Interplay between discretization and algebraic computation in adaptive numerical solution of elliptic PDE problems

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Received ..., revised ..., accepted ...
Published online ...

Key words adaptive finite element methods, boundary value problems, eigenvalue problems, a posteriori error analysis, linear algebraic solvers, balancing of errors, stopping criteria
MSC (2000) 65F10, 65F15, 65N22, 65N25, 65N30

The Adaptive Finite Element Method (AFEM) for approximating solutions of PDE boundary value and eigenvalue problems is a numerical scheme that automatically and iteratively adapts the finite element space until a sufficiently accurate approximate solution is found. The adaptation process is based on a posteriori error estimators, and at each step of this process an algebraic problem (linear or nonlinear algebraic system or eigenvalue problem) has to be solved. In practical computations the solution of the algebraic problem cannot be obtained exactly. As a consequence, the algebraic error should be incorporated in the context of the AFEM and its a posteriori error estimators. The goal of this paper is to survey some existing approaches in the AFEM context that consider the interplay between the finite element discretization and the algebraic computation. We believe that a better understanding of this interplay is of great importance for the future development in the area of numerically solving large-scale real-world motivated problems.

1 Introduction

The finite element method (FEM) is widely used in order to discretize variational formulations of partial differential equations representing boundary value or eigenvalue problems. In this method an approximation to the exact PDE solution is found as a linear combination of basis vectors (functions) from a finite dimensional function space, called the *finite element space*. The coefficients in this linear combination are determined by solving a linear algebraic problem (linear algebraic system or algebraic eigenvalue problem). The construction of the finite element space is based on a mesh that discretizes the domain on which the PDE is formulated.

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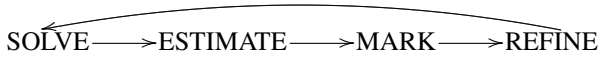
The basis functions typically have a local support consisting of several mesh elements. Usually, a finer mesh leads to a better approximation. However, there is a trade-off: finer meshes mean more finite element basis functions, hence larger algebraic problems, and consequently a higher computational effort for determining the approximate solution.

To balance accuracy of numerical approximation and cost of computation one can use the following idea: start with a coarse mesh, compute an approximate solution, refine the mesh only in regions where this approximation is not good enough, and then compute a new approximation using the refined mesh. What we have just described is one iteration of the *Adaptive Finite Element Method (AFEM)*, which starts with setting the mathematical model and its initial approximation, and which can schematically be written as follows:



Here "SOLVE" means solving the linear algebraic problem (linear algebraic system or eigenvalue problem) and "ESTIMATE" means the *local a posteriori* estimation of the error between the exact solution and its numerical approximation. The steps "MARK" and "REFINE" refer to the actual refinement of the mesh; they are not in the focus of this paper. In short, the AFEM can be described as a numerical scheme that automatically and iteratively adapts the finite element space until a sufficiently accurate approximate solution is found.

The AFEM is no new development. This is documented, e.g., by a special issue of *Computing* devoted to "adaptive techniques" published in 1995, where Hackbusch wrote in the Editorial:

> Adaptivity is a further development. Instead of solving problems with a discretization of very high dimension, it is more reasonable to obtain the same solution quality by a lower dimensional but adapted discretization. Adaptivity has created a new paradigm in mathematical computation. In traditional numerical mathematics, the fields "discretization" (e.g., FEM), its "numerical analysis" (e.g., error estimates), and "solution algorithms" (e.g., solvers for linear systems) are well separated. Adaptive techniques, however, require a combination of all three. For example, the error estimation has become a part of the algorithm. The concrete discretization is now an outgrowth of the algorithm.

The special issue of *Computing* contains recommendable contributions, among them the paper of Becker, Johnson and Rannacher [22], which affected further development related, in particular, to multigrid finite element methods. In the Introduction, which can be considered a rigorous formulation of the new research program, the authors write:

> [F]or large size problems, in particular in three dimensions, direct methods are too work-intensive and only iterative methods such as multigrid methods or preconditioned conjugate gradient type methods may be used. ... Usually, ad hoc stopping criteria are used, e.g. requiring an initial (algebraic) residual to be reduced by a certain ad hoc factor, but these criteria have no clear connection to the actual error in the corresponding approximate solution, which is the quantity of interest. This leaves the user of iterative solutions methods in a serious dilemma: With no objective stopping criterion available, one has either to continue the iterations until the discrete solution error is practically "zero", which increases the computational

> cost with possibly no gain in the overall precision, or take the risk of stopping the iterations prematurely. In the first case there would be a loss of efficiency and in the second a loss of reliability. ... A solution to this problem can only be obtained by combining aspects of the underlying partial differential equations and the corresponding finite element discretization with aspects of the iterative discrete solution algorithm. A "pure" numerical linear algebra point of view, for instance based on the condition number of the stiffness matrix, does not appear to be able to lead to a balance of discretization and solution errors.

It is remarkable that only a relatively small percentage of the research devoted to adaptive finite element methods has adopted this point of view. In fact, in the vast majority of publications on the AFEM (and on the FEM in general) it is assumed that the step "SOLVE" is performed *exactly*. Moreover, in almost all publications considering inexact solution of the algebraic problem, the inexactness is identified with iterative methods and their premature stopping, while it is assumed that the algebraic computations are performed in exact arithmetic. As a consequence, in the majority of publications on the AFEM it is assumed that direct solvers are "exact" (irrespectively of the numerical properties of the problems to be solved), and maximum attainable accuracy as well as delay of convergence of iterative methods are excluded from consideration. These assumptions, however, cannot be satisfied in practical computations; see, e.g. [123]. Their violation can lead to discrepancies between proven statements for arbitrary error tolerance on the one hand, and computational results on the other; see, e.g. Theorem 3.11 and experimental results presented in [97].

We believe that a better understanding of the interplay between discretization and algebraic computation (including rounding errors) in the adaptive numerical solution of PDEs is of great importance for the future development in the area of numerically solving large-scale real-world problems. Our main intention in this paper is to survey some approaches that consider this interplay. To illustrate the main results and algorithms we use the setting of standard *linear, elliptic and selfadjoint* model problems. We state these problems in Section 2. In Section 3 we recall adaptive discretization and a posteriori error analysis for both boundary value and eigenvalue problems. Section 4 then discusses coupling of the discretization and the linear algebraic computation in the AFEM context. Some concluding remarks are given in Section 5.

Our presentation is addressed to nonspecialists, and therefore we keep technical details at a minimum. Such details can be found in the references that are cited throughout the text.

2 Model problems, the FEM, and a priori analysis

In this section we introduce basic notation, standard model problems, and the general context of the results stated in the following sections. Many readers are certainly familiar with the presented concepts, but we believe it is useful to recall them here for completeness. As mentioned above, we restrict ourselves to linear, elliptic and selfadjoint model problems, and we focus on the Galerkin-FEM rather than on more general (Petrov-Galerkin) methods. Extended treatments of the FEM and its many variants can be found in numerous books devoted to this method and its applications; see, e.g. [15, 35, 50, 51, 62, 70, 106, 121, 125].

2.1 Boundary value model problem and the Galerkin method

We start with the standard variational formulation of a linear boundary value problem:

$$\text{Find } u \in V \text{ such that } \mathfrak{a}(u,v) = \ell(v) \text{ for all } v \in V, \tag{1}$$

where V is a real Hilbert space with scalar product $(\cdot,\cdot)_V$ and the associated norm $\|\cdot\|_V$, $\mathfrak{a} : V \times V \to \mathbb{R}$ is a bilinear form, and $\ell : V \to \mathbb{R}$ is a bounded linear functional. Throughout this paper we assume that $\mathfrak{a}(\cdot,\cdot)$ satisfies the following conditions:

1. $\mathfrak{a}(\cdot,\cdot)$ is *symmetric*: $\mathfrak{a}(v,w) = \mathfrak{a}(w,v)$ for all $v, w \in V$.
2. $\mathfrak{a}(\cdot,\cdot)$ is *continuous (or bounded)*:
   There exists a real constant $\alpha > 0$ such that $\mathfrak{a}(w,v) \le \alpha \|w\|_V \|v\|_V$ for all $w, v \in V$.
3. $\mathfrak{a}(\cdot,\cdot)$ is *coercive (or V-elliptic)*:
   There exists a real constant $\beta > 0$ such that $\mathfrak{a}(w,w) \ge \beta \|w\|_V^2$ for all $w \in V$.

Because of conditions 2. and 3., the classical Lax-Milgram Lemma [86] (see, e.g. [62, Theorem 2.12, p. 52], [70, Theorem 6.5.9, p. 140] or [106, Theorem 5.5.1, p. 133]), implies that the variational problem (1) has a unique solution that depends continuously on the given data. Since the bilinear form $\mathfrak{a}(\cdot,\cdot)$ is coercive and symmetric, it defines a scalar product on V. The associated norm

$$|\!|\!| v |\!|\!| \equiv \mathfrak{a}(v,v)^{1/2}$$

is called the *energy norm* on V.

