ADAPTIVE MODELING IN COMPUTATIONAL MECHANICS

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

Keywords: Nonlinear continuum mechanics, hierarchical modeling, a posteriori modeling 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 object, 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 [6, 10, 3, 5].

Initially, model error estimation methods were confined to global estimates [11, 7]; recently, extensions of the theories related to approximation error 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 [8, 4]. 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, 2]).

In this paper, we develop a general theory of a posteriori estimates of modeling error for models of phenomena in solid and fluid mechanics. The approach is based on the idea
that a highly sophisticated mathematical model of a collection of events of interest can be
developed which may be validated by observation or experiment, which may be intractable
or impractical to solve, but which can be used as a datum with respect to which coarser or
simplified models can be compared. We develop a general framework for comparing coarse
and fine models, and, thus, produce a basis for computing modeling error. The theory is a
generalization of the theory for approximation error, developed in [2]. Applications of the
theory require different developments for each application. We demonstrate applications
of modeling error estimation on specific classes of problems, including the analyses of
heterogeneous materials, incompressible viscous fluids, and nonlinear viscoelastic solids.
The framework for a posteriori error estimates of approximation errors can be obtained as
special cases of the theory.

2 PRELIMINARIES: DIFFERENTIATION AND LINEARIZATION

A key tool in our analysis of nonlinear problems is linearization, by which we mean the
representation of nonlinear functions as Taylor or mean-value expansions in certain function
spaces in terms of abstract derivatives and well-defined remainders. Thus, we assume from
the outset that the functionals and forms of interest are differentiable up to a sufficiently
high order, generally two or three. To lay the groundwork for such analyses, we record for
future reference representative forms of such expansions in the setting of general functions
spaces.

Let $\mathcal{V}$ denote a Banach space and $\mathcal{B}(\cdot; \cdot)$ and $Q(\cdot)$ a differentiable semilinear and possibly nonlinear differentiable functional, respectively, defined on $\mathcal{V}$:

$$ B : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R} $$

$$ Q : \mathcal{V} \rightarrow \mathbb{R} $$

Following common practice, we use the convention that semilinear forms such as $\mathcal{B}(\cdot; \cdot)$ are linear in all arguments that follow the semicolon; thus $\mathcal{B}(u; v)$ is linear in $v$ but possibly nonlinear in $u$. By differentiability of $\mathcal{B}(\cdot; \cdot)$, we mean that limits such as:

$$ B'(u; v, w) = \lim_{\theta \to 0} \theta^{-1} [B(u + \theta v; w) - B(u; w)] $$

$$ B''(u; v, p, w) = \lim_{\theta \to 0} \theta^{-1} [B'(u + \theta p; v, w) - B'(u; v, w)] $$

$$ B'''(u; v, p, q, w) = \lim_{\theta \to 0} \theta^{-1} [B''(u + \theta q; v, p, w) - B''(u; v, p, w)] $$

exist. Thus, for fixed $u$, $\mathcal{B}'(u; \cdot, \cdot)$, $\mathcal{B}''(u; \cdot, \cdot, \cdot)$, for instance, are bilinear and trilinear forms in the arguments following the semicolon. Analogously, if $Q(\cdot)$ is a differentiable
functional on $V$, we use the following notations for its Gâteaux derivatives:

$$Q'(u;v) = \lim_{\theta \to 0} \theta^{-1}[Q(u + \theta v) - Q(u)]$$
$$Q''(u;v,w) = \lim_{\theta \to 0} \theta^{-1}[Q'(u + \theta w;v) - Q'(u;v)]$$

\[\vdots\]

etc.

It is known that Taylor expansions with integral remainders can be constructed for such functionals and semilinear forms. Among such expansions, we list the following:

$$Q(u + v) - Q(u) = \int_0^1 Q'(u + sv;v) \, ds$$
$$Q(u + v) - Q(u) = Q'(u;v) + \int_0^1 Q''(u + sv;v,v)(1 - s) \, ds$$
$$Q(u + v) - Q(u) = \frac{1}{2}Q'(u;v) + \frac{1}{2}Q'(u + v;v)$$
$$+ \frac{1}{2} \int_0^1 Q'''(u + sv;v,v,v)(s - 1)s \, ds$$

(1)

We also have:

$$B(u + v;w) - B(u;w) = \int_0^1 B'(u + sv;v,w) \, ds$$
$$B(u + v;w) - B(u;w) = B'(u;v,w)$$
$$+ \int_0^1 B''(u + sv;v,v,w)(1 - s) \, ds$$

(2)

Many alternative forms of such expansions can be derived.

\section{A GENERAL FRAMEWORK FOR RESIDUAL ERROR ESTIMATION}

In an important series of papers that inspired portions of the present work, Becker and Rannacher developed the Dual-Weighted Residual (DWR) method as a general approach for deriving residual-based estimates of approximation error in finite element approximations of a broad class of nonlinear problems (for a detailed summary and references to other work, see [2]).

We present in this section a straightforward generalization of the DWR framework, valid for deriving error estimates of modeling error that, formally, reduce to the original DWR of [2] as a specific case. The details of application of this framework to obtain modeling error estimates in specific cases are, of course, much different and, in some cases, more involved than those for approximation error.
We begin with the abstract nonlinear problem,

\[
\text{Find } u \in V \text{ such that } \quad B(u; v) = F(v), \quad \forall \ v \in V
\]  

(3)

where, again, \( B(\cdot; \cdot) \) is a semilinear form defined on the Banach space \( V \) and \( F(\cdot) \) is a linear functional on \( V \). We assume that (3) admits a unique solution \( u \) in \( V \).

Our goal is to determine specific features of the solution characterized by another functional \( Q(\cdot) \) defined on \( V \). Thus, for example, if (3) characterized a nonlinear boundary-value problem in, say, finite elasticity or viscous flow, \( Q(u) \) represents a specific “quantity of interest” such as average stress on an interior interface or the average vorticity near an obstacle in the flowfield. A theory for estimating approximation errors in such quantities of interest for linear elliptic problems can be found in the work of Oden and Prudhomme [8, 4].

