Verification for PCMM

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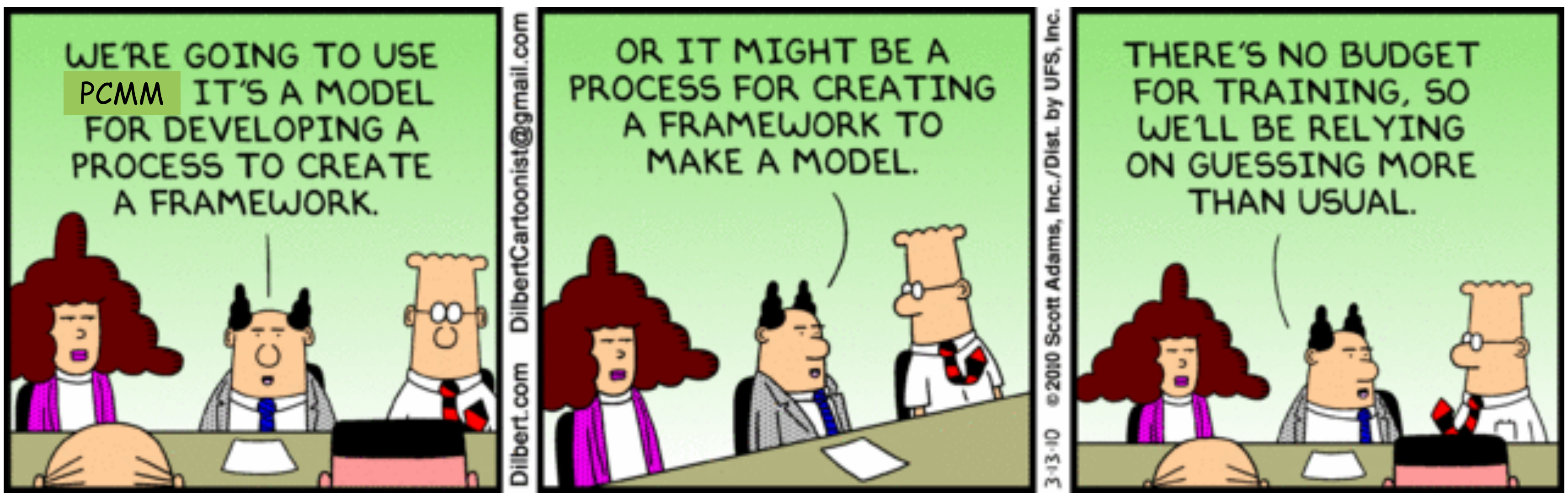
"...what can be asserted without evidence can also be dismissed without evidence."

by Christopher Hitchens



Who Am I ?

- I’m a staff member in 1431, and I’ve been at SNL for 3 years. Prior to that I was at LANL for 18 years. I’ve worked in ASC since its beginning and in the ASC V&V program since it began (@LANL).

- In addition, I have expertise in hydrodynamics (incompressible to shock), numerical analysis, interface tracking, turbulence modeling, nonlinear coupled physics modeling, nuclear engineering…
- I’ve written two books and lots of papers on these, and other topics.

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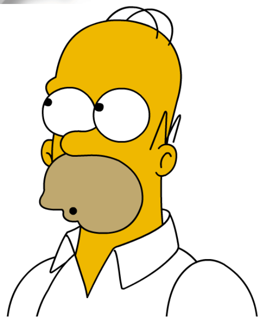
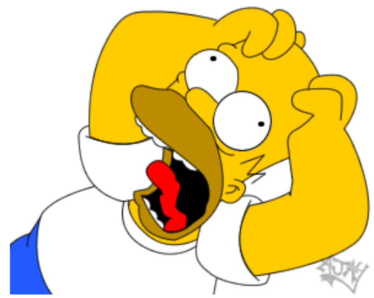
Don't be alarmed if you see a cartoon on my slide, its just for fun!

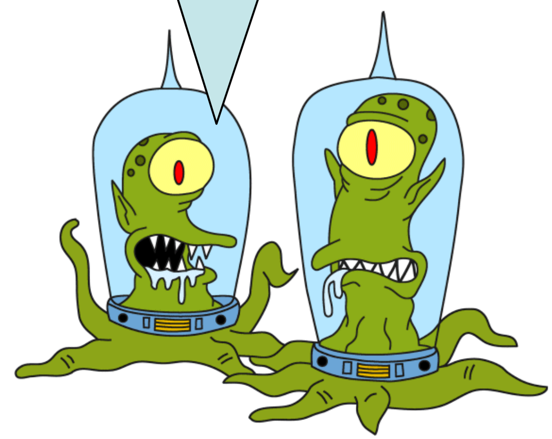


Its usually something inane, like Homer Simpson's probable reaction to this material.



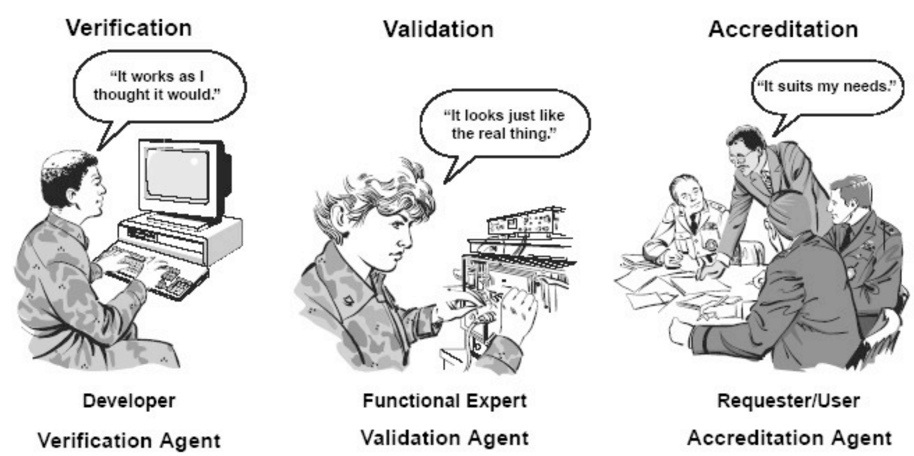
Homer doesn't do verification!