A widely used example where all conditions on $\mathfrak{a}(\cdot,\cdot)$ are satisfied is the Poisson equation $-\Delta u = f$ in a polyhedral domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2$, or 3) with a given function $f \in L^2(\Omega)$ and with homogeneous Dirichlet boundary conditions, $u = 0$ on $\partial\Omega$. The variational formulation of this problem is of the form (1) with

$$\begin{aligned} V &\equiv H_0^1(\Omega) \equiv \{v \in L^2(\Omega) \,|\, \nabla v \in [L^2(\Omega)]^d,\ v = 0 \text{ on } \partial\Omega \text{ in the sense of traces}\}, \\ \mathfrak{a}(w,v) &\equiv \int_\Omega \nabla w \cdot \nabla v \, d\Omega, \\ \ell(v) &\equiv \int_\Omega f\, v \, d\Omega. \end{aligned} \tag{2}$$

Many results stated in this paper were (first) derived in the context of this model problem.

Note that continuous bilinear forms on $V \times V$ can be identified with continuous linear mappings from V to its dual space V'. Denoting by $\langle\cdot,\cdot\rangle$ the $V' \times V$ duality pairing, this is done by considering, for a fixed u, the linear mapping T from V to V' given by

$$\langle Tu, v\rangle = \mathfrak{a}(u,v) = \ell(v) = \langle f, v\rangle. \tag{3}$$

This mapping is coercive and continuous if the bilinear form $\mathfrak{a}(\cdot,\cdot)$ is. Given the mapping, it can of course be used to define the bilinear forms. Summarizing, using $T : V \to V'$, the variational formulation (1) can be written as an operator equation in the dual space V', i.e.

$$Tu = f, \text{ where } f \in V'; \tag{4}$$

for a concise description see [80, Section 2] and for details see, e.g. [35, Section 2.7], [36, p. 81] or [59, Section 5.9.1 and Chapter 6]. The formulation (4) is conveniently used in numerical analysis of PDE boundary value problems.

Using the inequalities of the Lax-Milgram Lemma one can show that the V-norm of the discretization error is bounded as

$$\|u - u_h\|_V \leq \frac{\alpha}{\beta} \min_{v_h \in V_h} \|u - v_h\|_V. \tag{5}$$

This result is known as Céa's Lemma [47, Proposition 3.1]; see, e.g. [62, p. 61], [70, Theorem 8.2.1, p. 168] or [106, Theorem 5.2.1, p. 137].

For $V = H^1(\Omega) \equiv \{v \in L^2(\Omega) \,|\, \nabla v \in [L^2(\Omega)]^d\}$ and the corresponding norm,

$$\|w\|_{H^1(\Omega)} \equiv \left(\int_\Omega (w^2 + \nabla w \cdot \nabla w)\, d\Omega \right)^{1/2} \quad \text{for all } w \in H^1(\Omega),$$

it can be shown that

$$|\!|\!| w |\!|\!| \leq \|w\|_{H^1(\Omega)} \leq c\, |\!|\!| w |\!|\!| \quad \text{for all } w \in H^1_0(\Omega), \tag{6}$$

where the energy norms on the left and right correspond to the bilinear form $\mathfrak{a}(\cdot,\cdot)$ from the Poisson model problem (2), and $c > 0$ is some generic constant[1] that is independent of w. In the context of the Poisson model problem the norm equivalence expressed in (6) allows to derive error bounds with respect to the $H^1(\Omega)$-norm from those for the energy norm, and vice versa.

Here it is important to point out some differences between analysis of PDEs and numerical solution of PDEs. While in analysis the (topological) equivalence of norms represents a basic tool, in computations one should always specify the possible size of any unspecified constant. As an example, if we solve the discretized problem iteratively, it does make a difference in which norm (or, more generally, in which way) we measure the distance of the computed approximation to the true solution. The algebraic error should, as a rule, be measured in a norm conforming to the underlying PDE or its variational formulation. Hence, in particular, the algebraic residual norm should not be used for stopping the algebraic iterations unless there is a well justified reason for doing so; for further comments on this issue see Section 4 below.

We will now consider the *Galerkin method* for finding an approximation to the solution of a variational problem of the form (1). In this method one chooses a finite dimensional subspace $V_h \subset V$ and then solves the variational problem on V_h:

$$\text{Find } u_h \in V_h \text{ such that } \mathfrak{a}(u_h, v_h) = \ell(v_h) \text{ for all } v_h \in V_h. \tag{7}$$

By the assumptions on $\mathfrak{a}(\cdot,\cdot)$ and $\ell(\cdot)$, and since V_h is a subspace of V, the Lax-Milgram Lemma implies that (7) has a uniquely determined solution u_h. For any $v_h \in V_h$ we have the *Galerkin orthogonality property*

$$\mathfrak{a}(u - u_h, v_h) = \mathfrak{a}(u, v_h) - \mathfrak{a}(u_h, v_h) = \ell(v_h) - \ell(v_h) = 0, \tag{8}$$

[1] Throughout this paper we use, for ease of notation, the letter c to denote a constant independent of the solution u. The actual values of c will be different in different contexts.

which means that the *discretization error* $u - u_h \in V$ is orthogonal to the subspace V_h with respect to the scalar product $\mathfrak{a}(\cdot,\cdot)$ on V. This implies that the method is optimal with respect to the energy norm, i.e. the discretization error satisfies

$$|||u - u_h||| \;=\; \min_{v_h \in V_h} |||u - v_h|||. \tag{9}$$

The bounds (5) and (9) are essential ingredients in the *a priori error analysis* of the FEM for boundary value problems; see Section 2.3 below.

Let V_h be of dimension n_h, and let $\phi_1, \phi_2, \ldots, \phi_{n_h}$ be a basis of V_h. Then we can write

$$u_h = \sum_{j=1}^{n_h} \mu_{h,j}\phi_j, \tag{10}$$

where the coefficients in this linear combination are to be determined. This can be done by rewriting the problem (7) in the form

Find $\mu_{h,1}, \mu_{h,2}, \ldots, \mu_{h,n_h} \in \mathbb{R}$ such that
$\sum_{j=1}^{n_h} \mathfrak{a}(\phi_j, \phi_i)\mu_{h,j} = \ell(\phi_i)$ for all $i = 1, 2, \ldots, n_h$,

which is equivalent to finding the solution $\mathbf{u}_h = [\mu_{h,i}] \in \mathbb{R}^{n_h}$ of the linear algebraic system

$$\mathbf{A}\mathbf{u}_h = \mathbf{b}, \;\; \mathbf{A} = [a_{ij}] = [\mathfrak{a}(\phi_j, \phi_i)] \in \mathbb{R}^{n_h \times n_h}, \;\; \mathbf{b} = [b_i] = [\ell(\phi_i)] \in \mathbb{R}^{n_h}. \tag{11}$$

The matrix $\mathbf{A}$, which by our assumptions on $\mathfrak{a}(\cdot,\cdot)$ is symmetric and positive definite, is often called the *stiffness matrix*. This term goes back to early applications of the method in structural mechanics.

Suppose that

$$\mathbf{u}_h^{(n)} = [\mu_{h,i}^{(n)}] \in \mathbb{R}^{n_h}$$

is an approximation of the vector $\mathbf{u}_h$, with the corresponding approximation of the function $u_h \in V_h$ given by

$$u_h^{(n)} \equiv \sum_{j=1}^{n_h} \mu_{h,j}^{(n)}\phi_j \;\in\; V_h.$$

Then the *algebraic error* is

$$\mathbf{u}_h - \mathbf{u}_h^{(n)} \;\in\; \mathbb{R}^{n_h} \quad \text{or} \quad u_h - u_h^{(n)} \;\in\; V_h.$$

The *total error* is given by the the sum of the discretization error and the algebraic error, i.e.

$$u - u_h^{(n)} = (u - u_h) \;+\; (u_h - u_h^{(n)}). \tag{12}$$

Since $u_h - u_h^{(n)} \in V_h$, the Galerkin orthogonality property (8) implies that

$$|||u - u_h^{(n)}|||^2 = |||u - u_h|||^2 + |||u_h - u_h^{(n)}|||^2. \tag{13}$$

This equality for the energy norms of the respective quantities indicates that in practical applications the discretization error and the algebraic error should be in a reasonable balance,

so that neither one of them dominates the total error. This observation has important consequences for coupling of the linear algebraic computations with the FEM discretization in particular in the AFEM context. We will explore these consequences in Section 4 below.

It is worth to point out that in (13) the relation between the total error, the discretization error and the algebraic error is described in terms of their global norms. In the context of adaptive numerical solution of PDEs this is not sufficient. For an instructive discussion of this point we refer to the book [15], where Babuška and Strouboulis state on p. 417:

> In engineering practice it is not sufficient to estimate only the energy norm of the error because *a small value of the global energy norm of the error does not necessarily imply that the error in the outputs of interest is also small* (e.g. a 5% relative error in the global energy norm does not imply 5% relative error in the maximum stress in a region of interest). ... An essential requirement is that the quantity of interest has to be well defined; for example, it is meaningless to ask for an estimate of the maximum error in the derivative, flux, or stress for a problem set in a polygonal non-convex domain, because the exact value does not exists (the derivative, flux, or stress in the neighborhood of a corner point is usually unbounded).