In [2], an “optimal control” approach to this problem is proposed based on the constrained minimization problem,

\[
\text{Find } u \in V \text{ such that } \quad Q(u) = \inf_{v \in M} Q(v)
\]

where

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

(4)

The minima \( u \) correspond to a saddle point \( (u, p) \in V \times V \) of the Lagrangian,

\[
L(u, p) = Q(u) + F(p) - B(u; p)
\]

(5)

with \( p \) the influence function (or Lagrange multiplier or adjoint variable) corresponding to the choice \( Q \) of the quantity of interest. The critical points \( (u, p) \) of \( L(\cdot, \cdot) \) are such that

\[
L'((u, p); (v, q)) = 0, \quad \forall (v, q) \in V \times V.
\]

(6)

Since, for all \( (v, q) \in V \times V \),

\[
L'((u, p); (v, q)) = Q'(u; v) - B'(u; v, p) + F(q) - B(u; q),
\]

(7)

to solve (4), we seek \( (u, p) \in V \times V \) such that

\[
\begin{align*}
B(u; q) &= F(q), \quad \forall q \in V \\
B'(u; v, p) &= Q'(u; v), \quad \forall v \in V
\end{align*}
\]

(8)

Equation (8)\(^1\) is the primal problem for \( u \); (8)\(^2\) is the adjoint or dual problem for \( p \), and, with \( u \) specified, is a linear variational equation for the influence function \( p \) corresponding to the choice \( Q \) of the quantity of interest.
Now let us suppose that problem (3) is, for practical purposes, intractable and that we are led to consider a related but possibly simplified problem using a different bilinear form $B_0(\cdot;\cdot)$ (a different model of the physical event abstracted by model (3)) defined on a subspace $V_0 \subseteq V$. Instead of (4), we consider:

$$
\begin{align*}
\text{Find } u_0 & \in V_0 \text{ such that } Q(u_0) = \inf_{v \in M_0} Q(v) \\
\text{where } M_0 & = \{ v \in V_0; B_0(v;q) = F(q), \forall q \in V_0 \}
\end{align*}
$$

Instead of (8), we now have

$$
\begin{align*}
B_0(u_0;q) & = F(q), \quad \forall q \in V_0 \\
B'_0(u_0;v,p_0) & = Q'(u_0;v), \quad \forall v \in V
\end{align*}
$$

If $V_0 = V$, $u_0$ may correspond to an approximation of $u$ using a simplified model (e.g. using homogenized coefficients to approximate heterogeneous media). If $V_0 = V^h$, a finite element subspace of $V$, then $u_0 = u_h$, the corresponding Galerkin-finite-element approximation of $u$. We are concerned with the former case, and hereafter, take $V_0 = V$.

We regard (8) and (10) as different models of the same events, with $(u,p)$ a “fine” solution to the problem (corresponding to a model with finer detail) and $(u_0,p_0)$ as a “coarse” (or simplified) solution to the problem.

Assuming that solutions $(u,p)$ and $(u_0,p_0)$ exist to (8) and (10), respectively, we define the primal and adjoint errors $(\epsilon_0, \epsilon_0)$ as

$$
\epsilon_0 = u - u_0 \quad \text{and} \quad \epsilon_p = p - p_0.
$$

Also, the degree to which $(u_0,p_0)$ fail to satisfy the fine problem (8) is characterized by the residual functionals:

$$
\begin{align*}
\mathcal{R}(u_0;q) & = F(q) - B(u_0;q), \quad q \in V \\
\mathcal{R}(u_0,p_0;v) & = Q'(u_0;v) - B'(u_0;v,p_0), \quad v \in V
\end{align*}
$$

Our goal is to relate the modeling error in the quantity of interest, $Q(u) - Q(u_0)$, to the residual functionals (12). This is accomplished in the following general result.

**Theorem 1** Given any approximation $(u_0,p_0)$ of the solution $(u,p)$ of system (8), we have the a posteriori error representation

$$
Q(u) - Q(u_0) = \mathcal{R}(u_0;p_0) + \frac{1}{2} \left( \mathcal{R}(u_0;\epsilon_0) + \mathcal{R}(u_0,p_0;\epsilon_0) \right) + r(\epsilon_0,\epsilon_p),
$$
where

\[
r(e_0, e_0) = \frac{1}{2} \int_0^1 \left\{ Q''(u_0 + se_0; e_0, e_0, e_0) - 3B''(u_0 + se_0; e_0, e_0, e_0) \right. \\
- B''(u_0 + se_0; e_0, e_0, p_0 + s e_0) \left\} (s - 1) s \, ds.
\]

(14)

**Proof.** For the Lagrangian defined in (5), and using the fact that \((u, p)\) is a solution of (8), we observe that

\[
Q(u) = L(u, p) - (F(p) - B(u; p)) = L(u, p),
\]

\[
Q(u_0) = L(u_0, p_0) - (F(p_0) - B(u_0; p_0)) = L(u_0, p_0) - R(u_0; p_0).
\]

Therefore:

\[
Q(u) - Q(u_0) = R(u_0; p_0) + L(u, p) - L(u_0, p_0).
\]

(15)

By virtue of the last expansion in (1), with \(Q\) as \(L\) and \(u\) as \((u_0, p_0)\), \(v\) as \((e_0, e_0)\), we have:

\[
L(u, p) - L(u_0, p_0) = \frac{1}{2} L'((u_0, p_0); (e_0, e_0)) + \frac{1}{2} L'((u, p); (e_0, e_0)) \\
+ \frac{1}{2} \int_0^1 L'''((u_0, p_0) + s(e_0, e_0); (e_0, e_0), (e_0, e_0)) (s - 1) s \, ds.
\]

Since \((u, p)\) is a stationary point of \(L\), it follows that \(L'((u, p); (e_0, e_0)) = 0\). On the other hand, using the expression of \(L'\) given in (7), we have, for any \((v, q) \in V \times V\),

\[
L'((u_0, p_0); (v, q)) = \underbrace{Q'((u_0, p_0); (e_0, e_0)) - B'((u_0, p_0); (v, q))}_{\mathcal{R}(u_0, p_0; v)} \underbrace{+ F(q) - B((u_0, q))}_{\mathcal{R}(u_0, q)}.
\]

It is not difficult, but tedious, to show that:

\[
L'''((u_0, p_0) + s(e_0, e_0); (e_0, e_0), (e_0, e_0), (e_0, e_0)) = \\
Q'''((u_0 + se_0; e_0, e_0, e_0) - 3B'''((u_0 + se_0; e_0, e_0, e_0) \\
- B'''((u_0 + se_0; e_0, e_0, p_0 + se_0).
\]

Hence

\[
L(u, p) - L(u_0, p_0) = \frac{1}{2} \mathcal{R}(u_0; e_0) + \frac{1}{2} \mathcal{R}(u_0, p_0; e_0) + r(e_0, e_0),
\]

where \(r(e_0, e_0)\) is given by (14). Substituting this last equality into (15) gives the stated result. 

