On Computational Simulations and Predictions

Boris Jeremić

Department of Civil and Environmental Engineering
University of California, Davis

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 do we use experiments to develop and improve models?
- How much can (should) we trust model implementations (verification)?
- How much can (should) we trust numerical simulations (validation)?
- How good are our predictions?

Verification, Validation and Prediction

- 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: 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: 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

Outline

Importance of V & V

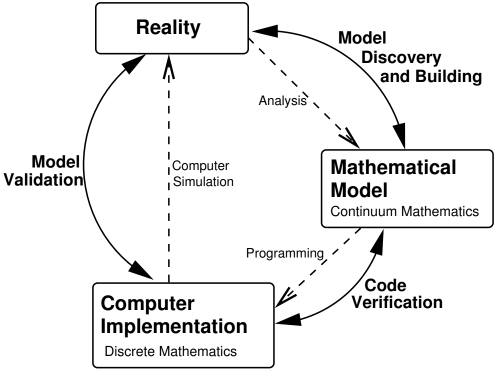
- V & V procedures are the primary means of assessing accuracy in modeling and computational simulations
- V & V procedures are the tools with which we build confidence and credibility in modeling and computational simulations

Maturity of Computational Simulations

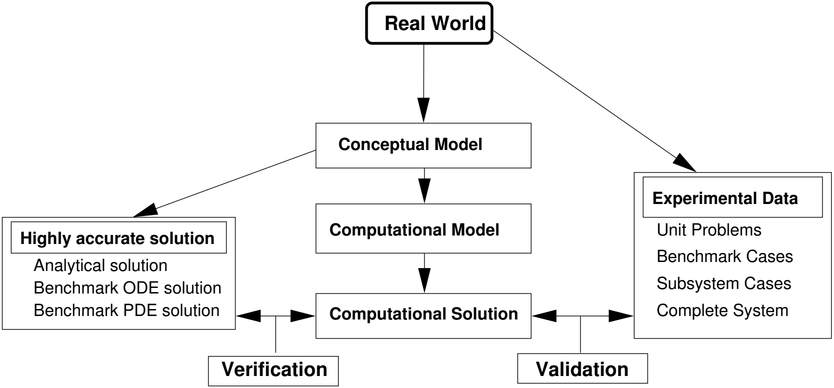
NRC committee (1986) identified stages of maturity in CFD

- **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)

Role of Verification and Validation



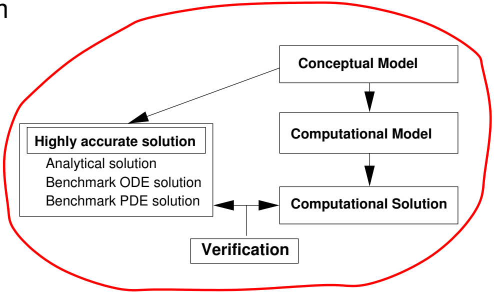
Fundamentals of Verification and Validation



Verification: Model is solved correctly (Mathematics)

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

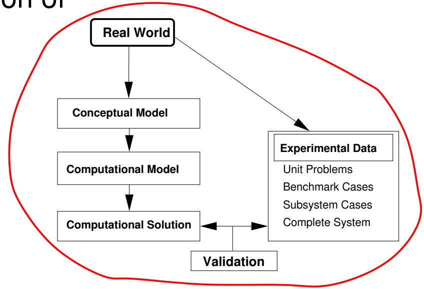
- Identify and remove errors in computer coding
  - Numerical algorithm verification
  - Software quality assurance practice
- Quantification of the numerical errors in computed solution



Validation: Correct model is solved (Physics)

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.