We introduce advanced topics!



Outline

- Types of verification
- A bit about SQA
- Theoretical expectations (brief & sketchy)
- Code verification
- Solution verification
- Verification in context



SAND2007-5948: Predictive Capability Maturity Model for Computational Modeling and Simulation

Increasing completeness and rigor

Decreasing risk

Content

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Slide from Marty Pilch's PCMM overview talk

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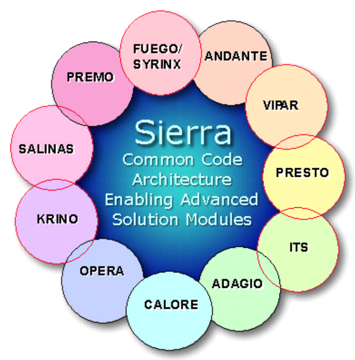
Attributes of Code and Solution Verification

Demonstrating Convergence to Correct Answer for the Intended Application

Solution Verification: Convergence for intended application, *but is it the right answer?*

• *Address adequacy of spatial AND temporal AND other discretizations AND numerical knobs*

Inference → Application



Coupled Multi-Physics Across Codes

Coupled Multi-Physics Within Code

Separate Physics

Issues: non-smooth solutions, contact, constitutive laws, internal constraints, multiscale physics, global/local norms, etc.

Inference

Regression Testing

Code Verification: Convergence to correct answer, *wrong application*

• Eliminate code bugs *AND* inadequate algorithms

SQE(A)

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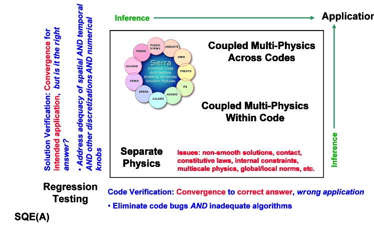
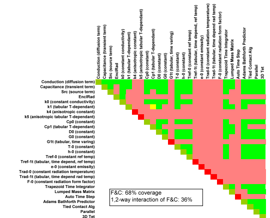
Code Verification

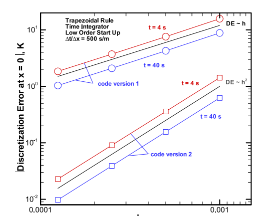
Are software errors or algorithm deficiencies corrupting simulation results?

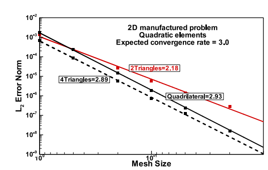


- Apply good SQE processes
  - Do you have a mature code development process?
- Assess SQE processes
  - Verify that codes are developed with an appropriate level SQE maturity?
- Provide adequate test coverage
  - Can the user be confident that the code is adequately tested for the intended application?
- Quantify computation errors
  - What is the impact of undetected code or algorithm deficiencies on simulation results?

~~Code1:Code2 Comparisons~~







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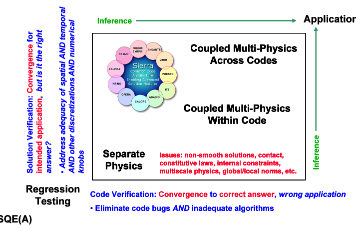
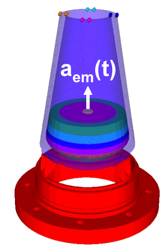
Solution Verification

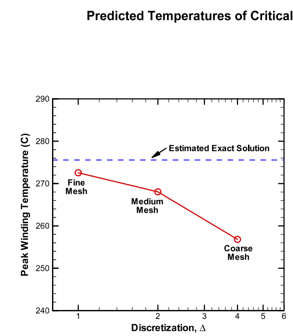
Are human procedural errors or numerical solution errors corrupting simulation results?



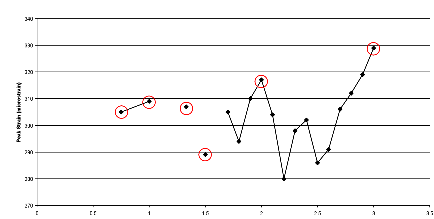
- Quantify numerical solution errors
  - What is the impact of numerical solution errors on relevant system response quantities (SRQs)

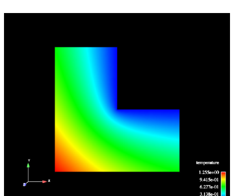


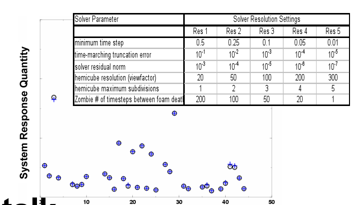
- Verify all simulation inputs and outputs
  - Have we corrupted simulation results with incorrect inputs or post processing errors?



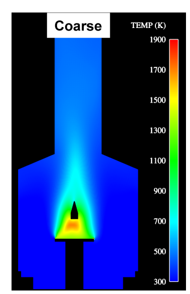
- Perform technical review
  - Verify that the solution verification activities are relevant, adequate, and executed in a technically sound manner







Solver Parameter	Solver Resolution Settings				
	Res 1	Res 2	Res 3	Res 4	Res 5
minimum time step	0.5	0.25	0.1	0.05	0.01
time-marching truncation error	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
solver residual norm	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
hemicube resolution (viewfactor)	20	50	100	200	300
hemicube maximum subdivisions	1	2	3	4	5
Zombie # of timesteps between foam deat	200	100	50	20	1



Slide from Marty Pilch's PCMM overview talk

“The plural of 'anecdote' is not ‘evidence’.”

