsymbol{\alpha}}_k$, $k=1,2,\ldots,K$ of the applied parametrized prismatic ($K=6$) element

$$\overset{fe}{\boldsymbol{\alpha}}=\sum_k \overset{fe}{\boldsymbol{\alpha}}_k\,\lambda_k \tag{5.4}$$

where λ_k represents the vertex node shape functions of the element.

In the electric field, the unknown scalar equilibrated interelement equivalent charge $\langle\overset{e}{h}(u^{h\pi\rho})\rangle$ is proposed by us to be determined by the scalar electric potential $\phi^{h\pi\rho}$ taken from the global problem

$$\langle\overset{e}{h}(\phi^{h\pi\rho})\rangle=\overset{fee}{\beta}h(\phi^{h\pi\rho})+\overset{eff}{\beta}h(\phi^{h\pi\rho}) \tag{5.5}$$

Above

$$\overset{e}{h}(\phi^{h\pi\rho})=\overset{e}{\boldsymbol{\nu}}\mathbf{d}\,\overset{e}{(}\phi^{h\pi\rho}) \qquad \overset{f}{h}(\phi^{h\pi\rho})=\overset{e}{\boldsymbol{\nu}}\mathbf{d}\,\overset{f}{(}\phi^{h\pi\rho}) \tag{5.6}$$

The terms $\overset{e}{\mathbf{d}}$ and $\overset{f}{\mathbf{d}}$ are three-component electric displacement vectors of the element e and its any neighbour f. The quantity $\overset{fe}{\beta}$ is the scalar splitting function, while $\overset{fe}{\beta} = 1 - \overset{ef}{\beta}$. For the first-order equilibration, we suggest to define the splitting function $\overset{fe}{\beta}$ as a linear one, by means of the vertex nodes splitting factors $\overset{fe}{\beta}_k$, i.e.

$$\overset{fe}{\beta} = \sum_k \overset{fe}{\beta}_k \, \lambda_k \tag{5.7}$$

where $k = 1, 2, \ldots, K$ and $K = 6$ again.

5.2. Determination of the splitting factors

The procedure starts with the standard version of the first-order equilibration condition for elasticity (see Ainsworth and Oden, 1993a; Ainsworth *et al.*, 1994) extended by us to the case of piezoelectricity

$$\begin{aligned} &- \overset{e}{B}(\mathbf{u}^{hpq}, \boldsymbol{\lambda}_k) + \overset{e}{C}(\phi^{hpq}, \boldsymbol{\lambda}_k) + \overset{e}{L}(\boldsymbol{\lambda}_k) + \int\limits_{\overset{e}{S}\backslash S} \boldsymbol{\lambda}_k^{\mathrm{T}} \langle \overset{e}{\mathbf{r}}(\mathbf{u}^{hpq}) \rangle \, d\overset{e}{S} = 0 \\ &\overset{e}{b}(\phi^{h\pi\rho}, \lambda_k) + \overset{e}{C}(\mathbf{u}^{hpq}, \lambda_k) - \overset{e}{l}(\lambda_k) + \int\limits_{\overset{e}{S}\backslash S} \lambda_k \langle \overset{e}{h}(\phi^{h\pi\rho}) \rangle \, d\overset{e}{S} = 0 \end{aligned} \tag{5.8}$$

by taking into consideration the coupling form $\overset{e}{C}$ in mechanical condition $(5.8)_1$ and adding electrical condition $(5.8)_2$, where $\boldsymbol{\lambda}_k = \operatorname{diag}[\lambda_k, \lambda_k, \lambda_k]$ due to vectorial character of the displacement field. It is worth noticing that $\sum_{k=1}^{6} \lambda_k = 1$, i.e. the sums of the first and second equation (5.8) gives (4.1) and (4.2), and the load and/or charge compatibility conditions are fulfilled for the elements in the Neumann or mixed (Dirichlet-Neumann) local problems.

