COMPLEMENTARITY – THE WAY TOWARDS GUARANTEED ERROR ESTIMATES*

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Abstract

This paper presents a review of the complementary technique with the emphasis on computable and guaranteed upper bounds of the approximation error. For simplicity, the approach is described on a numerical solution of the Poisson problem. We derive the complementary error bounds, prove their fundamental properties, present the method of hypercircle, mention possible generalizations and show a couple of numerical examples.

1 Introduction

Reliability of numerical schemes is a crucial topic in the scientific and technical computing. There is a general agreement that an approximate solution alone is not sufficient as an output of the computations. The user needs certain information about its accuracy.

An ultimate goal of numerical algorithms is to provide an approximate solution with accuracy within a prescribed tolerance in an efficient way. In the framework of numerical methods for partial differential equation this goal can be achieved. The needed tool is an *adaptive algorithm* equipped with an efficient and reliable error indicator for mesh refinements and with a *computable guaranteed upper bounds on the error* for the stopping criterion.

In this contribution we concentrate on the guaranteed upper bounds on the error in the context of the finite element method for linear elliptic problems. As a model problem we use the Poisson equation with homogeneous Dirichlet boundary conditions. We point out that the complementary approach is not limited to finite elements only and can be used for arbitrary numerical method.

To illustrate the adaptive approach we introduce certain notation motivated by the finite element method. The finite element approximation u_h of an exact solution u is typically constructed on a finite element mesh $\mathcal{T}_h$. In order to employ the adaptive algorithm, we need an error indicator η_K which estimates a suitable norm of the error $(u - u_h)|_K$ in the element $K \in \mathcal{T}_h$. In order to fulfill the goal and provide an approximation which is guaranteed to be under the user prescribed tolerance TOL, it is necessary to use certain guaranteed upper bound η on a suitable norm of the

*This work was supported by grant No. IAA100760702 of the Grant Agency of the Academy of Sciences of the Czech Republic and by the institutional research plan no. AV0Z10190503 of the Academy of Sciences of the Czech Republic.

error. The error bound η is said to be the *guaranteed upper bound* of the error if $\|u - u_h\| \le \eta$. Let us remark that the error bound η is often computed from the error indicators as $\eta^2 = \sum_{K\in\mathcal{T}_h} \eta_K^2$. Now, we can present the general adaptive algorithm:

1. *Initialize*: Construct the initial mesh $\mathcal{T}_h$.
2. *Solve*: Find approximate solution u_h on $\mathcal{T}_h$.
3. *Indicators*: Compute error indicators η_K for all $K \in \mathcal{T}_h$.
4. *Estimator*: Compute error estimator η.
5. *Stop*: If $\eta \le \mathrm{TOL}$ then STOP.
6. *Mark*: If $\eta_K \ge \Theta \max\limits_{K\in\mathcal{T}_h} \eta_K$ then mark K.
7. *Refine*: Refine the marked elements and build the new mesh $\mathcal{T}_h$.
8. Go to 2.

The parameter $\Theta \in (0, 1)$ in Step 6 is given by the user and determines the fraction of elements to be refined in each adaptive cycle.

In this adaptive algorithm we can clearly distinguish the different roles of error indicators η_K and the error estimator η. If the estimator η provides guaranteed upper bound of the error and the algorithm stops in Step 5 then $\|u - u_h\| \le \eta \le \mathrm{TOL}$ and the goal is fulfilled – the error is below the prescribed tolerance.

The computation of fully computable guaranteed upper bounds on the error seems to be a more difficult problem than construction of local error indicators η_K. The guaranteed error bounds can be successfully obtained by the *complementary approach*. The idea is fairly old. It goes back to the method of hypercircle from 1950's [21]. Further development came in 1970's and 1980's with the dual (or equilibrium) finite elements, see e.g. [4, 6, 8, 9, 11, 22, 28]. Later, the idea was worked out even further in the approach of error majorants, see e.g. [3, 13, 14, 17, 18, 16, 19]. Anyway, the idea can be traced in many other works, see e.g. [2, 5, 27].

In the rest of the paper we would like to give a brief review of the complementary approach for the Poisson problem. The emphasis is put on the derivation, properties, and practical implementation of computable guaranteed upper bounds on the energy norm of the error. The organization is the following. Section 2 introduces the classical and weak formulation of the Poisson equation. Section 3 contains derivation of the complementary guaranteed error bound and Section 4 presents the corresponding complementary problem and the theoretical properties of the complementary solution including the method of hypercircle. Section 5 briefly describes the concurrent approach of error majorants. Section 6 provides hints for practical evaluation of the obtained error bounds. Section 7 briefly lists possible generalizations of the complementary approach to various especially non-elliptic problems. Section 8 presents numerical examples to show the practical implementation and to compare the described variants of the error bounds mainly by their accuracy. Section 9 contains concluding remarks.

2 Model problem

Let us consider a domain $\Omega \subset \mathbb{R}^d$ with Lipschitz continuous boundary. The classical formulation of the Poisson problem reads: find $u \in C^2(\Omega) \cap C(\overline{\Omega})$ such that

$$-\Delta u = f \quad \text{in } \Omega, \tag{1}$$
$$u = 0 \quad \text{on } \partial\Omega. \tag{2}$$

In order to introduce the complementary approach, it is advantageous to formulate problem (1)–(2) in the weak sense. Therefore, we consider the standard Sobolev space $V = H_0^1(\Omega)$ of square-integrable functions with square-integrable derivatives and vanishing traces on the boundary $\partial\Omega$.

The weak formulation of problem (1)–(2) reads: find $u \in V$ such that

$$\mathcal{B}(u, v) = \mathcal{F}(v) \quad \forall v \in V. \tag{3}$$

The bilinear form $\mathcal{B}$ and the linear functional $\mathcal{F}$ are given as

$$\mathcal{B}(u, v) = (\boldsymbol{\nabla} u, \boldsymbol{\nabla} v) \quad \text{and} \quad \mathcal{F}(v) = (f, v),$$

where

$$(\boldsymbol{v}, \boldsymbol{w}) = \int_\Omega \boldsymbol{v} \cdot \boldsymbol{w} \, \mathrm{d}x \quad \text{and} \quad (v, w) = \int_\Omega vw \, \mathrm{d}x$$

stand for the vector and scalar version of the $L^2(\Omega)$ inner product. We point out that within the paper we denote the vector quantities by bold symbols.

