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Adaptive mesh refinement and *a posteriori* error estimates

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Abstract: This short contribution is intended mainly for mathematicians who are not specialists in numerical analysis but would like to understand better the fundamental features of the finite element method. First, we review the finite element method for linear elliptic partial differential equations of second order. Then we concentrate on the main ideas of *a priori* and *a posteriori* error estimates, convergence and adaptive mesh refinement. We especially emphasize the pioneering convergence result of Professor Miloš Zlámal and present some modern results from the theory of the finite element method. We use several numerical examples to illustrate the presented results.

Keywords: finite element method, convergence, *a priori* error bounds, *a posteriori* error estimates, adaptivity.

AMS classification: 65N30, 65N15.

1 Introduction

The finite element method developed gradually and independently in different parts of the world. It does not have a single inventor and it is hard to say when it was discovered. Its beginnings can be traced back to the work of Alexander Hrennikoff and Richard Courant in the 1940s. Its popularity and importance gained momentum worldwide in the 1950s with the development of computers. Several pioneering works also appeared in the former Czechoslovakia and a prominent place among them was the seminal paper [18] of Professor Miloš Zlámal published in 1968. In this paper, he proved one of the first convergence results for finite elements under a novel minimal angle condition.

Later on, the convergence theory of the finite element method developed into an elegant and versatile theory. One of the first, recommendable and still influential monographs on the finite element theory are [8] and [15].

In this short contribution, we first review Zlámal's *a priori* error bound as an example of the convergence result. We will comment on its aspects to motivate interest in *a posteriori* error bounds. A pioneer in *a posteriori* error analysis is Professor Ivo Babuška, another prominent Czech mathematician. His papers [2] and [3] belong among the very first ones on *a posteriori* error estimates in the finite element method. *A posteriori* error estimates are crucial in adaptive algorithms for automatic mesh refinement. This procedure enables us to construct nearly optimal finite element meshes during the computation and, thus, achieve nearly optimal computational performance in numerical solution of partial differential equations. The adaptive algorithm is the final concept we present in this short contribution.

To ease the understanding, we illustrate all these prominent features of the finite element method on simple numerical examples with numerous illustrations. For clarity, we do not comment on some technical mathematical assumptions and subtle theoretical details.

The rest of this contribution is organized as follows. Section 2 introduces an elliptic linear problem of second order and briefly explains how to solve it by the finite element method.

Section 3 reviews the *a priori* error estimates on an example of Zlámal's result and explains its relevance for the convergence of the finite element method. Section 4 is devoted to *a posteriori* error estimates and Section 5 provides a brief introduction to the mesh adaptive algorithms. Finally, Section 6 draws the conclusions.

2 Linear elliptic problem of second-order and the finite element method

As a model problem, let us consider a simple diffusion-reaction linear elliptic partial differential equation of second order in a two-dimensional domain with homogeneous Dirichlet boundary conditions. If $\Omega \subset \mathbb{R}^2$ is a domain with sufficiently smooth boundary $\partial\Omega$ and if $f = f(x_1, x_2)$ is a suitable right-hand side function defined in Ω then we seek the solution function $u = u(x_1, x_2)$ such that it satisfies

$$\begin{aligned} -\Delta u + u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{1}$$

Here, Δ stands for the Laplace differential operator defined as

$$\Delta u = \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2}.$$

As an example, let us consider a square $\Omega = (-1/2, 1/2)^2$, right-hand side function and the corresponding exact solution

$$f(x_1, x_2) = \cos(\pi x_1)\cos(\pi x_2) \quad \text{and} \quad u(x_1, x_2) = \frac{\cos(\pi x_1)\cos(\pi x_2)}{2\pi^2 + 1}.$$

Note that it is easy to verify by differentiation that this u satisfies the differential equation and the boundary condition in (1). Further, note that we have chosen the solution u as the first eigenfunction of the Laplace operator with homogeneous Dirichlet boundary conditions and, therefore, functions u and f differ by a constant multiple only. For illustration, Figure 1 (left) shows a three-dimensional graph of the function $u(x_1, x_2)$ over the square Ω.