The residuals \(\mathcal{R}(u_0; e_0)\) and \(\overline{\mathcal{R}}(u_0, p_0; e_0)\) can be related as shown in the next lemma:
Lemma 2  Given any approximation \((u_0, p_0)\) of the solution \((u, p)\) of system (8), the following equality holds:
\[
\mathcal{R}(u_0, p_0; \epsilon_0) = \mathcal{R}(u_0; \epsilon_0) + \Delta \mathcal{R}
\]  (16)
where
\[
\Delta \mathcal{R} = \int_0^1 B''(u_0 + se_0; e_0, p_0 + se_0) \, ds - \int_0^1 Q''(u_0 + se_0; e_0, \epsilon_0) \, ds.
\]  (17)

Proof.  Since \(u\) is the solution of (8), we can replace \(F(q)\) by \(B(u; q)\) in the definition of the residual of the primal equation (12). Hence:
\[
\mathcal{R}(u_0; q) = B(u; q) - B(u_0; q), \quad \forall q \in V.
\]  (18)
and, using one of the Taylor expansions, we get:
\[
\mathcal{R}(u_0; q) = B'(u_0; e_0, q) + \int_0^1 B''(u_0 + se_0; e_0, e_0, q)(1 - s) ds.
\]  (19)
Likewise, the residual associated with the dual equation can be written as:
\[
\mathcal{R}(u_0, p_0; v) = Q'(u_0; v) - B'(u_0; v, p_0)
\]
\[
= Q'(u_0; v) - Q'(u_0; v) + Q'(u_0; v) - B'(u_0; v, p_0)
\]
\[
= Q'(u_0; v) - Q'(u_0; v) + B'(u_0; v, p) - B'(u_0; v, p_0)
\]
\[
= -[Q'(u_0; v) - Q'(u_0; v)] + [B'(u_0; v, p) - B'(u_0; v, p)] + B'(u_0; v, \epsilon_0).
\]
Using the following Taylor expansions
\[
Q'(u; v) - Q'(u_0; v) = \int_0^1 Q''(u_0 + s \epsilon_0; e_0, v) \, ds,
\]
\[
B'(u_0; v, p) - B'(u_0; v, p) = \int_0^1 B''(u_0 + s \epsilon_0; e_0, v, p) \, ds,
\]
we obtain:
\[
\mathcal{R}(u_0, p_0; v) = B'(u_0; v, \epsilon_0) - \int_0^1 Q''(u_0 + s\epsilon_0; e_0, v) \, ds
\]
\[
+ \int_0^1 B''(u_0 + s\epsilon_0; e_0, v, p) \, ds.
\]  (20)
Taking \(q = \epsilon_0\) in (19) and \(v = \epsilon_0\) in (20), we arrive at the following relationship
\[
\mathcal{R}(u_0, p_0; \epsilon_0) = \mathcal{R}(u_0; \epsilon_0) - \int_0^1 Q''(u_0 + s\epsilon_0; e_0, \epsilon_0) \, ds
\]
\[
+ \int_0^1 B''(u_0 + s\epsilon_0; e_0, \epsilon_0, p - (1 - s)\epsilon_0) \, ds,
\]
and observing that \(p - (1 - s)\epsilon_0 = p_0 + s\epsilon_0\) gives the stated result. 

A companion simplified representation of the error is embodied in the following theorem.
Theorem 3 With same notation as above:
\[ Q(u) - Q(u_0) = \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; \varepsilon_0) + \frac{1}{2} \Delta \mathcal{R} + r(\varepsilon_0, \varepsilon_0). \] (21)

Proof. This immediately follows from Theorem 1 and Lemma 2. ■

Our proofs of Theorem 1, and to a lesser extent, of Lemma 2, follow more or less the same lines as that of Propositions 2.2 and 2.3 in Becker and Rannacher [2], except that for modeling error, we cannot take advantage of the orthogonality property of the error to a finite-element subspace, as can be exploited in the case of Galerkin approximations. By setting \( V_0 = V^h \subset V \) and \( B_0(\cdot; \cdot) = B(\cdot; \cdot) \), \( \mathcal{R}(u_0; p_0) = \mathcal{R}(u_0; p_h) = 0 \) and (13) reduces to equation (2.18) of [2]. Likewise, for these choices, (21) reduces to (2.22) of [2].

Remark 1 Since the residual \( \mathcal{R}(u_0; \cdot) \) is a linear functional in the second argument, result (21) can be rewritten as:
\[ Q(u) - Q(u_0) = \mathcal{R}(u_0; p) + \frac{1}{2} \Delta \mathcal{R} + r(\varepsilon_0, \varepsilon_0). \] (22)
In other words, it “suffices” to use the exact influence function \( p \) to obtain a very accurate estimate of the error.

Remark 2 In the proof of Lemma 2, we unraveled the relationships between the errors \( \varepsilon_0 \) and \( \varepsilon_0 \) and the residuals \( \mathcal{R}(u_0; q) \) and \( \overline{\mathcal{R}}(u_0, p_0; v) \). Indeed, dropping the high-order terms in (19) and (20), we respectively obtain the governing equation for the modeling error \( \varepsilon_0 \) and for the error \( \varepsilon_0 \) in the influence function, i.e.
\[ B'(u_0; \varepsilon_0, q) = \mathcal{R}(u_0; q), \quad \forall q \in V, \] (23)
\[ B'(u_0; v, \varepsilon_0) = \overline{\mathcal{R}}(u_0, p_0; v), \quad \forall v \in V. \] (24)

Remark 3 We note that \( (u_0, p_0) \) in Theorems 1 and 3 do not necessarily need to be the solution of (10) in order for the Theorems to be satisfied. Indeed, \( (u_0, p_0) \) are simply approximations of \( (u, p) \) and Problem (10) was introduced as a possible means to obtain \( (u_0, p_0) \).