Moreover, there is no guarantee that the spatial distributions of the (properly measured) discretization error and algebraic error are similar; see [87, Chapter 5] and [102] for illustrations of this fact. When evaluating the local error indicators in practice one should therefore consider *local* distributions of the appropriately measured *individual* errors $u-u_h^{(n)}$ and $u_h-u_h^{(n)}$.

2.2 Eigenvalue model problem and the Galerkin method

The standard variational formulation of a linear PDE eigenvalue (and eigenfunction) problem considered in this paper can be written as follows:

$$\text{Find } u \in V \setminus \{0\} \text{ and } \lambda \in \mathbb{R} \text{ such that } \mathfrak{a}(u,v) = \lambda\,(u,v)_W \text{ for all } v \in V. \tag{14}$$

Here V, W are two real Hilbert spaces such that the embedding $V \subset W$ is compact and V is dense in W, $(\cdot,\cdot)_W$ is the scalar product on W, and $\mathfrak{a} : V \times V \to \mathbb{R}$ is a (symmetric, continuous and coercive) bilinear form.

A standard example is given by the Poisson eigenvalue (and eigenfunction) model problem formulated in a polyhedral domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2,$ or 3) with homogeneous Dirichlet boundary conditions. The task is to find a nonzero function $u : \overline{\Omega} \to \mathbb{R}$ and a scalar $\lambda \in \mathbb{R}$, such that $-\Delta u = \lambda u$ in Ω, where $u = 0$ on $\partial\Omega$. The variational formulation of this problem is given by (14) with

$$\begin{aligned} &V \equiv H_0^1(\Omega) \subset W \equiv L^2(\Omega),\\ &\mathfrak{a}(w,v) \equiv \textstyle\int_\Omega \nabla w \cdot \nabla v \, d\Omega,\\ &(w,v)_W \equiv \textstyle\int_\Omega w\, v \, d\Omega. \end{aligned} \tag{15}$$

Consider, for any given $f \in V$, the following (variational) boundary value problem:

$$\text{Find } z \in V \text{ such that } \mathfrak{a}(z,v) = (f,v)_W \text{ for all } v \in V.$$

By our assumptions on $\mathfrak{a}(\cdot,\cdot)$ this problem has a unique solution $z \in V$. Hence we can introduce the (linear and compact) *solution operator* $S : V \to V$ such that

$$\mathfrak{a}(Sf, v) = (f, v)_W \quad \text{for all} \quad v \in V. \tag{16}$$

Since $\mathfrak{a}(\cdot,\cdot)$ is symmetric and coercive, which holds in particular for $\mathfrak{a}(\cdot,\cdot)$ in (15), the operator S has countably many eigenvalues that are real and positive. Their reciprocals, denoted by

$$0 < \lambda_1 \le \lambda_2 \le \cdots \le \lambda_m \le \cdots ,$$

give the eigenvalues of the problem (14); see, e.g. [13, p. 650], [59, p. 355] or [70, Theorem 11.1.2, p. 253–254]. The corresponding (normalized) eigenfunctions u_j form an orthonormal basis for the space W; see, e.g. [59, p. 355]. Using the operator S with $f = u$ and (14) we get

$$\mathfrak{a}(Su, v) = (u, v)_W = \frac{1}{\lambda}\mathfrak{a}(u, v) = \mathfrak{a}(\frac{1}{\lambda}u, v) \quad \text{for all} \quad v \in V.$$

Hence $\{\lambda, u\}$ is a solution of the eigenvalue problem (14) if and only if $\{\frac{1}{\lambda}, u\}$ is an eigenpair of the operator S. For further details see, e.g. [48, Chapter 4, pp. 203–204], [59, p. 355–356] or [31, 82, 117].

Analogously to the Galerkin method for boundary value problems, the Galerkin method for the eigenvalue problem (15)–(14) consists in solving the variational problem on a finite dimensional subspace $V_h \subset V$:

$$\begin{aligned} &\text{Find } u_h \in V_h \setminus \{0\} \text{ and } \lambda_h \in \mathbb{R} \text{ such that} \\ &\mathfrak{a}(u_h, v_h) = \lambda_h\,(u_h, v_h)_W \text{ for all } v_h \in V_h. \end{aligned} \tag{17}$$

As in the previous section, let n_h be the dimension of V_h, and let $\phi_1, \phi_2, \ldots, \phi_{n_h}$ be a basis of V_h. Writing the function u_h as a linear combination of the basis functions (as in (10)), the problem (17) can be transformed into the equivalent *generalized algebraic eigenvalue problem*

$$\begin{aligned} &\mathbf{A}\mathbf{u}_h = \lambda_h \mathbf{M}\mathbf{u}_h, \quad \text{where} \\ &\mathbf{A} = [a_{ij}] = [\mathfrak{a}(\phi_j, \phi_i)] \in \mathbb{R}^{n_h \times n_h}, \;\; \mathbf{M} = [m_{ij}] = [(\phi_j, \phi_i)_W] \in \mathbb{R}^{n_h \times n_h}, \end{aligned}$$

for the eigenvalue $\lambda_h \in \mathbb{R}$ and a corresponding eigenvector $\mathbf{u}_h \in \mathbb{R}^{n_h}$. The matrix $\mathbf{A}$ is (as above) called the stiffness matrix, and $\mathbf{M}$ is the *mass matrix*.

Both $\mathbf{A}$ and $\mathbf{M}$ are symmetric positive definite (since both $\mathfrak{a}(\cdot,\cdot)$ and $(\cdot,\cdot)_W$ are scalar products), and hence the problem (17) has a finite sequence of eigenvalues

$$0 < \lambda_{h,1} \le \lambda_{h,2} \le \cdots \le \lambda_{h,n_h}$$

with the corresponding eigenvectors $\mathbf{u}_{h,1}, \mathbf{u}_{h,2}, \ldots, \mathbf{u}_{h,n_h} \in \mathbb{R}^{n_h}$ that can be chosen $\mathbf{M}$-orthonormal, i.e. $\mathbf{u}_{h,i}^T \mathbf{M} \mathbf{u}_{h,j} = \delta_{ij}$. They determine, analogously to (10), the respective eigenfunction approximations $u_{h,1}, u_{h,2}, \ldots, u_{h,n_h} \in V_h$. The eigenvalue $\lambda_{h,j}$ and the corresponding function $u_{h,j}$ are called the *Galerkin approximation* of the j-th eigenvalue λ_j and the corresponding eigenfunction u_j of the problem (14). From the Courant-Fischer minimax theorem it directly follows that

$$\lambda_j \le \lambda_{h,j}, \quad j = 1, 2, \ldots, n_h;$$

see, e.g. [13, equation (8.42), p. 699] or [125, equation (23), p. 223].

If we solve the generalized eigenvalue problem inexactly, and hence obtain an eigenvector approximation $\mathbf{u}_{h,j}^{(n)}$ and a corresponding eigenvalue approximation $\lambda_{h,j}^{(n)}$, we get the *algebraic errors*

$$\mathbf{u}_{h,j} - \mathbf{u}_{h,j}^{(n)} \in \mathbb{R}^{n_h} \quad \text{or} \quad u_{h,j} - u_{h,j}^{(n)} \in V_h, \quad \text{and} \quad \lambda_{h,j} - \lambda_{h,j}^{(n)}.$$

The *total errors* are then given by

$$u_j - u_{h,j}^{(n)} = (u_j - u_{h,j}) + (u_{h,j} - u_{h,j}^{(n)}) \quad \text{and} \tag{18}$$

$$\lambda_j - \lambda_{h,j}^{(n)} = (\lambda_j - \lambda_{h,j}) + (\lambda_{h,j} - \lambda_{h,j}^{(n)}). \tag{19}$$

In both cases the total error is the sum of the discretization error and the algebraic error.

All this looks very similar to the formulations for the boundary value problems in the previous section. However, results obtained for boundary value problems can typically not be directly transferred because eigenvalue problems are by their nature *nonlinear*. In particular, there exists no simple analogy to the Galerkin orthogonality property (8) for the boundary value problems: When $\{\lambda, u\}$ and $\{\lambda_h, u_h\}$ are eigenpairs of (14) and (17), respectively, we get

$$\mathfrak{a}(u - u_h, v_h) = (\lambda u - \lambda_h u_h, v_h)_W. \tag{20}$$

This is usually nonzero for any nonzero $v_h \in V_h$.

