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Computer methods in applied mechanics and engineering
Comput. Methods Appl. Mech. Engrg. 194 (2005) 195–204
www.elsevier.com/locate/cma

Theory and methodology for estimation and control of errors due to modeling, approximation, and uncertainty

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Received 24 June 2003; accepted 24 June 2003

Abstract

The reliability of computer predictions of physical events depends on several factors: the mathematical model of the event, the numerical approximation of the model, and the random nature of data characterizing the model. This paper addresses the mathematical theories, algorithms, and results aimed at estimating and controlling modeling error, numerical approximation error, and error due to randomness in material coefficients and loads. *A posteriori* error estimates are derived and applications to problems in solid mechanics are presented.

Keywords: Modeling error estimation; Stochastic partial differential equations; Adaptive modeling

1. Introduction

The reliability of computer simulations has become one of the most critical subjects in computational science. The expectations of users of computer predictions to make decisions about many events and processes that affect broad areas of technology has risen due to advances in computing and computational methods. The mere calculation of qualitative information on global trends of physical systems is no longer viewed as the primary goal of simulations. Today's analysts expect to obtain quantitative information on system performance and outputs, and this expectation has put stringent demands on the sophistication and accuracy of computer simulations and on the use of effective methods of estimation and control of errors in computed results.

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0045-7825/$ - see front matter
doi:10.1016/j.cma.2003.06.003

In this paper, we review recent developments in the estimation and control of errors encountered in computer predictions in computational mechanics. Three error sources are considered: modeling error, due to use of simplified models of physical events, discretization error, due to use of discrete approximations of mathematical models of the events, and error due to uncertainty, due to scatter in data, particularly data involving material coefficients in the various models. The estimation of modeling error follows the theory developed in [1,3,6] and discretization error, the theory in [2,4,5,7–9] and elsewhere. To estimate errors due to uncertainty, we employ first-order perturbation methods for stochastic partial differential equations. In this analysis, the "worst-case-scenario" is used to obtain upper and lower bounds on errors in quantities of interest in situations in which the material coefficients are random variables. Some applications to three-dimensional elasticity models are presented.

2. Preliminaries: The base model

We consider the following mathematical models of the deformation of a material body in equilibrium under the action of applied forces: find the displacement field $\mathbf{u} \in V$ such that

$$B_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{v}) = F(\mathbf{v}) \quad \forall \mathbf{v} \in V. \tag{2.1}$$

Here

$$\left.\begin{aligned} B_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{v}) &= \textstyle\int_D \boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{u}) : \nabla\mathbf{v}\,\mathrm{d}x, \\ F(\mathbf{v}) &= \textstyle\int_D \mathbf{f}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + \int_{\Gamma_1} \mathbf{g}\cdot\mathbf{v}\,\mathrm{d}s. \end{aligned}\right\} \tag{2.2}$$

Here V is the space of admissible functions,

$$V = \{\mathbf{v} : \ \boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{v}) : \nabla\mathbf{v} \ \in \ L^1(D), \ \mathbf{v} = \mathbf{0} \text{ on } \Gamma_0\}, \tag{2.3}$$

$\boldsymbol{\beta}$ is a vector of material coefficients provided as data to the model, $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{f}$ and $\mathbf{g}$ are prescribed body forces and surface tractions of sufficient regularity that $F(\cdot)$ is a continuous linear functional on V, D is an open bounded domain in $\mathbb{R}^d$ $(d = 1, 2, \text{ or } 3)$ with boundary $\partial D = \overline{\Gamma}_0 \cup \overline{\Gamma}_1$, $\int_{\Gamma_0} \mathrm{d}s > 0$. The semicolon notation in the definition of $B_{\boldsymbol{\beta}}(\cdot\,;\cdot)$ is intended to imply that $B_{\boldsymbol{\beta}}(\cdot\,;\cdot)$ may be a nonlinear function of $\mathbf{u}$ but is linear in arguments to the right side of the semicolon ($\mathbf{v}$ in this case). Problem (2.1) characterizes the *primal base model* (or "fine" model; cf [1]) of the physical event of interest.

Of particular interest are specific features of the solution $\mathbf{u}$, the so-called *target outputs* or *quantities of interest*, defined by functionals Q on V. For instance, we may be particularly interested in the average shear stress on a material surface area ω within D with unit normal $\mathbf{n}$ and tangential vector $\boldsymbol{\nu}$. In this case,

$$Q(\mathbf{u}) = |\omega|^{-1} \int_\omega \boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{u})\ \mathbf{n}\cdot\boldsymbol{\nu}\,\mathrm{d}s. \tag{2.4}$$

The *dual base model* consists of finding an influence function $\mathbf{p} \in V$ such that

$$B'_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{v},\mathbf{p}) = Q'(\mathbf{u};\mathbf{v}) \quad \forall \mathbf{v} \ \in V. \tag{2.5}$$

Here

$$\begin{aligned} B'_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{v},\mathbf{p}) &= \lim_{\theta\to 0^+} \theta^{-1}[B_{\boldsymbol{\beta}}(\mathbf{u}+\theta\mathbf{v};\mathbf{p}) - B_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{p})] \\ &= \int_D \boldsymbol{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u})\ \nabla\mathbf{v} : \nabla\mathbf{p}\,\mathrm{d}x, \end{aligned} \tag{2.6}$$

where

$$\mathbf{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u}) = \frac{\partial\boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{u})}{\partial\nabla_s\mathbf{u}}, \tag{2.7}$$

