COST TU0904 Integrated Fire Engineering and Response
MC and WG´s meetings
2012 October 8-9, Zadar, CROATIA

Principles of benchmark studies (Verification & Validation)

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Plan for presentation

- Main question
- Spectacular example
- Some facts
- Predictive capabilities
- Verification & Validation
    - General aspects
    - Errors & Uncertainties
    - Definitions
    - Verification
    - Mesh density study
    - Validation
    - Domains
    - Calibration
    - SRQ
    - Validation Metrics
- Example
- Databases of benchmark problems
- Summary

What are the predictive capabilities of our computer simulations (in Structural Fire Engineering)?

Computational Science and Engineering (CS&E)
Computational Engineering and Physics (CE&P)


George E. P. Box

„Essentially, all models are wrong, but some are useful''

Box G.E.P., Draper N.R. (1987) Empirical model-building and response surfaces, *John Wiley & Sons*., pp. 669

Spectacular example of a software bug

F-22 Squadron Shot Down by the International Date Line (2007)

Maj. Gen. Don Sheppard (ret.):

”...At the international date line, whoops, all systems dumped and when I say all systems, I mean all systems, their navigation, part of their communications, their fuel systems.


$120 million F-22 Raptor

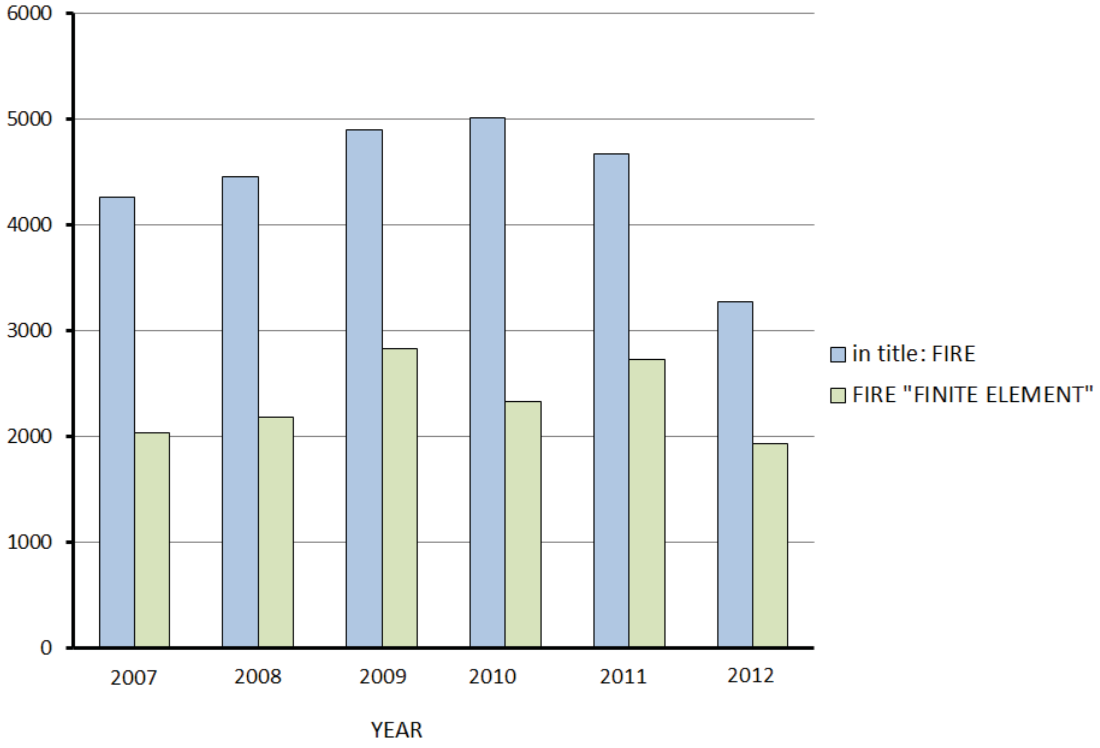
……

It was a computer glitch in the millions of lines of code, somebody made an error in a couple lines of the code and everything goes.”