Taking advantage of (5.1) and (5.4), and (5.5) and (5.7) as well, substituted into (5.8), we get

$$\begin{aligned} 0 = &- \overset{e}{B}(\mathbf{u}^{hpq}, \boldsymbol{\lambda}_k) + \overset{e}{C}(\phi^{h\pi\rho}, \boldsymbol{\lambda}_k) + \overset{e}{L}(\boldsymbol{\lambda}_k) \\ &+ \sum_f \left[\overset{fe}{\boldsymbol{\alpha}}_k \int\limits_{\overset{ef}{S}} \boldsymbol{\lambda}_k \, \overset{e}{\mathbf{r}}(\mathbf{u}^{hpq}) \, d\overset{ef}{S} + \overset{ef}{\boldsymbol{\alpha}}_k \int\limits_{\overset{ef}{S}} \boldsymbol{\lambda}_k \, \overset{f}{\mathbf{r}}(\mathbf{u}^{hpq}) \, d\overset{ef}{S} \right] \\ 0 = &\ \overset{e}{b}(\phi^{h\pi\rho}, \lambda_k) + \overset{e}{C}(\mathbf{u}^{hpq}, \lambda_k) - \overset{e}{l}(\lambda_k) \\ &+ \sum_f \left[\overset{fe}{\beta}_k \int\limits_{\overset{ef}{S}} \lambda_k \, \overset{e}{h}(\phi^{h\pi\rho}) \, d\overset{ef}{S} + \overset{ef}{\beta}_k \int\limits_{\overset{ef}{S}} \lambda_k \, \overset{f}{h}(\phi^{h\pi\rho}) \, d\overset{ef}{S} \right] \end{aligned} \tag{5.9}$$

where $\overset{fe}{\boldsymbol{\alpha}}_k$ includes three directional stress splitting factors at node k of the element e, while $\overset{fe}{\beta}_k$ denotes scalar charge splitting factor for node k of the element e. Above, the integration over the internal part of element boundary $\overset{e}{S}\backslash S$ from (5.8) was replaced with the integrations over the common sides $\overset{ef}{S}$ of the element e and any of its neighbours f. It is worth noticing that three displacement and one potential equations (5.9) are independent. The procedure for calculation of the four splitting factors may be proposed to take advantage of the sets of equations (5.9) written for the element patches composed of elements surrounding any node of the domain V, at which the element vertex nodes meet (cf. Ainsworth and Oden, 1993b, Ainsworth *et al.*, 1994).

In the case of higher-order equilibration, relations (5.8) and (5.9) have to be modified by introduction of the shape functions $\lambda_{l,m}$ corresponding to any higher-order nodal dof (l,m) at the element edges and sides, where l stands for the edge or side number, and m defines the dof number at this edge or side, instead of the linear vertex node shape functions λ_k. The searched splitting factors $\overset{fe}{\boldsymbol{\alpha}}_{l,m}$ and $\overset{fe}{\beta}_{l,m}$ can be obtained from the sets of modified equations (5.8) and (5.9) written for the element patches composed of elements surrounding any edge or side node (l,m) of the domain V. The method is presented in (Zboiński, 2020) for the elasticity case. Its application to dielectricity is analogous.

6. Numerical experiments

In this Section, we will check the effectivity of ERM error estimation applied to coupled problems of piezoelectricity. We will show that such effectivity is different in the cases of direct, inverse and general piezoelectricity. These results will be compared to the analogous effectivity for the reference problems of uncoupled elasticty (elastostatics) and uncoupled dielectricity (electrostatics). In these tests, the global effectivity indices θ for the modeling, approximation and total errors of the model piezoelectric plate problem will be presented. Such indices are defined as a ratio of the estimated error, expressed by the ERM estimator η and the exact value of the potential energy error e:

$$\theta = \frac{\eta}{\mathrm{e}} \tag{6.1}$$

Three components e_M, e_C, e_E of the potential energy error e will be introduced by us, i.e. related to the mechanical, coupling and electric parts of this energy

