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Maxim Frolov

Reliable Control Over Approximation Errors by Functional Type a Posteriori Estimates

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ABSTRACT

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This thesis is focused on the development and numerical justification of a modern computational methodology that provides guaranteed upper bounds of the energy error norms. The methodology considered is based on the so-called *functional* type a posteriori error estimates, which have been recently suggested for problems that can be represented as problems of minimization of convex functionals. For boundary-value problems arising in the theory of plates, several new a posteriori error estimates (Duality Error Majorants) are derived on purely functional grounds either by the methods of duality theory in the calculus of variations or by modifying respective integral identities. This important feature makes it possible to take into account not only "pure" approximation errors, but also all other errors contained in the approximate solution (including also the errors caused by possible defects of a computer code).

Numerical tests are performed for elliptic type boundary-value problems of the second and fourth order. In particular, the method is compared with some other (classical) error indicators and estimators, which are based on gradient recovery or an explicit estimation of residuals. It is shown that functional type a posteriori error estimates provide accurate and reliable upper bounds of the energy norm of the actual error and, also, indicate elements with relatively large local errors.

Keywords: Reliable modelling, functional type a posteriori error estimates, efficient adaptive algorithms.

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Jyväskylä, 15 November, 2004
Maxim Frolov

LIST OF INCLUDED ARTICLES

[A]. Repin, S. and Frolov, M. *A posteriori error estimates for approximate solutions to elliptic boundary value problems*, Computational Mathematics and Mathematical Physics, 42(12), 2002, 1704–1716.

[B]. Frolov, M., Neittaanmäki, P., and Repin, S. *On the reliability, effectivity and robustness of a posteriori error estimation methods*, Numerical Methods for Scientific Computing. Variational problems and applications, CIMNE, Barcelona, 2003, 153–175.

[C]. Frolov, M., Neittaanmäki, P., and Repin, S. *On computational properties of a posteriori error estimates based upon the method of duality error majorants*, Numerical Mathematics and Advanced Applications (ENUMATH, 2003), Springer-Verlag, Berlin, Heidelberg, 2004, 346–357.

[D]. Frolov, M., Neittaanmäki, P., and Repin, S. *On practical implementation of duality error majorants for boundary-value problems arising in the theory of plates*, Proc. of the European Congress on Computational Methods in Applied Sciences and Engineering, Jyväskylä, Finland, 2004.

[E]. Frolov, M. *On efficiency of the dual majorant method for the quality estimation of approximate solutions of fourth-order elliptic boundary value problems*, Russian J. Numer. Anal. Math. Modelling, 19(5), 2004, 407–418.

CONTENTS

1 INTRODUCTION

Reliable control over approximation errors is one of the key questions in modern numerical analysis. This thesis is focused on the development of computational methodology able to present guaranteed upper bounds of the energy error norms and on the verification of its efficiency. The methodology considered is based on a posteriori error estimates of a new type, which have been recently suggested for problems that can be represented as problems of minimization of convex functionals. The method is compared with some other (classical) error indicators and estimators, which are based on gradient recovery or an explicit estimation of residuals. Numerical tests are performed for elliptic type boundary-value problems of the second and fourth order.

It was shown that the method provides accurate and guaranteed upper bounds of the energy norm of the actual error and, also, indicates elements with relatively large local errors, which makes it possible to create adaptively refined meshes in a highly efficient way.

For several decades the attention of a number of authors has been focused on questions of reliability and efficiency of calculations in computational engineering. Nowadays, it has become a matter of common knowledge that accurate approximation of real life problems arising in various applications can be obtained only on the basis of algorithms combining efficient numerical methods (finite element method, finite difference method, mixed and boundary element methods) with mesh-refinement. Such procedures require reliable error control, which is based on the analysis of solutions computed. On the one hand, it is necessary to have guaranteed upper bounds of the errors computed in a suitable norm. On the other hand, it is very desirable to have also a qualitative indication of their local behavior. These efforts are aimed at decreasing computational costs, while ensuring an accurate and reliable modelling of physical phenomena.

Nowadays, in the context of finite element methods several approaches to error control are widely used. The first of them was stated at the end of 70s in the papers of I. Babuška and W.C. Rheinboldt (see [6, 7]). Further investigations on this subject were pursued by a number of authors and the amount of relevant literature is very large. The most complete description of the methods and related literature are given, for instance, in the monographs of R. Verfürth [49], M. Ainsworth and J.T. Oden [2], I. Babuška and T. Strouboulis [9].

Residual type a posteriori error estimates form a well-known approach to estimation of errors arising in finite element approximations. This approach has been proposed in the papers of I. Babuška and W.C. Rheinboldt [6, 7, 8]. Further investigations of this approach were made by many authors (see, e.g., I. Babuška and A. Miller [5], R.E. Bank and A. Weiser [11], R. Durán and R. Rodríguez [25], R. Rodríguez [44], K. Eriksson and C. Johnson [27], C. Johnson and P. Hansbo [28], R. Verfürth [47, 48], J.R. Stewart and T. J.R. Hughes [45], C. Carstensen and R. Verfürth [19], C. Carstensen [17], and many other authors).

The first residual-based technique is presented by the so-called explicit residual methods, which are based on a special construction of an interpolation operator (see Ph. Clément [21], C. Bernardi and V. Girault [13], and C. Carstensen and R. Verfürth [19]). It maps the functions from the energy space of a problem to a respective subspace formed by finite element approximations. In this case, a posteriori error estimates usually include a great quantity of mesh-dependent constants. Therefore, it is necessary either to find their exact values or to have a numerical procedure able to estimate them accurately. However, attempts at providing upper estimates for these constants may lead to a significant overestimation of the error (see, for example, C. Carstensen and S.A. Funken [18]). The second group of residual-based estimators is related to solution of a set of local problems of the Dirichlet (see I. Babuška and W.C. Rheinboldt [7]) or Neumann type (see R.E. Bank and A. Weiser [11], R. Durán and R. Rodríguez [25], R. E. Bank and B.D. Welfert [12], and R. Verfürth [47]). Right-hand sides of these problems are formed by respective element residuals and by approximations of interelement fluxes of the true solution. It is known that a proper setting (equilibration) of the normal fluxes leads to a significant improvement of the quality of error estimates. For various numerical tests, see U. Brink and E. Stein [16], P. Díez, N. Parés, and A. Huerta [22], I. Babuška, T. Strouboulis, C.S. Upadhyay, S.K. Gangaraj, and K. Copps [10].

A further approach, which is based on different grounds has been an outgrowth of the so-called *superconvergence phenomenon* (see, e.g., L.A. Oganesyan and L.A. Rukhovets [35], M. Křížek and P. Neittaanmäki [29, 30], L.B. Wahlbin [50], M.F. Wheeler and J.R. Whiteman [51], M. Zlámal [55, 56]) and various *gradient averaging techniques*. Among the earliest works devoted to this type of error estimation methods we refer to O.C. Zienkiewicz and J.Z. Zhu [53], E. Rank and O.C. Zienkiewicz [37]. Nowadays this approach is widely used. Various procedures of a gradient recovery are described, for example, in M. Ainsworth and J.T. Oden [2], M. Ainsworth and A. Craig [1], R. Durán, M.A. Muschietti, and R. Rodríguez [23, 24], and O.C. Zienkiewicz and J.Z. Zhu [54].

However, a rigorous mathematical justification of the approach was obtained under the assumption of higher regularity of weak solutions, which (especially in nonlinear problems) may not hold. Nevertheless, there are known examples demonstrating that such simple averaging procedures can give realistic results for a wider class of problems (see O.C. Zienkiewicz and J.Z. Zhu [52, 53, 54], I. Babuška, T. Strouboulis, C.S. Upadhyay, S.K. Gangaraj, and K. Copps [10]).

It should be emphasized that both residual-based and postprocessing-based error estimation techniques rest crucially on the assumption that an approximate solution is the Galerkin approximation in a respective finite element subspace.

The first a posteriori error estimates of the functional type were proposed by W. Prager and J.L. Synge [36], J.L. Synge [46], and S.G. Mikhlin [32]. Estimates of this type are valid not only for Galerkin approximations but for any conforming approximate solution of a boundary-value problem. The first approach was called the hypercircle method. It has its origin in geometric analogies. At the same time, in the book of S.G. Mikhlin, the derivation of the error estimate is justified by the calculus of variations. However, in the case of the Poisson equation with a Dirichlet type boundary condition both methods give an estimate of the same form. It includes a free additional variable. A proper selection of its value provides guaranteed upper bounds of the energy norm of the actual error. Unfortunately, estimates of this type are difficult for practical implementation, because the abovementioned free variable must satisfy exactly a very essential restriction.

