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A Posteriori Error Estimation

J. Tinsley Oden

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No matter how sophisticated or how appropriate a mathematical model can be for characterizing certain physical phenomena of interest, all computational results obtained using it will be in error. Fundamentally, the discretization process of transforming a model characterized by partial differential or integral equations into one manageable by digital devices naturally loses information, the result being that the numerical approximations differ from those of continuum models. This approximation error can be enormous; it can completely invalidate numerical predications; it is often pervasive and difficult to detect or evaluate by intuitive or heuristic means. Over the last two decades, mathematical theories and computational procedures have been under development for estimating approximation error in numerical solutions of boundary - and initial - value problems in mechanics. The general subject is referred to as *a posteriori error estimation*; basically, it involves post-processing numerical solutions in such a way that important and useful information can be obtained on the actual error present in the numerical solutions themselves. This information can manifest itself in several forms; typically, as rigorous upper and lower bounds on the approximation error measured in appropriate norms, but also as quantitative estimates of actual local features of the error in principal quantities of interest, such as stresses, strains, displacements, fluxes, natural frequencies, *etc.* Clearly, if the error can be estimated, then it should be possible to enhance the approximation so as to reduce the error; *i.e.* error estimation makes feasible error control. This fact is at the heart of *adaptive computational methods*, those which allow modification of the mesh, the order of the approximation, time steps, or other features of numerical algorithms so as to reduce and control numerical error.

In a typical computational situation, the approximation error is a function of position x and time t and is defined simply as,

$$e = u - u_h$$

where u is the exact solution of the equations, inequalities, boundary - and initial - conditions characterizing the mathematical model of the phenomena of interest and u_h is the numerical approximation of u obtained, for example, by finite element, finite difference, or boundary element approximations of the model. Obviously, for models involving systems of equations and many dependent variables, e can be a vector - or tensor - valued function.

In most engineering applications, we are not only interested in assessing the magnitude of $\|e\|$ of the error in some appropriate norm, but also the error in some specific, real-valued quantity of interest Q that depends on the solution u. Thus, we wish to estimate the error

$$\mathcal{E} = Q(u) - Q(u_h).$$

The quantity $Q(u)$ may be a "local" feature of u, such as the value of u at a point x_0 in the domain of u, $Q(u) = u(x_0)$ or the value of the stress $\sigma(u)$ in the direction ν on a material surface with unit normal n,

$$Q(u) = \nu \cdot \sigma(u) \cdot n$$

or the average stress in the direction ν over a material interface of area ω:

$$Q(u) = \frac{1}{|\omega|} \int_\omega \nu \cdot \sigma(u) \cdot n \, ds$$

etc. Importantly, the analyst may specify a list of quantities of interest Q; then the goal of methods of *a posteriori* error estimation is to assess the error $Q(u) - Q(u_h)$ or to obtain upper and lower bounds, η_{low} and η_{upp}, on this error:

$$\eta_{\text{low}} \leq Q(u) - Q(u_h) \leq \eta_{\text{upp}}.$$

The function $Q(u)$ may be a linear or nonlinear function of u. If Q is a linear functional, then

$$Q(u) - Q(u_h) = Q(e) \qquad \text{or} \qquad Q(u) = Q(e) + Q(u_h).$$

Of course, the exact solution u is, in general, unknown and impossible to compute, but if $Q(e)$ can be well approximated, the actual value of $Q(u)$ can also be approximated. The error bounds η_{low} and η_{upp} are computed using the numerical approximation u_h.