Alan Leshner, publisher of <u>Science</u>

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An Introduction to Verification

References for this Lectures

- Richtmyer & Morton, "Difference Methods for Initial Value Problems," Wiley Interscience, 1967.
- R. J. Leveque, "Nonlinear Conservation Laws," Birkauser, or his more recent Cambridge Book. 1990.
- Oberkampf & Trucano, "Verification and Validation in Computational Fluid Dynamics," Progress in Aerospace Sciences, 2002.
- Pat Roache's paper in Annual Reviews in Fluid Mechanics, 1998.
- Pat Roache's books, "*Verification and Validation in Computational Science and Engineering*"
- Go to the SAND reports and search for Trucano, Oberkampf, Pilch, Knupp,…

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A few good reports

Verification, validation, and predictive capability in computational engineering and physics

William L Oberkampf
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Developers of computer codes, analysts who use the codes, and decision makers who rely on the results of the analyses face a critical question: How should confidence in modeling and simulation be critically assessed? Verification and validation (V&V) of computational simulations are the primary methods for building and quantifying this confidence. Briefly, verification is the assessment of the accuracy of the solution to a computational model. Validation is the assessment of the accuracy of a computational simulation by comparison with experimental data. In verification, the relationship of the simulation to the real world is not an issue. In validation, the relationship between computation and the real world, ie, experimental data, *is* the issue. This paper presents our viewpoint of the state of the art in V&V in computational physics. (In this paper we refer to all fields of computational engineering and physics, eg, computational fluid dynamics, computational solid mechanics, structural dynamics, shock wave physics, computational chemistry, etc, as computational physics.) We describe our view of the framework in which predictive capability relies on V&V, as well as other factors that affect predictive capability. Our opinions about the research needs and management issues in V&V are very practical: What methods and techniques need to be developed and what changes in the views of management need to occur to increase the usefulness, reliability, and impact of computational physics for decision making about engineering systems? We review the state of the art in V&V over a wide range of topics, for example, prioritization of V&V activities using the Phenomena Identification and Ranking Table (PIRT), code verification, software quality assurance (SQA), numerical error estimation, hierarchical experiments for validation, characteristics of validation experiments, the need to perform nondeterministic computational simulations in comparisons with experimental data, and validation metrics. We then provide an extensive discussion of V&V research and implementation issues that we believe must be addressed for V&V to be more effective in improving confidence in computational predictive capability. Some of the research topics addressed are development of improved procedures for the use of the PIRT for prioritizing V&V activities, the method of manufactured solutions for code verification, development and use of hierarchical validation diagrams, and the construction and use of validation metrics incorporating statistical measures. Some of the implementation topics addressed are the needed management initiatives to better align and team computationalists and experimentalists in conducting validation activities, the perspective of commercial software companies, the key role of analysts and decision makers as code customers, obstacles to the improved effectiveness of V&V, effects of cost and schedule constraints on practical applications in industrial settings, and the role of engineering standards committees in documenting best practices for V&V. There are 207 references cited in this review article. [DOI: 10.1115/1.1767847]

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nted October 2007

redictive Capability Maturity Model for omputational Modeling and Simulation

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SAND2008-7813
Unlimited Release
Printed July 2009

Enhanced Verification Test Suite For Physics Simulation Codes

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Los Alamos National Laboratory

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Lawrence Livermore National Laboratory

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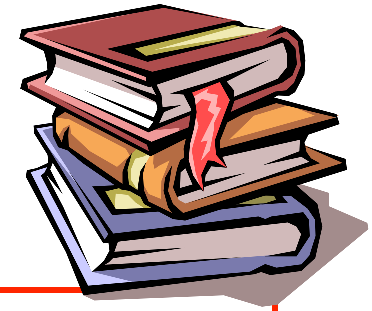
Some definitions used in V&V



complementary

- Verification ≈ **Solving the equations <u>correctly</u>**
  - **Mathematics/Computer Science issue**
  - **Applies to both codes and calculations**
- Validation ≈ **Solving the <u>correct</u> <u>equations</u>**
  - **Physics/Engineering (i.e., modeling) issue**
  - **Applies to both codes and calculations**

- Calibration ≈ **Adjusting (“tuning”) parameters**
  - **Parameters chosen for a specific <u>class</u> of problems**

- Benchmarking ≈ **Comparing with other codes**
  - **“There is no democracy in physics.”***

*L.Alvarez, in D. Greenberg, *The Politics of Pure Science*, U. Chicago Press, 1967.

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Types of verification

- Software: there is formal verification ala software engineering.
  - I won’t have much to say about this
  - Regression testing is a part of this area
- Code: means comparing the results of the code with an analytical solution
  - Usually means refine meshes/grids, compute normed errors and convergence rates
- Solution: means computing a solution on multiple grids, estimating errors in quantities of interest and the rate of convergence. It is similar in intent to, but not identical to mesh sensitivity (its better! but takes more effort).

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Hieronymus Bosch. 1485

The 7 Deadly Sins of V&V*

Otto Dix, 1933

- **Assume the code is correct**
- **Only do a qualitative comparison (e.g., *the viewgraph norm*!)**
- **Use problem specific special methods or settings**
- **Use code-to-code comparisons (benchmarks)**
- **Use only one mesh**
- **Only show the results that make the code look good - the ones that appear correct**
- **Don't differentiate between accuracy and robustness**

- Lust
- Gluttony
- Envy
- Wrath
- Sloth
- Pride
- Avarice

Traditional "7 Deadly Sins"

*these three slides were shown at the first tri-Lab V&V workshop in 2001.

Code to Code Comparisons Are a Poor Substitute for Formal Verification

Code Comparison Principle (CCP)

Code 1 = assessed code   Code 2 = benchmark code

What if this term is not negligible?

- **Could be that Code 1 models are different from Code 2 models**
- **Could be a bug in Code 1 or Code 2**
- **Could be an algorithm flaw in Code 1 or Code 2**
- **Could be that Code 1 or Code 2 model is not converged**

Points to path for better code-to-code comparisons; but if Code 2 is formally verified, why not verify Code 1 to the same verification test suite? And if not, why bother with the code-to-code comparison?

