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Introduction to Model Validation

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ABSTRACT
The discipline of mathematical model validation is increasing in importance as the value of accurate models of physical systems increases. The fundamental activity of model validation is the comparison of predictions from a mathematical model of a system to the measured behavior of the system. This discussion motivates the need for model validation and introduces some preliminary elements of model validation. This is the first in a sequence of six tutorial presentations on model validation, and will introduce five presentations to follow.

Motivation and Introduction

Mathematical model validation is defined as the “process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model applications.” (ASME, 2006, U.S. DOE, 2000, AIAA, 1998). It is accomplished through the comparison of predictions from a model to experimental results.

There are numerous, related reasons for performing validations of mathematical models. For example:

- There may be a need or desire to replace experimentation with model predictions, and, of course, a corresponding requirement that the model predictions have some degree of accuracy. The need for a model may arise from the fact that it is impossible to test system behavior or survivability in some regimes of operation. For example, a requirement of a building structure may be that it must survive a blast load, yet, for regulatory reasons, it may be impossible to test the structure in blast.
- Alternately, the need for validation may arise from a necessity to prove the reliability of a structure under a broad range of operating conditions or environments. Because it may be expensive to simulate the conditions in the laboratory or realize them in the field, an accurate model is required.
- Another reason for model validation is that a system may be undergoing changes in design that require analyses to assure that the design modifications yield acceptable system behavior. A validated model can be used to assess the system behavior. In all these situations it is useful to confirm analysts’ abilities to produce accurate models.

The sections that follow introduce some ideas and terminology from model validation and list some steps that can be followed to perform a model validation. The paper introduces an example structure with a model to be validated, and carries it through steps involving planning, experiments, and validation comparisons.

There are normally several parties or groups involved in performance of a validation. These are:

- Analysts/modelers. These are persons capable of creating computational models from mathematical and conceptual models, when details of the latter are established. They are capable of anticipating the behaviors of computational models that include specific features.
- Experimentalists. These are persons capable of planning and performing the calibration and validation experiments required in a validation. The experiments may be performed in the laboratory or field, and must normally be high precision experiments with high-accuracy measurements.
- Validation analysts (Persons performing validation comparisons). These are persons knowledgeable about validation procedures, including means for comparing model predictions to experimental outcomes. They should possess intuition regarding the difficulty of obtaining positive validation results given various system measures of response and various means of comparison.

- Customers. These are the persons who authorize a validation analysis – the persons for whom a validation analysis is performed. They are critical to the validation specification because they understand the engineering decision that is required of a model.
- Stakeholders. These are persons with an interest in the outcome of a validation comparison.

All these parties or groups should cooperatively participate in the detailed specification of the validation plan.

This is the first in a sequence of tutorial papers involving the validation of structural dynamic models. The other papers are included in these *Proceedings* and involve:

- Selection of response features and adequacy criteria of structural dynamic systems that can be used to compare predictions from mathematical models to experimental results based on the requirements of the model. (Mayes, 2009a)
- Uncertainty quantification (UQ) of the outcomes of laboratory and field experiments and the parameters and predictions of mathematical models using the theories of probability and statistics. (Paez and Swiler, 2009.)
- UQ of the outcomes of laboratory and field experiments and the parameters and predictions of mathematical models using epistemic modeling and analysis. (Swiler and Paez, 2009.)
- The role of model correlation and calibration in structural dynamics. (Mayes, 2009b)
- An example of model validation based on experiments on a real structure that is modeled with a large, complex finite element model. (Mayes, et al., 2009)

Validation – Definition and Operations

The validation of a mathematical model of a structural dynamic system entails the comparison of predictions from the model to measured results from experiments. Before a well-structured validation comparison can be performed there are several decisions that must be made and criteria defined. This section is a brief summary of items to be considered before commencement of calibration and validation experiments, and model predictions. And those three activities must be completed before validation comparisons can be performed.

The following is a list of activities and decisions – along with a brief description of each – to be completed prior to experimentation, modeling, and validation comparisons. Many of the terms used here have a specific meaning in the framework of validation; those terms are given in *italics* and their definitions are taken from the *Guide for Verification and Validation in Computational Solid Mechanics* (ASME, 2006). Although the activities and decisions listed here are given in order, there is interplay among elements that may require iterative modification to obtain a realistic and useful plan for validation.