http://www.defenseindustrydaily.com

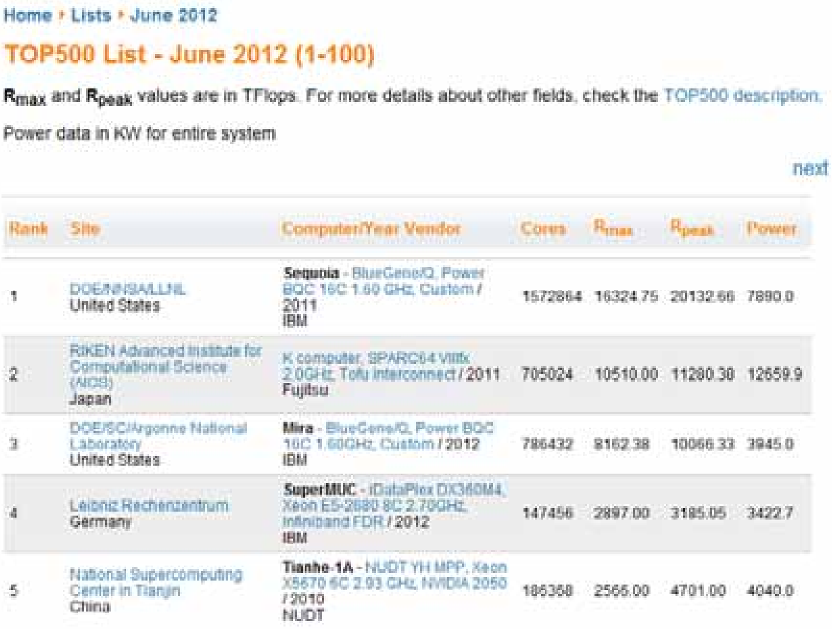
Some facts

Number of articles according Google Scholar
with FIRE in the title
with FIRE + "FINITE ELEMENT" anywhere in the article



Some facts

„In the 1970s, a 20 ms crash test simulation using a 300-element vehicle model took about 30 hours of computer time at a cost equivalent to the three-year salary of a university professor.''



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TOP500 List - June 2012 (1-100)

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

Power data in KW for entire system

next

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom / 2011 IBM	1572864	16324.75	20132.66	7890.0
2	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect / 2011 Fujitsu	705024	10510.00	11280.38	12659.9
3	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	786432	8162.38	10066.33	3945.0
4	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR / 2012 IBM	147456	2897.00	3185.05	3422.7
5	National Supercomputing Center in Tianjin China	**Tianhe-1A** - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050 / 2010 NUDT	186368	2566.00	4701.00	4040.0

Moore's law states that computer power increases by a factor of two every eighteen months

Some facts

LS-DYNA® - a finite element (FE) based simulation software - had originally 50,000 lines of code and then approached 2 million lines in little more than a decade.

"…for many years the Journal of Applied Mechanics shunned papers on the finite element method because it was considered of no scientific substance.

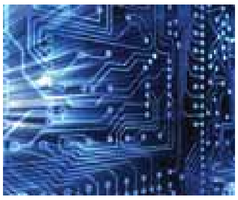
T. Belytschko, W.K. Liu, B. Moran, Nonlinear Finite Elements for Continua and Structures, John Wiley & Sons, LTD, Chichester, England, 2000

Barriers to computability - smoothness and stability of the response, uncertainties, coupled physics, …

The number of execution paths in a typical commercial code is often so large that some paths are never explored, even after years of service.

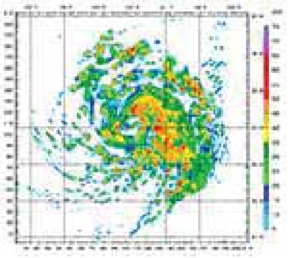
Belytschko T., Mish K., "Computability in nonlinear solid mechanics"
http://www.tam.northwestern.edu/tb/computability_w_figs.pdf

What are the predictive capabilities of our computer simulations?