7 Virtuous Practices in V&V

- **Assume the code has flaws, bugs, and errors then FIND THEM!**
- **Be quantitative**
- **Verify and Validate the same thing**
- **Use analytic solutions & experimental data**
- **Use systematic mesh refinement**
- **Show all results - reveal the shortcomings**
- **Assess accuracy and robustness separately**

- Prudence
- Temperance
- Faith
- Hope
- Fortitude
- Justice
- Charity

Traditional “7 Cardinal Virtues”

*these three slides were shown at the first tri-Lab V&V workshop in 2001.

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The Corollaries to the Virtues

- V&V helps to ensure quality. We help determine where the codes need to be improved. We help determine the codes' limits. This should help allocate resources.
- Make an unambiguous and clear statement of results. V&V is rigorous and systematic and self-consistent.
- Base results on unambiguous, high quality standards.
- We want codes that are consistent, stable, and <u>convergent</u>. Better computers yield better solutions!
- Show everything, be honest and open.
- Make sure you know what you are looking at.

*these three slides were shown at the first tri-Lab V&V workshop in 2001.

Software Quality Assurance

- **Software quality is important, and a deep topic unto itself, *which I am not qualified to talk about!***
- **It contains regression testing, which should cover the intended use and features of the code.**
- ***A code can be "fully" verified in the software sense and be completely incorrect from a mathematical, engineering or physics perspective.***
  - ***The opposite might be less so.***

Software Testing, Verification and Code Verification: Compare & Contrast

- There is a lot of confusion about which is which, for example, regression testing, test coverage and test-driven development.
- Generally, the test suites used in code development are NOT code verification.
- The coverage with regression testing is not any measure of the quality of code verification.
- Automatic code verification is in its infancy, but in the future the two areas may come together, but we're not there yet.

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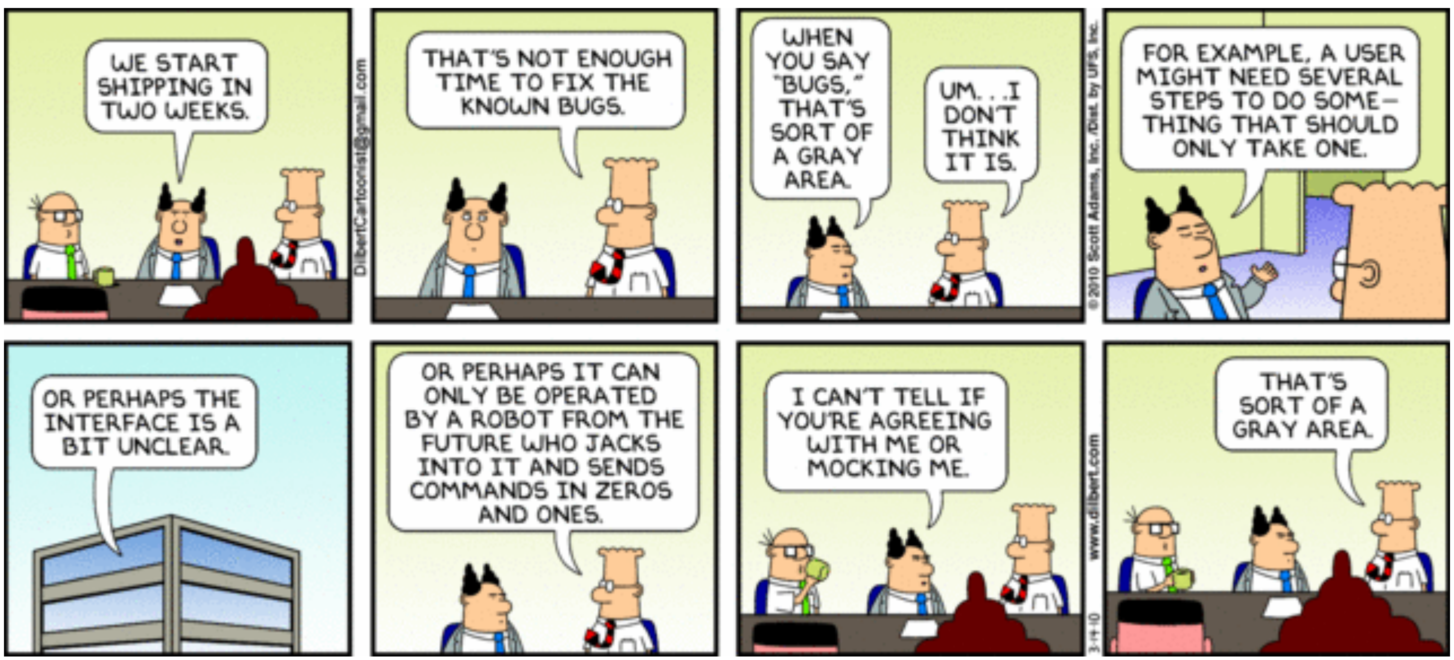
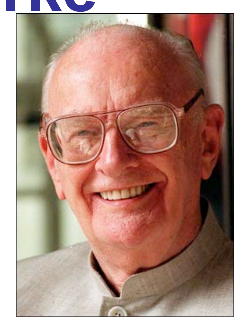
- **How to tell the forms of testing apart?**
  - **For code verification there needs to be a comparison made with either an analytical solution, or a refined grid, and**
  - **there needs to be a grid refinement.**
  - **For example, this is why the patch test is NOT code verification (more later!).**



The nature of the code development is a key aspect to consider.

- How well do the code developers understand what they are working on.
- In some cases the key developers have moved on and are not available…

- … leading to the "magic" code issue,
  - "Any sufficiently advanced technology is indistinguishable from magic." Arthur C. Clarke [Clarke's Third Law]



  - Understanding problems can be nearly impossible, or prone to substantial errors,
  - Fixing problems become problematic (bad choices are often made!) as a consequence.

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Example of Verification in Engineering Practice

I’m going to go through a set of examples next from the literature.

Disclaimer

- The examples are taken from the current (2009) literature for a small subset of journals.
- They *do not* reflect a comprehensive study, the articles were simply chosen from a recent issue of the journal.
- My working thesis is that any issues *are not an indictment of the authors*, but rather a reflection of accepted practice within the communities represented by the journals chosen.