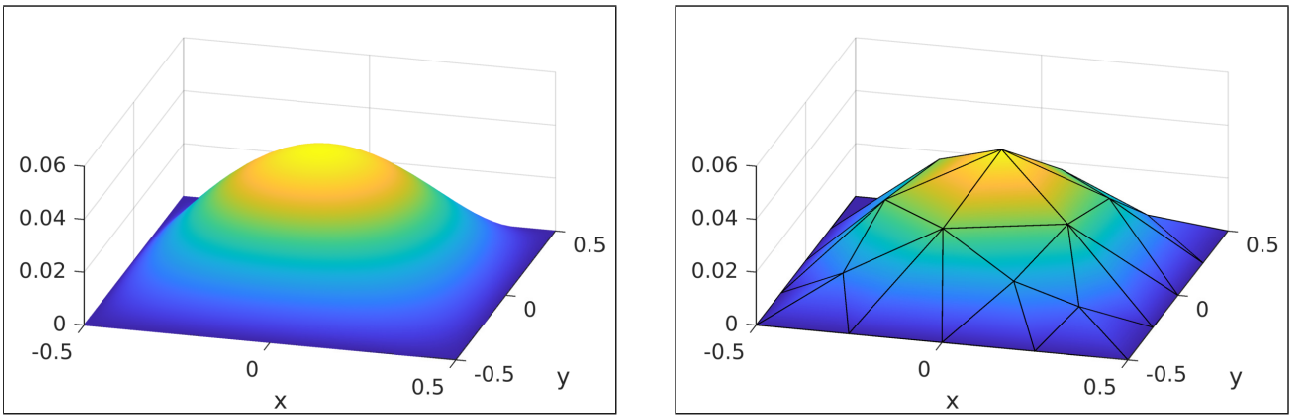

Fig. 1: Exact (left) and finite element (right) solutions of problem (1).

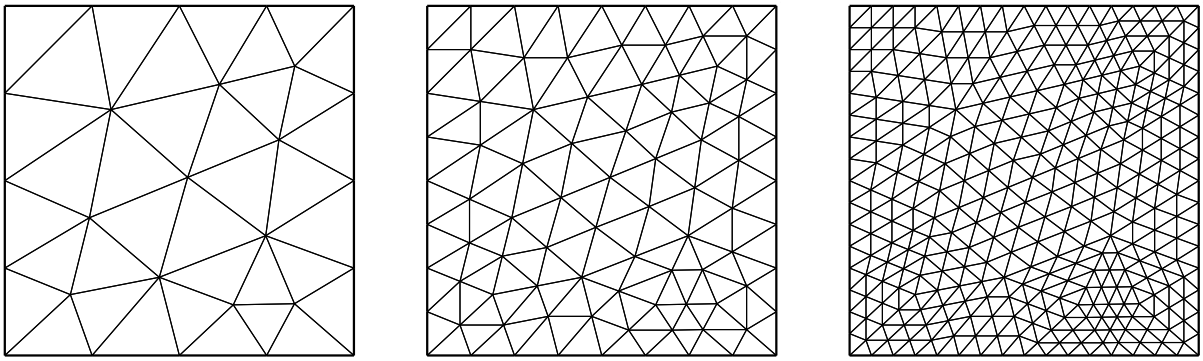

Fig. 2: Sequence of three uniformly refined finite element mesh.

Most often, for a given right-hand side function f, the exact solution cannot be expressed analytically in a closed form, especially, in the case of domains Ω with more complex geometries. Therefore, we have to employ numerical methods and solve problems like (1) numerically.

A very popular approach for numerical solution of partial differential equations is the finite element method. It is flexible and can handle complicated geometries of Ω. On top of that it has an elegant convergence theory and various error estimates. To apply the finite element method, we first construct a triangulation (or mesh) of the domain Ω. Triangulation is simply a splitting of the domain into triangles or other geometrically simple objects called elements. The finite element solution is then sought as a continuous and piecewise linear function over this triangulation.

Mathematically, the finite element method is a special case of the Galerkin method built on the weak formulation of problem (1). After the discretization one obtains a system of linear algebraic equations for unknown values of the approximate solution at the nodal points of the triangulation. This system can be large, but the distinctive feature of the finite element method is the sparsity of the system matrix. Hence, iterative methods together with suitable preconditioning enable us to solve resulting linear systems with millions of equations on usual personal computers. Figure 1 (right) shows an example of the approximate finite element solution. Note that this solution was computed on the mesh depicted in the left panel of Figure 2.

