A Toolbox for Validation of Nonlinear Finite Element Models

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Abbreviations

DTRA	Defense Threat Reduction Agency
HFPB	High fidelity, physics-based
PCD	Principal components decomposition
SVD	Singular value decomposition

Keywords
Model-test correlation, Model updating, Modeling uncertainty, Predictive accuracy, Surrogate model

ABSTRACT

With increasingly powerful computational resources at our disposal, it is becoming commonplace to use analytical predictions in lieu of experimentation for characterization of physical systems and events. This trend, with its perceived potential for reducing costs, is the basis for the simulation-based procurement initiatives currently gaining momentum within the Government and industry. However, a simulation-based approach is often sold to decision-makers via plausible visualizations of model simulation results; the simulations themselves having only been validated in an ad hoc manner using anecdotal comparisons with real events. Experience has shown that, while simulation using physics-based models may lead to *qualitatively correct* results, there can be large *quantitative discrepancies* between simulation and experimental results for a given physical event, and between simulation results from different analysts for the same event. Obviously, for simulation-based procurement to be a viable alternative to more traditional test-based procurement, the quantitative accuracy of the simulations must be insured. To do this requires at least a modicum of experimental data (perhaps at the component or subsystem level) to serve as a yardstick with which the accuracy of simulation results can be measured. And it requires minimizing the differences between corresponding analytical and experimental results in physically meaningful ways, as well as characterizing the ability of the models to predict future events. This paper describes a toolbox for the validation of nonlinear finite element models. The toolbox includes tools for quantitatively updating model parameters based on the differences between test results and analytical predictions, as well as estimating the predictive accuracy of the model based on generically similar comparisons. Use of the toolbox is illustrated for a DYNA model of a reinforced concrete wall subjected to blast loading.

INTRODUCTION

The Defense Threat Reduction Agency (DTRA) has promoted the verification and validation of nonlinear dynamic codes and models for many years. Numerous precision tests have been conducted over the years to support this effort, leading to codes such as SHARC (Hikida, et al., 1988), AUTODYN (Century Dynamics, 1989), and DYNA3D (Whirley and Engleman, 1993) that generate high fidelity physics-based (HFPB) models of explosive loads on structures and of structural response to those loads in terms of structural damage and residual strength. The purpose of verification and validation is to confirm the stability and accuracy of numerical algorithms and the behavior of material models under controlled conditions, so that the codes may be used with greater confidence to extrapolate limited test experience to a range of practical applications. The difficulty with this approach has been the lack of a coherent methodology and computational tools for its implementation, especially tools for model-test correlation, model updating, and predictive accuracy assessment.

The organization of the tools developed under this project is shown in Figure 1. The model-test correlation portion includes tools for statistical analysis of the differences between model predictions and test measurements based on difference analysis or principal component comparisons. The model updating section includes tools for parameter sensitivity analysis, parameter effects analysis, and response surface modeling. It also includes tools for the generation of surrogate models, as well as various continuous and discrete parameter estimation algorithms. The predictive accuracy assessment portion includes a tool for evaluating modeling uncertainty based on principal components derived from analysis and test data, and a tool for propagating these statistics through models to evaluate their predictive accuracy. Tools for preparation of data for these analyses are also included.

