Verification and Validation (V&V) of Computational Models

A Two-day Short-course of Introduction to, and Implementation of, V&V Concepts

Instructor: **François Hemez, Los Alamos Dynamics, L.L.C.**

Synopsis:

This short-course on the Verification and Validation (V&V) of computational models teaches techniques to quantify prediction uncertainty which includes the broad classes of, first, numerical uncertainty caused by truncation effects in the discretization of partial differential equations and, second, parametric uncertainty caused by the variability of model parameters. The quantification includes the propagation and assessment of how much uncertainty is present in the simulation of an application of interest (*"what are the sources, how much uncertainty is present?"*). It includes understanding which effects control the uncertainty (*"is it predominantly the mesh discretization, parameter variability, or other phenomena?"*) and what can be done to reduce the overall uncertainty (*"should the mesh be refined, should small-scale experiments be performed, should model parameters be calibrated and how?"*).

Technical topics addressed include: 1) code and solution verification, 2) numerical uncertainty, 3) the design of computer experiments, 4) sensitivity analysis and variance decomposition, 5) surrogate modeling, 6) sampling and the propagation of parametric uncertainty, 7) metrics for test-analysis correlation, and 8) model calibration and the assessment of predictive capability.

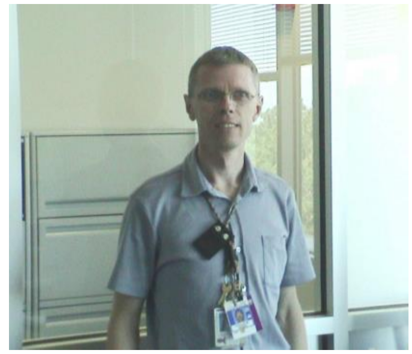
Definitions and concepts of V&V are not discussed in detail; the short-course focuses, instead, on the implementation and application of well-established techniques. Two pre-requisites are, first, a basic knowledge of V&V concepts and, second, familiarity with a computational method (finite element, finite volume, transport method, etc.) and the types of uncertainty that numerical simulations introduce. Many of the illustrations emphasize structural dynamics even though the techniques presented are general-purpose and can be applied to any numerical simulation. Applications include finite element simulations for nonlinear vibrations, transient dynamics, wind turbine blade vibrations and hydrodynamics simulations of smooth or shocked fluid flows.

The short-course has been taught over 20 times since 2001 at private companies, government institutions or in conjunction with technical conferences in Europe and the United States. It is organized jointly by the Israel Institute of Technology (Technion), Haifa, Israel, and Los Alamos Dynamics, L.L.C.

Instructor:

François Hemez, Los Alamos Dynamics, L.L.C.

François Hemez has been technical staff member at Los Alamos National Laboratory since 1997. François graduated from Ecole Centrale (Paris, France) in 1989 and earned a Ph.D. from the University of Colorado in 1993 (aerospace engineering). At Los Alamos, François spent seven years in the Engineering Division, one of which as leader of the Validation Methods team. In 2005, he joined the X-Division for nuclear weapons design. He managed the verification project and the predictive capability assessment project of the Advanced Scientific Computing program. His research interests revolve around the development of methods for Verification and Validation (V&V), uncertainty quantification and decision-making, and their applications to material modeling, engineering, energy and weapon physics projects. François is also adjunct professor at the University of California San Diego (UCSD). He developed and taught the first-ever, graduate-level course offered in a U.S. University in the discipline of V&V (UCSD, 2006). François received the Junior Research Award of the European Association of Structural Dynamics in 2005; four U.S. Department of Energy Defense Program Awards of Excellence for applying V&V to programmatic work at Los Alamos (2006, 2010, 2012); and the D.J. DeMichele Award of the Society for Experimental Mechanics in 2010. Since 1994, he has authored 360+ reports and technical publications, including 39 peer-reviewed journal articles, and given 120+ invited lectures and short-courses.



Course Goals:

Upon completion of this course, attendees will be able to:

- Understand the objectives of code verification, model validation, uncertainty quantification
- Develop procedures for practical code verification and solution verification
- Select a particular mesh size, or time step, to discretize the equations-of-motion
- Quantify the effects of truncation error in numerical simulations
- Assess the trade-offs between more computing resources and more small-scale testing
- Describe the validation paradigm of sensitivity analysis, correlation, uncertainty analysis
- Describe the process to select and compute appropriate features from simulation outputs
- Understand techniques for global sensitivity analysis and effect screening
- Explain the role of designs-of-experiments and analysis-of-variance in model validation
- Define appropriate test-analysis correlation metrics for model revision and calibration
- Discuss when model calibration might, or not, be needed

Who Should Attend?

