# AN UPDATED TOOLBOX FOR VALIDATION AND UNCERTAINTY QUANTIFICATION OF NONLINEAR FINITE ELEMENT MODELS

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*Abbreviations*

| | |
|---|---|
| DIF | Dynamic Increase Factor |
| DTRA | Defense Threat Reduction Agency |
| FEM | Finite Element Model |
| HFPB | High Fidelity, Physics-Based |
| PC | Principal Components |
| PCD | Principal Components Decomposition |
| RC | Reinforced Concrete |
| SVD | Singular Value Decomposition |

*Keywords: Model-Test Correlation, Model Updating, Validation, and Verification, Uncertainty Quantification* Predictive Accuracy, Nonlinear Finite Element Model (FEM), Surrogate Model

## ABSTRACT

It is becoming commonplace to use numerical simulations supported by limited experimentation for the characterization of physical phenomena. 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. Insuring the quantitative viability of a simulation-based procurement still requires some experimental data upon which the assessment of simulation accuracy can be based. In addition, it requires minimizing the differences between corresponding analytical and experimental results in physically meaningful ways, and characterizing the ability of the models to predict future events. The purpose of model validation and uncertainty quantification is to confirm the correctness and credibility of numerical simulations, so that the underlying models may be used with greater confidence to extrapolate limited test experience to a range of practical applications.

In this paper, an advanced principal components-based computational procedure is demonstrated by validating the DYNA models used to achieve HFPB numerical simulations of physical processes important to assessing weapon-target interaction. Bayesian statistical parameter estimation is used to estimate material parameters that cannot be measured directly, such as strain rate enhancement and shear dilatency in reinforced concrete structures. This demonstration is performed using an updated MATLAB® Nonlinear Model Validation and Verification Toolbox. The work reported in this paper has resulted in improvements to the original Toolbox. A multi-level parameter estimation procedure is implemented to sequentially accumulate information from prior estimates in a Fisher information matrix for use in subsequent parameter estimates. The use of a generic uncertainty model in estimating the predictive accuracy of future DYNA simulations is enhanced through the use of a reduced set of principal component metrics and a basis augmentation technique.

## 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 comparison, model updating, and predictive accuracy assessment.

The organization of the tools developed under this project is shown in Figure 1. The model-test comparison portion includes tools for statistical analysis of the differences between model predictions and test measurements based on either direct or principal components 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 generic 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, such as scaling, shifting, interpolation, etc., are also included.