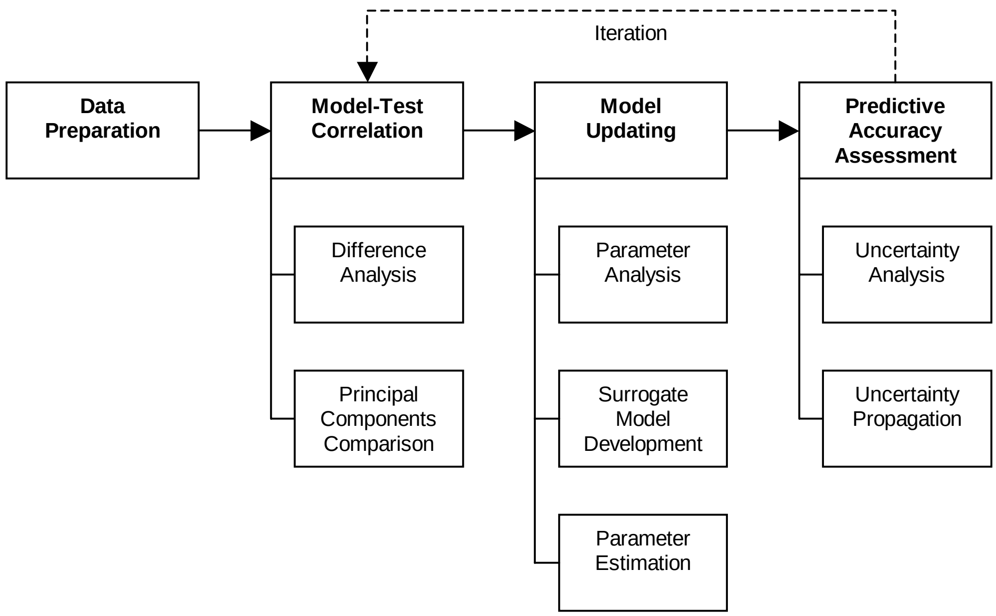


Figure 1. Design for Nonlinear Model Validation Toolbox

APPROACH

The tools for model validation are based on principal components analysis of model predictions and experimental measurements. Principal components analysis facilitates comparisons of data useful for model-test correlation and uncertainty analysis. It also provides a simple means of generating local, surrogate models useful for parameter estimation with computationally intensive finite element models.

Principal Components Analysis

Principal components analysis is based on the singular value decomposition (SVD) of a collection of time-histories (Klema and Laub, 1980). Let $x(t)$ denote a response time-history, where x may be displacement, velocity, or any time-dependent quantity of interest. A response matrix, X, is a collection of discretized time-histories,

$$X = \begin{bmatrix} x_1(t_1) & \cdots & x_1(t_n) \\ \vdots & \ddots & \vdots \\ x_m(t_1) & \cdots & x_m(t_n) \end{bmatrix} \tag{1}$$

where each row corresponds to either a different measurement location or set of physical parameters, and each column corresponds to response at a specific time. The SVD of X may be written

$$X = U \Sigma V^T \tag{2}$$

where U is an orthonormal $m \times m$ matrix whose columns are the left singular vectors of X, Σ is an $m \times n$ matrix containing the singular values of X along the main diagonal and zeros elsewhere, and V is an $n \times n$ orthonormal matrix whose columns correspond to the right singular vectors of X.

The matrices on the right hand side of (2) may be partitioned so that

$$X = \left[\phi \;\vdots\; {}^{\perp}\phi \right] \left[\begin{array}{c|c} D & 0 \\ \hline 0 & 0 \end{array} \right] \left[\begin{array}{c} \eta \\ \hline {}^{\perp}\eta \end{array} \right] \tag{3}$$

where D is the diagonal matrix of nonzero singular values, d_i ($i = 1, \ldots, p \leq \min(m,n)$), ϕ and η are the matrices of left and right principal vectors, respectively, corresponding to the nonzero singular values, and ${}^{\perp}\phi$ and ${}^{\perp}\eta$ span the orthogonal complements of the respective subspaces spanned by ϕ and η. By (3),

$$X = \phi D \eta \tag{4}$$

The columns (rows) of ϕ (η) are pairwise orthonormal, i.e.,

$$\phi^T \phi = \eta \eta^T = I_p \tag{5}$$

where I_p is the *p*-dimensional identity matrix. The factorization given by (4) is called the principal components decomposition (PCD) of the response matrix (Hasselman, Anderson, and Gan, 1998).

Model-Test Correlation

Principal components methods are useful for nonlinear model-test correlation for the same reason that modal properties are useful in linear structural dynamics. In nonlinear models, however, the interpretation of these "modal" properties depends on the selection of response data included in $X(t)$. Nevertheless, there are certain properties of the PCD that can be exploited for purposes of model-test correlation. These properties are suggested by the following equations:

$$\psi = {}^{0}\phi^{T} \phi \tag{6a}$$

$$\Delta D = D - {}^{0}D \tag{6b}$$

$$v = \eta \, {}^{0}\eta^{T} \tag{6c}$$

where ${}^{0}\phi$, ${}^{0}D$, and ${}^{0}\eta$ represent "modal" parameters derived from analysis for comparison with the corresponding "modal" parameters ϕ, D, and η derived from experimental data.

