Verification and Validation in Computational Geomechanics

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Outline

Important Sources

- W. L. OBERKAMPF, T. G. TRUCANO, AND C. HIRSCH. Verification, validation and predictive capability in computational engineering and physics. In *Proceedings of the Foundations for Verification and Validation on the 21st Century Workshop*, pages 1–74, Laurel, Maryland, October 22-23 2002. Johns Hopkins University / Applied Physics Laboratory.
- P. J. ROACHE. *Verification and Validation in Computational Science and Engineering*. Hermosa publishers, 1998. ISBN 0-913478-08-3.
- Material from *Verification and Validation in Computational Mechanics* web site `http://www.usacm.org/vnvcsm/` at the USACM.

Motivation

- How much can (should) we trust model implementations (verification)?
- How much can (should) we trust numerical simulations (validation)?
- How good are our numerical predictions?
- Can simulation tools (SimTool) be used for assessing **public safety**?

Verification

- Verification: the process of determining that a model implementation accurately represents the developer's conceptual description and specification. Mathematics issue. *Verification provides evidence that the model is solved correctly.*

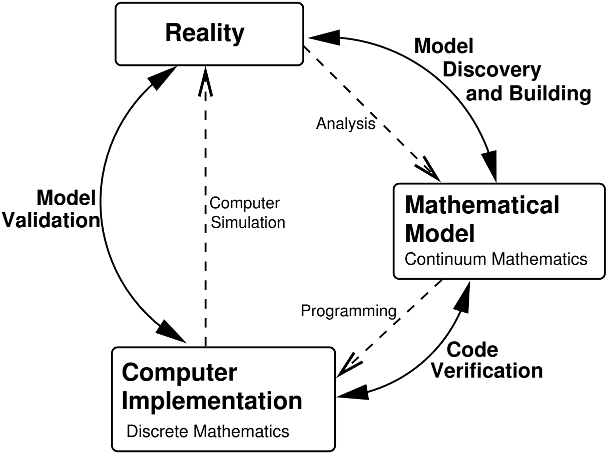
Validation

- Validation: The process of determining the degree to which a model is accurate representation of the real world from the perspective of the intended uses of the model. Physics issue. *Validation provides evidence that the correct model is solved.*

Prediction

- Prediction: use of computational model to foretell the state of a physical system under consideration under conditions for which the computational model has not been validated

Role of Verification and Validation



Outline

Importance of V & V

- V & V procedures are the primary means of assessing accuracy in modeling and computational simulations
- V & V procedures are the tools with which we build confidence and credibility in modeling and computational simulations

Maturity of Computational Simulations

National Research Council committee (1986) identified five stages of maturity in computational fluid dynamics

- **Stage 1:** Developing enabling technologies (scientific papers published)
- **Stage 2:** Demonstration of and Confidence in technologies and tools (capabilities and limitations of technology understood)
- **Stage 3:** Compilation of technologies and tools (capabilities and limitations of technology understood)
- **Stage 4:** Spreading of the effective use (changes the engineering process, value exceeds expectations)
- **Stage 5:** Mature capabilities (fully dependable, cost effective design applications)

Alternative V & V Definitions

IEEE V & V definitions (1984):

- **Verification:** The process of determining whether the products of a given phase of the software development cycle fulfill the requirements established during the previous phase
- **Validation:** The process of evaluating software at the end of the software development process to ensure compliance with software requirements.
- Other organization have similar definitions:
  - Software quality assurance community
  - American Nuclear Society (safety analysis of commercial nuclear reactors)
  - International Organization for Standardization (ISO)