- 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



Validation Procedure Uncertainty

- Aleatory uncertainty → inherent variation associated with the physical system of the environment (variation in external excitation, material properties...). Also know known as 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...). Also known as reducible uncertainty, model form uncertainty and subjective uncertainty

Types of Physical Experiments

- **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
- A validation Experiment should be designed to capture the relevant physics
- A validation experiment should use any possible synergism between experiment and computational approaches
- Maintain independence between computational and experimental results
- Validate experiments on unit level problems, hierarchy of experimental measurements should be made which present an increasing range of computational difficulty
- Experimental uncertainty analysis should be developed and employed

Outline

Prediction

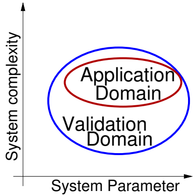
- Prediction: use of computational model to foretell the state of a physical system under consideration under conditions for which the computational model has not been validated
- Validation does not directly make a claim about the accuracy of a prediction
  - Computational models are easily misused (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

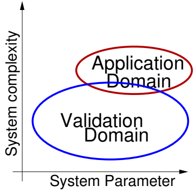
Relation Between Validation and Prediction

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 experiments in my validation database from my physical system of interest?

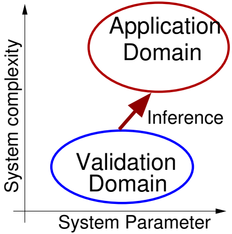
Application Domain Complete or Partial Overlap





- Rarely applicable to engineering systems, certainly not for bridges, buildings, port facilities, dams...
- Even if the engineering system is small, environmental influences (generalized loads, conditions, wear and tare) are hard to predict
- Human factors (Mars rover example: memory overflow, operator **forgot** to flush the memory...)

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)
- Experimental facilities provide for validation domain that are exclusively non–overlapping with the application domain.

Importance of Models and Numerical Simulations

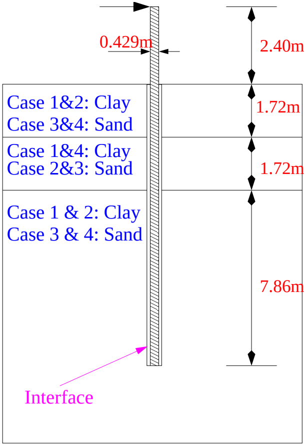
- Verified and Validated models can be used for assessing behavior of
  - components or
  - complete systems,
- with the understanding that the environmental influences cannot all be taken into the account prior to operation
- but with a good model, their influence on system behavior can be assessed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

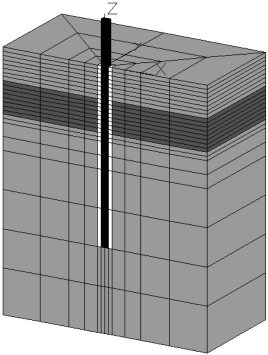
Prediction under Uncertainty

- Ever present uncertainty needs to be estimated for predictions
- Identify all relevant sources of uncertainty
- Create mathematical representation of individual sources
- Propagate representation of sources through modeling and simulation process

Outline

Single Pile in Layered Soils: Model

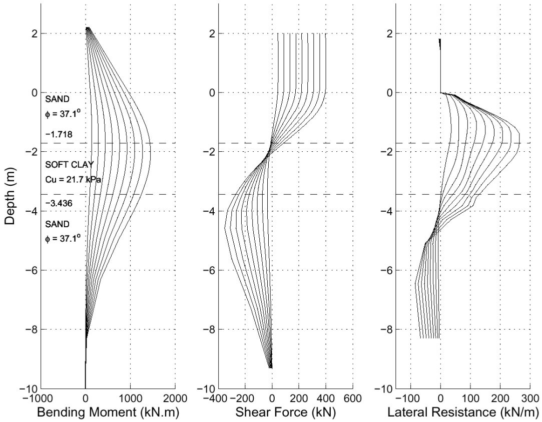




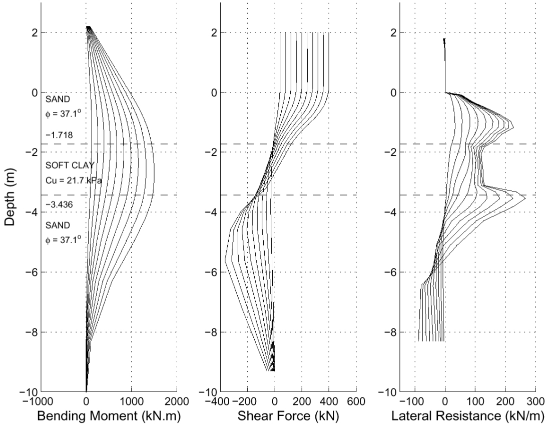
Available Data for Prototype

- Sand:
  - friction angle ϕ of 37.1^o,
  - Shear modulus at a depth of 13.7 m of 8960 kPa (E_o = 17400 kPa),
  - Poisson ratio of 0.35
  - Unit weight of 14.50 kN/m^3.
  - Dilation angle 0^o
- Clay (made up)
  - Shear strength 21.7 kPa
  - Young's modulus 11000 kPa
  - Poisson ratio 0.45
  - Unit weight 13.7 $\mathrm{kN/m^3}$

