ADAPTIVE MODELING IN COMPUTATIONAL SOLID MECHANICS

J.T. Oden and S. Prudhomme

The Texas Institute for Computational and Applied Mathematics
The University of Texas at Austin
201 E. 24th St.
Austin, TX 78712, USA
e-mail: oden@ticam.utexas.edu
web page: http://www.ticam.utexas.edu

Abstract. We review and extend the theory and methodology of a posteriori error estimation and adaptivity for both modeling error and approximation error for certain classes of problems in nonlinear mechanics.

Keywords: Hierarchical modeling, nonlinear continuum mechanics, a posteriori error estimation, goal-oriented methods.

1 INTRODUCTION

In principle, there are two major sources of error in computer simulations of physical events: approximation error, due to the inherent inaccuracies incurred in the discretization of mathematical models of the events, and modeling error, due to the natural imperfections in abstract models of actual physical phenomena. The estimation and control of the first of these has been the subject of research for two decades; the estimation and control of the second error source, modeling error, is a relatively new subject, studied in recent years in connection with heterogeneous materials, large deformation of polymers, and inelastic behavior of materials. A summary of the theory of a posteriori error estimates of finite element approximations is given in the recent monograph.1 Hierarchical modeling and model error estimation and control are discussed in references.3,5,6,10

For many years, error estimation methods were confined to global
estimates (e.g. 7, 11); recently, extensions of the theories have made possible the calculation of upper and lower bounds of error in linear functionals of the solutions, thereby making it possible to estimate errors in quantities of interest to the analyst, such as pointwise stresses and displacements and average stresses over interfaces between dissimilar materials. 4, 8 These types of estimates and the adaptive control procedures they make possible are referred to as “goal-oriented” methods. Extensions of certain types of goal-oriented methods to estimation of approximation errors encountered in nonlinear boundary-value problems have also been reported in recent literature (e.g. 9).

In the present work, the theory of a posteriori error estimation of approximation and modeling error is reviewed and a general framework for estimation of both approximation and modeling error is presented.

2 THE STRUCTURE OF RESIDUAL-BASED ERROR ESTIMATES

We derive here a formal and general setting for estimating both approximation and modeling errors in quantities of interest. We choose as a mode of presentation the optimal control setting adapted by Becker and Rannacher, 2 but we generalize slightly that theory to include model error estimation as well. We begin with the linear case.

Let \( V \) denote a reflexive Banach space (a Hilbert space for the moment), \( B(\cdot, \cdot) \) a continuous bilinear form from \( V \times V \) into \( \mathbb{R} \), \( F \in V' \) a bounded linear functional, and \( Q \in V' \) a functional representing a specific quantity of interest. We seek \( u \in V \) such that

\[
B(u, v) = F(v), \quad \forall \, v \in V
\]  

(1)

and then wish to calculate specifically \( Q(u) \). As noted by Becker and Rannacher, 2 this can be set up as the optimal control problem: find \( u \in V \) such that

\[
Q(u) = \inf_{v \in M} Q(v);
\]  

(2)

where

\[
M = \{ v \in V; \, B(v, w) = F(w), \, \forall \, w \in V \}.
\]  

(3)

The Lagrangian associated with this control problem is

\[
L(v, q) = Q(v) + F(q) - B(v, q), \quad (v, q) \in V \times V.
\]  

(4)
The saddle point \((u, p)\) of \(L(\cdot, \cdot)\), therefore, satisfies the system of equations,

\[
Q(v) = B(v, p), \quad \forall v \in V \tag{5a}
\]
\[
F(q) = B(u, q), \quad \forall q \in V \tag{5b}
\]

Equation (5a) is the adjoint or dual equation corresponding to the choice \(Q\) of the quantity of interest, \(p\) is the influence function or dual solution, and (5b) is the primal problem.

Now let us suppose that a related problem can be formulated using either a different bilinear form, say \(B_0(\cdot, \cdot)\) (a different model) on a subspace \(V_0 \subseteq V\) (possibly a Galerkin approximation space for (5a) and (5b)):

\[
Q(u) = \inf_{v \in M_0} Q(v); \tag{6}
\]

where

\[
M_0 = \{v \in V_0; B_0(v, w) = F(w), \forall w \in V_0\}. \tag{7}
\]

We then have, instead of (5a) and (5b):

\[
Q(v) = B_0(v, p_0), \quad \forall v \in V_0 \tag{8a}
\]
\[
F(q) = B_0(u_0, q), \quad \forall q \in V_0 \tag{8b}
\]

