On the Calibration and Validation of Mathematical Models

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A fundamental question of computational engineering is whether it is possible to *predict* the response of some physical system or process to various kinds of excitation by means of numerical simulation with a high degree of *reliability*. This question is addressed in a document published by ASME [1]. In this note the main considerations are outlined and the relevant capabilities of the finite element analysis software product StressCheck® [2] are summarized.

Numerical simulation

The main elements of numerical simulation are illustrated in Fig. 1.

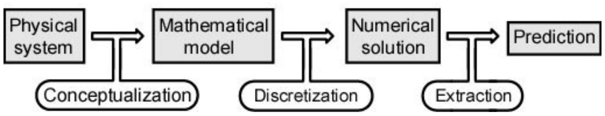

Figure 1: The main elements of numerical simulation.

The first and most important task in numerical simulation is to define a mathematical model. The process leading to the definition of a mathematical model is called conceptualization. This involves decisions about the level of topological details to be incorporated, material properties, boundary conditions, solution procedures, etc. At present, the formulation of mathematical models is largely left to the experience and judgment of analysts. As the complexity of models increases, necessitated (for example) by the use of advanced composite materials, reliance on experience and judgment alone becomes increasingly impractical and risky. Therefore it is necessary to establish a process for ascertaining that the mathematical model meets necessary conditions for acceptance from the perspective of its intended uses. This process is called *validation.*

The choice of a mathematical model depends on the goals of computation and the level of accuracy required. Associated with a mathematical model is an exact solution $\mathbf{u}_{EX}$. The goal of computation is to determine some engineering data from $\mathbf{u}_{EX}$, such as the maximum normal stress, the maximum shear stress, the maximum displacement, etc. In the following we denote the data of interest by $\Phi_i(\mathbf{u}_{EX})$, i=1,2,… In the finite element method $\mathbf{u}_{EX}$ is approximated by the finite element solution $\mathbf{u}_{FE}$ and the data of interest are approximated by $\Phi_i(\mathbf{u}_{FE})$, i=1,2,… It is important to ensure that $\Phi_i(\mathbf{u}_{FE})$ are sufficiently close to $\Phi_i(\mathbf{u}_{EX})$ from the point of view of the objectives of simulation.

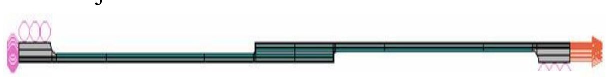

Figure 2: Asymmetric lap-joint specimen.

Virtual experiments

Virtual experiments play an important role in the selection of mathematical model. This is illustrated with a simple example in the following. The goal is to determine the extent of yielding in the adhesive layer of an asymmetric lap-joint specimen shown in Fig. 3.

Contours of the von Mises stress in the neighborhood of the adhesive run-out are shown for three models in Fig. 3. Model 1 is based on the linear theory of elasticity (plane strain). Model 2 is based on small strain plasticity in the adhesive layer, associative flow rule and the deformation theory. Model 3 is based on large strain theory plasticity in the adhesive layer, associative flow rule and the deformation theory.

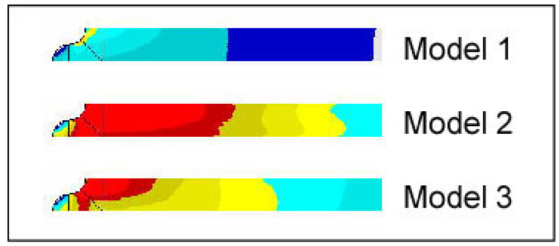

Figure 3: Stress distribution in the adhesive layer.

It is seen that the distribution of the von Mises stress changes substantially with the choice of the model. Only mathematical models that do not show sensitivity to restrictive assumptions incorporated in them can be considered suitable for the interpretation of experiments.

Calibration

Having chosen a mathematical model, certain material properties and criteria are needed. For example, in connection with the design of airframe components made of composite materials it is necessary to determine allowable stress or strain values. This is done by interpretation of the results of coupon tests. Of interest is the identification of some combination of strain values that are predictive of onset of failure events. Thus the purpose of coupon tests is to calibrate some hypothesis of failure under standard conditions. A large number of failure models have been proposed. As new material systems are developed, continuous testing and refinement of the relevant failure models are necessary.

Let us assume that the failure model being calibrated predicts the occurrence of onset of failure events when some functional $\Phi(\mathbf{u}_{EX}) > 0$ reaches a critical value Φ_{CRIT}. Thus the tentative design rule states that

$$\Phi(\mathbf{u}_{EX}) < \Phi_{CRIT}.$$

We compute $\mathbf{u}_{FE}$ and report $\Phi(\mathbf{u}_{FE})$. Adding and subtracting:

$$[\Phi(\mathbf{u}_{EX}) - \Phi(\mathbf{u}_{FE})] + \Phi(\mathbf{u}_{FE}) \le \Phi_{CRIT}$$

we see that the calibration can be considered reliable only if the error $|\Phi(\mathbf{u}_{EX}) - \Phi(\mathbf{u}_{FE})|$ is smaller than the experimental error. That this condition is not violated is tested through verification [3].

