Verification and Validation of FEA Software for Dams and Nuclear Containment Buildings

A Personal Perspective

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1. Preface
2. Preliminary Remarks
   - Dams
   - Nuclear Containment Buildings
   - Lexicon of Key Terms (Part I)
3. Who Cares
   - (and who does not care)
   - The Status Quo
4. My Experience
5. AAR
   - Verification (Basic Requirements)
6. Nonlinear Dynamics
   - Limitations of Pointwise Measurements
   - Transfer Functions, Far Better
   - Analytical formulation of the TF
   - Illustrative Example
   - Matlab Code
   - Python Code
   - So What now?
7. 2-a Validation: Dam
   - Background
   - Centrifuge Testing 101
   - Dam Model
   - Representative figures
   - Validation approved by sponsor ☺
   - Proposal
8. Bibliography

Preface

This is a preliminary draft of a white paper on Verification and Validation (V&V) in two fields familiar to me: concrete dams and nuclear containment structures.

I will focus on the proper modeling of nonlinear analyses in two key areas: 1) Alkali Aggregate Reactions (AAR), and 2) dynamic analysis. Both are critically important for the safety—not serviceability—assessment of the structures studied.

In addition to general considerations and remarks, I will highlight how I have conducted V&V for both AAR-affected structures and nonlinear dynamic analysis of dams using my computer program, Merlin.

For the nonlinear dynamic analysis, validation was achieved through transfer functions derived from unique tests conducted in Japan, where a dam model was mounted on a shake table, which was, in turn, mounted on a centrifuge.

In my opinion, the V&V of AAR is now well-established and widely adopted by many researchers, though, not yet by industry or government agencies.

Conversely, I argue for the use of transfer functions to validate nonlinear dynamic analysis, as they provide a more representative approach than simple pointwise measurement comparisons.

- In the past, many ICOLD International Benchmark workshops have focused on the numerical analysis of dams.
  - For the most part, the terms verification and validation were used interchangeably, without a clear, accepted definition of these terms.
  - Rarely, if ever, did a participant clearly articulate both the verification and the validation process.
  - Ultimately, participants' results were tabulated, plotted, and commented on, often with little attention to the inner workings of the finite element models (i.e., the "black box").
  - Could it be that at times, the end (matching) justified the mean ("whatever it takes")
  - In some cases, statistical analyses were expected.
  - In all cases, participants were asked to capture pointwise measurements.

- Only recently, there has been an attempt to clearly separate verification from validation.
  - Verification *a priori* is the easier of the two. However, I am not yet convinced about the “adjudication” process for determining what constitutes an acceptable model. What is likely missing is a clear list of minimum requirements that an FEA code should meet.
  - Validation remains a stumbling block, as obtaining reliable data is not easy.

- To the best of my knowledge, there have not been widely publicized benchmark studies assessing the performance of FEA codes in nuclear engineering.
- Following are some pertinent remarks:

AAR: The NRC has guidances for verification (NRC, 2013). Yet there is no indication that those guidelines were followed for the verification of the FEA codes used for the analysis of Seabrook (suffering from AAR).

Nonlinear Static: there is an excellent report on "Beyond Design Basis Failure" (Hessheimer and Dameron, 2006) which contains a trove of data that could be used for verification. I am not aware if any computer code has even attempted to use them for validation. This report has been summarized by (Saouma, 2017).

Nonlinear Dynamic: (Randy, Cherry, Rashid, and Chokshi, 2000) performed a 1:8 scale RCCV model constructed in Japan and subjected to seismic simulation tests. First, design-level seismic ground motions was initially conducted. These were followed by a series of tests in which progressively larger base motions were applied until structural failure was induced. It is not clear how extensively, if ever, has it been used for validation.

- Over the years, I have primarily consulted two primary references which comprehensively address the V&V processes.... One stemming from the Department of Energy (Thacker, Doebling, Hemez, et al., 2004) and the other from the Nuclear Regulatory Commission (NRC, 2013).
- To ensure a more productive discussion of V&V and to avoid the misuse of terms, it is important to use the correct terminology. Below are some key terms, with a more comprehensive list provided in the appendix.