A posteriori error estimates of different type have been proposed by S.I. Repin in [38, 39, 40, 41] and in a number of other papers. Most of the references are given in the book of P. Neittaanmäki and S. Repin [34]. The estimates have been derived on purely functional grounds either by the methods of duality theory in the calculus of variations or by modifying respective integral identities. They are valid for conforming approximations of all types and contain only global constants, which come from the embedding theorems for respective functional spaces. For these reasons, it is natural to call them *functional type a posteriori error estimates.*

By this method, guaranteed error estimates are also obtained for any approximations regardless of whether or not they satisfy the Galerkin orthogonality condition. The upper bound of the error is given by a new functional, which, in addition to an approximate solution and external data, also involves a new free variable. The difference between the exact solution and its approximation is estimated by analyzing the primal problem together with its dual counterpart. A posteriori error estimates of such a type are valid for all deviations from the exact solutions lying in an admissible class of functions. This important feature makes it possible to take into account not only "pure" approximation errors (arising due to the inconvenience between the approximation subspace and the respective functional space), but also all other errors contained in the approximate solution (including the errors caused by possible defects of a computer code). Thus, the majorant gives an "independent checker" for verification of the actual accuracy of a computed solution. It is clear that such a "checker" can be regarded as an efficient numerical tool if it is (a) reliable, (b) exact, and (c) robust. Reliability means that the estimate always gives a guaranteed upper bound of the error, and exactness means that it is possible to make this computed upper bound close to the true value of the error. By "robustness" we mean that the estimate adequately accounts errors of various types. In this thesis, we aim at showing that the method of duality error majorants possesses the properties (a), (b), and (c).

2 OUTLINE OF THE THESIS

The thesis includes papers A-D, which have been already published. These papers are devoted to a numerical justification of the method of duality error majorants by various tests. In addition, we present theoretical results based on the summary of two articles (paper E and paper of S. Repin and M. Frolov [42]) with some extensions. Let us begin with these papers. In subsections below we present the material in the sequence, which differs from the chronological one but better reflects logic of the whole research and gives its principal summary.

2.1 New duality error majorants for conforming approximate solutions of the biharmonic problem

In this subsection, a variational formulation of the biharmonic problem is considered. We call it the *primal* problem. With the example of this primal problem, we describe some general features of all estimates obtained by the method of duality error majorants for various elliptic boundary-value problems of divergent type.

The variational formulation of the biharmonic problem is as follows.
Problem $\mathcal{P}$. Find an element $u \in V_0$ such that

$$J(u) = \inf \mathcal{P} = \inf_{w \in V_0} J(w),$$

where

$$J(w) = \int\limits_{\Omega} \left(\frac{1}{2} (\Delta w)^2 - f w \right) dx$$

and

$$V_0 = \overset{\circ}{\mathbf{W}}{}^2_2(\Omega).$$

We assume that Ω is a bounded connected domain with a Lipschitz continuous boundary $\partial\Omega$ and $f \in \mathbf{L}_2(\Omega)$. These are quite standard assumptions that guarantee the existence and uniqueness of a solution. With an approximation $v \in V_0$ obtained, we come up against the problem of controlling the accuracy for this approximate solution. It is necessary to find guaranteed upper bounds of the energy norm of the error $e = v - u$. One of the modern approaches to reliable error control is based on duality theory in the calculus of variations.

Using the scheme proposed by P. Neittaanmäki and S. Repin in [33], we show how one can apply this method to the case considered. We represent the difference between the values of the functional J at elements v and u in the form

$$J(v) - \inf \mathcal{P} = \int\limits_\Omega \left(\frac{1}{2}(\Delta v)^2 - fv \right) dx - \int\limits_\Omega \left(\frac{1}{2}(\Delta u)^2 - fu \right) dx$$
$$= \int\limits_\Omega \frac{1}{2}(\Delta v - \Delta u)^2 \, dx + \int\limits_\Omega \left(\Delta u(\Delta v - \Delta u) - f(v-u)\right) dx$$
$$= \frac{1}{2}|\!|\!| e |\!|\!|^2 + \int\limits_\Omega (\Delta u \Delta e - fe) \, dx,$$

where

$$|\!|\!| e |\!|\!|^2 = \int\limits_\Omega (\Delta e)^2 \, dx.$$

It is well known that the weak solution u satisfies the relation

$$\int\limits_\Omega \Delta u \Delta w \, dx = \int\limits_\Omega fw \, dx, \quad \forall w \in V_0. \tag{2.1}$$

From (2.1) it follows that

$$\frac{1}{2}|\!|\!| e |\!|\!|^2 = J(v) - \inf \mathcal{P}. \tag{2.2}$$

Therefore, knowledge of the exact lower bound of the primal problem provides exact error estimates for any conforming approximate solution v. Unfortunately, this bound is generally unknown. But we can obtain the desired estimate, taking into account the so-called *dual* variational Problem $\mathcal{P}^*$. It can be obtained from the reformulation

$$J(u) = \inf_{w \in V_0} \left\{ \sup_{n^* \in \mathbf{L}_2(\Omega)} L(w, n^*) \right\},$$

of the primal problem in terms of the Lagrangian L, where

$$L(w, n^*) = \int\limits_\Omega \left(n^* \, \Delta w - \frac{1}{2}(n^*)^2 - fw \right) dx,$$

and has the following form.

Problem $\mathcal{P}^*$. Find an element $m^* \in N_f^*$ such that

$$I^*(m^*) = \sup \mathcal{P}^* = \sup_{n^* \in N_f^*} I^*(n^*),$$

where

$$I^*(n^*) = -\int_\Omega \frac{1}{2}(n^*)^2\, dx$$

and

$$N_f^* = \left\{ n^* \in \mathbf{L}_2(\Omega) \mid \int_\Omega n^* \Delta w\, dx = \int_\Omega f w\, dx, \quad \forall w \in V_0 \right\}.$$

It is known that the exact lower bound of the primal problem coincides with the exact upper bound of the dual one, namely,

$$\inf \mathcal{P} = \sup \mathcal{P}^*.$$

To prove this statement, we consider the difference

$$J(w) - I^*(n^*) = \int_\Omega \left(\frac{1}{2}(\Delta w)^2 - fw + \frac{1}{2}(n^*)^2 \right) dx =$$
$$= \int_\Omega \left(\frac{1}{2}(\Delta w - n^*)^2 + (n^* \Delta w - fw) \right) dx = \int_\Omega \frac{1}{2}(\Delta w - n^*)^2\, dx \geq 0.$$

The last-mentioned inequality holds for any $w \in V_0$ and $n^* \in N_f^*$, therefore, $\inf \mathcal{P} \geq \sup \mathcal{P}^*$.

On the other hand, from (2.1) it follows that Δu is an element of the set N_f^*. Thus,

$$\sup \mathcal{P}^* \geq I^*(\Delta u) = -\int_\Omega \frac{1}{2}(\Delta u)^2\, dx$$
$$= \int_\Omega \left(\frac{1}{2}(\Delta u)^2 - \Delta u \Delta u \right) dx = \int_\Omega \left(\frac{1}{2}(\Delta u)^2 - fu \right) dx = \inf \mathcal{P},$$

and we obtain the desired result.

Substituting the relation between the primal and the dual problems in (2.2), we arrive at the estimate

$$\frac{1}{2} \| e \|^2 \leq J(v) - I^*(n^*), \quad \forall n^* \in N_f^*.$$

The right-hand side of this estimate can be rearranged as follows:

$$\int_\Omega \left(\frac{1}{2}(\Delta v)^2 - fv + \frac{1}{2}(n^*)^2 \right) dx = \int_\Omega \frac{1}{2}(\Delta v - n^*)^2\, dx,$$

and we obtain the a posteriori error estimate

$$|\!|\!| e |\!|\!|^2 \leq \|\Delta v - n^*\|_\Omega^2, \tag{2.3}$$

which is valid for any element $n^* \in N_f^*$.

Unfortunately, the estimate (2.3) is mainly of theoretical significance. The problem of obtaining approximations n^* from the admissible set N_f^* for an arbitrary right-hand side f is rather hard, and this approach is not efficient in practice.

Let us transform the right-hand side of the estimate (2.3) substituting a free element $\varkappa^* \in \mathbf{L}_2(\Omega)$:

$$\|\Delta v - n^*\|_\Omega^2 \leq (\|\Delta v - \varkappa^*\|_\Omega + \|\varkappa^* - n^*\|_\Omega)^2.$$

Applying the well-known inequality

$$2 \mid ab \mid \leq \beta a^2 + \beta^{-1} b^2,$$

we have

$$|\!|\!| e |\!|\!|^2 \leq (1+\beta) D(v, \varkappa^*) + (1+\beta^{-1}) R(\varkappa^*), \quad \forall \beta > 0,$$

where

$$D(v, \varkappa^*) = \|\Delta v - \varkappa^*\|_\Omega^2,$$

$$R(\varkappa^*) = \inf_{n^* \in N_f^*} \|\varkappa^* - n^*\|_\Omega^2.$$

Now, it is necessary to obtain a computable upper estimate of the value of the functional R. By substituting $\sigma^* = \varkappa^* - n^*$, we arrive at the problem

$$R(\varkappa^*) = \inf_{n^* \in N_f^*} \|\varkappa^* - n^*\|_\Omega^2 = -2 \sup_{\sigma^* \in N_r^*} \left\{ - \int_\Omega \frac{1}{2} (\sigma^*)^2 \, dx \right\},$$

where

$$N_r^* = \left\{ \sigma^* \in \mathbf{L}_2(\Omega) \mid \int_\Omega \sigma^* \Delta w \, dx = \int_\Omega (\varkappa^* \Delta w - f w) \, dx, \quad \forall w \in V_0 \right\}.$$

