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Complementarity based a posteriori error estimates and their properties

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Abstract: The paper is devoted to complementary approaches in a posteriori error estimation for a diffusion-reaction model problem. These approaches provide sharp and guaranteed upper bounds for the energy norm of the error and they are independent from the way how the approximate solution is obtained. In particular, the estimator naturally includes all sources of errors of any conforming approximation, like the discretization error, the error in the solver of linear algebraic systems, the quadrature error, etc. The paper recapitulates three complementarity approaches, proves sufficient and necessary conditions for the efficiency and asymptotic exactness of the error estimators, constructs an approximation by the method of hypercircle such that its error can be computed exactly, and presents numerical tests showing robustness of these approaches.

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1 Introduction

There is a general agreement that just a numerical solution of a partial differential equation is not sufficient. An information about the error is needed. The usage of a priori error estimates for these purposes is limited to the verification of the asymptotic

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rate of convergence. On the other hand, the a posteriori error estimates are capable to quantify the size of the error. In addition, they play an irreplaceable role in mesh adaptation processes. They serve as local indicators of the error for the mesh refinement and as the global estimators for the stopping criteria.

The topic of a posteriori error estimates for numerical solutions of partial differential equations has a long tradition going back to 1960s. The pioneering works [4, 6] introduce explicit residual error estimators. This kind of estimators was generalized for many types of problems and today it is probably the most popular strategy. However, during the time, people develop several different approaches like implicit residual estimates, hierarchical estimates, estimates based on postprocessing, and complementarity based error estimates. For general information we refer to books [2, 5, 16, 17, 24].

In general, the *a posteriori error estimator* is a quantity η, which approximates or bounds a suitable norm $\|e\|$ of an error e. There is several desirable properties the error estimator should satisfy. The estimator η can be a *guaranteed upper* or *lower* bound of the error ($\|e\| \leq \eta$ or $\eta \leq \|e\|$). The estimator is *efficient* and/or *reliable* if there exist constants C_1 and C_2 (independent from the discretization parameter h) such that $C_1\eta \leq \|e\|$ and/or $\|e\| \leq C_2\eta$, respectively. The estimator is *robust* if constants C_1 and C_2 are independent from parameters of the problem (e.g. coefficients in the equation, mesh aspect ratio, etc.). The estimator is *asymptotically exact* if $\lim_{h\to 0} I_{\mathrm{eff}} = 1$, where $I_{\mathrm{eff}} = \eta/\|e\|$ is the *index of effectivity* and h stand for the discretization parameter. Finally, we distinguish *local* and *global* estimators, depending whether they can be computed locally (e.g. element by element) or whether a solution of a global problem is required. The evaluation of an local estimator is fast in comparison with the computation of the approximate solution, while the effort for evaluation of the global estimator is comparable to the computation of the approximate solution.

A useful estimator should be efficient and reliable, because these two properties are necessary for convergence of adaptive procedures [8]. In addition, it should provide the guaranteed upper bound, because then it can be used for reliable stopping criterion. It also should be robust, because otherwise it can be used for a narrow range of parameters only. Pleasant properties are the asymptotic exactness and the locality of the estimator. An estimator meeting all these requirements is not know, up to the author's knowledge. However, in this contribution, we are going to present an approach which is a good candidate to satisfy all these criteria.

This approach is based on the method of error majorants of S. Repin and others, see e.g. [16, 17, 18, 19, 20, 12], however the idea origins much deeper in the history. Very similar idea was utilized in the dual (finite element) methods (or complementary energy approaches) by I. Hlaváček and his followers, see e.g. [9, 10, 11, 22, 13]. The idea is also connected to the method of hypercircle which goes back to J.L. Synge

[21], see also [3]. This idea is however used by other authors as well, see e.g. [7, 25].

In the current contribution we introduce a model diffusion-reaction problem and its FEM discretization in Section 2. Section 3 defines the a posteriori error estimator and proves the upper bound property. Section 4 shows the connection with a dual problem. Section 5 presents the sufficient and necessary conditions for the efficiency and asymptotic exactness of the estimator and, in addition, a result about the method of hypercircle. Section 6 is devoted to the generalization of the presented approach to the Poisson (i.e. pure diffusion) problem. Section 7 illustrates the numerical performance of the described estimators on two test cases. Finally, Section 8 draws the conclusions.

2 Model problem

The complementarity approach we are going to present is fairly general and it can be used for various linear and nonlinear problems. However, to simplify the exposition, we intentionally choose the following simple model problem.

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain. The classical formulation of the model problem reads: find $u \in C^2(\Omega) \cap C^0(\overline{\Omega})$ such that

$$\begin{aligned} -\Delta u + \kappa^2 u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

For simplicity, we assume κ to be a nonnegative constant. In Sections 3–5 we consider $\kappa > 0$, because the case $\kappa = 0$ brings additional technical difficulties which are treated in Section 6. Anyway, the complementarity approach can be generalized in a straightforward way to the case of variable coefficient κ, the Laplacian can be replaced by a general diffusion operator with nonhomogeneous and anisotropic diffusion tensor, and we may consider any combination of the standard boundary conditions.

The complementarity a posteriori error estimator is based on the following weak formulation: find $u \in V$, $V = H^1_0(\Omega)$, such that

$$\mathcal{B}(u, v) = \mathcal{F}(v) \quad \forall v \in V, \tag{1}$$

where

$$\mathcal{B}(u, v) = \int_\Omega (\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v + \kappa^2 uv) \,\mathrm{d}x, \qquad \mathcal{F}(v) = \int_\Omega fv \,\mathrm{d}x.$$

Here we assume $f \in L^2(\Omega)$ to ensure integrability. The existence and uniqueness of the weak solution u is guaranteed by the Lax-Milgram lemma.

We conclude this section by a regularity result for the weak solution. We denote by $\mathbf{H}(\mathrm{div}, \Omega)$ the usual space of L^2 vector fields with divergence in L^2.

Lemma 1 *Let $\Omega \subset \mathbb{R}^d$ be Lipschitz domain and let $u \in H_0^1(\Omega)$ be the weak solution of problem* (1). *Then $\boldsymbol{\nabla} u \in \mathbf{H}(\mathrm{div}, \Omega)$.*

Proof By definition, a vector field $\mathbf{g}$ is in $\mathbf{H}(\mathrm{div}, \Omega)$ if $\mathbf{g} \in [L^2(\Omega)]^d$ and if exists $z \in L^2(\Omega)$ such that

$$\int_\Omega zv \,\mathrm{d}x = -\int_\Omega \mathbf{g} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x \quad \forall v \in C_0^\infty(\Omega).$$

From (1) we immediately see that $\mathbf{g} = \boldsymbol{\nabla} u \in [L^2(\Omega)]^d$ satisfies this definition for $z = \kappa^2 u - f \in L^2(\Omega)$, because $C_0^\infty(\Omega) \subset H_0^1(\Omega)$. □

3 Complementarity based a posteriori error estimator

The complementarity approach is independent from the way how the approximate solution is obtained. We simply consider any function $u_h \in V$ and we estimate the error $e = u - u_h$, where $u \in V$ is the weak solution (1). Further in this section and also in Sections 4–5 we assume $\kappa > 0$. See Section 6 for the case $\kappa = 0$.