Verification deals with the mathematics of the problem and is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model by comparing numerical solutions to analytical or highly accurate benchmark solutions.

Validation on the other hand deals with the physics of the problem and is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. It compares numerical solutions to experimental data.

Calibration is the process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with experimental data.

Code Verification Process of determining that the computer code is correct and functioning as intended.

From my (limited) experience:

Who cares

- **Academics** who by definition should be first and foremost address V&V before any analysis
- **Few "illuminati"** from advocacy groups (ICOLD and others)....
- **National laboratories** that focus on scientific and technological research to support national goals (e.g., Los Alamos, Oak Ridge).

Who does not care

- **Industry** whether consulting firms or utility companies, lacks the qualified personnel sensitive to this issue, and they also do not have the financial resources that can be justifiably allocated for such a process prior to analysis.

Federal Agencies (such as the NRC and BoR) are primarily responsible for regulating industries and providing public services, focusing on oversight, policy, and regulation. While some of these agencies are more aware of this issue, they often pay only lip service to V&V. They also lack qualified personnel and, to a lesser extent, qualified engineers.

Dams:

- In most cases (related to concrete), federal agencies do not perform nor mandate V&V.
- As a substitute to V&V industry gravitates toward the software which is fashionable (Ansys $\rightarrow$ Abaqus $\rightarrow$ LS-Dyna. While these are all excellent tools, possibly validated for applications outside of concrete (such as AAR or nonlinear analysis), they are chosen largely for their popularity. Their ability to generate visually appealing figures and their reputation also contribute to their appeal.
- In many instances, verification, validation, and calibration are often conflated.
- No one got fired for using LS-Dyna, no matter whether the analysis is credible or not for the true believers in V&V.

Nuclear:

- From personal experience, I have no indication that FEA codes were validated for either AAR, or dynamic analysis in the only case I am familiar with (Seabrook).
- Seabrook, and presumably all containment buildings in the US are designed in accordance with the LRFD (load resistance factor Design) philosophy of the American Concrete Institute (ACI 318, 2019) design code in which only linear elastic analysis is to be performed!

Over the years, I have encountered the need to perform V&V in two different contexts.

- Nonlinear Dynamic Analysis
- Alkali Aggregate Reaction

I will start succinctly with the second context,... as it is well-documented, and then proceed to the nonlinear dynamic analysis, which is the primary focus of this white paper.

There is a broad consensus that the following factors should be considered in the finite element analysis of a structure:

- AAR Model
  - Kinetics (expansion *vs time).*
  - *Gel absorption due to micro/macro cracking.*
  - *Effect of temperature.*
  - *Effect of constraints.*
  - *Degradation of* f'_c *and* E.
  - *Stress redistribution.*
- Environmental Conditions of the concrete
  - Temperature
  - Humidity
- Constitutive models
  - Ttension, compression, creep, shrinkage
  - Cracks/joints/interfaces.
- Load history
  - Temperature.
  - Relative humidity.
- Mechanical Boundary Conditions
  - Structural Arrangement
  - Reinforcement
  - Anchorage
- Restart following an AAR analysis for a nonlinear dynamic analysis with different BC.

- We can only reliably validate with "Experimental Data"
- In the past, many have attempted to "validate" using existing dams afflicted with AAR, but such efforts are absurd given the overwhelming number of interfering factors. At best, the so-called "validator" is merely *calibrating* the FEA code due to:
  - Reducible uncertainties (more data)
  - Irreducible uncertainties (can not control some variables such as time, temperature)
  - Parasitic effects such as shrinkage cracks which may be attributed to AAR.
- Unlikely to have a reliable and sufficient field measurement (other than pendulum measurements)
- If we have a potential dam for validation,
  - It is likely to be the dam we want to analyze.

