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TWO-SIDED A POSTERIORI ERROR ESTIMATES FOR LINEAR ELLIPTIC PROBLEMS WITH MIXED BOUNDARY CONDITIONS*

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Abstract. The paper is devoted to verification of accuracy of approximate solutions obtained in computer simulations. This problem is strongly related to a posteriori error estimates, giving computable bounds for computational errors and detecting zones in the solution domain where such errors are too large and certain mesh refinements should be performed. A mathematical model consisting of a linear elliptic (reaction-diffusion) equation with a mixed Dirichlet/Neumann/Robin boundary condition is considered in this work. On the base of this model, we present simple technologies for straightforward constructing computable upper and lower bounds for the error, which is understood as the difference between the exact solution of the model and its approximation measured in the corresponding energy norm. The estimates obtained are completely independent of the numerical technique used to obtain approximate solutions and are "flexible" in the sense that they can be, in principle, made as close to the true error as the resources of the used computer allow.

Keywords: a posteriori error estimation, error control in energy norm, two-sided error estimation, differential equation of elliptic type, mixed boundary conditions

MSC 2000: 65N15, 65N30

1. Introduction

Many physical phenomena can be described by means of mathematical models presenting boundary value problems of elliptic type [9], [18]. Various numerical techniques (such as the finite difference method, the finite element method, the finite volume method etc.) are well developed for finding approximate solutions for such problems, see, e.g., [7] and references therein.

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However, in order to be practically meaningful, computer simulations always require an accuracy verification of computed approximations. Such a verification is the main purpose of a posteriori error estimation methods. Several approaches for deriving various a posteriori estimates for elliptic problems for errors measured in global (energy) norms ([1], [2], [3], [10], [13], [19], [24], [31], [32], [33]), or in terms of various local quantities ([4], [8], [11], [12], [16], [17], [23], [25], [29], [30]) have been suggested (see also references in the above mentioned works).

However, most of the estimates proposed strongly use the fact that the computed solutions are true finite element (FE) approximations which, in fact, rarely happens in real computations, e.g., due to quadrature rules, forcibly stopped iterative processes, various round-off errors, or even bugs in computer codes.

In this note, on the base of a model linear elliptic problem (diffusion-reaction equation), we present relatively simple technologies for obtaining *computable guaranteed bounds* needed for reliable control of the overall accuracy of computed approximations. Such bounds are *two-sided* and are valid for *any conforming approximations* independently of the numerical method used to obtain them. The bounds obtained can be made *arbitrarily close* to the true error. In real calculations this closeness only depends on resources of the concrete computer. We also shortly discuss some issues of the practical realization of the proposed error estimation procedures.

We notice that the estimates proposed in this work can be viewed as a certain generalization of the estimates presented for the first time in [24] (see also [21]). However, our way of constructing the error estimates is somewhat different and much simpler. In particular, it does not require complicated tools of the duality theory and is purely based on the integral identities related to the problem. Moreover, the equations and the boundary conditions analysed in our work are of considerably more general type than those in [24], [21]. The first variants of the present paper were published as preprints [15], [12] in February–March, 2006.

2. Formulation of the problem

Consider the following classical formulation of the reaction-diffusion problem: Find a function u such that

$$-\operatorname{div}(A\nabla u) + cu = f \quad \text{in } \Omega, \tag{1}$$

$$u = u_0 \quad \text{on } \Gamma_D, \tag{2}$$

$$\nu^T \cdot A\nabla u = g \quad \text{on } \Gamma_N, \tag{3}$$

$$\nu^T \cdot A\nabla u + \sigma u = h \quad \text{on } \Gamma_R, \tag{4}$$

where Ω is a bounded domain in $\mathbb{R}^d$ with a Lipschitz continuous boundary $\partial\Omega$, such that $\overline{\partial\Omega} = \overline{\Gamma}_D \cup \overline{\Gamma}_N \cup \overline{\Gamma}_R$, $\operatorname{meas}_{d-1} \Gamma_D > 0$, ν is the outward normal to the boundary, and Γ_D, Γ_N and Γ_R are disjoint sets.

In order to formulate the above problem in the weak form, we further assume that $f \in L_2(\Omega)$, $u_0 \in H^1(\Omega)$, $g \in L_2(\Gamma_N)$, $h \in L_2(\Gamma_R)$, $\sigma \in L_\infty(\Gamma_R)$, $c \in L_\infty(\Omega)$, the coefficient matrix A is symmetric, with entries $a_{ij} \in L_\infty(\Omega)$, $i, j = 1, \ldots, d$, and is uniformly positive definite, i.e.,

$$C_1|\xi|^2 \leqslant A(x)\xi \cdot \xi \leqslant C_2|\xi|^2 \quad \forall\, \xi \in \mathbb{R}^d \quad \text{a.e. in } \Omega, \tag{5}$$

where C_1 and C_2 are positive constants. In addition, we assume that

$$c \geqslant 0 \quad \text{a.e. in } \Omega, \qquad \sigma \geqslant \sigma_0 > 0 \quad \text{a.e. on } \Gamma_R, \tag{6}$$

introduce the set

$$\Omega^c := \{x \in \Omega\colon\ c(x) \geqslant c_0 > 0\}, \tag{7}$$

where σ_0 and c_0 are fixed positive constants, and assume that $c = 0$ almost everywhere in $\Omega \setminus \overline{\Omega^c}$. We notice that Ω^c can be, in particular, an empty set or equal to Ω.