Let us first derive the a posteriori error estimator. The derivation is based on the divergence theorem

$$\int_\Omega v \,\mathrm{div}\, \mathbf{y} \,\mathrm{d}x + \int_\Omega \mathbf{y} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x - \int_{\partial\Omega} v\mathbf{y} \cdot \mathbf{n} \,\mathrm{d}x = 0 \quad \forall v \in H^1(\Omega)\ \forall \mathbf{y} \in \mathbf{H}(\mathrm{div}, \Omega), \quad (2)$$

where $\mathbf{n}$ stands for the unit outward normal to $\partial\Omega$. For brevity, we denote $\mathbf{W} = \mathbf{H}(\mathrm{div}, \Omega)$ in what follows. Taking any $v \in V$ and any $\mathbf{y} \in \mathbf{W}$, using the fact that v vanishes on $\partial\Omega$, using $\kappa > 0$, (1), (2) and the Cauchy-Schwarz inequality, we can obtain the following estimate

$$\begin{aligned}
\mathcal{B}(u - u_h, v) &= \int_\Omega fv \,\mathrm{d}x - \int_\Omega \boldsymbol{\nabla} u_h \cdot \boldsymbol{\nabla} v \,\mathrm{d}x - \int_\Omega \kappa^2 u_h v \,\mathrm{d}x + \int_\Omega v \,\mathrm{div}\, \mathbf{y} \,\mathrm{d}x + \int_\Omega \mathbf{y} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x \\
&= \int_\Omega \kappa^{-1}(f - \kappa^2 u_h + \mathrm{div}\, \mathbf{y})\kappa v \,\mathrm{d}x + \int_\Omega (\mathbf{y} - \boldsymbol{\nabla} u_h) \cdot \boldsymbol{\nabla} v \,\mathrm{d}x \\
&\le \left\| \kappa^{-1}(f - \kappa^2 u_h + \mathrm{div}\, \mathbf{y}) \right\|_0 \|\kappa v\|_0 + \|\mathbf{y} - \boldsymbol{\nabla} u_h\|_0 \|\boldsymbol{\nabla} v\|_0 \\
&\le \left(\left\| \kappa^{-1}(f - \kappa^2 u_h + \mathrm{div}\, \mathbf{y}) \right\|_0^2 + \|\mathbf{y} - \boldsymbol{\nabla} u_h\|_0^2 \right)^{1/2} |||v||| \qquad (3)
\end{aligned}$$

where $\|\cdot\|_0$ stands for the $L^2(\Omega)$ norm and $|||v|||^2 = \mathcal{B}(v, v) = \|\boldsymbol{\nabla} v\|_0^2 + \|\kappa v\|_0^2$ is the energy norm. Setting $v = u - u_h$ in (3), we immediately obtain the following upper bound for the energy norm of the error

$$|||u - u_h|||^2 \le \left\| \kappa^{-1}(f - \kappa^2 u_h + \mathrm{div}\, \mathbf{y}) \right\|_0^2 + \|\mathbf{y} - \boldsymbol{\nabla} u_h\|_0^2 \quad \forall \mathbf{y} \in \mathbf{W}. \qquad (4)$$

This the fundamental result for our subsequent considerations. The right-hand side of (4) serves as the error estimator. Thus, let us define

$$\eta^2(u_h, \mathbf{y}) = \left\|\kappa^{-1}(f - \kappa^2 u_h + \operatorname{div} \mathbf{y})\right\|_0^2 + \|\mathbf{y} - \boldsymbol{\nabla} u_h\|_0^2 \tag{5}$$

for $\kappa > 0$ and summarize our findings in the following theorem.

Theorem 1 *Let $\kappa > 0$, let $u \in V$ be the weak solution of* (1)*, and let $u_h \in V$ be arbitrary. Then*

$$|\!|\!| u - u_h |\!|\!| \le \eta(u_h, \mathbf{y}) \quad \forall \mathbf{y} \in \mathbf{W}. \tag{6}$$

Hence, the estimator $\eta(u_h, \mathbf{y})$ provides the guaranteed upper bound for any choice of $\mathbf{y} \in \mathbf{W}$. However, in order to obtain a sharp upper bound the vector field $\mathbf{y}$ must be chosen in an appropriate way. This issue is discussed in the following section.

4 Minimization of the estimator – the dual problem

Naturally, we may ask what is the minimum of $\eta(u_h, \mathbf{y})$ over $\mathbf{W}$ for the fixed u_h. Let us define the minimization problem: find $\mathbf{y}^* \in \mathbf{W}$ such that

$$\eta(u_h, \mathbf{y}^*) \le \eta(u_h, \mathbf{y}) \quad \forall \mathbf{y} \in \mathbf{W}. \tag{7}$$

Since $\eta^2(u_h, \mathbf{y})$ is a quadratic functional in $\mathbf{y}$, we may infer in a standard way the equivalent variational problem – the dual problem to (1). The dual problem reads: find $\mathbf{y}^* \in \mathbf{W}$ such that

$$\mathcal{B}^*(\mathbf{y}^*, \mathbf{w}) = \mathcal{F}^*(\mathbf{w}) \quad \forall \mathbf{w} \in \mathbf{W}, \tag{8}$$

where

$$\mathcal{B}^*(\mathbf{y}^*, \mathbf{w}) = \int_\Omega \kappa^{-2} \operatorname{div} \mathbf{y}^* \operatorname{div} \mathbf{w} \, \mathrm{d}x + \int_\Omega \mathbf{y}^* \cdot \mathbf{w} \, \mathrm{d}x, \qquad \mathcal{F}^*(\mathbf{w}) = -\int_\Omega \kappa^{-2} f \operatorname{div} \mathbf{w} \, \mathrm{d}x,$$

and $\kappa > 0$. Notice that the bilinear form $\mathcal{B}^*$ induces the inner product in $\mathbf{W}$. The corresponding norm is $|\!|\!| \mathbf{w} |\!|\!|_*^2 = \mathcal{B}^*(\mathbf{w}, \mathbf{w}) = \left\|\kappa^{-1} \operatorname{div} \mathbf{w}\right\|_0^2 + \|\mathbf{w}\|_0^2$.

The following lemma presents the crucial complementarity result for the estimator $\eta(u_h, \mathbf{y})$. The subsequent theorems show the equivalence of problems (7) and (8) and their unique solvability.

Lemma 2 *Let $\kappa > 0$, let $\mathbf{y}^* \in \mathbf{W}$ be the solution of the dual problem* (8)*, and let $u_h \in V$ and $\mathbf{y} \in \mathbf{W}$ be arbitrary then*

$$\eta^2(u_h, \mathbf{y}) = \eta^2(u_h, \mathbf{y}^*) + |\!|\!| \mathbf{y}^* - \mathbf{y} |\!|\!|_*^2.$$

Proof Putting $\mathbf{w} = \mathbf{y}^* - \mathbf{y}$ and using (5), we may directly compute

$$\eta^2(u_h, \mathbf{y}) = \eta^2(u_h, \mathbf{y}^* - \mathbf{w}) = \left\|\kappa^{-1}(f - \kappa^2 u_h + \operatorname{div} \mathbf{y}^*)\right\|_0^2$$
$$- 2 \int_\Omega \kappa^{-2}(f - \kappa^2 u_h + \operatorname{div} \mathbf{y}^*) \operatorname{div} \mathbf{w} \, \mathrm{d}x + \left\|\kappa^{-1} \operatorname{div} \mathbf{w}\right\|_0^2$$
$$+ \|\mathbf{y}^* - \boldsymbol{\nabla} u_h\|_0^2 - 2 \int_\Omega (\mathbf{y}^* - \boldsymbol{\nabla} u_h) \cdot \mathbf{w} \, \mathrm{d}x + \|\mathbf{w}\|_0^2 . \qquad (9)$$

Since $\mathbf{y}^*$ solves (8) and due to (2) we have the following orthogonality relation

$$\int_\Omega \kappa^{-2}(f - \kappa^2 u_h + \operatorname{div} \mathbf{y}^*) \operatorname{div} \mathbf{w} \, \mathrm{d}x + \int_\Omega (\mathbf{y}^* - \boldsymbol{\nabla} u_h) \cdot \mathbf{w} \, \mathrm{d}x = 0 \quad \forall \mathbf{w} \in \mathbf{W}. \qquad (10)$$

The proof is finished by substitution of (10) into (9). $\square$

Theorem 2 *There exists unique solution of the dual problem* (8)*.*

Proof The statement follows immediately from the Riesz representation theorem, because the bilinear form $\mathcal{B}^*$ is an inner product in $\mathbf{W}$ and $\mathcal{F}^*$ is a linear and continuous functional on $\mathbf{W}$. $\square$

Theorem 3 *Vector field $\mathbf{y}^* \in \mathbf{W}$ solves the minimization problem* (7) *if and only if it solves the dual problem* (8)*.*

Proof The proof is fairly standard. Let $\mathbf{y}^* \in \mathbf{W}$ solves (7) and let $\mathbf{w} \in \mathbf{W}$ be arbitrary. Then the function $J(t) = \eta^2(u_h, \mathbf{y}^* + t\mathbf{w})$ attains its minimum for $t = 0$. The derivative $J'(0)$ exists, it must vanish, and it can be explicitly computed from the definition of the derivative as

$$0 = J'(0) = 2 \int_\Omega \kappa^{-2}(f - \kappa^2 u_h + \operatorname{div} \mathbf{y}^*) \operatorname{div} \mathbf{w} \, \mathrm{d}x + 2 \int_\Omega (\mathbf{y}^* - \boldsymbol{\nabla} u_h) \cdot \mathbf{w} \, \mathrm{d}x.$$

Thus, using (2), we conclude that $\mathbf{y}^*$ solves (8).