It is easy to note that the problem

$$\sup \tilde{\mathcal{P}}^* = \sup_{\sigma^* \in N_r^*} \left\{ - \int_\Omega \frac{1}{2} (\sigma^*)^2 \, dx \right\}$$

is dual to Problem $\tilde{\mathcal{P}}$, which is of the same structure as Problem $\mathcal{P}$ with another right-hand side:

$$\inf \tilde{\mathcal{P}} = \inf_{w \in V_0} \int_\Omega \left(\frac{1}{2} (\Delta w)^2 - (\varkappa^* \Delta w - f w) \right) dx.$$

For the pair of problems $\tilde{\mathcal{P}}$ and $\tilde{\mathcal{P}}^*$, we have the same relation as in the above-mentioned case, namely,

$$\sup \tilde{\mathcal{P}}^* = \inf \tilde{\mathcal{P}}.$$

Therefore,

$$R(\varkappa^*) = - \inf_{w \in V_0} \int_\Omega \big((\Delta w)^2 - 2(\varkappa^* \Delta w - f w) \big) \, dx. \tag{2.4}$$

With the help of this relation, two different estimates of the term $R(\varkappa^*)$ can be found. Using these estimates, we arrive at various forms of duality error majorants for the biharmonic problem. The first of them is obtained and investigated in paper E, as is shown below.

Estimate 1. In addition, we assume that the variable $\varkappa^*$ belongs to the set

$$N^*_\Delta = \{ \varkappa^* \in \mathbf{L}_2(\Omega) \mid \Delta \varkappa^* \in \mathbf{L}_2(\Omega) \} .$$

Therefore, the identity

$$\int_\Omega \varkappa^* \Delta w \, dx = \int_\Omega \Delta \varkappa^* w \, dx, \quad \forall w \in V_0, \quad \forall \varkappa^* \in N^*_\Delta,$$

yields the following transformation of (2.4):

$$- \inf_{w \in V_0} \int_\Omega \big((\Delta w)^2 - 2(\Delta \varkappa^* - f) w \big) \, dx \leq$$
$$\leq - \inf_{w \in V_0} \big(\|\Delta w\|^2_\Omega - 2 \mathbb{C}_{2\Omega} \|\Delta \varkappa^* - f\|_\Omega \|\Delta w\|_\Omega \big),$$

where $\mathbb{C}_{2\Omega}$ is a constant from the inequality

$$\|w\|_\Omega \leq \mathbb{C}_{2\Omega} \|\Delta w\|_\Omega, \quad \forall w \in V_0,$$

which is related to the minimum eigenvalue of the biharmonic operator. The quantity $\|\Delta w\|_\Omega$ is nonnegative, whence,

$$R(\varkappa^*) \leq - \inf_{a \geq 0} \big(a^2 - 2 \mathbb{C}_{2\Omega} \|\Delta \varkappa^* - f\|_\Omega a \big) = \mathbb{C}^2_{2\Omega} \|\Delta \varkappa^* - f\|^2_\Omega,$$

and we arrive at the estimate

$$R(\varkappa^*) \leq \mathbb{C}^2_{2\Omega} \|\Delta \varkappa^* - f\|^2_\Omega.$$

Combining the above results, we obtain an a posteriori error estimate of the first type given by the method of duality majorants

$$|\!|\!| e |\!|\!|^2 \leq \mathcal{M}(v, \beta, \varkappa^*), \tag{2.5}$$

where

$$\mathcal{M}(v,\beta,\varkappa^*) = (1+\beta)\|\Delta v - \varkappa^*\|^2_\Omega + (1+\beta^{-1})\mathbb{C}^2_{2\Omega}\|\Delta\varkappa^* - f\|^2_\Omega. \qquad (2.6)$$

The functional $\mathcal{M}$ on the right-hand side is well defined for any $\beta > 0$ and $\varkappa^* \in N^*_\Delta$. For $\beta = 0$, it can be defined as follows:

$$\begin{cases} \mathcal{M}(v,0,\varkappa^*) = +\infty & \text{for } \varkappa^* \notin N^*_f, \\ \mathcal{M}(v,0,\varkappa^*) = \|\Delta v - \varkappa^*\|^2_\Omega & \text{for } \varkappa^* \in N^*_f. \end{cases}$$

The above estimate has a certain drawback: for the calculation of bounds of the actual error we cannot use the simplest approximations of the dual variable $\varkappa^*$, because they do not ensure the necessary condition $\Delta\varkappa^* \in \mathbf{L}_2(\Omega)$.

Estimate 2. In order to make the restriction on the dual variable $\varkappa^*$ weaker, we assume that this element belongs to the set N^*_∇, where

$$N^*_\nabla = \left\{\varkappa^* \in \mathbf{L}_2(\Omega) \mid \nabla\varkappa^* \in \mathbf{L}_2(\Omega,\mathbb{R}^2)\right\},$$

and introduce the second dual variable $y^* \in Q^*_{\mathrm{div}}$, where

$$Q^*_{\mathrm{div}} = \left\{y^* \in \mathbf{L}_2(\Omega,\mathbb{R}^2) \mid \mathrm{div} y^* \in \mathbf{L}_2(\Omega)\right\}.$$

Then,

$$\int\limits_\Omega \big((\Delta w)^2 - 2(\varkappa^*\Delta w - fw)\big)\,dx = \int\limits_\Omega \big((\Delta w)^2 - 2(y^*\cdot\nabla w - \nabla\varkappa^*\cdot\nabla w + \mathrm{div} y^* w - fw)\big)\,dx.$$

In this case, similarly to the derivation of the above estimate, we can continue the relation (2.4) by an upper estimate of the form

$$\begin{aligned} -\inf_{w\in V_0}\int\limits_\Omega &\big((\Delta w)^2 - 2(\varkappa^*\Delta w - fw)\big)\,dx \\ &\le -\inf_{w\in V_0}\big(\|\Delta w\|^2_\Omega - 2(\|\nabla\varkappa^* - y^*\|_\Omega + \mathbb{C}_{1\Omega}\|\mathrm{div} y^* - f\|_\Omega)\|\nabla w\|_\Omega\big) \\ &\le -\inf_{w\in V_0}\big(\|\Delta w\|^2_\Omega - 2\mathbb{C}_{1\Omega}(\|\nabla\varkappa^* - y^*\|_\Omega + \mathbb{C}_{1\Omega}\|\mathrm{div} y^* - f\|_\Omega)\|\Delta w\|_\Omega\big), \end{aligned}$$

where $\mathbb{C}_{1\Omega}$ is a constant in the Friedrichs inequality

$$\|w\|_\Omega \le \mathbb{C}_{1\Omega}\|\nabla w\|_\Omega, \quad \forall w \in \mathring{\mathbf{W}}^1_2(\Omega).$$

Thus, we obtain another estimate of the term $R(\varkappa^*)$:

$$R(\varkappa^*) \le \mathbb{C}^2_{1\Omega}(\|\nabla\varkappa^* - y^*\|_\Omega + \mathbb{C}_{1\Omega}\|\mathrm{div} y^* - f\|_\Omega)^2.$$

In practice, it is more convenient to represent the last-mentioned estimate with a free positive parameter that arises in the same manner as does the parameter β. The final estimate has the form

$$|\!|\!|e|\!|\!|^2 \leq \mathcal{M}(v, \beta_1, \beta_2, \varkappa^*, y^*), \tag{2.7}$$

where

$$\begin{aligned}\mathcal{M}(v, \beta_1, \beta_2, \varkappa^*, y^*) &= (1+\beta_1)\|\Delta v - \varkappa^*\|_\Omega^2 \\ &+ (1+\beta_1^{-1})\mathbb{C}_{1\Omega}^2 \left((1+\beta_2)\|\nabla\varkappa^* - y^*\|_\Omega^2 + (1+\beta_2^{-1})\mathbb{C}_{1\Omega}^2\|\mathrm{div} y^* - f\|_\Omega^2\right).\end{aligned} \tag{2.8}$$

In this estimate, the original parameter β is denoted by β_1.

Note that in paper [33] of P. Neittaanmäki and S. Repin, more general estimates of such a type have been derived. However, these estimates are more complicated in structure and include a symmetric second-order tensor as the dual variable $\varkappa^*$.

2.2 Efficiency of functional type a posteriori error estimates

Below, we consider computational properties of the majorant (2.6). As is known (see, for example, I. Ekeland and R. Temam [26]), the exact solution of the dual problem m^* satisfies the relations

$$m^* = \Delta u \quad \text{and} \quad \Delta m^* = f \quad \text{a.e. in } \Omega.$$

Therefore, the optimal value of the majorant, which occurs at a pair $(0, m^*)$, coincides with the square of the energy norm of the actual error:

$$\mathcal{M}(v, 0, m^*) \;=\; \|\Delta v - m^*\|_\Omega^2 \;=\; |\!|\!|e|\!|\!|^2.$$

Any pair $(\beta, \varkappa^*)$ from respective admissible sets provides a guaranteed upper bound of this quantity. Therefore, with an algorithm that is able to produce an element $\varkappa^*$, which is close enough to m^*, we can provide efficient error bounds with any prescribed accuracy. Following this argument, we arrive at the problem of minimization of the functional $\mathcal{M}(v, \beta, \varkappa^*)$ by $(\beta, \varkappa^*)$ for a given approximate solution v. It is natural to solve this problem by approximating the dual variable $\varkappa^*$ on the basis of a certain finite-dimensional subspace of N_Δ^*.