Let us remark that a method with a faster convergence rate can be obtained by approximating the solution u by a continuous and piecewise quadratic function over the finite element triangulation. In such a case, we speak about the finite element method of second order. The resulting system of linear algebraic equations is naturally larger, but the obtained approximate solution is more accurate. For problems with smooth solutions (without singularities), the higher order methods pay off, because the gain in the accuracy outweighs higher computational costs.

3 Convergence and *a priori* error estimates

As we mentioned above, there is an elegant convergence theory for the finite element method. One of the first convergent results for the finite element method was proved by Professor Miloš Zlámal in the 1960s. His result applies well to problem (1) discretized by finite elements of second order. Figure 3 literally quotes his famous result published in [18]. The first two lines of this quote formulate the assumption that the exact solution u must have all derivatives of order three bounded in Ω. Simply speaking, the exact solution must be sufficiently smooth for the validity of this convergence result.

If the solution $u(x_1, x_2)$ has bounded derivatives of the third order in Ω,

(10) $$|D^i u(x_1, x_2)| \leqq M_3, \quad |i| = 3,$$

then it holds

(11) $$\|u - U\|_{W_2^{(1)}(\Omega)} \leqq C \frac{1}{\sin \vartheta} M_3 h^2$$

where the constant C does not depend on the triangulation.

(11) means that if we refine the triangulation in such a way that $\vartheta \geqq \vartheta_0 > 0$ the approximate solution $U(x_1, x_2)$ converges to the exact solution in the norm $\| \|_{W_2^{(1)}(\Omega)}$, the convergence being of the order h^2.

Fig. 3: A quote of the famous Zlámal's convergence result from [18].

Inequality (11) in this quote is the main statement. On the left-hand side, we see the error, i.e., the difference between the exact solution u and the finite element solution U in the $W_2^{(1)}(\Omega)$ norm. This norm measures the size of involved functions in terms of both their values and derivatives. It is the most natural norm for the linear elliptic problems of the second order and it is defined as

$$\|v\|^2_{W_2^{(1)}(\Omega)} = \int_\Omega \left(v^2 + |\nabla v|^2\right) \,\mathrm{d}x_1 \,\mathrm{d}x_2, \quad \text{where} \quad \nabla v = \left(\frac{\partial v}{\partial x_1}, \frac{\partial v}{\partial x_2}\right)^T.$$

The $W_2^{(1)}$-norm of the error $u - U$ is bounded by the term on the right-hand side of (11). Important is the last factor h^2. Symbol h stands for the mesh parameter and it indicates the size of finite elements in the triangulation. In particular, h is the largest diameter out of all (triangular) elements. The first factor $C\frac{1}{\sin\vartheta}M_3$ on the right-hand side of (11) is a positive constant independent of h and we will comment on it later.

Zlámal's *a priori* error estimate (11) tells us that the finite element method converges and in addition that it converges quadratically fast. To understand the concept of convergence of finite element solutions, we have to consider a sequence of successively refined triangulation. For example, Figure 2 presents a sequence of three uniformly refined meshes. The coarsest mesh is depicted on the left-hand side. The refined mesh, depicted in the middle, is obtained from the coarsest one by splitting each triangle into four similar sub-triangles by connecting the centres of its edges. The finest mesh (on the right) is constructed by the same procedure applied to the already refined mesh. This refinement process can be repeated as many times as we wish and produces a sequence of uniformly refined meshes.

Note that if the first triangulation has the mesh parameter $h = h_0$ (the largest diameter out of all triangles) then the refined mesh has the mesh parameter $h_0/2$, the twice refined mesh $h_0/4$, etc. Looking back at Zlámal's *a priori* error estimate (11) in Figure 3, we see that if we uniformly refine the triangulation then the error bound in (11) drops by the factor 4. Indeed, if the bound on the right-hand side of (11) is $C\frac{1}{\sin\vartheta}M_3h_0^2$ for the first mesh then it will be $C\frac{1}{\sin\vartheta}M_3h_0^2/4$ on the refined mesh. This bound is optimal and, therefore, the error on the left-hand side behaves in the same manner during the process of uniform mesh refinement.

To sum up, Zlámal's *a priori* error estimate tells us, roughly speaking, that the error of the finite element approximation measured in the suitable norm will drop by a factor of 4 every time we uniformly refine the mesh. In other words, the error behaves like h^2 and we speak about the second-order convergence speed.

