New Computational Technologies for Reliable Computer Simulation: Ideas and Implementation

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Abstract

The present work is devoted to one of the most challenging problems in mathematical modelling and numerical analysis, which also has great importance for most of applications in industry: *reliable verification of accuracy of approximate solutions obtained via computer simulations*. This task is strongly related to the so-called *a posteriori error estimates*, giving computable bounds for modelling errors of various types and detecting zones, where such errors are excessively high and some mesh-refinement algorithm should be used.
On the base of a model boundary value problem of elliptic type we present effective technologies and discuss relevant implementation issues on how:

- to obtain two-sided (upper and lower) a posteriori error estimates for verifying the overall accuracy of computed solutions in the global energy norm
- to derive two-sided (upper and lower) a posteriori error estimates aimed at control of local errors
- to develop parallel numerical procedures for computing the above a posteriori estimates

The estimates derived in the paper are capable of giving bounds as close to exact errors as needed independently of the technique used to obtain approximate solutions. Two numerical tests, performed with a help of the PDE Toolbox of Matlab, clearly demonstrate high effectivity of the technologies proposed.

Keywords: reliable computations, a posteriori error estimation, error control in energy norm, local errors, differential equation of elliptic type, finite element method, PDE Toolbox of Matlab.

MSC: 65N15, 65N30

1 Introduction

Many physical phenomena can be described by means of mathematical models presenting *boundary value problems of elliptic type* (see, e.g., [13] for various examples). Several numerical techniques (such as the finite difference method (FDM), the finite element method (FEM), etc) are well developed for finding approximate solutions for these problems. Nowadays FEM [8] seems to be the most powerful and popular numerical method, which is successfully used in various industrial and educational codes (for example in such software product of Matlab as the PDE Toolbox [15]) for performing convenient computer simulations for problems of different types.

However, in order to be practically meaningful, simulations always require an accuracy verification of computed approximations, what is the main purpose of a posteriori error estimation methods. A number of approaches for deriving a posteriori estimates for errors measured in global energy norms and for various local errors have been suggested by many authors (see works [1], [2], [3], [4], [5], [6], [10], [11], [12], [16], [17], [19], [20] and references therein). Most of the estimates proposed rely strongly on the fact that

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the computed solutions are true finite element (FE) approximations which, in fact, rarely happens in real computations, e.g., due to quadrature rules, forcibly stopped iterative processes, various round-off errors, etc.

In this paper, on the base of a model linear elliptic problem, we present and test numerically relatively simple but effective technologies for obtaining *computable guaranteed two-sided (upper and lower) bounds* needed for reliable control of global and local computational errors arising in computer simulations. These bounds are valid for any conforming approximations independently of numerical method used to obtain them, and they can be made as close to the true errors as resources of a particular computer used allow. We shall also discuss main issues of corresponding practical realizations. Two numerical examples demonstrating high effectivity of the technologies proposed are presented.

2 Model Problem and Error Control

For definitions of functional spaces mentioned in this paper (and for another elliptic problems) we refer to the classical monograph [8].

Model problem: Find a function u such that

$$-\mathrm{div}(A\nabla u) = f \quad \text{in} \quad \Omega, \quad u = 0 \quad \text{on} \quad \partial\Omega, \tag{1}$$

where Ω is a bounded connected domain in $\mathbf{R}^d$ with a Lipschitz continuous boundary $\partial\Omega$, f is a square summable source function (from the space $L_2(\Omega)$), the matrix of coefficients A is symmetric, with bounded entries a_{ij} (from the space $L_\infty(\Omega)$), $i, j = 1, ..., d$, and is such that

$$c_2|\xi|^2 \geq A(x)\xi\cdot\xi \geq c_1|\xi|^2 \qquad \forall\xi \in \mathbf{R}^d \quad \forall x \in \Omega. \tag{2}$$

It is a common practice to use so-called *weak formulation* of the problem (1), which reads: Find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega A\nabla u\cdot\nabla w\,dx = \int_\Omega fw\,dx \quad \forall w \in H_0^1(\Omega). \tag{3}$$

Let $\overline{u}$ be *any function* from $H_0^1(\Omega)$ (e.g., computed by some numerical method) considered as an approximation of the exact solution u. We are interested in *reliable and diverse control* of the error $e := u - \overline{u}$ during computational process, depending on the user's needs. So far two general possibilities for the error control are well realized and used in mathematical and engineering communities.