Model Updating

The PCD furnishes a compact representation of the response of a nonlinear model. The scaled right principal vectors, $d_i \eta_i$, represent the response time-histories of the principal components. Each row of the left principal vector matrix, ϕ, denotes the specific linear combination of the principal component response time-histories which reproduces the total response time-history at the corresponding value of the parameter vector, θ, and spatial location of the response.

For example, when each row of the response matrix corresponds to the response at a single location and a unique set of parameters, then each left principal vector can be considered as a function of the parameter vector only. If the left principal vectors are considered as functions of the parameter vector, θ, then $x(t;\theta)$ may be approximated by

$$\hat{x}(t;\theta) = \hat{\phi}(\theta) D\eta(t) = \sum_{i=1}^{q\le p} \hat{\phi}_i(\theta) d_i \eta_i(t) \tag{7}$$

where the columns of $\hat{\phi}(\theta)$, $\hat{\phi}_j(\theta)$, are represented by individual response surfaces (Hasselman, Anderson, and Zimmerman, 1998).

Consequently, one may define a Bayesian objective function of the form

$$J = \left(x - {}^0\hat{x}\right) S_{\varepsilon\varepsilon}^{-1} \left(x - {}^0\hat{x}\right)^T + \left(\theta - \theta_o\right) S_{\theta\theta}^{-1} \left(\theta - \theta_o\right)^T \tag{8}$$

where θ and θ_o represent the current and initial estimates of the variable parameter vectors, respectively, and x and ${}^0\hat{x}$ represent the measured and currently predicted responses, respectively. The covariance matrices $S_{\theta\theta}$ and $S_{\varepsilon\varepsilon}$ represent uncertainties in the initial parameter estimates and response measurements, respectively. Bayesian estimation provides a revised covariance matrix of the updated parameter estimates given by

$$S_{\theta\theta}^* = \left(S_{\theta\theta}^{-1} + T_{x\theta}^T S_{\varepsilon\varepsilon}^{-1} T_{x\theta}\right)^{-1} \tag{9}$$

where $T_{x\theta}$ is the sensitivity matrix, $\partial x / \partial\theta$, relating the response vector to the parameter vector.

Uncertainty Analysis

When the principal components approach is used to represent a nonlinear model, the parameters are ϕ, D, and η, and modeling uncertainty is defined in terms of these parameters. Once a covariance matrix of the modal parameters is obtained, it can be transformed to obtain a covariance matrix of the response variables. The predictive accuracy of the model is thereby determined (Hasselman, Chrostowski, and Ross, 1992, and Anderson, Gan, and Hasselman, 1998).

A first order approximation of the experimental response matrix is given by

$$\Delta X_{ij} = \sum_{k=1}^{N_{mp}} \frac{\partial X_{ij}}{\partial \tilde{r}_k} \Delta\tilde{r}_k \tag{10}$$

where the parameter, $\tilde{r}_k$, is taken to represent any of the elements of the matrices ψ, $\tilde{D}$, or ν, $\tilde{D} = D/\mathrm{Trace}({}^0D)$, and N_{mp} denotes the number of modal parameters collectively contained in ψ, $\tilde{D}$, and ν. Here $\Delta\tilde{r}_k$ is an element of the vector $\Delta\tilde{r}$ with

$$\Delta\tilde{r} = \begin{Bmatrix} \mathrm{vec}\left(\Delta\psi\right) \\ \mathrm{vec}\left(\Delta\tilde{D}\right) \\ \mathrm{vec}\left(\Delta\nu\right) \end{Bmatrix} \tag{11}$$

where $\Delta\psi = \psi - I$, $\Delta\tilde{D} = (D - {}^0D)/\mathrm{Trace}({}^oD)$, and $\Delta\nu = \nu - I$. The derivative of X_{ij} with respect to $\tilde{r}_k$ is

$$\frac{\partial X_{ij}}{\partial \tilde{r}_k} = e_i^T \, {}^0\phi \left(\frac{\partial \psi}{\partial \tilde{r}_k} {}^0D + \frac{\partial \tilde{D}}{\partial \tilde{r}_k} {}^0D + {}^0D \frac{\partial v}{\partial \tilde{r}_k} \right) {}^0\eta_j \tag{12}$$