Excerpt from the editorial policy of JFE

"Journal of Fluids Engineering disseminates technical information in fluid mechanics of interest to researchers and designers in mechanical engineering. *The majority of papers present original analytical, numerical or experimental results and physical interpretation of lasting scientific value*. Other papers are devoted to the review of recent contributions to a topic, or the description of the methodology and/or the physical significance of an area that has recently matured."

Excerpt from the editorial policy of JFE (i.e. the fine print)

"Although no standard method for evaluating numerical uncertainty is currently accepted by the CFD community, there are numerous methods and techniques available to the user to accomplish this task. The following is a list of guidelines, enumerating the criteria to be considered for archival publication of computational results in the *Journal of Fluids Engineering*."

Then 10 different means of achieving this end are discussed, and a seven page article on the topic.

Excerpt from the editorial policy of JFE (digging even deeper, more fine print!)

"An uncertainty analysis of experimental measurements is necessary for the results to be used to their fullest value. Authors submitting papers for publication to this Journal are expected to describe the uncertainties in their experimental measurements and in the results calculated from those measurements and unsteadiness."

- *The numerical treatment of uncertainty follows directly from the need to assess the experimental uncertainty.*

- *This seems quite reasonable, but as we will see it is uncommon.*

Excerpt from the editorial policy of JFE

"The Journal of Fluids Engineering <u>will not</u> consider any paper reporting the numerical solution of a fluids engineering problem <u>that fails to address the task of systematic truncation error testing and accuracy estimation.</u> Authors should address the following criteria for assessing numerical uncertainty."

Its difficult to find language this strong for other publications, its also not clear that this policy is uniformly implemented.

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Example from JFE

Assessment of Large-Eddy Simulation of Internal Separated Flow

Marco Hahn[1]
e-mail: m.hahn@cranfield.ac.uk

Dimitris Drikakis

Department of Aerospace Sciences,
Fluid Mechanics and Computational Science Group,
Cranfield University,
Bedfordshire MK43 0AL, UK

This paper presents a systematic numerical investigation of different implicit large-eddy simulations (LESs) for massively separated flows. Three numerical schemes, a third-order accurate monotonic upwind scheme for scalar conservation laws (MUSCL) scheme, a fifth-order accurate MUSCL scheme, and a ninth-order accurate weighted essentially non-oscillatory (WENO) method, are tested in the context of separation from a gently curved surface. The case considered here is a simple wall-bounded flow that consists of a channel with a hill-type curvature on the lower wall. The separation and reattachment locations, velocity, and Reynolds stress profiles are presented and compared against solutions from classical LES simulations.

[DOI: 10.1115/1.3130243]

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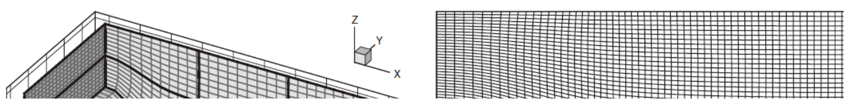
The numerical investigation of high-resolution methods for large-eddy simulation has been carried out using three different computational grids. The computational domain representing the constricted channel extents $9h$ and $4.5h$, and between $2h$ and $3.035h$ in x-, y-, and z-direction, also referred to as streamwise, cross-stream, and vertical directions, respectively. Here, h is the height of the hill-type shape at the lower wall. A H-H-type topology was chosen (Fig. 1(a)) and no-slip boundary conditions are applied at the top and bottom walls of the channel, while periodicity was assumed in the streamwise and cross-stream directions.

Three different grid resolutions have been investigated here: (i) a highly under-resolved grid, referred to as "coarse," comprising approximately 0.65×10^6 relative uniformly distributed points; (ii) a modified version of the coarse grid with an identical number of points, referred to as "modified," featuring a finer clustering near the top and bottom walls of the channel; and (iii) a moderately finer grid consisting of 1.03×10^6 points, referred to as "medium," where the refinement mainly affects the distribution around the hill crest and a slightly better resolution near the bottom wall is achieved; see Figs. 1(b)–1(d). The coarse and medium grids are basically identical to the ones used in previous wall-modeled LES [9]. The characteristic parameters for all three grids, including z^+ ... choice of ... Addition- ... simula-



This looks fairly good. Three grids and some degree of quantification. As we'll see its, much more than other papers, but in my opinion not quite enough.

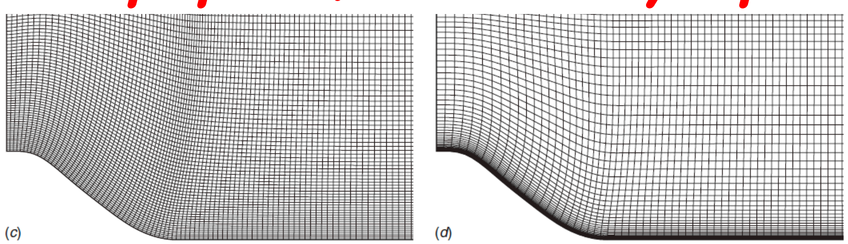


Fig. 1 The computational H-H-type grid topology and the three different grids employed in the simulations of the hill flow

Table 1 Characteristic parameters for the three grids employed here and for the highly resolved reference LES

Grid	$N_x\times N_y\times N_z$	Size	$\Delta x/h$	$\Delta y/h$	$\Delta z/h$	$z^+_{\min}$	$z^+_{\max}$
Coarse	$112\times91\times64$	0.65×10^6	0.08	0.049	0.032	≈7	≈14
Modified	$112\times91\times64$	0.65×10^6	0.08	0.049	0.0047	≈1	≈3
Medium	$176\times91\times64$	1.03×10^6	0.04	0.049	0.02	≈4	≈9
Reference	$196\times186\times128$	4.67×10^6	0.032	0.024	0.0033	≈0.5	≈1