$$\begin{aligned} &\Pi(\mathbf{u},\phi) - \Pi(\mathbf{u}^{hpq},\phi^{h\pi\rho}) \equiv \Pi(\mathbf{u}-\mathbf{u}^{hpq},\phi-\phi^{h\pi\rho}) = \frac{1}{2}B(\mathbf{u}-\mathbf{u}^{hpq},\mathbf{u}-\mathbf{u}^{hpq}) \\ &\quad - C(\mathbf{u}-\mathbf{u}^{hpq},\phi-\phi^{h\pi\rho}) - \frac{1}{2}b(\phi-\phi^{h\pi\rho},\phi-\phi^{h\pi\rho}) = \mathrm{e}_M - \mathrm{e}_C - \mathrm{e}_E = \mathrm{e} \end{aligned} \tag{6.2}$$

Above, the energy errors are defined as differences between potential energies. However, they and their components are proposed to be equivalently expressed by energies defined on differences $\mathbf{u}-\mathbf{u}^{hpq}$ and $\phi-\phi^{h\pi\rho}$ of the exact and numerical solutions. Derivation of the above equivalent formula required utilization of the potential energy definitions obtained from (2.1) and (2.3) by means of replacement of $\delta\mathbf{u}$ and $\delta\phi$ by $\mathbf{u}$ and ϕ and addition of coefficient 0.5 before the forms B and b. Then, elimination of the work of external forces L and charges l with use of stationarity conditions (2.2) was performed (with $\delta\mathbf{u}$ and $\delta\phi$ replaced by $\mathbf{u}$ and ϕ again). Finally, taking advantage of the mathematical properties of the quadratic forms B and b and mixed forms C was necessary.

For the thin- or thick-walled piezoelectric members considered in the paper, the hierarchical modelling is proposed by us (cf. Zboiński, 2010, 2016, 2018, 2019) where the mechanical, electric and electromechanical cases are considered. Such modelling implies division of the total energy error $\mathrm{e} \equiv \mathrm{e}^t$ into its modeling e^m and approximation e^a parts in accordance with the following relation describing the total, modeling and approximation errors of the solution displacements and electric potential

$$\begin{aligned} \mathbf{e}^t &= \mathbf{u} - \mathbf{u}^{hpq} = (\mathbf{u}-\mathbf{u}^q) + (\mathbf{u}^q - \mathbf{u}^{hpq}) = \mathbf{e}^m + \mathbf{e}^a \\ e^t &= \phi - \phi^{h\pi\rho} = (\phi-\phi^\rho) + (\phi^\rho - \phi^{h\pi\rho}) = e^m + e^a \end{aligned} \tag{6.3}$$

where $(\mathbf{u}^q,\phi^\rho)$ represents the exact solution to the hierarchical electromechanical (piezoelectric) model of the order (q,ρ) (Zboiński, 2016), with q and ρ denoting the mechanical and electric field transverse orders.

Substitution of (6.3) into (6.2) leads to nine global error components: e_M^t, e_M^m, e_M^a, e_C^t, e_C^m, e_C^a, e_E^t, e_E^m, e_E^a contributing to the energy error e. Also, the analogous division of the global error estimator η introduced in (3.1) is applied in the paper. Thus, nine resulting component effectivity indices can be defined. The analogous component quantities are defined for finite elements.

In the case of the total e^t and approximation e^a error calculations, the unknown values of the exact solutions $(\mathbf{u}, \phi)$ and $(\mathbf{u}^q, \phi^\rho)$ are replaced with their best numerical approximations $(\mathbf{u}^{ref}, \phi^{ref})$ and $(\mathbf{u}^{mod}, \phi^{mod})$, respectively, obtained from the *hpq*- and $h\pi\rho$-approximated version of (2.2). For the total η^t (or approximation η^a) error estimator, relations (6.2) and (6.3) hold, with $\mathbf{u}$ and ϕ (or $\mathbf{u}^q$ and ϕ^ρ) replaced by their proper ERM approximations $\mathbf{u}^{HPQ}$ and $\phi^{H\Pi P}$. Global values of the modeling error and estimator are obtained from $\mathrm{e}^m = \mathrm{e}^t - \mathrm{e}^a$ and $\eta^m = \eta^t - \eta^a$.