Let us consider a sequence of subspaces $\{N_k^*\}_{k=1}^\infty \subset N_\Delta^*$ and define a sequence of the corresponding pairs $(\beta_k, \varkappa_k^*)$ in the following way:

- Step 1: fix a value of the parameter β as a small positive δ.
- Step 2: find an element $\varkappa_k^*$ that minimizes the functional $\mathcal{M}$ over N_k^*:

$$\mathcal{M}(v, \delta, \varkappa_k^*) = \inf_{\varkappa^* \in N_k^*} \mathcal{M}(v, \delta, \varkappa^*).$$

– Step 3: calculate the optimal value β_k of the parameter for a given $\varkappa_k^*$:

$$\mathcal{M}(v, \beta_k, \varkappa_k^*) = \inf_{\beta \geq 0} \mathcal{M}(v, \beta, \varkappa_k^*).$$

Note that the optimal value β_k can be computed easily and practically does not equal to zero. It satisfies the relation

$$\beta_k = \mathbb{C}_{2\Omega} \frac{\|\Delta \varkappa_k^* - f\|_\Omega}{\|\Delta v - \varkappa_k^*\|_\Omega}.$$

Because a solution v has second derivatives that are piecewise continuous, but an approximation $\varkappa^*$ is continuous, the denominator of this ratio does not equal to zero. The majorant (2.6) with the optimal value of the parameter β is equivalently represented in the form

$$\mathcal{M}(v, \beta_k, \varkappa_k^*) = \left(\|\Delta v - \varkappa_k^*\|_\Omega \ + \ \mathbb{C}_{2\Omega}\|\Delta \varkappa_k^* - f\|_\Omega\right)^2. \tag{2.9}$$

Finally, we define a sequence

$$\mathcal{M}_k(v) = \mathcal{M}(v, \beta_k, \varkappa_k^*).$$

Proposition 1. If a sequence of subspaces $\{N_k^*\}_{k=1}^\infty$ possesses the limit density property in N_Δ^*, then for any positive δ we can find a number k_δ such that for $k > k_\delta$ the following two-sided estimate is valid:

$$0 \leq \mathcal{M}_k(v) - \|\!|e|\!\|^2 \leq \ \delta C(e, \delta, \mathbb{C}_{2\Omega}).$$

Proof.

By the definition of the limit density, for any $\delta > 0$ there exists a number k_δ such that for $k > k_\delta$ in a subspace N_k^* we can find an element m_k^* that satisfies the inequality

$$\|m_k^* - m^*\|_\Delta < \delta,$$

where

$$\|.\|_\Delta^2 = \ \|.\|_\Omega^2 + \|\Delta.\|_\Omega^2.$$

By the algorithm proposed, for the value $\mathcal{M}_k(v)$ we have

$$\begin{aligned}\mathcal{M}_k(v) &= (1 + \beta_k)\|\Delta v - \varkappa_k^*\|_\Omega^2 + (1 + \beta_k^{-1})\mathbb{C}_{2\Omega}^2\|\Delta \varkappa_k^* - f\|_\Omega^2 \\ &\leq (1 + \delta)\|\Delta v - \varkappa_k^*\|_\Omega^2 + (1 + \delta^{-1})\mathbb{C}_{2\Omega}^2\|\Delta \varkappa_k^* - f\|_\Omega^2 \\ &\leq (1 + \delta)\|\Delta v - m_k^*\|_\Omega^2 + (1 + \delta^{-1})\mathbb{C}_{2\Omega}^2\|\Delta m_k^* - f\|_\Omega^2 = (*).\end{aligned}$$

Using the relations $m^* = \Delta u$ and $\Delta m^* = f$ and the triangle inequality, we obtain

$$\begin{aligned}(*) &\leq (1 + \delta)\left(\|\Delta e\|_\Omega + \|m^* - m_k^*\|_\Omega\right)^2 + (1 + \delta^{-1})\mathbb{C}_{2\Omega}^2\|\Delta(m_k^* - m^*)\|_\Omega^2 \\ &\leq (1 + \delta)\|\!|e|\!\|^2 + (1 + \delta)\left(2\|\!|e|\!\|\delta + \delta^2\right) + \mathbb{C}_{2\Omega}^2\left(\delta + \delta^2\right).\end{aligned}$$

Thus, we arrive at the desired result

$$0 \leq \mathcal{M}_k(v) - |||e|||^2 \leq \ \delta \ \left\{|||e|||^2 + (1+\delta)\ (2|||e||| + \delta + \mathbb{C}^2_{2\Omega})\right\}.$$

□

Proposition 1 justifies an important property of the duality error majorant (2.6). By this proposition, the effectivity index of the estimator

$$I_{eff} = \frac{\sqrt{\mathcal{M}_k(v)}}{|||e|||}$$

will tends to the optimal value (which is equal to one) in the process of minimization for any given approximate solution. In practice, this property is superior of the asymptotic exactness. We can obtain error estimates of high accuracy not only in the case where the corresponding mesh size h is small enough.

Proposition 2. If a sequence of optimal values β_k, which we obtain in the process of minimization, tends to zero for $k \to \infty$, then the sequence $\varkappa^*_k$ tends to the exact solution of the dual problem m^* in N^*_Δ.

Proof.

From Proposition 1 it follows that the sequence $\{\mathcal{M}_k(v)\}_{k=1}^{\infty}$ is bounded. Both terms of the majorant are nonnegative; therefore, the sequence of values of the second term is also bounded. Consequently,

$$\Delta\varkappa^*_k \to f = \Delta m^* \quad \text{in } \mathbf{L}_2(\Omega) \quad \text{as } \beta_k \to 0.$$

On the one hand,

$$\sqrt{\mathcal{M}_k(v)} \to \|\Delta v - \Delta u\|_\Omega.$$

On the other hand, from (2.9) we conclude that

$$\sqrt{\mathcal{M}_k(v)} = \|\Delta v - \varkappa^*_k\|_\Omega \, + \, \mathbb{C}_{2\Omega}\|\Delta\varkappa^*_k - f\|_\Omega.$$

We obtain the following result:

$$\|\Delta v - \varkappa^*_k\|_\Omega \ \to \ \|\Delta v - \Delta u\|_\Omega = \|\Delta v - m^*\|_\Omega,$$

or, in terms of the dual functional I^*,

$$|I^*(\varkappa^*_k) - I^*(m^*)| \to 0 \quad \text{as } k \to \infty.$$

Let us consider the sequence of elements $\varkappa^*_{kf} \in N^*_f$, where $\varkappa^*_{kf}$ is the $\mathbf{L}_2$-projection of $\varkappa^*_k$ to N^*_f. Following similar arguments as those used for obtaining the estimate of the term $R(\varkappa^*)$, we have

$$\|\varkappa^*_k - \varkappa^*_{kf}\|_\Omega \leq \mathbb{C}_{2\Omega}\|\Delta\varkappa^*_k - f\|_\Omega$$

and, therefore,

$$\|\varkappa_k^* - \varkappa_{kf}^*\|_\Omega \to 0.$$

This result yields

$$|I^*(\varkappa_{kf}^*) - I^*(m^*)| \to 0 \qquad \text{as } k \to \infty.$$

It is known that a solution of the dual problem exists, and it is unique. Any element of the sequence $\varkappa_{kf}^*$ belongs to N_f^*; therefore, this sequence must tend to m^*. By the triangle inequality, $\varkappa_k^*$ also tends to m^* in $\mathbf{L}_2(\Omega)$ as $k \to \infty$. Therefore,

$$\begin{cases} \Delta\varkappa_k^* \to \Delta m^* & \text{in } \mathbf{L}_2(\Omega), \\ \varkappa_k^* \to m^* & \text{in } \mathbf{L}_2(\Omega). \end{cases}$$

□

Proposition 2 is used for justification of the efficiency of the approach under consideration for indicating a local error distribution over the domain Ω. Note that, from our experience, it is preferable to use as an error indicator only the first term of the majorant (2.6).

Proposition 3. Under the assumption of Proposition 2, we have

$$\int\limits_\Omega |d_k(x) - \varepsilon(x)|\, dx \to 0,$$

where

$$d_k(x) = |\Delta v(x) - \varkappa_k^*(x)|^2, \quad \varepsilon(x) = |\Delta v(x) - \Delta u(x)|^2.$$

Proof.

$$\begin{aligned} \int\limits_\Omega |d_k - \varepsilon|\, dx &= \int\limits_\Omega |(\Delta v - \varkappa_k^*)^2 - (\Delta v - \Delta u)^2|\, dx \\ &= \int\limits_\Omega |(\varkappa_k^*)^2 - (\Delta u)^2 - 2\Delta v(\varkappa_k^* - \Delta u)|\, dx \\ &= \int\limits_\Omega |(\varkappa_k^* + \Delta u - 2\Delta v)(\varkappa_k^* - \Delta u)|\, dx \\ &\le (\|\varkappa_k^* - m^*\|_\Omega + 2|\!|\!|e|\!|\!|)\|\varkappa_k^* - m^*\|_\Omega. \end{aligned}$$

From Proposition 2, we obtain the desired result.