The topics to be covered are:

- Specify the model use and purpose (What decision is to be made?)
- Specify validation experiments
- Specify the conceptual model
- Specify the mathematical model
- Specify the computational model
- Specify the physical system response measures of interest
- Specify the validation metrics
- Specify the domain of comparison
- Specify the calibration experiments
- Specify the adequacy criteria (validation requirements)

In addition to the listing of activities and definition of terms, an example that shows how the steps might be applied is included.

1. Specify the model use and purpose (What decision is to be made"):
The use and purpose of the model refer to the applications for which the model is developed. The current model and its validation may be one in a sequence of validation comparisons that will be performed to, eventually, validate a model for the ultimate system of interest. The ultimate system of interest is the physical system and its associated environment for which a computational model is being developed. It is useful to identify the current model and validation comparison relative to the ultimate system of interest because a particular level of accuracy

will be required of the computational model of the ultimate system of interest and the accuracy requirements of the current model must be compatible with the accuracy requirements of the model of the ultimate system of interest. The decision to be made normally considers whether model predictions are sufficiently accurate.

Example: The ultimate system of interest is an ensemble of shell-payload structures with interior hardware that will experience random vibration environments. Each shell-payload structure consists of an external layered shell plus interior components. The external layered shell consists of an exterior composite shell bonded to an internal aluminum shell. The interior components are substructure elements with mechanical properties.

Prior to validation of the ultimate system of interest it is desired to validate a model of the external layered shell, only. Figure 1 shows a schematic of the external layered shell, and the shell with interior components. The hierarchy includes two elements and difficulty of model validation increases from the first to the second. The validation considered here is the validation of the computational model of the shell structure.

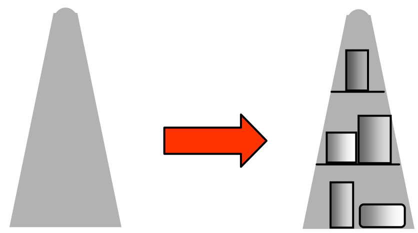


Figure 1. Validations to be performed during development of computational model of shell-payload structure. The schematic on the left denotes the shell structure. The schematic on the right denotes the shell structure with interior components.

2. Specify *validation experiments*:
Early in the planning process validation experiments must be specified. A validation experiment is an experiment that is designed and performed to generate data for the purpose of model validation. The validation experiments must be specified early in the planning process because details of the computational model to be developed for making predictions of validation experiment results will be specified during the validation planning phase, and the computational model needs to be sufficiently detailed, and contain the appropriate elements to make the required predictions with acceptable accuracy

It is emphasized that the validation experiments defined here differ from calibration experiments defined below. The calibration experiments are used to develop models for materials, sub-components, and connections in the physical system currently modeled.

Example: The validation experiments will subject eight nominally identical shell structures, described above, to base-excited, stationary random vibration. The random vibration load will be a band-limited white noise with frequency content in [10,2000] Hz, and it will be generated using an electrodynamic shaker. The input spectral density level is $5.25 \times 10^{-2} g^2 / Hz$. Each structure will be subjected to the random vibration environment for a duration of thee minutes. The structures will be attached to the electrodynamic shaker via a fixture during testing. Uniaxial acceleration responses will be measured in the axial direction, at three locations along the length of the shell, on the inside of the shell. Figure 2 shows a schematic of one structure under random vibration load. The load is primarily uni-directional and input at the base of the test structure. The squares denote the locations of the accelerometers.

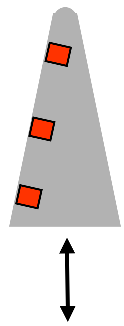


Figure 2. Shell structure subjected to random vibration load.

3. Specify the *conceptual model*:
The conceptual model of the physical system is the set of assumptions and descriptions of physical processes representing the behavior of the system of interest, and from which the mathematical model and the validation experiments can be constructed.

