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Estimation of Modeling Error in Computational Mechanics

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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. The basic idea is that for a given collection of physical phenomena a rich class of mathematical models can be identified, including models that are sufficiently refined and validated that they satisfactorily capture the events of interest. These fine models may be intractable, too complex to solve by existing means. Coarser models are therefore used. Moreover, as is frequently the case in applications, there are specific quantities of interest that are sought which are functionals of the solution of the fine model. In this paper, techniques for estimating modeling errors in such quantities of interest are developed. Applications to solid and fluid mechanics are presented.

Key Words: 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 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 recent monographs [2, 3]. Hierarchical modeling and model error estimation and control are discussed in Refs. [10, 12, 13, 18].

Initially, model error estimation methods were confined to global estimates [14, 19]; recently, extensions of the theories related to approximation error have made possible the

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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, 7, 8, 11, 15, 16]. 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., [5, 9, 17]). A type of modeling error considered in recent literature has to do with dimensional reduction, e.g., the use of two-dimensional models as approximations to three-dimensional models, as in the theory of plates and shells embedded in three-dimensional elasticity. Error estimation and adaptive modeling in this sense were discussed by several authors, e.g., Cho and Oden [6]. In particular, Ainsworth [1] addressed the problem of global estimates of both modeling error and discretization error for such problems.

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, and 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 [5]. 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.

Following this brief introduction, we recall in Section 2 some well-known results about differentiation and linearization of functionals. In Section 3, we present the general theory for residual error estimation with respect to quantities of interests. We briefly discuss in Section 4 how to derive computable error estimators and note that it is problem dependent. Finally, we apply the general theory to three problems, namely heterogeneous elastic materials in Section 5, incompressible fluid flows in Section 6, and nonlinear viscoelasticity in Section 7. This is followed by concluding remarks in Section 8.

2. PRELIMINARIES: DIFFERENTIATION AND LINEARIZATION OF FUNCTIONALS

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

$$B : V \times V \to \mathbb{R},$$
$$Q : V \to \mathbb{R}.$$

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

$$\begin{aligned}
B'(u;p,v) &= \lim_{\theta\to 0} \theta^{-1}[B(u+\theta p;v) - B(u;v)],\\
B''(u;p,q,v) &= \lim_{\theta\to 0} \theta^{-1}[B'(u+\theta q;p,v) - B'(u;p,v)],\\
B'''(u;p,q,r,v) &= \lim_{\theta\to 0} \theta^{-1}[B''(u+\theta r;p,q,v) - B''(u;p,q,v)],\ldots,
\end{aligned}$$

exist. Thus, for fixed u, $B'(u;\cdot,\cdot)$, $B''(u;\cdot,\cdot,\cdot)$, 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:

$$\begin{aligned}
Q'(u;p) &= \lim_{\theta\to 0} \theta^{-1}[Q(u+\theta p) - Q(u)],\\
Q''(u;p,q) &= \lim_{\theta\to 0} \theta^{-1}[Q'(u+\theta q;p) - Q'(u;p)],\\
Q'''(u;p,q,r) &= \lim_{\theta\to 0} \theta^{-1}[Q''(u+\theta r;p,q) - Q'(u;p,q)],\ldots.
\end{aligned}$$

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:

$$\left.\begin{aligned}
Q(u+v) - Q(u) &= \textstyle\int_0^1 Q'(u+sv;v)\,\mathrm{d}s,\\
Q(u+v) - Q(u) &= Q'(u;v) + \textstyle\int_0^1 Q''(u+sv;v,v)(1-s)\,\mathrm{d}s,\\
Q(u+v) - Q(u) &= \tfrac{1}{2}Q'(u;v) + \tfrac{1}{2}Q'(u+v;v)\\
&\quad + \tfrac{1}{2}\textstyle\int_0^1 Q'''(u+sv;v,v,v)(s-1)s\,\mathrm{d}s.
\end{aligned}\right\} \tag{1}$$

We also have

$$\left.\begin{aligned}
B(u+v;w) - B(u;w) &= \textstyle\int_0^1 B'(u+sv;v,w)\,\mathrm{d}s,\\
B(u+v;w) - B(u;w) &= B'(u;v,w) + \textstyle\int_0^1 B''(u+sv;v,v,w)(1-s)\,\mathrm{d}s.
\end{aligned}\right\} \tag{2}$$

Many alternative forms of such expansions can be derived.

3. 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 [5]).

We present in this section a straightforward generalization of the DWR framework, valid for deriving error estimates of modeling error that, formally, reduces to the original DWR of [5] 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

$$\boxed{\begin{aligned}&\text{Find } u \in V \text{ such that}\\ &\qquad B(u; v) = F(v), \quad \forall\, v \in V,\end{aligned}} \tag{3}$$

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 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 Prudhomme and Oden [11, 16]. The general framework for nonlinear problems was advanced by Becker and Rannacher [5].

In [5], an "optimal control" approach to this problem is proposed based on the following constrained minimization problem:

$$\boxed{\begin{aligned}&\text{Find } u \in V \text{ such that}\\ &\qquad Q(u) = \inf_{v \in M} Q(v),\\ &\text{where}\\ &\quad M = \{v \in V;\ B(v; q) = F(q),\ \forall\, q \in V\}.\end{aligned}} \tag{4}$$

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

$$L(u, p) = Q(u) + F(p) - B(u; p), \tag{5}$$

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

$$L'((u, p); (v, q)) = 0, \quad \forall\, (v, q) \in V \times V. \tag{6}$$

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

$$L'((u, p); (v, q)) = Q'(u; v) - B'(u; v, p) + F(q) - B(u; q), \tag{7}$$

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

$$\boxed{\begin{aligned}&B(u; q) = F(q), && \forall\, q \in V,\\ &B'(u; v, p) = Q'(u; v), && \forall\, v \in V.\end{aligned}} \tag{8}$$

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

$$\boxed{\begin{aligned}&\text{Find } u_0 \in V_0 \text{ such that}\\ &\qquad Q(u_0) = \inf_{v \in M_0} Q(v),\\ &\text{where}\\ &\quad M_0 = \{v \in V_0;\ B_0(v;q) = F(q),\ \forall\, q \in V_0\}.\end{aligned}} \tag{9}$$

Instead of (8), we now have

$$\boxed{\begin{aligned} B_0(u_0;q) &= F(q), && \forall\, q \in V_0,\\ B_0'(u_0;v,\,p_0) &= Q'(u_0;v), && \forall\, v \in V_0.\end{aligned}} \tag{10}$$

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 $(u_0,\,p_0)$ a "coarse" (or simplified) solution to the problem.