Vice versa, if $\mathbf{y}^* \in \mathbf{W}$ solves the dual problem (8) then Lemma 2 implies

$$\eta^2(u_h, \mathbf{y}^*) \le \eta^2(u_h, \mathbf{y}^*) + \|\mathbf{y}^* - \mathbf{y}\|_*^2 = \eta^2(u_h, \mathbf{y}) \quad \forall \mathbf{y} \in \mathbf{W}.$$

$\square$

The following theorem shows that the solution of the dual problem (8) is $\mathbf{y}^* = \boldsymbol{\nabla} u$.

Theorem 4 *Let $\kappa > 0$ and let $u \in V$ be the weak solution of* (1)*. Then $\mathbf{y}^* = \boldsymbol{\nabla} u$ solves the dual problem* (8) *and $\eta(u_h, \mathbf{y}^*) = \|u - u_h\|$.*

Proof By Lemma 1 we have $\boldsymbol{\nabla} u \in \mathbf{W}$. Using the divergence theorem (2) in (1), we obtain

$$\int_\Omega (-\operatorname{div} \boldsymbol{\nabla} u + \kappa^2 u - f) v \,\mathrm{d}x = 0 \quad \forall v \in V. \tag{11}$$

Thus $-\operatorname{div} \boldsymbol{\nabla} u + \kappa^2 u - f = 0$ a.e. in Ω. Consequently,

$$\int_\Omega \operatorname{div}(\boldsymbol{\nabla} u) \operatorname{div} \mathbf{w} \,\mathrm{d}x - \int_\Omega \kappa^2 u \operatorname{div} \mathbf{w} \,\mathrm{d}x = -\int_\Omega f \operatorname{div} \mathbf{w} \,\mathrm{d}x \quad \forall \mathbf{w} \in \mathbf{W}.$$

Since $-\int_\Omega \kappa^2 u \operatorname{div} \mathbf{w} \,\mathrm{d}x = \int_\Omega \kappa^2 \boldsymbol{\nabla} u \cdot \mathbf{w} \,\mathrm{d}x$ for all $\mathbf{w} \in \mathbf{W}$, we conclude that $\boldsymbol{\nabla} u$ solves (8). The equality $\eta(u_h, \boldsymbol{\nabla} u) = |\!|\!| u - u_h |\!|\!|$ is immediate from (5), because $f + \operatorname{div} \boldsymbol{\nabla} u = \kappa^2 u$ a.e. in Ω. $\square$

Theorem 4 and Lemma 2 immediately imply the following complementarity result.

Corollary 1 *Let $\kappa > 0$, let $u \in V$ be the weak solution of (1), and let $\mathbf{y}^* \in \mathbf{W}$ be the solution of the dual problem (8). Then*

$$|\!|\!| u - u_h |\!|\!|^2 + |\!|\!| \mathbf{y}^* - \mathbf{y}_h |\!|\!|_*^2 = \eta^2(u_h, \mathbf{y}_h) \quad \forall u_h \in V,\ \forall \mathbf{y}_h \in \mathbf{W}. \tag{12}$$

Thus, the quantity $\eta(u_h, \mathbf{y}_h)$ measures exactly the sum of the errors in the primal and dual problem. Consequently, taking $u_h = u$, we obtain

$$|\!|\!| \mathbf{y}^* - \mathbf{y}_h |\!|\!|_* = \eta(u, \mathbf{y}_h).$$

Hence, the $|\!|\!| \cdot |\!|\!|_*$-norm of the error $\mathbf{y}^* - \mathbf{y}_h$ in the dual problem is equal to the quantity $\eta(u, \mathbf{y}_h)$ with u being the exact solution of the primal problem (1). This statement is complementary to the equality $|\!|\!| u - u_h |\!|\!| = \eta(u_h, \mathbf{y}^*)$ proved in Theorem 4. Consequently, complementarity equality (12) can be written as

$$\eta^2(u_h, \mathbf{y}^*) + \eta^2(u, \mathbf{y}_h) = \eta^2(u_h, \mathbf{y}_h). \tag{13}$$

5 Properties of the estimator

Practical application of the estimator (5) requires suitable choice of the vector field $\mathbf{y} \in \mathbf{W}$. The best choice $\mathbf{y} = \boldsymbol{\nabla} u$, see Theorem 4, is apparently not accessible. A reasonable choice seems to be certain approximate solution $\mathbf{y}_h \in \mathbf{W}$ of the dual problem (8). At this point, we do not specify any particular choice of $\mathbf{y}_h$ and simply consider arbitrary $\mathbf{y}_h \in \mathbf{W}$.

Theorem 1 already proves that $\eta(u_h, \mathbf{y}_h)$ is a guaranteed upper bound of the energy norm of the error. However, this upper bound can be too large. Therefore, we have to require the estimator to be efficient and/or to be asymptotically exact. The following theorems present sufficient and necessary conditions for these two properties.

Theorem 5 *Let $\kappa > 0$, let $u \in V$ be the weak solution of* (1)*, let $\mathbf{y}^* \in \mathbf{W}$ be the solution of the dual problem* (8)*, and let $\mathbf{y}_h \in \mathbf{W}$ and $u_h \in V$ be arbitrary. The estimator $\eta(u_h, \mathbf{y}_h)$ given by* (5) *is efficient (i.e. there exists a constant $C_1 > 0$ such that $C_1\eta(u_h, \mathbf{y}_h) \leq |||u - u_h|||$) if and only if there exists a constant $C > 0$ such that*

$$|||\mathbf{y}^* - \mathbf{y}_h|||_* \leq C|||u - u_h|||. \tag{14}$$

Proof It follows immediately from (12). □

Hence, the estimator $\eta(u_h, \mathbf{y}_h)$ is efficient if and only if the error in the dual problem measured in the $|||\cdot|||_*$-norm is controlled by the error in the primal problem measured in the energy norm.

Theorem 6 *Let $\kappa > 0$, let $u \in V$ be the weak solution of* (1)*, let $\mathbf{y}^* \in \mathbf{W}$ be the solution of the dual problem* (8)*, and let $u_h \in V$ and $\mathbf{y}_h \in \mathbf{W}$ be defined for all $h > 0$. The estimator $\eta(u_h, \mathbf{y}_h)$ given by* (5) *is asymptotically exact if and only if*

$$\lim_{h \to 0} \frac{|||\mathbf{y}^* - \mathbf{y}_h|||_*}{|||u - u_h|||} = 0. \tag{15}$$

Proof It follows immediately from (12). □

Condition (15) requires the error $|||\mathbf{y}^* - \mathbf{y}_h|||_*$ in the dual problem to converge faster towards zero than the error $|||u - u_h|||$ in the primal problem. Further, notice that asymptotic exactness implies the efficiency, provided h is sufficiently small. Indeed, (15) implies $|||\mathbf{y}^* - \mathbf{y}_h|||_* \leq |||u - u_h|||$ for small enough h, which is the sufficient and necessary condition (14) for the efficiency.

The final property of the estimator (5) is connected with the method of hypercircle [21, 3]. This method is remarkable in the context of a posteriori error estimates, because it allows to compute the error of a certain approximation exactly. The method of hypercircle can be utilized in the presented framework as follows.