Example: The shell structures are, of course, nonlinear, to some extent, as are practically all real structures. But it is thought that the degree of nonlinearity is slight. In addition, the ensemble of structures from which the eight test structures are drawn is random in practically every respect. Material properties are random; the geometries of the outer shell and internal aluminum shell are random; the thickness of the bond layer is random; adhesion of the bond material to the outer shell and the internal shell is imperfect and random, etc. But expert opinion holds that the major source of randomness is the material properties of the bonding material that bonds the external shell to the internal aluminum shell; and those material properties are the only quantities conceptually considered to be random. Therefore, the bonding material modulus of elasticity and shear modulus, E and G, are modeled as jointly distributed random variables. All other facets of the physical system are conceptually considered capable of being accurately modeled as deterministic with nominal system dimensions and nominal material parameters.

4. Specify the *mathematical model*:
The mathematical model is the mathematical equations, boundary conditions, excitations, initial conditions, and other modeling data needed to describe the conceptual model. The mathematical model must be specified not only as a prelude to specification of the computational model, but also to assure that all phenomenology anticipated in the validation experiments is included.

When the computational model is to be implemented in an *uncertainty quantification* framework, the parameters and functions in the mathematical model intended to simulate the uncertainty are specified here.

Example: Within the frequency range of interest ([10,2000] *Hz*), and at the excitation levels specified, and at the corresponding response levels anticipated, it is assumed sufficiently accurate to model the structure with linear, partial differential equations. An analysis that does not require specification of initial conditions will be specified, so no initial conditions need be specified here. The excitation is a stationary, random, externally enforced acceleration, with spectral density provided in item 2, above.

Because the bonding material modulus of elasticity and shear modulus are assumed random, a probability model for their joint realizations will be developed using data obtained during calibration experiments. Both the modulus of elasticity and the shear modulus of the bonding layer are modeled as spatially constant throughout the bonding layer field.

5. Specify the *computational model*:
The computational model is the numerical implementation of the mathematical model, usually in the form of numerical discretization, solution algorithm, and convergence criteria. The computational model must be carefully defined (following code verification and solution verification) to assure that the features of the mathematical model are captured with sufficient accuracy to guarantee positive validation results if, indeed, the model should be validated.

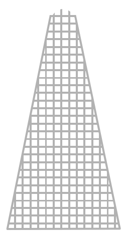
When the computational model is implemented in the *uncertainty quantification* framework, the specific implementations that permit simulation of uncertainty are specified here.

Example: The system will be modeled with a finite element model (FEM). The code to be used is Salinas, a Sandia National Laboratories-developed code for the simulation of linear (mostly) structural dynamics. (See Reese, et al., 2004) The outer shell, the inner aluminum shell, and the bonding layer, are all modeled using solid elements. Solution verification (See Roache, 1998) indicates that an FEM with approximately 1.1 million nodes is adequately converged to yield computation accuracy compatible with the measurement accuracy of the transducers used to make experimental measurements.

The FEM is deterministic, i.e., during any code run all model data – system geometry, parameters, loads, etc. – must be specified as constants. Probability analysis using the FEM is accomplished via Monte Carlo simulation. That is, randomness is introduced into the analysis by generating samples of the random modulus of elasticity and shear modulus from their probability model, then introducing them to the analysis via model data of the FEM. Each set of inputs – modulus of elasticity and shear modulus – yields a different response. The collection of responses forms the ensemble of the random response. (Some ideas of probability modeling are introduced in Paez and Swiler (2009), and some ideas of uncertainty quantification that is non-probabilistic are introduced in Swiler and Paez (2009), two papers in this tutorial sequence.) The ensemble of the random response can be used to develop a probability model of the response measures.

The computational model is shown schematically in Figure 4, along with the FEM equations of motion in matrix form.

$$\boldsymbol{m}\ddot{\boldsymbol{x}} + \boldsymbol{c}\ddot{\boldsymbol{x}} + \boldsymbol{k}\boldsymbol{x} = \boldsymbol{q}$$

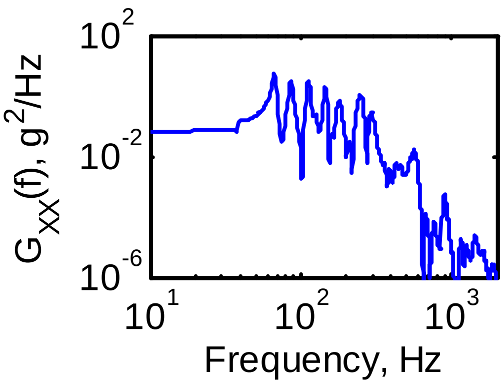


m mass matrix
c damping matrix
k stiffness matrix
q force
x response displacement
Dots denote differentiation with respect to time.