$\nabla_s\mathbf{u}$ being the symmetric part of $\nabla\mathbf{u}$ $(= (\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}})/2)$. Thus, $\mathbf{\Phi}$ is a fourth-order tensor with components $\Phi_{ijkl} = (\partial\sigma_{ij}/\partial u_{k,l} + \partial\sigma_{i,j}/\partial u_{l,k})/2$, $1 \leqslant i,j,k,l \leqslant d$. We shall assume that constants $\alpha_0, \alpha_1 > 0$ exist, independent of $\boldsymbol{\beta}$, such that at a.e. $\mathbf{x} \in D$,

$$\alpha_0\varepsilon_{ij}\varepsilon_{ij} \geqslant \Phi_{ijkl}(\boldsymbol{\beta};\nabla\mathbf{u})\varepsilon_{kl}\varepsilon_{ij} \geqslant \alpha_1\varepsilon_{ij}\varepsilon_{ij} \tag{2.8}$$

$\forall$ symmetric tensor ε_{ij}, where repeated indices are summed throughout their range. Of particular interest is the linear elasticity case in which

$$\mathbf{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u}) = \mathbf{C}(\boldsymbol{\beta}), \tag{2.9}$$

where $\mathbf{C}(\boldsymbol{\beta})$ is the fourth-order tensor of elasticities. The tensor $\mathbf{C}(\boldsymbol{\beta})$ has the symmetries, $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$, $1 \leqslant i,j,k,l \leqslant d$.

Returning to (2.5), the right-hand side is given by

$$Q'(\mathbf{u};\mathbf{v}) = \lim_{\theta\to 0^+} \theta^{-1}[Q(\mathbf{u}+\theta\mathbf{v}) - Q(\mathbf{u})]. \tag{2.10}$$

If Q is chosen to be the particular functional in (2.4), then

$$Q'(\mathbf{u};\mathbf{v}) = |\omega|^{-1}\int_\omega \mathbf{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u})\nabla\mathbf{v}\,\mathbf{n}\cdot\boldsymbol{v}\,\mathrm{d}s.$$

But Q, at this stage of the analysis, can be quite general. In much of the analysis and in examples given later, we consider cases in which Q is a linear functional; e.g. $Q(\mathbf{v}) = \int_\omega \mathbf{v}\cdot\boldsymbol{v}\,\mathrm{d}s$ or $Q(\mathbf{v}) = v_1(\mathbf{x}_0)$, $\mathbf{x}_0 \in D$. Then $Q'(\mathbf{u};\mathbf{v}) = Q(\mathbf{v})$. Note that the dual problem is linear in p.

3. The surrogate and the discrete problems

Instead of (2.1), we consider a simplified problem referred to as the *surrogate* (*or coarse*) *problem* which, contrary to (2.1), is tractable to numerical approximation:

Find $\mathbf{u}_0 \in V$ such that

$$B^0_{\boldsymbol{\beta}_0}(\mathbf{u}_0;\mathbf{v}) = F(\mathbf{v}) \quad \forall\mathbf{v}\in V, \tag{3.1}$$

where now

$$B^0_{\boldsymbol{\beta}_0}(\mathbf{u}_0;\mathbf{v}) = \int_D \boldsymbol{\sigma}_0(\boldsymbol{\beta}_0;\nabla\mathbf{u}_0) : \nabla\mathbf{v}\,\mathrm{d}x. \tag{3.2}$$

Here $\boldsymbol{\beta}_0$ belongs to a fixed deterministic bounded set of coefficients, and $\boldsymbol{\sigma}_0(\boldsymbol{\beta}_0;\nabla\mathbf{u}_0)$ is the stress tensor in the surrogate model, which can be characterized by a different, and simpler constitutive equation than that used in the base model. In the case that the surrogate model describes a linearly elastic homogeneous and isotropic material,

$$\boldsymbol{\sigma}_0(\boldsymbol{\beta}_0;\nabla\mathbf{u}_0) = \mathbf{C}(\boldsymbol{\beta}_0)\nabla\mathbf{u}_0, \tag{3.3}$$

where

$$\mathbf{C}(\boldsymbol{\beta}_0)\nabla\mathbf{u}_0 = \kappa_0\mathbf{I}\,\mathrm{div}\,\mathbf{u}_0 + G_0(\nabla\mathbf{u}_0 + \nabla\mathbf{u}_0^{\mathrm{T}}), \tag{3.4}$$

where κ_0 and G_0 are the bulk and shear moduli, respectively, and $\mathbf{I}$ is the unit tensor. Then $\boldsymbol{\beta}_0 = (\kappa_0, G_0)$. Throughout this analysis, $\mathbf{C}(\boldsymbol{\beta}_0)$ is assumed to have standard symmetry and ellipticity properties.