6.1. Model problem

The applied model problem concerns a uniformly loaded, hardly clamped, square piezoelectric (piezoceramic) plate. The plate is charged on its top surface, and grounded around its lateral sides. The length of the plate is equal to $l = 3.1415 \cdot 10^{-2}\,\mathrm{m}$. The plate thickness is $t = 0.15 \cdot 10^{-2}\,\mathrm{m}$. Young's modulus of the piezoelectric is $E = 0.5 \cdot 10^{11}\,\mathrm{N/m^2}$. Poisson's ratio equals 0.294. The dielectric permitivity (isotropic dielectric constant) under constant stress is $\delta = 0.1593 \cdot 10^{-7}\,\mathrm{F/m}$. The non-zero anisotropic piezoelectricity constants under constant stress are equal to: $c_{13} = c_{23} = -0.15 \cdot 10^{-9}\,\mathrm{C/N}$, $c_{33} = 0.3 \cdot 10^{-9}\,\mathrm{C/N}$, and $c_{52} = c_{61} = 0.5 \cdot 10^{-9}\,\mathrm{C/N}$. The way the measurable dielectric and piezoelectric constants under constant stress can be converted into the corresponding constants under constant strain, present in (2.1)-(2.3), can be found in (Preumont, 2006; Zboiński, 2020). The vertical pressure load is equal to $p = 4.0 \cdot 10^6\,\mathrm{N/m^2}$. The uniform charges applied to the top surface are equal to $c = 0.2 \cdot 10^{-1}\,\mathrm{C/m^2}$. Due to symmetry of the geometry, load, charge and boundary conditions, only a quarter of dimensions $l/2 \times l/2 \times t$ of the plate is analysed.

Due to space limitation, the applied electromechanical model is limited to one hierarchical model of orders $q = 2$ and $\rho = 2$. This is possible as the solution results for all models $q \geqslant 2$ and $\rho \geqslant 2$ is very close (qualitatively almost identical). Because of the same reason (qualitative similarity observed), only one examplary mesh $3 \times 3 \times 2$ of prismatic elements, is applied for three (direct, inverse and general) piezoelectricity cases and two uncoupled cases of elasticity and dielectrciity.

Our effectivity calculations are performed for changing values ($p = \pi = 2, 3, \ldots, p_{max} = \pi_{max}$, $p_{max} = \pi_{max} = 7$ or 8) of the longitudinal, displacement and electric potential, orders of approximation, as the error estimation is most sensitive to changes in these discretization parameters. The approximations $(\mathbf{u}^{ref}, \phi^{ref})$ and $(\mathbf{u}^{mod}, \phi^{mod})$ of the exact solutions are obtained from (3.1) with $m = 9$, $p = \pi = 9$ and $q = \rho = 6$ and $m = 9$, $p = \pi = 9$ and $q = \rho = 2$, respectively, where $m = l/2h$ and h is the characteristic length of the applied prismatic elements.

6.2. Results

In Table 1, the reference values of effectivity indices for two decoupled problems are presented. The ERM local problems results were obtained with initial tunning within the mechanical field due to thin-walled character of the plate domain. 18 vertex degrees of freedom within each element were constrained instead of constraining 6 such dofs and linear equilibration (cf. Zboiński, 2020). In the initial tuning, the longitudinal and transverse orders of approximation in ERM local problems were increased by 1 with respect to global problems for both the fields. For $p \geqslant 3$ or $\rho \geqslant 3$, all effectivities are close to the desired value of 1.0, i.e. the estimated errors are very close to the true errors.