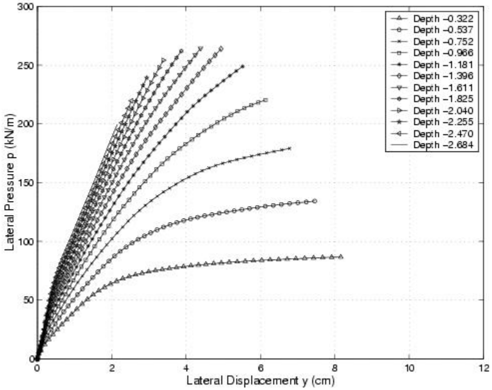
Single Pile in Sand: M, Q, p

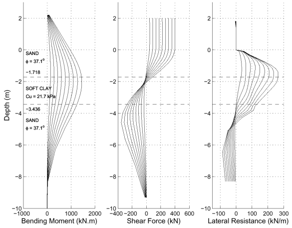


Single Pile in Sand with Clay Layer: M, Q, p

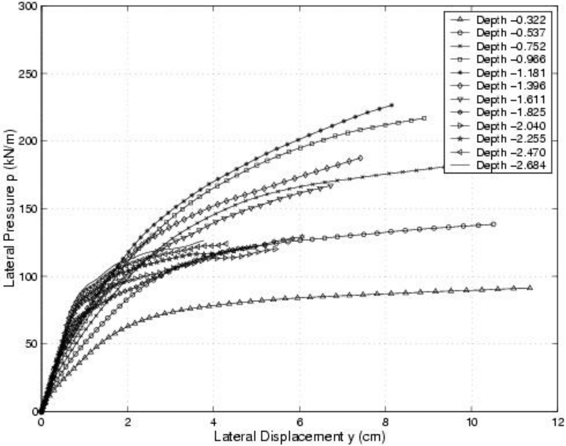


Single Pile in Sand: $p - y$ Response

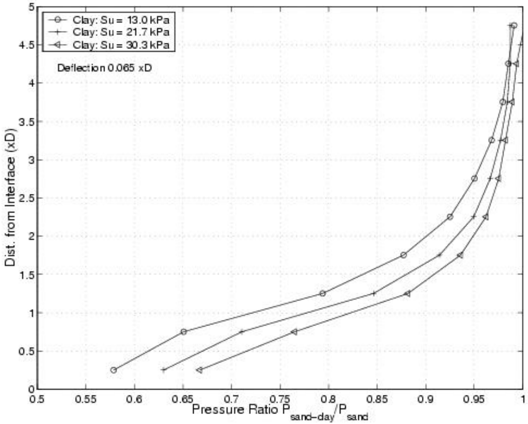


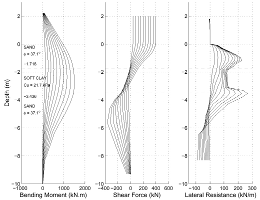


Single Pile in Sand with Clay Layer: $p - y$ Response