This second-order convergence does not appear unconditionally. Besides the assumption of the smoothness of u, the angle ϑ plays a crucial role here. Zlámal comments on it immediately below his celebrated result, see Figure 3. To explain, ϑ is the smallest angle within the given triangulation and it is important to guarantee that it stays bounded away from zero during the refinement process. In other words, the smallest angle ϑ in the triangulation cannot degenerate to zero. The point is that the mesh refinement needs not to be uniform. There are countless ways how triangular meshes can be refined and it is not difficult to imagine a refinement process that splits the angles. If such angle splitting happens infinitely many times then the smallest angle converges to zero and the factor $1/\sin\vartheta$ on the right-hand side of Zlámal's bound (11) blows up towards infinity. Therefore, we have to refine the meshes such that the smallest angle in all triangulations stays bounded away from zero.

Let us note here that this well-known Zlámal's minimum angle condition was generalized to arbitrary dimension in [7]. However, it is not an optimal condition for convergence. The finite element method can converge (even optimally fast) on a sequence of meshes where the smallest angle degenerates towards zero. The right-hand side of Zlámal's estimate will blow up to infinity but the error on the left-hand side will converge to zero.

More recent results showed that the finite element method converges under the assumption that the largest angles in triangulations are bounded away from π, see e.g. [6, 11, 12]. Notice that an obtuse triangle with one large angle has necessarily two small angles. On the other hand, if a triangle has one small angle then the other two angles can be close to $\pi/2$ and, hence, bounded well away from π. Therefore, Zlámal's minimal angle condition is indeed less general than the largest angle condition. On top of that, it turns out that the finite element method can converge even on certain sequences of meshes, where the largest angle converges to infinity. This brings us to a still unresolved question, what is the sufficient and necessary condition for the convergence of the finite element method. See [13, 14] for more details.

Zlámal's error bound (11) is a typical example of an *a priori* error estimate. We can hypothetically evaluate it even before any computation (hence *a priori*). However, and it is a characteristic feature of *a priori* error estimates, they contain unknown constants typically denoted by C. The right-hand side of Zlámal's bound contains two such constants. Besides C, it is M_3 that can be theoretically derived from the third derivatives of the exact solution u, but this solution is not known in practical applications and the value of constant M_3 is, thus, unreachable.

4 *A posteriori* error estimates

In contrast to *a priori* error estimates the *a posteriori* bounds can be evaluated from the knowledge of the approximate solution after it has been computed. Hence, the name *a posteriori*. There are various types of *a posteriori* error estimates with various properties. Here, we present one that currently seems most suitable for problem (1).

If $u = u(x_1, x_2)$ and $U = U(x_1, x_2)$ stand for the exact and finite element solutions of (1), respectively, then *a posteriori* error estimator η satisfying

$$\|u - U\|_{W_2^{(1)}(\Omega)} \leq \eta \tag{2}$$

can be computed as

$$\eta^2 = \|\sigma - \nabla U\|^2_{L^2(\Omega)} + \|f - U + \operatorname{div}\sigma\|^2_{L^2(\Omega)}, \quad \text{where} \quad \|v\|^2_{L^2(\Omega)} = \int_\Omega v^2 \,\mathrm{d}x_1\,\mathrm{d}x_2, \tag{3}$$

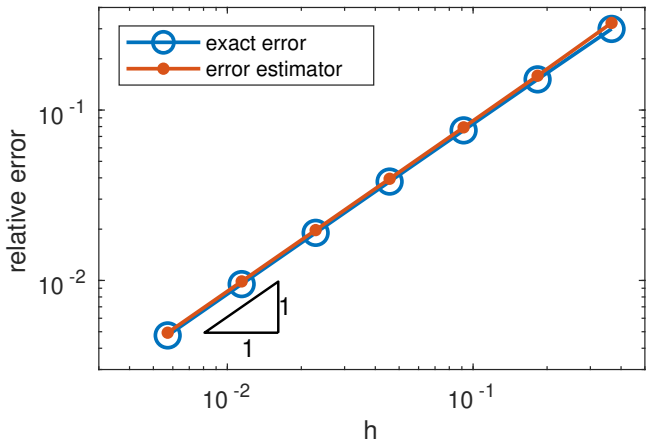

Fig. 4: Convergence of the exact error and the error estimator for uniformly refined meshes.

see e.g. [1]. Here, the flux reconstruction $\sigma = (\sigma_1(x_1, x_2), \sigma_2(x_1, x_2))^T$ is a two-dimensional vector field defined in Ω and $\operatorname{div} \sigma = \partial\sigma_1/\partial x_1 + \partial\sigma_2/\partial x_2$ stands for its divergence. Recall that gradient ∇ was already introduced above.