The following lemma presents a simple observation. It says that the gradient $\boldsymbol{\nabla} u$ of the weak solution of (3) lies in $\mathbf{H}(\mathrm{div}, \Omega)$. For the reader's convenience, we recall the definition

$$\mathbf{H}(\mathrm{div}, \Omega) = \left\{ \boldsymbol{y} \in [L^2(\Omega)]^d : \mathrm{div}\, \boldsymbol{y} \in L^2(\Omega) \right\}, \tag{4}$$

where the divergence is understood in the sense of distributions.

Lemma 1. *Let $u \in V$ be the weak solution given by* (3)*. If the corresponding right-hand side f is in $L^2(\Omega)$ then $\boldsymbol{\nabla} u \in \mathbf{H}(\mathrm{div}, \Omega)$.*

Proof. The divergence $\mathrm{div}\, \boldsymbol{y}$ is in $L^2(\Omega)$ in the sense of distributions if and only if there exists $z \in L^2(\Omega)$ such that $(v, z) = -(\boldsymbol{\nabla} v, \boldsymbol{y})$ for all $v \in C_0^\infty(\Omega)$. Thus, putting $z = -f$, we immediately conclude that $\boldsymbol{y} = \boldsymbol{\nabla} u$ lies in $\mathbf{H}(\mathrm{div}, \Omega)$ whenever f lies in $L^2(\Omega)$, see definitions (4) and (3). $\square$

We remind that the $z \in L^2(\Omega)$ from the above proof is called the distributional divergence of $\boldsymbol{y} \in [L^2(\Omega)]^d$ and we put $\mathrm{div}\, \boldsymbol{y} = z$.

3 Derivation of the complementary error estimate

The complementary error estimates can be easily derived using the divergence theorem:

$$\int_\Omega v \operatorname{div} \boldsymbol{y} \, \mathrm{d}x + \int_\Omega \boldsymbol{y} \cdot \boldsymbol{\nabla} v \, \mathrm{d}x - \int_{\partial\Omega} v \boldsymbol{y} \cdot \boldsymbol{n} \, \mathrm{d}x = 0 \quad \forall v \in H^1(\Omega), \ \forall \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega), \tag{5}$$

where $\boldsymbol{n}$ stands for the unit outward normal vector to the boundary $\partial\Omega$.

The definition of the weak solution (3) together with the divergence theorem yields the following identity for arbitrary $u_h \in V$, $v \in V$, and $\boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega)$:

$$\begin{aligned} \mathcal{B}(u - u_h, v) &= (f, v) - (\boldsymbol{\nabla} u_h, \boldsymbol{\nabla} v) + (v, \operatorname{div} \boldsymbol{y}) + (\boldsymbol{y}, \boldsymbol{\nabla} v) \\ &= (f + \operatorname{div} \boldsymbol{y}, v) + (\boldsymbol{y} - \boldsymbol{\nabla} u_h, \boldsymbol{\nabla} v). \end{aligned} \tag{6}$$

This is the main trick. Subsequent derivation of the complementary error estimates is based on more or less standard technical steps. Crucial point is the handling of the term $(f + \operatorname{div} \boldsymbol{y}, v)$. There are at least two possibilities. The first one is to restrict the set of admissible $\boldsymbol{y}$ such that this term vanishes. The second one is based on the Friedrichs' inequality. We postpone the second possibility to Section 5 and start with the first one.

We introduce an affine space

$$\boldsymbol{Q}(f) = \{ \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega) : (\boldsymbol{y}, \boldsymbol{\nabla} v) = (f, v) \quad \forall v \in V \}. \tag{7}$$

This is a set of vector fields $\boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega)$ satisfying $-\operatorname{div} \boldsymbol{y} = f$ in the weak sense. Below, we will use the consistent notation $\boldsymbol{Q}(0)$ for the space of divergence-free (solenoidal) vector fields.

Using identity (6) for any $\boldsymbol{y} \in \boldsymbol{Q}(f)$ and the Cauchy-Schwarz inequality, we immediately obtain

$$\mathcal{B}(u - u_h, v) = (\boldsymbol{y} - \boldsymbol{\nabla} u_h, \boldsymbol{\nabla} v) \le \|\boldsymbol{y} - \boldsymbol{\nabla} u_h\|_0 \, \|\boldsymbol{\nabla} v\|_0 \,, \tag{8}$$

where $\|\boldsymbol{w}\|_0^2 = (\boldsymbol{w}, \boldsymbol{w})$ is the norm in $[L^2(\Omega)]^d$. Introducing the energy norm $|||v|||^2 = \mathcal{B}(v, v) = \|\boldsymbol{\nabla} v\|_0^2$ and substituting $v = u - u_h$ into (8) yields finally the guaranteed upper bound on the approximation error of u_h:

$$|||u - u_h||| \le \eta(u_h, \boldsymbol{y}) \qquad \forall u_h \in V, \ \forall \boldsymbol{y} \in \boldsymbol{Q}(f), \tag{9}$$

where the complementary error estimate is given by

$$\eta(u_h, \boldsymbol{y}) = \|\boldsymbol{y} - \boldsymbol{\nabla} u_h\|_0 \,. \tag{10}$$

We point out that the error bound (9) holds true for arbitrary conforming approximation $u_h \in V$ of the weak solution u, regardless what numerical method has been used for it. In addition, the bound (9) is valid for any $\boldsymbol{y} \in \boldsymbol{Q}(f)$. Hence, practically, any vector field from $\boldsymbol{Q}(f)$ used in (9) provides guaranteed upper bound on the energy norm of the approximation error. However, this $\boldsymbol{y} \in \boldsymbol{Q}(f)$ must be chosen with care, otherwise the value $\eta(u_h, \boldsymbol{y})$ overestimates the error too much. A practical choice of a suitable $\boldsymbol{y} \in \boldsymbol{Q}(f)$ is discussed below in Section 6.

Let us conclude this section by summarizing the main statement into a theorem.