$p - y$ Pressure Ratio Reduction for Layered Soils

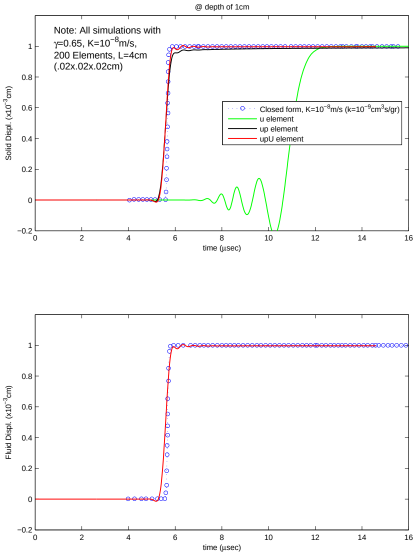




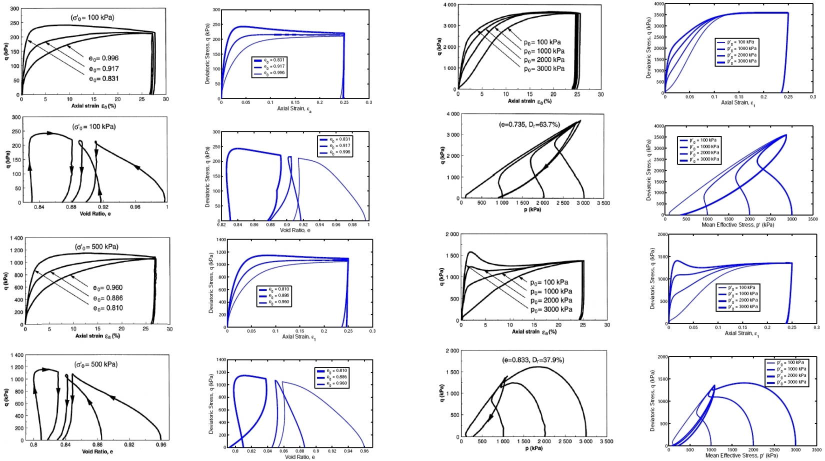
Outline

Verification

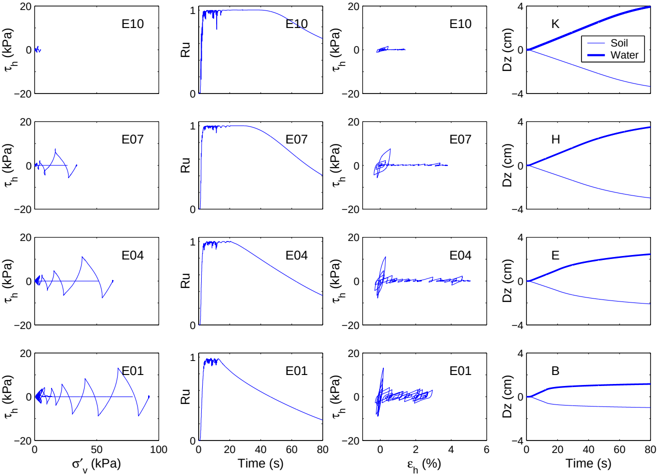
Number of closed form solutions used (elastic, coupled, static and dynamic)



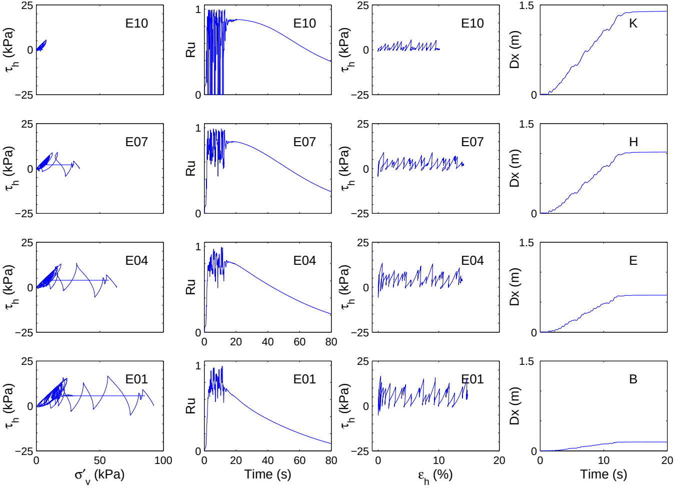
Material Model Validation (Dafalias-Manzari)