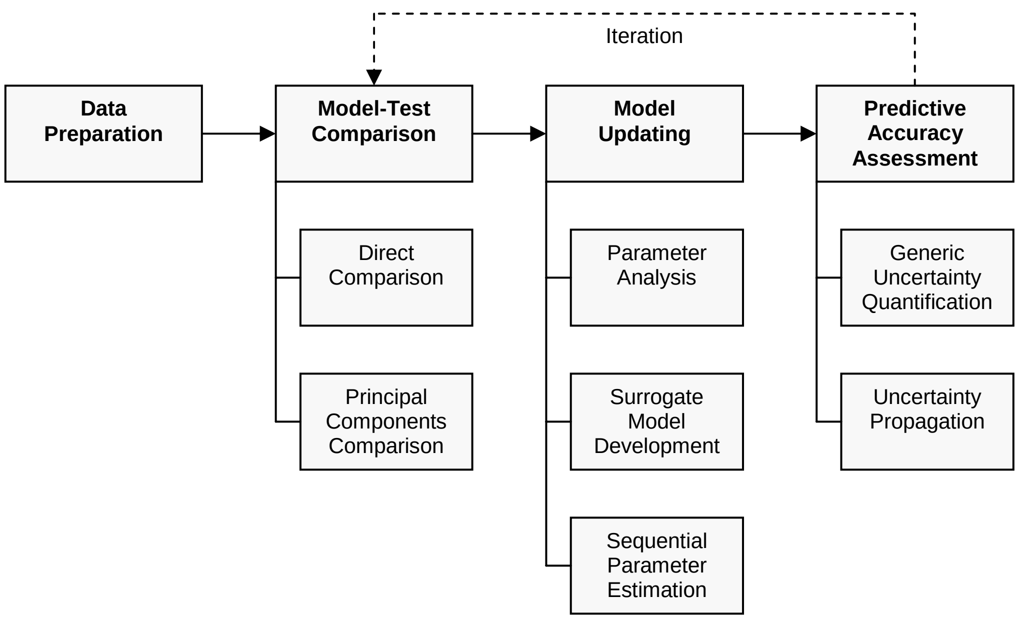



Figure 1. Design for Updated Nonlinear Model Validation Toolbox

## THEORETICAL 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 updating and uncertainty analysis. It provides a simple means of generating local, surrogate models useful for parameter estimation with computationally intensive finite element models.

The following subsections update the Theoretical Approach outlined in (Anderson, et al, 2000), using a more conventional notation. The basic approach is the same as that in (Anderson, et al, 2000), so that the same text and same equations can be used with the new notation. Updates to the previous methodology appear in Equations (6d,e), (9b) and (11) that introduce, respectively,

- Basis augmentation to the improve the accuracy of uncertainty analysis,
- The use of Fisher information matrices to accumulate information from prior estimates in sequential estimation, and
- The use of a reduced set of uncertainty metrics for uncertainty quantification. The reduced set removes redundancies in the original set, and reduces the number of metrics by nearly half.

This paper along with the earlier paper (Anderson, et al, 2000) constitute a complementary set in that the parallel development of the theory in two notational systems provide a link between previous papers, and those that will be published in the future. The numerical example presented in the next section is also an extension of the numerical example presented in (Anderson, et al, 2000), in the sense that this example takes up where the previous example ended.

*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 as

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

where $U$ is an orthonormal $m \times m$ matrix whose columns are the left singular vectors of $X$, $\Sigma$ 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

$$X = \left[ {}^{\circ}U \;\middle|\; {}^{\perp}U \right] \left[ \begin{array}{c|c} {}^{\circ}\Sigma & 0 \\ \hline 0 & 0 \end{array} \right] \left[ \begin{array}{c} {}^{\circ}V^T \\ \hline {}^{\perp}V^T \end{array} \right], \tag{3}$$

where ${}^{\circ}\Sigma$ is the diagonal matrix of nonzero singular values, $\sigma_i$ ($i = 1,\ldots, p \le \min(m,n)$), ${}^{\circ}U$ and ${}^{\circ}V$ are the matrices of left and right principal vectors, respectively, corresponding to the nonzero singular values, and ${}^{\perp}U$ and ${}^{\perp}V$ span the orthogonal complements of the respective subspaces spanned by ${}^{\circ}U$ and ${}^{\circ}V$. By (3),

$$X = {}^{\circ}U\,{}^{\circ}\Sigma\,{}^{\circ}V^T. \tag{4}$$

The columns (rows) of ${}^{\circ}U$ (${}^{\circ}V$) are pairwise orthonormal, i.e.,

$${}^{\circ}U^T\,{}^{\circ}U = {}^{\circ}V^T\,{}^{\circ}V = I_p, \tag{5}$$

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). **For notational simplicity and convenience, the left superscripts $^{\circ}$ in Eq. (4) will be dropped in subsequent formulations.**

*Model-Test Comparison*

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:

$$\tilde{U} = U_{mod}^{T} U_{exp} , \qquad (6a)$$

$$\tilde{\Sigma} = \Sigma_{mod}^{-1} \Sigma_{exp} , \qquad (6b)$$

$$\tilde{V} = V_{mod}^{T} V_{exp} , \qquad (6c)$$

provided that each of left and right singular vectors satisfies

$$1 - \tilde{U}_j^T \tilde{U}_j < \varepsilon , \qquad (6d)$$

$$1 - \tilde{V}_j^T \tilde{V}_j < \varepsilon , \qquad (6e)$$

where $U_{mod}$, $\Sigma_{mod}$, and $V_{mod}$ represent "modal" parameters derived from analysis for comparison with the corresponding "modal" parameters $U_{exp}$, $\Sigma_{exp}$, and $V_{exp}$ derived from experimental data. When (6d) and (6e) are not satisfied, usually because of too few rows in (1), then some form of basis augmentation is required as provided for in the toolbox.