Theorem 2. *If $u \in V$ is the exact solution of problem* (3) *and $u_h \in V$ its arbitrary approximation then estimate* (9)–(10) *holds true for any $\boldsymbol{y} \in \boldsymbol{Q}(f)$.*

4 The complementary problem

Let the approximation $u_h \in V$ be fixed. Since $\eta(u_h, \boldsymbol{y})$ is an upper bound of its error, it is natural to ask, what $\boldsymbol{y} \in \boldsymbol{Q}(f)$ minimizes this error bound. The problem of minimization of $\eta(u_h, \boldsymbol{y})$ with respect to $\boldsymbol{y} \in \boldsymbol{Q}(f)$ is called the complementary problem and its solution the complementary solution. It turns out that this problem can be formulated in several equivalent forms. Before, we state a theorem about this equivalence, let us introduce certain notation. Let us define the complementary bilinear form $\mathcal{B}^*(\boldsymbol{y}, \boldsymbol{w}) = (\boldsymbol{y}, \boldsymbol{w})$, the complementary energy norm $|||\boldsymbol{w}|||_*^2 = \mathcal{B}^*(\boldsymbol{w}, \boldsymbol{w})$, and the functional of the complementary energy $J^*(\boldsymbol{w}) = \frac{1}{2}\mathcal{B}^*(\boldsymbol{w}, \boldsymbol{w})$.

Theorem 3. *The following problems are equivalent*

$$\textit{find } \boldsymbol{y} \in \boldsymbol{Q}(f): \quad \eta(u_h, \boldsymbol{y}) \le \eta(u_h, \boldsymbol{w}) \quad \forall \boldsymbol{w} \in \boldsymbol{Q}(f), \tag{11}$$

$$\textit{find } \boldsymbol{y} \in \boldsymbol{Q}(f): \quad J^*(\boldsymbol{y}) \le J^*(\boldsymbol{w}) \quad \forall \boldsymbol{w} \in \boldsymbol{Q}(f), \tag{12}$$

$$\textit{find } \boldsymbol{y} \in \boldsymbol{Q}(f): \quad \mathcal{B}^*(\boldsymbol{y}, \boldsymbol{w}^0) = 0 \quad \forall \boldsymbol{w}^0 \in \boldsymbol{Q}(0). \tag{13}$$

Proof. First, we prove the equivalence of (11) and (12). Using (10) in (11), and utilizing the fact that $(\boldsymbol{y}, \boldsymbol{\nabla} u_h) = (\boldsymbol{w}, \boldsymbol{\nabla} u_h) = (f, u_h)$ for any $\boldsymbol{y} \in \boldsymbol{Q}(f)$ and $\boldsymbol{w} \in \boldsymbol{Q}(f)$, we can perform the following chain of simple equivalent adjustments:

$$\begin{gathered}
\eta(u_h, \boldsymbol{y}) \le \eta(u_h, \boldsymbol{w}), \\
\|\boldsymbol{y} - \boldsymbol{\nabla} u_h\|_0^2 \le \|\boldsymbol{w} - \boldsymbol{\nabla} u_h\|_0^2, \\
\|\boldsymbol{y}\|_0^2 - 2(\boldsymbol{y}, \boldsymbol{\nabla} u_h) + \|\boldsymbol{\nabla} u_h\|_0^2 \le \|\boldsymbol{w}\|_0^2 - 2(\boldsymbol{w}, \boldsymbol{\nabla} u_h) + \|\boldsymbol{\nabla} u_h\|_0^2, \\
\|\boldsymbol{y}\|_0^2 \le \|\boldsymbol{w}\|_0^2, \\
J^*(\boldsymbol{y}) \le J^*(\boldsymbol{w}).
\end{gathered}$$

Second, we prove that any solution of problem (12) is a solution of (13). Let $\boldsymbol{y} \in \boldsymbol{Q}(f)$ be a solution of (12) and let $\boldsymbol{w}^0 \in \boldsymbol{Q}(0)$ be arbitrary. Then $\boldsymbol{y} + t\boldsymbol{w}^0$ lies in $\boldsymbol{Q}(f)$ for any $t \in \mathbb{R}$ and the real function $\varphi(t) = \|\boldsymbol{y} + t\boldsymbol{w}^0\|_0^2$ has the global minimum at $t = 0$. If we compute the derivative of $\varphi(t)$ at $t = 0$ by definition, we obtain

$$\varphi'(0) = \lim_{t \to 0} \frac{\|\boldsymbol{y} + t\boldsymbol{w}^0\|_0^2 - \|\boldsymbol{y}\|_0^2}{t} = \lim_{t \to 0} \frac{2t(\boldsymbol{y}, \boldsymbol{w}^0) + t^2 \|\boldsymbol{w}^0\|_0^2}{t} = 2\mathcal{B}^*(\boldsymbol{y}, \boldsymbol{w}^0).$$

Hence, the derivative exists and since $\varphi(t)$ has the minimum at $t=0$, the derivative has to vanish: $\varphi'(0)=0$. This proves that $\boldsymbol{y}$ solves (13).

Finally, we prove that any solution of (13) is a solution of (12). Let $\boldsymbol{y} \in \boldsymbol{Q}(f)$ be the solution of (13) and let $\boldsymbol{w} \in \boldsymbol{Q}(f)$ be arbitrary. Let us set $\boldsymbol{w}^0 = \boldsymbol{w} - \boldsymbol{y}$. Clearly, $\boldsymbol{w}^0 \in \boldsymbol{Q}(0)$. Since $(\boldsymbol{y}, \boldsymbol{w}) = (\boldsymbol{y}, \boldsymbol{y} + \boldsymbol{w}^0) = \|\boldsymbol{y}\|_0^2$, see (13), we easily conclude that

$$0 \le \|\boldsymbol{w} - \boldsymbol{y}\|_0^2 = \|\boldsymbol{w}\|_0^2 - 2(\boldsymbol{y}, \boldsymbol{w}) + \|\boldsymbol{y}\|_0^2 = \|\boldsymbol{w}\|_0^2 - \|\boldsymbol{y}\|_0^2 .$$

This proves that $\boldsymbol{y}$ solves (12). □

Formulation (11) of the complementary problem is natural to derive. It is a straightforward minimization of η. Formulation (12) is variational. It is a minimization of a simple quadratic functional – the complementary energy J^*. Variant (13) is a weak formulation using the complementary bilinear form $\mathcal{B}^*$. Notice that in the simple case of Poisson equation (3), the complementary problem is just a problem of orthogonal projection. The following theorem finds the complementary solution and states that it is unique.