Figure 3. Schematic of the computational model and matrix equation of motion.

6. Specify the physical system *response measures* of interest:
The response measures of interest are the quantities that are functions of system behavior or response to be used in the comparison of model predictions to experimental system predictions. They need to be quantities that can be inferred from measured experimental excitations and responses, and from specified model excitations and computed model responses.

Example: The response measures of interest are obtained from the spectral densities of the responses at the three experimental measurement locations, denoted by squares in Figure 2. An acceleration record is obtained from each accelerometer, therefore, three spectral densities are computed. The spectral density of a random process defines the distribution of mean square signal content in the frequency domain. (See Wirsching, Paez, Ortiz, 1995.) The area under the spectral density function of a random process is the total mean square of a random process. Two response measures are defined for each spectral density. The first is the square root of the area under the spectral density curve over the frequency range [0,300] Hz; the second is the square root of the area under the spectral density curve over the frequency range [300,2000] Hz. The first response measure is the root-mean-square (RMS) of response due to “modes” in the response, up to 300 Hz; the second response measure is the RMS of response due to “modes” in the response in [300,2000] Hz. A typical acceleration response spectral density excited by a random vibration environment like the validation test environment is shown in Figure 4, along with the definitions of the response measures of interest, and the actual response measures from the spectral density curve.



$$R_1 = \left[\int_0^{300} G_{XX}(f)\,df \right]^{1/2} = 11.17\,g$$

$$R_2 = \left[\int_{300}^{2000} G_{XX}(f)\,df \right]^{1/2} = 2.02\,g$$

Figure 4. A typical acceleration response spectral density excited by a band-limited white noise acceleration environment. Definitions of the response measures of interest. Response measures for the spectral density shown.

7. Specify *validation metrics*:
These are the precise mathematical means for comparing model predicted response measures to response measures computed from experimental responses.

Example: There are numerous means for accomplishing validation comparisons. Of course, when results are available from multiple experiments, the approach should involve comparisons based on the theories of probability and statistics. Two of the papers in this tutorial sequence (Paez and Swiler, 2009, and Swiler and Paez, 2009) discuss methods for comparison of model predictions to experimental outcomes when both the predictions and the outcomes are uncertain. For now, we refer those interested in learning about such methods of comparison to those papers, and note that both the response measures from the eight validation experiments and multiple response measures from the model predictions will be computed and graphed.

8. Specify the *domain of comparison*:
The domain of comparison is the region of environment space and model and physical system parameter space within which experiment responses will be measured and model predictions will be made. Once a validation comparison is made over a particular domain, the results of the comparison are normally specified only for that domain, and the model is used only in that domain unless a careful extrapolation implies that the results are useful over an extended domain.

Example: The validation test environment is specified as a stationary random vibration with root-mean-square (RMS) value 10.2 *g*, and with frequency content up to about 2000 *Hz*. Figure 4 shows that the environment excites responses in the structure up to about 12 *g*'s RMS. Assuming that if a computational model that simulates the system at these levels could also do so at lower levels, the domain of comparison can be thought of as random vibration excitations up to 10 *g* RMS, with signal content up to 2000 *Hz*, exciting responses up to about 12 *g*'s RMS.

9. Specify the *calibration experiments*:
Calibration experiments are the experiments to be performed and used with the structural model to identify model parameters. Once the calibration experiment results are used to infer values for model parameters, they cannot be used to make inferences of model validity.

Example: Calibration experiments are required to develop the probability model for the bond material parameters, *E* and *G*, the modulus of elasticity and the shear modulus. Details of how this is accomplished are contained in Paez and Swiler (2009), and a summary of those results is provided in the section entitled "Perform Calibration Experiments," below. However, note that the calibration experiments must be specified prior to performance of the validation experiments and construction of the computational model.