The weak formulation of problem (1)–(4) then reads: Find $u \in u_0 + H^1_{\Gamma_D}(\Omega)$ such that

$$\begin{aligned} &\int_\Omega A\nabla u \cdot \nabla w \,\mathrm{d}x + \int_\Omega cuw \,\mathrm{d}x + \int_{\Gamma_R} \sigma uw \,\mathrm{d}s \\ &\qquad = \int_\Omega fw \,\mathrm{d}x + \int_{\Gamma_N} gw \,\mathrm{d}s + \int_{\Gamma_R} hw \,\mathrm{d}s \quad \forall\, w \in H^1_{\Gamma_D}(\Omega), \end{aligned} \tag{8}$$

where

$$H^1_{\Gamma_D}(\Omega) := \{v \in H^1(\Omega)\colon\ v = 0 \text{ on } \Gamma_D\}. \tag{9}$$

Let us define a bilinear form $a(\cdot,\cdot)$ and a linear form $F(\cdot)$ as

$$a(v, w) := \int_\Omega A\nabla v \cdot \nabla w \,\mathrm{d}x + \int_\Omega cvw \,\mathrm{d}x + \int_{\Gamma_R} \sigma vw \,\mathrm{d}s, \quad v, w \in H^1(\Omega), \tag{10}$$

$$F(w) := \int_\Omega fw \,\mathrm{d}x + \int_{\Gamma_N} gw \,\mathrm{d}s + \int_{\Gamma_R} hw \,\mathrm{d}s, \quad w \in H^1(\Omega). \tag{11}$$

Then the weak formulation (8) can be rewritten in a compact form: Find $u \in u_0 + H^1_{\Gamma_D}(\Omega)$ such that $a(u, w) = F(w)\ \forall\, w \in H^1_{\Gamma_D}(\Omega)$.

R e m a r k 2.1. The above conditions on the coefficients of the problem provide the existence and uniqueness of the weak solution u defined by (8) due to the well-known Lax-Milgram lemma [7]. However, it should be stressed here that this lemma is actually applied to the following problem: Find $u_\star \in H^1_{\Gamma_D}(\Omega)$ such that $a(u_\star, w) = \overline{F}(w)\ \forall\, w \in H^1_{\Gamma_D}(\Omega)$, where $\overline{F}(w) = F(w) - a(u_0, w)$, and setting $u := u_0 + u_\star$ after that.

The energy functional J of problem (8) is defined as

$$J(w) := \frac{1}{2}a(w,w) - \overline{F}(w), \quad w \in H^1(\Omega). \tag{12}$$

It is well known that problem (8) is equivalent to the problem of finding the minimizer (which is equal to the above introduced solution $u_\star$) of the above energy functional J over the set $H^1_{\Gamma_D}(\Omega)$ and setting again $u = u_0 + u_\star$.

In what follows we shall need the Friedrichs inequality

$$\|w\|_{0,\Omega} \leqslant C_{\Omega,\Gamma_D}\|\nabla w\|_{0,\Omega} \quad \forall\, w \in H^1_{\Gamma_D}(\Omega), \tag{13}$$

and the inequality in the trace theorem

$$\|w\|_{0,\partial\Omega} \leqslant C_{\partial\Omega}\|w\|_{1,\Omega} \quad \forall\, w \in H^1(\Omega), \tag{14}$$

where C_{Ω,Γ_D} and $C_{\partial\Omega}$ are positive constants, depending solely on Ω, Γ_D and $\partial\Omega$. Proofs of inequalities (13) and (14) can be found, e.g., in [22].

3. Two-sided estimation of the error

3.1. Measure for the global accuracy of approximations

Let $\bar{u}$ be *any function* from $u_0 + H^1_{\Gamma_D}(\Omega)$ (e.g., computed by some numerical method), which we shall consider as an approximation of u. We can easily show (see the proof of Proposition 3.2) that if $\bar{u} := u_0 + \bar{u}_\star$, where $\bar{u}_\star \in H^1_{\Gamma_D}(\Omega)$, then

$$J(\bar{u}_\star) - J(u_\star) = \frac{1}{2}a(u - \bar{u}, u - \bar{u}), \tag{15}$$

which is, probably, the reason for natural measurement of the overall accuracy of the approximations in terms of the bilinear form a, and also for calling it an estimation in the energy norm since the *energy norm* is defined as $\sqrt{a(\cdot,\cdot)}$ (cf. [1], [2], [3], [21], [32]).