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Example from JFE

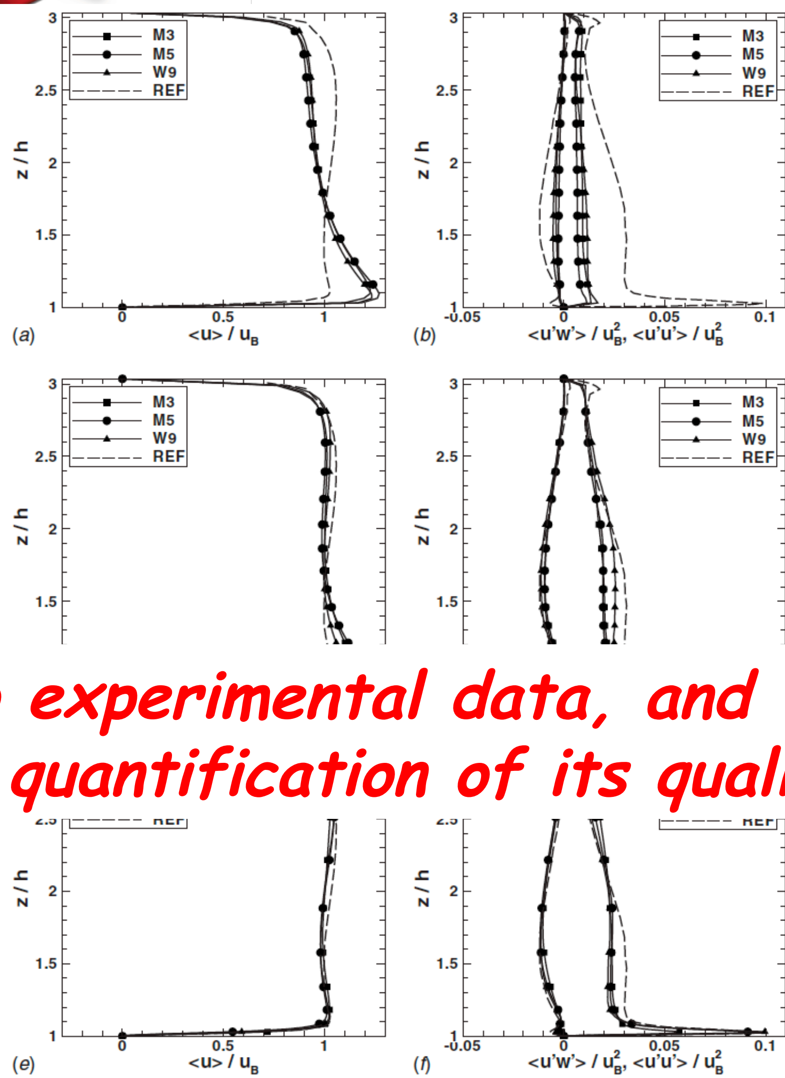

Fig. 3 Comparison of the averaged streamwise velocity and Reynolds stresses near the hill crest at $x/h = 0.05$ as obtained by different high-resolution methods on the coarse, medium and modified grids with the reference LES

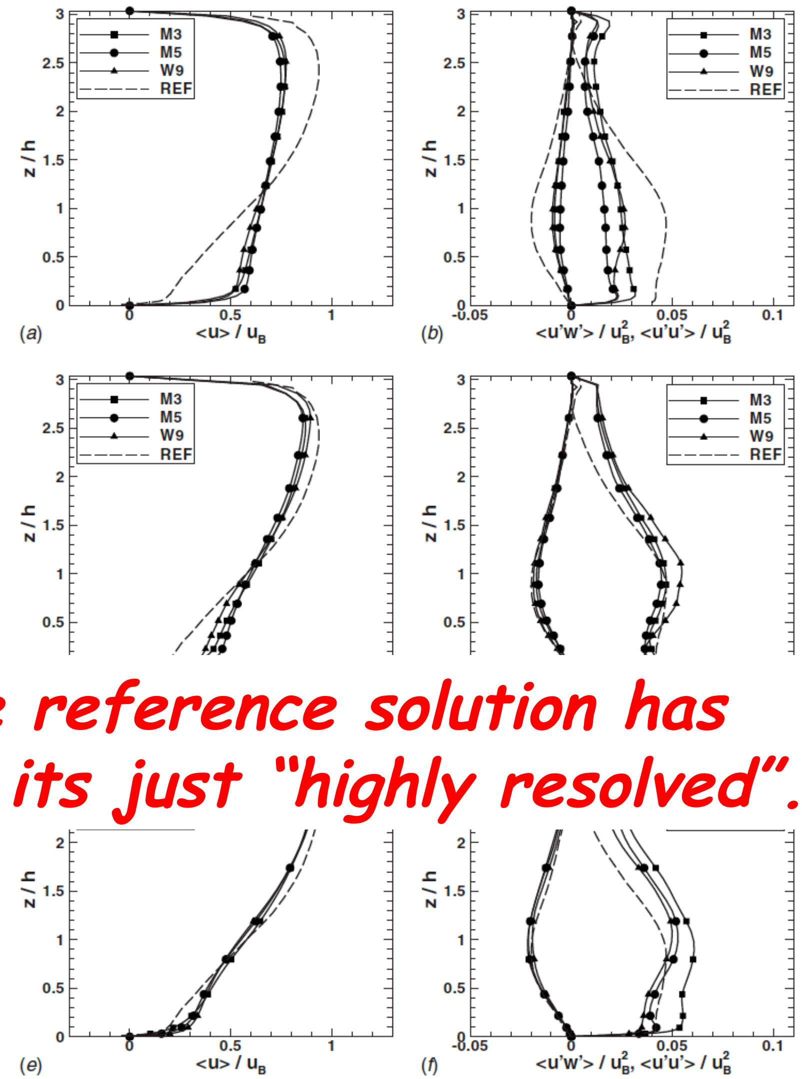

Fig. 5 Comparison of the averaged streamwise velocity and Reynolds stresses after reattachment at $x/h = 6$ as obtained by different high-resolution methods on the coarse, medium and modified grids with the reference LES

No experimental data, and the reference solution has no quantification of its quality its just "highly resolved".