Assuming that solutions $(u,\,p)$ and $(u_0,\,p_0)$ exist for (8) and (10), respectively, we define the primal and adjoint errors (e_0, ε_0) as

$$e_0 = u - u_0 \quad \text{and} \quad \varepsilon_0 = p - p_0. \tag{11}$$

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

$$\boxed{\begin{aligned} \mathcal{R}(u_0;q) &= F(q) - B(u_0;q), && q \in V,\\ \overline{\mathcal{R}}(u_0,\,p_0;v) &= Q'(u_0;v) - B'(u_0;v,\,p_0), && v \in V.\end{aligned}} \tag{12}$$

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*

$$Q(u) - Q(u_0) = \mathcal{R}(u_0;\,p_0) + \frac{1}{2}(\mathcal{R}(u_0;\varepsilon_0) + \overline{\mathcal{R}}(u_0,\,p_0;e_0)) + r(e_0,\,\varepsilon_0), \tag{13}$$

where

$$\begin{aligned} r(e_0,\varepsilon_0) = \frac{1}{2}\int_0^1 \{&Q'''(u_0 + se_0;e_0,e_0,e_0) - 3B''(u_0 + se_0;e_0,e_0,\varepsilon_0)\\ &- B'''(u_0 + se_0;e_0,e_0,e_0,\,p_0 + s\varepsilon_0)\}(s-1)s\,\mathrm{d}s.\end{aligned} \tag{14}$$

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

$$Q(u) = L(u, p) - (F(p) - B(u; p)) = L(u, p),$$
$$Q(u_0) = L(u_0, p_0) - (F(p_0) - B(u_0; p_0)) = L(u_0, p_0) - \mathcal{R}(u_0; p_0).$$

Therefore,

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p_0) + L(u, p) - L(u_0, p_0). \tag{15}$$

By virtue of the last expansion in (1), with Q as L, u as (u_0, p_0), and v as (e_0, ε_0), we have

$$L(u, p) - L(u_0, p_0) = \frac{1}{2}L'((u_0, p_0); (e_0, \varepsilon_0)) + \frac{1}{2}L'((u, p); (e_0, \varepsilon_0)) + \frac{1}{2}\int_0^1 L'''((u_0, p_0) + s(e_0, \varepsilon_0); (e_0, \varepsilon_0), (e_0, \varepsilon_0), (e_0, \varepsilon_0))(s - 1)s \, \mathrm{d}s.$$

Since (u, p) is a stationary point of L, it follows that $L'((u, p); (e_0, \varepsilon_0)) = 0$. On the other hand, using the expression of L' given in (7), we have, for any $(v, q) \in V \times V$,

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

It is not difficult, but tedious, to show that

$$\begin{aligned} &L'''((u_0, p_0) + s(e_0, \varepsilon_0); (e_0, \varepsilon_0), (e_0, \varepsilon_0), (e_0, \varepsilon_0)) \\ &\quad = Q'''(u_0 + se_0; e_0, e_0, e_0) - 3B''(u_0 + se_0; e_0, e_0, \varepsilon_0) \\ &\qquad - B'''(u_0 + se_0; e_0, e_0, e_0, p_0 + s\varepsilon_0). \end{aligned}$$

Hence

$$L(u, p) - L(u_0, p_0) = \frac{1}{2}\mathcal{R}(u_0; \varepsilon_0) + \frac{1}{2}\overline{\mathcal{R}}(u_0, p_0; e_0) + r(e_0, \varepsilon_0),$$

where $r(e_0, \varepsilon_0)$ is given by (14). Substituting this last equality into (15) gives the stated result.

The residuals $\mathcal{R}(u_0; \varepsilon_0)$ and $\overline{\mathcal{R}}(u_0, p_0; e_0)$ can be related, as shown in the following lemma.

LEMMA 1. *Given any approximation* (u_0, p_0) *of the solution* (u, p) *of system* (8), *the equality*

$$\overline{\mathcal{R}}(u_0, p_0; e_0) = \mathcal{R}(u_0; \varepsilon_0) + \Delta\mathcal{R} \tag{16}$$

holds where

$$\Delta\mathcal{R} = \int_0^1 B''(u_0 + se_0; e_0, e_0, p_0 + s\varepsilon_0) \, \mathrm{d}s - \int_0^1 Q''(u_0 + se_0; e_0, e_0) \, \mathrm{d}s. \tag{17}$$

Proof. Since u is the solution of $(8)^1$, we can replace $F(q)$ with $B(u;q)$ in the definition of the residual of the primal equation $(12)^1$. Hence,

$$\mathcal{R}(u_0;q) = B(u;q) - B(u_0;q), \quad \forall\, q \in V, \tag{18}$$

and using one of the Taylor expansions, we get

$$\mathcal{R}(u_0;q) = B'(u_0;e_0,q) + \int_0^1 B''(u_0+se_0;e_0,e_0,q)(1-s)\,\mathrm{d}s. \tag{19}$$

Likewise, the residual associated with the dual equation can be written as

$$\begin{aligned}
\overline{\mathcal{R}}(u_0,\,p_0;v) &= Q'(u_0;v) - B'(u_0;v,\,p_0)\\
&= Q'(u_0;v) - Q'(u;v) + Q'(u;v) - B'(u_0;v,\,p_0)\\
&= Q'(u_0;v) - Q'(u;v) + B'(u;v,\,p) - B'(u_0;v,\,p_0)\\
&= -[Q'(u;v) - Q'(u_0;v)] + [B'(u;v,\,p) - B'(u_0;v,\,p)] + B'(u_0;v,\varepsilon_0).
\end{aligned}$$

Using the following Taylor expansions

$$Q'(u;v) - Q'(u_0;v) = \int_0^1 Q''(u_0+s\varepsilon_0;\varepsilon_0,v)\,\mathrm{d}s,$$

$$B'(u;v,\,p) - B'(u_0;v,\,p) = \int_0^1 B''(u_0+se_0;e_0,v,\,p)\,\mathrm{d}s,$$

we obtain

$$\begin{aligned}
\overline{\mathcal{R}}(u_0,\,p_0;v) = B'(u_0;v,\varepsilon_0) &- \int_0^1 Q''(u_0+s\varepsilon_0;\varepsilon_0,v)\,\mathrm{d}s\\
&+ \int_0^1 B''(u_0+se_0;e_0,v,\,p)\,\mathrm{d}s.
\end{aligned} \tag{20}$$

Taking $q = \varepsilon_0$ in (19) and $v = e_0$ in (20), we arrive at the relationship

$$\begin{aligned}
\overline{\mathcal{R}}(u_0,\,p_0;e_0) = \mathcal{R}(u_0;\varepsilon_0) &- \int_0^1 Q''(u_0+s\varepsilon_0;\varepsilon_0,e_0)\,\mathrm{d}s\\
&+ \int_0^1 B''(u_0+se_0;e_0,e_0,\,p-(1-s)\varepsilon_0)\,\mathrm{d}s,
\end{aligned}$$

and observing that $p-(1-s)\varepsilon_0 = p_0 + s\varepsilon_0$ gives the stated result.

A companion simplified representation of the error is embodied in the following theorem.

THEOREM 2. *With same notation as above*,

$$Q(u) - Q(u_0) = \mathcal{R}(u_0;p_0) + \mathcal{R}(u_0;\varepsilon_0) + \frac{1}{2}\Delta\mathcal{R} + r(e_0,\varepsilon_0). \tag{21}$$

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

By setting $V_0 = V^h \subset V$ and $B_0(\cdot;\cdot) = B(\cdot;\cdot)$, $\mathcal{R}(u_0;p_0) = \mathcal{R}(u_h;p_h) = 0$ and (13) reduces to Eq. (2.18) of [5]. Likewise, for these choices, (21) reduces to (2.22) of [5].