□

Similar propositions for the Poisson equation with a Dirichlet type boundary condition was stated and proved in the paper [43] of S. Repin, S. Sauter and A. Smolianski and in paper B. Computational properties of the majorant (2.8) have been numerically investigated in paper D. The question of a rigorous efficiency justification for the corresponding error estimate is open.

2.3 Computational properties of a duality error majorant for Kirchhoff-Love plates

Further we consider a more general case of the primal variational formulation. Problem $\mathcal{P}$. Find an element $u \in V_0$ such that

$$J(u) = \inf_{w \in V_0} J(w),$$

where

$$J(w) = \int\limits_{\Omega} \left(\frac{1}{2} \mathrm{B} \nabla\nabla w : \nabla\nabla w - f w \right) dx$$

and

$$V_0 = \overset{\circ}{\mathbf{W}}{}^2_2(\Omega).$$

Assume that a fourth-order tensor B possesses the symmetry property and there exist positive constants α_1 and α_2 such that

$$\alpha_1 |\varkappa|^2 \leq \mathrm{B}\varkappa : \varkappa \leq \alpha_2 |\varkappa|^2, \quad \forall \varkappa \in \mathbb{M}_s^{2\times 2}, \quad |\varkappa|^2 = \varkappa : \varkappa,$$

where $\mathbb{M}_s^{2\times 2}$ denotes the space of symmetric 2×2 matrices.

We consider the case of Kirchhoff-Love plates that are clamped along the boundary. In particular, if the material of a plate is homogeneous and isotropic, then

$$\mathrm{B}\varkappa = \frac{E}{12(1-\nu^2)} \left((1-\nu)\varkappa + \nu \,\mathrm{tr}\varkappa \mathbb{I} \right),$$

where $\mathbb{I}$ is the identity matrix, E and ν are Young's modulus and the Poisson ratio, respectively. The variational statement of this problem is exactly the same as Problem $\mathcal{P}$. The tensor B is symmetric and possesses the necessary inequalities

$$\alpha_1 |\varkappa|^2 \leq \mathrm{B}\varkappa : \varkappa \leq \alpha_2 |\varkappa|^2$$

with

$$\alpha_1 = \frac{E}{12(1+\nu)}, \quad \alpha_2 = \frac{E}{12(1-\nu)}.$$

Proof.

Let us consider the product $\mathrm{B}\varkappa : \varkappa$ without a multiplicative constant:

$$
\begin{aligned}
(\,(1-\nu)\varkappa \,+\, \nu\,\mathrm{tr}\varkappa\mathbb{I}\,) : \varkappa &= (1-\nu)\varkappa : \varkappa + \nu\mathrm{tr}\varkappa\ (\mathbb{I} : \varkappa) \\
&= (1-\nu)\varkappa : \varkappa + \nu(\mathrm{tr}\varkappa)^2 \geq (1-\nu)\varkappa : \varkappa.
\end{aligned}
$$

Therefore, on the one hand, we obtain $\alpha_1 = E/(12(1+\nu))$. On the other hand,

$$
\begin{aligned}
(1-\nu)\varkappa : \varkappa + \nu\,(\varkappa_{11} + \varkappa_{22})^2 &\leq (1-\nu)\varkappa : \varkappa + 2\nu\,(\varkappa_{11}^2 + \varkappa_{22}^2) \\
&\leq (1-\nu)\varkappa : \varkappa + 2\nu\,(\varkappa_{11}^2 + 2\varkappa_{12}^2 + \varkappa_{22}^2) = (1+\nu)\varkappa : \varkappa
\end{aligned}
$$

and $\alpha_2 = E/(12(1-\nu))$.

□

Consequently, the variational statement for Kirchhoff-Love plates is a very important special case of Problem $\mathcal{P}$. In this case, the dual problem is as follows.
Problem $\mathcal{P}^*$. Find an element $m^* \in N_f^*$ such that

$$
I^*(m^*) = \sup_{n^* \in N_f^*} I^*(n^*),
$$

where

$$
I^*(n^*) = \int_\Omega \left(-\frac{1}{2}\mathrm{B}^{-1} n^* : n^* \right) dx,
$$

and

$$
N_f^* = \left\{ n^* \in \mathbf{L}_2(\Omega, \mathbb{M}_s^{2\times 2}) \mid \int_\Omega n^* : \nabla\nabla w \, dx = \int_\Omega f w \, dx \ , \quad \forall w \in V_0 \right\}.
$$

Problems $\mathcal{P}$ and $\mathcal{P}^*$, and their solutions are related as above:

$$
J(u) = I^*(m^*),
$$

and

$$
m^* = \mathrm{B}\nabla\nabla u \ , \quad \mathrm{div}(\nabla\cdot m^*) = f \quad \text{a.e. in } \Omega \, . \tag{2.10}
$$

A respective error estimate of the functional type has been derived by P. Neittaanmäki and S. Repin in [33] and has the form

$$
|\!|\!| e |\!|\!|^2 \leq M(v, \beta, \varkappa^*) = \mathcal{M}_D(v, \beta, \varkappa^*) + \mathcal{M}_R(\beta, \varkappa^*) \ , \tag{2.11}
$$

where

$$
|\!|\!| e |\!|\!|^2 = \int_\Omega \mathrm{B}\nabla\nabla e : \nabla\nabla e \, dx,
$$

$$\mathcal{M}_D(v, \beta, \varkappa^*) = (1+\beta) \int\limits_\Omega (\mathrm{B}\nabla\nabla v - \varkappa^*) : (\nabla\nabla v - \mathrm{B}^{-1}\varkappa^*)\, dx,$$

$$\mathcal{M}_R(\beta, \varkappa^*) = (1+\beta^{-1})\, \frac{\mathbb{C}^2_{3\Omega}}{\alpha_1} \int\limits_\Omega (\mathrm{div}(\nabla\cdot\, \varkappa^*) - f)^2\, dx.$$

In this case, β is a free positive parameter and the tensor-valued dual variable $\varkappa^*$ belongs to the set

$$N^*_{\mathbb{W}} = \{\varkappa^* \in \mathbf{L}_2(\Omega, \mathbb{M}^{2\times 2}_s) \mid \mathrm{div}(\nabla\cdot\, \varkappa^*) \in \mathbf{L}_2(\Omega)\}.$$

The constant $\mathbb{C}_{3\Omega}$ comes from the inequality

$$\|w\| \leq \mathbb{C}_{3\Omega}\|\nabla\nabla w\|, \qquad \forall w \in V_0,$$

and in the case of the boundary conditions considered coincides with $\mathbb{C}_{2\Omega}$.

Paper C provides a similar analysis of the efficiency of the majorant $\mathcal{M}$ in (2.11). From the results of the paper, it follows that the duality error majorant for the Kirchhoff-Love plates possesses the same computational properties as does a more trivial majorant (2.6).

2.4 A reliable a posteriori error estimate for Reissner-Mindlin plates

Below, we present some extensions of the previous analysis to the case of the theory of Reissner-Mindlin plates, which is a very interesting generalization of the classical Kirchhoff-Love model. We show how one can derive a functional type a posteriori error estimate for any conforming approximate solution of this problem. Mainly, our discussions are based of the results of paper [42].

In the Reissner-Mindlin model, the bending of a plate of thickness t with middle plane $\Omega \subset \mathbb{R}^2$ is described in terms of two variables: a scalar-valued function $w(x)$ (the transverse displacement) and a vector-valued function $\varphi(x)$ (the rotation of the fibers normal to the middle plane). The energy functional for this problem has the form

$$J(w, \varphi) = \int\limits_\Omega \left(\frac{1}{2}\mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) + \frac{1}{2\alpha}|\nabla w - \varphi|^2 - fw \right) dx,$$

where B is a fourth-order tensor,

$$\varepsilon(\varphi) = \frac{\nabla\varphi + (\nabla\varphi)^T}{2},$$

α is a positive parameter that is proportional to t^2, and the function ft^3 is related to the transverse loading of a plate. The existence of a pair $(u, \phi) \in \mathbf{W}^1_2(\Omega) \times$

$\mathbf{W}_2^1(\Omega, \mathbb{R}^2)$, which satisfies given boundary conditions and minimizes the functional $J(w, \varphi)$, follows from known results of the calculus of variations for convex coercive functionals. One can show that as $\alpha \to 0$ the minimizers of this variational problem tend to the corresponding solution of the variational problem related to Kirchhoff-Love plates (see F. Brezzi and M. Fortin [15]).

At the present time, this model is popular. It has wide ranges of applicability and does not require for an approximate solution to possess second generalized derivatives. But, unfortunately, a direct application of the simplest finite elements leads to poor performance and yields some numerical effects such as the locking phenomenon. In this thesis, we are not able to focus our attention on the problem of constructing finite element methods for this model. For reviews on this subject we refer to D.N. Arnold and R.S. Falk [3], D.N. Arnold, A.L. Madureira, and S. Zhang [4], J.H. Bramble and T. Sun [14], F. Brezzi and M. Fortin [15], and the literature cited therein.