10. Specify *adequacy criteria* (*validation requirements*):

(In this paper, the focus is on the process and not the actual validation criteria, so the details of specifying the adequacy criteria are omitted.) Adequacy criteria define the values that validation metrics must assume in order for the model to be judged valid.

Example: The adequacy criteria for a given validation comparison relate directly to the validation metric. Specifically, the validation metric must satisfy some quantitative requirement. Because the validation metric has not been specified, here, adequacy criteria will not be specified, either. Note, though, that the issue of validation requirements is covered in the example in Paez and Swiler (2009), Mayes (2009a), and Mayes et al. (2009).

This is the end of the preliminary activities – the planning activities – in a model validation analysis.

Validation – Experiments and Predictions

The experiments and model predictions that support a validation analysis are performed following the specification of system hierarchy, validation experiments, the model, response measures of interest, validation metric and calibration experiments. This section describes the latter activities and provides examples of the results that might be obtained.

1. Perform calibration experiments and calibrate model:
Calibration experiments are required to identify the parameters of component materials, boundary conditions, laws that govern mechanical joint mechanics, etc., or the probability laws of those parameters, for use in the computational model. When the computational model is used to help identify those parameters, the activity is known as calibration. When another, perhaps simpler, model is used to identify the parameters, the activity is sometimes called parameter identification.

Example: The discussion in the “Example” section of item 3, Conceptual Model, stated that the modulus of elasticity, E, and shear modulus, G, of the bond material would be considered random variables. Parameter identification experiments are required to obtain a probability law for the joint (simultaneous) behavior of the parameters. Paez and Swiler (2009) show, in detail, how the parameter identification is performed. To summarize, though, five experiments were performed on a simple structure like the one shown, schematically, in Figure 5a. The structure is a small (1.125 in diameter) sandwich of three disks – two steel, on the outside, and one bonding material disk in the center. Each structure was excited with a modal hammer, and its responses were measured. A modal analysis was performed on the measured responses, and modal frequencies were estimated.

An FEM of the simple structure in figure 5a was constructed, with specific E and G, and its modal frequencies were computed. The values of E and G were systematically modified to make the modal frequencies of the FEM match the experimental modal frequencies. In this way, five sets of experimental pairs of E and G were obtained. Those experimentally inferred quantities were modeled, and used to generate numerous other pairs of the parameters E and G. The generated values are shown in Figure 5b. They are clearly related, linearly, and that relation is discussed in the above mentioned reference.

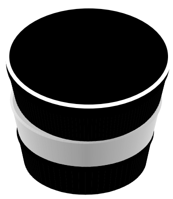


Figure 5a. Schematic of a simple structure used to infer the characteristics of a bond material.

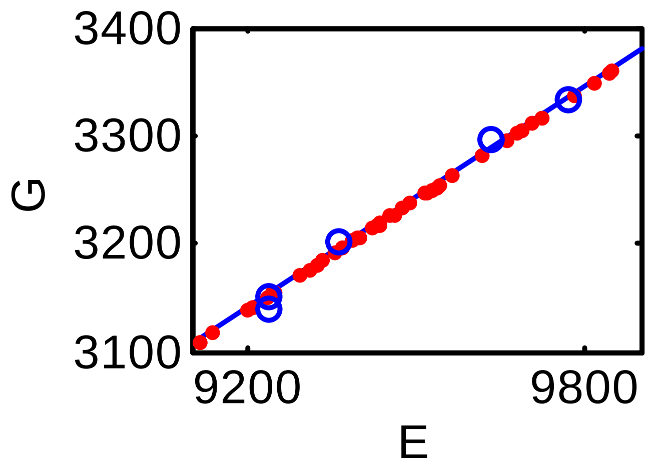


Figure 5b. Experimentally inferred values of *G* vs. *E* (circles), and generated values of *G* vs. *E* (dots).