Equation (10) has a particularly simple form when the matrix, ΔX, is also vectorized as $\Delta u = \text{vec}(\Delta X)$,

$$\Delta u = T_{u\tilde{r}} \Delta \tilde{r} \tag{13}$$

where the elements of $T_{u\tilde{r}}$ are populated by the scalar values given in (12).

The covariance matrix of the vector $\tilde{r}$ is given by

$$S_{\tilde{r}\tilde{r}} = \mathrm{E}\left[\Delta\tilde{r}\Delta\tilde{r}^T \right] = \frac{1}{N} \sum_{i=1}^{N} \Delta\tilde{r}_i \Delta\tilde{r}_i^T \tag{14}$$

where the index, *i*, is on a particular data set consisting of corresponding analysis-test pairs, *N* is the total number of data sets in the sample, and the analytical model is assumed to predict mean response. When the analytical model contains bias-type error, as may be indicated when replicate test measurements are available, then

$$S_{\tilde{r}\tilde{r}} = \mathrm{E}\left[\left(\Delta\tilde{r} - \mu_{\Delta\tilde{r}}\right)\left(\Delta\tilde{r} - \mu_{\Delta\tilde{r}}\right)^T \right] = \frac{1}{N-1} \sum_{i=1}^{N} \left[\left(\Delta\tilde{r}_i - \mu_{\Delta\tilde{r}}\right)\left(\Delta\tilde{r}_i - \mu_{\Delta\tilde{r}}\right)^T \right] \tag{15}$$

where $\mu_{\Delta\tilde{r}}$ is the mean of the vector $\Delta\tilde{r}$.

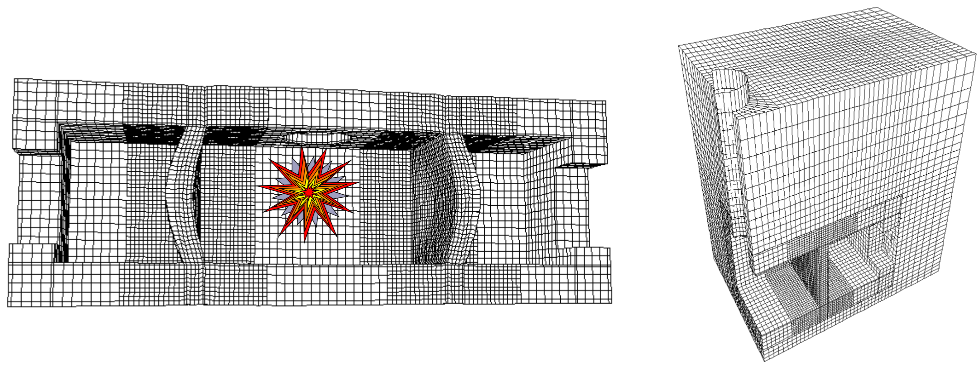
$S_{\tilde{r}\tilde{r}}$ represents the generic modeling uncertainty inherent in analytical predictions of the response matrix, *X*, based on normalized comparisons of previous analysis and test data. In order to evaluate the predictive accuracy of a new response prediction, Equation (13) is used, with the understanding that $T_{u\tilde{r}}$ is evaluated with respect to the new model, i.e., the values of ${}^0\phi$, ${}^0D$, and ${}^0\eta$ representing the modal parameters of the *new* model, rather than those of the models that have been correlated with previous test data. Then

$$S_{uu} = \mathrm{E}\left[\Delta u \Delta u^T \right] = T_{u\tilde{r}} S_{\tilde{r}\tilde{r}} T_{u\tilde{r}}^{\ T} \tag{16}$$

DISCUSSION OF RESULTS

To illustrate these concepts the parameters of a complex, nonlinear system model were updated using available test data. The physical scenario for the example is depicted in Figure 2a and consists of a three-room, buried, reinforced concrete structure subjected to blast loading in the center room. Experimental measurements included blast overpressures inside the room and accelerations of the two interior walls. Accelerations were integrated to obtain displacements.