An oldie, but a goodie…

“The purpose of computing is insight, not pictures”–Richard Hamming

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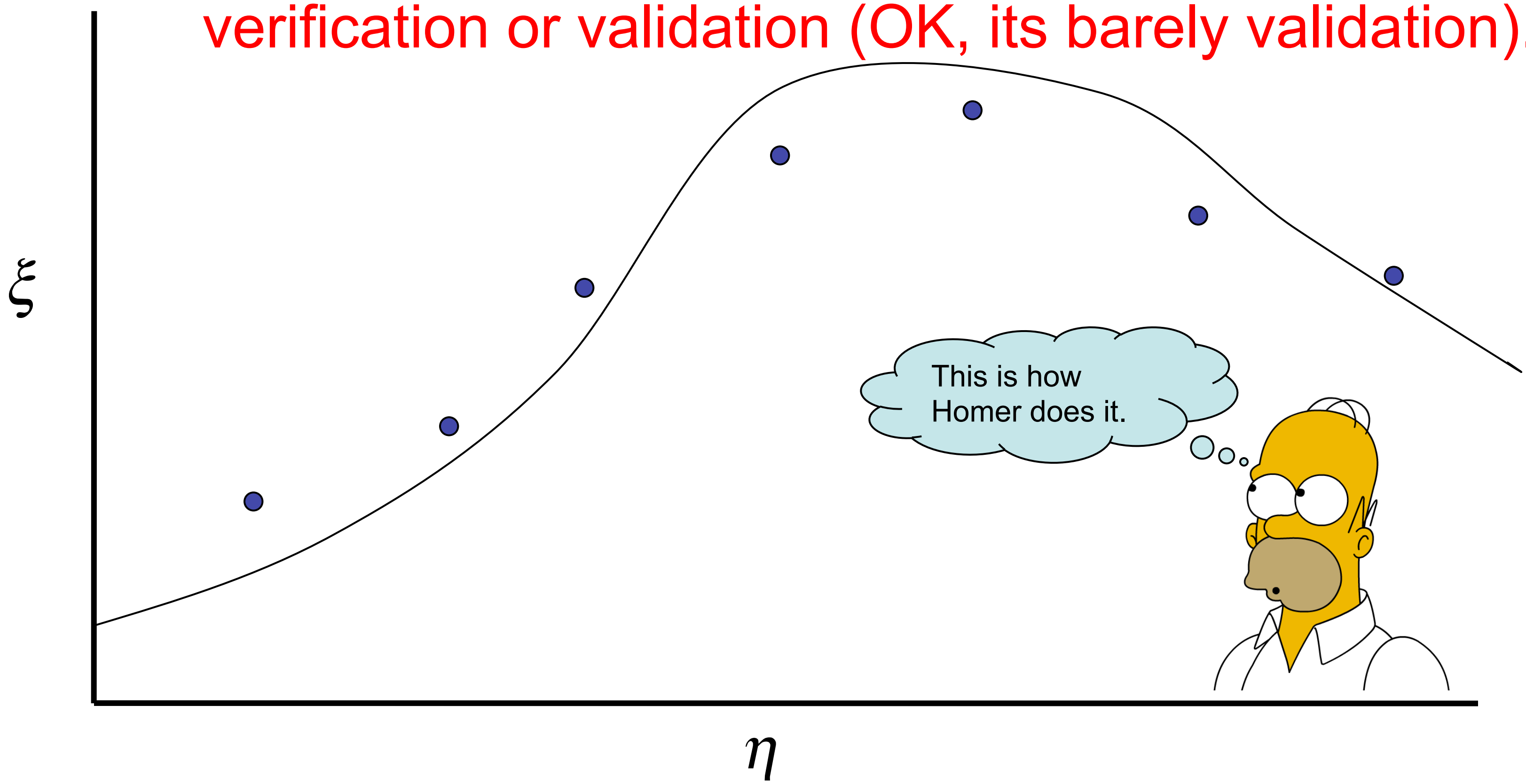
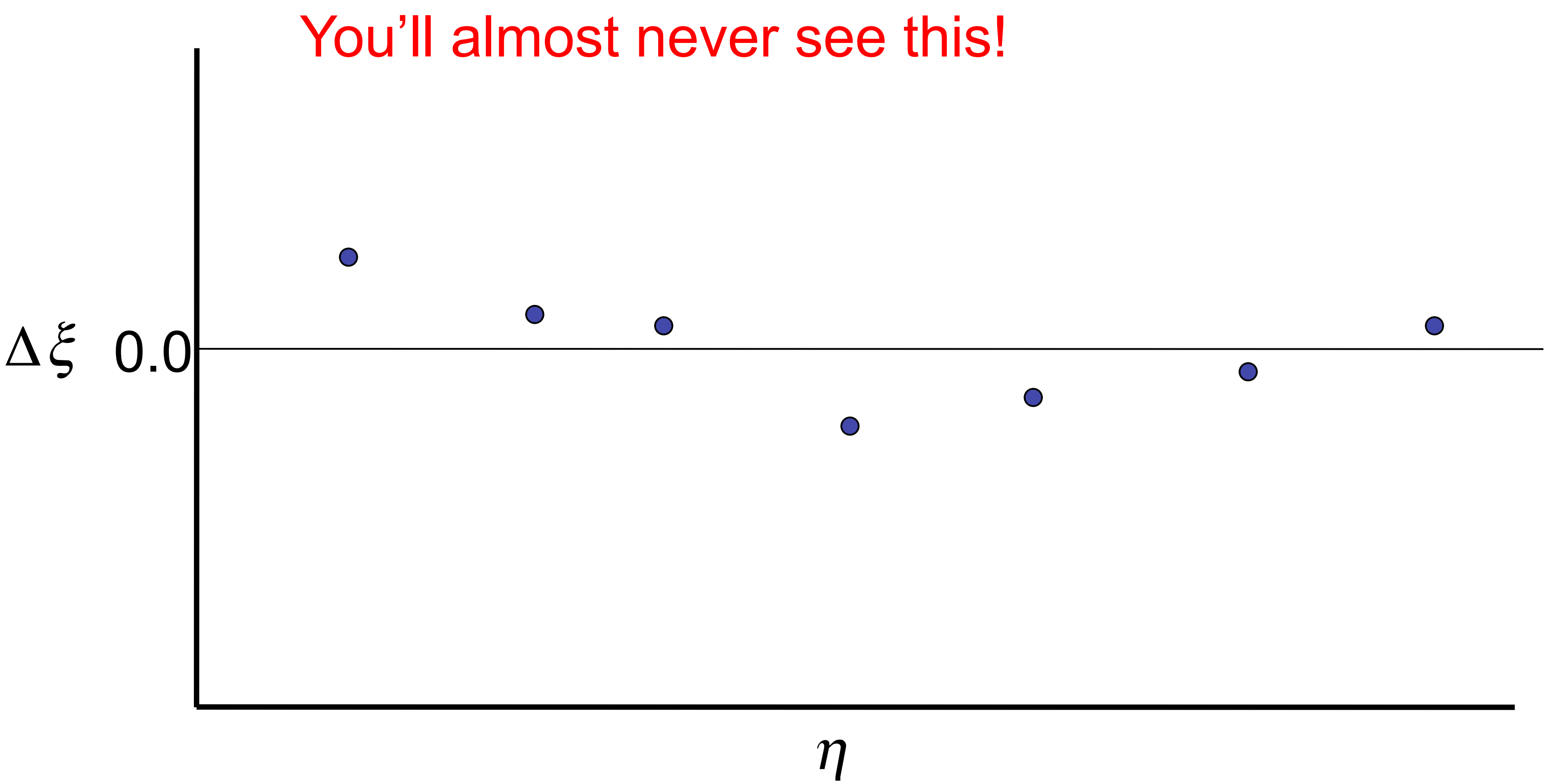
This is the way validation is usually presented in the literature.

