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## FUNCTIONAL-TYPE A POSTERIORI ERROR ESTIMATES FOR SOLUTIONS OF PROBLEMS IN DEFORMABLE SOLID MECHANICS

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The paper provides a historical review and recent developments on theoretical justification and numerical implementations of functional a posteriori error estimates and adaptive algorithms for approximate solutions to problems in deformable solid mechanics. The efficient practical implementation of such methods is a relevant objective, including for modern engineering practice.

**Keywords:** error estimates, finite element method, adaptive algorithms, solid mechanics

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### Introduction

Different issues related to construction of methods for numerically solving boundary-value problems and for a posteriori control of the error of the obtained approximate solutions have been the focus of attention from scientists and engineers for several decades. Today, there are thousands of publications on this subject. Due to high significance of the topic cluster *Finite Element Method*, *Galerkin Methods*, and *Errors*, it is very important to continue investigations in this direction. The issues addressed by the theory of a posteriori error control go beyond computational mathematics or engineering analysis, raising questions of mathematical modeling in general, and even philosophy.

Modern engineering practices now customarily rely on huge computational resources; the physical processes simulated become incredibly sophisticated. Problems are considered in a complex, multidisciplinary manner, at different scales of physical phenomena, with practically no simplifications, generating large amounts of data and solutions. Such problems are being successfully solved, in particular, at Peter the Great St. Petersburg Polytechnic University (see, for example, [1–3]). Since closed-source commercial software products by well-known developers are often used for these purposes, it is impossible to have a proper ‘look inside’ such systems to assess all the mathematical and algorithmic aspects

of their implementation. This motivates experts working at the intersection of computational mathematics, physics, mechanics, engineering sciences to search for universal methods for objective estimation of the results obtained. Both technical methods and rigorous, mathematically sound approaches are being developed for this purpose, concerning in one way or another two key issues:

1. What is the accuracy of the solution obtained for a specific problem and is it always possible to estimate it reliably?

2. In which regions does the solution need to be refined (it is highly preferable that such a procedure is automated)?

Unfortunately, there can be simply no common, universal approach to estimating the error, which would have low computational complexity, making it easy to obtain new theoretical results and implement them algorithmically. Therefore, the choice of priorities is hardly a simple matter, since it is a problem extending to the philosophical domain.

### Classical a posteriori estimates

It is generally agreed that modern methods for constructing a posteriori estimates have been intensively developing thanks to the groundwork laid in [4, 5], published in the late 1970s. The interest aroused by these studies was so great that several approaches aimed at estimating the accuracy of the results obtained by mathematical



and engineering simulation were formulated in the early to mid-1980s. In the decade following the mid-1990s, several monographs have been published by various authors (see, in particular, [6–9] and references therein), summarizing the experience accumulated over this time.

Thus, a separate branch evolved within the theory on the finite element method, considering the verification of numerical solutions and the validation of mathematical models. Since a posteriori estimates allow to evaluate the deviation of the approximate solution from the unknown exact solution, the error introduced by the mathematical model can be separated from the error of the numerical solution. It is only in this case that it is possible to correctly assess whether the mathematical model is suitable and adequate for analysis of a particular object.

Several groups of methods became the most popular at that time and were even implemented in commercial software products (ANSYS, MATLAB, etc.) for a number of simple boundary-value problems. Let us consider, in particular, explicit and implicit residual methods, and methods for post-processing of derivatives of an approximate solution.

While the first group of methods is much simpler than the second one, it requires for auxiliary constants to be computed so that the estimates adequately reflect not only the local distribution of the error over the computational domain (i.e., serve as indicators), but also its global value (i.e., provide reliable guaranteed upper bounds of the error). In practice, this simplistic approach faces significant difficulties, so the methods of this group are applied specifically to the adaptation of meshes.

Implicit methods circumvent the problem of computing constants by introducing the solution of a sequence of local problems with boundary conditions of different types into the structure of the methods, which increases their computational complexity but does not always yield an upper bound of the error norm.