Thus, the main goal in what follows is to show how to effectively estimate the value

$$a(u-\bar{u},u-\bar{u}) = \int_\Omega A\nabla(u-\bar{u})\cdot\nabla(u-\bar{u})\,\mathrm{d}x + \int_\Omega c(u-\bar{u})^2\,\mathrm{d}x + \int_{\Gamma_R}\sigma(u-\bar{u})^2\,\mathrm{d}s \tag{16}$$

from above and from below for an arbitrary approximation $\bar{u}\in u_0+H^1_{\Gamma_D}(\Omega)$.

3.2. Upper bound for the error

First, we demonstrate how to estimate (16) from above. Let us use the notation $|\!|\!|y|\!|\!|_\Omega := \left(\int_\Omega Ay\cdot y\,\mathrm{d}x\right)^{1/2}$ for $y\in L_2(\Omega,\mathbb{R}^d)$ and define

$$H_{N,R}(\mathrm{div},\Omega) := \{y\in L_2(\Omega,\mathbb{R}^d)\colon\ \mathrm{div}\,y\in L_2(\Omega),\ \nu^T\cdot y\in L_2(\Gamma_N\cup\Gamma_R)\}.$$

In what follows, we shall also employ the notation χ_S for the characteristic function of a set $S\subset\Omega$, i.e., $\chi_S(x)=1$ if $x\in S$, and $\chi_S(x)=0$ if $x\notin S$.

Proposition 3.1. *The following upper estimate for the global error* (16) *holds:*

$$\begin{aligned} a(u-\bar{u},u-\bar{u}) \leqslant{}& \Big\|\frac{1}{\sqrt{c}}(f+\mathrm{div}\,y^*-c\bar{u})\Big\|^2_{0,\Omega^c} \\ &+ \Big\|\frac{1}{\sqrt{\sigma}}(h-\sigma\bar{u}-\nu^T\cdot y^*)\Big\|^2_{0,\Gamma_R} + (1+\alpha)|\!|\!|A^{-1}y^*-\nabla\bar{u}|\!|\!|^2_\Omega \\ &+ \Big(1+\frac{1}{\alpha}\Big)(1+\beta)\frac{C^2_{\Omega,\Gamma_D}}{C_1}\|\chi_{\Omega\setminus\overline{\Omega}^c}(f+\mathrm{div}\,y^*-c\bar{u})\|^2_{0,\Omega} \\ &+ \Big(1+\frac{1}{\alpha}\Big)\Big(1+\frac{1}{\beta}\Big)C^2_{\Omega,\partial\Omega}\|g-\nu^T\cdot y^*\|^2_{0,\Gamma_N}, \end{aligned} \tag{17}$$

where α and β are arbitrary positive numbers, y^* is any function from the set $H_{N,R}(\mathrm{div},\Omega)$, and the constant $C_{\Omega,\partial\Omega}$ satisfies

$$C_{\Omega,\partial\Omega} := \frac{C_{\partial\Omega}\sqrt{1+C^2_{\Omega,\Gamma_D}}}{\sqrt{C_1}}. \tag{18}$$

Proof. First of all, we notice that

$$a(u-\bar{u},u-\bar{u}) = |\!|\!|\nabla(u-\bar{u})|\!|\!|^2_\Omega + \|\sqrt{c}(u-\bar{u})\|^2_{0,\Omega^c} + \|\sqrt{\sigma}(u-\bar{u})\|^2_{0,\Gamma_R}, \tag{19}$$

see (7) for the definition of the set Ω^c. Further, using the fact that $u-\bar{u}\in H^1_{\Gamma_D}(\Omega)$ and taking $w=u-\bar{u}$ in the integral identity (8), we get

$$
\begin{aligned}
a(u-\bar{u},u-\bar{u}) = &\int_\Omega f(u-\bar{u})\,\mathrm{d}x + \int_{\Gamma_N} g(u-\bar{u})\,\mathrm{d}s + \int_{\Gamma_R} h(u-\bar{u})\,\mathrm{d}s \\
&- \int_\Omega A\nabla\bar{u}\cdot\nabla(u-\bar{u})\,\mathrm{d}x - \int_\Omega c\bar{u}(u-\bar{u})\,\mathrm{d}x \\
&- \int_{\Gamma_R} \sigma\bar{u}(u-\bar{u})\,\mathrm{d}s.
\end{aligned} \tag{20}
$$