Validation

The next step is to validate the mathematical model, for example by predicting onset of failure events in sub-components. An example of a sub-component is shown in Fig. 4.

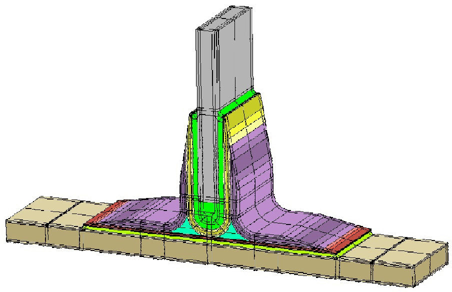

Figure 4: Example of a sub-component.

Once again it is necessary to compute $\Phi(\mathbf{u}_{FE})$ and ensure that $|\Phi(\mathbf{u}_{EX})- \Phi(\mathbf{u}_{FE})|$ is sufficiently small. If the failure model is correct then failure will occur when $\Phi(\mathbf{u}_{FE})$ is approximately equal to Φ_{CRIT}. The criterion for rejection is based on the error between the predicted and observed failure events. Statistical considerations apply, see, for example, [4].

Generally speaking, the results of validation experiments are evaluated on the basis of one or more metrics and the corresponding criteria. The metrics are the data of interest, the criteria are the conditions on the basis of which it is decided whether the model being validated satisfies necessary conditions for acceptance. Validation is an inductive process.

Confidence in a mathematical model is established through successful prediction of the outcome of experiments (e.g., the onset of failure events) in several sub-components subjected to various loading conditions. On the other hand, if a model fails to predict the outcome of even one validation experiment then that model must be rejected.

The next steps are to perform validation experiments at the component level, then at sub-assembly and finally at the assembly level. The costs of experiments rapidly increase with the complexity of test articles. Usually only very few tests can be performed at the sub-assembly and assembly levels. Therefore it is very important to plan and execute validation at the coupon, sub-component and component levels utilizing best practices in numerical simulation and experimentation. The goal is to have the very few tests that can be performed at the sub-assembly and assembly levels confirm the predictions based on the mathematical model. The mathematical model that passed the validation tests can then be used for evaluating responses to load cases for which experimental information is not available.

Sources of error

In validation we have to be concerned with (a) errors in the mathematical model or hypothesis being tested, (b) errors in the numerical approximation (c) errors in the experiment and statistical variations. Unless the errors in the experiment and the numerical approximation are controlled, it will not be possible to judge whether the model or hypothesis being tested should be rejected or not.

Unfortunately, the use of “tuned” finite element solutions is far too common. In that practice the finite element mesh is adjusted until the experimental observations are closely matched by the corresponding data computed from the finite element solution. Implied is the absurd assumption that errors in the model can be compensated by errors in the finite element approximation. Clearly, one cannot make reliable predictions based on the assumption that two large errors will consistently cancel one another.

The hierarchic view of mathematical models

A mathematical model should be viewed as a special case of a more comprehensive mathematical model. For example, a mathematical model based on the linear theory of elasticity is a special case of a mathematical model that accounts for material non-linearity based on small strain theory which, in turn, is a special case of a model that accounts for material non-linearity as well as large strain formulation, etc. Therefore any mathematical model is a member of a hierarchic sequence of models. One is interested in selecting the simplest model from the hierarchy that accounts for all of the data of interest within the prescribed criteria.

Therefore it is necessary to have software tools available that support seamless transition from one mathematical model to another. StressCheck® was designed with this goal in mind. The finite elements, the polynomial degrees associated with the elements and the formulation are treated separately, allowing *independent control* of the errors of approximation and the errors associated with model selection. This is either not possible or very difficult to do with conventional finite element libraries where these attributes are combined.

References

[1] Guide for Verification and Validation in Computational Solid Mechanics. V&V 10-2006 American Society of Mechanical Engineers, New York, 2006.

[2] StressCheck® is trademark of Engineering Software Research and Development, Inc., 111 West Port Plaza, Suite 825, St. Louis, MO 63146 www.esrd.com

[3] Szabó, B. The p-Version of the Finite Element Method. ESRD Technical Brief 12/19/06, 2006.

[4] Hills, R. G. and Trucano, T. G. Statistical Validation of Engineering and Scientific Models: Background. Technical Report SAND99-1256, Sandia National Laboratories, 1999.