Loose Sand, Level Ground



Loose Sand, Sloping Ground



Outline

Detailed 3D, FEM model

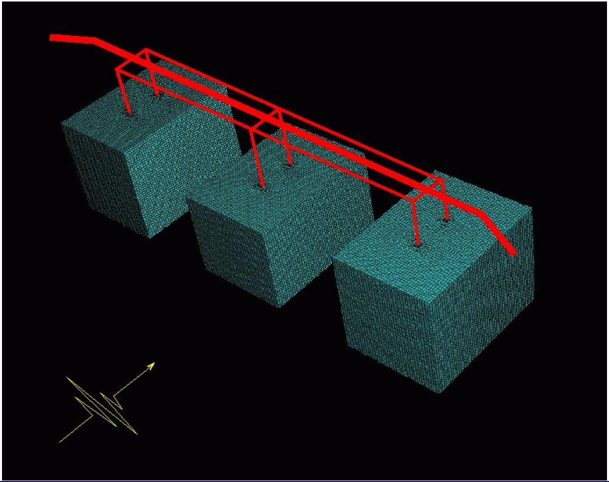
- Construction process
- Two types of soil: stiff soil (UT, UCD), soft soil (Bay Mud)
- Deconvolution of given surface ground motions
- Use of the DRM (Bielak et al.) for seismic input
- Soil:
  - Sand (single monotonic triax test from UT...)
  - Clay (made up, bay mud, total stress)
- Piles $\rightarrow$ beam-column elements in soil holes
- Structural model: collaboration UCD, UCB and UW
- No artificial damping (only mat. dissipation, radiation)

Element Size Issue

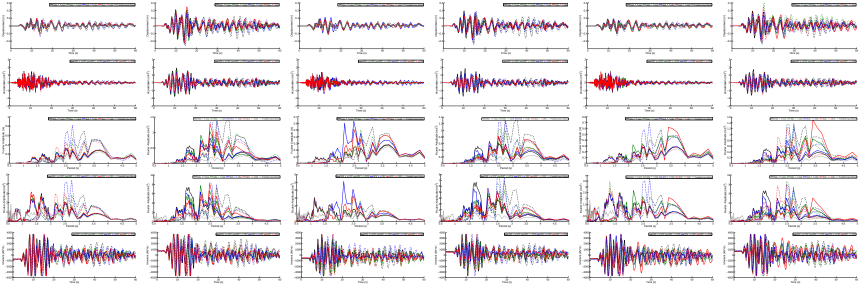
Filtering of frequencies depending on element size (want at least 10 nodes per full wave form)

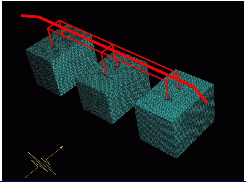
model size (el)	el. size	f_{cutoff}	min. $G/Gmax$	γ
12K	1.0 m	10 Hz	1.0	<0.5 %
15K	0.9 m	>3 Hz	0.08	1.0 %
150K	0.3 m	10 Hz	0.08	1.0 %
500K	0.15 m	10 Hz	0.02	5.0 %

FEM Mesh (one of)