2.3 The FEM and a priori error estimation

The FEM (more precisely, the Galerkin-FEM) generates the subspace V_h in order to obtain a *sparse* matrix $\mathbf{A}$, respectively *sparse* matrices $\mathbf{A}$ and $\mathbf{M}$. The method is based on a decomposition of $\overline{\Omega}$ into a finite number of subdomains τ_j, called the *elements*. In case Ω is a polyhedral domain one typically considers simplicial elements. Popular choices are triangles when $\Omega \subset \mathbb{R}^2$, and tetrahedra when $\Omega \subset \mathbb{R}^3$. We denote by $\mathcal{T}_h$ the set of all the elements in the decomposition $\overline{\Omega} = \cup_j \tau_j$. This decomposition is called the *mesh*, with the *mesh size* h given by the maximal diameter of any element. A standard assumption is that each intersection of two distinct elements is either empty, or a common vertex, or a common edge in $\mathbb{R}^2$ (a common face or a common edge in $\mathbb{R}^3$) of the two elements.

In the standard FEM, the finite element basis functions $\phi_1, \phi_2, \ldots, \phi_{n_h}$ are globally (i.e. throughout Ω) continuous functions that are piecewise (i.e. on individual elements) polynomials, and that are nonzero only on a few of the elements. Considering higher-degree polynomials but preserving the geometry of the mesh is called a *p-refinement*. Below we will mostly consider *h-refinements*, also called *mesh refinements*, where the decomposition of $\overline{\Omega}$ is refined by subdividing elements.

When the supports of ϕ_i and ϕ_j do not overlap, the corresponding entries $a_{ij} = \mathfrak{a}(\phi_j, \phi_i)$ of $\mathbf{A}$ and $m_{ij} = (\phi_j, \phi_i)_W$ of $\mathbf{M}$ will be zero. Hence the local nature of the FEM basis functions guarantees sparsity of the stiffness and mass matrices. At the same time it means that the solutions u_h of the variational problem (7) or $u_{h,j}$ of the problem (17) are linear combinations of functions with significantly local supports. The global approximation properties of u_h or $u_{h,j}$ have to be obtained by solving the linear algebraic system or the algebraic eigenvalue problem.

Standard *a priori convergence theory* for the FEM is concerned with bounding the discretization error of the boundary value or the eigenvalue problem *globally* in some norm. We point out that the choice of the polynomial degree used for the basis of the FEM approximation is linked with the *regularity of the solution* of the boundary value problem or of the eigenfunctions we want to approximate; see, e.g. [69] for an extensive analysis of the regularity of the solutions when Ω is not convex, and [11, 125] for the convergence analysis for Sobolev spaces $H^s(\Omega)$ for real s (so-called fractional order Sobolev spaces [1]). Under some *regularity assumptions on the mesh*, the usual goal of an a priori analysis is to find bounds on the discretization error that depend on the mesh size h. For example, a standard regularity assumption used in the context of triangular meshes is a minimum angle condition to guarantee that the interior angles of the elements do not become too acute; see, e.g. [56, Definition 1.15, p. 44] or [125, Chapter 3, Section 3.1 and 3.2].

A classical result for boundary value problems of the form (1) on a polygonal domain $\Omega \subset \mathbb{R}^2$ can be formulated as follows: If $\mathfrak{a}(\cdot,\cdot)$ and $\ell(\cdot)$ satisfy the Lax-Milgram conditions, the solution satisfies $u \in H^s(\Omega)$ for some integer $s > 1$, the FEM basis functions are (locally) polynomials of degree k, where $1 \leq k < s$, and the triangular mesh is regular, then

$$\|u - u_h\|_{H^1(\Omega)} \;\leq\; c\,\|u\|_{H^{r+1}(\Omega)}\, h^r, \quad \text{where } r \equiv \min(k, s-1). \tag{21}$$

Here $c > 0$ is a constant depending on the ratio α/β (from the Lax-Milgram conditions) and on the minimum angle in the mesh, but c does not depend on the mesh size h and the solution u. This result can be generalized to real values of s [11]; see also [70, Theorem 8.4.8, p. 189] for the case $1 < s \leq 2$, [106, Theorem 6.2.1, p. 171] for the case $s \geq 2$, and the classical book [51] for a general treatment. A less technical presentation valid for integer $s > 1$ is given in [62, Section 5.3]. The exponent r on the right hand side of (21) is called the method's *rate of convergence*. The inequality indicates that when the solution is sufficently smooth, higher degree finite elements (i.e. p-refinement) yield a larger rate of convergence. Results of the form (21) are derived by bounding the minimization problem on right hand side of (5) or (9).

In eigenvalue problems the analysis is complicated due to the lack of a Galerkin-type orthogonality property; see Section 2.2 above. Nevertheless, one can derive a priori bounds on the discretization error that depend on the regularity of the eigenfunction and hence, in particular, on the geometry of the domain Ω; see, e.g. [125, Chapter 8] or [69] for details on the regularity of eigenfunctions.

One of the first a priori error results for eigenvalues and eigenfunctions of elliptic operators was obtained by Strang and Fix in [125, Chapter 6], where the eigenfunction approximations are determined by the Rayleigh-Ritz method, i.e. as the stationary (fixed) points of the Rayleigh-quotient $\mathfrak{a}(\cdot,\cdot)/(\cdot,\cdot)_W$. Improvements for selfadjoint operators were made in [48, 81, 112], and for compact operators in [12, 13].

To state a well known a priori error bound for the problem (14) with $\mathfrak{a}(\cdot,\cdot)$ symmetric and satisfying the Lax-Milgram conditions, suppose that $\{\lambda, u\}$ is an eigenpair, where λ is a simple eigenvalue and the eigenfunction satisfies $u \in H^s(\Omega)$ for some (real) $s \in (1, 2]$. When the triangular mesh is regular and linear finite elements are used, there exists an eigenpair $\{\lambda_h, u_h\}$ of the discretized problem (17) such that

$$\|u - u_h\|_{H^1(\Omega)} \leq c\, h^{s-1} \quad \text{and} \quad |\lambda - \lambda_h| \leq c\, h^{2(s-1)}, \tag{22}$$

where the constant $c > 0$ depends on the eigenvalue λ, the eigenfunction u, and on the mesh; see, e.g. [70, Corollary 11.2.21, p. 264]. A key observation to be made in (22), which is also made in the standard matrix perturbation theory, is that the eigenvalue approximation is usually much more accurate than the corresponding eigenfunction approximation. A generalization of this result to the case of multiple eigenvalues is given by Babuška and Osborn in [13]; see also the recent survey paper [31].

3 Adaptivity and a posteriori estimators

A priori bounds of the form (21) or (22) indicate that the discretization error decreases (at least asymptotically) with a decreasing mesh size h. Since h is the maximum diameter of any element, we get $h \to 0$ only if the mesh is refined *everywhere*. Such refinement, however, is costly and it is usually prohibitive in challenging practical applications. The key idea of adaptive mesh refinement is to refine the mesh only where it is necessary. This requires information on the local distribution of the error within the domain, which is provided by a locally efficient and computable *a posteriori error estimator*. In the following we will summarize main ideas of a posteriori error estimation in the FEM context. For further details we refer in particular to the books [3, 15, 17, 129], or the surveys given in [57, 67, 97, 100, 118].

Using an appropriate norm induced by a scalar product on $L^2(\Omega)$ or $H^1(\Omega)$, an a posteriori error estimator for a stationary boundary value problem like (1)–(3) is typically written as

$$\|u - u_h\| \approx \eta, \qquad \eta \equiv \left(\sum_{\tau \in \mathcal{T}_h} \eta_\tau^2 \right)^{1/2} \tag{23}$$

(similarly for the eigenvalue problem), where η_τ is an indicator for the local error on the element τ. This indicator depends on u_h and some known information about the problem, for example the domain Ω and its boundary. Other forms of a posteriori error estimators can be found, e.g., in [3, Section 2.5].

A posteriori error estimators should be computable from u_h at a low cost, and they should ideally satisfy the following additional properties:

1. *Reliability* (*guaranteed upper bound*): The right hand side in the approximation (23) represents an upper bound on the left hand side,

$$\|u - u_h\| \leq \left(\sum_{\tau \in \mathcal{T}_h} \eta_\tau^2 \right)^{1/2}.$$

   This definition of reliability corresponds to the ideal situation where the estimator on the right hand side is not multiplied by a constant $c > 0$. Some important estimators satisfy a weaker form of reliability, where a constant c is present; see, e.g. (25)–(26) below.

2. *Local efficiency*: For each element $\tau \in \mathcal{T}_h$ the corresponding η_τ represents a lower bound on the error in the vicinity $\widehat{\tau}$ of τ (typically $\widehat{\tau}$ is the union of τ and its neighbors) up to a mesh size independent constant $c > 0$,

$$\eta_\tau \leq c\|u - u_h\|_{\widehat{\tau}} + h.o.t. \quad \text{for all } \tau \in \mathcal{T}_h.$$

The constant c should not be close to zero and it should not be substantially (orders of magnitude) larger than one; $h.o.t.$ represents a higher order term related to data oscillations.

3. *Asymptotic exactness*: The ratio of the error and its estimator in (23) approaches one when the estimators are used to locally refine the mesh within the AFEM loop (cf. the Introduction).

It is highly desirable that the a posteriori estimators are also *robust*, i.e. the above mentioned properties should hold for a wide range of parameters defining the practical problems. Not every existing a posteriori estimator satisfies all these desirable properties. In the following we will give examples of some techniques and mention which properties have been shown for them.