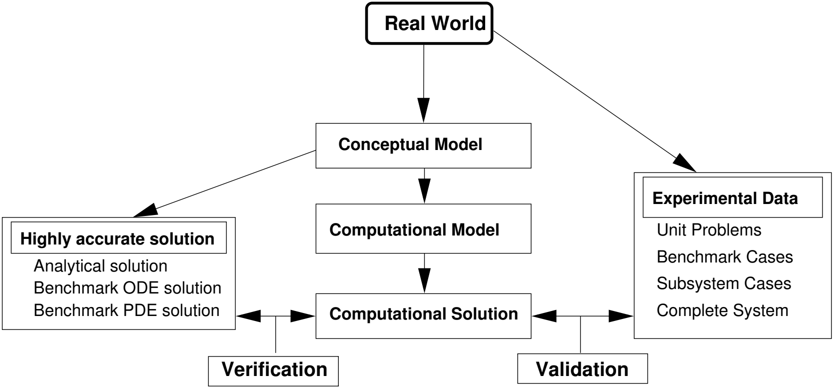
Certification and Accreditation

- **Certification:** A written guarantee that a system or component complies with its specified requirements and is acceptable for operational use (IEEE (1990)).
  - Written guarantee can be issued by anyone (code developer, code user, independent code evaluator)
  - Code certification is more formal than validation documentation
- **Accreditation:** The official certification that a model or simulation is acceptable for use for a specific purpose (DOD/DMSO (1994))
  - Only officially designated entities can accredit
  - Normally appointed by the customers/users of the code or legal authority
  - Appropriate for major liability or public safety applications

Independence of Computational Confidence Assessment

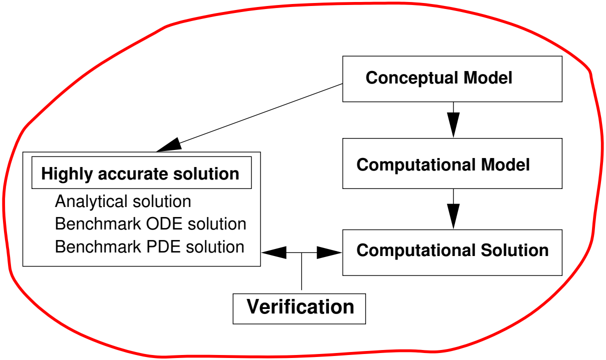
1. V&V conducted by the computational tool developer, *No Independence*
2. V&V conducted by a user from same organization
3. V&V conducted by a computational tool evaluator contracted by developer's organization
4. V&V conducted by a computational tool evaluator contracted by the customer
5. V&V conducted by a computational tool evaluator contracted by the a legal authority *High Independence*

Fundamentals of Verification and Validation



Verification

The process of determining that a model implementation accurately represents the developer's conceptual description and specification.



Verification

Mathematics issue. *Verification provides evidence that the model is solved correctly.*

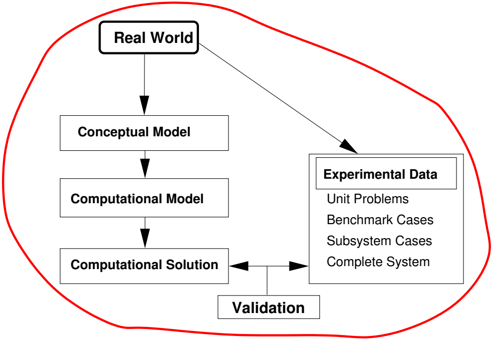
- Identify and remove errors in computer coding
    - Numerical algorithm verification
    - Software quality assurance practice
- Quantification of the numerical errors in computed solution

Verification

- Improving software quality through development process
- Application Programming Interface (API) defines software services developed by **Developers** that are used by **Users**
  - Public API is forever (asset, liability)
  - Realistically, API evolves
  - API design is tough (perfection unachievable, try anyway)
  - Literate programming for API
- Two sided software platform connect Developers AND users through positive feedback (through API)

Validation

The process of determining the degree to which a model is accurate representation of the real world from the perspective of the intended uses of the model.



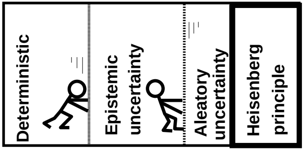
Validation

Quantification of uncertainties and errors in the computational model and the experimental measurements

- Goals on validation
  - Tactical goal: Identification and minimization of uncertainties and errors in the computational model
  - Strategic goal: Increase confidence in the quantitative predictive capability of the computational model
- Strategy is to reduce as much as possible the following:
  - Computational model uncertainties and errors
  - Random (precision) errors and bias (systematic) errors in the experiments
  - Incomplete physical characterization of the experiment

Validation Procedure Uncertainty

- Aleatory uncertainty → inherent variation associated with the physical system (variation in external excitation, material properties...). AKA irreducible uncertainty, variability and stochastic uncertainty.
- Epistemic uncertainty → potential deficiency in any phase of the modeling process that is due to lack of knowledge (poor understanding of mechanics...). AKA reducible uncertainty, model form uncertainty and subjective uncertainty.