Control of error in global norm: First of all, engineers are usually interested in estimation of the gradient of the error in the so-called *energy norm*, i.e., in estimation of the value

$$|||\nabla e||| := \left(\int_\Omega A\nabla(u-\overline{u})\cdot\nabla(u-\overline{u})\,dx\right)^{1/2}, \tag{4}$$

which gives a general presentation on the quality of the computed approximation $\overline{u}$. Such type of the error control has been in the focus of research work since 1978 (see the first works on this subject [2], [3]).

Control of local errors: There is also a new trend in a posteriori error estimation (see, e.g., [1], [6], [10], [11], [12], [14]), which is based on the concept of local error control in addition to the classical control in the global energy norm. This approach is strongly motivated by practical needs, in which analysts are often interested not only in the value of the overall error, but also in controlling errors over certain parts of the solution domain, or relative to some interesting characteristics ("quantities of interest"). Common way to perform such type of control is to introduce a certain linear functional ℓ associated with particular subdomain of interest (and/or with a "quantity of interest") and to obtain a computable estimate for $\ell(u-\overline{u})$. For example, we can be interested in estimation of

$$\ell(e) = \ell(u-\overline{u}) \;=\; \int_\Omega \varphi(u-\overline{u})\,dx, \tag{5}$$

where $\varphi \in L_2(\Omega)$ and $\mathrm{supp}\,\varphi = \omega \subseteq \Omega$, which provides us with a certain information on the behaviour of the error e locally, in subdomain ω. The estimates for $\ell(u-\overline{u})$ can also be used for estimation of unknown "quantity of interest" $\ell(u)$ in a view of the representation $\ell(u) = \ell(\overline{u}) + \ell(u-\overline{u})$, where $\ell(\overline{u})$ is computable and $\ell(u-\overline{u})$ is estimated. It is worth to mention that certain "quantities of interest" (e.g., in linear elasticity problems) are often more interesting to practitioners than the solution itself.

3 Two-Sided Estimates of Error Measured in Global Energy Norm

3.1 Description of technology

Upper Estimate. Using the fact that $u-\bar{u}\in H_0^1(\Omega)$, from (3) and (4) we obtain

$$|||\nabla e|||^2 = \int_\Omega f(u-\bar{u})dx - \int_\Omega A\nabla\bar{u}\cdot\nabla(u-\bar{u})\,dx =$$

$$= \int_\Omega f(u-\bar{u})\,dx - \int_\Omega (A\nabla\bar{u}-y^*)\cdot\nabla(u-\bar{u})\,dx - \int_\Omega y^*\cdot\nabla(u-\bar{u})\,dx =$$

$$= \int_\Omega (f+\mathrm{div}y^*)(u-\bar{u})\,dx - \int_\Omega A(\nabla\bar{u}-A^{-1}y^*)\cdot\nabla(u-\bar{u})\,dx \le$$

$$\le \|f+\mathrm{div}y^*\|\,\|u-\bar{u}\| + \Big(\int_\Omega A(\nabla\bar{u}-A^{-1}y^*)\cdot(\nabla\bar{u}-A^{-1}y^*)\,dx\Big)^{1/2} |||\nabla(u-\bar{u})|||,$$

where $y^*\in H(\mathrm{div};\Omega)$, $\|\cdot\|$ is a standard norm in $L_2(\Omega)$ and $|||\cdot|||$ is norm defined in (4). From the Friedrichs inequality

$$\|w\| \le c_\Omega \|\nabla w\| \quad \forall w\in H_0^1(\Omega), \tag{6}$$

and (2) we observe that

$$\|u-\bar{u}\|^2 \le c_\Omega^2 \|\nabla(u-\bar{u})\|^2 \le \frac{c_\Omega^2}{c_1}|||\nabla(u-\bar{u})|||^2. \tag{7}$$