For a typical example we consider the variational boundary value model problem (1)–(2) in a bounded polygonal domain $\Omega \subset \mathbb{R}^2$ and its Galerkin discretization as in (7). Let $\mathcal{T}_h$ be a regular triangulation of Ω. Considering the discretization error $u - u_h$ and any given $v \in V$ we can write

$$\mathfrak{a}(u - u_h, v) = \ell(v) - \mathfrak{a}(u_h, v) = \sum_{\tau \in \mathcal{T}_h} \left(\int_\tau f\, v d\tau - \int_\tau \nabla v \cdot \nabla u_h \right). \tag{24}$$

Let $\mathcal{E}_h$ be the set of edges in the triangulation $\mathcal{T}_h$ excluding the boundary of Ω. For a scalar function w that is defined in an open neighborhood of $\varepsilon \in \mathcal{E}_h$ one defines the *jump across* ε by

$$[w](x) \equiv \lim_{t \to 0} \left(w(x - t\mathbf{n}_\varepsilon) - w(x + t\mathbf{n}_\varepsilon) \right), \quad x \in \varepsilon,$$

where $\mathbf{n}_\varepsilon$ denotes the outward normal of ε (this is defined analogously in $\mathbb{R}^3$ for element faces). Let h_τ and h_ε denote the mesh sizes of the element τ and the edge ε, respectively. Substituting $v = u - u_h \in V$ in (24), and using the Galerkin orthogonality property, integration by parts and some subtle technical ingredients, one obtains the *a posteriori bound*

$$|\!|\!| u - u_h |\!|\!|^2 \leq \; c\, \eta^2_{res,\mathcal{T}_h}, \quad \text{where} \tag{25}$$

$$\eta_{res,\mathcal{T}_h} \equiv \left(\sum_{\tau \in \mathcal{T}_h} h_\tau^2 \|\Delta u_h + f\|^2_{L^2(\tau)} + \sum_{\varepsilon \in \mathcal{E}_h} h_\varepsilon \| \left[\nabla u_h \cdot \mathbf{n}_\varepsilon\right] \|^2_{L^2(\varepsilon)} \right)^{1/2}; \tag{26}$$

see the original work of Babuška and Rheinboldt in [14] or, e.g. the books [35, Section 9.2], [62, Section 15.2], or [129, Section 1.2].

In (25)–(26) the energy norm of the discretization error is bounded by the sums of local contributions of the *residual* $\Delta u_h + f$ on the individual elements and of the jumps of the gradient of u_h at the element edges. The expression (26) is called *residual a posteriori error estimator*. The value of the constant c is in principle computable (even if quite costly). It depends on the minimal angle allowed in the mesh elements, on the Poincaré-Friedrichs inequality constant (which is a function of the volume of Ω and the area of the portion of $\partial\Omega$ where the Dirichlet condition are imposed; see [129, p. 11]), and, in an analogous estimator for a more general $\mathfrak{a}(\cdot,\cdot)$, on the constants α and β from the Lax-Milgram conditions. However, the possibly large value of c can produce a significant overestimate of the error; see,

e.g. [40, 49]. The residual a posteriori error estimator satisfies the property 1. (reliability) in a weaker form, namely with the estimator multiplied by a suitable constant $c > 0$ (see (25)–(26) and the evaluation of c in, e.g. [40, 41, 127]), and it satisfies the property 2. (local efficiency); for the proofs see, e.g. [3, 129]. The third property (asymptotic exactness) usually does not hold in practical computations.

Analogous residual estimators can be derived for the variational eigenvalue model problem (14)–(15) and its Galerkin discretization (17). Here the interior element residual is given by the function $\Delta u_h + \lambda_h u_h$, and one obtains the bound

$$|||u - u_h|||^2 \leq c\, \eta_{res,\mathcal{T}_h} |||u - u_h||| + \frac{\lambda + \lambda_h}{2} \|u - u_h\|^2_{L^2(\Omega)}\,, \tag{27}$$

$$\eta_{res,\mathcal{T}_h} \equiv \left(\sum_{\tau \in \mathcal{T}_h} h_\tau^2 \|\Delta u_h + \lambda_h u_h\|^2_{L^2(\tau)} + \sum_{\varepsilon \in \mathcal{E}_h} h_\varepsilon \| \left[\nabla u_h \cdot \mathbf{n}_\varepsilon\right] \|^2_{L^2(\varepsilon)} \right)^{1/2}, \tag{28}$$

where for c the above considerations are valid; see [32, Section 6.3], [55, Theorem 3.1], [133, Section 4], or the earlier work of Larson [85]. It was shown that the L^2-norm of the error is of higher order than the energy norm of the error (see [55]), so that (27)–(28) indeed represents an a posteriori estimate for the energy norm of the error. As for the properties 1.–3., the situation is analogous to (25)–(26) for the boundary value problem; for a proof see, e.g. [55].

The residual a posteriori estimators, though well-understood and well-established in practice, may significantly overestimate the actual error. The reason is that the constant c present in the bounds may be very large. Therefore, several other techniques were introduced over the last years, and they can be classified as follows (see, e.g. [3, 50, 129]):

Local problem-based estimators (implicit estimators): Instead of considering the original discrete problem, local analogues of the residual equations are solved and suitable norms of the local solutions are used for the error estimation. The local problems usually involve only small subdomains of Ω and more accurate finite element approximations. In terms of cost, the solution of all local problems should be much less demanding than assembling the stiffness matrix of the original discrete problem. More details for boundary value problems are given in [3, Chapter 3], [50, Section 6.3.2], [62, Section 15.3], [129, Section 1.3] and [2, 34, 45]. A proof of the property 2. for this type of estimator can be found, e.g., in [3]. The properties 1. and 3. are, in general, not formally proved, but they are often satisfied, in a bit relaxed form, in practical computations. We are not aware of any local problem-based error estimators designed specifically for eigenvalue problems.

Averaging estimators (recovery-based estimators): These error estimators use a local extrapolation or averaging technique. The error of the approximation can be controlled by a difference of a low-order approximation (e.g., a piecewise constant function) and a finite element solution obtained in the space of higher-order elements (e.g., globally continuous piecewise linear functions), which additionally satisfy more restrictive continuity conditions than the approximation itself; see, e.g. [3, Chapter 4], [50, Section 6.3.3] or [129, Section 1.5]. Carstensen gives in [39] a nice overview of averaging techniques in a posteriori finite element error analysis in general. Particular error estimators are discussed in [42, 90, 139]. The property 1. can, in general, not be proved for averaging estimators. The proof of property 3. can be found, e.g., in [3, 129], and the property 2. is often satisfied in practice.

Hierarchical estimators (multilevel estimators): The main idea of a hierarchical error estimator is to evaluate the residual for the finite element solution $u_H \in V_H$ with respect to another finite element space V_h that satisfies $V_H \subset V_h \subset V$. Then the error $\|\!|u - u_H|\!\|$ can be bounded by $\eta \equiv \|\!|u_h - u_H|\!\|$, where $u_h \in V_h$; see [19, 53, 60], [50, Chapter 6], or [129, Section 1.4] for details. Usually V_h corresponds to a refinement $\mathcal{T}_h$ of $\mathcal{T}_H$ or consists of higher-order finite elements. This approach takes advantage of the so-called *saturation assumption*; see, e.g. [20]. The error of a fine discrete solution u_h is supposed to be smaller than the error of the coarse solution u_H in the sense of an error reduction property, i.e.

$$\|\!|u_h - u|\!\| \leq \gamma \, \|\!|u_H - u|\!\|, \quad \text{where } \gamma \in (0,1).$$

Hierarchical error estimators for eigenvalue problems are discussed in [91, 99].

Estimators based on equilibrated flux reconstruction: A recent general framework for a posteriori error estimators founded on potential and equilibrated flux reconstruction, which can be traced back to the ideas of Prager and Synge [105] and to the hypercircle method [126], is described in [77, 130, 131]. As recalled in [71], the flux reconstruction idea has been used for construction of a posteriori error estimators by many authors, possibly starting with [84]. The resulting estimators consist of the residual part, the flux part and the so-called nonconformity part, and they can be applied to various discretization methods and inexact computations; see [71, 132]. The following section will present more details. The estimators are proved to satisfy properties 1. and 2., while property 3. typically holds, in a bit relaxed form, in practice.

As an example from the classical approaches based on the flux reconstruction we point out the *equilibrated residual method*, which is comprehensively described (with many references to the original papers) in [3, Chapter 6]. Here the fluxes are reconstructed using the discretized solution u_h, i.e. it is assumed that the algebraic problems are solved exactly.