4 ERROR ESTIMATORS FOR QUANTITIES OF INTEREST

Theorems 1 and 3 provide us with exact representations of the error in the quantity of interest \( Q(u) - Q(u_0) \). In this section, we describe how to derive computable error estimates. We first note that the term \( \mathcal{R}(u_0; p_0) \) is readily computable assuming that the functions \( u_0 \) and \( p_0 \) are explicitly known. On the other hand, the high-order terms \( r(\varepsilon_0, \varepsilon_0) \) and \( \Delta \mathcal{R}/2 \) may be neglected if the errors \( \varepsilon_0 \) and \( \varepsilon_0 \) are known to be small. It therefore follows that error estimates of \( Q(u) - Q(u_0) \) can be introduced as:
\[ Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p_0) + \frac{1}{2} (\mathcal{R}(u_0; \varepsilon_0) + \overline{\mathcal{R}}(u_0, p_0; \varepsilon_0)), \] (25)
\[ Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; \varepsilon_0). \] (26)
If \( \varepsilon_0 \) and \( \varepsilon_0 \) were known, these estimates would be computable and the first estimate would be expected to yield more accurate results than the second one. Unfortunately, these errors are in general not known and need to be estimated. In doing so, we naturally introduce additional errors. The first estimate is then not guaranteed to provide a more accurate result on estimates of \( Q(u) - Q(u_0) \).

Methods to obtain estimates of \( \varepsilon_0 \) and \( \varepsilon_0 \) are usually problem dependent. We present in the following sections three different applications for which we describe various approaches to derive computable error estimators for the quantity of interest.

5 HETEROGENEOUS ELASTIC MATERIALS

One of the most important applications of the modeling error estimates has to do with the analysis of heterogeneous elastic materials. The subject was studied in some depth by Oden and Vemaganti [6, 10].

5.1 Notation and Preliminaries

In the case of heterogeneous elastic materials, we have:

\[
V = \{ v \in (H^1(\Omega))^N : \ v|_{\Gamma_D} = 0 \} \tag{27}
\]

\[
B(u, v) = \int_{\Omega} \nabla v : E \nabla u \, dx \tag{28}
\]

\[
B_0(u_0, v) = \int_{\Omega} \nabla v : E_0 \nabla u_0 \, dx \tag{29}
\]

\[
F(v) = \int_{\Omega} f \cdot v \, dx \int_{\Gamma_N} g \cdot v \, ds \tag{30}
\]

\[
Q(v) = \frac{1}{|\omega|} \int_{\omega} \sigma_{11}(v) \, ds \tag{31}
\]

Here \( V \) is the space of admissible displacements of a linearly elastic body occupying a domain \( \Omega \subset \mathbb{R}^N \) with boundary \( \partial \Omega = \Gamma_D \cup \Gamma_N \), displacements prescribed on \( \Gamma_D \) and tractions prescribed on \( \Gamma_N \), with meas \( \Gamma_D > 0 \), the body being subject to body forces \( b \) and surface tractions \( g \) on \( \Gamma_N \). The elasticity tensor \( E = E(x) \in (L^\infty(\Omega))^{N^2 \times N^2} \) is a highly oscillatory function of position exhibiting standard ellipticity and symmetry properties; e.g. \( \exists \alpha_0, \alpha_1 > 0 \) such that for a.e. \( x \in \Omega \),

\[
\alpha_0 \varepsilon_{ij} \varepsilon_{ij} \leq \varepsilon_{ij} E_{ijkl}(x) \varepsilon_{kl} \leq \alpha_1 \varepsilon_{ij} \varepsilon_{ij}
\]

\[
E_{ijkl}(x) = E_{jikl}(x) = E_{ijlk}(x) = E_{klij}(x)
\]

a.e. \( x \in \Omega, 1 \leq i, j, k, l \leq N, \forall \varepsilon_{ij} = \varepsilon_{ji} \)
(repeated indices summed over their range). The tensor $E_0$ is an approximation of $E$ obtained through some homogenization process. Thus, the fine model problem is:

Find $u \in V$ such that

$$B(u, v) = F(v), \quad \forall v \in V \quad (32)$$

and the coarse model corresponds to the homogenized problem,

Find $u_0 \in V$ such that

$$B_0(u_0, v) = F(v), \quad \forall v \in V \quad (33)$$

It follows that $e = u - u_0$ represents the modeling error due to using “homogenized” coefficients in the equilibrium equations for linear elastostatics.

The example of the quantity of interest $Q$ is the average normal stress component $\sigma_{11}(v) = E_{ijkl}(x) \partial u_k(x)/\partial x_l$ over an (internal) surface $\omega$ (such as an interface between dissimilar materials).

### 5.2 General Modeling Error Estimates

Returning to (13), we observe that in this application,

$$\mathcal{R}(u_0; \varepsilon_0) = F(\varepsilon_0) - B(u_0, \varepsilon_0)$$

$$= B(u, \varepsilon_0) - B(u_0, \varepsilon_0)$$

$$= B(\varepsilon_0) \quad (34)$$

$$\mathcal{R}(p_0; e_0) = Q(e_0) - B(e_0, p_0)$$

$$= B(e_0, p) - B(e_0, p_0)$$

$$= B(e_0) \quad (35)$$

$$\mathcal{R}(u_0; p_0) = B(e_0, p_0) + \int_{\omega} \nabla p_0 : E I_0 \nabla u_0 \, dx$$

$$r(e_0, \varepsilon_0) = 0 \quad (36)$$

where $I_0 = I - E^{-1} E_0$, $e_0 = u - u_0$, $\varepsilon_0 = p - p_0$. Hence, the general estimate (13) reduces to:

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p_0) + B(e_0, \varepsilon_0) = \mathcal{R}(u_0; p_0) + B(e_0, s \varepsilon_0) \quad (38)$$

for all $s > 0$. 

5.3 Error Estimates, Upper and Lower Bounds

In this example, $B(\cdot, \cdot)$ is a symmetric, positive definite, bilinear form (i.e. an inner product) on the space of admissible functions of finite energy. Thus, we can use the parallelogram identity

$$B(se_0, s^{-1}e_0) = \frac{1}{4} \| se_0 + s^{-1}e_0 \|^2 - \frac{1}{4} \| se_0 - s^{-1}e_0 \|^2$$

(39)

where $s \in \mathbb{R}$ is an arbitrary scaling factor and $\| \cdot \|$ denotes the energy norm,

$$\|v\|^2 = (v, v) = B(v, v).$$

(40)

But

$$B(se_0 \pm s^{-1}e_0, v) = sR(u_0; v) \pm s^{-1}R(p_0; v), \quad \forall \ v \in V,$$

(41)

so that

$$\|se_0 \pm s^{-1}e_0\| \leq \eta_{\text{upp}}^\pm,$$

(42)

where $\eta_{\text{upp}}^\pm$ is the computable bound (assuming $u_0$ and $p_0$ are known):

$$\eta_{\text{upp}}^\pm = \left\{ \int \Omega \nabla (su_0 \pm s^{-1}p_0) : E I_0 \nabla (su_0 \pm s^{-1}p_0) \, dx \right\}^{1/2}$$