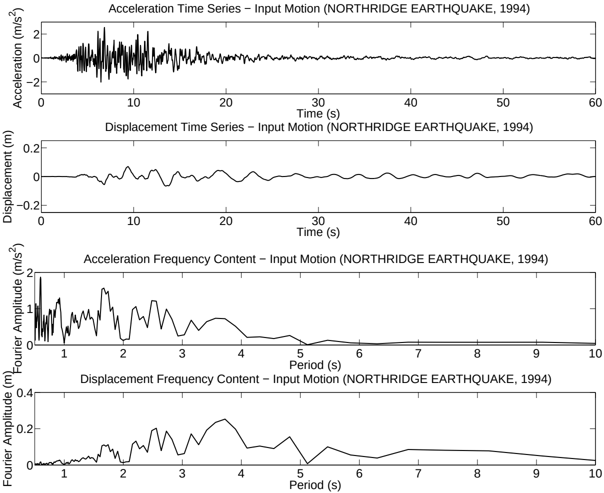


Simulation Results

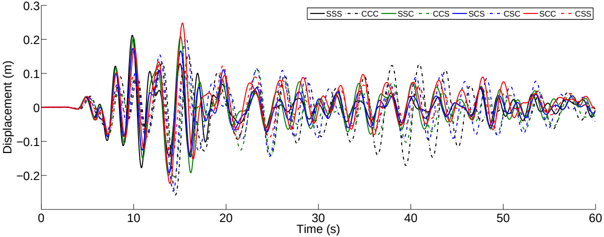


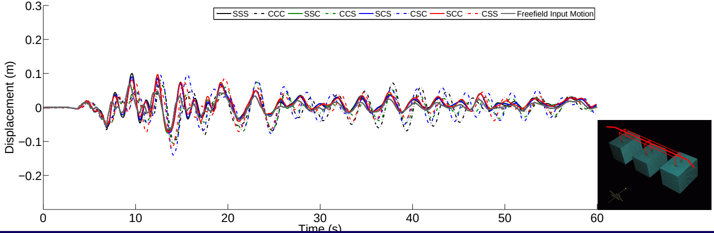


Northridge Input Motions

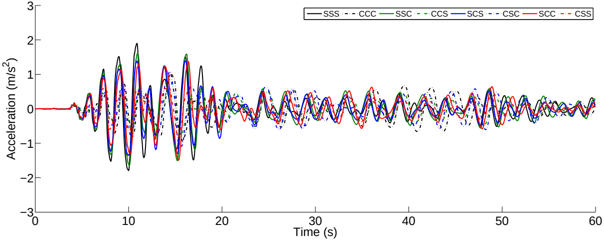


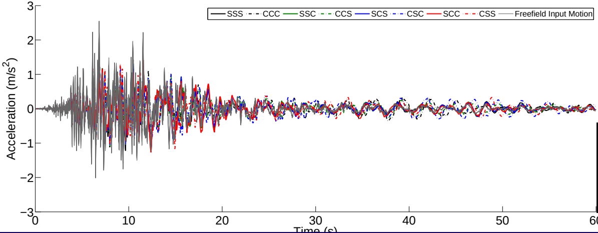
Short Period E.: Left Bent, Structure and Soil, Disp.

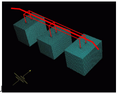




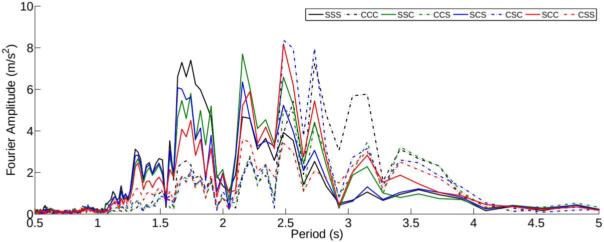
Short Period E.: Left Bent, Structure and Soil, Acc.

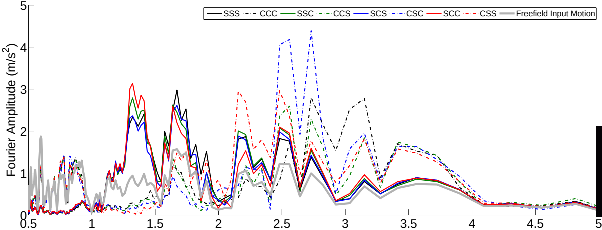


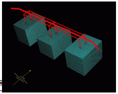




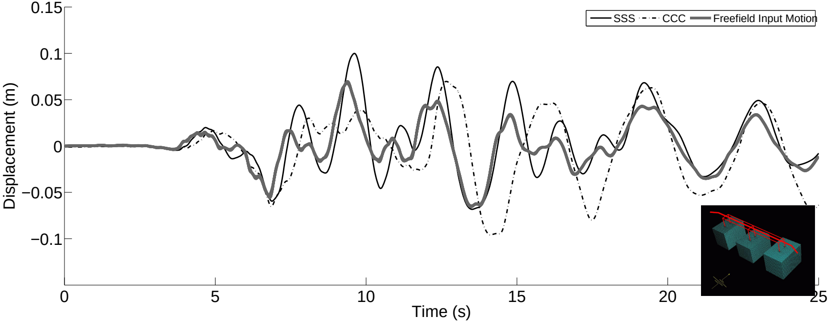
Short Period E.: Left Bent, Structure and Soil, Acc.Sp.







Short Period E.: Left Bent, Free Field vs Real Disp.



Summary

- Importance of verification and validation for numerical prediction (simulations)
- Detailed treatment in new courses:
  - Spring '08 ECI280A, Nonlinear Finite Elements
  - Spring '09 ECI280B, Nonlinear Dynamic Finite Elements
- Would you (and others) trust simulations if you followed V and V procedures?