Theorem 7 *Let $\kappa > 0$, let $u \in V$ be the weak solution of* (1) *and let $\mathbf{y}_h \in \mathbf{W}$ be arbitrary. Further, let $\bar{u}_h = [\kappa^{-2}(f + \operatorname{div} \mathbf{y}_h) + u_h]/2$ and $\boldsymbol{\mathcal{G}}\bar{u}_h = (\mathbf{y}_h + \boldsymbol{\nabla} u_h)/2$ be approximations of u and $\boldsymbol{\nabla} u$, respectively. Then*

$$\|\boldsymbol{\nabla} u - \boldsymbol{\mathcal{G}}\bar{u}_h\|_0^2 + \|\kappa(u - \bar{u}_h)\|_0^2 = \frac{1}{4}\eta^2(u_h, \mathbf{y}_h). \tag{16}$$

Proof Since $\mathbf{y}^* = \boldsymbol{\nabla} u$, we can modify the first term in (16) as follows

$$\begin{aligned} 4\,\|\boldsymbol{\nabla} u - \boldsymbol{\mathcal{G}}\bar{u}_h\|_0^2 &= \|\boldsymbol{\nabla}(u - u_h) + \boldsymbol{\nabla} u - \mathbf{y}_h\|_0^2 \qquad (17) \\ &= \|\boldsymbol{\nabla}(u - u_h)\|_0^2 + \|\mathbf{y}^* - \mathbf{y}_h\|_0^2 + 2\int_\Omega \boldsymbol{\nabla}(u - u_h) \cdot (\mathbf{y}^* - \mathbf{y}_h)\,\mathrm{d}x \end{aligned}$$

To adjust the second term in (16) in a similar way, we have to use the equality $\kappa u = \kappa^{-1}(f + \operatorname{div}\mathbf{y}^*)$ a.e. in Ω which follows from (11) and from the fact that $\boldsymbol{\nabla} u \in \mathbf{W}$:

$$\begin{aligned} 4\left\|\kappa(u-\bar{u}_h)\right\|_0^2 &= \left\|\kappa(u-u_h) + \kappa u - \kappa^{-1}(f + \operatorname{div}\mathbf{y}_h)\right\|_0^2 \\ &= \left\|\kappa(u-u_h) + \kappa^{-1}\operatorname{div}(\mathbf{y}^* - \mathbf{y}_h)\right\|_0^2 \\ &= \left\|\kappa(u-u_h)\right\|_0^2 + \left\|\kappa^{-1}\operatorname{div}(\mathbf{y}^* - \mathbf{y}_h)\right\|_0^2 + 2\int_\Omega (u-u_h)\operatorname{div}(\mathbf{y}^* - \mathbf{y}_h)\,\mathrm{d}x. \end{aligned} \tag{18}$$

Summing up (17) and (18), using the divergence theorem (2) and equality (12), we conclude

$$4\left\|\boldsymbol{\nabla} u - \boldsymbol{\mathcal{G}}\bar{u}_h\right\|_0^2 + 4\left\|\kappa(u-\bar{u}_h)\right\|_0^2 = |||u-u_h|||^2 + |||\mathbf{y}^* - \mathbf{y}_h|||_*^2 = \eta^2(u_h, \mathbf{y}_h).$$

□

6 Poisson problem

The estimator (5) is not defined for $\kappa = 0$ due to the factor κ^{-1}. Moreover, the numerical experiments show that it is not robust for small values of κ (it overestimates the error by a factor proportional to κ^{-1}). Therefore, the case with small or zero coefficient κ has to be treated in a different way. There are two principal possibilities how to handle this case. In Section 6.1 we describe the approach of error majorants, while in Section 6.2 we present the approach based on a complementarity technique.

6.1 Error majorant

This approach is presented e.g. in [16, 17, 18, 19, 20, 12]. The idea is to use the Friedrichs' inequality

$$\|v\|_0 \le C_\Omega \left\|\boldsymbol{\nabla} v\right\|_0 \quad \forall v \in V, \tag{19}$$

where the smallest possible value C_Ω^{F} of C_Ω is known as the Friedrichs' constant. In the case $V = H_0^1(\Omega)$, several upper bounds of the Friedrichs' constant are known. For example, the following bound is presented in [15]:

$$C_\Omega^{\mathrm{F}} \le \frac{1}{\pi}\left(\frac{1}{a_1} + \cdots + \frac{1}{a_d}\right)^{-1/2}, \tag{20}$$

where $a_1, \ldots, a_d$ are lengths of edges of a rectangular cuboid such that the domain Ω is contained in it. However, in the case of mixed boundary conditions, i.e. if the space V consists of functions from $H^1(\Omega)$ which vanish on a part of the boundary $\partial\Omega$ only, the bounds on C_Ω are not known, in general.

The error estimator can be derived similarly as in (3) but instead of introducing the factor κ^{-1}, we use the Friedrichs' inequality:

$$\begin{aligned}\mathcal{B}(u-u_h,v) &= \int_\Omega (f-\kappa^2 u_h + \operatorname{div}\mathbf{y})v \,\mathrm{d}x + \int_\Omega (\mathbf{y}-\boldsymbol{\nabla} u_h)\cdot\boldsymbol{\nabla} v\,\mathrm{d}x \\ &\le \left(C_\Omega \left\|f-\kappa^2 u_h + \operatorname{div}\mathbf{y}\right\|_0 + \|\mathbf{y}-\boldsymbol{\nabla} u_h\|_0\right) |\!|\!| v |\!|\!| \quad \forall \mathbf{y}\in\mathbf{W}.\end{aligned}$$

This yields the error estimate

$$|\!|\!| u-u_h |\!|\!| \le \widehat{\eta}(u_h,\mathbf{y}) \quad \forall \mathbf{y}\in\mathbf{W}, \tag{21}$$

where

$$\widehat{\eta}(u_h,\mathbf{y}) = C_\Omega \left\|f-\kappa^2 u_h + \operatorname{div}\mathbf{y}\right\|_0 + \|\mathbf{y}-\boldsymbol{\nabla} u_h\|_0 . \tag{22}$$

Notice that

$$\widehat{\eta}^2(u_h,\mathbf{y}) \le 2C_\Omega^2 \left\|f-\kappa^2 u_h + \operatorname{div}\mathbf{y}\right\|_0^2 + 2\|\mathbf{y}-\boldsymbol{\nabla} u_h\|_0^2 . \tag{23}$$

The bound (23) has certain practical advantages in comparison with (22), because it represents a simple quadratic functional in $\mathbf{y}$ with the same structure as (5). On the other hand, the error bound (22) is sharper.

6.2 Complementarity approach

An alternative approach how to handle the case $\kappa = 0$ was worked out in [9, 10, 11, 13]. They treat the case $\kappa > 0$ by introducing the factor κ^{-1} as described in Section 3. The case $\kappa = 0$ is handled in the way we present below. However, we generalize this approach in a new way also for $\kappa > 0$, see also [23].

The idea is to choose $\mathbf{y}$ in (5) such that $f - \kappa^2 u_h + \operatorname{div}\mathbf{y}$ vanishes. Therefore, we define the affine space

$$\mathbf{Q}(f,u_h) = \left\{ \mathbf{y}\in[L^2(\Omega)]^d : \int_\Omega \mathbf{y}\cdot\boldsymbol{\nabla} v\,\mathrm{d}x = \int_\Omega (f-\kappa^2 u_h)v\,\mathrm{d}x \quad \forall v\in V \right\}. \tag{24}$$

Notice that $\mathbf{Q}(f,u_h)\subset\mathbf{H}(\operatorname{div},\Omega)$, because $f-\kappa^2 u_h \in L^2(\Omega)$. In analogy with (5) we define

$$\widetilde{\eta}(u_h,\widetilde{\mathbf{y}}) = \|\widetilde{\mathbf{y}}-\boldsymbol{\nabla} u_h\|_0 \quad \text{for } \widetilde{\mathbf{y}}\in\mathbf{Q}(f,u_h). \tag{25}$$

Clearly, $\widetilde{\eta}(u_h,\widetilde{\mathbf{y}}) = \eta(u_h,\widetilde{\mathbf{y}})$ for all $\widetilde{\mathbf{y}}\in\mathbf{Q}(f,u_h)$ and for $\kappa > 0$. However, $\widetilde{\eta}(u_h,\widetilde{\mathbf{y}})$ is well defined also for $\kappa = 0$. In addition, $\widetilde{\eta}(u_h,\widetilde{\mathbf{y}})$ provides a guaranteed upper bound for the energy norm of the error even in the case $\kappa = 0$. This fact follows from the following complementarity result which uses a special norm

$$|\!|\!| v |\!|\!|_\sim^2 = |\!|\!| v |\!|\!|^2 + \|\kappa v\|_0^2 = \|\boldsymbol{\nabla} v\|_0^2 + 2\|\kappa v\|_0^2 \quad \text{for } v\in V.$$