The corresponding model shown if Figure 2b was a quarter-symmetry, nonlinear finite element model. This model consisted of approximately 80,000 continuum elements for the concrete and surrounding soil, and roughly 20,000 structural beam elements for the steel reinforcement. A cold joint near the bottom of the interior wall was explicitly modeled. The material models contained dozens of parameters, many of which were candidates for estimation. Since the loading was distributed and available input measurements were few, an intermediate input model was required. This model was a computational fluid dynamics model of the interior room pressure. A preliminary validation of the input model was performed by a third party using available pressure data.



(a) Physical scenario (without soil) (b) HFPB quarter-symmetry model

Figure 2. Example Problem

The pre-update predictive accuracy of the model is illustrated in Figure 3. The predicted and measured responses at the center of the wall are shown, along with $\pm 2\sigma$ uncertainty bands. These bands were based on an unbiased estimate of the measurement uncertainty for the center wall response using principal components analysis. Note that the measured response generally falls within the uncertainty bands, but that the bands fail to capture the experimental behavior in the neighborhood of 0.002 seconds.

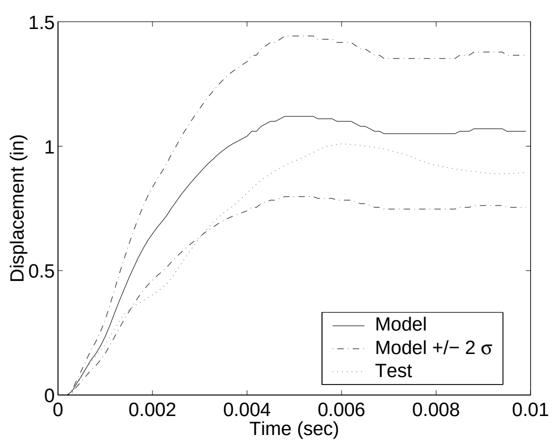
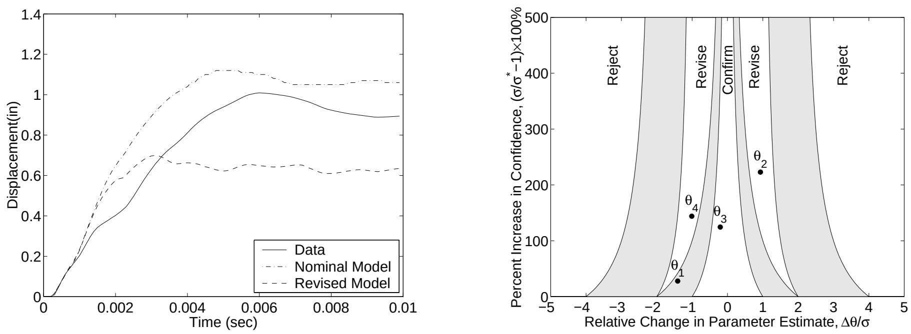


Figure 3. Pre-Update Predictive Accuracy

The estimation problem consisted of using measurements of the displacement of the interior wall to update some of the concrete and steel material parameters so that the predicted response matched the test data. Measurements used for estimation included sampled displacement histories at four locations on the wall. Estimation parameters were chosen by a three-stage process comprised of engineering judgement, sensitivity analysis, and parameter effects analysis. The results of this process indicated that the concrete strain rate enhancement and shear dilatancy, the steel reinforcement tensile strength, and the cold joint friction were the most significant parameters. Since the input model was tentatively validated, input parameters were excluded from consideration for the initial estimation.