Finally, another group of classical methods is based on the superconvergence phenomenon, which is used to construct error indicators for different problems and provides the theoretical justification for this approach. These methods involve averaging derivatives or stresses at the points of superconvergence. They are not computationally expensive and are quite simple to implement, yielding good local indication of the regions with large errors even when they do not have a rigorous mathematical justification;

however, these methods do not give reliable upper bounds of the error.

In addition to the above monographs, a more detailed review of the results in Russian can be found in [10].

The key feature of the classical methods for a posteriori error control is that their rigorous mathematical justification is fundamentally based on the assumption that the given solution is not arbitrary and approximate but rather the exact solution of the corresponding finite-dimensional problem, the Galerkin approximation. This is by no means always the case in commercial packages, where the solution may not have this property due to the specifics of numerical algorithms. For example, to solve problems in the theory of plates, it is necessary to overcome the computational locking phenomenon. This is achieved, in particular, by using numerical integration formulas that are coarser in accuracy on some of the elements, producing non-Galerkin solutions.

#### **Classical a posteriori estimates in deformable solid mechanics**

Finding effective solutions to engineering problems is no less important on its own than developing the theory of numerical methods. For this reason, along with the general theory of a posteriori accuracy control as an independent branch of computational mathematics, researchers have long focused on constructing methods for adaptively solving mechanical problems. As advances were made almost simultaneously, the methods were proposed and theoretically justified based on the example of classical elliptical boundary-value problems (Poisson's equation or stationary diffusion problem), while successful concepts were extended to plane or spatial problems of linear elasticity theory, plate theory, etc. (see, for example, [11–13] and the collection in [14]).

The method of hypercircles appeared in the late 1940s [15]; it was later generalized in other studies and called the method of errors in constitutive relations (see, for example, monograph [16]). The gradient averaging method [12, 17, 18] was also extended to problems of deformable solid mechanics in 1987–1992 and is currently included in the ANSYS package as a built-in procedure for analyzing the accuracy of solutions in a number of simple problems. Different aspects of numerical implementation of the averaging procedures are discussed in detail in the literature. References to early

publications extending the explicit and implicit residual-based methods to mechanical problems are given, in particular, in monographs [6, 19] and review [20]. Details can also be found in later monographs [21, 22] and the relatively recent work [23].

### Functional-type a posteriori estimates

The functional approach is based on rigorous mathematical methods, including mathematical physics, functional analysis, calculus of variations (in particular, the duality theory), theory of partial differential equations, using weak (generalized) formulations of the problems under consideration. By design, it includes an arbitrary solution of the problem from the corresponding functional space as an element whose error must be estimated. This makes the approach sufficiently general and reliable, since it allows analyzing errors in solutions regardless of how the procedures for computing these solutions are specifically implemented in commercial packages.

The Galerkin orthogonality, which is the key property for classical methods, does not play much of a role in the theory here, although it can be used in practical implementations. The estimates remain (guaranteed) upper bounds for all conforming approximations, which is true not only in theory but also in numerical implementation: this important property implies that the a posteriori error control method is reliable. This versatile and general approach is characteristic for Mikhlin's studies [24]. The functional approach was proposed and is currently developed by Prof. Sergey Repin (principal investigator at the St. Petersburg Department of the Steklov Mathematical Institute of the Russian Academy of Sciences and professor of Peter the Great St. Petersburg Polytechnic University) together with colleagues in Russia and several European countries, including Finland, Czech Republic, Austria, Switzerland and Germany. A detailed review of the advances in this direction can be found in monograph [22].

The key aspect of the approach is that it not only yields guaranteed upper bounds (that are not violated in practical implementation) but is also suitable for a wide range of approximate solutions. At the same time, the functional approach differs from the geometric arguments of the method of hypercircles, does not require construction of equilibrated fields, and has been successfully extended to nonlinear problems in theoretical aspects.

The formal starting point for this direction is 1996, when the first study [25] appeared; the approach was subsequently developed by Repin in a series of works [26–29]. Further history of the approach can be traced by the sources described in monographs [9, 22, 30].