Lemma 3 *Let $u \in V$ be the weak solution of* (1) *and let $\widetilde{\mathbf{y}} \in \mathbf{Q}(f, u_h)$ and $u_h \in V$ be arbitrary. Then*

$$\|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u\|_0^2 + |\!|\!| u - u_h |\!|\!|_\sim^2 = \widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}).$$

Proof Since $\widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}) = \|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u_h\|_0^2$, we express

$$\|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u_h\|_0^2 - \|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u\|_0^2 = 2 \int_\Omega \widetilde{\mathbf{y}} \cdot \boldsymbol{\nabla}(u - u_h) \,\mathrm{d}x + \|\boldsymbol{\nabla} u_h\|_0^2 - \|\boldsymbol{\nabla} u\|_0^2 . \tag{26}$$

Definitions (24) and (1) yield

$$\int_\Omega \widetilde{\mathbf{y}} \cdot \boldsymbol{\nabla}(u - u_h) \,\mathrm{d}x = \int_\Omega (f - \kappa^2 u_h)(u - u_h) \,\mathrm{d}x = \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla}(u - u_h) \,\mathrm{d}x + \int_\Omega \kappa^2 (u - u_h)^2 \,\mathrm{d}x$$
$$= \|\boldsymbol{\nabla} u\|_0^2 - \int_\Omega \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} u_h \,\mathrm{d}x + \|\kappa(u - u_h)\|_0^2 .$$

Inserting this into (26), we end up with the desired equality

$$\|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u_h\|_0^2 - \|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u\|_0^2 = \|\boldsymbol{\nabla}(u - u_h)\|_0^2 + 2 \|\kappa(u - u_h)\|_0^2 .$$

$\square$

Lemma 3 is analogous to Corollary 1 and it yields the following upper bound for the energy norm of the error

$$|\!|\!| u - u_h |\!|\!| \le |\!|\!| u - u_h |\!|\!|_\sim \le \widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}) \quad \forall \widetilde{\mathbf{y}} \in \mathbf{Q}(f, u_h), \ \forall u_h \in V. \tag{27}$$

Further, we can proceed in analogy with Section 4. The vector field $\widetilde{\mathbf{y}} \in \mathbf{Q}(f, u_h)$ which minimizes $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}})$ for a fixed $u_h \in V$ also minimizes $\|\widetilde{\mathbf{y}}\|_0$, because

$$\widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}) = \|\widetilde{\mathbf{y}} - \boldsymbol{\nabla} u_h\|_0^2 = \|\widetilde{\mathbf{y}}\|_0^2 - 2 \int (f - \kappa^2 u_h) u_h \,\mathrm{d}x + \|\boldsymbol{\nabla} u_h\|_0^2 .$$

Hence, the dual problem reads: find $\widetilde{\mathbf{y}}^* \in \mathbf{Q}(f, u_h)$ such that $\|\widetilde{\mathbf{y}}^*\|_0 \le \|\widetilde{\mathbf{w}}\|_0$ for all $\widetilde{\mathbf{w}} \in \mathbf{Q}(f, u_h)$. Or equivalently: find $\widetilde{\mathbf{y}}^* \in \mathbf{Q}(f, u_h)$ such that

$$\int_\Omega \widetilde{\mathbf{y}}^* \cdot \widetilde{\mathbf{w}} \,\mathrm{d}x = 0 \quad \forall \widetilde{\mathbf{w}} \in \mathbf{Q}_0, \tag{28}$$

where we denote $\mathbf{Q}_0 = \mathbf{Q}(0, 0) = \left\{ \mathbf{y} \in [L^2(\Omega)]^d : \int_\Omega \mathbf{y} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x = 0 \quad \forall v \in V \right\}$. Notice that the dual problem (28) possesses unique solution $\widetilde{\mathbf{y}}^* = \boldsymbol{\nabla} \tilde{z}$, where $\tilde{z} \in V$ satisfies

$$\int_\Omega \boldsymbol{\nabla} \tilde{z} \cdot \boldsymbol{\nabla} v \,\mathrm{d}x = \int_\Omega (f - \kappa^2 u_h) v \,\mathrm{d}x \quad \forall v \in V.$$

Hence, the minimal value the estimator $\widetilde{\eta}$ can attain for a given $u_h \in V$ is $\widetilde{\eta}(u_h, \nabla\tilde{z})$. However, Lemma 3 yields the following estimate

$$|\!|\!| u - u_h |\!|\!|^2 \leq \|\nabla\tilde{z} - \nabla u\|_0^2 + |\!|\!| u - u_h |\!|\!|_\sim^2 = \widetilde{\eta}^2(u_h, \nabla\tilde{z}).$$

Thus, if $\kappa > 0$ and $u \neq u_h$ then the estimator (25) is not exact. There are two sources of this inexactness First, $\|\nabla\tilde{z} - \nabla u\|_0^2$ is positive for $\kappa > 0$ and $u \neq u_h$. Second, $|\!|\!| u - u_h |\!|\!| < |\!|\!| u - u_h |\!|\!|_\sim$ for $\kappa > 0$ and $u \neq u_h$. However, in the following we show that the estimator (25) is exact for $\kappa = 0$ and in addition that there is the same theory as for the estimator (5), see Section 4.

Indeed, if $\kappa = 0$ then $|\!|\!| v |\!|\!| = |\!|\!| v |\!|\!|_\sim$ for all $v \in V$ and $\tilde{z} = u$, where u is the weak solution of (1), i.e. the exact solution to the dual problem (28) is $\widetilde{\mathbf{y}}^* = \nabla u$. Thus, the complementarity identity from Lemma 3 reshapes into a complementarity relation analogous to (12), namely:

$$\|\widetilde{\mathbf{y}}_h - \widetilde{\mathbf{y}}^*\|_0^2 + |\!|\!| u - u_h |\!|\!|^2 = \widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}_h) \quad \forall \widetilde{\mathbf{y}}_h \in \mathbf{Q}(f), \tag{29}$$

where we use the notation $\mathbf{Q}(f)$ instead of $\mathbf{Q}(f, u_h)$, because $\kappa = 0$. Further, trivially $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}}^*) = |\!|\!| u - u_h |\!|\!|$ which is an analogy to the exactness result presented in Theorem 4 for the estimator (5). Finally, identity $\widetilde{\eta}(u, \widetilde{\mathbf{y}}_h) = \|\widetilde{\mathbf{y}}^* - \widetilde{\mathbf{y}}_h\|_0$ is also trivial in case $\kappa = 0$ and it enables to rewrite (29) as follows

$$\widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}^*) + \widetilde{\eta}^2(u, \widetilde{\mathbf{y}}_h) = \widetilde{\eta}^2(u_h, \widetilde{\mathbf{y}}_h) \quad \forall \widetilde{\mathbf{y}}_h \in \mathbf{Q}(f).$$

which is an analogy to equality (13).

These facts immediately yield the sufficient and necessary conditions for the efficiency and asymptotic exactness of $\widetilde{\eta}$ for $\kappa = 0$, see Theorems 5 and 6.

Theorem 8 *Let $\kappa = 0$, let $u \in V$ be the weak solution of* (1)*, let $\widetilde{\mathbf{y}}^* \in \mathbf{Q}(f)$ be the solution of the dual problem* (28)*, and let $\widetilde{\mathbf{y}}_h \in \mathbf{Q}(f)$ and $u_h \in V$ be arbitrary. The estimator $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}}_h)$ given by* (25) *is efficient if and only if there exists a constant $C > 0$ such that*

$$\|\widetilde{\mathbf{y}}_h - \widetilde{\mathbf{y}}^*\|_0 \leq C |\!|\!| u - u_h |\!|\!|.$$

Proof It follows immediately from (29). □

Theorem 9 *Let $\kappa = 0$, let $u \in V$ be the weak solution of* (1)*, let $\widetilde{\mathbf{y}}^* \in \mathbf{Q}(f)$ be the solution of the dual problem* (28)*, and let $u_h \in V$ and $\widetilde{\mathbf{y}}_h \in \mathbf{Q}(f)$ be defined for all $h > 0$. The estimator $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}}_h)$ given by* (25) *is asymptotically exact if and only if*

$$\lim_{h \to 0} \frac{\|\widetilde{\mathbf{y}}_h - \widetilde{\mathbf{y}}^*\|_0}{|\!|\!| u - u_h |\!|\!|} = 0.$$