Remark 1. Since the residual $\mathcal{R}(u_0; \cdot)$ is a linear functional in the second argument, result (21) can be rewritten as

$$Q(u) - Q(u_0) = \mathcal{R}(u_0; p) + \frac{1}{2}\Delta\mathcal{R} + r(e_0, \varepsilon_0). \tag{22}$$

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 1, we unraveled the relationships between the errors e_0 and ε_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 obtain the governing equations for the modeling error e_0 and for the error ε_0 in the influence function; i.e.,

$$B'(u_0; e_0, q) = \mathcal{R}(u_0; q), \qquad \forall\, q \in V, \tag{23}$$

$$B'(u_0; v, \varepsilon_0) = \overline{\mathcal{R}}(u_0, p_0; v), \quad \forall\, v \in V. \tag{24}$$

The above equations are linear with respect to the errors. We note that their solutions are approximations of e_0 and ε_0 rather than the exact errors themselves.

Remark 3. We note that (u_0, p_0) in Theorems 1 and 2 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 2 provide us with exact representations of the error in the quantity of interest $Q(u) - Q(u_0)$. In this section, we discuss means 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 $r(e_0, \varepsilon_0)$ and $\Delta\mathcal{R}/2$ may be neglected if the errors e_0 and ε_0 are known to be small. It therefore follows that error estimates of $Q(u) - Q(u_0)$ can be introduced as

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p_0) + \frac{1}{2}(\mathcal{R}(u_0; \varepsilon_0) + \overline{\mathcal{R}}(u_0, p_0; e_0)), \tag{25}$$

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; \varepsilon_0). \tag{26}$$

Estimate (25) involves omitting remainders that are cubic in the errors e_0, ε_0, while (26) omits second-order terms in the error. One might, therefore, expect (25) to yield more accurate results than (26), but this may not be the case. 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 e_0 and ε_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 [13, 18].

5.1. Notation and Preliminaries

In the case of heterogeneous elastic materials, we have

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

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

$$B_0(\boldsymbol{u}_0, \boldsymbol{v}) = \int_\Omega \nabla \boldsymbol{v} : \boldsymbol{E}_0 \nabla \boldsymbol{u}_0\, dx, \tag{29}$$

$$F(\boldsymbol{v}) = \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}\, dx + \int_{\Gamma_N} \boldsymbol{g} \cdot \boldsymbol{v}\, ds, \tag{30}$$

$$Q(\boldsymbol{v}) = \frac{1}{|\omega|} \int_\omega \sigma_{11}(\boldsymbol{v})\, ds. \tag{31}$$

Here $\boldsymbol{V}$ is the space of admissible displacements of a linearly elastic body occupying a domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, with boundary $\partial\Omega = \overline{\Gamma_D \cup \Gamma_N}$, displacements prescribed on Γ_D, and tractions prescribed on Γ_N, with meas $\Gamma_D > 0$, and with the body being subject to body forces $\boldsymbol{b}$ and surface tractions $\boldsymbol{g}$ on Γ_N. For highly heterogenous materials, the elasticity tensor $\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{x}) \in (L^\infty(\Omega))^{d^2 \times d^2}$ 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. $\boldsymbol{x} \in \Omega$,

$$\alpha_0 \varepsilon_{ij} \varepsilon_{ij} \leq \varepsilon_{ij} E_{ijkl}(\boldsymbol{x}) \varepsilon_{kl} \leq \alpha_1 \varepsilon_{ij} \varepsilon_{ij},$$

$$E_{ijkl}(\boldsymbol{x}) = E_{jikl}(\boldsymbol{x}) = E_{ijlk}(\boldsymbol{x}) = E_{klij}(\boldsymbol{x}),$$

$$\text{a.e. } \boldsymbol{x} \in \Omega,\ 1 \leq i, j, k, l \leq d, \forall\, \varepsilon_{ij} = \varepsilon_{ji}$$

(repeated indices summed over their range). The tensor $\boldsymbol{E}_0$ is an approximation of $\boldsymbol{E}$ obtained through some homogenization process. Thus, the fine model problem is

$$\boxed{\begin{array}{l}\text{Find } \boldsymbol{u} \in \boldsymbol{V} \text{ such that} \\ \qquad B(\boldsymbol{u}, \boldsymbol{v}) = F(\boldsymbol{v}), \quad \forall\, \boldsymbol{v} \in \boldsymbol{V},\end{array}} \tag{32}$$

and the coarse model corresponds to the homogenized problem

$$\boxed{\begin{array}{l}\text{Find } \boldsymbol{u}_0 \in \boldsymbol{V} \text{ such that} \\ \qquad B_0(\boldsymbol{u}_0, \boldsymbol{v}) = F(\boldsymbol{v}), \quad \forall\, \boldsymbol{v} \in \boldsymbol{V}.\end{array}} \tag{33}$$

It follows that $\boldsymbol{e} = \boldsymbol{u} - \boldsymbol{u}_0$ 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 $\sigma_{11}(\boldsymbol{v}) = E_{11kl}(\boldsymbol{x})\partial v_k(\boldsymbol{x})/\partial x_l$ over an (internal) surface ω (such as an interface between dissimilar materials).

5.2. General Modeling Error Estimates

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

$$\begin{aligned}\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{\varepsilon}_0) &= F(\boldsymbol{\varepsilon}_0) - B(\boldsymbol{u}_0,\boldsymbol{\varepsilon}_0)\\ &= B(\boldsymbol{u},\boldsymbol{\varepsilon}_0) - B(\boldsymbol{u}_0,\boldsymbol{\varepsilon}_0)\\ &= B(\boldsymbol{e}_0,\boldsymbol{\varepsilon}_0),\end{aligned} \tag{34}$$

$$\begin{aligned}\overline{\mathcal{R}}(\boldsymbol{p}_0;\boldsymbol{e}_0) &= Q(\boldsymbol{e}_0) - B(\boldsymbol{e}_0,\boldsymbol{p}_0)\\ &= B(\boldsymbol{e}_0,\boldsymbol{p}) - B(\boldsymbol{e}_0,\boldsymbol{p}_0)\\ &= B(\boldsymbol{e}_0,\boldsymbol{\varepsilon}_0),\end{aligned} \tag{35}$$

$$\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{p}_0) = B(\boldsymbol{e}_0,\boldsymbol{p}_0) = -\int_\Omega \nabla\boldsymbol{p}_0 : \boldsymbol{E}\boldsymbol{I}_0\nabla\boldsymbol{u}_0\,\mathrm{d}x, \tag{36}$$

$$r(\boldsymbol{e}_0,\boldsymbol{\varepsilon}_0) = 0, \tag{37}$$

where $\boldsymbol{I}_0 = \boldsymbol{I} - \boldsymbol{E}^{-1}\boldsymbol{E}_0$, $\boldsymbol{e}_0 = \boldsymbol{u} - \boldsymbol{u}_0$, $\boldsymbol{\varepsilon}_0 = \boldsymbol{p} - \boldsymbol{p}_0$. Hence, the general estimate (13) reduces to

$$Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0) = \mathcal{R}(\boldsymbol{u}_0;\boldsymbol{p}_0) + B(\boldsymbol{e}_0,\boldsymbol{\varepsilon}_0). \tag{38}$$