Finally, we wish to mention *goal-oriented estimators*, which are more general than the previous approches estimating (23). The objective in goal-oriented error estimation is to determine the accuracy of the finite element solution u_h with respect to some physically relevant scalar quantity of the solution u, the so-called "quantity of interest" $J(\cdot)$, e.g., velocity or flow rates. The error in the quantity of interest is then related to the residual, i.e.

$$|J(u) - J(u_h)| \approx \sum_{\tau \in \mathcal{T}_h} \rho_\tau(u_h)\omega_\tau,$$

where $\rho_\tau(u_h)$ denotes the so-called "cell residuals" of the approximate solution, and ω_τ a corresponding "cell weights". The latter are obtained from the solution of the so-called *dual problem*. The solution of this problem is typically not available, and in practice it is replaced by some local postprocessing of the computed discrete approximation. One of the well-known techniques of goal-oriented error estimation is the *Dual Weighted Residual (DWR)* method introduced by Rannacher in [107]. More details on this method and many further references are given in the following section. Approaches based on goal oriented estimators such as DWR do not typically aim at proving the properties 1.–3. from above. They, however, target a much more difficult result and allow complicated settings without strong assumptions on the problem to be solved, and they are very sucessful in most of their practical applications.

4 Coupling discretization with algebraic computation

As described in the Introduction, the AFEM is an iterative procedure consisting of the four steps SOLVE, ESTIMATE, MARK, and REFINE. It starts with an initial (usually coarse) mesh $\mathcal{T}_{h_0}$ and a corresponding finite element space V_{h_0}. The finite element approximation of the continuous solution obtained in the first SOLVE step is used in the following ESTIMATE step for the local a posteriori estimation of the error. This estimation yields a set of elements on which the local error is indicated too large, so that a refinement is necessary. The actual refinement procedure happens in the steps MARK and REFINE (see [17, 34, 54] for details), and it leads to a mesh $\mathcal{T}_{h_1}$ and a corresponding finite element space V_{h_1}. The AFEM loop is continued in this way until the a posteriori estimator indicates that no further refinement is necessary. It should also be pointed out that although the last step is called REFINE, it can also include a possible coarsening of the mesh in the areas where the error appears to be small.

This description, the bounds in the previous section, and the majority of the AFEM publications are based on *exact* solutions of the linear algebraic problems. This is an acceptable assumption when the cost for solving these problems is small and the problems are well conditioned independently of the mesh refinement (results in this direction can be found, e.g., in [18] and [35, Section 9.5]). In real-world applications, however, adaptive finite element methods can lead to very large and possibly ill-conditioned linear algebraic problems. Consequently, in practical applications an exact (i.e. to machine precision) solve of the related linear algebraic problems is not possible. Here it is important to point out that the accuracy can not be measured by the algebraic residual; cf. the quote from the paper by Becker, Johnson and Rannacher [22] in the Introduction. Some works suggest the algebraic residual as a measure of convergence in the numerical PDE context even for the Conjugate Gradient (CG) method [73]; see, e.g. [104]. It should be understood that unless the problem is easily preconditioned, this approach hardly can work in practice. The arguments can be found already in [73]; for a recent discussion we refer to, e.g., [5, Section 4]. For numerically challenging problems even residuals proportional to machine precision (such as those obtained by direct solvers) do not necessarily guarantee any reasonably accuracy of the computed approximate solution. Moreover, solving the linear algebraic problems to a (much) higher accuracy than the order of the discretization error usually does not improve the overall computed approximate solution and it just inadequately increases the computational cost; see the quote from [22] or [62, Section 13.4.1]. We have also mentioned this fact in our discussion of equations (12)–(13) above.

In practical applications of the AFEM the algebraic error should be considered a part of the estimation of the total error, i.e. one should use some appropriate norm and aim at estimates of the form

$$\|u - u_h^{(n)}\| \approx \eta_n, \tag{29}$$

where η_n is a function of the approximate solution $u_h^{(n)}$ (or $\lambda_h^{(n)}$ and $u_h^{(n)}$) of the linear algebraic problem. Moreover, the fact that the algebraic problems are not solved exactly (and the Galerkin orthogonality does not hold when u_h is replaced by $u_h^{(n)}$) should be in an adequate way taken into account in the *derivation* of (29). The last point is of principal importance. Formulas derived under restrictive assumptions should, in general, only be used when the assumptions are satisfied. Here the situation is somewhat analogous to the algebraic error estimation in the CG method [73], where for a long time formulas were practically used without being justified by a proper rounding error analysis.

An instructive work on adaptive error control in the FEM combined with the multigrid method for solving the discretized problems was published in 1995 by Becker, Johnson, and Rannacher [22], which we already quoted several times above. The authors consider the Poisson problem on a polygonal domain Ω and prove a posteriori error estimates in the $H^1(\Omega)$- and $L^2(\Omega)$-norms that incorporate algebraic errors and design of the adaptive algorithm, and they suggest stopping criteria for the multigrid computations. Although the paper does not explicitly consider quadrature and rounding errors, its approach can be generalized to cover those as well. The only assumption, standard in multigrid computations, which might require further substantial analysis in extension to difficult problems, is that the algebraic problem on the coarsest grid is solved exactly. The authors also point out that the adaptive error control for the multigrid computations is different from the one for CG computations. An extension of the approach from [22] to the Stokes problem was given by Becker in [21]; see also [27].

An interesting framework for construction of a posteriori error estimates of the total error which allows for local estimates and adaptive refinement follows from the first-order system least-squares formulation (FOSLS); see, e.g. [29]. This methodology is now applied for solving a large variety of problems.

Guaranteed upper bounds for the total error based on the so-called Repin majorant and not assuming Galerkin orthogonality are thoroughly described by Repin in [113]; see also the nice survey [128]. This approach naturally includes all sources of error (including the discretization and the algebraic error); for another example with this property (though somewhat hidden in the text) we refer to the recent work of Ainsworth and Vejchodský [4]. On the other hand, the general character of the results not taking into account the specifics of the error origin does not allow to distinguish, analyze, and compare parts of the error corresponding to different sources. In particular, these approaches do not consider constructing stopping criteria for algebraic iterative solvers. Results considering balancing the discretization and the algebraic error will be recalled below.

4.1 Results for boundary value problems

For a general variational boundary value problem of the form (1) based on a symmetric and coercive bilinear form $\mathfrak{a}(\cdot,\cdot)$, the squared energy norm of the total error is the sum of the squared energy norm of the discretization error and the squared energy norm of the algebraic error; see (13). The second term in (13) is equal to the squared $\mathbf{A}$-norm of the error of the linear algebraic system (11), i.e.

$$|||u_h - u_h^{(n)}|||^2 \;=\; \|\mathbf{u}_h - \mathbf{u}_h^{(n)}\|_{\mathbf{A}}^2 \;\equiv\; (\mathbf{u}_h - \mathbf{u}_h^{(n)})^T \mathbf{A} (\mathbf{u}_h - \mathbf{u}_h^{(n)}). \tag{30}$$

It is well known that $\mathbf{A}$-norm of the error is minimized over a Krylov subspace when the CG method is applied to (11); see [73]. This fact makes CG a natural choice for solving (symmetric positive definite) linear algebraic systems in the finite element context; see [56, Chapters 1 and 2] and [87, Chapter 5]. However, due to the presence of the exact Galerkin solution u_h in the first term on the right hand side of (13), this splitting can not be directly used for practical error evaluation. It also does not allow *a local* comparison of the different parts of the total error (that would require a knowledge of the spatial distribution of the discretization and algebraic parts of the error). This goal can be achieved, to a certain extent, by the following approaches.

The DWR method for boundary value problems: This approach, developed by Rannacher, Becker and their collaborators, does not require the bilinear form $\mathfrak{a}(\cdot,\cdot)$ being symmetric and coercive, and it has been successfully applied to many problems. Based on theoretically supported heuristics, it allows to compare the estimators for the discretization error and the algebraic error, and to construct adequate stopping criteria for algebraic iterative solvers. In order to outline the main ideas we consider the variational boundary value problem (1). Let the error be controlled by some linear (goal) functional $J(\cdot)$ defined on V representing the quantity of interest. The DWR method considers the associated *dual problem*:

$$\text{Find } \; z \in V \;\; \text{such that } \; \mathfrak{a}(v,z) = J(v) \;\; \text{for all } \; v \in V.$$

Since $J(\cdot)$ is linear,

$$J(u - u_h^{(n)}) = J(u - u_h) + J(u_h - u_h^{(n)}). \tag{31}$$

For any $v_h \in V_h \subset V$ we can write, using the Galerkin orthogonality property,

$$\begin{aligned} J(u - u_h) &= \mathfrak{a}(u - u_h, z) = \mathfrak{a}(u - u_h, z - v_h) = \ell(z - v_h) - \mathfrak{a}(u_h, z - v_h) \\ &\equiv \rho(u_h)(z - v_h). \end{aligned} \tag{32}$$

The function

$$\rho(u_h)(\cdot) \equiv \ell(\cdot) - \mathfrak{a}(u_h, \cdot)$$

is called the *residual functional* corresponding to the problem (1). Similarly,

$$\begin{aligned} J(u - u_h^{(n)}) &= \mathfrak{a}(u - u_h^{(n)}, z) = \mathfrak{a}(u - u_h^{(n)}, z - v_h) + \mathfrak{a}(u - u_h^{(n)}, v_h) \\ &= \ell(z - v_h) - \mathfrak{a}(u_h^{(n)}, z - v_h) + \ell(v_h) - \mathfrak{a}(u_h^{(n)}, v_h) \\ &\equiv \rho(u_h^{(n)})(z - v_h) + \rho(u_h^{(n)})(v_h)\,. \end{aligned} \tag{33}$$