It is also emphasized that the validity of results producible by a mathematical model can only be measured to within some arbitrary preset tolerance provided by the analyst. Thus, the model has been solved "correctly" (*i.e.*, the goal of verification has been reached) when

$$|Q(u) - Q(u_h)| \leq \gamma_{\text{tol}}.$$

Notice that if the error $\mathcal{E}$ is, in fact, estimated by computable bounds η_{low}, η_{upp} generated through post-processing u_h, then

$$\mathcal{E} \approx \frac{1}{2}\eta_{\text{low}} + \frac{1}{2}\eta_{\text{upp}} = \eta \qquad \text{and} \qquad Q(u) \approx Q(u_h) + \eta.$$

1. Global Estimates

Let us first review the idea of obtaining so-called global estimates of numerical error. Global methods have dominated the literature on this subject for nearly two decades and can be obtained through straightforward, well-known, efficient, post-processing procedures. Presuming, for simplicity, that the domains of u and u_h coincide, the classical goal of methods of *a posteriori* error estimation is to obtain a number η, the global error estimate of

e, which provides bounds on e in certain meaningful norms $\|\cdot\|$. Thus, one uses to compute a number η, which approximates or bounds $\|e\|$. A major requirement of any successful error estimator η is that positive constants C_1 and C_2 exist such that

$$C_1\|e\| \leq \eta \leq C_2\|e\|.$$

Then, when $\|e\|$ is small, we are confident that η is also small, provided C_2 is not too large. Conversely, when η is small, we know that $\|e\|$ is small, provided C_1 is not too small. The quantity

$$\theta = \frac{\eta}{\|e\|}$$

is referred to as an *effectivity index*. Obviously, θ is a measure of the quality of the estimator η: when $\theta = 1$, η is close to $\|e\|$. Of course, $\|e\|$ is seldom known, so that it is customary to compute for special benchmark problems where e or u is known or can be accurately approximated. Then, the robustness and accuracy of various estimators can be experimentally assessed. Barring such experiments, the quality of an estimator can also be assessed theoretically, but then only asymptotically as certain mesh parameters are refined or as $e \longrightarrow 0$.

The estimate $C_1\|e\| \leq \eta \leq C_2\|e\|$ is a *global* error estimate, meaning that the total error over the entire computational domain is measured in the particular norm appearing in these inequalities. In general, for a computational mesh containing N cells (elements), cellwise (elementwise) error indicators η_K are computed using restrictions of the approximate solution u_h to each cell K. Then the global estimator is given by

$$\eta = \left\{ \sum_{K=1}^{N} \eta_K^2 \right\}^{1/2}$$

The local (or elementwise) effectivity index is then

$$\theta_K = \frac{\eta_K}{\|e\|_K},$$

$\|e\|_K$ being the norm of functions restricted to cell K. It should be understood that the element indicators η_K for an element K do not represent the local error in this element. All that can be said is that η_K is the contribution from element K to the global error estimate η.

Indeed, the actual local error $\|e\|_K$ in element K is "polluted" by errors in elements remote from K. Thus, local refinements of an element in a mesh can only reduce error to a certain threshold; the pollution of the error from remote sources can only be controlled by appropriate mesh refinements or enrichments relevant to those remote sources. Despite the existence of pollution effects, the quantities η_K are nevertheless frequently used effectively as a basis for mesh adaptivity procedures for controlling and reducing the global error.

There are several distinct methods for computing the element error indicators η_K. We mention two broad classes:

(1) Residual Methods
(2) Recovery Methods.

For an abstract problem, $Au = f$ (plus boundary and initial conditions), A being a linear operator and f the source data, we observe that since $u = u_h + e$, the error satisfies the equation $Ae = R$, where R is the residual: $R = f - Au_h$. Thus, the residual defines the degree with which the approximate solution u_h fails to satisfy the equations, boundary - and initial - conditions of the original problem. Residual methods of error estimation are based on the idea of determining efficient (and sometimes rough) approximate solutions to $Ae = R$. In the same spirit as explicit and implicit methods for numerically solving ordinary differential equations, residual error estimation methods can be explicit or implicit. The explicit methods produce estimators η_K by function evaluations and substitutions, they do not involve the solution of linear systems of equations, while implicit methods involve the solution of local equations over K for local error indicators.