(43)

Likewise, a lower bound on $se_0 \pm s^{-1}e_0$ is obtained by noting that

$$\|se_0 \pm s^{-1}e_0\| \geq \sup_{v \in V \setminus \{0\}} \frac{|sR(u_0; v) \pm s^{-1}R(p_0; v)|}{\|v\|} \geq \frac{|sR(u_0; v_0) \pm s^{-1}R(p_0; v_0)|}{\|v_0\|}$$

for any $v_0 \in V \setminus \{0\}$. Selecting $v_0 = u_0 + \theta^\pm p_0$, where $\theta^\pm$ is chosen to provide an optimal lower bound, we get

$$\|se_0 \pm s^{-1}e_0\| \geq \eta_{\text{low}}^\pm$$

(44)

$$\eta_{\text{low}}^\pm = \frac{|sR(u_0; u_0 + \theta^\pm p_0) \pm s^{-1}R(p_0; u_0 + \theta^\pm p_0)|}{\|u_0 + \theta^\pm p_0\|}$$

(45)

$$\theta^\pm = \frac{((u_0, p_0))R(u_0; su_0 \pm s^{-1}p_0) - \|u_0\|^2R(p_0; su_0 \pm s^{-1}p_0)}{((u_0, p_0))R(p_0; su_0 \pm s^{-1}p_0) - \|p_0\|^2R(u_0; su_0 \pm s^{-1}p_0)}$$

(46)

Thus, introducing (39) into (38) and making use of inequalities (42) and (44), we have the upper and lower bounds,

$$\eta_{\text{low}} \leq Q(u) - Q(u_0) \leq \eta_{\text{upp}}$$

(47)

where

$$\eta_{\text{low}} = R(u_0; p_0) + \frac{1}{4}(\eta_{\text{upp}}^+) - \frac{1}{4}(\eta_{\text{upp}}^-)^2$$

(48)

$$\eta_{\text{upp}} = R(u_0; p_0) + \frac{1}{4}(\eta_{\text{upp}}^+) - \frac{1}{4}(\eta_{\text{low}}^-)^2$$

(49)
For the parameter $s$, we take:

$$s = \sqrt{\frac{\|I_0 \nabla p_0\|}{\|I_0 \nabla u_0\|}} \approx \sqrt{\frac{\|\epsilon_0\|}{\|e_0\|}}$$

(50)

The bounds (47) were derived by Oden and Vemaganti in [6] and used in [10] to develop an adaptive modeling strategy for controlling modeling error in heterogeneous elastic bodies due to the use of averaged coefficients.

### 6 INCOMPRESSIBLE FLUID FLOWS

In the second example, we consider the simulation of incompressible Newtonian fluid flows at low Reynolds numbers. We assume that such flows can be accurately predicted using the steady-state Navier-Stokes equations. A coarse model is provided by the linear Stokes equations. Our main motivation in this example is to illustrate some aspects of the theory rather than introducing a new approach to predict quantities of interest of the solutions of the Navier-Stokes equations. These equations at low Reynolds numbers are generally simple enough to be directly solved using the Newton-Raphson method.

#### 6.1 Preliminaries

Let $\Omega$ denote an open bounded domain in $\mathbb{R}^d$, $d = 2$ or $3$ with boundary $\partial \Omega$. The flow of an incompressible Newtonian fluid in modeled by:

$$-\nu \Delta u + \nabla p + (u \cdot \nabla) u = f, \quad \text{in } \Omega$$

$$\nabla \cdot u = 0, \quad \text{in } \Omega$$

$$u = 0, \quad \text{on } \partial \Omega$$

where the velocity $u$ and pressure $p$ are respectively a vector and scalar field, and $f$ a body force per unit volume. Moreover, $\nu$ represents the kinematic viscosity and the density is assumed to be equal to unity. We emphasize here that $p$ denotes the hydrostatic pressure (and not the influence function introduced earlier). Thus, the fine model problem is:

$$\text{Find } (u, p) \in V \times Q \text{ such that}$$

$$B((u, p), (v, q)) = F(v), \quad \forall (v, q) \in V \times Q$$

(51)

where

$$V = \{ v \in (H^1(\Omega))^d; \ v = 0 \text{ on } \partial \Omega \},$$

$$Q = \{ q \in L^2(\Omega); \ \int_{\Omega} q \, dx = 0 \},$$

$$B((u, p), (v, q)) = a(u, v) + b(u, q) + b(v, p) + c(u, u, v),$$

$$F(v) = \int_{\Omega} f \cdot v \, dx,$$
and

\[ a(u, v) = \int_{\Omega} \nu \nabla u : \nabla v \, dx, \]
\[ b(v, q) = \int_{\Omega} q \nabla \cdot v \, dx, \]
\[ c(u, v, w) = \int_{\Omega} (u \cdot \nabla)v \cdot w \, dx. \]

The Stokes equations are derived from the Navier-Stokes equations by neglecting the convective term, i.e. the solution of the coarse model satisfies:

\[-\nu \Delta u_0 + \nabla p_0 = f, \quad \text{in } \Omega \]
\[ \nabla \cdot u_0 = 0, \quad \text{in } \Omega \]
\[ u_0 = 0, \quad \text{on } \partial \Omega \]

and the corresponding weak form of the problem is given by:

\[
\begin{align*}
\text{Find } (u_0, p_0) & \in V \times Q \text{ such that } \\
B_0((u_0, p_0), (v, q)) & = F(v), \quad \forall (v, q) \in V \times Q
\end{align*}
\]

(52)

where the bilinear form \( B_0(\cdot, \cdot) \) reads:

\[
B_0((u_0, p_0), (v, q)) = a(u_0, v) + b(u_0, q) + b(v, p_0).
\]

We denote by \((e_0^u, e_0^p)\) the error in the solution \((u_0, p_0)\) of the coarse model.