Here the first term is analogous to (32) with replacing the Galerkin solution u_h by the computed approximation $u_h^{(n)}$, and the second term can be considered as accounting for the deviation from the Galerkin orthogonality. Taking for v_h the computed approximation to the dual solution, i.e. $v_h = z_h^{(n)}$, and replacing the unknown exact dual solution z by its approximation obtained using the higher-order interpolation $I_{2h}^{(2)}$ applied to $z_h^{(n)}$, i.e.

$$z - z_h^{(n)} \approx I_{2h}^{(2)} z_h^{(n)} - z_h^{(n)}\,, \tag{34}$$

we get

$$J(u - u_h^{(n)}) \approx \rho(u_h^{(n)})(I_{2h}^{(2)} z_h^{(n)} - z_h^{(n)}) + \rho(u_h^{(n)})(z_h^{(n)}). \tag{35}$$

The two terms on the right hand side account for the discretization and the algebraic error, respectively. The criterion balancing the discretization and the algebraic part of the error is then based on the requirement that the second term is significantly smaller than the first one. The practical implementations depend on the particular applications and the numerical methods used for discretization and algebraic computation; see [107], the later works [17, 28,

75, 76, 92, 101, 108, 109], and the recent instructive exposition in [110]. The DWR method should be given credit not only for its pioneering coupling of the discretization error and the algebraic error estimators, but also for its practical applications to solving linear as well as nonlinear problems, and for opening doors for further developments.

Stopping criteria for Krylov subspace methods inspired by estimating the $H^{-1}(\Omega)$ norm of the residual: Krylov subspace methods, in combination with their *acceleration techniques* (commonly, but inaccurately, called preconditioning), belong to the very efficient tools for solving large-scale linear algebraic problems arising from the discretization of PDEs. As mentioned above, in case of $\mathfrak{a}(\cdot,\cdot)$ symmetric and coercive and thus $\mathbf{A}$ symmetric positive definite, the CG method minimizes the $\mathbf{A}$-norm of the algebraic error over the Krylov subspaces generated by the powers of $\mathbf{A}$ with respect to the initial residual.

Up to now, the majority of stopping criteria used in practical CG computations are based on the (relative) *Euclidean norm* of the algebraic residual $\mathbf{r}^{(n)} = \mathbf{b} - \mathbf{A}\mathbf{u}_h^{(n)}$ (here $\mathbf{u}_h^{(n)}$ denotes the approximation of $\mathbf{u}_h$ computed at the nth CG iteration). Even without the mathematical modeling and numerical PDE context, this situation is most alarming. Already Hestenes and Stiefel warned in [73] against using the Euclidean residual norm as a base for CG stopping criteria, and they gave a hint on how the estimator for the energy norm of the error, i.e.

$$\|\mathbf{u}_h - \mathbf{u}_h^{(n)}\|_{\mathbf{A}} = \|\mathbf{r}^{(n)}\|_{\mathbf{A}^{-1}},$$

can be constructed using the computed quantities. Their recommendation was, however, overlooked for almost five decades.

A revived interest in estimating the (energy) norm of the error in CG and other iterative methods is due to Golub and his collaborators. Golub suggested (independently of [73]) to use for that purpose the family of (appropriately modified) Gauss-Christoffel quadrature approximations of the related quadratic formulas; see, e.g. [63, 64]. In [66] it was argued that since CG is based on short recurrences, any such estimate must take into account effects of rounding errors in CG computations. A few years later the story turned back to the original work of Hestenes and Stiefel [73]. The paper [124] highlighted the overlooked formulas presented by Hestenes and Stiefel and derived the estimator for $\|\mathbf{r}^{(n)}\|_{\mathbf{A}^{-1}}$ using only the *local orthogonality* among the successive CG residuals and direction vectors. Since this local orthogonality is close to machine precision, the resulting estimate is numerically stable; for the proof see [124]. It should be pointed out, however, that while this holds for the lower bound on $\|\mathbf{r}^{(n)}\|_{\mathbf{A}^{-1}}$, which can be evaluated at almost no additional cost, a reliable upper bound can not be obtained without substantial a priori assumptions and/or an additional cost which may be significant. Details can be found in the survey paper [94], in the books [65, Chapter 12], [87, Chapter 5, in particular Sections 5.6 and 5.9], and in the original references presented there.

The energy norm of the Galerkin FEM discretization error in solving elliptic selfadjoint PDEs was coupled with the energy norm of the error in the corresponding algebraic computations in the so-called *cascadic CG method* by Deuflhard [52] published in 1994; see also, e.g. [119]. The algorithmic realisations of the cascadic CG do not take into account rounding errors and they could not use the results of estimating the algebraic energy norm of the error in CG published later. Therefore the idea is worth revisiting and further investigation.

A fundamental step in incorporating the state-of-the-art techniques of algebraic error estimation in CG (as well as other Krylov subspace methods) into the numerical PDE context

is due to Arioli and his coworkers. They emphasized in [9] that the algebraic residual $\mathbf{r}^{(n)}$ should be considered as the discrete counterpart of the functional residual which belongs to the dual of the space containing the solution; see (3) and the related discussion above. Therefore the algebraic stopping criteria should be based on the analogy of the dual norm of the functional residual. For the Poisson model problem (1)–(2) this reduces to the algebraic energy norm of the error discussed above. The stopping criterion suggested in [5] then combines some *a priori* knowledge about the problem with the *a posteriori* error estimates; see also [65, Sections 12.3 and 12.7]. This approach has been extended to non-selfadjoint problems [7, 8] and it has motivated further ongoing investigations.

BPX preconditioning and the residual a posteriori estimator without Galerkin orthogonality: Harbrecht and Schneider [72] combined the idea of the standard residual a posteriori error estimator (see (25)–(26) above) with the multilevel Bramble, Pasciak and Xu preconditioning scheme (BPX) [33]. The infinite BPX scheme provides a frame for bounding the residual norm in the dual space $H^{-1}(\Omega)$. In practice the BPX scheme is truncated at a certain level. Neglecting the data oscillations, the resulting hierarchical estimator is composed of the discrete part $BPX(\mathbf{r}^{(n)})^2$, which can be evaluated using the BPX hierarchical scheme, and the standard residual a posteriori error estimator, giving

$$\eta_n \equiv \left(BPX(\mathbf{r}^{(n)})^2 + \sum_{\tau\in\mathcal{T}_h} h_\tau^2 \|\Delta u_h^{(n)} + f\|^2_{L^2(\tau)} + \sum_{\varepsilon\in\mathcal{E}_h} h_\varepsilon \| \left[\nabla u_h^{(n)} \cdot \mathbf{n}_\varepsilon\right] \|^2_{L^2(\varepsilon)} \right)^{1/2} . \tag{36}$$

The recent paper [72] recalls the earlier literature on the subject and investigates a rigorous background for this estimator.

Estimators based on the equilibrated flux reconstruction: Using a locally conservative cell-centered finite volume discretization, the a posteriori estimators of Vohralík mentioned above (cf. the end of Section 3) were in [77] extended in order to take into account the algebraic error. The resulting a posteriori error estimator is given as a sum of three quantities,

$$\eta_n \equiv \eta_{NC} + \eta_O + \eta_{AE} \,. \tag{37}$$

Here η_{NC}, η_O and η_{AE} are called *nonconformity estimator*, *oscillation estimator* and *algebraic error estimator*, respectively; see [77, Theorem 5.2]. The nonconformity estimator indicates the departure of the approximate solution from the space $H^1(\Omega)$; it depends on the approximation $u_h^{(n)}$ of the solution u_h (and not only on the discretization error). The algebraic error estimator accounts for the error arising from the inexact solution of the algebraic system (11); its value is determined using the algebraic residual vector $\mathbf{r}^{(n)}$. Finally, the oscillation estimator measures the interpolation error in the right-hand side of the PDE (this value is significant only on coarse grids and for PDEs with highly varying coefficients). It is also shown in [77, Theorems 6.2 and 6.3] that the estimator (37) is locally and globally efficient (see Section 3) and therefore it is suitable for adaptive mesh refinement which takes into account the inaccurate algebraic computations. The results were successfully used for construction of stopping criteria in CG computations. Further work of Vohralík and his collaborators is outlined in [131]; the paper [58] extends the results from [77] to more general settings.