The *surrogate dual* problem is to find $\mathbf{p}_0 \in V$ such that

$$B^{0\prime}_{\boldsymbol{\beta}_0}(\mathbf{u}_0; \mathbf{v}; \mathbf{p}_0) = Q_0'(\mathbf{u}_0; \mathbf{v}) \quad \forall \mathbf{v} \in V, \tag{3.5}$$

where, for example, $Q_0(\mathbf{v}) = |\omega|^{-1} \int_\omega \boldsymbol{\sigma}_0(\boldsymbol{\beta}_0; \nabla \mathbf{u}_0) \nabla \mathbf{v}\, \mathbf{n} \cdot \boldsymbol{\nu}\, \mathrm{d}s$ and $B^{0\prime}_{\boldsymbol{\beta}_0}(\mathbf{u}_0; \mathbf{p}, \mathbf{v})$ and $Q'(\mathbf{u}_0; \mathbf{v})$ are defined in (2.6) and (2.10) with $\boldsymbol{\Phi}(\boldsymbol{\beta}; \nabla \mathbf{u})$ replaced by $\boldsymbol{\Phi}_0(\boldsymbol{\beta}_0; \nabla \mathbf{u}_0) = \partial \boldsymbol{\sigma}_0 / \partial \nabla_s \mathbf{u}_0$.

In general, we regard the base problems (2.1) and (2.5) as intractable, and surrogate problems (3.1) and (3.5) as amendable to numerical approximation using finite element methods. Thus, we consider a family of finite-dimensional subspaces $\{V^h\}$, $V^h \subset V$, constructed using standard conforming piecewise-polynomial, finite element approximation, and develop finite element approximation of (3.1) and (3.5) of the form:

Find $\mathbf{u}_0^h$, $\mathbf{p}_0^h \in V^h$ such that

$$B^0_{\boldsymbol{\beta}_0}(\mathbf{u}_0^h; \mathbf{v}^h) = F(\mathbf{v}^h) \quad \text{and} \quad B^{0\prime}_{\boldsymbol{\beta}_0}(\mathbf{u}_0^h; \mathbf{v}_0^h, \mathbf{p}^h) = Q'(\mathbf{u}_0^h; \mathbf{v}^h) \quad \forall \mathbf{v}^h \in V^h. \tag{3.6}$$

4. Error estimation

For simplicity, we confine our attention to the case in which the output functional Q is linear and $Q_0(\mathbf{v}) = Q(\mathbf{v})$, $\mathbf{v} \in V$, assuming that $Q(\cdot)$ depends on $\boldsymbol{\beta}$ through the solution $\mathbf{u}$ only. We consider three sources of error.

Modeling error

$$\left.\begin{aligned} Q(\mathbf{u}) - Q(\mathbf{u}_0) &= Q(\mathbf{e}_0), \\ \mathbf{e}_0 &= \mathbf{u} - \mathbf{u}_0. \end{aligned}\right\} \tag{4.1}$$

Discretization error

$$\left.\begin{aligned} Q(\mathbf{u}_0) - Q(\mathbf{u}_0^h) &= Q(\mathbf{e}_0^h), \\ \mathbf{e}_0^h &= \mathbf{u}_0 - \mathbf{u}_0^h. \end{aligned}\right\} \tag{4.2}$$

Error due to uncertainty

$$Q(\mathbf{u}(\boldsymbol{\beta})) - Q(\bar{\mathbf{u}}) = Q(\delta \mathbf{u}). \tag{4.3}$$

In (4.3), the coefficients $\boldsymbol{\beta}$ are assumed to be random variables with bounded variances, and $\bar{\boldsymbol{\beta}}$ is the mean or expected value of $\boldsymbol{\beta} = [\beta_1, \beta_2, \ldots, \beta_m]$. With obvious notation,

$$\bar{\beta}_i = E[\beta_i] = \int_{-\infty}^{\infty} \rho \beta_i \, \mathrm{d}\boldsymbol{\beta}; \quad \beta_{\text{mini}} \leqslant \beta_i \leqslant \beta_{\text{maxi}}, \quad i = 1, 2, \ldots, m,$$

where ρ is the joint PDF of the random vector $\boldsymbol{\beta}$. Then, $\mathbf{u}(\boldsymbol{\beta}) = \mathbf{u}(\bar{\boldsymbol{\beta}}) + \delta \mathbf{u}(\bar{\boldsymbol{\beta}}, \delta \boldsymbol{\beta}, \mathbf{x}) (= \bar{\mathbf{u}} + \delta \mathbf{u})$. Thus, the error in Q due to uncertainty, based on first-order perturbation theory, is $Q(\delta \mathbf{u})$.

According to [1, Theorem 2, p. 502], to within quadratic terms in the error components $\mathbf{e}_0 = \mathbf{u} - \mathbf{u}_0$ and $\boldsymbol{\varepsilon}_0 = \mathbf{p} - \mathbf{p}_0$,

$$Q(\mathbf{e}_0) = R_{\boldsymbol{\beta}}(\mathbf{u}_0; \mathbf{p}_0) + R_{\boldsymbol{\beta}}(\mathbf{u}_0; \boldsymbol{\varepsilon}_0) = R_{\boldsymbol{\beta}}(\mathbf{u}_0; \mathbf{p}), \tag{4.4}$$

where $R(\cdot\,;\cdot)$ is the residual functional,

$$R_{\boldsymbol{\beta}}(\mathbf{u}_0; \mathbf{v}) = F(\mathbf{v}) - B_{\boldsymbol{\beta}}(\mathbf{u}_0; \mathbf{v}) \tag{4.5}$$

for $\mathbf{v} \in V$. Likewise,

$$Q(\mathbf{e}_0^h) = R_{\boldsymbol{\beta}}(\mathbf{u}_0^h; \mathbf{p}_0) = R_{\boldsymbol{\beta}}(\mathbf{u}_0^h; \boldsymbol{\epsilon}_0), \tag{4.6}$$

where $\boldsymbol{\epsilon}_0 = \mathbf{p}_0 - \mathbf{p}_0^h$ the orthogonality condition, $R_{\boldsymbol{\beta}}(\mathbf{u}_0^h; \mathbf{v}^h) = 0$ has been used.