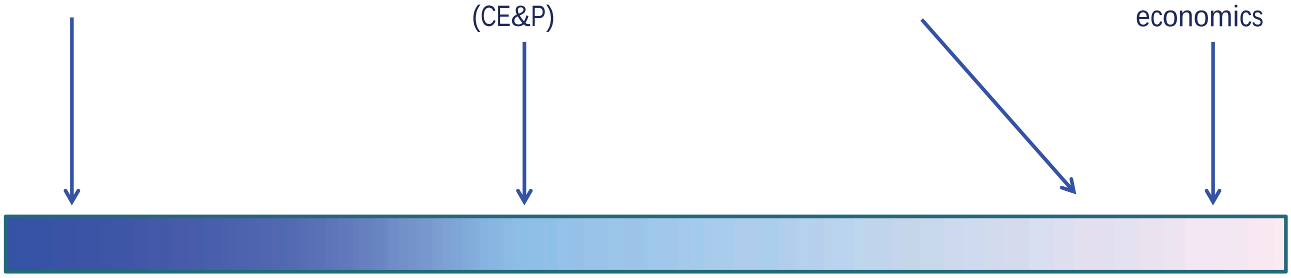
Modeling
electronic
systems
e.g. Verilog

Computational Science
and Engineering (CS&E)
Computational
Engineering and Physics
(CE&P)



Numerical
weather
prediction

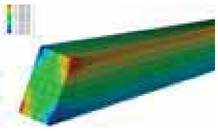
Numerical
models
in
economics



VERY GOOD

POOR

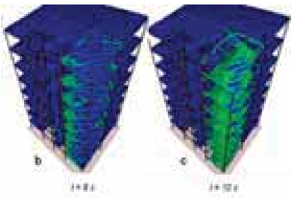
What are the predictive capabilities of our computer simulations (Computational Science and Engineering (CS&E))?



Linear FE static analysis

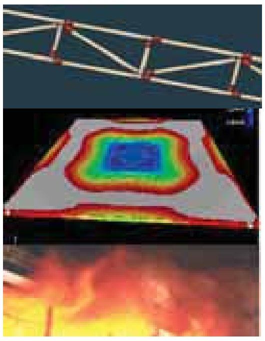
Linear FE dynamic analysis

Transient dynamics (crash tests)



Nonlinear static (stability)

Computational Fluid Dynamics CFD



Structural Fire Engineering

BETTER

MORE DIFFICULT

Verification & Validation

What are the recommended procedures?

ASME V&V 10-2006

Guide for Verification and Validation in Computational Solid Mechanics

AN AMERICAN NATIONAL STANDARD

The American Society of Mechanical Engineers

Simulation Verification, Validation and Accreditation Guide

Australian Defence Simulation Office

Department of Defence, Canberra

Concepts of Model Verification and Validation

Los Alamos NATIONAL LABORATORY

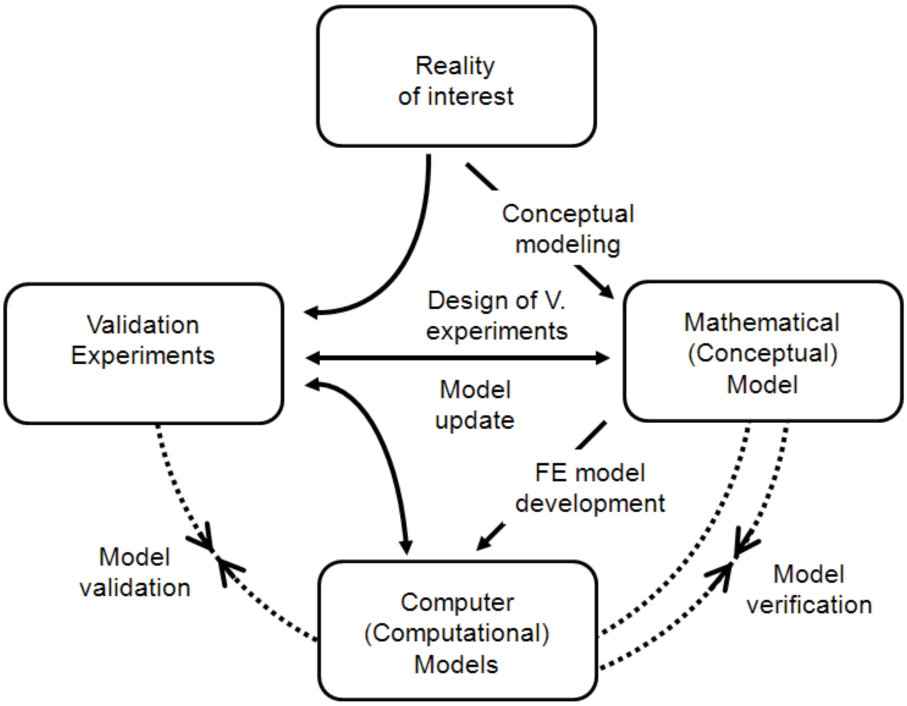
AIAA G-077-1998

Guide

Guide for the Verification and Validation of Computational Fluid Dynamics Simulations