Global convergence: The standard a priori convergence theory for the FEM requires that $h \to 0$, i.e. that the mesh is refined everywhere, so that for each value of h the approximation error is of the required order of accuracy. This obviously does not hold in the context of the AFEM, where the main point is to avoid refining the mesh everywhere. Here the goal is to show that the method is a contraction (for some appropriate norm of the error and/or error estimator) between two consecutive loops . Under the assumption of the *exact solution of the algebraic finite dimensional problem*, such a proof is given, e.g., in the paper of Morin, Nochetto, and Siebert [97]; see also the earlier work of Babuška and Vogelius [16] and of Dörfler [54]. In [97, p. 631] the authors conclude that "[a]ny prescribed error tolerance is thus achieved in a finite number of steps", which is certainly true under the assumptions in their Theorems 3.1 and 3.11, and, in particular, under the assumption of exact algebraic computations; see also [26, 46, 83, 93, 98].

The fact that in practice we cannot compute the exact algebraic solution is addressed by Binev, Dahmen, and DeVore in [30]. They modify the method of [97] and prove that for the Poisson problem in two dimensions with piecewise linear finite elements their adaptive method has an optimal convergence rate with respect to the energy norm (and hence also the H^1-norm). One of the building blocks of their method is the application of preconditioned CG to the discretized problem. Their convergence proof of the AFEM requires that the (BPX-preconditioned) CG method gives an algebraic error norm below a given tolerance that depends on several parameters; see [30, Sections 3 and 8] for details.

Whether such tolerance can be met in practice depends, in general, on the *maximal attainable accuracy* of the iterative solver; see, e.g. [87, Section 5.9.3] and the references given there. This accuracy, in turn, depends on the properties of the problem, and also on the numerical stability of the solver itself. As an example we refer, e.g., to Example 6 in the book on iterative methods by Axelsson [10, Appendix A, pp. 608–609] and to the numerical experiments in [97]. This issue requires a complete rounding error analysis of the adaptive algorithms, a work that is still to be done. The existing approaches consider an inexact solution of algebraic problems in the sense of prematurely stopping the iterative computation (using an appropriate stopping criterion). Whether a maximal attainable accuracy has been reached is not considered an issue that affects the adaptive computations.

A highly recommendable paper by Stevenson [122] considers the Poisson model problem in two dimensions with piecewise linear finite elements. It presents a nice review of previous relevant work and it extends the approach in [97] by allowing an inexact solution of the discretized algebraic system. Its main result, presented in Theorem 6.3, holds under the assumption that the algebraic solver deviates from an ideal exact computation in a sufficiently small way. This assumption is mathematically specified, and it refers to a paper by Wu and Chen [137] on uniform convergence of multigrid V-cycle algorithms. The last paper assumes exact arithmetic and, in particular, it assumes that the operator on the coarsest grid is exactly invertible. Hence, as mentioned above, there still remains some work in order to account for all aspects of practical computations.

Assuming that a maximal attainable accuracy has not been approached, a result analogous to [46] has been proved in [6]. In that paper the algebraic problem is solved using the CG method and the energy norm of the finite dimensional error is estimated by the techniques described above. In particular, the global convergence result in [6] is based on the use of a well justified (although not strictly formally proved) upper bound for the energy norm of the algebraic error using the technique proposed in [88] for estimating an accurate lower bound

of the smallest eigenvalue of the matrix $\mathbf{A}$ in (11). A different approach which includes an adaptive stopping criterion for iterative solution of the algebraic problem has been used in [23, 24] for investigating the so-called quasi-optimal complexity of the AFEM; see also [25].

Finally, we want to mention that among the approaches to a posteriori error analysis which do not assume the exact solution of the discretized algebraic problem are the works of Wohlmuth and Hoppe [135], Rüde [114, 115, 116], Burstede and Kunoth [37, 38], Maday and Patera [89], and Patera and Rönquist [103]. Indefinite and non-selfadjoint problems have been extensively addressed by Elman, Kay, Silvester, Simoncini, Wathen, and Wu; see, e.g. [56, 79, 120, 134, 136]. Lacking in space we can not describe their approaches and refer an interested reader to the original literature.

4.2 Results for eigenvalue problems

Minimizing the total errors (18)–(19) for eigenvalue problems is more complicated than minimizing (12) for boundary value problems where the CG method naturally minimizes the algebraic energy norm of the error. Even the definition of an appropriate (in the physical sense) norm to measure the error for the eigenvalue problem is not an easy task. We will briefly outline several recently investigated approaches.

The concept of a *functional backward error and condition number* introduced in [9] for boundary value problems were used in [95] for selfadjoint eigenvalue problems in order to analyze the continuous dependence of the inexact solution on the data, in particular to analyze the approximation error and the backward stability of the algebraic eigenvalue problem. This resulted in a combined residual a posteriori error estimator and a balanced AFEM algorithm, where the stopping criteria are based on the variant of the shift-invert Lanczos method introduced by Hetmaniuk and Lehoucq in [74]. A similar direction was considered by Gratton, Mouffe, and Toint [68] in the context of bound-constrained optimization; the ideas introduced there can be applied to the minimization of the Rayleigh-quotient in the case of eigenvalue computations.

Carstensen and Gedicke [43] combined an adaptive finite element scheme with an iterative algebraic eigenvalue solver and obtained a method of quasi-optimal computational complexity. Under the assumption that the iteration error $\|\!|u_h - u_h^{(n)}|\!\|^2 + |\lambda_h - \lambda_h^{(n)}|$ for two consecutive AFEM steps is small in comparison with the size of the residual a posteriori error estimate, they showed the contraction property for the quasi-error up to higher-order terms. Checking the condition on the size of the iteration error is based on some heuristic arguments. A similar analysis of convergence and a quasi-optimality of the inexact inverse iteration coupled with adaptive finite element methods was presented by Zeiser [138].

The results above have been derived in the context of eigenvalue problems that usually are of the form (14) with $\mathfrak{a}(\cdot,\cdot)$ symmetric and coercive. To deal with non-selfadjoint problems, one can follow Rannacher and Becker [28] and their DWR approach. Here duality techniques are used to estimate the error in the target quantities in terms of the weighted primal and dual residuals,

$$\rho(u_h, \lambda_h)(v) \equiv \mathfrak{a}(u_h, v) - \lambda_h(u_h, v), \tag{38}$$

$$\rho^*(u_h^*, \lambda_h^*)(v) \equiv \mathfrak{a}(v, u_h^*) - \lambda_h^*(v, u_h^*), \tag{39}$$

respectively. The resulting estimates can be written as

$$\lambda - \lambda_h^{(n)} \approx \frac{1}{1-\sigma_n} \left(\eta_n + \eta_n^* + \eta_n^{(it)} \right), \tag{40}$$

where the primal and the dual eigenvalue residual estimators are given by

$$\eta_n \equiv \frac{1}{2} \rho(u_h^{(n)}, \lambda_h^{(n)})(I_{2h}^{(2)} u_h^{*(n+1)} - u_h^{*(n)}), \tag{41}$$

$$\eta_n^* \equiv \frac{1}{2} \rho^*(u_h^{*(n)}, \lambda_h^{*(n)})(I_{2h}^{(2)} u_h^{(n+1)} - u_h^{(n)}), \tag{42}$$

the term

$$\eta_n^{(it)} = \rho(u_h^{(n)}, \lambda_h^{(n)})(u_h^{*(n)}) \tag{43}$$

represents an indicator for the iteration error, and the reminder term σ_n is assumed to be sufficiently small. The derivation is based on a perturbation argument and the application requires a careful monitoring of the computed quantities. For more details we refer to [111]. In practice the DWR method can be used in both boundary value and eigenvalue parts of various problems. An application to the stationary Navier-Stokes equations is given in [109], the studies in the context of the hydrodynamic stability analysis can be found in [76].

Finally, an algorithm based on a *homotopy method* which allows adaptivity in space, in the homotopy stepsize as well as in the stopping criteria for the iterative algebraic eigenvalue solvers is described in [44]; see also [61, 96].

5 Concluding remarks

This text gives a very brief introduction to the issues related to adaptive numerical solving of linear elliptic PDEs. Obviously, the work in the outlined directions has been extended to more general as well as to nonlinear problems. Many researchers are attracted by the fundamental character of the related applications, the difficulty of the mathematical problems, as well as the discretization and computational challenges (for an early account of the difficulties associated with the error control in the particularly intriguing area of computational fluid dynamics we refer to, e.g., [78]). We believe that this effort, with combination of expertise from fields such as mathematical modeling, mathematical and numerical PDE analysis and discretization, and matrix computations including numerical stability analysis, will lead to further remarkable results. Rigorous theoretical analysis complemented with soundly justified heuristics will bring adaptivity into the center of numerical computations.

Acknowledgments. The authors are grateful to Martin Vohralík, Vít Dolejší, Pavel Jiránek, Jan Papež, Gerhard Starke, and three anonymous referees for correcting several errors in a previous version of the manuscript, for pointing out numerous important references, and for many valuable suggestions which improved the text.

Mario Arioli was supported by the EPSRC Grant EP/I013067/1. Jörg Liesen was supported by the Heisenberg-Programm of the Deutsche Forschungsgemeinschaft (DFG). Agnieszka Międlar was supported by the DFG Research Center MATHEON and by the Berlin Mathematical School. Zdeněk Strakoš was supported by the ERC-CZ project LL1202.

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