Further, inserting another identity

$$
\int_\Omega y^*\cdot\nabla(u-\bar{u})\,\mathrm{d}x + \int_\Omega \operatorname{div} y^*(u-\bar{u})\,\mathrm{d}x - \int_{\Gamma_N\cup\Gamma_R} \nu^T\cdot y^*(u-\bar{u})\,\mathrm{d}s = 0 \tag{21}
$$

valid for any function $y^*\in H_{N,R}(\mathrm{div},\Omega)$ into (21) we get

$$
\begin{aligned}
&a(u-\bar{u},u-\bar{u}) \\
&\quad= \int_\Omega A(A^{-1}y^*-\nabla\bar{u})\cdot\nabla(u-\bar{u})\,\mathrm{d}x + \int_\Omega (f+\operatorname{div} y^*-c\bar{u})(u-\bar{u})\,\mathrm{d}x \\
&\qquad+ \int_{\Gamma_N} (g-\nu^T\cdot y^*)(u-\bar{u})\,\mathrm{d}s + \int_{\Gamma_R} (h-\sigma\bar{u}-\nu^T\cdot y^*)(u-\bar{u})\,\mathrm{d}s \\
&\quad= \mathbf{T_1}+\mathbf{T_2}+\mathbf{T_3}+\mathbf{T_4},
\end{aligned} \tag{22}
$$

and estimate each of the terms in (22) separately.

First, using the Cauchy-Schwarz inequality, we have

$$
\mathbf{T_1} \leqslant |\!|\!| A^{-1}y^*-\nabla\bar{u} |\!|\!|_\Omega \, |\!|\!| \nabla(u-\bar{u}) |\!|\!|_\Omega. \tag{23}
$$

Now we decompose and estimate the second term as

$$
\begin{aligned}
\mathbf{T_2} = &\int_{\Omega^c} \frac{1}{\sqrt{c}}(f+\operatorname{div} y^*-c\bar{u})\sqrt{c}(u-\bar{u})\,\mathrm{d}x \\
&+ \int_{\Omega\setminus\overline{\Omega}^c} (f+\operatorname{div} y^*-c\bar{u})(u-\bar{u})\,\mathrm{d}x \\
\leqslant &\frac{1}{2}\|\sqrt{c}(u-\bar{u})\|^2_{0,\Omega^c} + \frac{1}{2}\Big\|\frac{1}{\sqrt{c}}(f+\operatorname{div} y^*-c\bar{u})\Big\|^2_{0,\Omega^c} \\
&+ \frac{C_{\Omega,\Gamma_D}}{\sqrt{C_1}}\|\chi_{\Omega\setminus\overline{\Omega}^c}(f+\operatorname{div} y^*-c\bar{u})\|_{0,\Omega}\, |\!|\!| \nabla(u-\bar{u}) |\!|\!|_\Omega,
\end{aligned} \tag{24}
$$

where the simple inequality

$$
2ab \leqslant a^2+b^2 \quad \forall\, a,b\in\mathbb{R}^1 \tag{25}
$$

was used. Further, by the Cauchy-Schwarz inequality, the trace inequality (14), (13) and (5), we obtain

$$\mathbf{T_3} \leqslant \|g - \nu^T \cdot y^*\|_{0,\Gamma_N} \|u - \bar{u}\|_{0,\Gamma_N} \leqslant C_{\Omega,\partial\Omega} \|g - \nu^T \cdot y^*\|_{0,\Gamma_N} \|\!|\nabla(u - \bar{u})|\!\|_{\Omega}, \tag{26}$$

where $C_{\Omega,\partial\Omega}$ is defined in (18). Using (25) for the fourth term, we get the estimate

$$\begin{aligned} \mathbf{T_4} &= \int_{\Gamma_R} (h - \sigma\bar{u} - \nu^T \cdot y^*)(u - \bar{u}) \, \mathrm{d}s \\ &= \int_{\Gamma_R} \frac{1}{\sqrt{\sigma}} (h - \sigma\bar{u} - \nu^T \cdot y^*) \sqrt{\sigma}(u - \bar{u}) \, \mathrm{d}s \\ &\leqslant \frac{1}{2} \|\sqrt{\sigma}(u - \bar{u})\|^2_{0,\Gamma_R} + \frac{1}{2} \Big\| \frac{1}{\sqrt{\sigma}} (h - \sigma\bar{u} - \nu^T \cdot y^*) \Big\|^2_{0,\Gamma_R}. \end{aligned} \tag{27}$$