In the following, we suppose that we are interested in the kinetic energy of the flow in the whole domain; that is, since the density is unity, the quantity of interest is half the square of the \(L^2\) norm of the velocity:

\[
Q(u, p) = \frac{1}{2} \int_{\Omega} u \cdot u \, dx
\]

(53)

Thus, \(Q(\cdot)\) is a functional of the velocity only and since it is nonlinear, we compute its derivatives up to the third order; i.e.

\[
Q'(u_0, p_0; (e_0^u, e_0^p)) = \int_{\Omega} u_0 \cdot e_0^u \, dx,
\]
\[
Q''(u_0, p_0; (e_0^u, e_0^p), (e_0^u, e_0^p)) = \int_{\Omega} e_0^u \cdot e_0^p \, dx,
\]
\[
Q'''(u_0, p_0; (e_0^u, e_0^p), (e_0^u, e_0^p), (e_0^u, e_0^p)) = 0
\]
and, for the form $B(\cdot, \cdot)$, the derivatives, with respect to the first variable, are

$$
B'(\langle u_0, p_0 \rangle; (e_0^u, e_0^p), (v, q)) = a(e_0^u, v) + b(v, e_0^p) + b(e_0^u, q) + c(u_0, e_0^u, v) + c(e_0, u_0^u, v),
$$

$$
B''((u_0, p_0); (e_0^u, e_0^p), (e_0^u, e_0^p), (v, q)) = 2c(e_0^u, e_0^u, v),
$$

$$
B'''((u_0, p_0); (e_0^u, e_0^p), (e_0^u, e_0^p), (e_0^u, e_0^p), (v, q)) = 0.
$$

We denote by $(\omega, \mu)$ and $(\omega_0, \mu_0)$ the influence functions with respect to the quantity of interest $Q$ associated with the fine and coarse model, respectively. These are the solutions of the adjoint problems:

Find $(\omega, \mu) \in V \times Q$ such that

$$
B'(\langle u, p \rangle; (v, q), (\omega, \mu)) = Q'(\langle u, p \rangle; (v, q)), \quad \forall (v, q) \in V \times Q \tag{54}
$$

and

Find $(\omega_0, \mu_0) \in V \times Q$ such that

$$
B_0((v, q), (\omega_0, \mu_0)) = Q'(\langle u_0, p_0 \rangle; (v, q)), \quad \forall (v, q) \in V \times Q \tag{55}
$$

In explicit form, these problems consist in finding $(\omega, \mu)$ and $(\omega_0, \mu_0)$ in $V \times Q$ such that, for all $(v, q) \in V \times Q$,

$$
a(v, \omega) + b(v, \mu) + b(\omega, q) + c(v, v, \omega) + c(v, u, \omega) = \int_\Omega u \cdot v \, dx,
$$

$$
a(v, \omega_0) + b(v, \mu_0) + b(\omega_0, q) = \int_\Omega u_0 \cdot v \, dx.
$$

We note that, since $B_0(\cdot, \cdot)$ is a bilinear form, the right-hand side of the above equation does not depend on $u_0$. We are now in a position to derive estimates for the modeling error.

### 6.2 Estimates of the modeling error

We denote by $(e_0^u, e_0^p)$ and $(\epsilon_0^u, \epsilon_0^p)$ the error in $(u_0, p_0)$ and $(\omega_0, \mu_0)$ respectively. From the definition of the residual $R((u_0, p_0); \cdot)$ of (12), we obtain:

$$
R((u_0, p_0); (\epsilon_0^u, \epsilon_0^p)) = F(\epsilon_0^u) - B((u_0, p_0); (\epsilon_0^u, \epsilon_0^p)) = B_0((u_0, p_0); (\epsilon_0^u, \epsilon_0^p)) - B((u_0, p_0); (\epsilon_0^u, \epsilon_0^p)) = -c(u_0, u_0, \epsilon_0^u) \tag{56}
$$

$$
R((u_0, p_0); (\omega_0, \mu_0)) = F(\omega_0) - B((u_0, p_0); (\omega_0, \mu_0)) = -c(u_0, u_0, \omega_0) \tag{57}
$$
Meanwhile, the remainders are found to be:

\[ r((e^n_0, e^n_0), (\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)) = \frac{1}{2} \int_0^1 -6c(e^n_0, e^n_0, \varepsilon^{\omega}_0) (s - 1) s \, dx = \frac{1}{2} c(e^n_0, e^n_0, \varepsilon^{\omega}_0), \]

and

\[ \Delta \mathcal{R} = \int_0^1 c(e^n_0, e^n_0, \omega_0 + s \varepsilon^{\omega}_0) \, ds - \int_\Omega e^n_0 \cdot \nu_0 \, dx. \]

It immediately follows that an estimate of the modeling error, in terms of the unknown error \( \varepsilon^{\omega}_0 \), is given by:

\[ Q(u, p) - Q(u_0, p_0) \approx -c(u_0, u_0, \omega_0) - c(u_0, u_0, \varepsilon^{\omega}_0). \quad (58) \]

The problem governing the error \( \varepsilon^{\omega}_0 \) in the influence function, following (24) of Remark 2, reads:

\[ B'((u_0, p_0); (v, q), (\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)) = \mathcal{R}((u_0, p_0); (v, q)), \quad \forall (v, q) \in V \times Q, \]

that is:

\[ a(v, \varepsilon^{\omega}_0) + b(v, \varepsilon^{\omega}_0) + b(\varepsilon^{\omega}_0, q) + c(u_0, v, \varepsilon^{\omega}_0) + c(v, u_0, \varepsilon^{\omega}_0) = \mathcal{R}((u_0, p_0); (v, q)). \]

Replacing \((v, q)\) by \((\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)\) in the above equation and observing that \( \nabla \cdot u_0 = 0 \) and \( \nabla \cdot \varepsilon^{\omega}_0 = 0 \), we obtain:

\[ a(\varepsilon^{\omega}_0, \varepsilon^{\omega}_0) + c(u_0, \varepsilon^{\omega}_0) = \mathcal{R}((u_0, p_0); (\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)). \quad (59) \]

Then, assuming that the term \( c(u_0, \varepsilon^{\omega}_0) \) is negligible with respect to \( a(\varepsilon^{\omega}_0, \varepsilon^{\omega}_0) \), we obtain

\[ \| \varepsilon^{\omega}_0 \| \leq \| \mathcal{R} \| \quad (60) \]

where

\[ \| \varepsilon^{\omega}_0 \| = \sqrt{a(\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)}, \quad \text{and} \quad \| \mathcal{R} \| = \sup_{v \in V \setminus \{0\}} \frac{\mathcal{R}((u_0, p_0); v)}{\| v \|}. \]