Thus, we immediately get the following estimate

$$|||\nabla e||| \le \frac{c_\Omega}{\sqrt{c_1}}\|f+\mathrm{div}y^*\| + \Big(\int_\Omega A(\nabla\bar{u}-A^{-1}y^*)\cdot(\nabla\bar{u}-A^{-1}y^*)\,dx\Big)^{1/2}, \tag{8}$$

or, in another form, after squaring and using definition (4),

$$|||\nabla e|||^2 \le \left(1+\frac{1}{\beta}\right)\frac{c_\Omega^2}{c_1}\|f+\mathrm{div}y^*\|^2 + (1+\beta)\,|||\nabla\bar{u}-A^{-1}y^*|||^2, \tag{9}$$

where both estimates are valid for any $y^*\in H(\mathrm{div};\Omega)$ and any $\beta>0$.

The upper bound (9) was first obtained in [16] in a general form using the duality theory (see also [17]), and later it was obtained in a more simplified way using the Helmholtz decomposition of $L_2(\Omega,\mathbf{R}^d)$ in [19]. The comparison of such obtained upper bound and its properties with the other existing a posteriori estimates and indicators was performed in [18].

Lower Estimate. It is easy to show that

$$|||\nabla(u-v)|||^2 = 2(J(v)-J(u)) \quad \forall v\in H_0^1(\Omega), \tag{10}$$

where $J(w)=\frac{1}{2}\int_\Omega A\nabla w\cdot\nabla w\,dx - \int_\Omega fw\,dx$ is the so-called *energy functional*. The solution u minimises the energy functional, so $J(u)\le J(w)\quad\forall w\in H_0^1(\Omega)$. Using this fact, one can get a lower bound for the error as follows

$$|||\nabla e|||^2 \ge 2(J(\bar{u})-J(w)), \tag{11}$$

where w is *any function* from $H_0^1(\Omega)$. We note that this form of the lower estimate is different from that one presented in [17].

3.2 Practical realization

In this section we shall shortly consider several relevant practical issues, mainly in the framework of the finite element method. Thus, the approximation $\bar{u}$ is further assumed to be obtained by FEM, and denoted as u_h, where h is the standard (positive) discretization parameter usually denoting the length of the smallest edge in the corresponding mesh [8]. Nevertheless, we do not use any immanent properties of FE approximations in what follows and use FEM terminology only for convenience.

We also assume that computations are performed on a series of successive meshes $\mathcal{T}_{h_1}$, $\mathcal{T}_{h_2}$, $\mathcal{T}_{h_3}$, ..., where $h = h_1 > h_2 > h_3 > \ldots$, and, thus, we always have in hands several successive approximations u_{h_1}, u_{h_2}, u_{h_3}, ... Such a situation is quite typical in most of practical calculations.

On computation of constant c_Ω. The upper bound (9) contains the only unknown constant c_Ω. In the general case, this constant is determined by the smallest eigenvalue λ_Ω of the Laplacian for Ω, namely $c_\Omega = \frac{1}{\sqrt{\lambda_\Omega}}$. We refer to the work [18] for more details on how to estimate c_Ω from above. It is worth to note that the other existing estimation techniques (of residual-type) commonly involve *many unknown constants* usually related to patches of the computational meshes used. Those constants are very hard to estimate (from above) and their computation, in general, leads to a very big overestimation of the error even in simple cases (see, e.g.,[7]). Moreover, such constants have to be always recomputed if we perform adaptive computations and change the computational mesh. On the contrary, the constant c_Ω remains the same under any change in computational mesh.