*Model Updating*

The PCD furnishes a compact representation of the response of a nonlinear model. The scaled right principal vectors, $\sigma_i V_i$, represent the response time-histories of the principal components. Each row of the left principal vector matrix, $U$, 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, $\theta$, 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, $\theta$, then $x(t;\theta)$ may be approximated by

$$\hat{x}(t;\theta) = \hat{U}(\theta) \Sigma V^T(t) = \sum_{i=1}^{q \le p} \hat{U}_i(\theta) \Sigma_{ii} V^T{}_i(t) , \qquad (7)$$

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

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

$$J = \left(\vec{X} - {}^{\circ}\vec{X}\right) S_{XX}^{-1} \left(\vec{X} - {}^{\circ}\vec{X}\right)^T + (\theta - \theta_o) S_{\theta\theta}^{-1} (\theta - \theta_o)^T , \qquad (8)$$

where $\theta$ and $\theta_o$ represent the current and initial estimates of the variable parameter vectors, respectively, and $\vec{X}$ and ${}^{\circ}\vec{X}$ represent the measured and currently predicted vectorized responses, respectively. The covariance matrices $S_{\theta\theta}$ and $S_{XX}$ represent uncertainties in the initial parameter estimates and test data, respectively. The corresponding Fisher information matrices, $F_{\theta\theta}$ and $F_{XX}$, are the inverses (or pseudoinverses) of $S_{\theta\theta}$ and $S_{XX}$, respectively. Bayesian estimation provides a revised covariance matrix and a corresponding revised Fisher information matrix of the updated parameter estimates given respectively by

$$S_{\theta\theta}^{*} = \left( S_{\theta\theta}^{-1} + T_{X\theta}^{T} \, S_{XX}^{-1} \, T_{X\theta} \right)^{-1} \tag{9a}$$

and

$$F_{\theta\theta}^{*} = F_{\theta\theta} + T_{X\theta}^{T} \, F_{XX} \, T_{X\theta} \, . \tag{9b}$$

where $T_{X\theta}$ is the sensitivity matrix, $\partial X / \partial \theta$, relating the response vector to the parameter vector, and $F$ denotes the Fisher information matrix.

The Fisher information matrix is defined as the inverse of the corresponding covariance matrix (Walter and Pronzato, 1997). When the symmetric non-negative-definite covariance matrix is rank-deficient (i.e. singular), the inverse implies a pseudo-inverse satisfying the Moore-Penrose conditions (Golub and Van Loan, 1989). Information content may be quantified in terms of a scalar *information index*, defined as the trace of the Fisher information matrix normalized by pre and post-multiplying it by a diagonal matrix of the mean values of the metrics used to define the covariance matrix. For example, in the case of a one-by-one covariance matrix, i.e. a scalar, the information index is simply the inverse of the coefficient of variation squared.

Information content is relative to the metrics used to define the covariance matrix. Therefore, the information content of the measurement information matrix and that of the parameter information matrix may not be compared directly. However, if the measurement information matrix is transformed to the parameter space by the proper sensitivity matrix, then the information index of the transformed measurement information matrix, and the prior and updated parameter information matrices, may be compared. The additive nature of information matrices resulting from Bayesian sequential estimation as indicated in Equation (9b) suggests that information is cumulative from one Bayesian update of the parameters to the next.