Now, combining all the above estimates, we conclude that

$$\begin{aligned} & a(u - \bar{u}, u - \bar{u}) \\ &\leqslant \Big(\|\!|A^{-1}y^* - \nabla\bar{u}|\!\|_{\Omega} + C_{\Omega,\partial\Omega} \|g - \nu^T \cdot y^*\|_{0,\Gamma_N} \\ &\quad + \frac{C_{\Omega,\Gamma_D}}{\sqrt{C_1}} \|\chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u})\|_{0,\Omega} \Big) \|\!|\nabla(u - \bar{u})|\!\|_{\Omega} \\ &\quad + \frac{1}{2} \|\sqrt{c}(u - \bar{u})\|^2_{0,\Omega^c} + \frac{1}{2} \Big\| \frac{1}{\sqrt{c}} (f + \operatorname{div} y^* - c\bar{u}) \Big\|^2_{0,\Omega^c} \\ &\quad + \frac{1}{2} \|\sqrt{\sigma}(u - \bar{u})\|^2_{0,\Gamma_R} + \frac{1}{2} \Big\| \frac{1}{\sqrt{\sigma}} (h - \sigma\bar{u} - \nu^T \cdot y^*) \Big\|^2_{0,\Gamma_R} \\ &\leqslant \frac{1}{2} \Big(\|\!|A^{-1}y^* - \nabla\bar{u})|\!\|_{\Omega} + C_{\Omega,\partial\Omega} \|g - \nu^T \cdot y^*\|_{0,\Gamma_N} \\ &\quad + \frac{C_{\Omega,\Gamma_D}}{\sqrt{C_1}} \|\chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u})\|_{0,\Omega} \Big)^2 \\ &\quad + \frac{1}{2} \|\!|\nabla(u - \bar{u})|\!\|^2_{\Omega} + \frac{1}{2} \|\sqrt{\sigma}(u - \bar{u})\|^2_{0,\Gamma_R} + \frac{1}{2} \|\sqrt{c}(u - \bar{u})\|^2_{0,\Omega^c} \\ &\quad + \frac{1}{2} \Big\| \frac{1}{\sqrt{c}} (f + \operatorname{div} y^* - c\bar{u}) \Big\|^2_{0,\Omega^c} + \frac{1}{2} \Big\| \frac{1}{\sqrt{\sigma}} (h - \sigma\bar{u} - \nu^T \cdot y^*) \Big\|^2_{0,\Gamma_R}. \end{aligned} \tag{28}$$

Multiplying the inequality (28) by two and regrouping, we immediately get that

$$\begin{aligned} & a(u - \bar{u}, u - \bar{u}) \\ &= \|\!|\nabla(u - \bar{u})|\!\|^2_{\Omega} + \|\sqrt{c}(u - \bar{u})\|^2_{0,\Omega^c} + \|\sqrt{\sigma}(u - \bar{u})\|^2_{0,\Gamma_R} \\ &\leqslant \Big\| \frac{1}{\sqrt{c}} (f + \operatorname{div} y^* - c\bar{u}) \Big\|^2_{0,\Omega^c} + \Big\| \frac{1}{\sqrt{\sigma}} (h - \sigma\bar{u} - \nu^T \cdot y^*) \Big\|^2_{0,\Gamma_R} \\ &\quad + \Big(\|\!|A^{-1}y^* - \nabla\bar{u}|\!\|_{\Omega} + \frac{C_{\Omega,\Gamma_D}}{\sqrt{C_1}} \|\chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u})\|_{0,\Omega} \\ &\qquad + C_{\Omega,\partial\Omega} \|g - \nu^T \cdot y^*\|_{0,\Gamma_N} \Big)^2. \end{aligned} \tag{29}$$

Now using twice the obvious inequality

$$(a+b)^2 \leqslant (1+\lambda)a^2 + \Big(1+\frac{1}{\lambda}\Big)b^2 \quad \forall\,\lambda > 0 \tag{30}$$

for the terms in the parentheses in the above inequality, we finally get the estimate (17). $\square$

3.3. Lower estimate for the error

Proposition 3.2. *For the error in the energy norm* (16) *we have the lower bound*

$$a(u-\bar{u}, u-\bar{u}) \geqslant 2(J(\bar{u}_\star) - J(w_\star)), \tag{31}$$

where $w_\star$ is any function from $H^1_{\Gamma_D}(\Omega)$ and the functional J is defined in (12).

P r o o f. First, we prove that (cf. (15))

$$a(u-\bar{u}, u-\bar{u}) = 2(J(\bar{u}_\star) - J(u_\star)). \tag{32}$$

Indeed, we have

$$\begin{aligned} 2(J(\bar{u}_\star) - J(u_\star)) &= a(\bar{u}_\star, \bar{u}_\star) - 2\overline{F}(\bar{u}_\star) - a(u_\star, u_\star) + 2\overline{F}(u_\star) \\ &= a(\bar{u}_\star, \bar{u}_\star) - a(u_\star, u_\star) + 2\overline{F}(u_\star - \bar{u}_\star) \\ &= a(\bar{u}_\star, \bar{u}_\star) - a(u_\star, u_\star) + 2a(u_\star, u_\star - \bar{u}_\star) \\ &= a(\bar{u}_\star, \bar{u}_\star) + a(u_\star, u_\star) - 2a(u_\star, \bar{u}_\star) \\ &= a(u_\star - \bar{u}_\star, u_\star - \bar{u}_\star) = a(u-\bar{u}, u-\bar{u}). \end{aligned}$$

Since $u_\star$ minimizes the energy functional, we have $J(u_\star) \leqslant J(w_\star)$ for any $w_\star$ from $H^1_{\Gamma_D}(\Omega)$, which immediately proves (31). $\square$

R e m a r k 3.1. We note that the above proposed form of the lower estimation is quite natural and is different from that presented in Sect. 6.2 in [25] and in Sect. 6.4.4 in [21] for Dirichlet and Dirichlet/Neumann boundary conditions.