AIAA

General aspects of modeling, experimentation, verification, and validation



Kwasniewski L. (2009) On practical problems with verification and validation of computational models, Archives of Civil Engineering, vol. LV, no. 3, pp. 323-346

Errors & Uncertainties

“**Error** of measurement (calculation) - the result of a measurement (calculation) minus the value of the measurand” (accurate solution),

“**Uncertainty** - a parameter associated with the result of a measurement (solution) that characterizes the dispersion of the values that could reasonably be attributed to the measurand” (accurate solution).

An **error** is the difference between our result and the value (given or imaginable) that is considered to be accurate.

The **uncertainties** can be thought as the bounds of the **errors** which can be irreducible (aleatory) or reducible (epistemic).

Errors in testing usually have two components, random (precision) and systematic (bias)

ISO, Guide to the Expression of Uncertainty in Measurement, ISO Geneva, 1993.

Errors & Uncertainties

Most of the literature point out at five primary sources of errors in computational solutions:

- insufficient spatial discretization,
- insufficient time discretization,
- insufficient iterative convergence,
- computer round-off,
- computer programming.

W.L. Oberkampf, T.G. Trucano, C. Hirsch, Verification, validation, and predictive capability in computational engineering and physics, Appl. Mech. Rev. 57 (5), 345–384, 2004

In the nonlinear computation there are also errors which are not the result of a programmer's mistakes or improper use of the code but are an inherent part of the solution procedures.

Kwasniewski L. (2009) On practical problems with verification and validation of computational models, Archives of Civil Engineering, vol. LV no 3 pp 323-346

Definitions of Verification & Validation

Verification is supposed to deliver evidence that mathematical models are properly implemented and that the numerical solution is correct with respect to the mathematical model.

Verification uses comparison of computational solutions with highly accurate (analytical or numerical) **benchmark** solutions and among themselves, whereas **validation** compares the numerical solution with the experimental data.

Verification should precede **validation.**

Experimental **validation** is the final check to reveal possible errors and to estimate the accuracy of the simulation.

Validation can be practically split into three tasks:

- to detect and separate the model's significant discrepancies,
- to remove and reduce removable and unavoidable errors,
- to evaluate uncertainties in the results.

„**Verification** deals with **mathematics**; **validation** deals with **physics**''

Roache P.J. (1998) Verification and validation in computational science and engineering, Hermosa Publishers Albuquerque, NM

Verification

A „posteriori” approach where the reasoning is based on the experience coming from repeated calculations.

Benchmarking and comparison with simplified models

- question about the sufficient mesh resolution
- the mesh size should be dependent of specific quantities of interest
- simple checks: mass, reactions (Equations of Equilibrium must be always satisfied)
- simple check: conservation laws for mass, momentum, and energy (non-physical energy components < 5%)
- simplify FE model: simle loading, simplified BC, materials
- Quasi-static loading as a special case for transient analysis
- importance of the databases collecting well-documented **benchmark** problems

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Mesh density study

- Discretization error

$$E = f_h - f_{exact} = Ch^p + H.O.T.$$

…….

- Order of convergence

$$p = \frac{ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{ln(r)}$$

- Estimate of the asymptotic solution

$$f_{h=0} \cong f_1 + \frac{f_1 - f_2}{r^2 - 1}$$

- E_1 is the estimator of the relative error

$$E_1 = \frac{\varepsilon}{r^p - 1}, \qquad \varepsilon = \frac{f_1 - f_2}{f_1}$$

- Grid Convergence Index – GCI procedure (Richardson extrapolation)

$$GCI = \frac{F_s|\varepsilon|}{r^p - 1} 100\%$$

P.J. Roache "Verification and validation in computational science and engineering", Computing in Science Engineering, Hermosa publishers, pp. 8-9 (1998)

Verification

Sensitivity study

- determine the crucial input parameters
- evaluate the possible range of their variation
- helps to identify the sources of errors
- can reveal if the considered problem is extremely sensitive to the input variation (imperfection sensitive structures or the on-off processes)
- imperfections can be applied to geometry, loading (as eccentricities), boundary conditions, and material properties