*Uncertainty Analysis*

When the principal components approach is used to represent a nonlinear model, the parameters are $U$, $\Sigma$, and $V$, 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 response error matrix is given by

$$\Delta X_{ij} = \sum_{k=1}^{N_{mp}} \frac{\partial X_{ij}}{\partial \vec{Y}_k} \Delta \vec{Y}_k \, , \tag{10}$$

where the parameter, $\vec{Y}_k$, is taken to represent any of the elements of the vector $\vec{Y}$, and $N_{mp}$ denotes the number of modal parameters collectively contained in $\vec{Y}$, and $\Delta\vec{Y}_k$ is an element of the vector

$$\Delta\vec{Y} = \begin{Bmatrix} \Delta\vec{\tilde{\Psi}} \\ \Delta\vec{\tilde{\Sigma}} \end{Bmatrix} \in \mathbb{R}^{\,r+r^2} \, , \tag{11}$$

where $\Delta\tilde{\Psi} = \tilde{\Psi} - I$, $\Delta\tilde{\Sigma} = \tilde{\Sigma} - I$, and $\tilde{\Psi} = \Sigma_{mod}{}^{-1}\tilde{U} \quad \Sigma_{mod} \; \tilde{V}^T$. The derivative of $X_{ij}$ with respect to $\vec{Y}_k$ is

$$\frac{\partial X_{ij}}{\partial \vec{Y}_k} = e_i{}^T U_{mod} \left( \frac{\partial \tilde{U}}{\partial \vec{Y}_k} \Sigma_{mod} + \frac{\partial \tilde{\Sigma}}{\partial \vec{Y}_k} \Sigma_{mod} + \Sigma_{mod} \frac{\partial \tilde{V}^T}{\partial \vec{Y}_k} \right) V_{mod_j}^{T} \, . \tag{12}$$

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

$$\Delta \vec{X} = T_{\vec{X}\vec{Y}} \Delta \vec{Y}, \tag{13}$$

where the elements of $T_{\vec{X}\vec{Y}}$ are populated by the scalar values given in (12).

The covariance matrix of the vector $\vec{Y}$ is given by

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

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 the case when a single FEM is used to simulate a range of test conditions, then

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

where $\mu_{\Delta \vec{Y}}$ is the mean of the vector $\Delta \vec{Y}$.

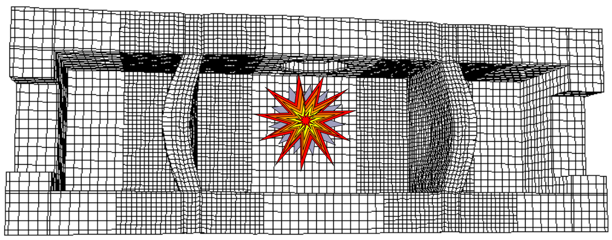
$S_{\vec{Y}\vec{Y}}$ represents the generic modeling uncertainty inherent in analytical predictions of the response matrix, *X*, based on normalized comparisons of previous analysis and test data. In order to evaluate the predictive accuracy of a new response prediction, Equation (13) is used, with the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

$$S_{\vec{X}\vec{X}} = \mathrm{E}\left[ \Delta \vec{X} \Delta \vec{X}^T \right] = T_{\vec{X}\vec{Y}} S_{\vec{Y}\vec{Y}} T_{\vec{X}\vec{Y}}^T . \tag{16}$$

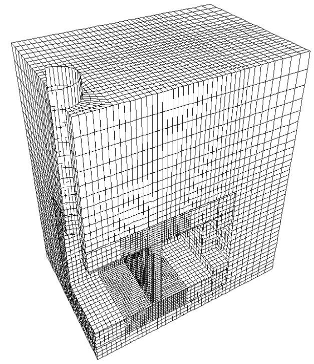
## DISCUSSION OF NUMERICAL EXAMPLE

To illustrate these concepts the parameters of a complex, nonlinear system model were updated using available test data (Anderson, et al., 2000). 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 in Figure 2b is 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)