On minimisation of upper bound. For convenience we shall use a short denotation for the upper bound (9) as follows

$$M^{\oplus}(u_h, \beta, y^*) := \left(1 + \frac{1}{\beta}\right) \frac{c_\Omega^2}{c_1} \| f + \operatorname{div} y^* \|^2 + (1+\beta) \| \nabla u_h - A^{-1} y^* \|^2. \tag{12}$$

A "coarse" upper bound can be "cheaply and fast" computed using, e.g., values $y^* = G_\mu(\nabla u_\mu) \in H(\operatorname{div}, \Omega)$, where $\mu = h_1, h_2, h_3, \ldots$, and G_μ is some commonly used and computationally "inexpensive" *gradient averaging operator* [9]. However, more sharp estimates require real minimisation of the upper bound $M^{\oplus}(u_h, \beta, y^*)$ with respect to the "free" variables y^* and β, which can be performed by a direct minimisation of it or by finding the minimiser as a solution of the respective system of linear equations.

On computation of lower bound. The estimate (11) has a practical meaning only if it provides with a positive lower bound for the (positive) error $\|\nabla e\|$. This can be obtained if we recall that one normally tries to have $J(u_{h_1}) > J(u_{h_2}) > J(u_{h_3}) > \ldots$, in a series of successive computations, which immediately suggests obtaining meaningful lower bounds as follows

$$\|\nabla e\|^2 = \|\nabla (u - u_h)\|^2 \geq 2(J(u_h) - J(u_\mu)) > 0, \tag{13}$$

where $\mu = h_2, h_3, \ldots$. In what follows, we shall use the following denotation $M^{\ominus}(u_h, u_\mu) := 2(J(u_h) - J(u_\mu))$ for the lower bound of type (13).

3.3 Test 1

We consider the problem (1) posed in L-shaped domain Ω (see Fig. 1). Let A be the unit matrix and $f \equiv 10$. The FE solution u_h is computed on the mesh $\mathcal{T}_h$ having 258 nodes. To obtain sufficiently sharp upper and lower bounds we employ three successive meshes $\mathcal{T}_h, \mathcal{T}_{\frac{h}{2}}, \mathcal{T}_{\frac{h}{4}}$. The behaviour of the two-sided bounds is presented in Fig. 1 (right), the upper bound is easily seen to be of sufficiently high quality already on the same mesh and is only slightly decreasing from 0.5054 to 0.5021 later on. The lower bound grows from 0 to 0.3943. For the sake of completeness we also computed the "exact error" using the so-called *reference solution* (obtained by solving the problem (1) on a very fine mesh, in our example – on 5 times globally refined mesh $\mathcal{T}_h$ instead of the exact solution u), which approximates the squared error $\|\nabla e\|^2$ by the value 0.4252.

4 Two-Sided Estimates for Local Errors

4.1 Description of technology

The second technology is developed for controlling the error $e = u - \bar{u}$ measured in terms of the following simple functional (cf. (5))

$$\ell(e) = \int_\Omega \varphi (u - \bar{u})\, dx, \tag{14}$$

where $\varphi \in L_2(\Omega)$ and $\operatorname{supp} \varphi = \omega \subseteq \Omega$.

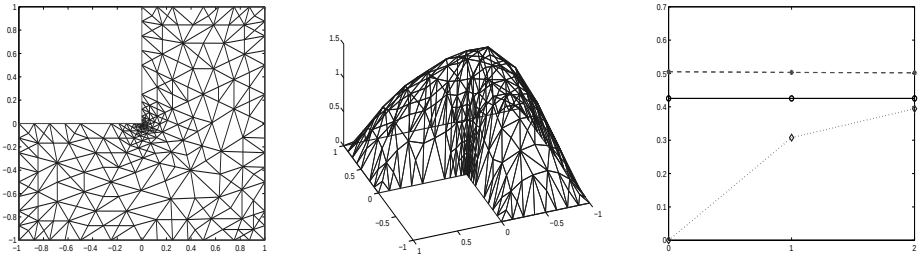

Figure 1: Mesh $\mathcal{T}_h$ with 258 nodes (left), the finite element solution u_h (center), and behaviour of the upper (9), and the lower (13), bounds versus the squared exact error $|||\nabla e|||^2$ (right) in Test 1.