Theorem 4. *Let $u \in V$ be the exact solution of problem* (3). *Then $\boldsymbol{y} = \boldsymbol{\nabla} u$ lies in $\boldsymbol{Q}(f)$ and it is the unique solution of complementary problems* (11)–(13).

Proof. Lemma 1 implies that $\boldsymbol{\nabla} u$ lies in $\mathbf{H}(\mathrm{div}, \Omega)$. Weak formulation (3) guarantees that $\boldsymbol{\nabla} u$ is in $\boldsymbol{Q}(f)$. Substituting $\boldsymbol{y} = \boldsymbol{\nabla} u$ into (13) and using the definition (7) of $\boldsymbol{Q}(0)$ we immediately find that

$$(\boldsymbol{y}, \boldsymbol{w}^0) = (\boldsymbol{\nabla} u, \boldsymbol{w}^0) = 0 \quad \forall \boldsymbol{w}^0 \in \boldsymbol{Q}(0).$$

Thus, $\boldsymbol{y} = \boldsymbol{\nabla} u$ is a solution of problem (13).

To prove the uniqueness, we consider two solutions $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \boldsymbol{Q}(f)$ of problem (13). Then of course $(\boldsymbol{y}_1 - \boldsymbol{y}_2, \boldsymbol{w}^0) = 0$ for all $\boldsymbol{w}^0 \in \boldsymbol{Q}(0)$. Since $\boldsymbol{y}_1 - \boldsymbol{y}_2 \in \boldsymbol{Q}(0)$, we can set $\boldsymbol{w}^0 = \boldsymbol{y}_1 - \boldsymbol{y}_2$ and obtain $\|\boldsymbol{y}_1 - \boldsymbol{y}_2\|_0 = 0$. Thus, $\boldsymbol{y}_1 = \boldsymbol{y}_2$.

Theorem 3 finishes the proof. □

Sometimes, we call problem (3) the primal problem, in order to distinguish it from the complementary problem. Notice that this primal problem can also be equivalently formulated as energy minimization. The corresponding functional of primal energy is $J(v) = \frac{1}{2}\mathcal{B}(v,v) - \mathcal{F}(v)$. Interestingly, if we sum up the functionals of primal and complementary energy evaluated at the exact primal and complementary solutions u and $\boldsymbol{y} = \boldsymbol{\nabla} u$, we obtain zero:

$$J(u) + J^*(\boldsymbol{y}) = -\frac{1}{2}\mathcal{B}(u,u) + \frac{1}{2}\mathcal{B}^*(\boldsymbol{\nabla} u, \boldsymbol{\nabla} u) = 0.$$

The next theorem provides an interesting result. It reminds the Pythagoras' theorem and it is based on the orthogonality of the spaces $\boldsymbol{Q}(0)$ and $\boldsymbol{\nabla} V$, i.e.,

$$(\boldsymbol{w}^0, \boldsymbol{\nabla} v) = 0 \quad \forall \boldsymbol{w}^0 \in \boldsymbol{Q}(0),\ \forall v \in V, \tag{14}$$

see (7). Figure 1 (left) illustrates this orthogonality.

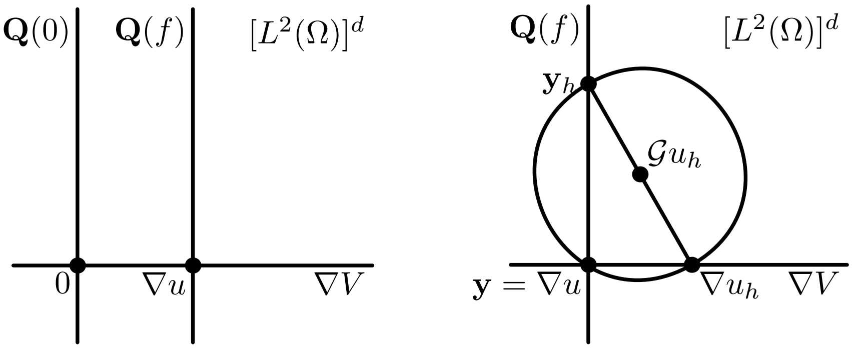

Figure 1: Orthogonality of spaces $\boldsymbol{Q}(f)$ and $\boldsymbol{\nabla} V$ in $[L^2(\Omega)]^d$ (left). An illustration of the method of hypercircle (right).

Theorem 5. *Let $u \in V$ and $\boldsymbol{y} \in \boldsymbol{Q}(f)$ be exact solutions of problems* (3) *and* (11)–(13)*, respectively. Then*

$$\eta^2(u, \boldsymbol{y}_h) + \eta^2(u_h, \boldsymbol{y}) = \eta^2(u_h, \boldsymbol{y}_h) \quad \forall u_h \in V,\ \forall \boldsymbol{y}_h \in \boldsymbol{Q}(f). \tag{15}$$

Proof. We use the fact that $\boldsymbol{y} = \boldsymbol{\nabla} u$, see Theorem 4, and the orthogonality (14) in the form $(\boldsymbol{y}_h - \boldsymbol{\nabla} u, \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h) = 0$ to compute

$$\begin{aligned}\eta^2(u_h, \boldsymbol{y}_h) &= \|\boldsymbol{y}_h - \boldsymbol{\nabla} u + \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 \\ &= \|\boldsymbol{y}_h - \boldsymbol{\nabla} u\|_0^2 + \|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 = \eta^2(u, \boldsymbol{y}_h) + \eta^2(u_h, \boldsymbol{y}).\end{aligned}$$

□

Notice that using definition (10) and Theorem 4, equality (15) can be stated in the form

$$\|\boldsymbol{y}_h - \boldsymbol{y}\|_0^2 + \|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\|_0^2 = \|\boldsymbol{y}_h - \boldsymbol{\nabla} u_h\|_0^2 . \tag{16}$$