A posteriori error estimates for this model have been proposed by several authors. These estimates are based on the arguments of explicit residual methods (see C. Carstensen [17], C. Carstensen and K. Weinberg [20], and E. Liberman [31]).

In paper [42], we obtain a computable error majorant of the functional type that provides guaranteed upper bounds of the error for any conforming approximate solution of the Reissner-Mindlin plate bending problem. The derivation of this majorant is based purely on functional grounds and does not require any additional specification of the finite element method or properties of respective approximate solutions.

For the sake of simplicity, we consider the case of homogeneous boundary conditions where the pair of elements u and ϕ satisfies the conditions

$$\begin{cases} u = 0 & \text{on } \partial\Omega, \\ \phi = 0 & \text{on } \partial\Omega. \end{cases} \tag{2.12}$$

However, the approach can also be applied in the case of various boundary conditions.

The weak formulation of the problem is as follows: find a triple $(u, \phi, \gamma) \in V_0 \times Y_0 \times Q$ such that

$$\begin{cases} \int\limits_\Omega \mathrm{B}\varepsilon(\phi) : \varepsilon(\varphi)\, dx - \int\limits_\Omega \gamma \cdot \varphi\, dx = 0 & , \ \forall \varphi \in Y_0, \\ \int\limits_\Omega \gamma \cdot \nabla w\, dx = \int\limits_\Omega f w\, dx & , \ \forall w \in V_0, \\ \int\limits_\Omega (\alpha\gamma - (\nabla u - \phi)) \cdot q\, dx = 0 & , \ \forall q \in Q, \end{cases} \tag{2.13}$$

where

$$V_0 = \mathring{\mathbf{W}}_2^1(\Omega), \quad Y_0 = \mathring{\mathbf{W}}_2^1(\Omega, \mathbb{R}^2), \quad Q = \mathbf{L}_2(\Omega, \mathbb{R}^2).$$

At the same time, the pair of elements (u, ϕ) minimizes the above-mentioned functional

$$J(w, \varphi) = \int\limits_\Omega \left(\frac{1}{2} \mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) + \frac{1}{2\alpha} |\nabla w - \varphi|^2 - f w \right) dx$$

on a set $S = V_0 \times Y_0$. Thus,

$$J(u,\phi) = \inf_{(w,\varphi)\in S} J(w,\varphi) = \inf \mathcal{P}.$$

We call this variational statement *primal.*

Consider a pair (v,ψ) that provides a conforming approximation of the true solution (u,ϕ) in S (it this case, the element $\gamma = \frac{\nabla u-\phi}{\alpha}$ is approximated in $\mathbf{L}_2(\Omega,\mathbb{R}^2)$ by the element $y = \frac{\nabla v-\psi}{\alpha}$). Define the corresponding deviations from the exact values: $e_v = v - u$, $e_\psi = \psi - \phi$ and $e_y = y - \gamma$. The errors e_v, e_ψ, and e_y are restricted by the relation

$$e_\psi + \alpha e_y = \psi - \phi + (\nabla v - \psi) - (\nabla u - \phi) = \nabla v - \nabla u = \nabla e_v. \tag{2.14}$$

Using this relation, the following proposition is proved.

Proposition 4. The relation

$$|||e_\psi|||^2 + \alpha \|e_y\|^2_\Omega = 2\left(J(v,\psi) - \inf \mathcal{P}\right) \tag{2.15}$$

holds for any approximation $(v,\psi) \in S$, where

$$\|e_y\|^2_\Omega = \int\limits_\Omega |e_y|^2\, dx$$

and

$$|||e_\psi|||^2 = \int\limits_\Omega \mathrm{B}\varepsilon(e_\psi) : \varepsilon(e_\psi)\, dx.$$

The element γ and its approximation y in (2.15) have an independent physical meaning and present the so-called shear stress vector. The left-hand side of (2.15) is a norm in the space $Y_0 \times Q$, which is natural to use for measuring the error in terms of the deviations e_ψ and e_y. As is shown in the concluding part of the section, the estimates of these two deviations and the relation (2.14) enable us to control the norm of the deviation e_v as well. Thus, the accuracy of any approximation (v,ψ) can be estimated if the quantity $\inf \mathcal{P}$ is known. Although the exact lower bound of the problem under consideration is unknown in the general case, below we show that the right-hand side of (2.15) is estimated from above by invoking the dual variational formulation.

Consider the Lagrangian:

$$L(w,\varphi,q^*) = \int\limits_\Omega \left(\frac{1}{2}\mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) - fw + q^* \cdot (\nabla w - \varphi) - \frac{\alpha|q^*|^2}{2}\right) dx,$$

where

$$\inf \mathcal{P} = \inf_{(w,\varphi)\in S}\, \sup_{q^*\in Q^*} L(w,\varphi,q^*),$$

and $Q^* = \mathbf{L}_2(\Omega, \mathbb{R}^2)$. The dual problem $\mathcal{P}^*$ generated by the Lagrangian L, has the form: find an element $p^* \in Q^*$ such that

$$I^*(p^*) = \sup_{q^* \in Q^*} I^*(q^*) = \sup \mathcal{P}^*,$$

where

$$I^*(q^*) = \inf_{(w,\varphi) \in S} L(w, \varphi, q^*).$$

Using the known results of convex analysis, one can prove that the relation $\inf \mathcal{P} = \sup \mathcal{P}^*$ is valid, i.e.

$$\inf_{(w,\varphi) \in S} \sup_{q^* \in Q^*} L(w, \varphi, q^*) = \sup_{q^* \in Q^*} \inf_{(w,\varphi) \in S} L(w, \varphi, q^*). \tag{2.16}$$

With the help of the relations (2.15) and (2.16), we obtain the estimate

$$|||e_\psi|||^2 + \alpha \|e_y\|_\Omega^2 \leq 2 \left(J(v, \psi) - I^*(q^*) \right), \tag{2.17}$$

which is valid for any element $q^* \in Q^*$.

As follows from the definition of the dual functional,

$$I^*(q^*) = \inf_{w \in V_0, \varphi \in Y_0} L(w, \varphi, q^*) =$$
$$= \inf_{w \in V_0, \varphi \in Y_0} \int_\Omega \left(\frac{1}{2} \mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) - q^* \cdot \varphi - \frac{\alpha |q^*|^2}{2} + q^* \cdot \nabla w - f w \right) dx.$$

If the element q^* does not lie in the set Q_f^*, where

$$Q_f^* = \left\{ q^* \in \mathbf{L}_2(\Omega, \mathbb{R}^2) \mid \int_\Omega q^* \cdot \nabla w \, dx = \int_\Omega f w \, dx, \quad \forall w \in \mathring{\mathbf{W}}{}_2^1 \right\},$$

then the value of $I^*(q^*)$ is not bounded from below. Therefore, in fact the functional is well defined for $q^* \in Q_f^*$ and has the form

$$I^*(q^*) = \inf_{\varphi \in Y_0} \int_\Omega \left(\frac{1}{2} \mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) - q^* \cdot \varphi \right) dx - \int_\Omega \frac{\alpha |q^*|^2}{2} \, dx.$$

The first term in the above expression can be represented as follows:

$$\inf_{\varphi \in Y_0} \int_\Omega \left(\frac{1}{2} \mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) - q^* \cdot \varphi \right) dx = \sup_{\tau^* \in N_q^*} \int_\Omega \left(-\frac{1}{2} \mathrm{B}^{-1} \tau^* : \tau^* \right) dx,$$

where

$$N_q^* = \left\{ \tau^* \in \mathbf{L}_2(\Omega, \mathbb{M}_s^{2\times 2}) \mid \int_\Omega \tau^* : \varepsilon(\varphi) \, dx = \int_\Omega q^* \cdot \varphi \, dx, \quad \forall \varphi \in Y_0 \right\}.$$

This relation connects the primal and dual problems of a special form. As a result, we arrive at the expression

$$I^*(q^*) = \sup_{\tau^* \in N_q^*} \int\limits_\Omega \left(-\frac{1}{2} \mathrm{B}^{-1} \tau^* : \tau^* \right) dx - \int\limits_\Omega \frac{\alpha |q^*|^2}{2} \, dx.$$

Taking into account the inequality

$$I^*(q^*) \geq \mathcal{J}^*(q^*, \tau^*),$$

where

$$\mathcal{J}^*(q^*, \tau^*) = -\int\limits_\Omega \left(\frac{1}{2} \mathrm{B}^{-1} \tau^* : \tau^* + \frac{\alpha |q^*|^2}{2} \right) dx,$$

and using (2.17), we obtain the estimate

$$|\!|\!| e_\psi |\!|\!|^2 + \alpha \| e_y \|_\Omega^2 \leq 2 \left(J(v, \psi) - \mathcal{J}^*(q^*, \tau^*) \right), \tag{2.18}$$

which is valid for any $q^* \in Q_f^*$ and $\tau^* \in N_q^*$.