Two remarks are in order: (1) the errors (4.4) and (4.6) in $Q(\cdot)$ depend upon the influence functions $\mathbf{p}$ and $\mathbf{p}_0$; thus to estimate or bound these errors, estimates or bounds on $\mathbf{p}$ and $\mathbf{p}_0$ must be obtained; (2) in any application, only $\mathbf{u}_0^h(\bar{\boldsymbol{\beta}}) = \bar{\mathbf{u}}_0^h$ and $\mathbf{p}_0^h(\bar{\boldsymbol{\beta}}) = \bar{\mathbf{p}}_0^h$ are known, moreover, the residual functional $R_{\boldsymbol{\beta}}(\cdot\,;\cdot)$ also depends upon the random variable $\boldsymbol{\beta}$. Thus, we compute

$$\left.\begin{aligned} Q(\mathbf{u}) - Q(\bar{\mathbf{u}}_0^h) = Q(\mathbf{u}) - Q(\mathbf{u}_0) &\qquad \text{(modeling)} \\ + & \\ Q(\mathbf{u}_0) - Q(\mathbf{u}_0^h) &\qquad \text{(discretization)} \\ + & \\ Q(\mathbf{u}_0^h(\boldsymbol{\beta})) - Q(\bar{\mathbf{u}}_0^h) &\qquad \text{(uncertainty)} \end{aligned}\right\} \tag{4.7}$$

To estimate the modeling error, we use the procedures described in [2,3] to compute a estimator $\eta(\mathbf{u}_0, \mathbf{p}_0, \boldsymbol{\beta})$; and to estimate the discretization error, we compute an estimator $\zeta(\mathbf{u}_0^h, \mathbf{p}_0^h, \boldsymbol{\beta})$. Since only $\bar{\mathbf{u}}_0^h$, $\bar{\mathbf{p}}_0^h$ and $\bar{\boldsymbol{\beta}}$ are known, we set

$$\left.\begin{aligned} Q(\mathbf{u}) - Q(\mathbf{u}_0) \approx \eta(\bar{\mathbf{u}}_0^h, \bar{\mathbf{p}}_0^h, \bar{\boldsymbol{\beta}}) := \bar{\eta}, \\ Q(\mathbf{u}_0) - Q(\mathbf{u}_0^h) \approx \zeta(\bar{\mathbf{u}}_0^h, \bar{\mathbf{p}}_0^h, \bar{\boldsymbol{\beta}}) := \bar{\zeta}. \end{aligned}\right\} \tag{4.8}$$

To estimate the error due to uncertainty, we use first-order perturbation theory to obtain the approximation,

$$Q(\mathbf{u}_0^h(\boldsymbol{\beta})) \approx Q(\mathbf{u}_0^h(\bar{\boldsymbol{\beta}})) - \int_D \partial_{\boldsymbol{\beta}} \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}}; \nabla \bar{\mathbf{u}}_0^h) \cdot \delta\boldsymbol{\beta} : \nabla \bar{\mathbf{p}}_0^h \, \mathrm{d}x. \tag{4.9}$$

A derivation of this result is given in Appendix A. Let

$$\left.\begin{aligned} \mathbf{G}(\mathbf{x}) := \partial_{\boldsymbol{\beta}} \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}}; \nabla \bar{\mathbf{u}}_0^h) : \nabla \bar{\mathbf{p}}_0^h \in [L^1(D)]^m, \\ \|\delta\beta_i\|_{L^\infty(D)} \leqslant M_i, \quad \delta\boldsymbol{\beta} \in \Omega \subset [L^\infty(D)]^m, \end{aligned}\right\} \tag{4.10}$$

then

$$|Q(\mathbf{u}_0^h(\boldsymbol{\beta})) - Q(\mathbf{u}_0^h(\bar{\boldsymbol{\beta}}))| \leqslant \Delta Q(\bar{\mathbf{u}}_0^h, \bar{\mathbf{p}}_0^h) = \sup_{\|\delta\boldsymbol{\beta}_i\|_{L^\infty(D)} \leqslant M_i} \left| \int_D \mathbf{G} \cdot \delta\boldsymbol{\beta} \, \mathrm{d}x \right|. \tag{4.11}$$

Finally,

$$|Q(\mathbf{u}) - Q(\bar{\mathbf{u}}_0^h)| \leqslant \bar{\eta} + \bar{\zeta} + \Delta Q(\bar{\mathbf{u}}_0^h, \bar{\mathbf{p}}_0^h). \tag{4.12}$$

5. First-order perturbation analysis of error due to uncertainty

We recount here the determination of bounds on the error component $Q(\delta\mathbf{u})$ given by (4.11) for the case in which $\boldsymbol{\sigma}$ is a linear function of $\nabla\mathbf{u}$:

$$\boldsymbol{\sigma}(\boldsymbol{\beta}, \nabla\mathbf{u}) = \mathbf{C}(\boldsymbol{\beta})\nabla\mathbf{u}. \tag{5.1}$$

For a sufficiently refined mesh, the following result shows that we can use $\mathbf{u}_0^h \approx \mathbf{u}_0$ and $\mathbf{p}_0^h \approx \mathbf{p}_0$.