If \(V_0 = V\), \(u_0\) may correspond to an approximation of \(u\) using a simplified model of the event of interest (e.g., using homogenized coefficients). If \(V_0 = V^h\), a finite element subspace, then \(u_0 = u_h\) is the Galerkin approximation of \(u\). In either case, we define the errors:

\[
e_0 = u - u_0 \quad \text{and} \quad e_0 = p - p_0. \tag{9}
\]

From the governing equation for \((u, p)\) and \((u_0, p_0)\), we easily show that:

\[
B(v, e_0) = \mathcal{R}_{p_0}(v), \quad \forall v \in V_0 \tag{10a}
\]
\[
B(e_0, q) = \mathcal{R}_{u_0}(q), \quad \forall q \in V_0 \tag{10b}
\]

where the right-hand sides are the residual functionals,

\[
\mathcal{R}_{p_0}(v) = Q(v) - B(v, p_0) = B(v, p) - B(v, p_0),
\]
\[
\mathcal{R}_{u_0}(q) = F(q) - B(u_0, q) = B(u, q) - B(u_0, q).
\]

It is not difficult to establish the following:
Proposition 1 With above notation and definitions, the following relations hold:

\[ F(\varepsilon_0) = B(\varepsilon_0, \varepsilon_0) + \overline{R}_{p_0}(u_0), \quad (11a) \]
\[ Q(\varepsilon_0) = B(\varepsilon_0, \varepsilon_0) + R_{u_0}(p_0). \quad (11b) \]

In order to evaluate \( Q(e_0) \), only the term \( B(\varepsilon_0, \varepsilon_0) \) needs to be estimated as \( R_{u_0} \). \( u_0 \) and \( p_0 \) are known.

Example 1 Following Oden and Vemaganti,\(^6,^{10}\) the general framework in (11) can be used to estimate error due to homogenization of heterogeneous materials. Let

\[ B(u, v) = \int_{\Omega} \nabla v : E \nabla u \, dx \quad (12a) \]
\[ F(v) = \int_{\Omega} f \cdot v \, dx \int_{\Gamma_i} g \cdot v \, ds \quad (12b) \]
\[ B_0(u_0, v) = \int_{\Omega} \nabla v : E^0 \nabla u_0 \, dx \quad (12c) \]
\[ Q(v) = \frac{1}{\omega} \int_{\omega} n \cdot \sigma(v) \cdot n \, ds \quad (12d) \]
\[ V = \{ v \in H^1(\Omega)^N : v|_{\Gamma_D} = 0 \} \quad (12e) \]

Here \( V \) is the space of admissible displacements of a linearly elastic body \( \Omega \) with tractions \( g \) on \( \Gamma_i \subset \partial \Omega \) and body forces \( f \); \( E = E(x) \) is the elasticity tensor for a highly heterogeneous multiphase material and \( E^0 \) is a constant tensor obtained through standard homogenization procedures. The quantity of interest \( Q \) is the average normal stress over a surface area \( \omega \).

We assume that the "homogenized solution" \( u_0 \) is known as is the "homogenized influence function" \( p_0 \) corresponding to the adjoint problem, (8a). According to (11b), the error in the quantity of interest is:

\[ Q(e_0) = Q(u) - Q(u_0) \\
= B(e_0, \varepsilon_0) + R_{u_0}(p_0) \\
= \frac{1}{4} \| s e_0 + s^{-1} \varepsilon_0 \|_E^2 - \frac{1}{4} \| s e_0 - s^{-1} \varepsilon_0 \|_E^2 + R_{u_0}(p_0) \quad (13) \]
where \[ \|v\|^2_E = B(v, v) \] is the (squared) energy norm and \( s \in (0, 1) \) is a scaling factor. It is shown in\(^6\) that

\[
\| s e_0 \pm s^{-1} e_0 \|_E \leq \eta_{\text{upp}}
\]

where

\[
\eta_{\text{upp}} = \left\{ \int_{\Omega} I_0 \nabla (s u_0 \pm s^{-1} p_0) : E I_0 (s u_0 \pm s^{-1} p_0) \, dx \right\}^{1/2}
\]

where \( I_0 = I - E^{-1} E_0 \). Also, a lower bound is provided by:

\[
\eta_{\text{low}} = \frac{|R_{su0 \pm s^{-1} p_0} (u_0 + \theta^\pm p_0)|}{\|u_0 + \theta^\pm p_0\|_E}
\]

Computable choices for the parameters \( s \) and \( \theta^\pm \) are given in.\(^2\) We then immediately have the following estimates from (13), (15) and (16):

\[
\eta_{\text{low}} \leq Q(e_0) \leq \eta_{\text{upp}}
\]

where

\[
\eta_{\text{low}} = \frac{1}{4} (\eta_{\text{low}}^+)^2 - \frac{1}{4} (\eta_{\text{upp}}^-)^2 + R_{u0}(p_0)
\]

\[
\eta_{\text{upp}} = \frac{1}{4} (\eta_{\text{upp}}^+)^2 - \frac{1}{4} (\eta_{\text{low}}^-)^2 + R_{u0}(p_0)
\]