4. Error estimation and adaptivity procedures

In this section we shall briefly give some comments and suggestions on the usage of the proposed estimates in practical calculations.

4.1. On computation of the error estimates

First of all, it is clear that both the upper and lower estimates (17) and (31) are easily computable immediately after we fix (or find) concrete values for the free parameters $y^\star$, α, β, and $w_\star$ in their respective admissible sets, and also compute (or estimate from above, which is, in fact, sufficient) two global constants C_{Ω,Γ_D} and $C_{\partial\Omega}$.

In this subsection we shall assume that those two constants are given. Actually, those constants are not involved in the process of computation of any approximations, etc., as they are of functional type and can be often found or estimated by purely analytical methods, just after the solution domain is given and the original problem is posed. Even if the estimation of those constants is to be performed numerically, it can be done independently and in parallel to finding the approximations and to the construction of the error estimators (as they are just multipliers of integrals-to-be-computed in the upper estimates). More details on computation of global constants will be given in the next two subsections.

Now we demonstrate that the upper estimate (17) is sharp in principle, i.e., there are certain values of the parameters for which the estimate is equal to the exact error. Indeed, if one takes $y^* = A\nabla u$, which obviously belongs to $H_{N,R}(\mathrm{div},\Omega)$, then the last two terms on the right-hand side of (17) vanish. Further, taking $\alpha = 0$ (the parameter β is not needed at all), we finally observe that (17) holds as an equality for such a choice of the parameters. The lower estimate (31) is also sharp since it holds as an equality for the (acceptable) choice $w_\star = u_\star$.

Obviously, we do not know the exact solution u (or, equivalently, the function $u_\star$). Hence, the above comments on the sharpness of the estimates are somehow of pure mathematical nature and real computational procedures for finding concrete "good" values of the parameters have to be proposed. Such procedures are presented and discussed quite well in the monograph [21, Chapt. 6] (see also papers [27], [28], [12]) for simpler problems ($c \equiv 0$ in Ω and no Robin type boundary condition is imposed). Obviously, in our case we should take into account a more general form of the main equation and of the boundary conditions and, correspondingly, the presence of more terms in the estimates.

However, for completeness we propose below one simple way of possible usage of our two-sided estimates that can be easily employed if we perform computations on a series of meshes, which is a quite typical situation in the engineering practice. Thus, let us have a sequence of simplicial meshes $\mathcal{T}^{h_1}, \mathcal{T}^{h_2}, \ldots, \mathcal{T}^{h_k}$

($k \geqslant 2$) with the corresponding computed piecewise linear continuous FE solutions $u^{h_1}, u^{h_2}, \ldots, u^{h_k}$, where $u^{h_i} = u_0 + u_\star^{h_i}$, $i = 1, \ldots, k$. Further, for simplicity, we assume that $J(u_\star^{h_1}) > J(u_\star^{h_2}) > \ldots > J(u_\star^{h_k})$. These assumptions immediately lead to the following meaningful estimation of the (positive) error from below:

$$a(u - u^{h_i}, u - u^{h_i}) \geqslant 2(J(u_\star^{h_i}) - J(u_\star^{h_j})) > 0 \tag{33}$$

for $1 \leqslant i \leqslant k-1$ and $j > i$, i.e., we take $w_\star = u_\star^{h_j} \in H^1_{\Gamma_D}(\Omega)$ in (31). For the construction of reasonable upper estimates we can use the concept of averaged gradients. Namely, we prescribe $y^* := AG_{h_i}(\nabla u^{h_i})$, $i = 1, \ldots, k$, where G_{h_i} is a suitable *gradient averaging operator* (see [5], [14] for exact definitions), and use trivial calculations of values of the parameters α and β which minimize the upper bound for the above choices of y^*. Since, normally, $G_{h_i}(\nabla u^{h_i})$ presents quite a good approximation of the true gradient ∇u, we can expect that the estimates obtained in the above described manner shall represent a quite acceptable estimation of the error from above. The just described strategies for the error estimation are not computationally expensive and have been used, e.g., in [11], [12].

It is also natural to ask whether we could use our estimates for the mesh adaptation purposes. Here, we describe a general strategy for such a goal. The upper estimate (17) is, in fact, an integral over the solution domain Ω plus surface integrals over the Neumann and Robin portions of the boundary. Thus, we can represent the value of this integral as the sum $\sum\limits_{T \in \mathcal{T}^{(i)}} I_T$, where each contribution I_T is the value of the total domain integral taken over a particular element T of the current mesh $\mathcal{T}^{(i)}$ plus the relevant parts of surface integrals for elements T adjacent to Γ_N or Γ_R. To construct the next mesh $\mathcal{T}^{(i+1)}$ in order to obtain a more accurate approximation, we could use the following scheme. First, we find the maximum among all terms I_T and, secondly, mark up those elements T which have their contributions larger than the "user-given threshold" θ ($\theta \in [0,1]$) times that maximum value. Refining the marked elements (and making the mesh conforming), we obtain the next mesh $\mathcal{T}^{(i+1)}$.