2. Perform validation experiments and transmit required information to modelers.
The validation experiments described in item 2 of the previous section were performed on the eight nominally identical realizations of the structure shown, schematically, in Figure 2. During each experiment, acceleration responses were measured at the three instrumented locations to obtain response time histories. The response time histories were used to estimate response spectral densities at the three locations on the eight structures. The acceleration response spectral densities at one location on the eight structures are shown in Figure 6a. As expected, random variation in the structures is reflected in the response spectral densities. (The acceleration response spectral densities at the other two locations on the eight structures are similar.)

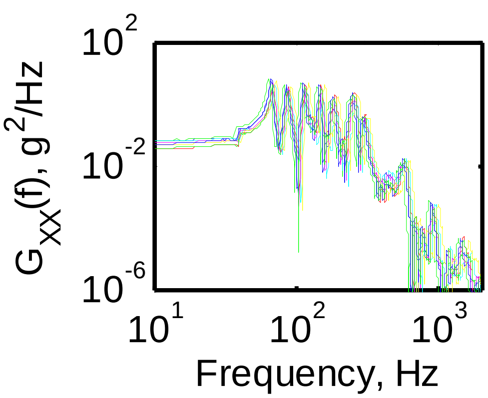


Figure 6a. Acceleration response spectral densities at one location on the eight validation structures subjected to random excitation.

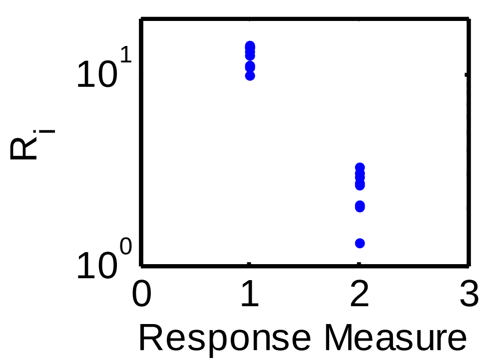


Figure 6b. RMS response measures corresponding to response spectral densities in Figure 6a.

The RMS response measures defined in item 6 of the previous section were computed for each response spectral density shown in Figure 6a. They are shown in Figure 6b. These quantities (and four more like them, from the responses at the other two locations on the structure) form the basis for validation comparisons.

The spectral density of the stationary, random base excitation needs to be transmitted to the modelers for use in response computations because the white noise spectrum specified in the validation test item is not perfectly realized. Following the validation tests, the transmission the excitation spectral density to the modelers took place.

3. Create model and generate model-based predictions:

The computational model described in element 5 in the previous section was constructed and excited with the test spectral density from the experiment. The response spectral densities of fifty computational structures with the modulus of elasticity and shear modulus values shown by the red dots in Figure 5b were computed at three locations, and ten response spectral densities at one location (corresponding the location considered in Figure 6a) are shown in Figure 7a. (For the sake of visual clarity, all 50 response spectral densities are not shown.) The RMS response measures defined in item 6 in the previous section were computed for each model-predicted response spectral density, and they are shown in Figure 7b. These are the quantities to be compared to the experimentally obtained response measures shown in Figure 6b to establish the validity of the model.

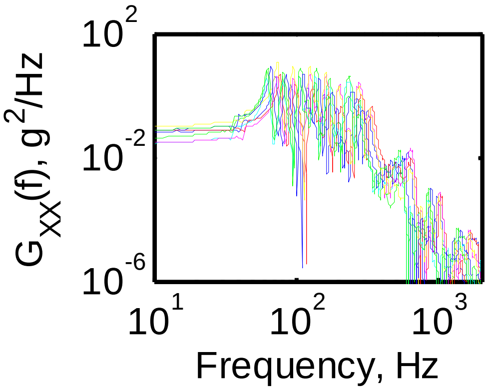


Figure 7a. Acceleration response spectral densities at one location on 10 of 50 model structures subjected to random excitation.

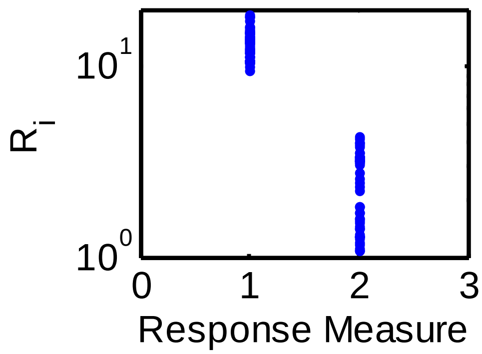


Figure 7b. RMS response measures corresponding to response spectral densities in Figure 7a.