For example, in a linear elliptic boundary-value problem solved by finite elements, the equation $Ae = R$ takes on as a "weak" form for element K,

$$a_K(\psi_K, v) = r_K(v)$$

for arbitrary test functions v, $a_K(\cdot,\cdot)$ being the local bilinear form characterizing the problem over element K, ψ_K is the local error estimator, and $r_K(\cdot)$ is the functional produced by the residual restricted to element K. It is argued that the solutions ψ_K of these local problems exist and satisfy bounds of the type

$$\|\psi_K\| \leq C|r_K|$$

where C is a positive constant, possibly dependent on mesh size h_k and $|r_K|$ is an appropriate norm of the local residual. In an explicit error estimator, the easily computable quantity $|r_K|$ can be obtained directly from calculations of r_K and one sets $\eta_K = |r_K|$ as the local indicator. In implicit estimators, one solves

$$a_K(\psi_K, v) = r_K(v)$$

for ψ_K and sets

$$\eta_K = \sqrt{a_K(\psi_K, \psi_K)} = \|\psi_K\|_K.$$

Of course, these local equations are rarely solvable exactly, so that instead of ψ_K one obtains an approximation ψ_K^h generally computed using polynomial approximations of higher degree than those used to compute the approximation u_h itself. To solve the local equations for ψ_K^h, it is often necessary to process the right-hand side (the residuals) so that they balance; *i.e.* so that they are *equilibrated.* Then, for sufficiently accurate approximations ψ_K^h of

ψ_K, one can sometimes prove that the global error bound

$$\|e\| \leq C_2 \left\{ \sum_{K=1}^{N} \eta_K^2 \right\}^{1/2}$$

holds with constant $C_2 = 1$.

In general, the explicit residual error estimators can be calculated easily and efficiently, but they may be useful in only giving trends of error distributions in computational grids and do not furnish quantitative measures of the error. They produce *error indicators*, as opposed to error estimators. They are well suited for use in adaptive meshing algorithms. The implicit residual estimators, on the other hand, require more computational effort but can sometimes yield remarkably accurate estimates of the global error.

Another type of error estimator is that of the recovery type. In these approaches, the approximate solution u_h is post-processed to obtain an enhanced solution u_h^* that is presumably more accurate than u_h. Then the function $e^* = u_h^* - u_h$ provides a computable approximation of the error $e \approx e^*$. In some cases, u_h^* can be obtained by extrapolation, but more commonly, other techniques must be employed. One of the most popular recovery methods is the so-called ZZ Super Convergence Patch Recovery Method (after Zienkiewicz and Zhu). In this technique, a higher-order polynomial is fit over nodal values of u_h (or ∇u_h) over a patch of elements surrounding the element of interest K, and a least-square fit is calculated to determine an enhanced approximation $G \approx \nabla u$. Then the L_2-norm of $G - \nabla u_h$ over K is used as the local error indicator η_K. The ZZ indicator has the attractive property that it can be implemented independently of the actual operators characterizing the problem being solved. Thus, it is applicable to nonlinear problems as well as linear problems.

2. Local Estimates and Errors in Quantities of Interest

One of the most important developments in *a posteriori* error estimation in recent years is the discovery of methods for obtaining estimates of error in local quantities of interest $Q(u)$ discussed earlier. As noted earlier, these local quantities could be, for example, averaged stresses or displacements on surfaces within a structure or material body or mollifications of pointwise stresses or displacements. Whatever the desired quantity, the idea is to characterize it as a functional on the class of admissible displacements for which the problem of interest is posed. For example, consider the weak form of a linear elliptic boundary-value problem such as

$$a(u, v) = (f, v)$$

for any v in a class V of admissible functions, $a(\cdot, \cdot)$ being the global bilinear form and $(f, \cdot)$ the data functional. Suppose $Q(v)$ defines a quantity of

interest, *e.g.* for the average stress component σ_{11} on a surface ω,

$$Q(v) = \frac{1}{|\omega|} \int_{\omega} \sigma_{11}(v)\, \mathrm{d}s.$$

Then, an auxiliary adjoint problem is set up in the form

$$a(v, w) = Q(v)$$

for any v in V. The solution w is the *influence function* for the particular choice of Q. We obtain numerical approximations of both the primal and the adjoint problems and we use the numerical solution u_h of the primal problem and w_h of the adjoint problem to compute the estimate of the error in $Q(u_h)$:

$$\mathcal{E} = Q(u) - Q(u_h) \approx \zeta.$$

The local effectivity index is then

$$\theta_Q = \frac{\zeta}{\mathcal{E}} \qquad \left(\text{or } \frac{|\zeta|}{|\mathcal{E}|}\right).$$