First, we introduce an auxiliary (called *adjoint*) problem (and name the problem (3) as the *primal problem* in what follows, we shall also use the term *primal mesh* for the mesh $\mathcal{T}_h$ used to compute u_h), which reads: Find $v \in H_0^1(\Omega)$ such that

$$\int_\Omega A\nabla v \cdot \nabla w\, dx = \int_\Omega \varphi w\, dx \quad \forall w \in H_0^1(\Omega). \tag{15}$$

The adjoint problem is uniquely solvable due to the assumption $\varphi \in L_2(\Omega)$. However, its exact solution v is usually unknown in analytical form, so we can only have some approximation $\bar{v}$ (e.g., computed by FEM on *adjoint mesh* $\mathcal{T}_\tau$ with a discretization parameter τ, however, we again assume, in fact, only that $\bar{v} \in H_0^1(\Omega)$). Then it can be easily shown (see [12] and [17] for the proof) that

$$\ell(u-\bar{u}) = E_0(\bar{u},\bar{v}) + E_1(e,e_\varphi), \tag{16}$$

where

$$E_0(\bar{u},\bar{v}) = \int_\Omega f\bar{v}\, dx - \int_\Omega A\nabla\bar{v}\cdot\nabla\bar{u}\, dx, \tag{17}$$

and

$$E_1(e,e_\varphi) = \int_\Omega A\nabla e \cdot \nabla e_\varphi\, dx, \tag{18}$$

with $e_\varphi := v - \bar{v}$.

The first term E_0 is, obviously, directly computable once we have $\bar{u}$ and $\bar{v}$ computed, but the term E_1 contains unknown gradients ∇u and ∇v. In order to estimate it, we use the following identity

$$2E_1(e,e_\varphi) = |||\nabla(\alpha e + \frac{1}{\alpha}e_\varphi)|||^2 - \alpha^2|||\nabla e|||^2 - \frac{1}{\alpha^2}|||\nabla e_\varphi|||^2, \tag{19}$$

valid for any positive α. Further, we notice that the above identity contains errors in the energy norm for both, primal and adjoint problems, and we can use the two-sided estimates from Section 3, written in somewhat simplified form:

$$M_f^\ominus \le |||\nabla e|||^2 \le M_f^\oplus, \quad M_\varphi^\ominus \le |||\nabla e_\varphi|||^2 \le M_\varphi^\oplus. \tag{20}$$

As far it concerns the first term in the right-hand side of (19), we observe that

$$|||\nabla(\alpha e + \frac{1}{\alpha}e_\varphi)|||^2 = |||\nabla(\alpha u + \frac{1}{\alpha}v) - \nabla(\alpha\bar{u} + \frac{1}{\alpha}\bar{v})|||^2. \tag{21}$$

The function $\alpha u + \frac{1}{\alpha}v$ can be perceived as the solution of the following problem: Find $u_\alpha \in H_0^1(\Omega)$ such that

$$\int_\Omega A\nabla u_\alpha \cdot \nabla w\, dx = \int_\Omega (\alpha f + \frac{1}{\alpha}\varphi) w\, dx \quad \forall w \in H_0^1(\Omega), \tag{22}$$

and the function $\alpha\bar{u} + \frac{1}{\alpha}\bar{v}$ can be considered as an approximation of u_α. Then we can again apply the techniques of Section 3 and obtain the following two-sided estimates (written below in simplified form)

$$M^{\ominus}_{\alpha,f,\varphi} \le |||\nabla(\alpha e + \frac{1}{\alpha} e_\varphi)|||^2 \le M^{\oplus}_{\alpha,f,\varphi}, \tag{23}$$