Proof It follows immediately from (29). □

The error estimator by the method of hypercircle is particularly interesting for $\kappa = 0$, see e.g. [3, 22, 14, 21]. If the goal is an approximation of the gradient ∇u of the weak solution u of (1), then we can compute a conforming approximation $u_h \in V$ and an approximation $\widetilde{\mathbf{y}}_h \in \mathbf{Q}(f)$ of the dual problem (28). The arithmetic average $(\widetilde{\mathbf{y}}_h + \nabla u_h)/2$ is then a better approximation of ∇u and its error is known exactly, because

$$\|\nabla u - (\widetilde{\mathbf{y}}_h + \nabla u_h)/2\|_0 = \frac{1}{2} \|\widetilde{\mathbf{y}}_h - \nabla u_h\|_0 \quad \forall u_h \in V, \ \forall \widetilde{\mathbf{y}}_h \in \mathbf{Q}(f).$$

In general, a practical difficulty of this complementarity approach lies in the fact, that the approximate solution $\widetilde{\mathbf{y}}_h$ of the dual problem (28) must be in $\mathbf{Q}(f, u_h)$, i.e. its divergence must be exactly equal to $-f + \kappa^2 u_h$ in the weak sense. This difficulty can be easily overcome if an antiderivative of the function $f = f(x_1, \dots, x_d)$ is known at least with respect to one of its variables. Indeed, let us assume without loss of generality that the antiderivative is known with respect to x_1. Then we construct a vector field $\mathbf{F} \in \mathbb{R}^d$ as follows

$$\mathbf{F}(x_1, \dots, x_d) = \left(\int_0^{x_1} f(s, x_2, \dots, x_d) \,\mathrm{d}s, 0, \dots, 0 \right)^\top . \tag{30}$$

Then, clearly, $\operatorname{div} \mathbf{F} = f$. Theoretically, a vector field $\mathbf{U}_h \in \mathbb{R}^d$ such that $\operatorname{div} \mathbf{U}_h = u_h$ can be constructed in the same way as $\mathbf{F}$. Practically, it is advantageous to use special properties of u_h known from its construction, e.g. the fact that u_h is piecewise linear. Anyway, vector field $\mathbf{q} = -\mathbf{F} + \kappa^2 \mathbf{U}_h$ lies in $\mathbf{Q}(f, u_h)$ and we can express the affine space $\mathbf{Q}(f, u_h)$ as $\mathbf{Q}(f, u_h) = \mathbf{q} + \mathbf{Q}_0$. Furthermore, $\mathbf{Q}_0 = \mathbf{curl}\, H^1(\Omega)$ for $d = 2$ and Ω being Lipschitz with finitely many holes [13]. Here, $\mathbf{curl}\, v = (\partial v/\partial x_2, -\partial v/\partial x_1)^\top$. This enable to find an approximate solution of the dual problem (28) in a convenient way, see [13, 23] for more details.

7 Numerical examples

In this section we compare the performance of estimators η, $\widehat{\eta}$, and $\widetilde{\eta}$ given by (5), (22), and (25), respectively, for two-dimensional model problem (1) for values of κ ranging from 0 to 10^6. The approximate solution u_h is obtain by the finite element method (FEM) of the lowest order. Thus, we consider a triangulation $\mathcal{T}_h$ of a polygonal approximation Ω_h of Ω and define a space V_h of piecewise linear and globally continuous functions on $\mathcal{T}_h$, i.e.

$$V_h = \{v \in V : v|_K \in P^1(K), \ K \in \mathcal{T}_h\},$$

where $P^1(K)$ stands for the space of linear functions on K. The Galerkin solution $u_h \in V_h$ of (1) is then uniquely determined by the requirement

$$\mathcal{B}(u_h, v_h) = \mathcal{F}(v_h) \quad \forall v_h \in V_h. \tag{31}$$

7.1 Approximate solution of the dual problems

The dual problems are solved in a similar way as the primal one using the same mesh $\mathcal{T}_h$. In the case of $\eta\left(u_h, \mathbf{y}_h^{p_*}\right)$ given by (5), we compute $\mathbf{y}_h^{p_*} \in \mathbf{W}_h^{p_*} \subset \mathbf{W}$ as a Galerkin solution of (8). The finite dimensional space $\mathbf{W}_h^{p_*}$ is defined as

$$\mathbf{W}_h^{p_*} = \left\{ \mathbf{w} \in \mathbf{W} : \mathbf{w}|_K \in [P^{p_*}(K)]^d,\ K \in \mathcal{T}_h \right\},$$

where $P^{p_*}(K)$ stands for the space of polynomials of degree at most p_* on K. Thus, the approximate solution $\mathbf{y}_h^{p_*} \in \mathbf{W}_h^{p_*}$ of the dual problem (8) satisfies

$$\mathcal{B}^*(\mathbf{y}_h^{p_*}, \mathbf{w}_h) = \mathcal{F}^*(\mathbf{w}_h) \quad \forall \mathbf{w}_h \in \mathbf{W}_h^{p_*}, \quad \kappa > 0. \tag{32}$$

In the case of $\widehat{\eta}(u_h, \widehat{\mathbf{y}}_h^{p_*})$ given by (22), we proceed in a very similar way. We minimize the upper bound (23) in the space $\mathbf{W}_h^{p_*}$. This is equivalent to the variational problem of finding $\widehat{\mathbf{y}}_h^{p_*} \in \mathbf{W}_h^{p_*}$ such that

$$\widehat{\mathcal{B}}^*(\widehat{\mathbf{y}}_h^{p_*}, \mathbf{w}_h) = \widehat{\mathcal{F}}^*(\mathbf{w}_h) \quad \forall \mathbf{w}_h \in \mathbf{W}_h^{p_*}, \tag{33}$$

where

$$\widehat{\mathcal{B}}^*(\mathbf{y}, \mathbf{w}) = C_\Omega^2 \int_\Omega \operatorname{div} \mathbf{y} \operatorname{div} \mathbf{w} \,\mathrm{d}x + \int_\Omega \mathbf{y} \cdot \mathbf{w} \,\mathrm{d}x, \qquad \widehat{\mathcal{F}}^*(\mathbf{w}) = -C_\Omega^2 \int_\Omega f \operatorname{div} \mathbf{w} \,\mathrm{d}x.$$

Notice that problems (32) and (33) only differ in the constant factors κ^{-2} and C_Ω^2, respectively. Furthermore, we stress that we minimize the quadratic functional (23) and use the obtained $\widehat{\mathbf{y}}_h^{p_*}$ in (22) to compute the error estimator $\widehat{\eta}(u_h, \widehat{\mathbf{y}}_h^{p_*})$.

Finally, in the case of $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}}_h^{p})$ given by (25), we obtain $\widetilde{\mathbf{y}}_h^{p} \in \mathbf{Q}(f, u_h)$ by Galerkin approximation of the dual problem (28). We use the technique described at the end of Section 6.2. In particular, we define $\mathbf{q} = -\mathbf{F} + \kappa^2 \mathbf{U}_h$, where $\mathbf{F}$ is given by (30) and the piecewise quadratic vector field $\mathbf{U}_h$ satisfies $\operatorname{div} \mathbf{U}_h = u_h$. Clearly, $\mathbf{q} \in \mathbf{Q}(f, u_h)$. Further, since $\mathbf{Q}_0 = \mathbf{curl}\, H^1(\Omega)$, we can express the solution of the dual problem (28) as $\widetilde{\mathbf{y}}^* = \mathbf{q} + \mathbf{curl}\, z$, where $z \in H^1(\Omega)$ satisfies

$$\int_\Omega \mathbf{curl}\, z \cdot \mathbf{curl}\, v \,\mathrm{d}x = -\int_\Omega \mathbf{q} \cdot \mathbf{curl}\, v \,\mathrm{d}x \quad \forall v \in H^1(\Omega). \tag{34}$$

Notice that $\mathbf{curl}\, z \cdot \mathbf{curl}\, v = \boldsymbol{\nabla} z \cdot \boldsymbol{\nabla} v$ and hence problem (34) is just the Poisson problem with homogeneous Neumann boundary conditions. Solution of this problem is unique up to an additive constant. The value of this constant is irrelevant, because we use $\mathbf{curl}\, z$ only. We solve problem (34) approximately by the p-version of the FEM using the same mesh $\mathcal{T}_h$. In particular, we define a finite dimensional space $\widetilde{V}_h^p = \{v \in H^1(\Omega) : v|_K \in P^p(K),\ K \in \mathcal{T}_h\}$ and find $z_h \in \widetilde{V}_h^p$ such that

$$\int_\Omega \boldsymbol{\nabla} z_h \cdot \boldsymbol{\nabla} v_h \,\mathrm{d}x = -\int_\Omega \mathbf{q} \cdot \mathbf{curl}\, v_h \,\mathrm{d}x \quad \forall v_h \in \widetilde{V}_h^p. \tag{35}$$

The approximate solution of the dual problem (28) is then given by $\widetilde{\mathbf{y}}_h^p = \mathbf{q} + \mathbf{curl}\, z_h$.