Numerous examples of applications of these estimates are given in.\(^10\)

**Example 2** The results of Oden and Prudhomme\(^4\) and Becker and Rannacher\(^2\) are obtained from (10) and (11) as follows. Set

\[
V_0 = V^h \subset V
\]

\( V^h \) being a finite-element subspace of \( V \). Then \( e_0 = u - u_h = e_h \) and \( e_0 = p - p_h = e_h \) are the errors in Galerkin finite element approximations of \( u \) and \( p \), i.e. now \( u_0 = u_h \) and \( p_0 = p_h \). In this case,

\[
R_{p_h}(v_h) = 0, \ R_{u_h}(v_h) = 0 \quad \forall v_h \in V^h
\]

Then, essentially the same procedure leading to (17) now gives upper and lower bounds on \( Q(e_h) \) when \( B(\cdot, \cdot) \) is a symmetric bilinear form.\(^6\)
3 CONCLUDING COMMENTS

The concepts of modeling error, error estimation, and adaptive modeling provide a framework for systematically selecting appropriate models of physical phenomena. Additional advances are needed if these methods are to have a useful role in model validation. First, the predictive qualities of computational models will always depend upon the goals of the simulation. In other words, the particular physical event(s) of interest must be clearly specified before it is meaningful to compare the effectiveness of various models of it. Second, the modeling error is, as noted earlier, a random variable. Thus, the adaptive modeling process should be embedded in an appropriate stochastic framework or in something equivalent. Thirdly, modeling error and approximation error must be simultaneously estimated and controlled for a completed, verified and validated predictive tool to be created. Finally, adaptive modeling should be integrated into a larger framework that provides an interaction and feedback with physical experiments and tests to allow dynamic updating of the parameters that define models within a hierarchy of possible models.

Acknowledgements The support of this work through the Office of Naval Research under grant N00014-95-0401, and of the Sandia National Laboratories under grant BF-2070 are gratefully acknowledged.

4 REFERENCES


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estimates (e.g. 7, 11); recently, extensions of the theories have made possible the calculation of upper and lower bounds of error in linear functionals of the solutions, thereby making it possible to estimate errors in quantities of interest to the analyst, such as pointwise stresses and displacements and average stresses over interfaces between dissimilar materials. 4, 8 These types of estimates and the adaptive control procedures they make possible are referred to as "goal-oriented" methods. Extensions of certain types of goal-oriented methods to estimation of approximation errors encountered in nonlinear boundary-value problems have also been reported in recent literature (e.g. 9).

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and then wish to calculate specifically $Q(u)$. As noted by Becker and Rannacher, 2 this can be set up as the optimal control problem: find $u \in V$ such that

$$Q(u) = \inf_{v \in M} Q(v);$$

where

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The Lagrangian associated with this control problem is

$$L(v, q) = Q(v) + F(q) - B(v, q), \quad (v, q) \in V \times V.$$
The saddle point \((u, p)\) of \(L(\cdot, \cdot)\), therefore, satisfies the system of equations,

\[
\begin{align*}
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F(q) &= B(u, q), \quad \forall \ q \in V \tag{5b}
\end{align*}
\]

Equation (5a) is the adjoint or dual equation corresponding to the choice \(Q\) of the quantity of interest, \(p\) is the influence function or dual solution, and (5b) is the primal problem.

Now let us suppose that a related problem can be formulated using either a different bilinear form, say \(B_0(\cdot, \cdot)\) (a different model) on a subspace \(V_0 \subseteq V\) (possibly a Galerkin approximation space for (5a) and (5b)):

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We then have, instead of (5a) and (5b):

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Q(v) &= B_0(v, p_0), \quad \forall \ v \in V_0 \tag{8a} \\
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If \(V_0 = V\), \(u_0\) may correspond to an approximation of \(u\) using a simplified model of the event of interest (e.g. using homogenized coefficients). If \(V_0 = V^k\), a finite element subspace, then \(u_0 = u_h\) is the Galerkin approximation of \(u\). In either case, we define the errors:

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e_0 = u - u_0 \quad \text{and} \quad \varepsilon_0 = p - p_0. \tag{9}
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From the governing equation for \((u, p)\) and \((u_0, p_0)\), we easily show that:

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\begin{align*}
B(v, e_0) &= \overline{R}_{p_0}(v), \quad \forall \ v \in V_0 \tag{10a} \\
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\end{align*}
\]

where the right-hand sides are the residual functionals,

\[
\begin{align*}
\overline{R}_{p_0}(v) &= Q(v) - B(v, p_0) = B(v, p) - B(v, p_0), \\
\mathcal{R}_{u_0}(q) &= F(q) - B(u_0, q) = B(u, q) - B(u_0, q).
\end{align*}
\]