- Partial validation may be performed to capture events unequivocally attributed to AAR (histogram of crest displacements and possible structural cracks). Others (such as surface cracks) may have multiple causes.
- AAR validation is, therefore, best performed with simple, well-executed laboratory experiments.
- RILEM TC-59 (Saouma, Sellier, Multon, and Le Pape, 2021) has proposed the following test problems for FEA validation

Cylindrical Specimen

P0 Mathematical description of the finite element constitutive model used.

P1 Calibration and prediction of the constitutive Models (tension, compression, reverse loading) without any AAR.

P2 Drying and shrinkage.

P3 Effect of creep on expansion.

P4 Temperature dependent expansion.

P5 Relative humidity dependent expansion

Structures

P7 Effect of Internal Reinforcement

P8 Reinforced concrete beam (France).

P9 Reinforced concrete panel (Tennessee).

P10 Large reinforced concrete beam (Texas).

P11 Reinforced concrete shear wall (Toronto).

P12 Idealized dam.

- Author's AAR model (Saouma and Perotti, 2006) widely adopted, has been validated through Merlin computer program with most of the above problems. ☺

In all benchmarks that I have seen, the participants are asked to record *point displacements and stresses* for comparison with laboratory experiment. This is an exceedingly difficult task because

- Material nonlinearities: Nonlinear FEA can accurately account for complex material behaviors like cracking, plasticity, and stress-strain relationships and those are very difficult to replicate in physical models.
- Boundary condition differences: In FEA, boundary conditions can be idealized, while in shake table tests, physical limitations of the setup, such as imperfect constraints or supports, can introduce additional discrepancies.
- Complexities in Nonlinear Dynamic Loading: Nonlinear dynamic FEA handles complex loading patterns, including time-varying forces and material degradation over time, in a highly controlled manner. In contrast, shake table tests might introduce additional noise or inaccuracies in the applied loads due to equipment limitations or physical imperfections, affecting how stresses and displacements are measured.

- Inconsistent Measurement Techniques:: In shake table tests, physical measurements (such as strain gauges and displacement sensors) are limited to discrete points and can be prone to noise or error. FEA, on the other hand, computes results at any point within the model, allowing for higher resolution but making direct comparisons at specific points difficult due to measurement discrepancies.

Japanese compared *Transfer functions* between base and crest, which in my opinion is a far more realistic, comprehensible and ultimately intelligent process because

- Captures global dynamic response: The transfer function describes how the entire structure responds to dynamic excitation at different frequencies. It provides a holistic view of how energy is transmitted through the structure. This integrative approach captures not just local effects but the overall structural behavior, including resonance, damping, and dynamic amplification, which a pointwise assessment of stress or displacement cannot fully represent.
- Accouns for nonlinear and complex interactions: In nonlinear dynamic systems, the relationship between input and output can be highly complex, involving multiple interactions between elements, modes of vibration, and material nonlinearity. The transfer function inherently incorporates these nonlinear effects over the entire structure, offering a more stable and averaged assessment of the dynamic performance, as opposed to pointwise measurements, which may fluctuate or misrepresent localized behavior.

- Frequency-dependent analysis: The transfer function provides information across a range of frequencies, allowing for an assessment of how the structure responds to dynamic loads at different spectral components. This is especially useful in identifying resonant frequencies and understanding how the structure's stiffness and damping change dynamically. Pointwise assessments typically do not provide this frequency-dependent insight and can miss critical dynamic phenomena.
- Minimizes localized noise and errors: Pointwise measurements of stresses and displacements are susceptible to localized anomalies, such as measurement noise, small-scale material defects, or inaccuracies in modeling local boundary conditions. The transfer function, by focusing on the relationship between the base and crest (two major points in the system), averages out these local fluctuations, leading to a more stable and robust assessment of the structure's overall dynamic response.
- Integrative over entire structural height: The transfer function measures the variation between the base and the crest, thus inherently integrating the behavior of the structure along its entire height. This gives a comprehensive assessment of how forces and displacements are distributed through the entire structure, rather than focusing on a single point, which could overlook significant structural dynamics occurring elsewhere.