Theorem. ([8]). *Let* $\partial_{\boldsymbol{\beta}} \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}}, \nabla\mathbf{u}_0) = (\partial\mathbf{C}/\partial\boldsymbol{\beta})\nabla\mathbf{u}_0$. *Then, there exists a constant* $C > 0$ *such that*

$$\left|\Delta Q(\mathbf{u}_0, \mathbf{p}_0) - \Delta Q(\mathbf{u}_0^h, \mathbf{p}_0^h)\right| \leqslant C(\|\nabla(\mathbf{u}_0 - \mathbf{u}_0^h)\|_{L^2(D)} + \|\nabla(\mathbf{p}_0 - \mathbf{p}_0^h)\|_{L^2(D)}), \tag{5.2}$$

where $\Delta Q(\mathbf{u}_0^h, \mathbf{p}_0^h)$ (*resp.* $\Delta Q(\mathbf{y}_0, \mathbf{p}_0)$) *is given in* (4.11).

Consider the following three different sets of perturbations with bounds $\Delta_G Q$, $\Delta_L Q$ and $\Delta_W Q$, respectively.

$$|Q(\mathbf{u}_0(\bar{\boldsymbol{\beta}} + \delta\boldsymbol{\beta})) - Q(\mathbf{u}_0(\bar{\boldsymbol{\beta}}))| \leqslant$$

$$(1) \quad \Delta_G Q(\bar{\mathbf{u}}_0, \bar{\mathbf{p}}_0) = \sum_i M_i \left| \int_D G_i \, \mathrm{d}x \right| \tag{5.3a}$$

and $\delta\beta_i = \text{constant}$.

$$(2) \quad \Delta_L Q(\bar{\mathbf{u}}_0, \bar{\mathbf{p}}_0) = \sum_i M_i \sum_{K \in \mathscr{P}^h} \left| \int_K G_i \, \mathrm{d}x \right| \tag{5.3b}$$

and $\delta\beta_i = \text{piecewise constant}$.

$$(3) \quad \Delta_W Q(\bar{\mathbf{u}}_0, \bar{\mathbf{p}}_0) = \sum_i M_i \int_D |G_i| \, \mathrm{d}x \tag{5.3c}$$

and $\delta\beta_i \in L^\infty(\mathbf{D}), \quad \|\delta\beta_i\|_{L^\infty} \leqslant M_i$.

where, again, $G_i = \partial_{\beta_i}\boldsymbol{\sigma}(\bar{\beta}_i; \nabla\bar{\mathbf{u}}_0^h) : \nabla\bar{\mathbf{p}}_0^h \approx \nabla\bar{\mathbf{u}}_0(\partial\mathbf{C}/\partial\beta_i)\nabla\bar{\mathbf{p}}_0, i = 1, 2, \ldots, m$. The bound (5.3a) describes the case in which the perturbation $\delta\boldsymbol{\beta}$ of the coefficients is constant over D; that of (5.3b) describes a piecewise constant variation of $\delta\boldsymbol{\beta}$ over a partition $\mathscr{P}^h$ of D into a mesh of finite element K, and (5.3c) is the general case in which $\delta\boldsymbol{\beta}$ can vary arbitrarily over D so long as $\|\beta_i\|_{L^\infty(D)} \leqslant M_i, i = 1, 2, \ldots, m$. In this case, the worst distribution of the coefficient β_i (i.e. the distribution of the coefficient that leads to the largest uncertainty ΔQ for the quantity of interest) is given by:

$$\beta_i = \bar{\beta}_i + \delta\beta_i^*, \quad \text{with } \delta\beta_i^* = M_i \,\mathrm{sign}(G_i). \tag{5.4}$$

As an application of these estimates, we consider a "bulky" prismatic, linear elastic isotropic body cantilevered at one end and loaded by a uniform shear at its free end that produces a net force of 1.0 MPa (Fig. 1). Let $\mathbf{u} = \mathbf{u}(x, y, z)$ be the displacement field in the body, (x, y, z) being the Cartesian coordinate system shown. As quantities of interest, we take the average displacements (see Fig. 2).

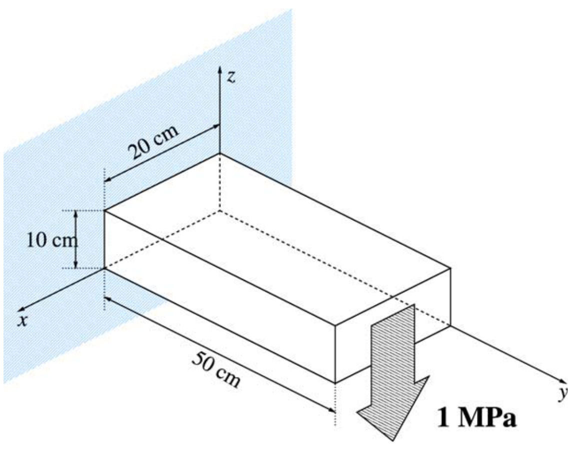

Fig. 1. Geometry of "bulky" prismatic body.