Use of Physical Experiments for Validation

- **Traditional Experiments**
  - Improve the fundamental understanding of physics involved
  - Improve the mathematical models for physical phenomena
  - Assess component performance
- **Validation Experiments**
  - Model validation experiments
  - Designed and executed to quantitatively estimate mathematical model's ability to simulate well defined physical behavior
  - The simulation tool (SimTool) (conceptual model, computational model, computational solution) is the customer

Validation Experiments

- A validation experiment should be jointly designed and executed by experimentalist and computationalist
  - Need for close working relationship from inception to documentation
  - Elimination of typical competition between each
  - Complete honesty concerning strengths and weaknesses of both experimental and computational simulations
- A validation experiment should be designed to capture the relevant physics
  - Measure all important modeling data in the experiment
  - Characteristics and imperfections of the experimental facility should be included in the model

Validation Experiments (contd)

- A validation experiment should use any possible synergism between experiment and computational approaches
  - Offset strength and weaknesses of computations and experiments
  - Use high confidence simulations for simple physics to calibrate of improve the characterization of the experimental facility
  - Conduct experiments with a hierarchy of physics complexity to determine where the computational simulation breaks (remember, SimTool is the customer!)
- Maintain independence between computational and experimental results
  - Blind comparison, the computational simulations should be predictions
  - Neither side is allowed to use fudge factors, parameters

Validation Experiments (contd)

- Validate experiments on unit level problems, hierarchy of experimental measurements should be made which present an increasing range of computational difficulty
  - Use of qualitative data (e.g. visualization) and quantitative data
  - Computational data should be processed to match the experimental measurement techniques
- Experimental uncertainty analysis should be developed and employed
  - Distinguish and quantify random and correlated bias errors
  - Use symmetry arguments and statistical methods to identify correlated bias errors
  - Make uncertainty estimates on input quantities needed by the SimTool

Outline

Prediction

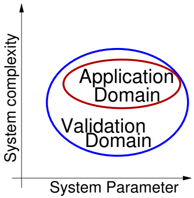
- Prediction: use of computational model to foretell the state of a physical system under consideration under conditions for which the computational model has not been validated
- Validation does not directly make a claim about the accuracy of a prediction
  - Computational models are easily misused (unintentionally or intentionally)
  - How closely related are the conditions of the prediction and specific cases in validation database
  - How well is physics of the problem understood

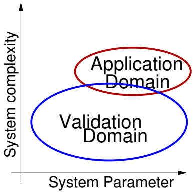
Relation Between Verification, Validation and Prediction

Quantification of confidence in a prediction:

- How do I quantify verification and its inference value in a prediction?
- How do I quantify validation and its inference value in a predictions?
- How far are individual validation experiments from physical system of interest?

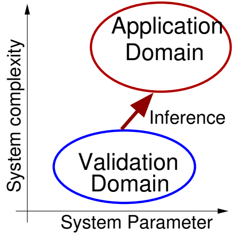
Application Domain Complete or Partial Overlap





- Rarely applicable to infrastructure objects
- Environmental influences (generalized loads, conditions, wear and tare) are hard to predict
- Human factors (I-35 bridge failure, **forgot** to multiply loads with safety factor...)

Application Domain – No Overlap



- Inference ⇒ Based on **physics** or **statistics** (or both)
- Validation domain is actually an aggregation of tests and thus might not be convex (bifurcation of behavior)
- Validation domain for infrastructure objects (bridges, dams, buildings, ports...) is exclusively non–overlapping with the application domain.