- More representative of real-world performance In real-world scenarios, the structural integrity of large structures like dams, bridges, or buildings under dynamic loading is not determined by local stresses but by how well the structure handles energy transfer and distribution as a whole. The transfer function provides a macro-level assessment that is more aligned with how the structure will behave in real-world dynamic events, such as earthquakes or wind loads, where the overall performance matters more than localized measurements.
- Transfer functions are perfectly aligned with the underlying concept of Performance Based Earthquake Engineering[1]

☺

[1] PBEE Takes a holistic approach to earthquake engineering by considering multiple performance objectives, such as life safety, damage control, and post-earthquake functionality. It does not rely solely on meeting specific stress or deformation criteria at particular points, but on how the entire building performs in terms of damage, repairability, and usability after an earthquake.

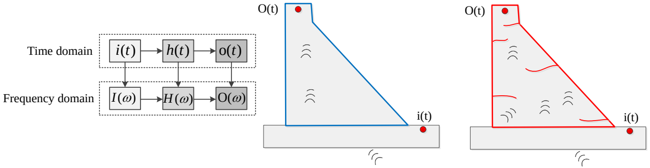
- Fourier transforms convert a signal from the time domain to the frequency domain (Saouma and Hariri-Ardebili, 2021)

$$X(\omega) = \int_{-\infty}^{\infty} x(t)e^{-2i\pi\omega t}\,\mathrm{d}t; \qquad x(t) \xrightarrow{\text{FFT}} X(\omega)$$

- The inverse FFT transforms a signal from the frequency domain back to the time domain

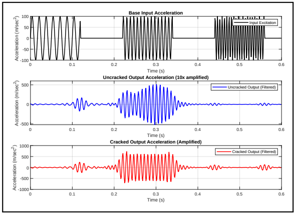
$$x(t) = \int_{-\infty}^{\infty} X(\omega)e^{2i\pi\omega t}\,\mathrm{d}\omega; \qquad X(\omega) \xrightarrow{\text{FFT}^{-1}} x(t)$$

- A transfer function relates an input signal, $i(t)$ (base acceleration), and its modification (structural response) through $h(t)$, resulting in an output signal (crest acceleration), $o(t)$.



- This relationship can also be expressed in the frequency domain, where the transfer function (TF) is simply the ratio of output to input:
  1. $i(t) \xrightarrow{\text{FFT}} I(\omega)$
  2. $o(t) \xrightarrow{\text{FFT}} O(\omega)$
  3. Transfer Function: $TF_{I-O} = \frac{O(\omega)}{I(\omega)}$

  Pretty simple
- Of course the transfer functions of uncracked and cracked dams will be different.



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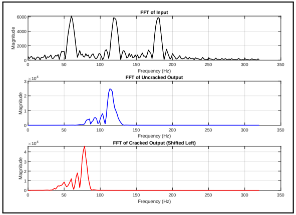

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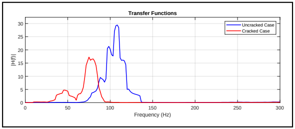