It is not difficult to establish the following:
Proposition 1 With above notation and definitions, the following relations hold:

\[
\begin{align*}
F(\varepsilon_0) &= B(\varepsilon_0, \varepsilon_0) + R_{\varepsilon_0}(u_0), \quad (11a) \\
Q(\varepsilon_0) &= B(\varepsilon_0, \varepsilon_0) + R_{u_0}(p_0). \quad (11b)
\end{align*}
\]

In order to evaluate \( Q(\varepsilon_0) \), only the term \( B(\varepsilon_0, \varepsilon_0) \) needs to be estimated as \( R_{\varepsilon_0}, u_0 \) and \( p_0 \) are known.

Example 1 Following Oden and Vemaganti, the general framework in (11) can be used to estimate error due to homogenization of heterogeneous materials. Let

\[
\begin{align*}
B(u, v) &= \int_{\Omega} \nabla v : E \nabla u \, dx \quad (12a) \\
F(v) &= \int_{\Omega} f \cdot v \, dx + \int_{\Gamma_t} g \cdot v \, ds \quad (12b) \\
B_0(u_0, v) &= \int_{\Omega} \nabla v : E^0 \nabla u_0 \, dx \quad (12c) \\
Q(v) &= \frac{1}{\omega} \int_{\omega} \mathbf{n} \cdot \varepsilon(v) \cdot \mathbf{n} \, ds \quad (12d) \\
V &= \{ v \in H^1(\Omega)^N : v|_{\Gamma_D} = 0 \} \quad (12e)
\end{align*}
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Here \( V \) is the space of admissible displacements of a linearly elastic body \( \Omega \) with tractions \( g \) on \( \Gamma_t \subset \partial \Omega \) and body forces \( f \); \( E = E(x) \) is the elasticity tensor for a highly heterogenous multiphase material and \( E^0 \) is a constant tensor obtained through standard homogenization procedures. The quantity of interest \( Q \) is the average normal stress over a surface area \( \omega \).

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\[
\begin{align*}
Q(\varepsilon_0) &= Q(u) - Q(u_0) \\
&= B(\varepsilon_0, \varepsilon_0) + R_{u_0}(p_0) \\
&= \frac{1}{4} \|s \varepsilon_0 + s^{-1} \varepsilon_0\|^2_E - \frac{1}{4} \|s \varepsilon_0 - s^{-1} \varepsilon_0\|^2_E + R_{u_0}(p_0) \quad (13)
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where \( \|v\|_E^2 = B(v, v) \) is the (squared) energy norm and \( s \in (0, 1) \) is a scaling factor. It is shown in\(^6\) that

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where

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\eta_{\text{upp}} = \left\{ \int_{\Omega} I_0 \nabla (s u_0 \pm s^{-1} p_0) : E I_0 (s u_0 \pm s^{-1} p_0) \, dx \right\}^{1/2}
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where \( I_0 = I - E^{-1} E_0 \). Also, a lower bound is provided by:

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\eta_{\text{low}} = \frac{|R_{su_0 \pm s^{-1} p_0} (u_0 \pm \theta \pm p_0)|}{\|u_0 + \theta \pm p_0\|_E}
\]

Computable choices for the parameters \( s \) and \( \theta \) are given in\(^2\). We then immediately have the following estimates from (13), (15) and (16):

\[
\eta_{\text{low}} \leq Q(e_0) \leq \eta_{\text{upp}}
\]

where

\[
\begin{align*}
\eta_{\text{low}} &= \frac{1}{4} (\eta_{\text{low}}^+)^2 - \frac{1}{4} (\eta_{\text{low}}^-)^2 + R_{u_0} (p_0) \\
\eta_{\text{upp}} &= \frac{1}{4} (\eta_{\text{upp}}^+)^2 - \frac{1}{4} (\eta_{\text{upp}}^-)^2 + R_{u_0} (p_0)
\end{align*}
\]

Numerous examples of applications of these estimates are given in\(^10\).

**Example 2** The results of Oden and Prudhomme\(^4\) and Becker and Rannacher\(^8\) are obtained from (10) and (11) as follows. Set

\[ V_0 = V^h \subset V \]

\( V^h \) being a finite-element subspace of \( V \). Then \( e_0 = u - u_h = e_h \) and \( e_0 = p - p_h = e_h \) are the errors in Galerkin finite element approximations of \( u \) and \( p \), i.e. now \( u_0 = u_h \) and \( p_0 = p_h \). In this case,

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4 REFERENCES