Numerous attempts to produce meaningful parameter estimates were made. The results of a typical attempt are shown for the center wall response in Figure 4. Figure 4a indicates that the revised model is noticeably worse than the nominal model with respect to the details of the response prediction. Figure 4b illustrates the quality of the parameter estimates.



(a) Time history comparison

(b) Quality of the estimates

Figure 4. Results of the Initial Estimation

The statistics of the initial parameter estimates are given in Table 1. Even though the posterior variances of the estimates are smaller than the prior variances, the posterior correlation matrix contains some large off-diagonal elements. Using an absolute correlation of 0.25 as a measure of significance implies that the concrete strain rate enhancement is correlated with the tensile strength of the steel reinforcement and the cold joint friction. An even higher degree of correlation can be noted between the concrete shear dilatancy and the steel reinforcement strength. These results are clearly unacceptable.

Table 1. Initial Prior and Posterior Estimate Statistics

Parameter		Concrete Strain Rate Enhance.	Steel Rein. Tensile Strength	Concrete Shear Dilatancy	Cold Joint Friction
Symbol		θ_1	θ_2	θ_3	θ_4
Prior Est. Posterior Est. Prior Var. Posterior Var.		0.0289 0.0434 1.06×10^{-4} 6.51×10^{-5}	64,000 60,273 1.60×10^{7} 1.53×10^{6}	0.500 0.531 2.25×10^{-2} 4.46×10^{-3}	0.200 0.339 1.89×10^{-2} 3.18×10^{-3}
Posterior Corr. Matrix	θ_1	1	0.388	-0.231	-0.597
	θ_2		1	-0.924	-0.148
	θ_2			1	-0.222
	θ_4	(Sym.)			1

After initial parameter estimation attempts failed, all available auxiliary information was reviewed to determine if it could be used to eliminate one or more of the parameters. This information included tensile test results for the steel reinforcement, as well as post-test measurements of the slip across the cold joint. Twenty-five independent measurements of the strength of steel reinforcing bars from the same batch used to construct the test structure were available. The results of these tests indicated that the prior value of the reinforcement strength was accurate, and this parameter was eliminated from further consideration. The measured cold joint slip was matched by the nominal model prediction, indicating that the cold joint friction may be a candidate for elimination.

Before proceeding with additional estimation attempts, the input model was reviewed to determine if any adjustments were required. Figure 5 compares the pressure and cumulative impulse measurements and predictions at one of the pressure gage locations. With the exception of the peak of the initial pulse, the predicted pressure history matched the data well, as indicated in the upper plot of the figure. However, the cumulative impulse data differed significantly from the model prediction, as shown in the lower plot. Simply scaling the predicted initial pulse by a factor of 0.6 rectified the problem at all locations for which data were available, as indicated in the figure. Similar scaling was applied to all inputs to the finite element model.

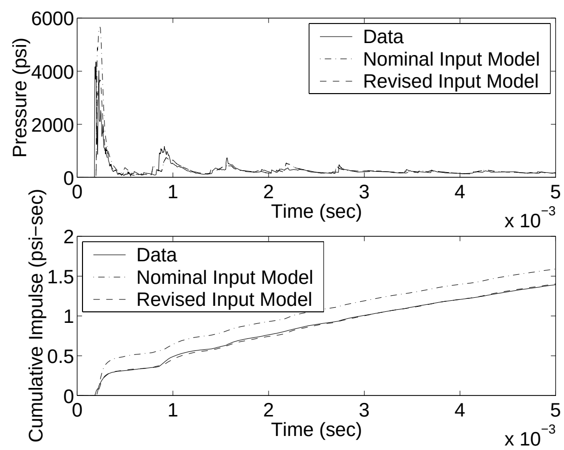
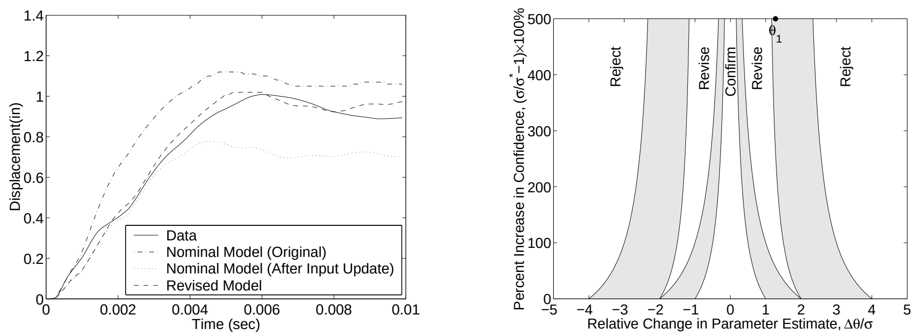