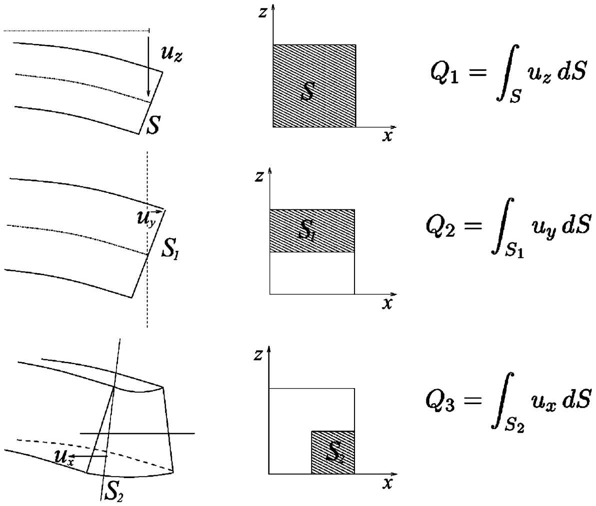

Fig. 2. Quantities of interest—average displacements at the free end.

$$\left.\begin{aligned} Q_1(\mathbf{u}) &= \int_0^{20}\int_0^{10} u_z(x,50,z)\mathrm{d}x\,\mathrm{d}z,\\ Q_2(\mathbf{u}) &= \int_0^{20}\int_5^{10} u_y(x,50,z)\mathrm{d}x\,\mathrm{d}z,\\ Q_3(\mathbf{u}) &= \int_{10}^{20}\int_5^{10} u_x(x,50,z)\mathrm{d}x\,\mathrm{d}z. \end{aligned}\right\} \quad (5.5)$$

The material is assumed to be isotropic. Based on laboratory tests on aluminum, the 2σ-variation (twice the standard deviation) in Young's modulus is 1.0%, and that in Poisson's ratio is 8.0%. These were used to define the bound M on $\delta\boldsymbol{\beta}$. In this case, $C_{ijkl}(\boldsymbol{\beta}) = \lambda(\boldsymbol{\beta})\delta_{ij}\delta_{kl} + \mu(\boldsymbol{\beta})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $1 \leqslant i,j,k,l \leqslant 3$, where $\lambda = \beta_1\beta_2/(1+\beta_2)(1-2\beta_2)$, $\mu = \beta_1/2(1+\beta_2)$, so that $\beta_1 = E$ and $\beta_2 = \nu$. A manually graded, anisotropically refined partition of D into the finite element mesh shown was used in evaluating the perturbations ΔQ of (5.3a)–(5.3c). The primal and dual problems were solved using a mesh of hexahedral elements with fourth-order polynomial shape functions, and $\mathbf{u}_0^h$ and $\mathbf{p}_0^h$ are believed to be highly accurate approximation of $\mathbf{u}_0$ and $\mathbf{p}_0$. Results of the calculation of perturbations are given in Table 1 below, where ΔQ_G, ΔQ_L, and ΔQ_W are given as a percentage of Q for each choice of the quantities of interest Q_i in (5.5).

We observe that Q_3 is a very small quantity, compared to Q_1, and Q_2, and it is relatively sensitive to the perturbation $\delta\boldsymbol{\beta}$. Figs. 3 and 4 show the worst distribution of the coefficients $\boldsymbol{\beta} = [\beta_1, \beta_2] = [E, \nu]$ for Q_1 and Q_2 defined in (5.5). The blue region corresponds to a negative perturbation of the coefficients, $\beta_i = \bar{\beta}_i - M_i$, $i = 1, 2$; while the red region corresponding to a positive perturbation $\beta_i = \bar{\beta}_i + M_i$, $i = 1, 2$. Figs. 5–7 show split-view of the regions with both positive and negative variation in quantities of interest (Q_1 and

Table 1
Computed variations in quantities of interest

Q (calculated)	$\Delta_G Q/Q$ (%)	$\Delta_L Q/Q$ (%)	$\Delta_W Q/Q$ (%)
Q_1 −6.98480E−04	1.45	1.55	1.56
Q_2 0.51221E−04	1.35	1.58	1.62
Q_3 0.00265E−04	7.27	1372	1382

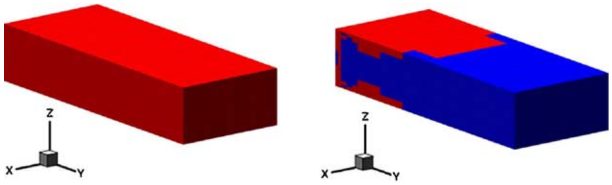

Fig. 3. Quantity of interest Q_1: worst distribution E (left) and v (right).

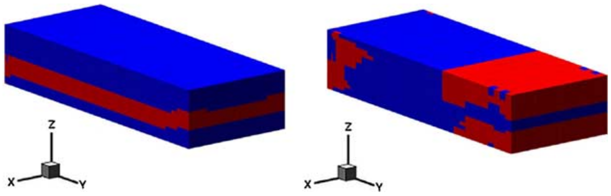

Fig. 4. Quantity of interest Q_2: worst distribution E (left) and v (right).

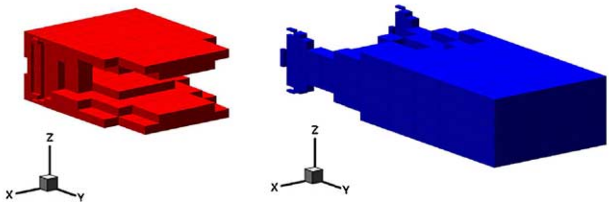

Fig. 5. Split-view of coefficient distribution v for Q_1: positive (left) and negative (right).