Table 1. Global effectivities for elasticity (E) and dielectricity (D) cases – global problem parameters: (E) $q = 2$, $p = \text{var}$, $m = 3$, (D) $\rho = 2$, $\pi = \text{var}$, $m = 3$; local problems characterization: (E) 18 dofs constrained within the mechanical field, $H = h$, $P = p + 1$, $Q = q + 1$; (D) 1 dof constrained and linear equilibration within the electric field, $H = h$, $\Pi = \pi + 1$, $P = \rho + 1$

Problem type	Estimator component	Component part	Effectivity symbol and values for varying p or π orders								
				1	2	3	4	5	6	7	8
uncoupled elasticity case	mechanical	total	θ_M^t	0.52	1.70	1.17	0.96	0.99	1.00	1.01	1.00
		approx.	θ_M^a	0.52	1.68	1.21	0.92	0.98	1.05	1.15	1.45
		modeling	θ_M^m	0.59	1.90	1.07	0.99	1.00	0.99	0.99	0.98
uncoupled dielectricity case	electric	total	θ_E^t	1.49	2.74	1.07	1.05	0.95	0.92	0.90	0.91
		approx.	θ_E^a	1.49	2.78	1.11	1.15	1.09	1.10	1.04	1.19
		modeling	θ_E^m	1.17	0.85	0.86	0.86	0.87	0.88	0.89	0.90

Table 2. Global effectivities for general (G), direct (D) and inverse (I) piezoelectricity cases – global problem parameters (G, D, I): $q = \rho = 2$, $p = \pi = \text{var}$, $m = 3$; local problems characterization (G, D, I)): 18 dofs constrained within the mechanical field, 1 dof constrained and linear equilibration within the electric field, $H = h$, $P = p + 1$, $Q = q + 1$, $\Pi = \pi + 1$, $P = \rho + 1$

Problem type	Estimator component	Component part	Effectivity symbol and values for following p or π							
				1	2	3	4	5	6	7
general piezoelectricity case	mechanical	total	θ_M^t	0.68	2.01	1.26	0.99	1.00	1.01	1.02
		approx.	θ_M^a	0.68	2.01	1.50	0.94	0.89	0.96	1.17
		modeling	θ_M^m	0.74	1.96	1.05	1.01	1.02	1.01	1.02
	coupling	total	θ_C^t	1.44	1.76	**0.81**	**0.72**	**0.76**	**0.73**	**0.70**
		approx.	θ_C^a	1.44	1.75	**0.79**	**0.73**	**0.77**	**0.85**	**1.06**
		modeling	θ_C^m	0.28	1.38	**0.37**	**0.32**	**0.39**	**0.30**	**0.35**
	electric	total	θ_E^t	1.13	1.58	**0.84**	**0.78**	**0.78**	**0.71**	**0.62**
		approx.	θ_E^a	1.13	1.63	**0.85**	**0.81**	**0.84**	**0.90**	**1.09**
		modeling	θ_E^m	0.67	0.83	**0.48**	**0.45**	**0.44**	**0.42**	**0.43**
direct piezoelectricity case	mechanical	total	θ_M^t	0.59	1.89	1.24	0.97	1.00	1.01	1.02
		approx.	θ_M^a	0.59	1.89	1.44	0.84	0.86	0.95	1.18
		modeling	θ_M^m	0.63	1.90	1.05	1.01	1.02	1.01	1.02
	coupling	total	θ_C^t	0.01	0.66	**0.80**	**0.74**	**0.77**	**0.74**	**0.73**
		approx.	θ_C^a	0.04	0.64	**0.79**	**0.74**	**0.77**	**0.85**	**1.06**
		modeling	θ_C^m	0.36	1.32	**0.49**	**0.45**	**0.48**	**0.40**	**0.44**
	electric	total	θ_E^t	0.73	1.28	**0.83**	**0.74**	**0.74**	**0.68**	**0.58**
		approx.	θ_E^a	0.73	1.33	**0.83**	**0.77**	**0.82**	**0.89**	**1.09**
		modeling	θ_E^m	0.21	0.79	**0.29**	**0.27**	**0.28**	**0.24**	**0.26**
inverse piezoelectricity case	mechanical	total	θ_M^t	1.45	3.09	**2.15**	**2.25**	**1.85**	**1.57**	**1.16**
		approx.	θ_M^a	1.44	3.10	**2.26**	**2.54**	**2.43**	**2.72**	**2.92**
		modeling	θ_M^m	8.82	3.66	1.27	1.17	0.94	0.89	0.83
	coupling	total	θ_C^t	1.43	2.82	1.10	1.14	1.06	1.05	1.02
		approx.	θ_C^a	1.43	2.83	1.15	1.21	1.17	1.22	1.32
		modeling	θ_C^m	1.14	0.99	1.08	1.09	1.02	1.00	1.00
	electric	total	θ_E^t	1.57	2.62	1.16	1.18	1.05	0.98	0.94
		approx.	θ_E^a	1.58	2.68	1.17	1.30	1.27	1.36	1.35
		modeling	θ_E^m	1.58	1.07	1.01	0.94	0.93	0.92	0.92