Interestingly, the error $u - U$ on the left-hand side of (2) is measured in the same $W_2^{(1)}(\Omega)$-norm as in Zlámal's *a priori* bound (11). The square of the *a posteriori* error estimator η is given by (3) as a sum of squares of two $L^2(\Omega)$-norms that can be evaluated from the knowledge of the finite element solution U, right-hand side f and the flux reconstruction σ.

The flux reconstruction σ plays a crucial role in the definition of estimator η. Technically, $\operatorname{div} \sigma$ is required to be square integrable over Ω, but otherwise σ can be arbitrary. However, to obtain a useful and accurate bound on the error, the flux reconstruction σ should approximate the gradient of the exact solution u. There are various possibilities, how the flux reconstruction σ can be computed. It can be a postprocessing of ∇U or it can be computed by minimizing the quadratic functional on the right-hand side of (3) for σ being in a suitable finite dimensional subspace. Although these approaches can be technically involved, fast and accurate algorithms for the flux reconstruction σ are known, see e.g. [4, 5, 10, 16, 17].

A posteriori error estimator (2) is especially useful in practical computations. It does not contain any unknown constant, can be fully computed and the resulting number η is proven to bound the (unknown) error from above. With this error estimator, we can guarantee that the error of our finite element solution is below the required tolerance.

Let us illustrate the convergence of the finite element method and the accuracy of *a posteriori* error estimator (3) on an example. As above, we will solve problem (1) on the square $\Omega = (-1/2, 1/2)$ with the right-hand side $f(x_1, x_2) = \cos(\pi x_1)\cos(\pi x_2)$. For simplicity, we use finite elements of the first order. In this case, the expected order of convergence is one. This means that every time we uniformly refine the triangulation, the error should drop by a factor of two. To verify this fact, we solve the problem on a sequence of uniformly refined meshes, as illustrated in Figure 2. For every mesh, we compute the $W_2^{(1)}(\Omega)$-norm of the error $u - U$ and plot it versus the mesh size h. Figure 4 shows these values in the log-log plot as the blue line with circular markers. We may observe that the error drops almost exactly as the theory predicts.

Note that we can compute this error and plot this convergence curve thanks to the knowledge of the exact solution u only. However, in practical computations the exact solution is unknown and, therefore, *a posteriori* error estimates such as (2) are needed. The red solid line with dot markers in Figure 4 plots the corresponding values of the error estimator η defined by (2). First,

we see that the estimator η is larger than the true error $\|u-U\|_{W_2^{(1)}(\Omega)}$, because of the result (2). Second, the estimator η is a very accurate approximation of the true error.

5 Adaptive mesh refinement

Zlámal's *a priori* error bound (11) assumes sufficient smoothness of the exact solution u, namely, the boundedness of its third derivatives. This is a typical and important assumption in *a priori* error analysis of the finite element method. If the exact solution is not smooth, the finite element method still converges but the convergence need not have the optimal speed. The optimal speed of convergence, even for non-smooth (singular) solutions, can be restored by applying the adaptive mesh refinement.

The main idea of the automatic mesh adaptation is to detect the size of the error on all elements in the mesh and refine those elements, where a large error is indicated while keeping the elements with small errors unchanged. The *a posteriori* error estimator described above is especially suitable for detecting the error on individual elements because it can be localized.

Let us assume that the flux reconstruction σ is already known. If we denote by K an element (triangle) from the finite element triangulation $\mathcal{T}_h$ then the local error indicator η_K is given by identity

$$\eta_K^2 = \|\sigma - \nabla U\|^2_{L^2(K)} + \|f - U + \operatorname{div}\sigma\|^2_{L^2(K)}. \tag{4}$$

Note that the definition of indicators η_K is the same as the definition of the estimator η but restricted from the global space $L^2(\Omega)$ on the entire domain Ω to the local space $L^2(K)$ on the single element K only. It can be easily shown that

$$\eta^2 = \sum_{K\in\mathcal{T}_h} \eta_K^2, \tag{5}$$

i.e., the square of the global error estimator η^2 can be computed by the sum of squares of all local error indicators η_K^2.

Local error indicators η_K given by (4) are essential for the following adaptive algorithm.