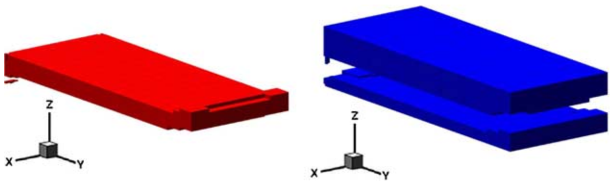

Fig. 6. Split-view of coefficient distribution E for Q_2: positive (left) and negative (right).

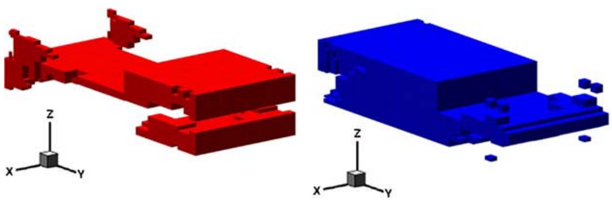

Fig. 7. Split-view of coefficient distribution v for Q_2: positive (left) and negative (right).

Q_2) with respect to E and v. We point out that a positive perturbation of E or v implies an increase in Q_1 or Q_2, illustrated in red on the left; and a negative perturbation implies a decrease, illustrated in blue on the right. The results in Table 1 suggest that, in the worst-case-scenario, small variations in E and v can lead to very large deviations in the values of rather benign quantities of interest.

Acknowledgments

This work has been supported by an ITR grant 0205181 from National Science Foundation and by grant N00014-95-0401 from the Office of Naval Research. The calculation presented were done by Drs. Fabio Nobile and Yusheng Feng who implemented algorithm to estimate error due to uncertainty based on software developed by Dr. Leszek Demkowicz. Drs. Nobile's and Tempone's work was supported by an ICES Post Doctoral Fellowship Program. The adaptive quadrature algorithm used to compute bound in (5.3c) on uncertainty error was developed and implemented by Drs. Nobile and Tempone. The bounds used on the variances in the coefficients were the result of experimental tests performed by Dr. Kenneth Liechti and P. Hosatte. Drs. Leszek Demkowicz, and James C. Browne provided valuable advice during the course of this work.

Appendix A. Derivation of the relation (4.9)

Recall the primal and dual problem seeking $(\mathbf{u},\mathbf{p}) \in V \times V$ are such that $\forall \mathbf{v} \in V$,

$$B_{\boldsymbol{\beta}}(\mathbf{u},\mathbf{v}) = \int_D \boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{u}) : \nabla\mathbf{v}\,\mathrm{d}x = F(\mathbf{v}) \tag{A.1}$$

and

$$B'_{\boldsymbol{\beta}}(\mathbf{u};\mathbf{v},\mathbf{p}) = \int_D \boldsymbol{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u})\nabla\mathbf{v} : \nabla\mathbf{p}\,\mathrm{d}x = Q(\mathbf{v}), \tag{A.2}$$

where $\boldsymbol{\Phi}$ is given by (2.7) and $Q(\mathbf{v})(= Q'(\mathbf{u};\mathbf{v}))$ is now a linear functional on V.

In the first-order perturbation method, we consider perturbations in $\boldsymbol{\beta}$, $\mathbf{u}$ and $\mathbf{p}$ about mean values $\bar{\boldsymbol{\beta}}, \bar{\mathbf{u}}$ and $\bar{\mathbf{p}}$ of the form,

$$\boldsymbol{\beta} = \bar{\boldsymbol{\beta}} + \delta\boldsymbol{\beta}(\mathbf{x}); \quad \mathbf{u} = \bar{\mathbf{u}} + \delta\mathbf{u}; \quad \mathbf{p} = \bar{\mathbf{p}} + \delta\mathbf{p}, \tag{A.3}$$

$(\bar{\mathbf{u}}(\mathbf{x}) = \mathbf{u}(\bar{\boldsymbol{\beta}},\mathbf{x}); \bar{\mathbf{p}}(\mathbf{x}) = \mathbf{p}(\bar{\boldsymbol{\beta}},\mathbf{x}))$ and we truncate expansions of the integrands in (A.1) and (A.2) by neglecting terms of quadratic or higher order terms in the perturbations. Noting that

$$\boldsymbol{\sigma}(\boldsymbol{\beta};\nabla\mathbf{u}) = \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}}) + \partial_{\boldsymbol{\beta}}\boldsymbol{\sigma}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}})\delta\boldsymbol{\beta} + \partial_{\nabla_s\mathbf{u}}\boldsymbol{\sigma}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}})\nabla\delta\mathbf{u} + \mathrm{HOT}, \tag{A.4}$$

$$\boldsymbol{\Phi}(\boldsymbol{\beta};\nabla\mathbf{u}) = \boldsymbol{\Phi}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}}) + \partial_{\boldsymbol{\beta}}\boldsymbol{\Phi}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}})\delta\boldsymbol{\beta} + \partial_{\nabla_s\mathbf{u}}\boldsymbol{\Phi}(\bar{\boldsymbol{\beta}};\nabla\bar{\mathbf{u}})\nabla\delta\mathbf{u} + \mathrm{HOT} \tag{A.5}$$