It follows that

\[ -c(u_0, u_0, \varepsilon^{\omega}_0) = \mathcal{R}((u_0, p_0); (\varepsilon^{\omega}_0, \varepsilon^{\omega}_0)) \leq \| \mathcal{R} \| \| \varepsilon^{\omega}_0 \| \leq \| \mathcal{R} \| \| \mathcal{R} \| \quad (61) \]

and thus

\[ -\| \mathcal{R} \| \| \mathcal{R} \| \leq -c(u_0, u_0, \varepsilon^{\omega}_0) \leq \| \mathcal{R} \| \| \mathcal{R} \|. \quad (62) \]

Finally, the error \( Q(u, p) - Q(u_0, p_0) \) is bounded above and below such as:

\[ \eta_{low} \leq Q(u) - Q(u_0) \leq \eta_{upp} \quad (63) \]

where

\[ \eta_{low} = -c(u_0, u_0, \omega_0) - \| \mathcal{R} \| \| \mathcal{R} \| \quad (64) \]

\[ \eta_{upp} = -c(u_0, u_0, \omega_0) + \| \mathcal{R} \| \| \mathcal{R} \| \quad (65) \]

in which the norms of the residuals can be replaced by computable estimates.
7 NONLINEAR VISCOELASTICITY

7.1 Notation and Preliminaries

The finite deformation of a nonlinear viscoelastic body under the action of time dependent loads is characterized by the following variational problem:

Find $u \in V$ such that

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

where now,

$$V = H^m(0, T; W)$$

$$B(u, v) = \int_0^T \int_{\Omega_0} \nabla v(t) : P(\nabla u^t(s)) F^T(u(t)) \, dX \, dt$$

$$+ \int_0^T \int_{\Omega_0} \rho_0 \dot{v}(t) \cdot u(t) \, dX \, dt + \int_{\Omega_0} \rho_0 (v(T) \cdot \dot{u}(T) - \dot{v}(T) \cdot u(T)) \, dX$$

$$F(v) = \int_0^T \left( \int_{\Omega_0} \rho_0 f_0(t) \cdot v(t) \, dX + \int_{\Gamma_0^f} g(t) \cdot v(t) \, dS \right) \, dt$$

$$+ \int_{\Omega_0} \rho_0 (v(0) \cdot V_0 - \dot{v}(0) \cdot U_0) \, dX$$

Here the displacement field $u = u(X, t)$ of a particle with material coordinates $X$ at time $t$ is sought in the Banach space $V$ of functions with time derivatives in $H^m(0, T), m \geq 2$, and values $u(\cdot, t)$ in a space of functions $W$ defined over the reference configuration characterized by the closure of an open bounded domain $\Omega_0 \subset \mathbb{R}^d$, $d = 1, 2, 3$; e.g. $W = (W^{1,p}(\Omega_0))^d, p \geq 2$; (the norm on $V$, is, in general, $\|u\|_V = \left\{ \int_0^T \|u(t)\|^2_W \, dt \right\}^{1/2}$).

In (67), $P(\cdot)$ is the constitutive functional for the second Piola-Kirchhoff stress tensor,

$$\nabla u^t(s) = \text{the history of the displacement gradient at time } t$$

$$= \{ \nabla u(\cdot, t - s) : u(\cdot, t - s) \in W; t \geq s \geq 0 \}$$

with $\nabla$ the gradient with respect to the material coordinates, and $F(u(t))$ is the deformation gradient,

$$F(u(t)) = I + \nabla u(t),$$

$I$ being the identity tensor, with $F^T$ the transpose of $F$.

We denote, for simplicity, $v(t) = v(X, t)$, test functions in $V$ at particle $X$ at time $t$; $\rho_0 = \rho_0(X)$ is the mass density referred to the (initial) reference configuration, $f_0(t)$ is
the body force density, and \( g(t) \) is the surface traction at time \( t \) referred to a portion \( \Gamma_N^t \) of the boundary \( \partial \Omega_0 \) at time \( t \). In (68), \( \dot{V}_0 = V_0(X) \) and \( \dot{U}_0 = U_0(X) \) are the initial velocity and displacement fields, respectively, experienced by the body at time \( t = 0 \). We use the notation \( \dot{\mathbf{v}}(t) = \partial \mathbf{v}(t)/\partial t \). We assume that the data are such that problem (66) is meaningful and well-posed in \( V \) with a unique (fine) solution \( \mathbf{u} \).

As an example of a quantity of interest in applications of the model (66), consider a material surface \( \omega \) that occupies a place \( \omega_0 \) in the reference configuration with orientation defined by a unit normal \( \mathbf{n}_0 \). The motion \( \chi = \mathbf{u} + X \) carries \( \Omega_0 \) into \( \Omega(t) = \chi(\Omega_0) \) and \( \omega_0 \) into a surface \( \omega(t) \) with normal \( \mathbf{n} \) in the current configuration of the body. The net normal force acting on the deformed area is \( \int_{\omega(t)} \mathbf{n} \cdot \mathbf{T} \, dS \), where \( \mathbf{T} \) is the Cauchy stress tensor.

A measure of the nominal force per unit undeformed area normal to \( \omega(t) \) is then

\[
Q(\mathbf{u}) = \frac{1}{|\omega_0|} \int_0^T \int_{\Omega_0} m(\mathbf{u}(t)) \cdot \mathbf{n}_0 \mathcal{P}(\nabla \mathbf{u}^t(s)) \mathbf{F}^T(\mathbf{u}(t)) \, dS_0 \, dt, \tag{70}
\]

where \( m \) is the unit vector, \( m = \mathbf{F}^{-T}\mathbf{n}_0 / \| \mathbf{F}^{-T}\mathbf{n}_0 \| \).

To simplify the presentation, we shall confine ourselves to the quasistatic case, so that the inertial terms, indicated in (67) and (68), are dropped. In addition, and only for simplicity in presentation, we assume that the body is stress free at \( t = 0 \) and the history \( \nabla \mathbf{u}(s) \) evolves from null gradients, \( \nabla \mathbf{u}(0) = 0 \) at \( t = 0 \). A coarse model of the phenomena of interest is then characterized by a semilinear form \( B(\mathbf{u}, \mathbf{v}, \mathbf{w}) \) obtained by replacing \( \mathcal{P}(\cdot) \) in (67) by a simplified constitutive functional, \( \mathcal{P}(\cdot) \) of the histories \( \nabla \mathbf{u}^t(s) \).