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

$$B(\boldsymbol{e}_0,\boldsymbol{\varepsilon}_0) = B(s\boldsymbol{e}_0, s^{-1}\boldsymbol{\varepsilon}_0) = \frac{1}{4}\|s\boldsymbol{e}_0 + s^{-1}\boldsymbol{\varepsilon}_0\|^2 - \frac{1}{4}\|s\boldsymbol{e}_0 - s^{-1}\boldsymbol{\varepsilon}_0\|^2, \tag{39}$$

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

$$\|\boldsymbol{v}\|^2 = (\!(\boldsymbol{v},\boldsymbol{v})\!) = B(\boldsymbol{v},\boldsymbol{v}). \tag{40}$$

But

$$B(s\boldsymbol{e}_0 \pm s^{-1}\boldsymbol{\varepsilon}_0, \boldsymbol{v}) = s\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{v}) \pm s^{-1}\mathcal{R}(\boldsymbol{p}_0;\boldsymbol{v}), \quad \forall\,\boldsymbol{v} \in \boldsymbol{V}, \tag{41}$$

so that

$$\|s\boldsymbol{e}_0 \pm s^{-1}\boldsymbol{\varepsilon}_0\| \le \eta^{\pm}_{upp}, \tag{42}$$

where $\eta^{\pm}_{upp}$ is the computable bound (assuming $\boldsymbol{u}_0$ and $\boldsymbol{p}_0$ are known):

$$\eta^{\pm}_{upp} = \left\{\int_\Omega \boldsymbol{I}_0\nabla(s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0) : \boldsymbol{E}\boldsymbol{I}_0\nabla(s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0)\,\mathrm{d}x\right\}^{1/2}. \tag{43}$$

Likewise, a lower bound on $s\boldsymbol{e}_0 \pm s^{-1}\boldsymbol{\varepsilon}_0$ is obtained by noting that

$$\|s\boldsymbol{e}_0 \pm s^{-1}\boldsymbol{\varepsilon}_0\| = \sup_{\boldsymbol{v}\in \boldsymbol{V}\setminus\{0\}} \frac{|s\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{v}) \pm s^{-1}\mathcal{R}(\boldsymbol{p}_0;\boldsymbol{v})|}{\|\boldsymbol{v}\|}$$
$$\geq \frac{|s\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{v}_0) \pm s^{-1}\mathcal{R}(\boldsymbol{p}_0;\boldsymbol{v}_0)|}{\|\boldsymbol{v}_0\|}$$

for any $\boldsymbol{v}_0 \in \boldsymbol{V}\setminus\{0\}$. Selecting $\boldsymbol{v}_0 = \boldsymbol{u}_0 + \theta^{\pm}\boldsymbol{p}_0$, where $\theta^{\pm}$ is chosen to provide an optimal lower bound, we get

$$\|s\boldsymbol{e}_0 \pm s^{-1}\boldsymbol{\varepsilon}_0\| \geq \eta^{\pm}_{low}, \tag{44}$$

$$\eta^{\pm}_{low} = \frac{|s\mathcal{R}(\boldsymbol{u}_0;\boldsymbol{u}_0 + \theta^{\pm}\boldsymbol{p}_0) \pm s^{-1}\mathcal{R}(\boldsymbol{p}_0;\boldsymbol{u}_0 + \theta^{\pm}\boldsymbol{p}_0)|}{\|\boldsymbol{u}_0 + \theta^{\pm}\boldsymbol{p}_0\|}, \tag{45}$$

$$\theta^{\pm} = \frac{(\!(\boldsymbol{u}_0, \boldsymbol{p}_0)\!)\mathcal{R}(\boldsymbol{u}_0; s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0) - \|\boldsymbol{u}_0\|^2\mathcal{R}(\boldsymbol{p}_0; s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0)}{(\!(\boldsymbol{u}_0, \boldsymbol{p}_0)\!)\mathcal{R}(\boldsymbol{p}_0; s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0) - \|\boldsymbol{p}_0\|^2\mathcal{R}(\boldsymbol{u}_0; s\boldsymbol{u}_0 \pm s^{-1}\boldsymbol{p}_0)}. \tag{46}$$

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

$$\eta_{low} \leq Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0) \leq \eta_{upp}, \tag{47}$$

where

$$\eta_{low} = \mathcal{R}(\boldsymbol{u}_0;\boldsymbol{p}_0) + \frac{1}{4}(\eta^{+}_{low})^2 - \frac{1}{4}(\eta^{-}_{upp})^2, \tag{48}$$

$$\eta_{upp} = \mathcal{R}(\boldsymbol{u}_0;\boldsymbol{p}_0) + \frac{1}{4}(\eta^{+}_{upp})^2 - \frac{1}{4}(\eta^{-}_{low})^2. \tag{49}$$

For the parameter s, we take

$$s = \sqrt{\frac{\|\boldsymbol{I}_0\nabla\boldsymbol{p}_0\|}{\|\boldsymbol{I}_0\nabla\boldsymbol{u}_0\|}} \approx \sqrt{\frac{\|\boldsymbol{\varepsilon}_0\|}{\|\boldsymbol{e}_0\|}}. \tag{50}$$

The bounds (47) were derived by Oden and Vemaganti in [13] and used in [18] to develop an adaptive modeling strategy for controlling modeling error in heterogeneous elastic bodies due to the use of averaged coefficients. Numerical experiments with a large number of diverse examples in two and three dimensions suggest that these estimates are quite sharp, typically yielding effectivity indices near 1.0 or 1.1 in cases in which the fine solution is known with good precision (see [18]).

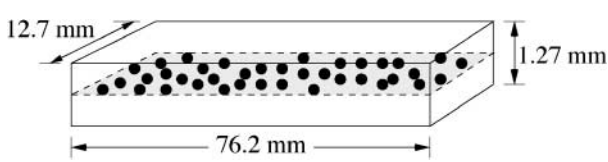

FIG. 1. Geometry and dimensions of the epoxy–glass specimen.

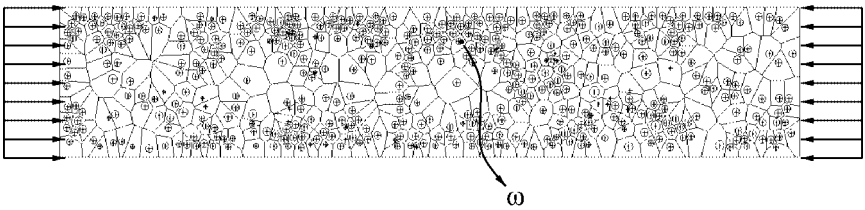

FIG. 2. Schematic for the 2D problem of a manufactured specimen under compressive loads.

5.4. Numerical Example

For illustrative purposes, we recall here some numerical experiments which were published in [18]. The study demonstrates the performance of adaptive material modeling and deals with the deformation of a fabricated composite material that has a single layer of glass beads distributed in an epoxy matrix. The geometry and dimensions of the specimen are shown in Fig. 1. The glass beads have an average diameter of 800 μm, a modulus of elasticity $E = 4.6$ GPa, and Poisson ratio $\nu = 0.36$. The parameters for the epoxy matrix are $E = 69$ GPa and $\nu = 0.22$.

We suppose in these experiments that we are interested in the σ_{11} component of the stress tensor averaged over the inclusion denoted by ω when the specimen is subjected to compressive loads, as shown in Fig. 2. The solutions $\boldsymbol{u}_0$ and $\boldsymbol{p}_0$ are then computed using a homogenized coarser problem. The adaptive modeling process suggested in Fig. 3 consists of the following steps.