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Validation Domains

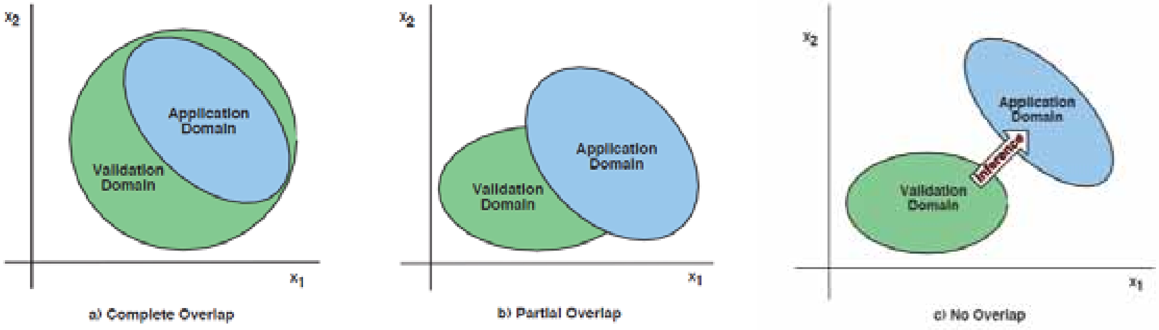
Experimental **validation** is the final check to reveal possible errors and to estimate the accuracy of the simulation.

- differences between mathematical and physical systems
- differences between computerized and mathematical models
- distinction between a physical system (our concept of it) and the subject of an experiment used for validation

Application and validation domains

Application domain defines the intended boundaries for the predictive capability of the computational model.

Validation domain characterizes the representation capabilities of the experiment.



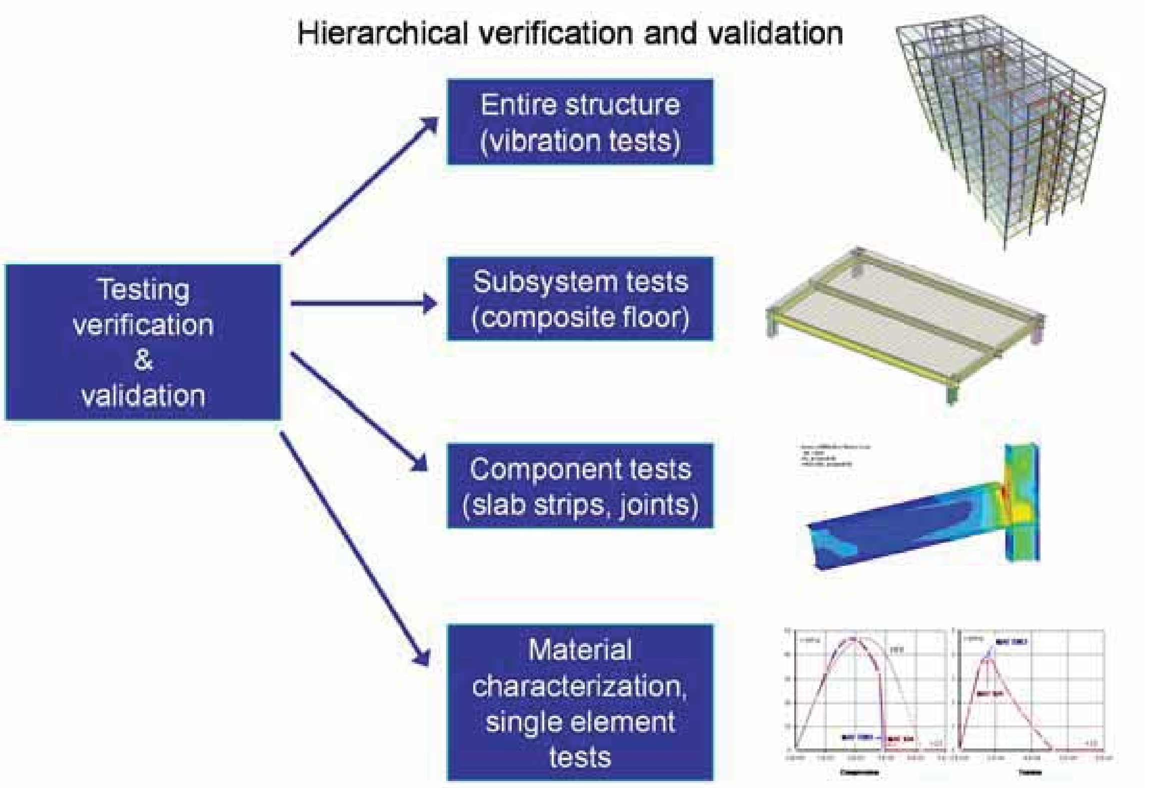
a) Complete Overlap b) Partial Overlap c) No Overlap