We show that the inequality (2.18) admits also the representation

$$|\!|\!| e_\psi |\!|\!|^2 + \alpha \| e_y \|_\Omega^2 \leq \inf_{q^* \in Q_f^*} \left\{ \inf_{\tau^* \in N_q^*} D(\psi, \tau^*) + \alpha \| y - q^* \|_\Omega^2 \right\}, \tag{2.19}$$

where

$$D(\psi, \tau^*) = \int\limits_\Omega \left(\mathrm{B} \varepsilon(\psi) : \varepsilon(\psi) + \mathrm{B}^{-1} \tau^* : \tau^* - 2 \tau^* : \varepsilon(\psi) \right) dx.$$

Indeed,

$$\begin{aligned} & 2 \left(J(v, \psi) - \mathcal{J}^*(q^*, \tau^*) \right) = \\ & \quad = \int\limits_\Omega \left(\mathrm{B} \varepsilon(\psi) : \varepsilon(\psi) + \frac{1}{\alpha} |\nabla v - \psi|^2 - 2 f v + \mathrm{B}^{-1} \tau^* : \tau^* + \alpha |q^*|^2 \right) dx = \\ & \qquad = D(\psi, \tau^*) + 2 \int\limits_\Omega \left(\tau^* : \varepsilon(\psi) - f v \right) \, dx + \int\limits_\Omega \alpha \left(|y|^2 + |q^*|^2 \right) \, dx. \end{aligned}$$

Using the relations

$$\int\limits_\Omega \tau^* : \varepsilon(\psi) \, dx = \int\limits_\Omega q^* \cdot \psi \, dx,$$

$$\psi + \alpha y = \nabla v,$$

and

$$\int\limits_\Omega q^* \cdot \nabla v \, dx = \int\limits_\Omega f v \, dx,$$

we conclude that

$$2\left(J(v,\psi) - \mathcal{J}^*(q^*,\tau^*)\right) = D(\psi,\tau^*) + \alpha\|y - q^*\|^2_\Omega + \\ + 2\int\limits_\Omega \left(q^* \cdot (\psi + \alpha y) - fv\right)\,dx = D(\psi,\tau^*) + \alpha\|y - q^*\|^2_\Omega.$$

Thus, the right-hand side of the estimate of the error, as well as its left-hand side, can be written in terms of the pair of approximations (ψ, y) rather than of the initial pair (v, ψ).

However, the practical application of the estimate (2.19) is hampered by the fact that, in computing upper bounds of the deviation, it is necessary to choose the elements q^* and τ^* in respective admissible classes Q^*_f and N^*_q. The problem of constructing approximations in these classes may be too labor consuming. For this reason, now our purpose is to modify the above inequality in such a way that the computation of the estimates of errors does not require complicated approximations.

Let us find an estimate of the deviation norm, in which the right-hand side is defined on $Q^*_{\rm div} \times N^*_{\rm div}$ instead of $Q^*_f \times N^*_q$, where

$$N^*_{\rm div} = \left\{\varkappa^* \in \mathbf{L}_2(\Omega, \mathbb{M}^{2\times 2}_s) \mid {\rm div}\varkappa^* \in \mathbf{L}_2(\Omega, \mathbb{R}^2)\right\}$$

and

$$Q^*_{\rm div} = \left\{y^* \in \mathbf{L}_2(\Omega, \mathbb{R}^2) \mid {\rm div} y^* \in \mathbf{L}_2(\Omega)\right\}.$$

Consider an arbitrary element $\varkappa^* \in N^*_{\rm div}$ and rewrite the term $D(\psi, \tau^*)$ in the form

$$D(\psi,\tau^*) = \int\limits_\Omega {\rm B}(\varepsilon(\psi) - {\rm B}^{-1}\tau^* \pm {\rm B}^{-1}\varkappa^*) : (\varepsilon(\psi) - {\rm B}^{-1}\tau^* \pm {\rm B}^{-1}\varkappa^*)\,dx.$$

By the properties of the tensor B, the quantity

$$\left(\int\limits_\Omega {\rm B}\varkappa : \varkappa\,dx\right)^{1/2}$$

is a norm in the space $\mathbf{L}_2(\Omega, \mathbb{M}^{2\times 2}_s)$ that is equivalent to the standard norm. Using the triangle inequality for this norm, we have

$$D(\psi,\tau^*)^{1/2} \le D(\psi,\varkappa^*)^{1/2} + \left(\int\limits_\Omega {\rm B}^{-1}(\tau^* - \varkappa^*) : (\tau^* - \varkappa^*)\,dx\right)^{1/2}.$$

Applying the inequality

$$2|ab| \le \beta_1\, a^2 + \beta_1^{-1}\, b^2,$$

we arrive at the estimate

$$D(\psi,\tau^*) \le (1+\beta_1) D(\psi,\varkappa^*) + \left(1+\beta_1^{-1}\right)\int\limits_\Omega {\rm B}^{-1}(\tau^* - \varkappa^*) : (\tau^* - \varkappa^*)\,dx,$$

which is valid for any positive value of the parameter β_1. Hence we conclude that

$$\inf_{\tau^*\in N_q^*} D(\psi,\tau^*) \le (1+\beta_1)D(\psi,\varkappa^*) + \left(1+\beta_1^{-1}\right) R(\varkappa^*), \tag{2.20}$$

where

$$R(\varkappa^*) = \inf_{\tau^*\in N_q^*} \int\limits_\Omega \mathrm{B}^{-1}(\tau^*-\varkappa^*) : (\tau^*-\varkappa^*)\, dx.$$

We show that for any element $\varkappa^*\in N^*_{\mathrm{div}}$, the estimate

$$R(\varkappa^*) \le \mathbb{C}^2_{4\Omega}\|q^* + \mathrm{div}\varkappa^*\|^2_\Omega,$$

holds, where $\mathbb{C}_{4\Omega}$ is a constant satisfying the inequality

$$\|\varphi\|_\Omega \le \mathbb{C}_{4\Omega}|\!|\!|\varphi|\!|\!|, \quad \forall\varphi\in Y_0.$$

<u>Proof.</u>

We make the change of variables $\sigma^* = \tau^* - \varkappa^*$ in the definition of $R(\varkappa^*)$. On the one hand,

$$\int\limits_\Omega \tau^* : \varepsilon(\varphi)\, dx = \int\limits_\Omega q^*\cdot\varphi\, dx, \quad \forall\varphi\in Y_0.$$

On the other hand,

$$-\int\limits_\Omega \varkappa^* : \varepsilon(\varphi)\, dx = \int\limits_\Omega \mathrm{div}\varkappa^*\cdot\varphi\, dx, \quad \forall\varphi\in Y_0.$$

Consequently, σ^* belongs to the set N_r^*, where $r = q^* + \mathrm{div}\varkappa^*$:

$$N_r^* = \left\{ \sigma^*\in \mathbf{L}_2(\Omega,\mathbb{M}_s^{2\times 2}) \mid \int\limits_\Omega \sigma^* : \varepsilon(\varphi)\, dx = \int\limits_\Omega r\cdot\varphi\, dx, \quad \forall\varphi\in Y_0 \right\}.$$

Hence, the required estimate is obtained on the basis of the same arguments as for the biharmonic problem. Indeed,

$$R(\varkappa^*) = \inf_{\sigma^*\in N_r^*}\int\limits_\Omega \mathrm{B}^{-1}\sigma^* : \sigma^*\, dx = -\sup_{\sigma^*\in N_r^*}\int\limits_\Omega \left(-\mathrm{B}^{-1}\sigma^* : \sigma^*\right)\, dx =$$

$$= -\inf_{\varphi\in Y_0}\int\limits_\Omega \left(\mathrm{B}\varepsilon(\varphi) : \varepsilon(\varphi) - 2r\cdot\varphi\right) dx \le -\inf_{\varphi\in Y_0}\left(|\!|\!|\varphi|\!|\!|^2 - 2\mathbb{C}_{4\Omega}\|r\|_\Omega|\!|\!|\varphi|\!|\!|\right) \le$$

$$\le -\inf_{a\ge 0}\left(a^2 - 2\mathbb{C}_{4\Omega}\|r\|_\Omega a\right) = \mathbb{C}^2_{4\Omega}\|q^* + \mathrm{div}\varkappa^*\|^2_\Omega.$$

□

The following estimate is a consequence of the inequalities (2.19) and (2.20) and the assertion proved above:

$$\|e_\psi\|^2 + \alpha\|e_y\|_\Omega^2 \le (1+\beta_1)D(\psi,\varkappa^*) + \\ + \inf_{q^*\in Q_f^*}\left\{\left(1+\beta_1^{-1}\right)\mathbb{C}_{4\Omega}^2\|q^*+\mathrm{div}\varkappa^*\|_\Omega^2 + \alpha\|y-q^*\|_\Omega^2\right\}.$$

It is valid for any $\beta_1 > 0$, $q^* \in Q_f^*$, and $\varkappa^* \in N_{\mathrm{div}}^*$. Thus, we have got rid of the first restriction — now we can choose the dual variable $\varkappa^*$ so that it satisfies the condition $\mathrm{div}\varkappa^* \in \mathbf{L}_2(\Omega,\mathbb{R}^2)$.