4.2. The number of required global constants versus the type of equation and of boundary conditions

Dirichlet boundary condition: In this case, $\Gamma_N = \emptyset$ and $\Gamma_R = \emptyset$, i.e., the second and fifth terms on the right-hand side of estimate (17) do not exist, and we get the following variant of estimate (17):

$$\begin{aligned} a(u - \bar{u}, u - \bar{u}) \leqslant{}& \Big\| \frac{1}{\sqrt{c}}(f + \operatorname{div} y^* - c\bar{u}) \Big\|^2_{0,\Omega^c} + (1+\alpha) \| A^{-1} y^* - \nabla \bar{u} \|^2_\Omega \\ &+ \Big(1 + \frac{1}{\alpha}\Big) \frac{C^2_{\Omega,\Gamma_D}}{C_1} \| \chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u}) \|^2_{0,\Omega}. \end{aligned} \tag{34}$$

Remark 4.1. In the case of pure Dirichlet boundary condition we need to compute one constant C_{Ω,Γ_D} only. However, if $c(x) \geqslant c_0 > 0$ in the whole solution domain Ω, then the third term in RHS of (34) disappears and we do not need any constant at all for the error estimation.

Remark 4.2. For the particular case $c \equiv 0$ in the whole Ω (i.e., $\Omega^c = \emptyset$), the estimate (34) reduces further to the bound derived in [24], but obtained there in a different way—via the duality theory. The estimate from [24] is also presented in [27], where it was derived via the Helmholtz decomposition of $L_2(\Omega, \mathbb{R}^d)$. Our way of obtaining the upper bound is much simpler and more straightforward.

Dirichlet/Neumann boundary condition: In this case $\Gamma_R = \emptyset$ and estimate (17) takes on the form

$$
\begin{aligned}
(35)\quad a(u-\bar{u}, u-\bar{u}) \leqslant{} & \Big\| \frac{1}{\sqrt{c}}(f + \operatorname{div} y^* - c\bar{u}) \Big\|_{0,\Omega^c}^2 + (1+\alpha) \| A^{-1} y^* - \nabla \bar{u} \|_{\Omega}^2 \\
& + \Big(1 + \frac{1}{\alpha}\Big)(1+\beta) \frac{C_{\Omega,\Gamma_D}^2}{C_1} \| \chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u}) \|_{0,\Omega}^2 \\
& + \Big(1 + \frac{1}{\alpha}\Big)\Big(1 + \frac{1}{\beta}\Big) C_{\Omega,\partial\Omega}^2 \| g - \nu^T \cdot y^* \|_{0,\Gamma_N}^2 .
\end{aligned}
$$

Remark 4.3. For such a mixed boundary condition one needs, in general, to compute already two (global) constants, C_{Ω,Γ_D} and $C_{\partial\Omega}$.

Remark 4.4. For the special case $c \equiv 0$ in Ω and a simple Poisson equation, the estimate (35) reduces to the estimate presented in [28] for this type of mixed boundary conditions, where it is again obtained using quite complicated tools of the duality theory.

Dirichlet/Robin boundary condition: For this type of boundary conditions, estimate (17) takes on the form (due to $\Gamma_N = \emptyset$)

$$
\begin{aligned}
(36)\quad a(u-\bar{u}, u-\bar{u}) \leqslant{} & \Big\| \frac{1}{\sqrt{c}}(f + \operatorname{div} y^* - c\bar{u}) \Big\|_{0,\Omega^c}^2 + \Big\| \frac{1}{\sqrt{\sigma}}(h - \sigma\bar{u} - \nu^T \cdot y^*) \Big\|_{0,\Gamma_R}^2 \\
& + (1+\alpha) \| A^{-1} y^* - \nabla \bar{u} \|_{\Omega}^2 \\
& + \Big(1 + \frac{1}{\alpha}\Big) \frac{C_{\Omega,\Gamma_D}^2}{C_1} \| \chi_{\Omega \setminus \overline{\Omega}^c} (f + \operatorname{div} y^* - c\bar{u}) \|_{0,\Omega}^2 .
\end{aligned}
$$

Remark 4.5. In this case one has to compute only one constant, namely, C_{Ω,Γ_D}, similarly to the case of the pure Dirichlet boundary condition. However, for the particular case $c(x) \geqslant c_0 > 0$ in Ω, no computation of any constant is needed.