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1. A “dam” is subjected to a sequence of three harmonics with triangular amplitude modulation and increasing frequencies. Input and output signals for both the uncracked and cracked dam.
2. The FFT of the three signals is shown below. Note the leftward shift in the FFT for the cracked dam (indicating reduced stiffness).
3. Transfer functions (TF) for the cracked and uncracked dams. TF for the cracked dam exhibits a leftward shift and a lower amplitude due to lower dynamic resistance to input accelerations.

```matlab
% Time parameters
Fs = 1000;              % Sampling frequency (Hz)
T = 1/Fs;               % Sampling period (s)
t_total = 0.6;          % Total time (s)
t = 0:T:t_total-T;          % Time vector
% Compute FFT of the input (excitation) and both filtered outputs
FFT_input = fft(excitation);
FFT_uncracked = fft(uncracked_output);
FFT_cracked = fft(cracked_output);
% Compute the frequency axis for FFT plots
f = Fs * (0:(length(t)/2)) / length(t);
% Take only the first half of the FFT (positive frequencies)
FFT_input_mag = abs(FFT_input(1:length(f)));
FFT_uncracked_mag = abs(FFT_uncracked(1:length(f)));
FFT_cracked_mag = abs(FFT_cracked(1:length(f)));
% Compute transfer functions (magnitude ratio)
transfer_function_uncracked = FFT_uncracked_mag ./ FFT_input_mag;
transfer_function_cracked = FFT_cracked_mag ./ FFT_input_mag;
```

```
import numpy as np
from scipy.fft import fft
# Time parameters
Fs = 1000              # Sampling frequency (Hz)
T = 1/Fs               # Sampling period (s)
t_total = 0.6          # Total time (s)
t = np.arange(0, t_total, T)  # Time vector
# Compute FFT of the input (excitation) and both filtered outputs
FFT_input = fft(excitation)
FFT_uncracked = fft(uncracked_output)
FFT_cracked = fft(cracked_output)
# Compute the frequency axis for FFT plots
f = Fs * np.arange(len(t)//2 + 1) / len(t)
# Take only the first half of the FFT (positive frequencies)
FFT_input_mag = np.abs(FFT_input[:len(f)])
FFT_uncracked_mag = np.abs(FFT_uncracked[:len(f)])
FFT_cracked_mag = np.abs(FFT_cracked[:len(f)])
# Compute transfer functions (magnitude ratio)
transfer_function_uncracked = FFT_uncracked_mag / FFT_input_mag
transfer_function_cracked = FFT_cracked_mag / FFT_input_mag
```

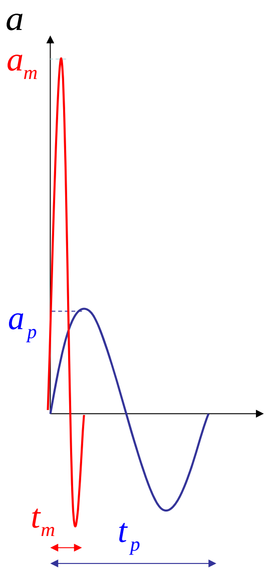
For Validation of nonlinear dynamic analysis FEA programs:

1. Capture the TF of the uncracked structure (laboratory or field); Any decent program should capture it.
2. Capture the TF of the cracked controlled test[2] test
   1. Shake table on a centrifuge for gravity sensitive structures
   2. Shake Table only if gravity can be ignored

Following is an example of a 2-a validation of a FEA (Merlin) for a gravity dam.

[2] It is not only nearly impossible, but no regulator would permit shaking a structure into the inelastic range.

- I was funded by the Tokyo Electric Power Company, to develop software for the nonlinear dynamic analysis of high arch dams (2000-2010; approximately $1.5 million).
- Around 2004, they sought to validate the software before continuing funding.
- A simple shake table test would not have sufficed, as it would not adhere to the laws of similitude for gravity. A centrifuge with a mounted shake table was needed.
- They contracted Obayashi, which had the world's largest centrifuge-mounted shaker, to design, build, and test a model.
- Prior to that, they, not I, conducted Merlin-based simulations to compare numerical results with the laboratory tests and then decide whether to continue funding.



Test characteristics

- Using centrifuge, similitude laws require that $\frac{L_p}{L_m} = \frac{t_p}{t_m} = \frac{a_m}{a_p} = N$, hence for $N = 100$, $t_p = 10$ sec., and $a_p = 0.5$ g, $\Rightarrow$ a 10 sec. excitation at 0.5g, will last 0.1 sec at 50 g acceleration in the centrifuge.
- Used a large shake table mounted on a centrifuge at Obayashi Corporation.