Without going into the specifics of each particular problem, the estimate has the following general form:

$$\|u - \tilde{u}\| \leq \mathcal{M}(\tilde{u}, D, \tilde{y}_1, \tilde{y}_2, \dots, C_1, C_2, \dots), \quad (1)$$

where the left-hand side contains a norm of the difference between the exact solution  $u$  and an approximation  $\tilde{u}$ , while the right-hand side includes the functional  $\mathcal{M}$  which is the deviation majorant.

The arguments of the functional are the approximate solution  $\tilde{u}$ , the parameters of the problem  $D$ , the set of real constants  $(C_1, C_2, \dots)$ , which are determined by the data of the problem but not by the properties of the solution or discretization. Finally,  $(\tilde{y}_1, \tilde{y}_2, \dots)$  is a set of free elements that control the accuracy of the upper bound. The functional  $\mathcal{M}$  vanishes if and only if  $\tilde{u}$  is the exact solution; it must be explicitly computable in practice, providing an accurate estimate of the error given a reasonable (from a physical viewpoint) choice of the set  $(\tilde{y}_1, \tilde{y}_2, \dots)$ .

Notably, there are local and global characteristics introduced in the literature for comparing various methods but only one of them, the efficiency index of an a posteriori estimate, has gained the widest popularity and is universally acclaimed as irrefutable. The efficiency index for the functional-type error majorants is calculated as the ratio of the functional  $\mathcal{M}$  to the norm of the error estimated by it. Thus, for guaranteed upper bounds, its value is never lower than 1.0 that is the optimal value at which the method exactly reproduces the unknown norm of error over the entire region. There are also various local characteristics (see, for example, [22] and the references therein) but they are not as common as the efficiency index.

Practically speaking, numerical implementation of the methods of this group is not as simple as for the classical error indicators discussed above. Greater computational complexity and the additional effort it takes to construct efficient algorithms for computing functional-type a posteriori estimates are the price for the versatility and reliability of the approach. Research in this direction is still ongoing and is far from completeness. Numerical



results for plane problems in the framework of classical linear elasticity were first obtained in [31], and in [32] using an alternative, more efficient implementation. An estimate for plane problems of the Cosserat elasticity theory was obtained in [33], modified in [34]; an overview of numerical studies can be found in [23].

The first theoretical result for problems of elastoplasticity was obtained in 1996 [25]; sufficient experience was subsequently accumulated in both theoretical and practical development of the estimates (see [35–38] and the references therein, as well as related studies [39, 40]).

Finally, studies into the functional approach to solving problems in the theory of plates started with [41], considering the theory of Kirchhoff–Love thin plates. The first version of such an estimate for Reissner–Mindlin plates was obtained in 2004 [42]. A review of further results, including those concerning numerical implementation, can be found in the recent work [43].

New interesting results have been obtained for obstacle problems [44–46] and for problems in exterior domains [47], as well as for parabolic equations [48, 49] and for norms differing from the energy norm [50]. A particularly noteworthy study [46] discussed a class of nonlinear problems with free boundaries, also confirming that majorants can control not only the error of the solution in the energy space but also some measures of the distance to the exact solution for nonlinear problems. Sufficiently efficient and explicitly computable two-sided estimates are obtained in this case, which is described in more detail in the next section.

Methodology for applying the approach

Effective numerical methods for obtaining solutions that do not have additional smoothness and contain singularities should involve adaptive approaches based on a posteriori estimates. In this case, the following steps, well known in the Western literature starting from the widely cited pioneering study [51] (see also [52]), are repeated cyclically:

$$\begin{aligned} \text{SOLVE} &\rightarrow \text{ESTIMATE} \rightarrow \\ &\rightarrow \text{MARK} \rightarrow \text{REFINE}. \end{aligned} \quad (2)$$

This approach is aimed at obtaining an approximate solution to the problem of higher accuracy with less computational efforts. However, the efficiency of the algorithm has to be substantiated for each class of problems, which does not automatically follow from the known a priori estimates of the convergence rate, because the latter were obtained under

the assumption of higher regularity of the exact solution and smoothness of the boundary of the computational domain.

It is well known that the Finite Element Method (FEM) can converge slowly even for typical elliptical problems. Thus, the true convergence rate of an adaptive numerical method largely depends on the algorithmic details of the implementation. Notably, the foundations of research into adaptive FEM (AFEM) were laid by the well-known work [53].