A straightforward calculation reveals that

\[
B'(\mathbf{u}; \mathbf{v}, \mathbf{w}) = \int_0^T \int_{\Omega_0} \nabla \mathbf{w}(t) : \mathcal{P}(\nabla \mathbf{u}^t(s)) \nabla \mathbf{v}(t) \, dX \, dt
+ \int_0^T \int_{\Omega_0} \nabla \mathbf{v}(t) : \partial \mathcal{P}(\nabla \mathbf{u}^t(s); \nabla \mathbf{v}^t(s)) \mathbf{F}^T(\mathbf{u}(t)) \, dX \, dt, \tag{71}
\]

where

\[
\partial \mathcal{P}(\nabla \mathbf{u}^t(s); \nabla \mathbf{v}^t(s)) = \lim_{\theta \to 0} 2^{-1} \left[ \mathcal{P}(\nabla \mathbf{u}^t(s) + \theta \nabla \mathbf{v}^t(s)) - \mathcal{P}(\nabla \mathbf{u}^t(s)) \right]. \tag{72}
\]

Likewise, for the functional in (70),

\[
Q'(\mathbf{u}; \mathbf{v}) = \frac{1}{|\omega_0|} \int_0^T \int_{\Omega_0} \frac{\partial m(\mathbf{u}(t))}{\partial \mathbf{u}} \cdot \mathbf{v}(t) \cdot \mathbf{n}_0 \mathcal{P}(\nabla \mathbf{u}^t(s)) \mathbf{F}^T(\mathbf{u}(t))
+ m(\mathbf{u}(t)) \cdot \mathbf{n}_0 \partial \mathcal{P}(\nabla \mathbf{u}^t(s); \nabla \mathbf{v}(t)^T) \mathbf{F}^T(\mathbf{u}(t))
+ m(\mathbf{u}(t)) \cdot \mathbf{n}_0 \mathcal{P}(\nabla \mathbf{u}^t(s)) \nabla \mathbf{v}(t)^T \, dS_0 \, dt. \tag{73}
\]

### 7.2 Modeling Error Analysis

In the present example, we note that:

\[
\mathcal{R}(\mathbf{u}_0; \mathbf{v}) = - \int_0^T \int_{\Omega_0} \nabla \mathbf{v}(t) : \Delta \mathcal{P}(\nabla \mathbf{u}^t_0(s)) \mathbf{F}^T(\mathbf{u}_0(t)) \, dX \, dt, \tag{74}
\]
where $\Delta \mathcal{P}$ is the stress error

$$
\Delta \mathcal{P}(\nabla u^f_0(s)) = \mathcal{P}(\nabla u^f_0(s)) - \mathcal{P}_0(\nabla u^f_0(s)),
$$

(75)

and $(u_0, p_0)$ are solutions of the equations (10) with $R_0(\cdot; \cdot; \cdot)$, $B'_0(\cdot; \cdot; \cdot)$ and $Q'(\cdot; \cdot)$ defined now by (67), (71) and (73) with the inertia terms dropped and $\mathcal{P}()$ replaced by $\mathcal{R}(\cdot)$. We have:

$$
\mathcal{R}(u_0, p_0; v) = B'_0(u_0; v, p_0) - B'(u_0; v, p_0)
= - \int_0^T \int_{\Omega_0} \nabla p_0 : \Delta \mathcal{P}(\nabla u^f_0(s)) \nabla v(t)^T dX dt
- \int_0^T \int_{\Omega_0} \nabla p_0 : \Delta \partial \mathcal{P}(\nabla u^f_0(s); \nabla v^f(t)) F'(u_0(t)) dX dt,
$$

(76)

where

$$
\Delta \partial \mathcal{P}(\nabla u^f_0(s); \nabla v^f(t)) = \partial \mathcal{P}(\nabla u^f_0(s); \nabla v^f(t)) - \partial \mathcal{P}_0(\nabla u^f_0(s); \nabla v^f(t)).
$$

(77)

Since $B'(u_0; v, \varepsilon_0) = \mathcal{R}(u_0, p_0; v)$, for all $v \in V$, we have:

$$
\int_0^T \int_{\Omega_0} \nabla \varepsilon_0(t) : \partial \mathcal{P}(\nabla u^f_0(s); \nabla v^f(t)) F'(u_0(t)) dX dt = \mathcal{R}(u_0, p_0; v)
$$

(78)

with $\mathcal{R}(u_0, p_0; v)$ as given in (76).

Equation (78) is a linear integro-differential equation for the error $\varepsilon_0$ in the influence function $p_0$. We shall assume that it is solvable using standard finite element methods, so that a good approximate solution $\varepsilon_0^h$ can be obtained. There we write

$$
\varepsilon_0^h(t) = \varepsilon_0^h(\nabla u^f_0(s)) \approx \varepsilon_0(t).
$$

(79)

With this result, we use (74) in (21), neglecting $\Delta \mathcal{R}$ and $r(\varepsilon_0, \varepsilon_0)$, to obtain the estimate:

$$
Q(u) - Q(u_0) \approx - \int_0^T \int_{\Omega_0} \nabla p_0(t) : \Delta \mathcal{P}(\nabla u^f_0(s)) F'(u_0(t)) dX dt
- \int_0^T \int_{\Omega_0} \nabla \varepsilon^h(\nabla u^f_0(s)) : \Delta \mathcal{P}(\nabla u^f_0(s)) F'(u_0(t)) dX dt.
$$

(80)

We hope to implement this theory in concrete applications in forthcoming work.

8 CONCLUDING COMMENTS

We have developed a general framework for the estimation of errors due to replacing a fine and possibly intractable model of physical phenomena with a coarse model that can yield
solutions by available computational methods, and we have provided several examples of applications to relevant problems in solid and fluid mechanics. These methods provide estimates in errors in quantities of interest, characterized by functionals $Q$ defined on the spaces on which the fine and coarse models are set. Thus, our methods are constructed to estimate the error

$$\mathcal{E} = Q(u) - Q(u_0)$$

assuming that $u_0$ is known exactly.

Of course, in applications, only an approximation $u_0^h$ of $u_0$ is known, so that we actually should seek estimates of the error

$$\mathcal{E}^h = Q(u) - Q(u_0^h).$$

But

$$Q(u) - Q(u_0^h) = Q(u) - Q(u_0) + Q(u_0) - Q(u_0^h).$$

The determination of modeling error is a goal of validation; that of approximation error is a goal of verification. Techniques for estimating approximation error have been developed in, e.g. [2, 4, 8, 9]; a combination of the methods of modeling error estimation developed herein and the techniques in [2, 4, 8, 9] should have an impact on broad issues of verification and validation for many classes of problems in mechanics.

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