W.L. Oberkampf, T.G. Trucano, C. Hirsch, Verification, validation, and predictive capability in computational engineering and physics, Appl. Mech. Rev. 57 (5), 345–384, 2004

Validation

Validation hierarchy

the experiments for the considered system are usually divided into three or four levels (tiers) representing different degrees of complexity.



Hierarchical verification and validation

Testing verification & validation

Entire structure (vibration tests)

Subsystem tests (composite floor)

Component tests (slab strips, joints)

Material characterization, single element tests

SRQ

Validation and calibration

The idea of the **calibration** procedure is to establish the quantities of modeling parameters that give the model's response closest to the actual experimental data.

The **calibration** is performed through comparison between an experiment and repeated calculations with modified input parameters.

It can happen that due to superimposing of errors we can get good correlation between experimental and numerical results for a wrong model defined by incorrect input parameters.

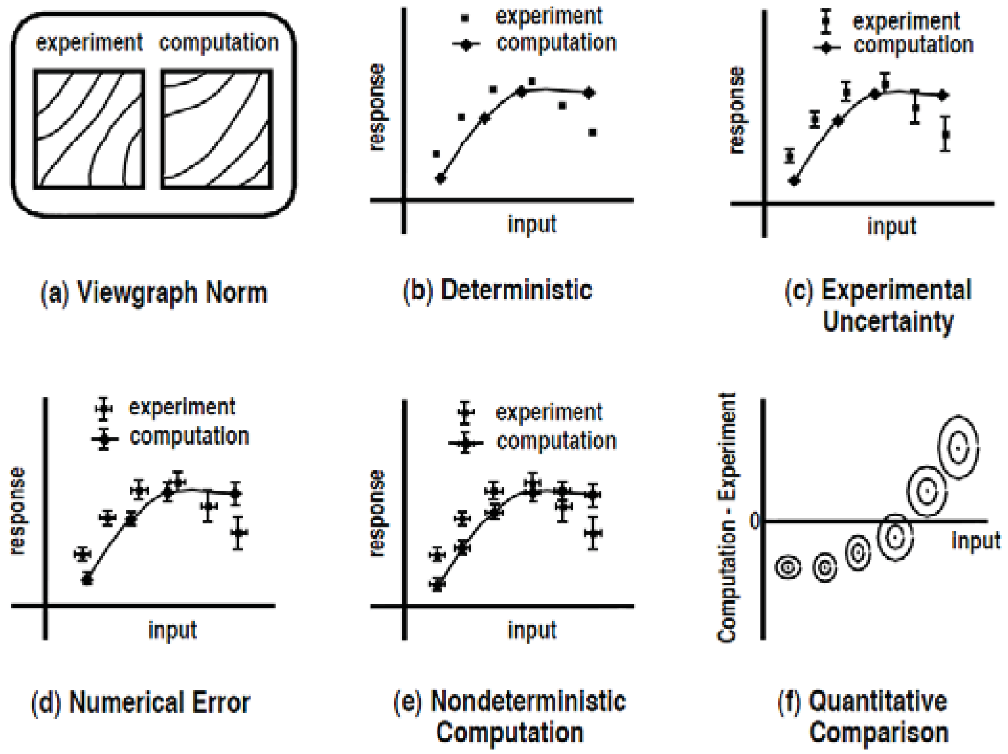
System response quantity SRQ

Validation is based on the comparison between computational results and experimental data.

An experiment can provide much less information than the calculation.

Selection of the system response quantity (SRQ) is often limited by the experiment output.