Further, we immediately observe that

$$\frac{1}{2}(M^{\ominus}_{\alpha,f,\varphi} - \alpha^2 M^{\oplus}_f - \frac{1}{\alpha^2} M^{\oplus}_\varphi) \le E_1(e, e_\varphi), \tag{24}$$

and

$$E_1(e, e_\varphi) \le \frac{1}{2}(M^{\oplus}_{\alpha,f,\varphi} - \alpha^2 M^{\ominus}_f - \frac{1}{\alpha^2} M^{\ominus}_\varphi), \tag{25}$$

which together with the computable term E_0 provide with two-sided estimates for the error (14).

4.2 Test 2

We consider the (primal) problem (1)–(3) posed in L-shaped domain Ω (see Fig. 1 and 2). Let A be the unit matrix, $f \equiv 10$, let the approximation $\overline{u}$ be the FE solution u_h computed on the mesh $\mathcal{T}_h$ having 249 nodes. The zone of interest ω is marked by bold line in Fig. 2 (left). Assume that the approximation $\overline{v}$ is the FE solution v_τ computed on the mesh $\mathcal{T}_\tau$ having 541 nodes. To obtain reasonably sharp upper and lower bounds for the approximations of the primal and adjoint problems, we perform relevant computations on three successive meshes ($\mathcal{T}_h, \mathcal{T}_{\frac{h}{2}}, \mathcal{T}_{\frac{h}{4}}$, and $\mathcal{T}_\tau, \mathcal{T}_{\frac{\tau}{2}}, \mathcal{T}_{\frac{\tau}{4}}$). The behaviour of the bounds is presented in Fig. 2 (right): the upper bound is decreasing from 0.04364 to 0.02433, the lower bound grows from -0.01606 to 0.005914. The "exact error" is computed by using the so-called reference solution (obtained by solving the problem (1) on a very fine mesh, in our example – on 4 times refined $\mathcal{T}_h$ instead of the exact solution u) which gave the value 0.01317 for the error (14).

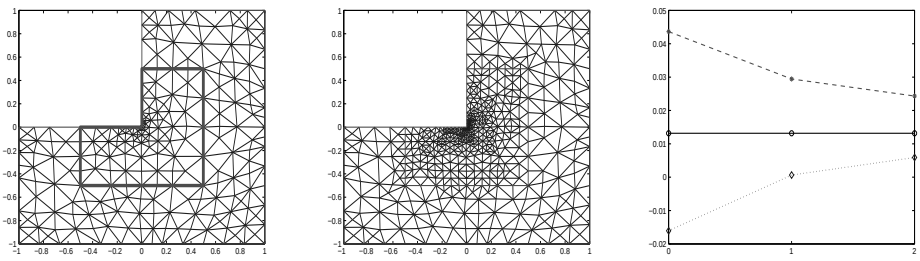

Figure 2: Solution domains Ω, zone of interest ω, primal mesh $\mathcal{T}_h$ with 249 nodes (left), corresponding adjoint mesh $\mathcal{T}_\tau$ with 541 nodes (center), and the behaviour of the upper and lower bounds versus the exact error (14) (right) in Test 2.

5 Final Comments

The techniques proposed can be straightforwardly adapted to treating the other boundary conditions and the other linear elliptic problems (e.g., in linear elasticity, biharmonic equation).

It is clear from the above considerations that for both types of control, the corresponding upper and lower bounds can be made arbitrary close to the true errors.

In decomposition (16), the unknown gradients ∇u and ∇v can be replaced by computable averaged gradients $G_h(\nabla u_h)$ and $G_\tau(\nabla u_\tau)$, which also leads to quite effective (and easily computable) indicators for error (14). More details on this approach can be found in [10], [11], [12].

The technologies can be easily coded and added as some block-checker to most of existing educational and industrial software products like MATLAB, FEMLAB, ANSYS, etc.

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