1. A highly accurate solution $\boldsymbol{u}_0$ of the coarse (homogenized) solution is obtained using an adaptive finite element method.
2. An initial "domain of influence" is identified that includes the particular features of interest (in this case, the average stress component σ_{11} over an inclusion).
3. The homogenized (coarse) solution $\boldsymbol{u}_0$ is supplied as boundary conditions on the domain of influence, and the problem is resolved with the full microstructure supplied within this subdomain.
4. The error estimate is computed using (47) (or $Q(\boldsymbol{e}) \approx \frac{1}{2}(\eta_{low} + \eta_{upp})$). If the error tolerance is met, the process stops. If not, a larger domain is selected, with more microscale information, and the process is updated until the error tolerance is met. This is the goal-oriented adaptive algorithm described in [18].

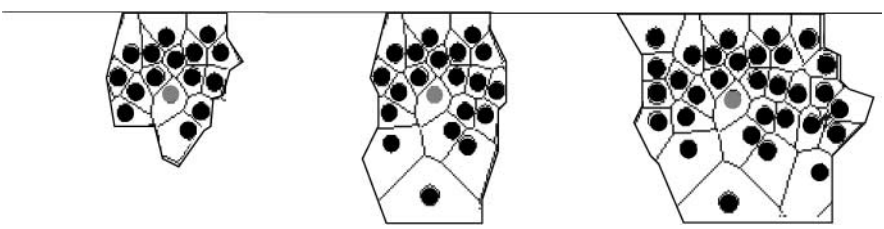

FIG. 3. Results of the adaptive modeling procedure: domains of influence and resulting modeling errors. By increasing the domain of influence, the modeling error is reduced from 17.0 to 9.05 and 2.1% (left to right).

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

$$\begin{aligned} -\nu\Delta\boldsymbol{u} + \nabla p + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} &= \boldsymbol{f}, \quad \text{in } \Omega, \\ \nabla\cdot\boldsymbol{u} &= 0, \quad \text{in } \Omega, \\ \boldsymbol{u} &= \boldsymbol{0}, \quad \text{on } \partial\Omega, \end{aligned}$$

where the velocity $\boldsymbol{u}$ and pressure p are, respectively, a vector and scalar field and $\boldsymbol{f}$ is a body force per unit volume. Moreover, ν 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

$$\boxed{\begin{aligned} &\text{Find } (\boldsymbol{u}, p) \in \boldsymbol{V}\times Q \text{ such that} \\ &\qquad B((\boldsymbol{u}, p), (\boldsymbol{v}, q)) = F(\boldsymbol{v}), \quad \forall\, (\boldsymbol{v}, q) \in \boldsymbol{V}\times Q, \end{aligned}} \tag{51}$$

where

$$\begin{aligned} \boldsymbol{V} &= \{\boldsymbol{v} \in (H^1(\Omega))^d;\ \boldsymbol{v} = \boldsymbol{0} \text{ on } \partial\Omega\}, \\ Q &= \left\{q \in L^2(\Omega);\ \int_\Omega q\,\mathrm{d}x = 0\right\}, \\ B((\boldsymbol{u}, p), (\boldsymbol{v}, q)) &= a(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{u}, q) + b(\boldsymbol{v}, p) + c(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{v}), \\ F(\boldsymbol{v}) &= \int_\Omega \boldsymbol{f}\cdot\boldsymbol{v}\,\mathrm{d}x, \end{aligned}$$

and

$$\begin{aligned} a(\boldsymbol{u}, \boldsymbol{v}) &= \int_\Omega \nu\nabla\boldsymbol{u} : \nabla\boldsymbol{v}\,\mathrm{d}x, \\ b(\boldsymbol{v}, q) &= \int_\Omega q\nabla\cdot\boldsymbol{v}\,\mathrm{d}x, \\ c(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) &= \int_\Omega (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{v}\cdot\boldsymbol{w}\,\mathrm{d}x. \end{aligned}$$

The Stokes equations are derived from the Navier–Stokes equations by neglecting the convective term; i.e., the solution $(\boldsymbol{u}_0,\, p_0)$ of the coarse model satisfies

$$\begin{aligned} -\nu\Delta\boldsymbol{u}_0 + \nabla p_0 &= \boldsymbol{f}, \quad \text{in } \Omega, \\ \nabla\cdot\boldsymbol{u}_0 &= 0, \quad \text{in } \Omega, \\ \boldsymbol{u}_0 &= \boldsymbol{0}, \quad \text{on } \partial\Omega, \end{aligned}$$

and the corresponding weak form of the problem is given by

$$\boxed{\begin{aligned} &\text{Find } (\boldsymbol{u}_0,\, p_0) \in \boldsymbol{V}\times Q \text{ such that} \\ &\qquad B_0((\boldsymbol{u}_0,\, p_0),(\boldsymbol{v},\, q)) = F(\boldsymbol{v}), \quad \forall\,(\boldsymbol{v},\, q)\in \boldsymbol{V}\times Q, \end{aligned}} \tag{52}$$

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

$$B_0((\boldsymbol{u}_0,\, p_0),(\boldsymbol{v},\, q)) = a(\boldsymbol{u}_0,\boldsymbol{v}) + b(\boldsymbol{u}_0,\, q) + b(\boldsymbol{v},\, p_0).$$

We denote by $(\boldsymbol{e}_0^u,\, e_0^p)$ the error in the solution $(\boldsymbol{u}_0,\, p_0)$ 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:

$$Q(\boldsymbol{u},\, p) = \frac{1}{2}\int_\Omega \boldsymbol{u}\cdot\boldsymbol{u}\,\mathrm{d}x. \tag{53}$$

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.,

$$\begin{aligned} Q'\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big)\big) &= \int_\Omega \boldsymbol{u}_0\cdot\boldsymbol{e}_0^u\,\mathrm{d}x, \\ Q''\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big)\big) &= \int_\Omega \boldsymbol{e}_0^u\cdot\boldsymbol{e}_0^u\,\mathrm{d}x, \\ Q'''\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big)\big) &= 0, \end{aligned}$$

and the derivatives of form $B(\cdot;\,\cdot)$ with respect to the first variable are

$$\begin{aligned} &B'\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big),(\boldsymbol{v},\, q)\big) \\ &\quad = a\big(\boldsymbol{e}_0^u,\boldsymbol{v}\big) + b\big(\boldsymbol{v},\, e_0^p\big) + b\big(\boldsymbol{e}_0^u,\, q\big) + c\big(\boldsymbol{u}_0,\boldsymbol{e}_0^u,\boldsymbol{v}\big) + c\big(\boldsymbol{e}_0,\boldsymbol{u}_0^u,\boldsymbol{v}\big), \\ &B''\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big),(\boldsymbol{v},\, q)\big) = 2c\big(\boldsymbol{e}_0^u,\boldsymbol{e}_0^u,\boldsymbol{v}\big), \\ &B'''\big((\boldsymbol{u}_0,\, p_0);\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big),\big(\boldsymbol{e}_0^u,\, e_0^p\big),(\boldsymbol{v},\, q)\big) = 0. \end{aligned}$$