Instead of an arbitrary element $q^* \in Q_f^*$, we insert an arbitrary element $y^* \in Q_{\mathrm{div}}^*$ in the a posteriori estimate:

$$\|y-q^*\|_\Omega^2 \le (1+\beta_2)\|y-y^*\|_\Omega^2 + \left(1+\beta_2^{-1}\right)\|q^*-y^*\|_\Omega^2,$$

$$\|q^*+\mathrm{div}\varkappa^*\|_\Omega^2 \le (1+\beta_3)\|y^*+\mathrm{div}\varkappa^*\|_\Omega^2 + \left(1+\beta_3^{-1}\right)\|q^*-y^*\|_\Omega^2,$$

where β_2 and β_3 are free positive parameters. Using the estimate

$$\inf_{q^*\in Q_f^*}\|q^*-y^*\|_\Omega^2 \le \mathbb{C}_{1\Omega}^2\|\mathrm{div}y^*+f\|_\Omega^2,$$

obtained in paper [41] of S.I. Repin, we arrive at the dual majorant of the following form for the Reissner–Mindlin plates:

$$\|e_\psi\|^2 + \alpha\|e_y\|_\Omega^2 \le \mathcal{M}(y,\psi,\beta_1,\beta_2,\beta_3,\varkappa^*,y^*) = \mathcal{M}_1+\mathcal{M}_2+\mathcal{M}_3+\mathcal{M}_4, \quad (2.21)$$

where

$$\mathcal{M}_1 = (1+\beta_1)\int_\Omega (\mathrm{B}\varepsilon(\psi)-\varkappa^*):(\varepsilon(\psi)-\mathrm{B}^{-1}\varkappa^*)\,dx,$$

$$\mathcal{M}_2 = \alpha(1+\beta_2)\|y-y^*\|_\Omega^2,$$

$$\mathcal{M}_3 = \left(1+\beta_1^{-1}\right)(1+\beta_3)\mathbb{C}_{4\Omega}^2\|y^*+\mathrm{div}\varkappa^*\|_\Omega^2,$$

$$\mathcal{M}_4 = \left\{\left(1+\beta_1^{-1}\right)\left(1+\beta_3^{-1}\right)\mathbb{C}_{4\Omega}^2 + \alpha\left(1+\beta_2^{-1}\right)\right\}\mathbb{C}_{1\Omega}^2\|\mathrm{div}y^*+f\|_\Omega^2.$$

Now we clarify the sense of the estimate (2.21). On the one hand, it contains the elements ψ and $y = \frac{\nabla v-\psi}{\alpha}$, in terms of which we control the accuracy of approximation of the solution of the problem under consideration. On the other hand, it also includes a pair of free functions $(y^*,\varkappa^*)$ and several positive parameters.

The right-hand side of the inequality (2.21) yields a guaranteed upper estimate of the norm of the deviation from the exact solution for any choice of y^*, $\varkappa^*$ and β_1, β_2, β_3 from respective admissible classes. However, a poor choice of these elements may lead to a significant overestimation of its value. On the other hand, it is easily seen that, with the help of the majorant, one can obtain an arbitrarily exact estimate of the quantity we are interested in. Indeed, for the pair $y^* = \gamma$ and

$\varkappa^* = \mathrm{B}\varepsilon(\phi)$ the terms $\mathcal{M}_3$ and $\mathcal{M}_4$ vanish. Consequently, we can set β_1, β_2, β_3 to be equal to zero, and the inequality is converted to equality.

It is easily seen that the estimate obtained implies also an estimate for the deviation $e_v = v - u$. Using relation (2.14), we get

$$\|\nabla e_v\|_\Omega \;\leq\; \|e_\psi\|_\Omega + \alpha\|e_y\|_\Omega \;\leq\; \mathbb{C}_{4\Omega}|\!|\!|e_\psi|\!|\!| + \alpha\|e_y\|_\Omega.$$

Hence it follows that

$$\|\nabla e_v\|^2_\Omega \leq (1+\beta)\mathbb{C}^2_{4\Omega}|\!|\!|e_\psi|\!|\!|^2 + \left(1+\beta^{-1}\right)\alpha^2\|e_y\|^2_\Omega,$$

where β is an arbitrary positive number. Putting $\beta = \alpha\mathbb{C}^{-2}_{4\Omega}$, we arrive at the inequality

$$\|\nabla e_v\|^2_\Omega \leq (\alpha + \mathbb{C}^2_{4\Omega})\left(|\!|\!|e_\psi|\!|\!|^2 + \alpha\|e_y\|^2_\Omega\right) \leq (\alpha + \mathbb{C}^2_{4\Omega})\left(\mathcal{M}_1 + ... + \mathcal{M}_4\right).$$

Thus, the dual majorant we have suggested enables us to control simultaneously the norms of all the deviations considered.

2.5 Summary of the numerical tests performed

In this subsection, we outline only numerical tests presented in papers A-D. These tests justify the method of duality error majorants as a robust and efficient approach.

Paper A was originally published in Russian and translated into English in the journal of Computational Mathematics and Mathematical Physics. The aim of this paper was to provide a short introduction to some classical methods of a posteriori error control and the method of duality error majorants. Three approaches have been discussed with an example of the Poisson equation with a Dirichlet type boundary condition. The first approach is known as the explicit residual method. The second technique is based on various procedures of gradient recovery and the so-called superconvergence phenomenon. The third one is provided by duality theory in the calculus of variations. In Sections 2–4 of the paper, the basic ideas of these approaches are described. The second part of the paper is devoted to numerical tests. Basic advantages and drawbacks and the ranges of applicability of the methods are examined with a set of boundary-value problems in polygonal domains with reentrant corners. We consider only the second term of the explicit residual estimator as an error indicator. This indicator includes only jumps on interelement boundaries and no longer depends on interpolation constants, but it does not provide any estimates of global errors. The second indicator is the so-called Zienkiewicz-Zhu indicator. The third one is the duality error majorant. For evaluation of the quality of the resulting estimates for the global norm of the error and its local indication some numerical characteristics have been introduced. Note that the first one, the so-called effectivity index, is a quite standard global measure of quality.

The numerical tests performed have shown that the method of duality error majorants furnishes accurate upper estimates of the global error and, also, yields qualitative local error indication. The results justify the theoretical prediction that this method does not depend on the type of approximation of the original problem and its accuracy. The quality of other indicators is degraded significantly for inaccurate approximate solutions, when the Galerkin orthogonality condition is not satisfied. For this reason, we can conclude that the ranges of robust applicability of duality error majorants are wider.

In paper B, a general scheme of the method of duality error majorants (see [41]) is applied to a certain class of nonlinear elliptic type boundary-value problems. Properties of the estimate presented are investigated from a theoretical point of view. It is shown that for a given conforming approximate solution the method, under natural assumptions, provides guaranteed upper bounds of the actual error with any prescribed accuracy. In some sense, this property is stronger than the well-known asymptotic exactness of an error estimate.

In numerical tests, we compare a special case of the estimator presented with several well-known error indicators. On the one hand, from the results we conclude that this approach furnishes global error estimates of higher quality. On the other hand, the sets of elements selected for further adaptive mesh refinement by the method and by the exact knowledge of error distribution are rather similar.

In paper C, we continue investigations that have been started in the previous paper. Certain analogs of the theorems of paper B are proved for an error estimator, which is valid for a wide class of fourth-order elliptic partial differential equations. This estimator has been proposed in [33] and, in particular, it can be applied to error control for Kirchhoff-Love plates.

The numerical tests are mostly devoted to the verification of the efficiency of the method in the course of mesh adaptation. Here, we combine the estimator, which has been considered in paper B, with a standard code of MATLAB PDE Toolbox. We have compared three error indicators. The first one is computed as the difference between a given approximate solution and the exact solution. It provides an objective judgement of the quality of indication of local errors and mesh adaptation. Then, the duality error majorant and the standard local indicator of the MATLAB PDE Toolbox are compared with this reference indicator. The main conclusion is as follows. The method of duality error majorants leads to a more efficient adaptation than the one obtained by the built-in indicator of the toolbox. The effectivity index of computed upper bounds for the majorant is very close to one at each step of adaptive refinement. At the same time, the standard approach leads to significantly worse results. Finally, the difference is clearly observed – the same accuracy of computed solutions is archived by the duality error majorant with approximately half the number of degrees of freedom.

It is important to emphasize that mesh adaptations based on the duality error majorant are very close to those that would be obtained on the basis of the exact knowledge of the error distribution.

In paper D, we present a new a posteriori error estimate of the functional type for the biharmonic problem. We continue investigations of [33] and of paper C. To derive the error majorant, we use methods of duality theory in the calculus of variations. Our analysis is focused on aspects of the practical application of this technique to error control in the process of adaptive mesh refinement. From this point of view, it is important to underline that the calculation of an approximate solution of the original problem requires C^1-elements. At the same time, the estimate proposed for the biharmonic problem includes a pair of dual variables, and both of them can be approximated by simple linear C^0-elements.

From numerical results, we conclude that in the case of higher order elliptic partial differential equations this approach also yields guaranteed error estimates of reasonable quality. In addition, meshes, which have been obtained in the process of adaptive refinement, reflect the local behavior of the true solution.

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