This relates the error in the complementary problem and the error in the primal problem with the computable difference of the approximate primal and complementary solutions. Consequently, the error estimate $\eta(u_h, \boldsymbol{y}_h)$ is also a guaranteed upper bound on the complementary energy norm of the error in the complementary problem:

$$|\!|\!|\boldsymbol{y} - \boldsymbol{y}_h|\!|\!|_* \le \eta(u_h, \boldsymbol{y}_h) \quad \forall u_h \in V,\ \forall \boldsymbol{y}_h \in \boldsymbol{Q}(f).$$

The final result of this section is called the method of hypercircle. It is a remarkable result in the field of the a posteriori error estimates, because it provides an approximation whose error is known exactly. More precisely, the arithmetic average of $\boldsymbol{\nabla} u_h$ (the gradient of the approximate primal solution) and $\boldsymbol{y}_h$ (the approximate complementary solution) yields an approximation $\boldsymbol{\mathcal{G}} u_h = (\boldsymbol{y}_h + \boldsymbol{\nabla} u_h)/2$ of $\boldsymbol{\nabla} u$ (the gradient of the exact solution). The error of $\boldsymbol{\mathcal{G}} u_h$ measured in the complementary energy norm can be computed exactly from the knowledge of u_h and $\boldsymbol{y}_h$. See Figure 1 (right) for an illustration.

Theorem 6 (Method of hypercircle)**.** *Let $u \in V$ be the exact solution of problem* (3)*. Consider arbitrary $u_h \in V$ and $\boldsymbol{y}_h \in \boldsymbol{Q}(f)$ and set $\boldsymbol{\mathcal{G}} u_h = (\boldsymbol{y}_h + \boldsymbol{\nabla} u_h)/2$. Then*

$$\|\!|\boldsymbol{\nabla} u - \boldsymbol{\mathcal{G}} u_h|\!\|_* = \frac{1}{2}\eta(u_h, \boldsymbol{y}_h).$$

Proof. Using the fact that $\boldsymbol{\nabla} u \in \boldsymbol{Q}(f)$ and again the orthogonality (14) in the form $(\boldsymbol{\nabla} u - \boldsymbol{y}_h, \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h) = 0$, the statement follows from (16) by direct computations:

$$\begin{aligned}4\left\|\boldsymbol{\nabla} u - \boldsymbol{\mathcal{G}} u_h\right\|_0^2 &= \left\|\boldsymbol{\nabla} u - \boldsymbol{y}_h + \boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\right\|_0^2 \\ &= \left\|\boldsymbol{\nabla} u - \boldsymbol{y}_h\right\|_0^2 + \left\|\boldsymbol{\nabla} u - \boldsymbol{\nabla} u_h\right\|_0^2 = \left\|\boldsymbol{y}_h - \boldsymbol{\nabla} u_h\right\|_0^2.\end{aligned}$$

□

5 Error majorants

As we announced above in Section 3, there is also another possibility how to derive a guaranteed upper bound from (6). It is based on *Friedrichs' inequality*:

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

see e.g. [15]. The optimal constant C_Ω is known as the *Friedrichs' constant.* Its determination is a difficult task and its exact value is known in exceptional cases only. However, various upper bounds for Friedrichs' constant C_Ω are known. For example, in [12] we can find the estimate

$$C_\Omega \le \frac{1}{\pi}\left(\frac{1}{|a_1|^2} + \cdots + \frac{1}{|a_d|^2}\right)^{-1/2}, \tag{17}$$

where $|a_1|$, …, $|a_d|$ are lengths of sides of a d-dimensional box, the domain Ω is contained in.

Using the Cauchy-Schwarz and the Friedrichs' inequality in (6), we obtain

$$\mathcal{B}(u - u_h, v) \le \left(C_\Omega \left\|f + \operatorname{div} \boldsymbol{y}\right\|_0 + \left\|\boldsymbol{y} - \boldsymbol{\nabla} u_h\right\|_0\right) \|\!|v|\!\|.$$

Substitution $v = u - u_h$ yields the error estimate

$$\|\!|u - u_h|\!\| \le \widehat{\eta}(u_h, \boldsymbol{y}) \quad \forall u_h \in V,\ \forall \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega), \tag{18}$$

where

$$\widehat{\eta}(u_h, \boldsymbol{y}) = C_\Omega \left\|f + \operatorname{div} \boldsymbol{y}\right\|_0 + \left\|\boldsymbol{y} - \boldsymbol{\nabla} u_h\right\|_0. \tag{19}$$

This is another guaranteed upper bound on the energy norm of error. The advantage of $\widehat{\eta}(u_h, \boldsymbol{y})$ in comparison with $\eta(u_h, \boldsymbol{y})$ given by (10) is that the estimate (19) is valid for any $\boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega)$ and the set $\boldsymbol{Q}(f)$, which might be difficult to handle in practice – see Section 6, is not needed. On the other hand evaluation of $\widehat{\eta}(u_h, \boldsymbol{y})$ requires the knowledge of the Friedrichs' constant C_Ω or of its upper bound.

The error bound $\widehat{\eta}(u_h, \boldsymbol{y})$ – as well as $\eta(u_h, \boldsymbol{y})$ – is sharp in the sense that the gradient of the exact solution $\boldsymbol{y} = \boldsymbol{\nabla} u$ yields the error exactly: $\widehat{\eta}(u_h, \boldsymbol{\nabla} u) = |||u - u_h|||$. Notice that the term with C_Ω in $\widehat{\eta}(u_h, \boldsymbol{y})$ vanishes for $\boldsymbol{y} = \boldsymbol{\nabla} u$. It means that the error bound $\widehat{\eta}(u_h, \boldsymbol{y})$ can provide sharp results even if the Friedrichs' constant C_Ω is estimated very roughly.