(HOT = high-order terms), we see that, to within first-order terms, and for any $\mathbf{v}$,

$$F(\mathbf{v}) \approx \int_D (\bar{\boldsymbol{\sigma}} : \nabla\mathbf{v} + \partial_{\boldsymbol{\beta}}\bar{\boldsymbol{\sigma}}\delta\boldsymbol{\beta} : \nabla\mathbf{v} + \partial_{\nabla_s\mathbf{u}}\bar{\boldsymbol{\sigma}}\nabla\delta\mathbf{u} : \nabla\mathbf{v})\,\mathrm{d}x, \tag{A.6}$$

$$Q(\mathbf{v}) \approx \int_D (\bar{\boldsymbol{\Phi}}\nabla\mathbf{v} : \nabla\bar{\mathbf{p}} + \partial_{\boldsymbol{\beta}}\bar{\boldsymbol{\Phi}}\delta\boldsymbol{\beta}\nabla\mathbf{v} : \nabla\bar{\mathbf{p}} + \partial_{\nabla_s\mathbf{u}}\bar{\boldsymbol{\Phi}}\nabla\delta\mathbf{u}\nabla\mathbf{v} : \nabla\bar{\mathbf{p}} + \bar{\boldsymbol{\Phi}}\nabla\mathbf{v} : \nabla\delta\bar{\mathbf{p}}) \tag{A.7}$$

and

$$\begin{aligned} Q(\mathbf{u}) &= Q(\bar{\mathbf{u}}) + Q(\delta\mathbf{u}) \\ &\approx \int_D (\bar{\boldsymbol{\Phi}}\nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \partial_{\boldsymbol{\beta}}\bar{\boldsymbol{\Phi}}\delta\boldsymbol{\beta}\nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \partial_{\nabla_s\mathbf{u}}\bar{\boldsymbol{\Phi}}\nabla\delta\mathbf{u}\nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \bar{\boldsymbol{\Phi}}\nabla\bar{\mathbf{u}} : \nabla\delta\bar{\mathbf{p}} + \bar{\boldsymbol{\Phi}}\nabla\delta\mathbf{u} : \nabla\bar{\mathbf{p}})\,\mathrm{d}x, \end{aligned} \tag{A.8}$$

where $\bar{\boldsymbol{\sigma}} \equiv \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}}; \nabla\bar{\mathbf{u}})$ and $\bar{\boldsymbol{\Phi}} \equiv \boldsymbol{\Phi}(\bar{\boldsymbol{\beta}}; \nabla\bar{\mathbf{u}})$, etc. From (A.6), we obtain the relations,

$$F(\mathbf{v}) = \int_D \bar{\boldsymbol{\sigma}} : \nabla\mathbf{v}\, \mathrm{d}x, \tag{A.9}$$

$$-\int_D \partial_\beta \bar{\boldsymbol{\sigma}} \delta\boldsymbol{\beta} : \nabla\mathbf{v}\, \mathrm{d}x = \int_D \bar{\boldsymbol{\Phi}} \nabla \delta\mathbf{u} : \nabla\mathbf{v}\, \mathrm{d}x, \tag{A.10}$$

$\forall \mathbf{v} \in V$, and from (A.8), we have

$$Q(\bar{\mathbf{u}}) = \int_D \bar{\boldsymbol{\Phi}} \nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}}\, \mathrm{d}x, \tag{A.11}$$

$$Q(\delta\mathbf{u}) = \int_D (\partial_\beta \bar{\boldsymbol{\Phi}} \delta\boldsymbol{\beta} \nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \partial_{\nabla_s \mathbf{u}} \bar{\boldsymbol{\Phi}} \nabla\delta\mathbf{u} \nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \bar{\boldsymbol{\Phi}} \nabla\bar{\mathbf{u}} : \nabla\delta\bar{\mathbf{p}} + \bar{\boldsymbol{\Phi}} \nabla\delta\mathbf{u} : \nabla\bar{\mathbf{p}})\, \mathrm{d}x \tag{A.12}$$

it being understood that these equations hold to within first-order terms.

Setting $\mathbf{v} = \bar{\mathbf{u}}$ in (A.7) and using (A.11) gives

$$\int_D \bar{\boldsymbol{\Phi}} \nabla\bar{\mathbf{u}} : \nabla\partial\bar{\mathbf{p}}\, \mathrm{d}x = -\int_D (\partial_\beta \bar{\boldsymbol{\Phi}} \delta\boldsymbol{\beta} \nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}} + \partial_{\nabla_s \mathbf{u}} \bar{\boldsymbol{\Phi}} \nabla\partial\mathbf{u} \nabla\bar{\mathbf{u}} : \nabla\bar{\mathbf{p}})\, \mathrm{d}x. \tag{A.13}$$

Thus, (A.12) reduces to

$$Q(\delta\mathbf{u}) = \int_D \bar{\boldsymbol{\Phi}} \nabla\delta\mathbf{u} : \nabla\bar{\mathbf{p}}\, \mathrm{d}x. \tag{A.14}$$

Introducing now (A.10) gives

$$Q(\delta\mathbf{u}) = -\int_D \partial_\beta \boldsymbol{\sigma}(\bar{\boldsymbol{\beta}}, \nabla\bar{\mathbf{u}}) \delta\boldsymbol{\beta} : \nabla\bar{\mathbf{p}}\, \mathrm{d}x. \tag{A.15}$$

as asserted.

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