Centrifuge

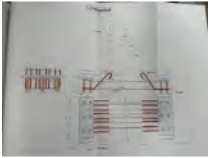
Max. Payload	7 t
Platform Size	2.2x2.2 m
Model height	2.5 m
Max. Accel.	120 g
Max. Payload	700 g-t

Shake Table

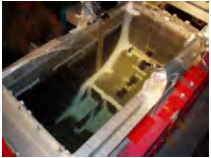
Max. Payload	3 t
Platform Size	2.2x1.07 m
Max. Accel.	500 m/s^2
Max. Freq.	200 Hz

Full technical paper: Uchita, Shimpo, and Saouma (2005)

- Representative Japanese dam geometry.
- Extensive instrumentation (strains and accelerations), as well as crack detection.
- Subjected dam to a sequence of

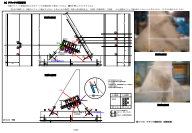


Construction drawings

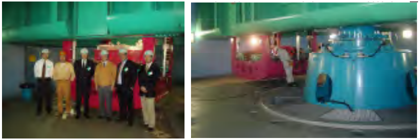


Container

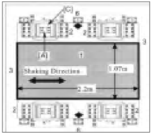
Instrumentation



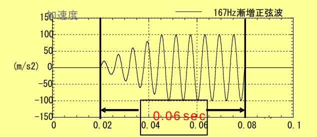
Strain gauges crack tip locators



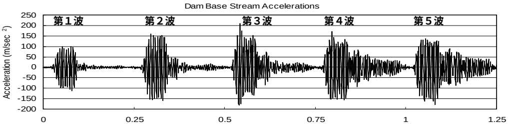
Centrifuge



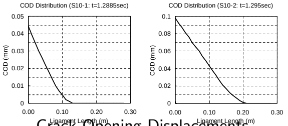
Platform



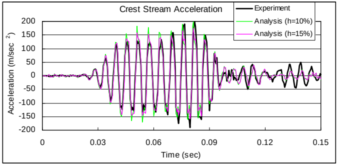
Representative signal



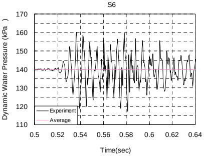
Base acceleration



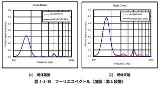
Crack Opening Displacements

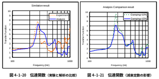


Crest acceleration

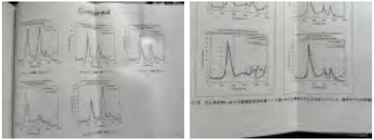


Dynamic water pressure





Transfer functions

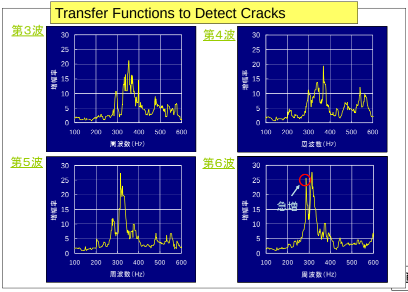


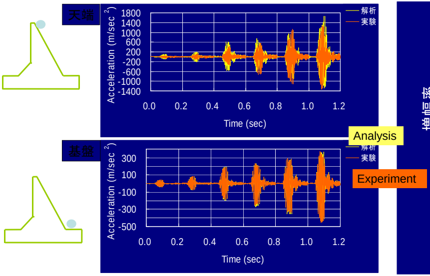
Transfer functions

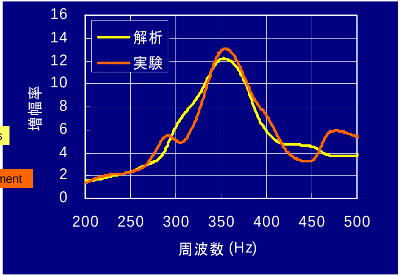
Pot Pourri of representative figures

2-a Validation: Dam

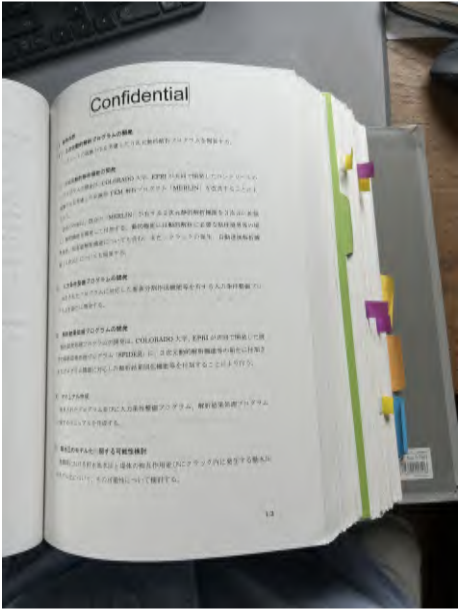
Validation approved by sponsor ☺







Proposal



- I have the final draft of the test program.
- It is approximately 3 inches thick, written in Japanese, and includes multiple figures.
- It can serve as a valuable resource for validating computer programs, specifically for their ability to perform nonlinear dynamic analysis of unreinforced concrete structures, such as dams.
- Open to sharing this report with interested parties (could request final report from TEPCO) under a formal agreement.

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Calibration Experiment Experiment performed for the purpose of fitting (calibrating) model parameters.

Computer Model Numerical implementation of the mathematical model, usually in the form of numerical discretization, solution algorithms, and convergence criteria.

Conceptual Model Collection of assumptions, algorithms, relationships, and data that describe the reality of interest from which the mathematical model and validation experiment can be constructed.

Confidence Probability that a numerical estimate will lie within a specified range.

Error is a recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge.

Experiment Observation and measurement of a physical system to improve fundamental understanding of physical behavior, improve mathematical models, estimate values of model parameters, and assess component or system performance.

Experimental Data Raw or processed observations (measurements) obtained from performing an experiment.

Experimental Outcomes Measured observations that reflect both random variability and systematic error.