1. Construct the initial mesh $\mathcal{T}_h^{(0)}$. Set $k=0$.
2. Find the finite element solution $U^{(k)}$ on $\mathcal{T}_h^{(k)}$.
3. By (4), compute error indicators η_K for all elements $K\in\mathcal{T}_h^{(k)}$.
4. Compute η by (5). If $\eta < TOL$, stop.
5. Mark elements with largest values of η_K.
6. Refine marked elements and construct new mesh $\mathcal{T}_h^{(k+1)}$.
7. Set $k=k+1$ and go to 2.

This adaptive algorithm enables us to find an approximate solution U with the error below the user-prescribed tolerance TOL (see Step 4). On top of that, this algorithm is nearly optimally efficient in terms of the computational costs. These favourable properties are connected to sophisticated theoretical results, such as the upper bound property (2). Most of these results are beyond the scope of this paper. We just mention that the efficiency of this algorithm is connected with the efficiency estimates of the error indicators (4). We do not comment on geometric issues connected with the construction of the mesh in Step 1 and its local refinement

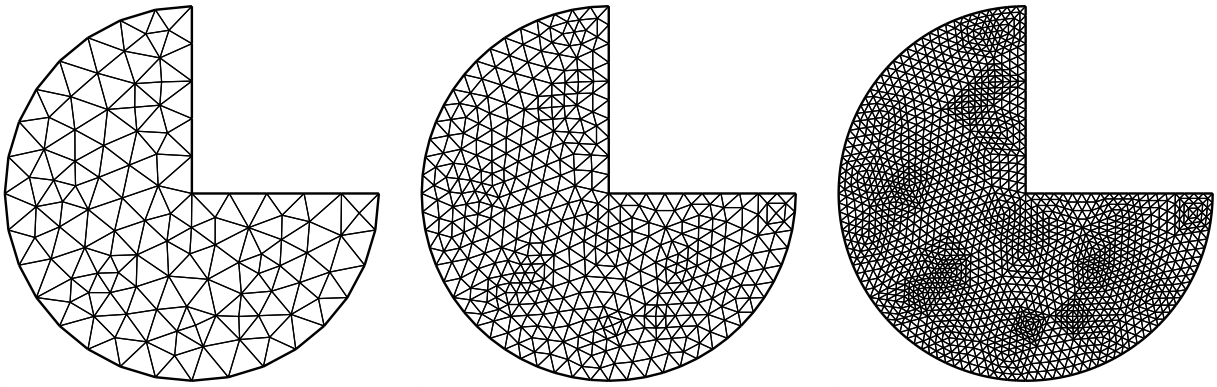

Fig. 5: Sequence of three uniformly refined finite element mesh.

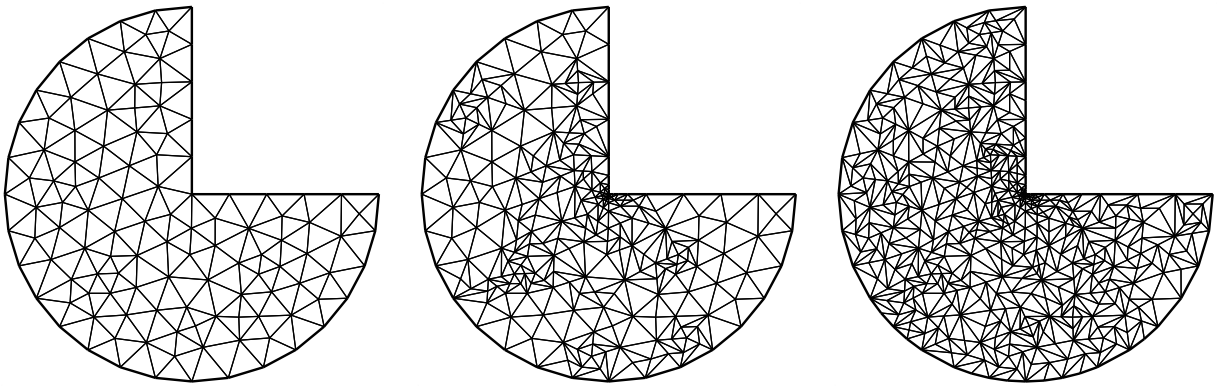

Fig. 6: Sequence of adaptively refined meshes. Initial mesh (left), 7th adaptive step (middle), and 10th adaptive step (right).

in Step 6. Finally, we note that the choice of suitable marking strategy in Step 5 is important for the convergence of this algorithm [9].