Algorithm (2) provides wide range of opportunities for implementation. The methods can differ in finite elements for the SOLVE step, engineering or rigorous approaches to estimating the error and indicating its local distribution over the computational domain for the ESTIMATE step; an a posteriori estimate of type (1) can be used in this case. The key difference at the REFINE step is that either the algorithm for mesh refinement (*h*-version) is used, or the order of approximation (*p*-version) is increased, or a more efficient combined method (*hp*-version) is used. There is another type of mesh improvement (*rp*-version) for nonlinear problems with unknown free boundaries (for example, unknown elastoplastic zones), when the element boundary is fitted to the free boundary. In this case, the nodes of the existing finite-element mesh are shifted so that discretization is improved without having to introduce additional degrees of freedom (see, for example, [54]). Finally, different criteria for selecting mesh elements at the MARK step also have an impact.

Implementation of the functional approach in software packages can be fairly sophisticated; successful examples done in the MATLAB package are described in recent works [55–57]. The generated codes implement low-order nodal and boundary elements, vectorized and providing reasonable assembly times in both plane and spatial cases, even for discretization with a large number of unknowns (up to several millions).

It seems interesting to apply the accumulated experience to various problems of mechanics, in particular, to computations of a posteriori estimates for plane problems of the Cosserat elasticity theory, also implemented in the MATLAB package [23].

In conclusion, let us focus more closely on the the effectiveness of the functional approach.

To compute the majorant in linear problems, it is necessary to additionally minimize the quadratic functional  $\mathcal{M}^2$ , which leads to solving a second system of linear algebraic

equations. In this case, it is not simple standard finite elements that are of interest but rather the elements related to mixed FEM (see, for example, [23, 32, 43] for more detail). The problem of estimating the error is much more difficult mathematically than the original boundary-value problem. For this reason, it is difficult to expect that it can always be solved with low computational costs compared to the original one. In some cases, this can be achieved, but estimating the error typically takes effort (requiring both resources and complex algorithmic solutions). The complexity of computing the a posteriori estimate is rarely less than that of the solution of the initial problem.

In most cases, it is possible to obtain the estimates that majorize the unknown error with an efficiency index no greater than 2.5 (see [22, 23, 32, 43] and the references therein). With certain additional computational costs, the overestimation obtained is by no more than 1.2–1.3 times (see [23, 36], etc.). In simple elliptical boundary-value problems, it is even possible to obtain an efficiency index close to the optimal value, namely 1.0. Then the functional approach provides a result close to the exact representation of the error that has been theoretically proved to be obtainable.

Consider an example of what this implies in practice. Let the criterion for stopping the computational process be chosen when a guaranteed global solution accuracy equal to 90% is generally reached. Then, with a true error of the approximate solution (which is actually unknown) of 7% and an efficiency index of 1.3, the computations on this mesh stop, since the majorant  $\mathcal{M}$ , computed in this case, shows an error of less than 10%. No additional computational costs are required for analysis

of mesh convergence, since there is no need to solve the problem on a finer mesh and make a comparison. With an efficiency index of up to 2.5, the estimate yields an error level of up to 20%, and a decision is made about one redundant iteration of uniform mesh refinement in order to reduce the error by half. This result is also considered acceptable, since, as noted above, the problem of estimating the accuracy is crucially more complicated than the original problem without such control.

As for adaptive algorithms, adapting the meshes allows to obtain solutions of the same level of accuracy as for uniform partitions, for a considerably smaller number of nodes. The difference reaches several tens of times even when compared with uniform partitions up to 100 thousand nodes [23]. This difference only grows subsequently, which fully compensates all computational costs required to construct estimates and error indicators.

### Conclusion

The paper outlines the main historical and modern approaches to constructing reliable (guaranteed) estimates of the accuracy of approximate solutions to the problems of deformable solid mechanics. The discussion largely revolves around the methods developed within the framework of the functional approach. Efficient implementation of the methods of this group is a complex and challenging task directly applicable to modern engineering practices. This is a direction demanding much further effort.

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