In many of the post-processing algorithms used to compute the estimates ζ, global error estimates η and $\bar{\eta}$ are computed for the primal and adjoint problems, respectively. Thus, the global methods remain useful in *a posteriori* error estimation, even in estimating local errors. However, it is also clear that estimating $Q(u) - Q(u_h)$ requires the solution of two problems, the primal problem characterized by the model we wish to verify and the adjoint problem that characterizes the quantity of interest Q. Once again, we emphasize that the original model can never be fully verified for all possible choices of Q: the best that can be done is to compare the estimated error $\mathcal{E} \approx \zeta$ with some preset tolerance γ_{tol}. If this tolerance is exceeded, one may resort to adaptive meshing to reduce (or control) the error in Q. Such adaptive schemes built around controlling errors in quantity of interest, as opposed to global bounds in energy norms, are called GOALS algorithms after "Goal-Oriented Adaptive Local Solutions".

3. The Role of A Posteriori Error Estimation in Verification

Verification is the process of assessing whether a model of a physical event or an engineering system is "solved" correctly - or, if not, with how accurately it is solved in a particular application. A key question that arises when stating this definition is: what is meant by the term "model"? The answer lies in the most basic notion of the mission of verification and validation: to assess the reliability of computer-based simulations and predictions of physical events and systems. Thus, it is fundamentally important to understand that the model referred to here is the mathematical model of the event: the system of equations (ordinary or partial differential, integral, integro-differential), inequalities, boundary and initial conditions, data (coefficients, source terms, geometry, load history), *etc.* that constitute the mathematical

abstraction of the physical phenomenon of interest. It is not the discrete version of the model fed into the computer. Verification and code verification are thus quite different subjects. Code verification is the process of assessing if a given computer code reliably solves the discrete versions of the class of mathematical models targeted in the application software. Code verification is the province of software engineering. It involves bug fixes, benchmarks, testing results against manufactured solutions, performance tests, and other technologies. It is, of course, a fundamentally important process in the broad area of verification and validation, but it is not, in itself, sufficient to complete the process of verification. In principle, the fact that a given code has been verified free of bugs and is highly efficient does not mean that the "model was solved correctly." Indeed, the accuracy with which the model is solved depends upon factors independent of the parameters used in code verification, such as the mesh used in the simulation, the order of the local approximations, time step size, *etc.* Verification, it is emphasized, has to do with the accuracy with which the mathematical model is solved. This fact means that assessing the accuracy of numerical approximations of solutions of the model is fundamentally the essence of verification. Implicit in the idea of verification is that models are somehow obtained and that we are bound to determine to what degree these simulations actually solve the model under study. This is *a posteriori* error estimation.

4. Summary and Recommendations

A posteriori error estimation provides a powerful tool for verification of results of computer simulations and predictions. Many techniques for *a posteriori* error estimation exist and they vary in cost, robustness, and quality of results, but virtually all available approaches give useful information on quality of computed solutions or on trends of the distribution of error as mesh parameters are varied. The theory and algorithms underlying *a posteriori* error analysis of finite element approximations have matured to a level that the technology can be used confidently to provide measures of the actual accuracy of computed solutions. Importantly, techniques for computing upper and lower bounds of errors in local features of computed solutions are now available for a significant class of problems. As an added benefit, error estimation provides a basis for adaptivity - the systematic alteration of the computational model, the mesh, the algorithms, *etc.* - to improve results and control the error.

References

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TICAM, The University of Texas at Austin, TX 78712, USA
E-mail address: oden@ticam.utexas.edu