Importance of Models and Numerical Simulations

- Verified and Validated models can be used for assessing behavior of
  - components or
  - complete systems,
- with the understanding that the environmental influences cannot all be taken into the account prior to operation
- but with a good model, their influence on system behavior can be assessed as need be (before or after the event)

Prediction under Uncertainty

- Ever present uncertainty needs to be estimated for predictions
- Identify all relevant sources of uncertainty (see next lecture on uncertain soils)
- Create mathematical representation of individual sources
- Propagate representation of sources through modeling and simulation process

Outline

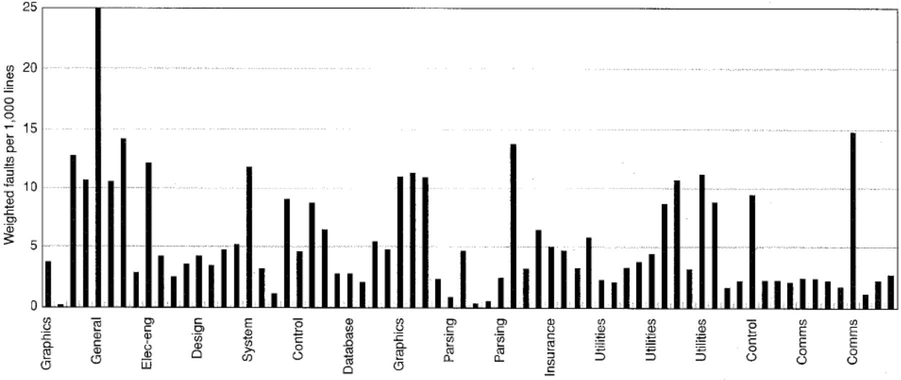
Errors in Scientific Software

- Les Hatton, Oakwood Computing
- "Extensive tests showed that many software codes widely used in science and engineering are not as accurate as we would like to think."
- "Better software engineering practices wold help solve this problem,"
- "Realizing that the problem exists is an important first step."
- Large experiment over 4 years measuring faults (T1) and failures (T2) of scientific and engineering codes

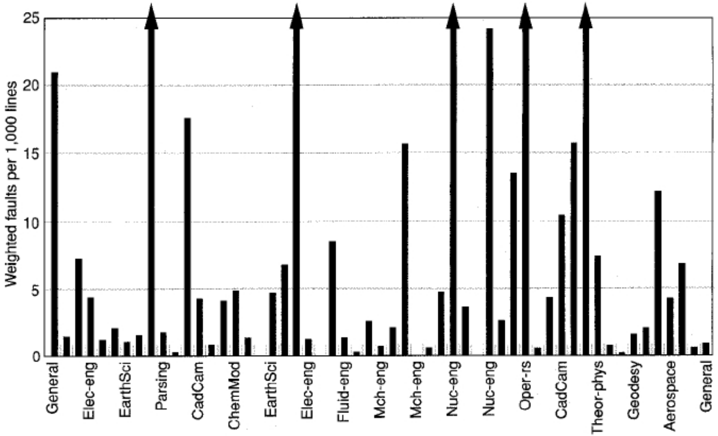
The T1 Experiments

- Measured defects without running the code, measuring formal consistency of 3,305,628 lines f77 and 1,928,011 lines of C
- 100 codes, 40 application areas: graphics, nuc. mech. chem. aero. civil engineering, comms, DBs, med. systems
- Safety–critical and non–safety–critical applications
- Applications with and without internationally standardized systems of quality control
- Mature codes (1 - 20 years old), in regular use
- Errors (select), arguments sequence in function calls, misunderstanding of finite precision arithmetic, code complexity

T1: C Sources


Weighted faults per 1,000 lines
25
20
15
10
5
0
Graphics
General
Elec-eng
Design
System
Control
Database
Graphics
Parsing
Parsing
Insurance
Utilities
Utilities
Utilities
Control
Comms
Comms