The short-course is intended for graduate students, researchers, practicing engineers and project managers seeking to understand, or implement, V&V techniques for their applications. Even though key techniques, such as sensitivity analysis and the propagation of uncertainty, are introduced, they are not discussed in depth. Their usefulness is motivated, instead, through the presentation of application examples. The emphasis is placed on explaining how methods can be organized into a process to verify and validate computational models.

The short-course contents are not designed to produce V&V experts. The goal is to provide a sufficient understanding of key techniques such that attendees are able to implement and apply them to their applications, discuss them with their peers and read the pertinent literature.

Graduate students and researchers will be pointed towards essential techniques without having to endure months of literature review. Practicing engineers will understand how to integrate them into a logical process for their applications. Project managers will be exposed to way to define quality controls for the numerical simulations that their projects and customers rely on.

Disclaimer:

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Short-course Outline:

The contents are presented in 12 lectures (one hour each), tentatively organized as shown. The two-day schedule allows for ample discussion and interaction with attendees. The instructor reserves the right to modify the contents to address the audience's needs and preferences.

Lecture 1) High-level Overview of Verification and Validation — Day-1

- High-level comments on modeling, simulation, and "predictability"
- Overview of Verification and Validation (V&V)
- Definitions, organization of V&V activities
- Which questions does V&V address? What can be learned from V&V?
- Examples of typical studies in structural dynamics

Lecture 2) Application of V&V to Wind Turbine Simulations — Day-1

- The "intelligent wind turbine" project at Los Alamos
- Code verification of the finite element software
- Simulation of blade vibration with bounds of numerical uncertainty
- Sensitivity analysis of the numerical simulations
- Calibration of the model using statistical emulators
- Final test-analysis correlation and validation assessment

Lecture 3) Code Verification — Day-1

- Definition of code verification, typical code verification activities
- How to define benchmark code verification problems?
- The Method of Manufactured Solutions (MMS)
- Examples of code verification studies

Lecture 4) Solution Verification — Day-1

- Definition of solution verification, typical solution verification activities
- The concepts of consistency, stability, and convergence
- Modified Equation Analysis (MEA)
- The representation and quantification of truncation error
- Richardson's extrapolation applied to numerical solutions
- The Grid Convergence Index (GCI)

Lecture 5) Feature Extraction for Structural Dynamics — Day-1

- What makes a good feature of the response analyzed?
- Features for linear, stationary dynamics
- Features for arbitrary time-series analysis
- Temporal moments and other features for fast, transient dynamics

- Application of Principal Component Analysis (PCA)
- Features that express a degree of correlation

(End of first day.)

Lecture 6) Design of Computer Experiments — Day-2

- Principles of the design of (physical or computer) experiments
- Full-factorial and fractional factorial designs
- Orthogonal arrays, central composite design
- Formulation of 2^(n-k) designs
- The concept of statistical aliasing
- Examples of applying various designs-of-experiments

Lecture 7) Sensitivity Analysis and Effect Screening — Day-2

- Rationale for effect screening (*"where is an observed variability coming from?"*)
- Simple, linear approaches to effect screening
- Analysis-of-variance (ANOVA) using a design-of-experiments
- Main-effect and linear interaction screening
- Application to Structural Dynamics simulations: what is learned?

Lecture 8) Development of Surrogate Models — Day-2

- Surrogate modeling using a design-of-experiments
- Diagnostics of quality of an emulator
- Low-order, polynomial emulators
- Kernel regression, Gaussian process modeling

Lecture 9) Sampling and Propagation of Parametric Uncertainty — Day-2

- Sampling methods for the forward propagation of (parametric) uncertainty
- Monte Carlo, stratified sampling, Latin Hypercube Sampling (LHS)
- Convergence of statistical estimates
- The concept of a confidence interval

Lecture 10) Test-analysis Correlation and Validation Metrics — Day-2

- Concepts of response features and validation metrics
- Metrics for Structural Dynamics and general-purpose test-analysis correlation
- Metrics based on Principal Component Analysis (PCA)
- Statistical tests that account for probabilistic uncertainty
- Model calibration and inference uncertainty quantification

Lecture 11) An End-to-end Example of Verification and Validation — Day-2

- Engineering example of transient dynamics simulations
- Verification of the finite element software
- Design and execution of computer experiments (predictions)
- Design of physical experiments (measurements)
- Effect screening and identification of statistically most-significant inputs
- Small-scale validation experiments: what is learned?
- Uncertainty propagation and final validation assessment

Lecture 12) Concluding Remarks Day-2

- Summary of main points, final remarks, discussion

(End of second day.)