7.2 Test problems

We present two test problems. Both fit into the framework of the model problem (1). The first problem is defined on a square $\Omega = (-1/2, 1/2)^2$. The right-hand side is $f(x_1, x_2) = \cos(\pi x_1)\cos(\pi x_2)$ and the exact solution is

$$u(x_1, x_2) = \frac{\cos(\pi x_1)\cos(\pi x_2)}{2\pi^2 + \kappa^2}.$$

The finite element mesh $\mathcal{T}_h$ is shown in Figure 1 (left). By (20), the Friedrichs' constant is bounded by $C_\Omega = (\pi\sqrt{2})^{-1}$ in this case. We use this value in estimator (22).

The second test problem is posed in a unit circle $\Omega = \{(x_1, x_2) : r < 1\}$ with $r = (x_1^2 + x_2^2)^{1/2}$. The right-hand side and the exact solution are $f(x_1, x_2) = 1$ and

$$u(x_1, x_2) = \frac{1}{\kappa^2}\left(1 - \frac{I_0(\kappa r)}{I_0(\kappa)}\right) \text{ for } \kappa > 0 \quad \text{and} \quad u(x_1, x_2) = \frac{1 - x_1^2 - x_2^2}{4} \text{ for } \kappa = 0,$$

where I_0 denotes the modified Bessel function. For the FEM solution, the circle Ω is approximated by an inscribed regular polyhedron Ω_h with 16 vertices. The used mesh $\mathcal{T}_h$ is sketched in Figure 1 (right). The estimate (20) yields the value $C_\Omega = 1/\pi$ for the second test problem.

7.3 Results

In this section we present the numerical performance of the estimators $\eta\left(u_h, \mathbf{y}_h^{p_*}\right)$, $\widehat{\eta}\left(u_h, \widehat{\mathbf{y}}_h^{p_*}\right)$, and $\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^{p}\right)$, given by (5), (22), and (25) with the vector fields $\mathbf{y}_h^{p_*}$, $\widehat{\mathbf{y}}_h^{p_*}$, and $\widetilde{\mathbf{y}}_h^p = \mathbf{q} + \mathbf{curl}\, z_h$ obtained by (32), (33), and (35), respectively. Tables 1 and 2 present the results for the first test problem while Tables 3 and 4 for the second test problem. In Tables 1 and 3 we provide the indices of effectivity $I_{\text{eff}} = \eta / |\!|\!| u - u_h |\!|\!|$ for the above estimators with $p_* = 1$ and $p = 1$. Tables 2 and 4 show the same results for $p_* = 2$ and $p = 2, 3$.

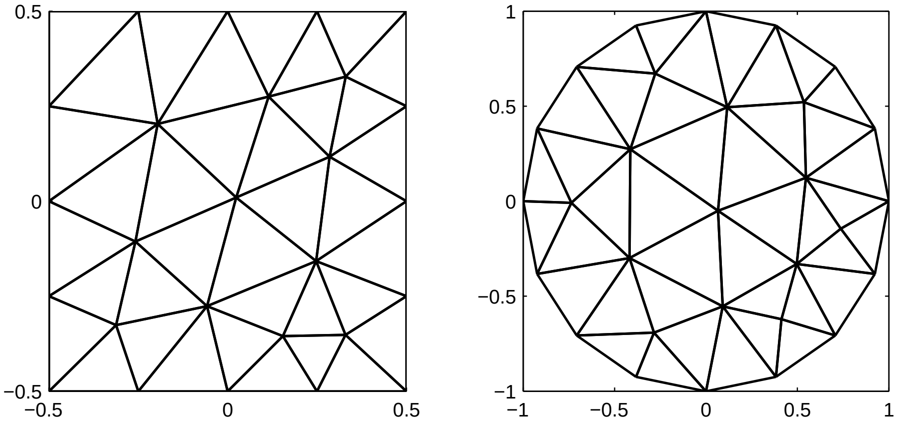

Figure 1: The meshes used for the first (left) and the second (right) test problem.

κ	$\eta\left(u_h, \mathbf{y}_h^1\right)$	$\widehat{\eta}\left(u_h, \widehat{\mathbf{y}}_h^1\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^1\right)$	η^{comb}
0	—	1.782	1.410	1.782
10^{-3}	$3.513 \cdot 10^3$	1.782	1.410	1.782
10^{-2}	$3.513 \cdot 10^2$	1.782	1.409	1.782
10^{-1}	$3.514 \cdot 10^1$	1.782	1.429	1.782
1	3.650	1.784	$5.041 \cdot 10^1$	1.784
10	1.058	1.889	$5.343 \cdot 10^3$	1.058
10^2	1.001	$2.219 \cdot 10^1$	$9.066 \cdot 10^4$	1.001
10^3	1.000	$2.292 \cdot 10^2$	$1.458 \cdot 10^6$	1.000
10^4	1.000	$2.293 \cdot 10^3$	$1.705 \cdot 10^7$	1.000
10^5	1.000	$2.293 \cdot 10^4$	$1.359 \cdot 10^8$	1.000
10^6	1.000	$2.293 \cdot 10^5$	$1.112 \cdot 10^9$	1.000

Table 1: Indices of effectivity for the first test problem with piecewise linear solutions of the dual problem.

κ	$\eta\left(u_h, \mathbf{y}_h^2\right)$	$\widehat{\eta}\left(u_h, \widehat{\mathbf{y}}_h^2\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^2\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^3\right)$	η^{comb}
0	—	1.161	1.008	1.000	1.161
10^{-3}	$4.937 \cdot 10^2$	1.161	1.008	1.000	1.161
10^{-2}	$4.939 \cdot 10^1$	1.161	1.009	1.000	1.161
10^{-1}	5.038	1.161	1.036	1.000	1.161
1	1.115	1.166	$4.496 \cdot 10^1$	1.003	1.166
10	1.001	1.640	$4.763 \cdot 10^3$	1.131	1.001
10^2	1.000	$1.732 \cdot 10^1$	$8.082 \cdot 10^4$	5.752	1.000
10^3	1.000	$1.771 \cdot 10^2$	$1.300 \cdot 10^6$	$5.744 \cdot 10^1$	1.000
10^4	1.000	$1.771 \cdot 10^3$	$1.520 \cdot 10^7$	$5.744 \cdot 10^2$	1.000
10^5	1.000	$1.771 \cdot 10^4$	$1.212 \cdot 10^8$	$5.744 \cdot 10^3$	1.000
10^6	1.000	$1.771 \cdot 10^5$	$9.908 \cdot 10^8$	$5.744 \cdot 10^4$	1.000

Table 2: Indices of effectivity for the first test problem with piecewise quadratic (and cubic in one case) solutions of the dual problem.

κ	$\eta\left(u_h, \mathbf{y}_h^1\right)$	$\widehat{\eta}\left(u_h, \widehat{\mathbf{y}}_h^1\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^1\right)$	η^{comb}
0	—	1.092	1.708	1.092
10^{-3}	1.000	1.092	1.708	1.092
10^{-2}	1.000	1.092	1.708	1.092
10^{-1}	1.001	1.092	1.711	1.092
1	1.086	1.166	7.789	1.148
10	1.223	3.712	$7.051 \cdot 10^1$	1.223
10^2	1.021	$2.641 \cdot 10^1$	$4.406 \cdot 10^2$	1.021
10^3	1.000	$2.579 \cdot 10^2$	$6.811 \cdot 10^3$	1.000
10^4	1.000	$2.579 \cdot 10^3$	$6.739 \cdot 10^4$	1.000
10^5	1.000	$2.579 \cdot 10^4$	$9.389 \cdot 10^5$	1.000
10^6	1.000	$2.579 \cdot 10^5$	$8.363 \cdot 10^6$	1.000

Table 3: Indices of effectivity for the second test problem with piecewise linear solutions of the dual problem.