We denote by $(\boldsymbol{\omega},\,\mu)$ and $(\boldsymbol{\omega}_0,\,\mu_0)$ 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:

$$\boxed{\begin{array}{l}\text{Find } (\boldsymbol{\omega}, \mu) \in \boldsymbol{V} \times Q \text{ such that} \\ B'((\boldsymbol{u}, p); (\boldsymbol{v}, q), (\boldsymbol{\omega}, \mu)) = Q'((\boldsymbol{u}, p); (\boldsymbol{v}, q)), \quad \forall\, (\boldsymbol{v}, q) \in \boldsymbol{V} \times Q,\end{array}} \tag{54}$$

and

$$\boxed{\begin{array}{l}\text{Find } (\boldsymbol{\omega}_0, \mu_0) \in \boldsymbol{V} \times Q \text{ such that} \\ B_0((\boldsymbol{v}, q), (\boldsymbol{\omega}_0, \mu_0)) = Q'((\boldsymbol{u}_0, p_0); (\boldsymbol{v}, q)), \quad \forall\, (\boldsymbol{v}, q) \in \boldsymbol{V} \times Q.\end{array}} \tag{55}$$

In explicit form, these problems consist of finding $(\boldsymbol{\omega}, \mu)$ and $(\boldsymbol{\omega}_0, \mu_0)$ in $\boldsymbol{V} \times Q$ such that for all $(\boldsymbol{v}, q) \in \boldsymbol{V} \times Q$,

$$a(\boldsymbol{v}, \boldsymbol{\omega}) + b(\boldsymbol{v}, \mu) + b(\boldsymbol{\omega}, q) + c(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\omega}) + c(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{\omega}) = \int_\Omega \boldsymbol{u} \cdot \boldsymbol{v}\, \mathrm{d}x,$$
$$a(\boldsymbol{v}, \boldsymbol{\omega}_0) + b(\boldsymbol{v}, \mu_0) + b(\boldsymbol{\omega}_0, q) = \int_\Omega \boldsymbol{u}_0 \cdot \boldsymbol{v}\, \mathrm{d}x.$$

We note that since $B_0(\cdot, \cdot)$ is a bilinear form, the left-hand side of the above equation does not depend on $\boldsymbol{u}_0$. We are now in a position to derive estimates for the modeling error.

6.2. Estimates of Modeling Error

We denote by $(\boldsymbol{e}_0^u, e_0^p)$ and $(\boldsymbol{\varepsilon}_0^\omega, \boldsymbol{\varepsilon}_0^\mu)$ the error in $(\boldsymbol{u}_0, p_0)$ and $(\boldsymbol{\omega}_0, \mu_0)$, respectively. From the definition of the residual $\mathcal{R}((\boldsymbol{u}_0, p_0); \cdot)$ of (12), we obtain

$$\begin{aligned}\mathcal{R}\big((\boldsymbol{u}_0, p_0); \big(\boldsymbol{\varepsilon}_0^\omega, \boldsymbol{\varepsilon}_0^\mu\big)\big) &= F\big(\boldsymbol{\varepsilon}_0^\omega\big) - B\big((\boldsymbol{u}_0, p_0); \big(\boldsymbol{\varepsilon}_0^\omega, \varepsilon_0^\mu\big)\big) \\ &= B_0\big((\boldsymbol{u}_0, p_0); \big(\boldsymbol{\varepsilon}_0^\omega, \varepsilon_0^\mu\big)\big) - B\big((\boldsymbol{u}_0, p_0); \big(\boldsymbol{\varepsilon}_0^\omega, \varepsilon_0^\mu\big)\big) \\ &= -c\big(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\varepsilon}_0^\omega\big), \end{aligned} \tag{56}$$

$$\begin{aligned}\mathcal{R}((\boldsymbol{u}_0, p_0); (\boldsymbol{\omega}_0, \mu_0)) &= F(\boldsymbol{\omega}_0) - B((\boldsymbol{u}_0, p_0); (\boldsymbol{\omega}_0, \mu_0)) \\ &= -c(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\omega}_0). \end{aligned} \tag{57}$$

Meanwhile, the remainders are found to be

$$r\big(\big(\boldsymbol{e}_0^u, e_0^p\big), \big(\boldsymbol{\varepsilon}_0^\omega, \varepsilon_0^\mu\big)\big) = \frac{1}{2}\int_0^1 -6c\big(\boldsymbol{e}_0^u, \boldsymbol{e}_0^u, \boldsymbol{\varepsilon}_0^\omega\big)(s-1)s\, \mathrm{d}s = \frac{1}{2}c\big(\boldsymbol{e}_0^u, \boldsymbol{e}_0^u, \boldsymbol{\varepsilon}_0^\omega\big)$$

and

$$\Delta\mathcal{R} = \int_0^1 c\big(\boldsymbol{e}_0^u, \boldsymbol{e}_0^u, \boldsymbol{\omega}_0 + s\boldsymbol{\varepsilon}_0^\omega\big)\, \mathrm{d}s - \int_\Omega e_0^u \cdot e_0^u\, \mathrm{d}x.$$

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

$$Q(\boldsymbol{u}, p) - Q(\boldsymbol{u}_0, p_0) \approx -c(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\omega}_0) - c\big(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\varepsilon}_0^\omega\big). \tag{58}$$

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

$$B'\big((\boldsymbol{u}_0,\, p_0);(\boldsymbol{v},\, q),\, \big(\boldsymbol{\varepsilon}_0^{\omega},\, \varepsilon_0^{\mu}\big)\big) = \overline{\mathcal{R}}((\boldsymbol{u}_0,\, p_0);(\boldsymbol{v},\, q)), \quad \forall\, (\boldsymbol{v},\, q) \in \boldsymbol{V} \times Q,$$

that is,

$$a\big(\boldsymbol{v},\, \boldsymbol{\varepsilon}_0^{\omega}\big) + b\big(\boldsymbol{v},\, \varepsilon_0^{\mu}\big) + b\big(\boldsymbol{\varepsilon}_0^{\omega},\, q\big) + c\big(\boldsymbol{u}_0, \boldsymbol{v},\, \boldsymbol{\varepsilon}_0^{\omega}\big) + c\big(\boldsymbol{v}, \boldsymbol{u}_0,\, \boldsymbol{\varepsilon}_0^{\omega}\big) = \overline{\mathcal{R}}((\boldsymbol{u}_0,\, p_0);(\boldsymbol{v},\, q)).$$

Replacing $(\boldsymbol{v}, q)$ with $(\boldsymbol{\varepsilon}_0^{\omega}, \varepsilon_0^{\mu})$ in the above equation and observing that $\nabla \cdot \boldsymbol{u}_0 = 0$ and $\nabla \cdot \boldsymbol{\varepsilon}_0^{\omega} = 0$, we obtain

$$a\big(\boldsymbol{\varepsilon}_0^{\omega},\, \boldsymbol{\varepsilon}_0^{\omega}\big) + c\big(\boldsymbol{\varepsilon}_0^{\omega},\, \boldsymbol{u}_0,\, \boldsymbol{\varepsilon}_0^{\omega}\big) = \overline{\mathcal{R}}\big((\boldsymbol{u}_0,\, p_0);\, \big(\boldsymbol{\varepsilon}_0^{\omega},\, \varepsilon_0^{\mu}\big)\big). \tag{59}$$

