Draft Outline

ROLE OF NON-DETERMINISM IN VERIFICATION AND VALIDATION OF COMPUTATIONAL SOLID MECHANICS MODELS

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Background

Computational solid mechanics (CSM) models are used to simulate the behavior of physical systems using numerical methods. Unless otherwise clear from the context, the term “model” is taken herein to include not only the computer software, but also all model inputs and analysis control options.

It is now widely understood and accepted that uncertainties, whether reducible or irreducible, arise due to the inherent randomness in physical systems, modeling idealizations, experimental variability, measurement inaccuracy, etc., and cannot be ignored. This complicates the already difficult process of model validation by creating an unsure target, where neither the simulated nor observed behavior of the system is known with certainty.

Because a non-deterministic analysis cannot improve the predictive capability of a flawed deterministic model, the first step of the validation process is to detect, identify and eliminate (if possible) any systematic error in the *formulation* of the model or the acquisition of experimental data.

The next step is to reduce and/or better characterize the remaining uncertainties, such as bias and random variations, to an acceptable level. This step may involve model updating or “calibration” to the extent that the updating results in improved predictive accuracy as defined below. All significant uncertainties associated with the model should be identified and quantified. As experience with a model or type of model accumulates, updating may be unnecessary, or may be required only occasionally or periodically. The inherent uncertainty of a model must also be quantified such that it may be used to assess predictive accuracy.

The final step of the model validation process then is to evaluate predictive accuracy. By definition, *predictive* accuracy refers to the accuracy of *future* simulations, which can only be verified by comparison with *new* experimental data (not used in any model updating or parameter characterization). The question of “how good is good enough?” may be answered by comparing the uncertainty of model predictions, based on the propagation of previously quantified modeling uncertainty through the model, with the new data. This comparison should not be done ad hoc, but rather follow a well-defined (statistical) procedure that results in reproducible measures of comparison.

Sources of Non-determinism

As previously stated, the real world is fundamentally non-deterministic, stemming from the following realizations:

1. Experimental data
    a. Test fixtures vary
    b. Installations vary
    c. Environmental conditions vary
    d. Measurements vary
2. As-built systems and structures
    a. There are design tolerances
    b. Material properties vary
    c. Methods of construction vary
3. Models
    a. Modeling decisions involve judgment that varies from modeler to modeler, and even from time to time.
    b. Modeling tools vary, e.g. different finite element (FE) methods, different FE analysis tools, and different versions of the same FE analysis tools.
    c. Modeling resources vary, leading to different degrees of fidelity.

Classification of Errors and Uncertainties

Errors produce reproducible, or deterministic bias in the simulation, and can in theory at least, be reduced or eliminated. Uncertainties, whether reducible or irreducible, produce non-deterministic effects.

1. Uncertainty
    a. Irreducible uncertainty
        i. Inherent variation associated with the physical system being modeled
        ii. Also referred to as variability or aleatory uncertainty
        iii. Probability theory is properly used to model irreducible uncertainty
    b. Reducible Uncertainty
        i. Potential deficiency that is due to incomplete information, e.g., lack of knowledge, poor understanding of physical process, imprecisely defined or non-specific description of failure modes, etc.
        ii. Also referred to as epistemic uncertainty
        iii. May or may not exist
        iv. Probability theory commonly applied, but non-probabilistic non-deterministic theories may be more appropriate
2. Error - Recognizable deficiency that is not due to lack of knowledge.
    a. Acknowledged Error
        i. Error that has been detected, and in principle can be quantified, although it may not be quantifiable in practice.
        ii. Blunders or mistakes: procedural methods are used to detect and eliminate these errors (quality control, reviews, etc.)
    b. Unacknowledged Error

    i. Error that has not been detected (including blunders or mistakes that have not been detected)

[Need to include several CSM examples within each category.]

Although unacknowledged error in principal may be classified as error rather than uncertainty, it may be a contributor to uncertainty if uncertainty is quantified in an ad hoc manner based on statistical differences between predicted and observed behavior. Traditionally, the term “uncertainty” has been used as a “catch-all” term to include all variations from “truth” that cannot be attributed to acknowledged (i.e. known) error. This is the definition of uncertainty adopted herein.