κ	$\eta\left(u_h, \mathbf{y}_h^2\right)$	$\widehat{\eta}\left(u_h, \widehat{\mathbf{y}}_h^2\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^2\right)$	$\widetilde{\eta}\left(u_h, \widetilde{\mathbf{y}}_h^3\right)$	η^{comb}
0	—	1.083	1.000	0.978	1.083
10^{-3}	0.978	1.083	1.000	0.978	1.083
10^{-2}	0.978	1.083	1.000	0.978	1.083
10^{-1}	0.978	1.083	1.002	0.978	1.083
1	0.976	1.093	6.642	0.978	1.049
10	1.013	1.674	$6.098 \cdot 10^1$	1.402	1.013
10^2	1.011	9.805	$3.821 \cdot 10^2$	8.219	1.011
10^3	1.000	$9.539 \cdot 10^1$	$5.906 \cdot 10^3$	$7.996 \cdot 10^1$	1.000
10^4	1.000	$9.539 \cdot 10^2$	$5.845 \cdot 10^4$	$7.996 \cdot 10^2$	1.000
10^5	1.000	$9.539 \cdot 10^3$	$8.100 \cdot 10^5$	$7.996 \cdot 10^3$	1.000
10^6	1.000	$9.539 \cdot 10^4$	$7.250 \cdot 10^6$	$7.996 \cdot 10^4$	1.000

Table 4: Indices of effectivity for the second test problem with piecewise quadratic (and cubic in one case) solutions of the dual problem.

Results in Tables 1–4 indicate that the estimator η is robust for great values of κ and the estimators $\widehat{\eta}$ and $\widetilde{\eta}$ are robust for small values of κ. Taking minimum of values η, $\widehat{\eta}$, and $\widetilde{\eta}$, we obtain a robust error estimator for the entire range of κ. In addition, such an estimator is sharp and provides the guaranteed upper bound of the error. However, computing all three values of η, $\widehat{\eta}$, and $\widetilde{\eta}$ could be too costly. It is possible to obtain sharp, robust, and guaranteed upper bound by a combination of η and $\widehat{\eta}$, only. This combined approach requires practically the same number of arithmetic operations as the evaluation of η and it can be expressed as follows

$$\eta^{comb} = \begin{cases} \min\{\eta(u_h, \mathbf{y}_h), \widehat{\eta}(u_h, \mathbf{y}_h)\} & \text{for } C_\Omega^2 \kappa^2 \geq 1, \\ \min\{\eta(u_h, \widehat{\mathbf{y}}_h), \widehat{\eta}(u_h, \widehat{\mathbf{y}}_h)\} & \text{otherwise,} \end{cases}$$

where $\mathbf{y}_h$ is computed by (32), $\widehat{\mathbf{y}}_h$ by (33), and $\eta(u_h, \widehat{\mathbf{y}}_h) = \infty$ for $\kappa = 0$. Notice that the same computer code can be used for both $\mathbf{y}_h$ and $\widehat{\mathbf{y}}_h$, because the corresponding dual problems differ in the constant factors κ^{-2} and C_Ω^2 only. Further notice that having the norms $\left\|f - \kappa^2 u_h + \operatorname{div} \mathbf{y}_h\right\|_0$ and $\|\mathbf{y}_h - \boldsymbol{\nabla} u_h\|_0$ computed, the evaluation of $\eta(u_h, \mathbf{y}_h)$ and $\widehat{\eta}(u_h, \mathbf{y}_h)$ by (5) and (22) is trivial and practically for free. The indices of effectivity for η^{comb} are presented in the last columns of Tables 1–4.

However, if an upper bound C_Ω of the Friedrichs' constant is not available then estimator $\widetilde{\eta}$ must be used instead of $\widehat{\eta}$. In that case a robust and automatic procedure requires evaluation of both η and $\widetilde{\eta}$. This is computationally more intensive than the approach combining η and $\widehat{\eta}$, because the estimators η and $\widetilde{\eta}$ have different structure and have to be computed independently.

Further, we observe in Tables 3 and 4 that the estimator η behaves in a robust way for the entire range of κ for the second test problem. This is exceptional and it is due to the constantness of the right-hand side f. Furthermore, in Tables 3 and 4 we observe indices of effectivity less than one contradicting the fact that the error estimators provide guaranteed upper bound of the error. This is caused by the error stemming from the approximation of the circular domain Ω by a polygon Ω_h. In fact, we compute $\mathbf{y}_h \in \mathbf{H}(\mathrm{div}, \Omega_h)$ but then $\mathbf{y}_h \notin \mathbf{H}(\mathrm{div}, \Omega)$ in general. If we treated the approximate dual problem properly such that $\mathbf{y}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ then the estimator $\eta(u_h, \mathbf{y}_h)$ would provide the upper bound. The same is true for $\widehat{\eta}$ and $\widetilde{\eta}$ as well.

The performance of all the estimators on finer meshes was tested as well. Uniform refinements of meshes depicted in Figure 1 have practically no influence on the values of the indices of effectivity presented in Tables 1–4. Exceptional are the indices of effectivity in Tables 3 and 4 smaller than one, which tend to one for finer approximations Ω_h of Ω.

Relations (12) and (29) confirm the intuitive statement that solving the dual problems with higher accuracy yields sharper bounds on the error. Tables 1–4 illustrate this fact. Interestingly, the lowest order approximations ($p_* = 1$ and $p = 1$) of the dual problems provide already quite good results. Quadratic and higher-order approximations ($p_* = 2$ and $p = 2, 3$) of the dual problems give the energy norm of the error almost exactly in the robust regime.

8 Conclusions

Interestingly, the error estimators η, $\widehat{\eta}$, and $\widetilde{\eta}$ given by (5), (22), and (25), respectively, are independent from the way how the approximation $u_h \in V$ is obtained. In particular, the error $u - u_h$ in the estimates (6), (21), and (27) includes the discretization error, the error in the solver of linear algebraic equations, quadrature errors, etc. Furthermore, the upper bounds (6), (21), and (27) are guaranteed up to the quadrature and round-off errors in the evaluation of L^2-norms in (5), (22), and (25).

The key point for the performance of the estimators $\eta(u_h, \mathbf{y}_h)$, $\widehat{\eta}(u_h, \widehat{\mathbf{y}}_h)$, and $\widetilde{\eta}(u_h, \widetilde{\mathbf{y}}_h)$ is the choice of the vector fields $\mathbf{y}_h$, $\widehat{\mathbf{y}}_h$, and $\widetilde{\mathbf{y}}_h$. We showed that they are connected with certain dual problems. In Section 7 we present numerical experiments, where the vector fields $\mathbf{y}_h$, $\widehat{\mathbf{y}}_h$, and $\widetilde{\mathbf{y}}_h$ are obtained as Galerkin approximations of the solution of the respective dual problems. This approach yields very sharp and robust a posteriori error estimates for all values of the reaction coefficient κ. On the other hand, this approach is not local. Galerkin method for the dual problems is computationally intensive. For example, the number of degrees of freedom needed in our tests in the discrete dual problems (32) and (33) is roughly 7–10 times (for $p_* = 1$) and 16–27 times (for $p_* = 2$) higher than the number of degrees of freedom needed for the computation of u_h by (31). In case of $\widetilde{\eta}$ the number of degrees of freedom in the dual problem (35) is comparable with the discrete problem (31) for $p = 1$, but its several times higher for $p = 2$ and 3.

A useful approximation of the solution of the dual problem can be obtained by a fast algorithm using a postprocessing of the approximate solution u_h. A promising approach is the method of equilibrated residuals described in [2]. This is a fast method which is robust for small values of κ. A generalization robust in the singularly perturbed case (κ large) is presented in [1]. A combination of this method with estimators η, $\widehat{\eta}$, and $\widetilde{\eta}$ can lead to an efficient, robust, fast, and fully computable upper bound for the energy norm of the error. Construction and analysis of such an estimator is still under research. However, a partial result was already published in [23], where a combination of the method of equilibrated residuals with the estimator $\widetilde{\eta}$ is presented.

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