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

$$\big\|\boldsymbol{\varepsilon}_0^{\omega}\big\| \leq \|\overline{\mathcal{R}}\|_*, \tag{60}$$

where

$$\big\|\boldsymbol{\varepsilon}_0^{\omega}\big\| = \sqrt{a\big(\boldsymbol{\varepsilon}_0^{\omega},\, \boldsymbol{\varepsilon}_0^{\omega}\big)} \quad \text{and} \quad \|\overline{\mathcal{R}}\|_* = \sup_{\boldsymbol{v} \in \boldsymbol{V} \setminus \{\boldsymbol{0}\}} \frac{|\overline{\mathcal{R}}((\boldsymbol{u}_0,\, p_0);\boldsymbol{v})|}{\|\boldsymbol{v}\|}.$$

It follows that

$$-c\big(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\varepsilon}_0^{\omega}\big) = \mathcal{R}\big((\boldsymbol{u}_0,\, p_0);\, \big(\boldsymbol{\varepsilon}_0^{\omega},\, \varepsilon_0^{\mu}\big)\big) \leq \|\mathcal{R}\|_* \big\|\boldsymbol{\varepsilon}_0^{\omega}\big\| \leq \|\mathcal{R}\|_* \|\overline{\mathcal{R}}\|_* \tag{61}$$

and thus

$$-\|\mathcal{R}\|_* \|\overline{\mathcal{R}}\|_* \leq -c\big(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\varepsilon}_0^{\omega}\big) \leq \|\mathcal{R}\|_* \|\overline{\mathcal{R}}\|_*. \tag{62}$$

Finally, the error $Q(\boldsymbol{u},\, p) - Q(\boldsymbol{u}_0,\, p_0)$ is bounded above and below,

$$\eta_{low} \leq Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0) \leq \eta_{upp}, \tag{63}$$

where

$$\eta_{low} = -c(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\omega}_0) - \|\mathcal{R}\|_* \|\overline{\mathcal{R}}\|_*, \tag{64}$$

$$\eta_{upp} = -c(\boldsymbol{u}_0, \boldsymbol{u}_0, \boldsymbol{\omega}_0) + \|\mathcal{R}\|_* \|\overline{\mathcal{R}}\|_*, \tag{65}$$

in which the norms of the residuals can be replaced by computable estimates (see, e.g., [2]).

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 variational problem

$$\boxed{\begin{array}{l}\text{Find } \boldsymbol{u} \in \boldsymbol{V} \text{ such that} \\ \qquad\qquad B(\boldsymbol{u}, \boldsymbol{v}) = F(\boldsymbol{v}), \quad \forall\, \boldsymbol{v} \in \boldsymbol{V},\end{array}} \tag{66}$$

where, now,

$$\boldsymbol{V} = H^m(0, T; \boldsymbol{W}),$$

$$B(\boldsymbol{u}, \boldsymbol{v}) = \int_0^T \int_{\Omega_0} \nabla \boldsymbol{v}(t) : \mathcal{P}(\nabla \boldsymbol{u}^t(s))\, \boldsymbol{F}^T(\boldsymbol{u}(t))\, \mathrm{d}X \mathrm{d}t + \underbrace{\int_0^T \int_{\Omega_0} \rho_0 \ddot{\boldsymbol{v}}(t) \cdot \boldsymbol{u}(t)\, \mathrm{d}X \mathrm{d}t + \int_{\Omega_0} \rho_0 \left(\boldsymbol{v}(T) \cdot \dot{\boldsymbol{u}}(T) - \dot{\boldsymbol{v}}(T) \cdot \boldsymbol{u}(T)\right) \mathrm{d}X}_{\text{Inertial Terms}}, \tag{67}$$

$$F(\boldsymbol{v}) = \int_0^T \left(\int_{\Omega_0} \rho_0 \boldsymbol{f}_0(t) \cdot \boldsymbol{v}(t)\, \mathrm{d}X + \int_{\Gamma_N^0} \boldsymbol{g}(t) \cdot \boldsymbol{v}(t)\, \mathrm{d}S \right) \mathrm{d}t + \underbrace{\int_{\Omega_0} \rho_0 (\boldsymbol{v}(0) \cdot \boldsymbol{V}_0 - \dot{\boldsymbol{v}}(0) \cdot \boldsymbol{U}_0)\, \mathrm{d}X}_{\text{Inertial Terms}}. \tag{68}$$

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

In (67), $\mathcal{P}(\cdot)$ is the constitutive functional for the second Piola–Kirchhoff stress tensor,

$$\begin{aligned} \nabla \boldsymbol{u}^t(s) &= \text{the history of the displacement gradient at time } t \\ &= \{\nabla \boldsymbol{u}(\cdot, t - s); \boldsymbol{u}(\cdot, t - s) \in \boldsymbol{W}; t \geq s \geq 0\}, \end{aligned}$$

where ∇ is the gradient with respect to the material coordinates and $\boldsymbol{F}(\boldsymbol{u}(t))$ is the deformation gradient,

$$\boldsymbol{F}(\boldsymbol{u}(t)) = \boldsymbol{I} + \nabla \boldsymbol{u}(t), \tag{69}$$

with $\boldsymbol{I}$ being the identity tensor and with $\boldsymbol{F}^T$ the transpose of $\boldsymbol{F}$.

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

As an example of a quantity of interest in applications of the model (66), consider a material surface ω that occupies a place ω_0 in the reference configuration with orientation defined by a unit normal $\boldsymbol{n}_0$. The motion $\boldsymbol{\chi} = \boldsymbol{u} + \boldsymbol{X}$ carries Ω_0 into $\Omega(t) = \boldsymbol{\chi}(\Omega_0)$ and ω_0 into a surface $\omega(t)$ with normal $\boldsymbol{n}$ in the current configuration of the body. The net normal force acting on the deformed area is $\int_{\omega(t)} \boldsymbol{n} \cdot \boldsymbol{n}\boldsymbol{T}\, \mathrm{d}S$, where $\boldsymbol{T}$ is the Cauchy stress tensor. A measure of the nominal force per unit undeformed area normal to $\omega(t)$ is then

$$Q(\boldsymbol{u}) = \frac{1}{|\omega_0|} \int_0^T \int_{\omega_0} \boldsymbol{m}(\boldsymbol{u}(t)) \cdot \boldsymbol{n}_0\, \mathcal{P}(\nabla \boldsymbol{u}^t(s)) \boldsymbol{F}^T(\boldsymbol{u}(t))\, \mathrm{d}S_0\, \mathrm{d}t, \tag{70}$$

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

To simplify the presentation, we shall confine ourselves to the quasi–static 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 $\nabla \boldsymbol{u}^t(s)$ evolves from null gradients, $\nabla \boldsymbol{u}(0) = \mathbf{0}$ at $t = 0$. A coarse model of the phenomena of interest is then characterized by a semilinear form $B_0(\boldsymbol{u}_0, \boldsymbol{v})$ obtained by replacing $\mathcal{P}(\cdot)$ in (67) with a simplified constitutive functional, $\mathcal{P}_0(\cdot)$ of the histories $\nabla \boldsymbol{u}_0^t(s)$.

