Verification and Validation (V&V) of Computational Models

A Three-day Short-course

Instructors: **François Hemez and Charles Farrar, 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. It focuses on applications in structural mechanics and structural dynamics. 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.

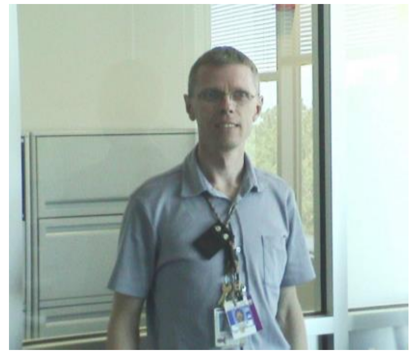
Definitions and concepts of V&V are not discussed in detail; the short-course focuses, instead, on the implementation and applications of well-established techniques. Two pre-requisites are, first, a basic knowledge of V&V concepts and, second, familiarity with the finite element method and the types of uncertainty that numerical simulations introduce. The illustrations emphasize solid mechanics and structural dynamics even though the techniques presented are general-purpose and can be applied to any simulation. The applications include finite element simulations for nonlinear vibrations, transient dynamics, and wind turbine blade vibrations.

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 7th European Workshop on Structural Health Monitoring and Los Alamos Dynamics, L.L.C., and offered in Nantes, France on July 5-7, 2014.

Instructors:

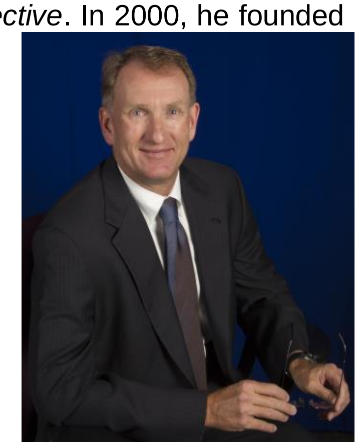
François Hemez, Los Alamos Dynamics, L.L.C.

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.



Charles Farrar, Los Alamos Dynamics, L.L.C.

Chuck Farrar is the President of Los Alamos Dynamics. He has 30 years of experience as a technical staff member, project leader and team leader at Los Alamos National Laboratory (LANL). He is currently the director of The Engineering Institute at LANL. While at Los Alamos, he earned a Ph.D. in civil engineering from the University of New Mexico in 1988. The first ten years of his career at LANL focused on performing experimental and analytical structural dynamics studies for a wide variety of systems including nuclear power plant structures subject to seismic loading and weapons components subject to various portions of their stockpile-to-target loading environments. Chuck Farrar's research interests focus on developing integrated hardware and software solutions to Structural Health Monitoring (SHM) problems and damage prognosis. The results of this research have been documented in over 300 refereed journal articles, book chapters, conference papers, Los Alamos reports, numerous keynote lectures at international conferences, and most recently in a book co-authored with Professor Keith Worden and entitled *Structural Health Monitoring: A Machine Learning Perspective*. In 2000, he founded the Los Alamos Dynamics Summer School. He has received the Los Alamos Fellows Prize for Technical Leadership and the Lifetime Achievement Award in SHM. Chuck Farrar is also adjunct professor at the University of California San Diego where he teaches a graduate-level course on SHM. Additional professional activities include an associated editor position for *Earthquake Engineering and Structural Dynamics* and the development of short-courses on SHM and model validation that have been offered numerous times to industry and government agencies in Asia, Australia, Europe and the United States. In January of 2007 Chuck Farrar was elected to Fellow of the American Society of Mechanical Engineers and in 2012 he was elected as a Fellow of Los Alamos National Laboratory.



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 train V&V experts. The goal is to provide a sufficient understanding of key techniques such that attendees are able to discuss them with their peers, read the pertinent literature implement and apply them to their applications.

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.

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

Short-course Outline:

The contents are presented in 18 lectures (one hour each), tentatively organized as shown. The three-day schedule allows for ample discussion and interaction with attendees. The instructors reserve 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 solid mechanics and 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 in structural dynamics

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) and its implication to quantify truncation effects
- Richardson's extrapolation applied to numerical solutions
- The Grid Convergence Index (GCI) and bounds of truncation error
- Examples of solution verification in structural dynamics

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 designs-of-experiments applied to structural dynamics simulations

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 gained?

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
- Application of statistical sampling to simulations in solid mechanics

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 finite element 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 gained?
- Uncertainty propagation and final validation assessment

Lecture 12) Discussion Session Day-2

- Question/answer session
- Discussion of attendees' applications of interest

(End of second day.)

Lecture 13) Hands-on Exercise: Code Verification Day-3

- Execute MATLAB® provided by the instructors
- Verification of a finite element beam element using an exact solution
- Estimation of the rate-of-convergence of the finite element

Lecture 14) Hands-on Exercise: Method of Manufactured Solutions Day-3

- Execute MATLAB® provided by the instructors
- Practice the Method of Manufactured Solutions (MMS)
- Implement a MMS for a beam bending problem
- Exercise the MMS to diagnose a programming mistake

Lecture 15) Hands-on Exercise: Quantification of Truncation Error Day-3

- Execute MATLAB® provided by the instructors
- Perform a mesh refinement study
- Estimate the Grid Convergence Index (GCI) and quantify truncation error
- Application to the vibration of a three-story frame structure

Lecture 16) Hands-on Exercise: Exploration of Parametric Uncertainty Day-3

- Execute MATLAB® provided by the instructors
- Propagate parametric uncertainty through a finite element model
- Observe differences obtained with different designs-of-experiments

- Perform an analysis-of-variance to identify the most influential parameters
- Application to the vibration of a mass-spring assembly

Lecture 17) Hands-on Exercise: Inference Uncertainty Quantification Day-3

- Execute MATLAB® provided by the instructors
- Perform an optimization of model parameters to reproduce measurements
- Perform an inference of parameter uncertainty to reproduce measurements
- Application to a three species model of radiation decay for medical isotopes

Lecture 18) Concluding Remarks Day-3

- Summary of main points, final remarks, discussion
- Exit survey and feed-back from attendees

(End of third day.)

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