4. Perform validation comparisons and judge validity of model

The validation comparisons are performed by establishing whether or not the model-predicted measures of response satisfactorily match the experimental measures of response, according to the adequacy criteria of item 10 in the previous section. Because no adequacy criterion was defined we cannot state whether the model is validated. The usual practice of validation typically requires that a quantitative metric be satisfied in order for validation to be confirmed.

We can, however, show a graphic comparison between the model-predicted measures of response and the experimentally inferred measures of response. Figure 8 shows the experimentally obtained measures of response from Figure 6b (blue circles). In addition Figure 8 shows the model-predicted measures of response (red x's). Some criteria would certainly validate the model predictions shown in Figure 8. We reiterate that Paez and Swiler (2009) provide some validations metrics and show how validation comparisons can be quantitatively performed.

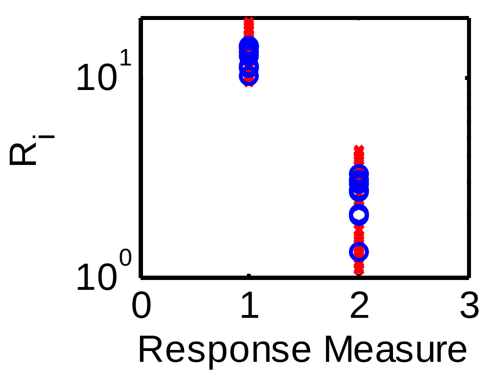


Figure 8. Response measures inferred from experiments (blue circles) and response measures from model predictions (red x's).

5. Take action regarding use of model:

Once it is established whether or not the model is valid, actions can be taken regarding its use or re-validation. If the model is not valid, there is a reason, and several possible options for making it valid exist.

- The model may not be valid because additional, un-modeled sources of randomness exist. An effort can be undertaken to identify the additional sources of randomness. Calibration testing can be performed and then used to specify the probability models for the additional sources of randomness. Then a revalidation may be performed.
- The model may not be valid because the physics included in the model may be insufficient. For example, nonlinear behavior may play a greater-than-expected role in structural response. The model physics may be augmented (if possible) and then calibration testing performed to identify the parameters of the physics model. Then a revalidation may be performed.
- The model may appear invalid because inadequate data may have been collected during calibration and/or validation experiments. Sensitivity of the validation conclusion to the amount of data may lead to incorrect or borderline conclusions. Collection of additional data and improvement of model parameters, followed by revalidation may lead to reversal of a conclusion regarding validity.
- The model may not be valid because the form of the response measure of interest may be too difficult for the model to predict correctly. For example, practically no structural dynamic model can be expected to accurately predict experimental response time histories using direct comparisons. The response measures used during validation comparisons can be modified and then revalidation may be performed. (However, modelers, experimentalists, and validation analysts should not simply change from one response measure to another, in search of a response measure that leads to a positive validation conclusion.)
- The model may not be valid because the adequacy criteria used during the validation comparisons are too stringent for the model to satisfy. That is, modelers, experimentalists, and validation analysts may have been too optimistic about the potential for model accuracy when specifying the adequacy criteria. The adequacy criteria may be modified and then revalidation may be performed.

If the model is valid then it can be used as the basis for development of the model in the next step of the hierarchy. Or it can be used to make predictions of structural response within the domain of comparison.

Summary and Conclusions

Any validation comparison performed using the guidelines specified here clearly leaves much to the judgment of (1) analysts, (2) experimentalists, (3) those performing the formal validation comparisons, (4) customers, and (5) stakeholders. Validation planning should be performed cooperatively by all five groups. The requirements specified during planning should be agreed to by all parties. Following planning, though, the three activities – analysis, experimentation, and validation comparisons – should ideally be performed by independent groups or individuals. Importantly, validation experiment results and validation model predictions should not be shared between experimentalists and analysts prior to the formal validation comparison so as to avoid the appearance of collusion and the actual temptation to tune the model.

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