In Table 2, the effectivity results are presented for three piezoelectric problems. The initial tunning of ERM was applied within the mechanical and electric fields as for the referrence elasticity and dielectricity problems, i.e. 18 mechanical vertex dofs were constrained and the ERM local approximation orders were higher by 1 in comparison to global problems. No other (additional) tuning was applied. In the case of general and direct piezoelectricity problems, considerable underestimation (effectivities lower than 1.0) of the modelling, approximation and total errors can be observed for the coupling and electric parts of the error. On the countrary, in the case of the inverse piezoelectricity, substantial overestimation (effectivities higher than 1.0) of the approximation and total errors can be seen for the mechanical part of the error. All unsatisfactory values are shown in bold in the table, for $p = \pi \geqslant 3$.

Table 3. Global effectivities for general (G), direct (D) and inverse (I) piezoelectricity cases – global problem parameters (G, D, I): $q = \rho = 2$, $p = \pi =$ var, $m = 3$; local problems characterization: (G) 18 dofs constrained within the mechanical field, 1 dof constrained and linear equilibration within the electric field, $H = h$, $P = p+1$, $Q = q+1$, $\Pi = \pi+2$, $P = \rho+2$, (D) 18 dofs constrained within the mechanical field, 1 dof constrained and linear equilibration within the electric field, $H = h$, $P = p+2$, $Q = q+2$, $\Pi = \pi+2$, $P = \rho+2$, (I) 18 dofs constrained and higher-order equilibration within the mechanical field, 1 dof constrained and linear equilibration within the electric field, $H = h$, $P = p+1$, $Q = q+1$, $\Pi = \pi+1$, $P = \rho+1$