However, from the point of the theory, the results of Theorems 3–6 are not valid for $\widehat{\eta}(u_h, \boldsymbol{y})$, in general. Moreover, the quantity $\widehat{\eta}^2(u_h, \boldsymbol{y})$ is not a quadratic functional in $\boldsymbol{y}$, any more. Nevertheless, there is a way how to transform it into a quadratic one. Introducing a real parameter $\beta > 0$, we can estimate $\widehat{\eta}^2(u_h, \boldsymbol{y})$ in an elementary way as

$$\widehat{\eta}(u_h, \boldsymbol{y}) \le \widehat{\eta}_\beta(u_h, \boldsymbol{y}) \quad \forall \beta > 0,\ \forall u_h \in V,\ \forall \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega),$$

where

$$\widehat{\eta}_\beta^2(u_h, \boldsymbol{y}) = \left(1 + \beta^{-1}\right) C_\Omega^2 \, \|f + \operatorname{div} \boldsymbol{y}\|_0^2 + (1 + \beta) \, \|\boldsymbol{y} - \boldsymbol{\nabla} u_h\|_0^2$$

is already quadratic in $\boldsymbol{y}$. Notice that there is always a suitable value of β such that $\widehat{\eta}_\beta(u_h, \boldsymbol{y}) = \widehat{\eta}(u_h, \boldsymbol{y})$.

In principle we should minimize $\widehat{\eta}_\beta(u_h, \boldsymbol{y})$ simultaneously with respect to $\boldsymbol{y}$ and β. This general nonlinear minimization problem might be difficult to solve. Anyway, for fixed $u_h \in V$ and fixed $\beta > 0$ the quadratic functional $\widehat{\eta}_\beta^2(u_h, \boldsymbol{y})$ can be minimized in a standard way. If we consider the minimization problem

$$\text{find } \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega) : \quad \widehat{\eta}_\beta(u_h, \boldsymbol{y}) \le \widehat{\eta}_\beta(u_h, \boldsymbol{w}) \quad \forall \boldsymbol{w} \in \mathbf{H}(\operatorname{div}, \Omega),$$

we find as above that it is equivalent to the problem

$$\text{find } \boldsymbol{y} \in \mathbf{H}(\operatorname{div}, \Omega) : \quad \widehat{\mathcal{B}}(\boldsymbol{y}, \boldsymbol{w}) = \widehat{\mathcal{F}}(\boldsymbol{w}) \quad \forall \boldsymbol{w} \in \mathbf{H}(\operatorname{div}, \Omega), \tag{20}$$

where

$$\begin{aligned} \widehat{\mathcal{B}}(\boldsymbol{y}, \boldsymbol{w}) &= (\operatorname{div} \boldsymbol{y}, \operatorname{div} \boldsymbol{w}) + \beta C_\Omega^{-2} (\boldsymbol{y}, \boldsymbol{w}), \\ \widehat{\mathcal{F}}(\boldsymbol{w}) &= (-f, \operatorname{div} \boldsymbol{w}) + \beta C_\Omega^{-2} (\boldsymbol{\nabla} u_h, \boldsymbol{w}). \end{aligned}$$

Notice that the upper bound $\widehat{\eta}(u_h, \boldsymbol{y})$ is more general than the upper bound $\eta(u_h, \boldsymbol{y})$ in the sense that $\eta(u_h, \boldsymbol{y})$ can be derived from $\widehat{\eta}(u_h, \boldsymbol{y})$. Indeed, $\widehat{\eta}(u_h, \boldsymbol{y}) = \eta(u_h, \boldsymbol{y})$ for all $\boldsymbol{y} \in \boldsymbol{Q}(f)$.

6 Practical computation of the complementary solution

The practical handling of the affine space $\boldsymbol{Q}(f)$ defined in (7) might be difficult in general. Here, we present a possible approach from [11]. For simplicity, we consider two dimensions only, i.e., $d = 2$.

First of all, we exploit the affine structure of $\boldsymbol{Q}(f)$. Any vector field $\boldsymbol{w} \in \boldsymbol{Q}(f)$, can be expressed as $\boldsymbol{w} = \overline{\boldsymbol{q}} + \boldsymbol{w}^0$, where $\overline{\boldsymbol{q}} \in \boldsymbol{Q}(f)$ is fixed and $\boldsymbol{w}^0$ lies in a linear space $\boldsymbol{Q}(0)$ of divergence-free vector fields. If an antiderivative of $f = f(x_1, x_2)$ with respect to one of its variables is known, we can construct $\overline{\boldsymbol{q}}$ for example as

$$\overline{\boldsymbol{q}}(x_1, x_2) = -\left(\int_0^{x_1} f(s, x_2)\,\mathrm{d}s, 0\right)^T. \tag{21}$$

Further, if the domain Ω is simply connected, then for any $\boldsymbol{w}^0 \in \boldsymbol{Q}(0)$ exists $v \in H^1(\Omega)$ such that $\boldsymbol{w}^0 = \mathbf{curl}\, v$, where $\mathbf{curl}\, v = (\partial v/\partial x_2, -\partial v/\partial x_1)^T$ is understood in the weak sense, see e.g. [11]. All together, any $\boldsymbol{w} \in \boldsymbol{Q}(f)$ can be expressed as $\boldsymbol{w} = \overline{\boldsymbol{q}} + \mathbf{curl}\, v$ for a $v \in H^1(\Omega)$. In terms of spaces, we can write

$$\boldsymbol{Q}(f) = \overline{\boldsymbol{q}} + \mathbf{curl}\, H^1(\Omega).$$

This structure enables to reformulate the complementary problem (13) as follows:

$$\text{find } z \in H^1(\Omega): \quad \mathcal{B}^*(\mathbf{curl}\, z, \mathbf{curl}\, v) = -\mathcal{B}^*(\overline{\boldsymbol{q}}, \mathbf{curl}\, v) \quad \forall v \in H^1(\Omega). \tag{22}$$

The corresponding complementary solution is then $\boldsymbol{y} = \overline{\boldsymbol{q}} + \mathbf{curl}\, z$. If we notice that $\mathcal{B}^*(\mathbf{curl}\, z, \mathbf{curl}\, v) = \mathcal{B}(z, v)$, problem (22) actually turns into the Poisson problem:

$$\text{find } z \in H^1(\Omega): \quad \mathcal{B}(z, v) = -\mathcal{B}^*(\overline{\boldsymbol{q}}, \mathbf{curl}\, v) \quad \forall v \in H^1(\Omega). \tag{23}$$

Let us remark that in contrast to (3), where we have prescribed the Dirichlet boundary conditions, problem (23) is equipped with Neumann boundary conditions. It is a consistent pure Neumann problem. Thus, it has infinitely many solutions and these solutions differ by a constant. Notice, that the actual value of this constant is irrelevant, because we only are interested in $\mathbf{curl}\, z$.