Experiment Revision The process of changing experimental test design, procedures, or measurements to improve agreement with simulation outcomes.

Fidelity The difference between simulation and experimental outcomes.

Field Experiment Observation of system performance under fielded service conditions.

Inference Drawing conclusions about a population based on knowledge of a sample.

Irreducible Uncertainty Inherent variation associated with the physical system being modeled.

Laboratory Experiment Observation of physical system performance under controlled conditions.

Mathematical Model The mathematical equations, boundary values, initial conditions, and modeling data needed to describe the conceptual model.

Model Conceptual/mathematical/numerical description of a specific physical scenario, including geometrical, material, initial, and boundary data.

Model Revision The process of changing the basic assumptions, structure, parameter estimates, boundary values, or initial conditions of a model to improve agreement with experimental outcomes.

Nondeterministic Method An analysis method that quantifies the effect of uncertainties on the simulation outcomes (also known as probabilistic method).

Performance Model A computational representation of a model's performance (or failure), based usually on one or more model responses.

Prediction Use of a model to foretell the state of a physical system under conditions for which the model has not been validated.

Pretest Calculations Use of simulation outcomes to help design the validation experiment.

Reality of Interest The particular aspect of the world (unit problem, component problem, subsystem or complete system) to be measured and simulated.

Reducible Uncertainty Potential deficiency that is due to lack of knowledge, e.g., incomplete information, poor understanding of physical process, imprecisely defined or nonspecific description of failure modes, etc.

Risk The probability of failure combined with the consequence of failure.

Risk Tolerance The consequence of failure that one is willing to accept.

Simulation The ensemble of models—deterministic, load, boundary, material, performance, and uncertainty—that are exercised to produce a simulation outcome.

Simulation Outcome Output generated by the computer model that reflect both the deterministic and nondeterministic response of the model.

Uncertainty A potential deficiency in any phase or activity of the modeling or experimentation process that is due to inherent variability (irreducible uncertainty) or lack of knowledge (reducible uncertainty).

Uncertainty Quantification The process of characterizing all uncertainties in the model and experiment, and quantifying their effect on the simulation and experimental outcomes.

Validation Experiment Experiments that are performed to generate high-quality data for the purpose of validating a model.

Validation Metric A measure that defines the level of accuracy and precision of a simulation.