Problem type	Estimator component	Component part	Effectivity symbol and values for the following p or π							
				1	2	3	4	5	6	7
general piezoelectricity case	mechanical	total	θ_M^t	0.66	2.03	1.24	0.97	0.98	0.99	1.00
		approx.	θ_M^a	0.66	2.02	1.49	0.93	0.89	0.90	1.17
		modeling	θ_M^m	1.13	2.22	1.02	0.97	1.00	1.00	1.00
	coupling	total	θ_C^t	1.18	1.92	**0.85**	0.83	**0.87**	**0.92**	**0.97**
		approx.	θ_C^a	1.14	1.80	**0.79**	**0.73**	**0.77**	**0.85**	**1.06**
		modeling	θ_C^m	1.89	5.38	**0.91**	**0.93**	**0.88**	**0.89**	**0.87**
	electric	total	θ_E^t	1.44	2.42	**1.01**	**0.93**	**0.92**	**0.96**	**0.99**
		approx.	θ_E^a	1.45	2.54	**0.99**	**0.88**	**0.89**	**0.94**	**1.12**
		modeling	θ_E^m	1.90	4.41	**0.98**	**0.90**	**0.88**	**0.92**	**0.94**
direct piezoelectricity case	mechanical	total	θ_M^t	0.73	2.28	1.34	1.01	1.03	1.03	1.04
		approx.	θ_M^a	0.71	2.28	1.55	0.96	1.00	1.10	1.35
		modeling	θ_M^m	1.40	2.28	1.14	1.02	1.03	1.02	1.03
	coupling	total	θ_C^t	0.35	1.03	**0.89**	**0.93**	**0.96**	**1.09**	**1.24**
		approx.	θ_C^a	0.35	1.07	**0.87**	**0.93**	**0.94**	**1.04**	**1.27**
		modeling	θ_C^m	1.53	1.68	**0.89**	**0.86**	**1.04**	**1.19**	**1.28**
	electric	total	θ_E^t	0.90	1.58	**1.00**	**0.93**	**0.96**	**1.06**	**1.17**
		approx.	θ_E^a	0.89	1.53	**0.99**	**0.93**	**0.96**	**1.04**	**1.26**
		modeling	θ_E^m	1.82	2.74	**0.93**	**0.86**	**0.96**	**1.09**	**1.16**
inverse piezoelectricity case	mechanical	total	θ_M^t	1.44	2.74	**1.48**	**1.22**	**1.20**	**0.97**	**0.91**
		approx.	θ_M^a	1.44	2.74	**1.54**	**1.30**	**1.45**	**1.27**	**1.63**
		modeling	θ_M^m	8.71	3.14	0.92	0.90	0.85	0.82	0.81
	coupling	total	θ_C^t	1.43	2.86	1.05	1.09	1.01	1.01	1.00
		approx.	θ_C^a	1.43	2.87	1.12	1.20	1.12	1.17	1.20
		modeling	θ_C^m	0.47	1.07	1.09	1.12	1.02	1.01	1.00
	electric	total	θ_E^t	1.57	2.57	1.16	1.18	1.06	0.98	0.94
		approx.	θ_E^a	1.58	2.63	1.17	1.27	1.26	1.32	1.35
		modeling	θ_E^m	1.67	1.20	1.07	0.99	0.94	0.92	0.92

So as to remove the mentioned under- or overestimation, an additional tuning of ERM was performed. The corresponding results are given in Table 3. In the case of the general piezoelectric problem, the additional tuning consisted in increasing the local approximation orders of the electric field by 2 with respect to their global counterparts. For the direct piezoelectricity, such increasing was performed within both mechanical and electric fields. In the inverse piezoelectricity case, higher-order equilibration was applied to the mechanical field. The corrected (previously unsatisfactory in Table 2) values of effectivity indices are marked in bold. They are closer to the desired value of 1.0 than in the cases without additional tuning.

The improvement of the effectivities for piezoelectricity cases of $p = \pi = 1, 2$ needs an individual approach as in the case of uncoupled elasticity (cf. Zboiński, 2020). For the general and direct piezoelectricity with $p = \pi = 1$ or $p = \pi = 2$, the additional tuning should be performed or skipped, repectively. In the case of the inverse piezoelectricity, for $p = \pi = 1, 2$, the local orders of approximation P and Q of the mechanical field should be increased by 3 or 4 with respect to the global values of p and q (cf. Zboiński, 2013).

Control of the tuning method for the piezoelectricity cases can be easily implemented into adaptive finite element analysis of complex electro-mechanical domains in the block-wise manner, by introduction of the control parameter for each geometrical or functional block of the analysed domain, analogusly to the case of complex mechanical systems (cf. Zboiński, 2010).

7. Conclusions

It was shown how to adapt the equilibrated residual method (ERM) of a posteriori error estimation, invented for elliptic problems, i.e. elasticity and dielectricity, to coupled problems including piezoelectricity ones.

Effective application of ERM to piezoelectric problems needs tuning of the error estimator. Different tuning procedures are necessary for general, direct and inverse piezoelectricity. Three such procedures were proposed, and their effectiveness was numerically demonstrated.

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