R e m a r k 4.6. To the author's knowledge, there exists a single work [31] where the mixed Dirichlet/Neumann/Robin boundary conditions are really analysed in detail. In that very recent paper a similar type of problems is considered and an efficient and close upper estimate is presented. However, the derivation of that estimate is still based on the assumption that the approximation is computed by the finite element method.

R e m a r k 4.7. We should also mention here that under the condition on the parameter y^*, that $-\operatorname{div} y^* = f$, which is often assumed in many papers devoted to the error control, the estimates presented here (for $c \equiv 0$) can assume a simpler form. However, this limitation on y^* is quite severe, since it is almost impossible to construct such parameters for real-life problems. On the contrary, a greater freedom for y^* provided by the weaker condition $y^* \in H_{N,R}(\operatorname{div}, \Omega)$ is very favourable for real calculations.

4.3. Computation of the global constants for the estimates

In general, the constant C_{Ω,Γ_D} satisfies $C_{\Omega,\Gamma_D} = (\lambda_{\Omega,\Gamma_D})^{-1/2}$, where $\lambda_{\Omega,\Gamma_D}$ is the smallest eigenvalue of the Laplacian in Ω with homogeneous mixed boundary conditions. However, for the error estimation purposes only an estimation of $\lambda_{\Omega,\Gamma_D}$ from below (i.e., estimation of C_{Ω,Γ_D} from above) is, in fact, sufficient.

In the case of pure homogeneous Dirichlet boundary condition (i.e., $\Gamma_D \equiv \partial\Omega$) this task can be easily solved as proposed by S. Mikhlin in [20, p. 8]. The idea consists of enclosing the solution domain into a rectangular parallelepiped, for which we can easily obtain the value of the smallest eigenvalue, which is known to be smaller than $\lambda_{\Omega,\Gamma_D}$. Thus, the following formula for the estimation of C_{Ω,Γ_D} ($\Gamma_D \equiv \partial\Omega$) holds:

$$C_{\Omega,\Gamma_D} \leqslant \frac{1}{\pi}\Big(\frac{1}{a_1^2} + \ldots + \frac{1}{a_d^2}\Big)^{-1/2}, \tag{37}$$

where $a_1, \ldots, a_d$ are the lengths of the edges of the parallelepiped.

Construction of the upper estimate of the constant $C_{\partial\Omega}$ is discussed in [28, Remark 3.3]. However, computation or estimation of this constant from above seems to be still an open problem for the general case.

Some new techniques for computation and estimation of C_{Ω,Γ_D} and $C_{\partial\Omega}$, suitable for the purposes of a posteriori error analysis, will be presented in our subsequent works.

5. Principal advantages of the proposed error estimation procedures

• First of all, we notice that in Propositions 3.1 and 3.2 we have no assumption that the approximation $\bar{u}$ is computed by the finite element method or by another numerical technique. In fact, it can be any function from the set of admissible functions $u_0 + H^1_{\Gamma_D}(\Omega)$, which is very advantageous since in real computations we never have "pure" Galerkin approximations due to various quadrature rules, forcibly stopped iterative processes, etc. We notice that in most of other existing approaches to the error control, the assumption that $\bar{u}$ is the finite element approximation is crucial.

• Further, the upper estimate (17) contains at most two (global) constants, C_{Ω,Γ_D} and $C_{\partial\Omega}$, which do not depend on the computational process and must be computed only after the problem (1)–(4) was posed. Many other existing estimation techniques (e.g., of the residual type) normally involve much more unknown constants (usually related to patches of computational meshes used). Such constants are very hard to compute (or even to estimate sufficiently accurately from above) and their evaluation normally leads to a very big overestimation of the error even in simple cases (cf. [6]). Moreover, those constants have to be always recomputed if we perform adaptive computations and change the computational mesh. On the contrary, the constants C_{Ω,Γ_D} and $C_{\partial\Omega}$ do remain the same regardless of any change of meshes during the whole computational process. Moreover, for computing the lower bound (31) we do not need any constants at all.

• It is also worth mentioning that, even though for the error estimates based on gradient averagings of different types (see, e.g., [17], [29], [30], [32], [33] and references therein) we do not require, in general, computations of any constants at all, such averaging-type estimates are not always reliable and can easily fail even for very simple problems in square domains (see [12] for an example). The averaging-type estimators work properly only if higher regularity of the solutions and special structures of the meshes are available.

• On the contrary, two-sided estimates presented in this work are really guaranteed and do not require any additional smoothness of solutions and any special regularity of meshes. Moreover, the bounds for the error can always be improved as much as needed using the freedom provided by the "free" parameters. Nonetheless, it should be stressed here that we assume that the estimates proposed are computed exactly, i.e., without round-off and quadrature errors.

R e m a r k 5.1. More details on comparison of the proposed type of error estimation with the other error control techniques can be found in [26] and [12].

R e m a r k 5.2. Two-sided estimates of the error in the global energy norm can be further employed to get two-sided computable bounds for the error measured in terms of linear bounded functionals, see [25], [11], [12].

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