Problem (23) can be approximately solved by any standard numerical method for Poisson equation. For example, we can use the same method as we have used for the approximate solution of (3).

7 Generalizations

The complementary approach seems to be quite special. From this point of view it might be surprising that it can be generalized to a wide variety of problems. However, for more complicated problems the complementary upper bounds loose some of their properties, we presented in Theorems 3–6.

Generalization of the complementary approach for diffusion-reaction equation

$$-\Delta u + \kappa^2 u = f$$

is of particular interest, because it requires an additional idea, see e.g. [2, 5, 10, 20, 23, 24, 25]. We will not describe it here in detail, we only introduce the resulting upper bound:

$$|\!|\!| u - u_h |\!|\!| \le \eta(u_h, \boldsymbol{y}) \quad \forall u_h \in V,\ \forall \boldsymbol{y} \in \mathbf{H}(\mathrm{div}, \Omega),$$

where

$$\eta(u_h, \boldsymbol{y})^2 = \|\boldsymbol{y} - \boldsymbol{\nabla} u_h\|_0^2 + \left\|\kappa^{-1}(f - \kappa^2 u_h + \operatorname{div} \boldsymbol{y})\right\|_0^2. \tag{24}$$

We point out that this upper bound cannot be used for the Poisson problem, i.e. for $\kappa = 0$. However, in the singularly perturbed case, i.e., for large values of κ, this upper bound provides very sharp results. In addition, for the upper bound (24) we can prove analogues of Theorems 3–6, see [25].

The presented complementary approaches (10), (19), and (24) can be generalized in more or less straightforward way to general linear elliptic problems with anisotropic diffusion, convection and reaction terms, equipped with a combination of Dirichlet, Neumann, and Robin boundary conditions. They can be generalized even to systems of such elliptic equations [26].

Nevertheless, the complementary approach is not limited to elliptic problems only. It has been generalized to linear elasticity [14], to system of thermo-elasticity [13], to stationary Navier-Stokes problem [17], to variational inequalities [7], to certain nonlinear problems [18], to equations with the curl operator [3], etc.

The complementary approach of error majorants for most of these problems is well described in the book [19]. The book [16] is devoted more to the general theory and derivation of the complementary error bounds based on the calculus of variation.

8 Numerical examples

In this section we present a few numerical examples showing the performance of the variants of the complementary upper bounds in the finite element method.

In these experiments, we consider the two-dimensional case (i.e. $d = 2$), polygonal domain Ω, a triangular finite element mesh $\mathcal{T}_h$ in Ω, and a space of continuous and piecewise linear functions in Ω:

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

where $P^1(K)$ stands for the space of linear functions on the triangle K. The finite element solution of (3) is then $u_h \in V_h$ such that

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

First, we use the error estimate $\eta(u_h, \boldsymbol{y}_h)$ given by (9)–(10). The approximate complementary solution $\boldsymbol{y}_h$ is computed as $\boldsymbol{y}_h = \overline{\boldsymbol{q}} + \mathbf{curl}\, z_h$, where $\overline{\boldsymbol{q}}$ is given by (21) and z_h is obtained as the finite element solution of problem (23). More precisely, we introduce a space

$$X_h = \{v_h \in H^1(\Omega) : v_h|_K \in P^p(K),\ \forall K \in \mathcal{T}_h\}$$

of piecewise polynomials of degree at most p over the same mesh $\mathcal{T}_h$ and define $z_h \in X_h$ such that

$$\mathcal{B}(z_h, v_h) = -\mathcal{B}^*(\overline{\boldsymbol{q}}, \mathbf{curl}\, v_h) \quad \forall v_h \in X_h.$$

In the experiments presented below we compare the values of $\eta(u_h, \boldsymbol{y}_h)$ for $p = 1$, $p = 2$, and $p = 3$.

As an alternative, we use the error bound $\widehat{\eta}(u_h, \widehat{\boldsymbol{y}}_h)$ given by (18)–(19). The corresponding approximate complementary solution $\widehat{\boldsymbol{y}}_h$ is computed as an approximate solution $\widehat{\boldsymbol{y}}_h$ of problem (20). The best results are obtained for small values of β, because the smaller the value of β is, the more the complementary solution is enforced to satisfy $-\operatorname{div} \boldsymbol{y}_h = f$. In the example, we use $\beta = C_\Omega^2\, 10^{-4}$. To solve the complementary problem (20) approximately, we use the Raviart-Thomas finite elements of degree $\widehat{p} = 1$ and $\widehat{p} = 2$ on the same mesh $\mathcal{T}_h$.

Finally, for comparison, we present results of $\eta(u_h, \boldsymbol{y}_h^{\mathrm{expl}})$, see (9)–(10), where $\boldsymbol{y}_h^{\mathrm{expl}}$ is obtained by a quite complicated but explicit formula from [2]. This formula is based on the so-called equilibrated residuals [1] and the approach utilizes the trick of so-called data oscillations.

In particular, we consider two specific examples. In the first example, the Poisson problem (1)–(2) is defined in a square $\Omega = (-1/2, 1/2)^2$ with the right-hand side $f(x_1, x_2) = \cos(\pi x_1)\cos(\pi x_2)$. The corresponding exact solution is then $u = \cos(\pi x_1)\cos(\pi x_2)/(2\pi^2)$. To use the error bound $\widehat{\eta}(u_h, \widehat{\boldsymbol{y}}_h)$, we estimate the Friedrichs' constant by (17) as $C_\Omega = 1/(\pi\sqrt{2})$. The finite element mesh is shown in Figure 2 (left).