At this point, we present a numerical example illustrating the performance of the mesh adaptive algorithm. Let us consider a domain consisting of three-quarters of the unite disc, i.e. the domain $\Omega = \{(r, \theta) : r < 1 \text{ and } \pi/2 < \theta < 2\pi\}$, where (r, θ) are the usual polar coordinates. In this domain, we define the right-hand side as $f = (32/9 + r^{2/3} - r^2)\sin(2\theta - \pi)/3$. It can be verified that the corresponding exact solution of (1) is $u = (r^{2/3} - r^2)\sin(2\theta - \pi)/3$. Notice that the derivative of u with respect to r tends to infinity at zero, i.e. in the re-entrant corner. We say that u has a singularity at this point.

First, we solve this problem on a sequence of uniformly refined meshes as we did above. The first three meshes in this sequence are presented in Figure 5. For every mesh in this sequence, we compute the error bound η by (2) and plot it versus the mesh size h in the log-log axis, see the blue solid line in Figure 7. Note that after every uniform refinement step, the error drops to about 70 % of its original value, while the optimal drop would be 50 %.

This suboptimal convergence rate is caused by the singularity of the exact solution and can be improved by employing adaptive mesh refinement. The above-described algorithm leads to a sequence of locally refined meshes illustrated in Figure 6. The corresponding convergence curve is shown in Figure 7 as the red line with dot markers. Observe that it approaches a straight line with a slope of 1, which corresponds to the optimal rate of convergence. In addition, using roughly the same computational resources, the adaptive algorithm reached considerably more

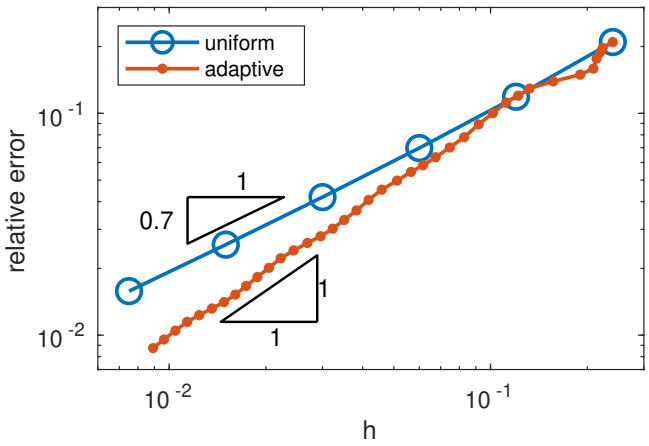

Fig. 7: Uniform and adaptive convergence curves.

accurate results. Note that the mesh size h does not have a good sense for locally refined meshes produced by adaptive algorithms. Therefore, to plot the adaptive convergence curve, we use $h \approx \sqrt{N}$, where N is the number of degrees of freedom, which is equal to the number of interior nodes in the triangulation in this case.

6 Conclusions

In this short contribution, we reviewed the convergence theory of the finite element method for a second-order linear elliptic problem for mathematicians without an expertise in the numerical analysis and finite element method. We emphasized the early *a priori* error bound of Professor Miloš Zlámal and used it as an illustrative example. Subsequently, we present more recent developments in the finite element method and described the concept of *a posteriori* error estimates and automatic mesh adaptation. These essential features of the finite element method are illustrated in several numerical examples by many graphs.

Especially, we explained the concept of convergence on a sequence of uniform meshes. We presented a problem with singularity in the re-entrant corner of the domain causing slower convergence than optimal. Therefore, we introduced the basic ideas of the adaptive algorithm and showed that it enables solving such problems efficiently even in the presence of singularities. We would like to emphasize the essential role of the *a posteriori* error estimates in this approach. First, their localized version indicates, where there are areas of large error within the computational domain and where we need to refine the finite element mesh. Second, they provide a guaranteed upper bound on the size of the error (measured in a suitable norm) and, thus, enable us to stop the adaptive algorithm at the moment, we reach the desired accuracy. As a result, we can confirm what is the error of the computed approximation and we also know that we stopped the calculations as soon as we reached it, so we did not use unnecessary computational resources.

In this contribution, we also touched on the still open problem of finding the sufficient and necessary conditions for the convergence of the finite element method and connected the pioneering result of Professor Miloš Zlámal with the current frontier research in the finite element theory.

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