Validation Metrics



(a) Viewgraph Norm (b) Deterministic (c) Experimental Uncertainty

(d) Numerical Error (e) Nondeterministic Computation (f) Quantitative Comparison

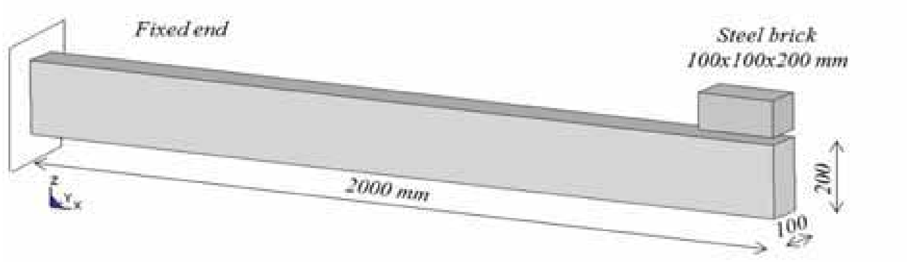
W.L. Oberkampf, T.G. Trucano, C. Hirsch, Verification, validation, and predictive capability in computational engineering and physics, Appl. Mech. Rev. 57 (5), 345–384, 2004.

Example

Steel cube dropped on a cantilever thin-walled steel beam

- input variation vs. output variation
- system response quantity
- on-off processes (zero-one switching)

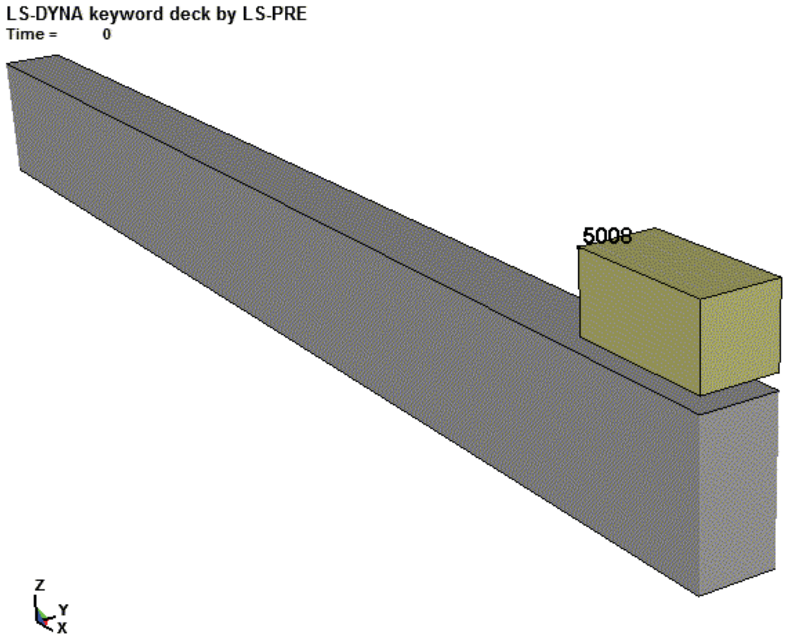
Drop heights 200.01 mm or 199.63 mm above the top flange.

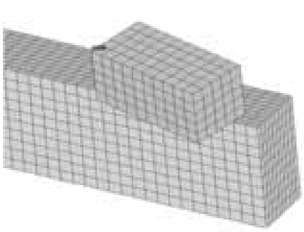


„If the answer is highly sensitive to perturbations, you have probably asked the wrong question''

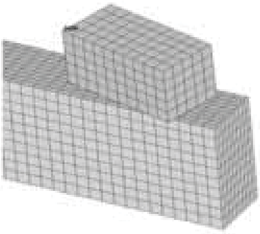
Elishakoff I. (2005) Controversy associated with the so-called “follower forces”: critical overview, Applied Mechanics Reviews, vol. 58, pp. 117