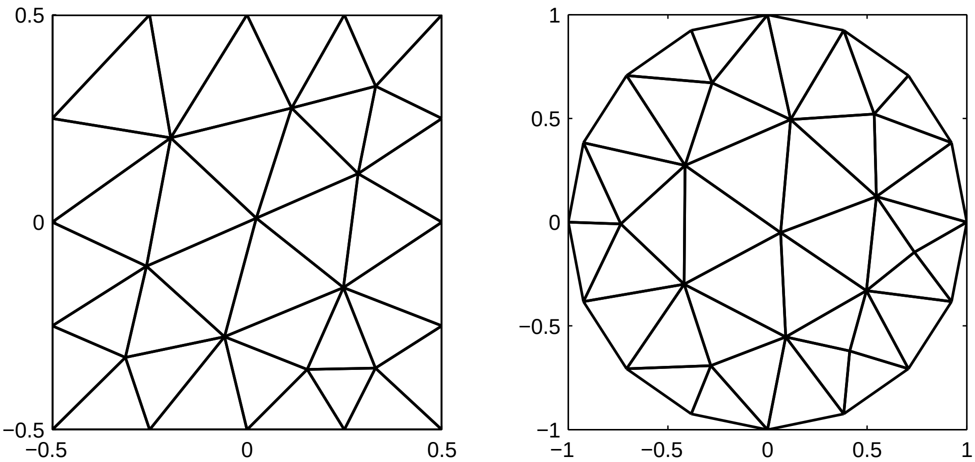

Figure 2: The finite element mesh used in the first (left) and in the second (right) example.

In the second example, we solve also the Poisson problem (1)–(2). In this case, the domain Ω is the unit disk $\Omega = \{(x_1, x_2) : r < 1\}$, where $r^2 = x_1^2 + x_2^2$. The right-hand side is $f = 1$ and the corresponding exact solution is $u = (1 - r^2)/4$. The Friedrichs' constant is estimated as $C_\Omega = \sqrt{2}/\pi$. Figure 2 (right) sketches the used finite element mesh.

Tables 1–2 present the indices of effectivity I_{eff}. It is the ratio of the estimate and the true value of the estimated quantity, for example $I_{\text{eff}} = \widehat{\eta}(u_h, \widehat{\boldsymbol{y}}_h)/|||u - u_h|||$. The first row corresponds to the mesh shown in Figure 2. The subsequent rows correspond to the subsequent uniform refinements of this mesh.

First of all, we do not see any substantial dependence of the values on the mesh refinement. This confirms the correctness of the approach and the correctness of the numerical implementation. Further, we observe that if the complementary problems are solved with the same orders of accuracy, i.e. with $p = 1$ and $\widehat{p} = 1$, then the complementary error bounds provide fair but not absolutely sharp results. They overestimate the error roughly by 40–80 %.

We point out that the number of degrees of freedom (DOFs) needed to compute z_h in the case $p = 1$ is comparable to the number of DOFs needed to compute u_h (i.e. to solve the primal problem). On the other hand, the number of DOFs needed for $\widehat{\boldsymbol{y}}_h$ is roughly six times higher. (There are two DOFs per edge and there is roughly three times more edges than vertices in triangular meshes.)

If we invest more DOFs into the solution of the complementary problem and use quadratic or even cubic finite elements, we obtain almost exact results. However, the solution of the complementary problem then requires much more computational time and such approach is not very practical. A remedy is presented in the last columns of Tables 1–2. They show the results obtained by a fast and explicit approach from [2]. The number of needed arithmetic operations is proportional to the number of DOFs in the primal problem. This is quite sharp and fast alternative.

The kind reader already noticed that certain values in Table 2 are less than one. This seems as a contradiction with Theorem 2 which states that the error estimate is an upper bound on the energy norm of the error. However, Theorem 2 assumes both u and u_h to be defined in the same domain Ω, but in the second example we actually approximate the circular domain Ω by a polygon Ω_h. Thus, strictly speaking the assumptions of Theorem 2 are not satisfied. Anyway, if we refine the mesh and use more precise approximation of the circular domain, we should obtain sharper results. In Table 2, we observe that this is indeed the case.

	$\eta(u_h, \overline{\boldsymbol{q}} + \mathbf{curl}\, z_h)$			$\widehat{\eta}(u_h, \widehat{\boldsymbol{y}}_h)$		$\eta(u_h, \boldsymbol{y}_h^{\text{expl}})$
	$p = 1$	$p = 2$	$p = 3$	$\widehat{p} = 1$	$\widehat{p} = 2$	
h	1.410	1.008	1.000	1.789	1.099	1.419
$h/2$	1.419	1.002	1.000	1.791	1.052	1.405
$h/4$	1.422	1.001	1.000	1.791	1.027	1.406
$h/8$	1.424	1.000	1.000	1.790	1.013	1.407
$h/16$	1.424	1.000	1.000	1.790	1.007	1.408

Table 1: Indices of effectivity obtained in the first example.

	$\eta(u_h, \overline{\boldsymbol{q}} + \mathbf{curl}\, z_h)$			$\widehat{\eta}(u_h, \widehat{\boldsymbol{y}}_h)$		$\eta(u_h, \boldsymbol{y}_h^{\mathrm{expl}})$
	$p=1$	$p=2$	$p=3$	$\widehat{p}=1$	$\widehat{p}=2$	
h	1.708	1.000	0.978	1.000	0.978	1.047
$h/2$	1.692	1.000	0.990	1.000	0.990	1.128
$h/4$	1.686	1.000	0.995	1.000	0.995	1.153
$h/8$	1.683	1.000	0.998	1.000	0.998	1.158
$h/16$	1.683	1.000	0.999	1.000	0.999	1.158

Table 2: Indices of effectivity obtained in the second example.

9 Conclusions

In this paper we surveyed the complementary approach yielding the computable and guaranteed upper bounds of the energy norm of error. A straightforward implementation of the complementary error bounds is computationally too expensive for practical purposes. However, there are fast approaches providing sufficiently accurate results.

From the point of view of reliability of numerical computations, the complementary approach is invaluable for its ability to provide computable and guaranteed upper bounds on the error. These errors bounds used in an adaptive algorithm enable to solve the given problem with prescribed accuracy. Up to the author's knowledge there is no available software, capable to solve for instance linear elliptic problems with guaranteed accuracy. The complementary framework provides theoretical background for the creation of such software.

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