A straightforward calculation reveals that

$$B'(\boldsymbol{u}; \boldsymbol{v}, \boldsymbol{w}) = \int_0^T \int_{\Omega_0} \nabla \boldsymbol{w}(t) : \mathcal{P}(\nabla \boldsymbol{u}^t(s)) \nabla \boldsymbol{v}(t)^T \, \mathrm{d}X \mathrm{d}t + \int_0^T \int_{\Omega_0} \nabla \boldsymbol{w}(t) : \partial \mathcal{P}(\nabla \boldsymbol{u}^t(s); \nabla \boldsymbol{v}^t(s)) \boldsymbol{F}^T(\boldsymbol{u}(t)) \, \mathrm{d}X \, \mathrm{d}t, \tag{71}$$

where

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

Likewise, for the functional in (70),

$$Q'(\boldsymbol{u}; \boldsymbol{v}) = \frac{1}{|\omega_0|} \int_0^T \int_{\omega_0} \frac{\partial \boldsymbol{m}(\boldsymbol{u}(t))}{\partial \boldsymbol{u}} \cdot \boldsymbol{v}(t) \cdot \boldsymbol{n}_0 \, \mathcal{P}(\nabla \boldsymbol{u}^t(s)) \, \boldsymbol{F}^T(\boldsymbol{u}(t)) + \boldsymbol{m}(\boldsymbol{u}(t)) \cdot \boldsymbol{n}_0 \partial \mathcal{P}(\nabla \boldsymbol{u}^t(s); \nabla \boldsymbol{v}(t)^T) \boldsymbol{F}^T(\boldsymbol{u}(t)) + \boldsymbol{m}(\boldsymbol{u}(t)) \cdot \boldsymbol{n}_0 \, \mathcal{P}(\nabla \boldsymbol{u}^t(s)) \nabla \boldsymbol{v}(t)^T \, \mathrm{d}S_0 \, \mathrm{d}t. \tag{73}$$

7.2. Modeling Error Analysis

In the present example, we note that

$$\mathcal{R}(\boldsymbol{u}_0; \boldsymbol{v}) = - \int_0^T \int_{\Omega_0} \nabla \boldsymbol{v}(t) : \Delta \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) \boldsymbol{F}^T(u_0(t)) \, \mathrm{d}X \, \mathrm{d}t, \tag{74}$$

where $\Delta \mathcal{P}$ is the stress error

$$\Delta \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) = \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) - \mathcal{P}_0\big(\nabla \boldsymbol{u}_0^t(s)\big) \tag{75}$$

and $(\boldsymbol{u}_0, \boldsymbol{p}_0)$ are solutions of the equations (10), with $B_0(\cdot;\cdot)$, $B_0'(\cdot;\cdot,\cdot)$, and $Q'(\cdot;\cdot)$ defined now by (67), (71), and (73) with the inertia terms dropped and $\mathcal{P}(\cdot)$ replaced by $\mathcal{P}_0(\cdot)$. We have

$$\begin{aligned} \overline{\mathcal{R}}(\boldsymbol{u}_0, \boldsymbol{p}_0; \boldsymbol{v}) &= B_0'(\boldsymbol{u}_0; \boldsymbol{v}, \boldsymbol{p}_0) - B'(\boldsymbol{u}_0; \boldsymbol{v}, \boldsymbol{p}_0) \\ &= - \int_0^T \int_{\Omega_0} \nabla \boldsymbol{p}_0 : \Delta \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) \nabla \boldsymbol{v}(t)^T \, \mathrm{d}X \, \mathrm{d}t \\ &\quad - \int_0^T \int_{\Omega_0} \nabla \boldsymbol{p}_0 : \Delta \partial \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s); \nabla \boldsymbol{v}^t(s)\big) \boldsymbol{F}^T(\boldsymbol{u}_0(t)) \, \mathrm{d}X \, \mathrm{d}t, \end{aligned} \tag{76}$$

where

$$\Delta \partial \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s); \nabla \boldsymbol{v}^t(s)\big) = \partial \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s); \nabla \boldsymbol{v}^t(s)\big) - \partial \mathcal{P}_0\big(\nabla \boldsymbol{u}_0^t(s); \nabla \boldsymbol{v}^t(s)\big). \tag{77}$$

Since $B'(\boldsymbol{u}_0; \boldsymbol{v}, \boldsymbol{\varepsilon}_0) = \overline{\mathcal{R}}(\boldsymbol{u}_0, \boldsymbol{p}_0; \boldsymbol{v})$, for all $\boldsymbol{v} \in \boldsymbol{V}$, we have

$$\int_0^T \int_{\Omega_0} \nabla \boldsymbol{\varepsilon}_0(t) : \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) \nabla \boldsymbol{v}(t)^T \, \mathrm{d}X \, \mathrm{d}t + \int_0^T \int_{\Omega_0} \nabla \boldsymbol{\varepsilon}_0(t) : \partial \mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s); \nabla \boldsymbol{v}^t(s)\big) \boldsymbol{F}^T(\boldsymbol{u}_0(t)) \, \mathrm{d}X \, \mathrm{d}t = \overline{\mathcal{R}}(\boldsymbol{u}_0, \boldsymbol{p}_0; \boldsymbol{v}), \quad (78)$$

with $\overline{\mathcal{R}}(\boldsymbol{u}_0, \boldsymbol{p}_0; \boldsymbol{v})$ as given in (76).

Equation (78) is a linear integrodifferential equation for the error $\boldsymbol{\varepsilon}_0$ in the influence function $\boldsymbol{p}_0$. We shall assume that it is solvable using standard finite element methods, so that a good approximate solution $\boldsymbol{\varepsilon}_0^h$ can be obtained. There we write

$$\boldsymbol{\varepsilon}_0^h(t) = \boldsymbol{\varepsilon}^h\big(\nabla \boldsymbol{u}_0^t(s)\big) \approx \boldsymbol{\varepsilon}_0(t). \quad (79)$$

With this result, we use (74) in (21), neglecting $\Delta\mathcal{R}$ and $r(\boldsymbol{e}_0, \boldsymbol{\varepsilon}_0)$, to obtain the estimate

$$Q(\boldsymbol{u}) - Q(\boldsymbol{u}_0) \approx -\int_0^T \int_{\Omega_0} \nabla \boldsymbol{p}_0(t) : \Delta\mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) \boldsymbol{F}^T(\boldsymbol{u}_0(t)) \, \mathrm{d}X \, \mathrm{d}t - \int_0^T \int_{\Omega_0} \nabla \boldsymbol{\varepsilon}^h\big(\nabla \boldsymbol{u}_0^t(s)\big) : \Delta\mathcal{P}\big(\nabla \boldsymbol{u}_0^t(s)\big) \boldsymbol{F}^T(\boldsymbol{u}_0(t)) \, \mathrm{d}X \, \mathrm{d}t. \quad (80)$$

Numerical examples for control of the modeling error in global norm were shown in [12]. 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 we actually should seek estimates of the error

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

But

$$Q(u) - Q\big(u_0^h\big) = \underbrace{Q(u) - Q(u_0)}_{\text{modeling error}} + \underbrace{Q(u_0) - Q\big(u_0^h\big)}_{\text{approximation error}}.$$

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,

for instance in [5, 11, 16, 17]; a combination of the methods of modeling error estimation developed herein and the techniques in [5, 11, 16, 17] should have an impact on broad issues of verification and validation for many classes of problems in mechanics.

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