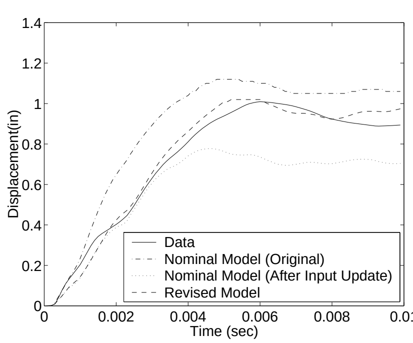


(b) HFPB quarter-symmetry model

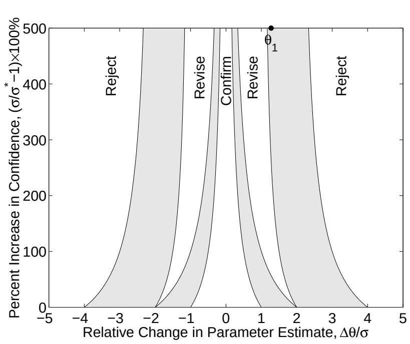
Figure 2. Example Problem

The final estimation process began by using a corrected 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 corrected 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 originally estimated shear dilatancy value of 0.5 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 shear dilatancy fixed at its nominal value.

The final estimated value of the strain rate enhancement parameter was 0.0158. 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 3. Figure 3a 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 3b shows the high quality of the parameter estimate. One is therefore 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 3. Results of the Final Estimation

Figure 4 depicts the pre-update predictive accuracy of the model, i.e., the predictive accuracy of the updated model based on a covariance metric of total modeling uncertainty derived from a generic class of pre-update models. 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, as do the earlier response predictions based on the pre-update (nominal) models shown in Figure 3a.

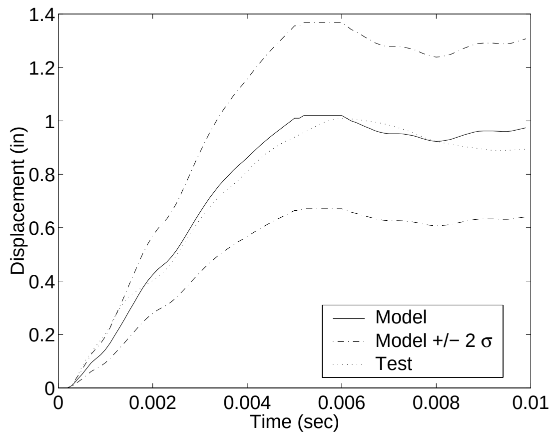



Figure 4. Post-Update Predictive Accuracy

In work performed subsequent to the foregoing as reported in the original paper, an attempt was made to determine how much additional information at the component level, or other lower level of assembly, would be required to obtain uncorrelated or at least weakly correlated estimates of concrete strain rate enhancement or dynamic increase factor (DIF) and concrete shear dilatancy ( $\omega$ ). A numerical experiment was conducted with the prior parameter covariance matrix and corresponding Fisher information matrix given in Equation (9). The original coefficient of variation of the shear dilatancy of 30% was first reduced to 6.5% consistent with information content from reinforced concrete (RC) column test data provided by Karagozian & Case. This increased the information index of the *prior* shear dilatancy estimate going into the system-level Bayesian update (based on the buried three-room RC structure) by a factor of 21.2. Unfortunately, this was not enough to obtain uncorrelated estimates of strain rate enhancement and shear dilatancy; the correlation coefficient was reduced from 0.983% to only 0.977%.

To demonstrate what it would take to reduce the correlation coefficient of the final Bayesian estimate to less than 50%, the information index of the prior estimate of shear dilatancy was artificially reduced progressively by an additional factor of 10, 100, and finally 1000. The results of this experiment on the correlation coefficient between strain rate enhancement and shear dilatancy are shown in Figure 5. Increasing the information content of the shear dilatancy estimate by a factor of 100 implies a reduction in the coefficient of variation by a factor of ten, i.e. an order of magnitude.