Figure 5. Input Model Update

The final estimation process began by using the revised input model to generate a new model prediction. This indicated that the cold joint friction had to be reduced to a lower level (0.05) so that the cold joint slip was accurately modeled. The finite element model was then used to generate the new nominal prediction using the revised inputs and cold joint friction. Parameter estimates were generated using the two remaining parameters, the concrete strain rate enhancement and shear dilatancy. The results of these efforts indicated that the shear dilatancy should not be revised even though the posterior correlation between the two parameters was high. The final estimation attempt used only the strain rate enhancement, with the dilatancy fixed at its nominal value.

The final estimated value of the strain rate enhancement parameter was 0.0158, or about 55 percent of the original nominal value. The posterior variance estimate was two orders of magnitude less than the prior estimate. The results of the final estimation process are illustrated in Figure 6. Figure 6a compares the measured displacement history at the center of the wall with that predicted by the model with the original nominal, modified nominal, and revised value of the parameters. Similar comparisons were made at other locations where data were available. The results clearly indicated that the revised model not only matched the data very well in a mean square sense, but also captured the character of the data significantly better than the original nominal model. Figure 6b shows the high quality of the parameter estimate. Therefore, one is led to conclude that the estimated parameter values are likely to provide accurate predictions for future analyses using the same materials.



(a) Time history comparison (b) Quality of the estimate

Figure 6. Results of the Final Estimation

Figure 7 depicts the pre-update predictive accuracy of the model. As before, the predicted and measured responses at the center of the wall are shown, along with $\pm 2\sigma$ uncertainty bands. Note that the measured response falls completely within the uncertainty bands.

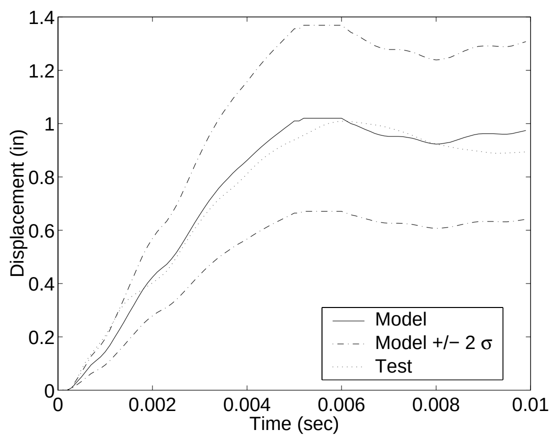


Figure 7. Post-Update Predictive Accuracy

SUMMARY

The principal components-based nonlinear model validation methodology summarized in this paper provides a means of systematically comparing model predictions with available data and updating model parameters to increase the fidelity of response predictions. This is a vast improvement over traditional ad hoc techniques. Included in the methodology are tools for evaluating the statistical significance and consistency of the parameter estimates, and the predictive accuracy of the updated model. These tools enable the analyst to confirm that the estimated parameter values are statistically meaningful, a prerequisite for true model improvement, and to quantify the degree of uncertainty associated with model simulations, based on structure-specific precision test data if replicate measurements are available, or historical data from generically similar structures and tests if they are not.

Application of the methodology to the air blast response of a reinforced concrete wall demonstrated statistical parameter estimation and predictive accuracy evaluation of a nonlinear HFPB model. Principal components analysis was instrumental in generating the fast-running approximate model used for function approximation in the nonlinear Bayesian parameter estimation, and as a means for quantifying modeling uncertainty in the evaluation of predictive accuracy. The same computational tools are currently being applied to other problems involving weapon-target interaction.

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