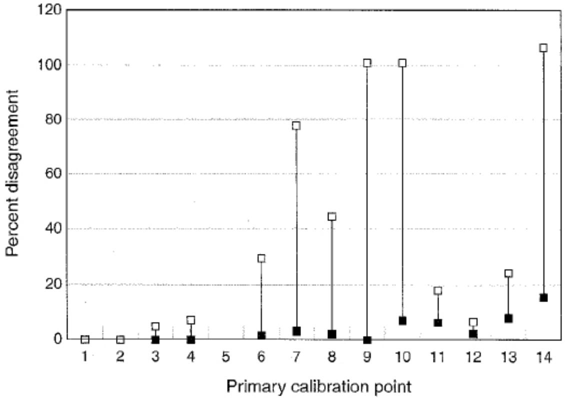
T1: f77 Sources



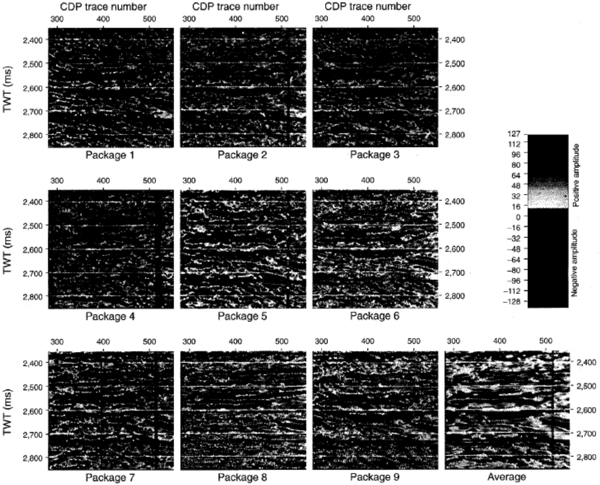
The T2 Experiments

- Specific application area: seismic data processing (inverse analysis)
- Echo sounding of underground and reconstructing "images" of subsurface geological structure
- Nine mature packages, using same algorithms were used on a same data set!
- 14 primary calibration points for results check
- Results "fascinating and disturbing"

T2: Disagreement at Calibration Points



T2: Stage 14, Interpretation of Data

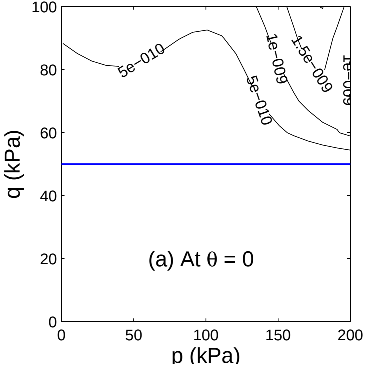


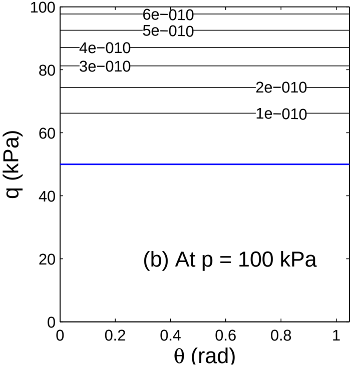
Outline

Constitutive Integration Error Maps

Normalized error: $\delta^r = \sqrt{(\sigma_{ij} - \sigma^*_{ij})(\sigma_{ij} - \sigma^*_{ij})} / \sqrt{\sigma^0_{pq}\sigma^0_{pq}}$

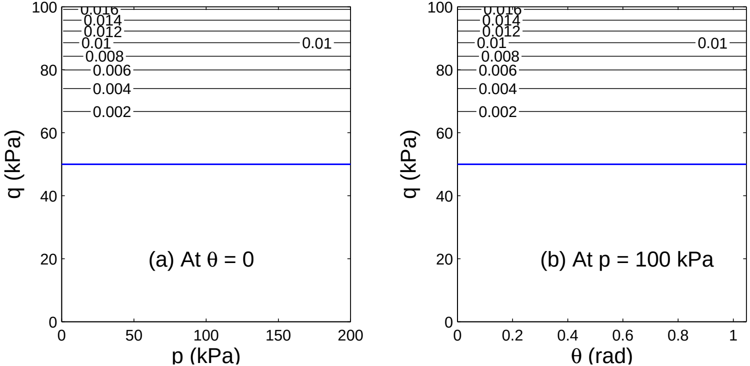
von Mises, linear isotropic hardening:





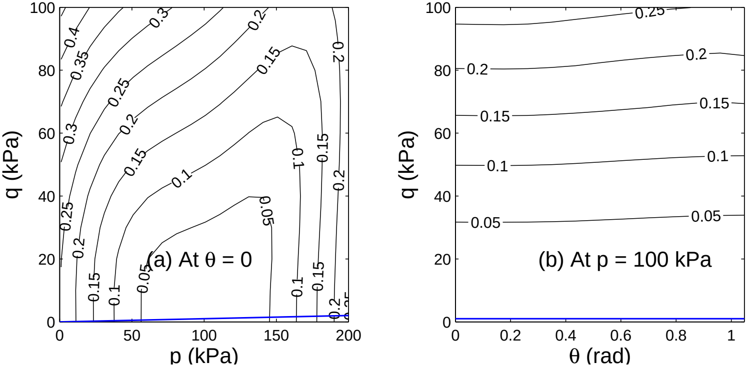
Constitutive Integration Error Maps

von Mises, non–linear kinematic hardening (Armstrong-Frederick):