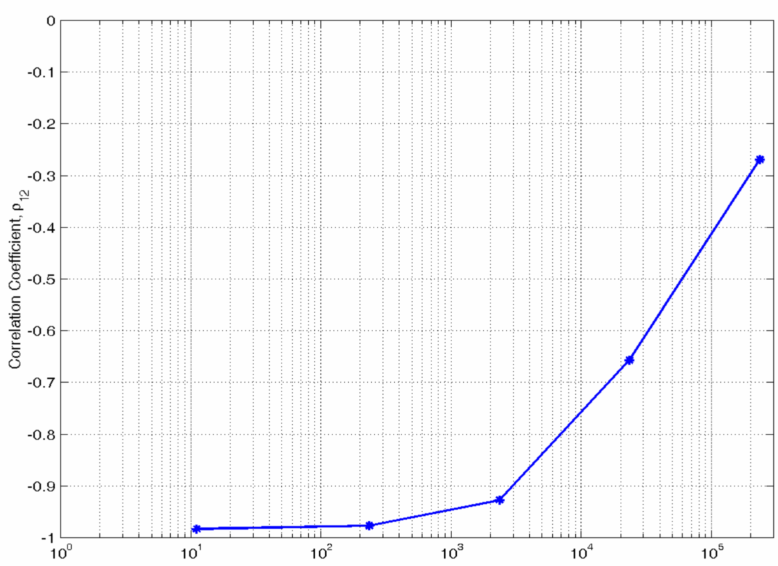
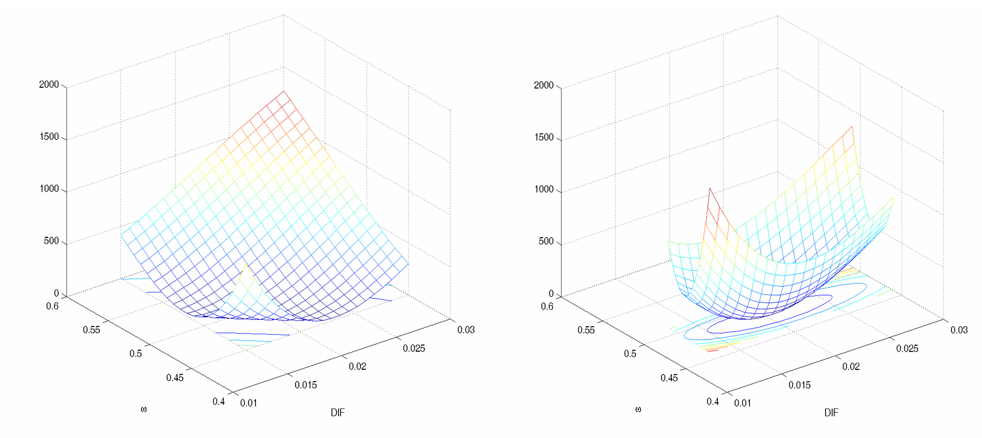



Figure 5. Variation of Correlation Coefficient, $\rho_{12}$ , with Increasing Input Information Content.

Surface plots of the original (1×) and final (1000×) Bayesian objective functions are shown in Figure 6. The strong negative correlation between the original estimates is apparent in Figure 6a, where the surface plot of the Bayesian objective function shows a long valley making an angle of approximately 45 degrees with the two parameter axes. The long valley in Figure 6a becomes a shallow dish in Figure 6b, with a distinct global minimum. The major axis of the elliptical contour plots is shown in Figure 6b to have rotated so as to be nearly parallel with the DIF axis, indicating weak correlation between the two parameters.




(a) Nominal Information Content (b) Enhanced Information Content

Figure 6. Bayesian Objective Functions.

## 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 assessment 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.

Finally, the benefits of a hierarchical or multi-level parameter estimation strategy were demonstrated by extending the example problem presented in Anderson, et al, 2000. The results were presented in terms of information content, and showed how much information would have been required from lower level component tests to significantly reduce the correlation of the estimated concrete strain rate enhancement and shear dilatancy parameters in the concrete constitutive model using system test data in a Bayesian update procedure.

## ACKNOWLEDGEMENTS

The work reported in this paper was sponsored by the Defense Threat Reduction Agency (DTRA). The nonlinear finite element models used in the numerical example were developed by Karagozian & Case, Structural Engineers.

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