Example

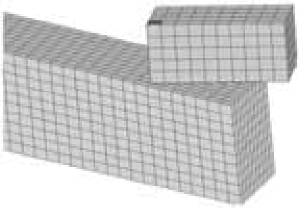




h=200.01 mm
single precision

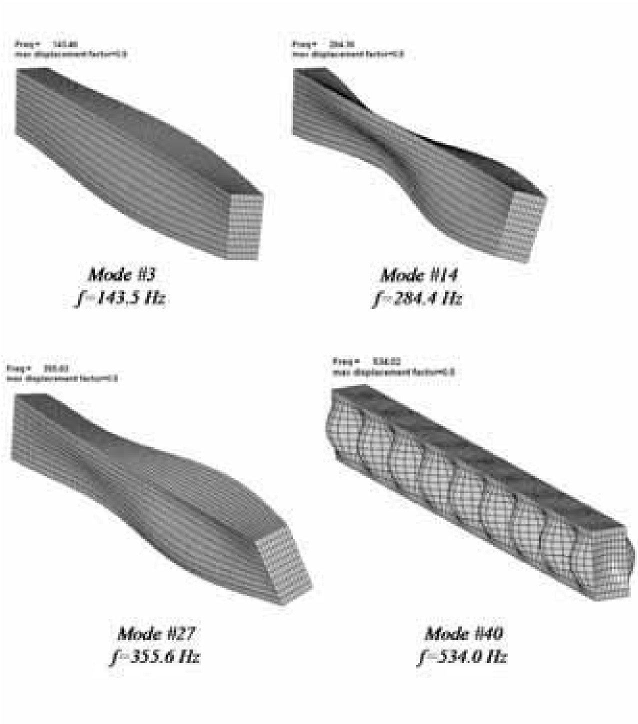


h=200.01 mm
double precision



h=199.63 mm
single precision

Example



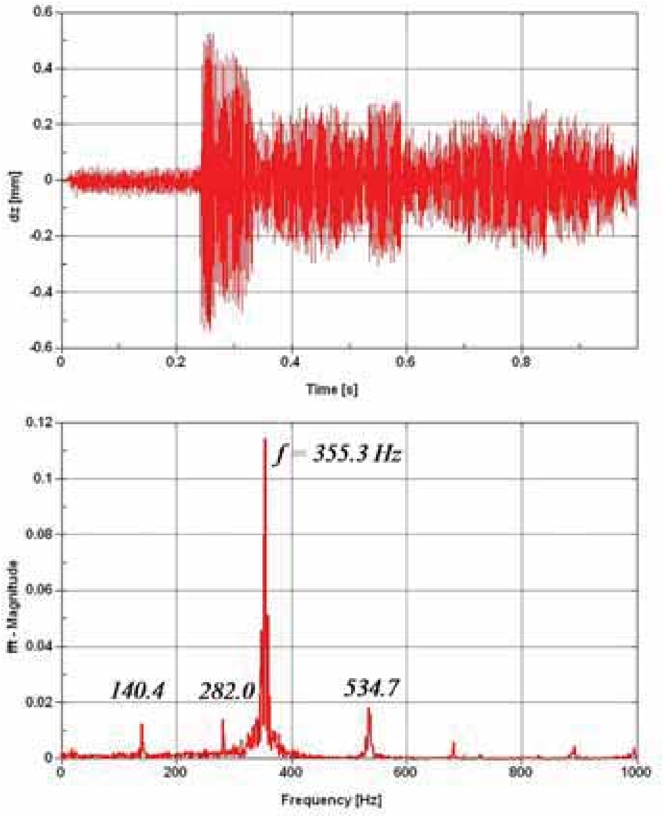
Mode #3
f=143.5 Hz

Mode #14
f=284.4 Hz

Mode #27
f=355.6 Hz

Mode #40
f=534.0 Hz

Eigenmodes corresponding to the identified frequency peaks.



Time history (top) of relative displacement for top corners at the beam and corresponding frequency spectrum (bottom).

Databases of benchmark problems

- National Agency for Finite Element Methods and Standards (NAFEMS) ~ 280 verification benchmarks (thermal analysis-14, thermal stress analysis-8)
- ABAQUS Benchmarks Manual – 264 (93-NAFEMS, 15-thermal analysis) Verification Manual, Example Problems Manual
- ANSYS® - around 250 problems
- SAFIR – significant amount of evidence presented in publications
- VULCAN, Fluent, ...
- DIN EN 1991-1-2 Raul ZAHARIA
- One Stop Shop in Structural Engineering http://www.mace.manchester.ac.uk/project/research/structures/strucfire/default.htm

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Summary

- For the non-linear problems there are unavoidable errors that are an inherent part of the solution procedures.
- Separation of all sources of errors is today impossible for many complex systems.
- Verification through the testing of different solution options is necessary.
- For the wide range of conditions found in practice, it is impossible to define general requirements guaranteeing satisfying accuracy.

Thank you for your attention!