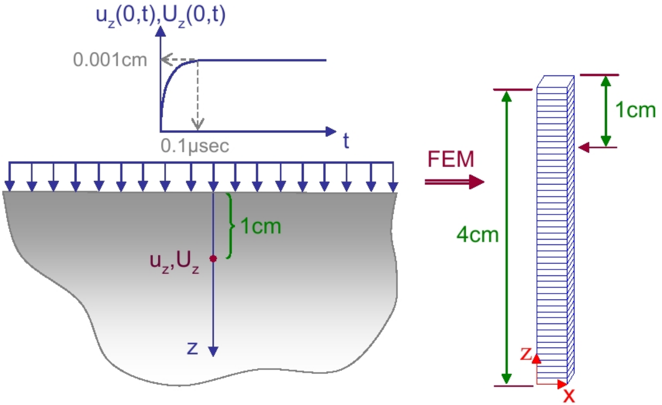


Constitutive Integration Error Maps

Dafalias-Manzari, rotational kinematic hardening, bounding surface:

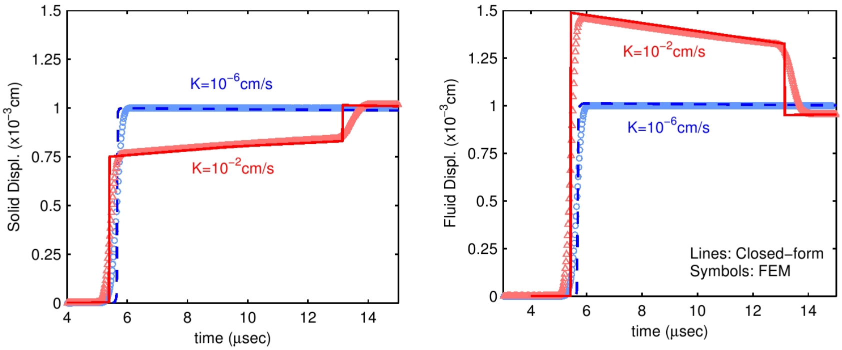


Coupled Formulation and Implementation

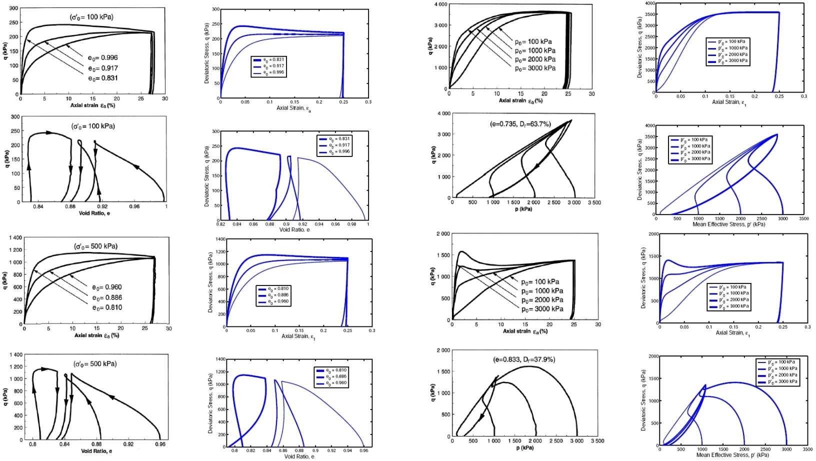


(after Gajo 1995)

Coupled Formulation and Implementation



Material Model Validation (Dafalias-Manzari)



Summary

- Importance of proper verification and validation for numerical predictions used in design of infrastructure objects
- Public (yours and mine) safety issue!
- Would you trust (design using) numerical simulations if SimTool did not follow (extensive) Verification and Validation procedures?