This is what you'll see in most Journals. It is neither verification or validation (OK, its barely validation).

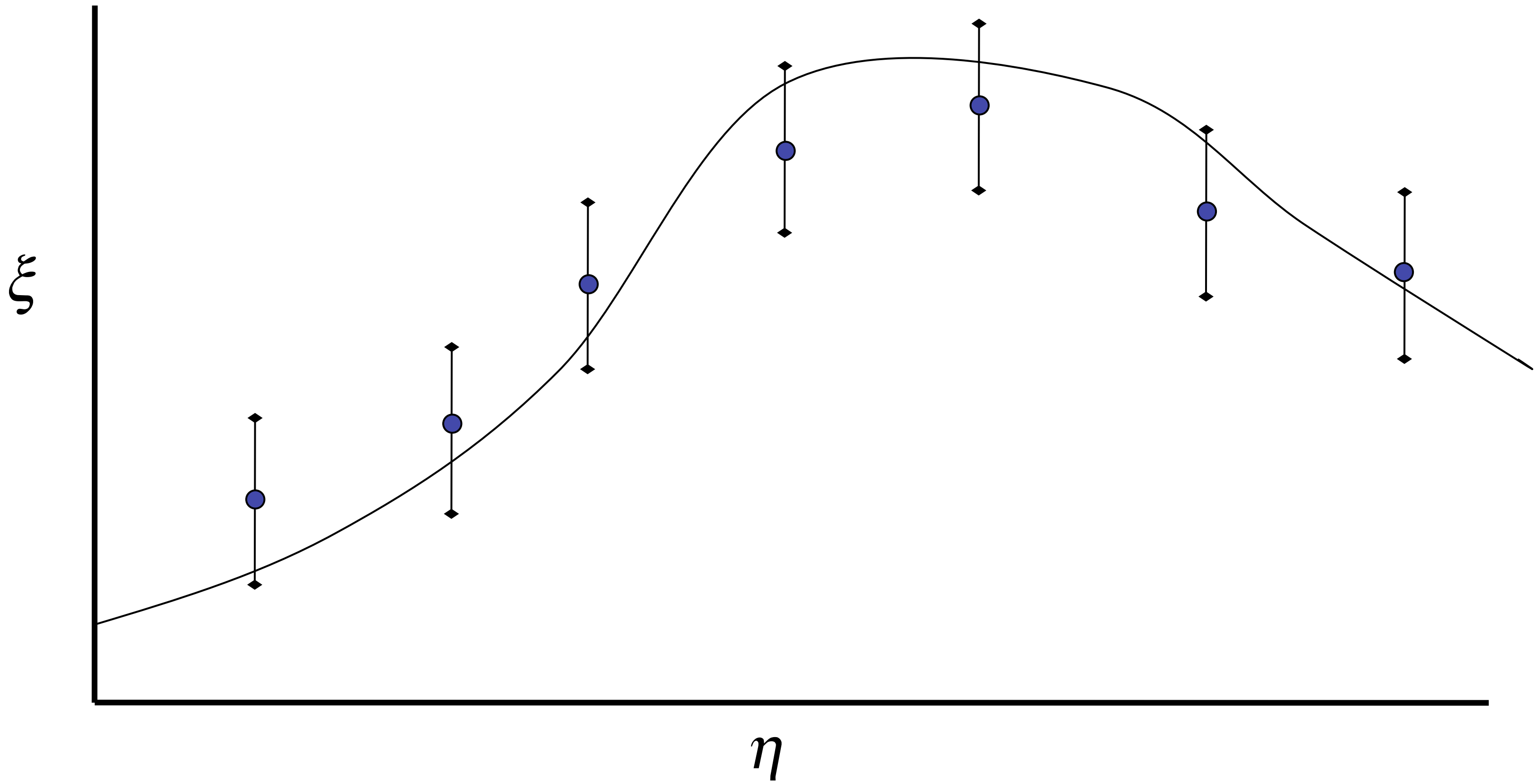


It might be even better if the figure was presented in terms of error too.



This presentation is an improvement because experimental error is shown.

This is *not* what you'll see in most Journals, but you should.



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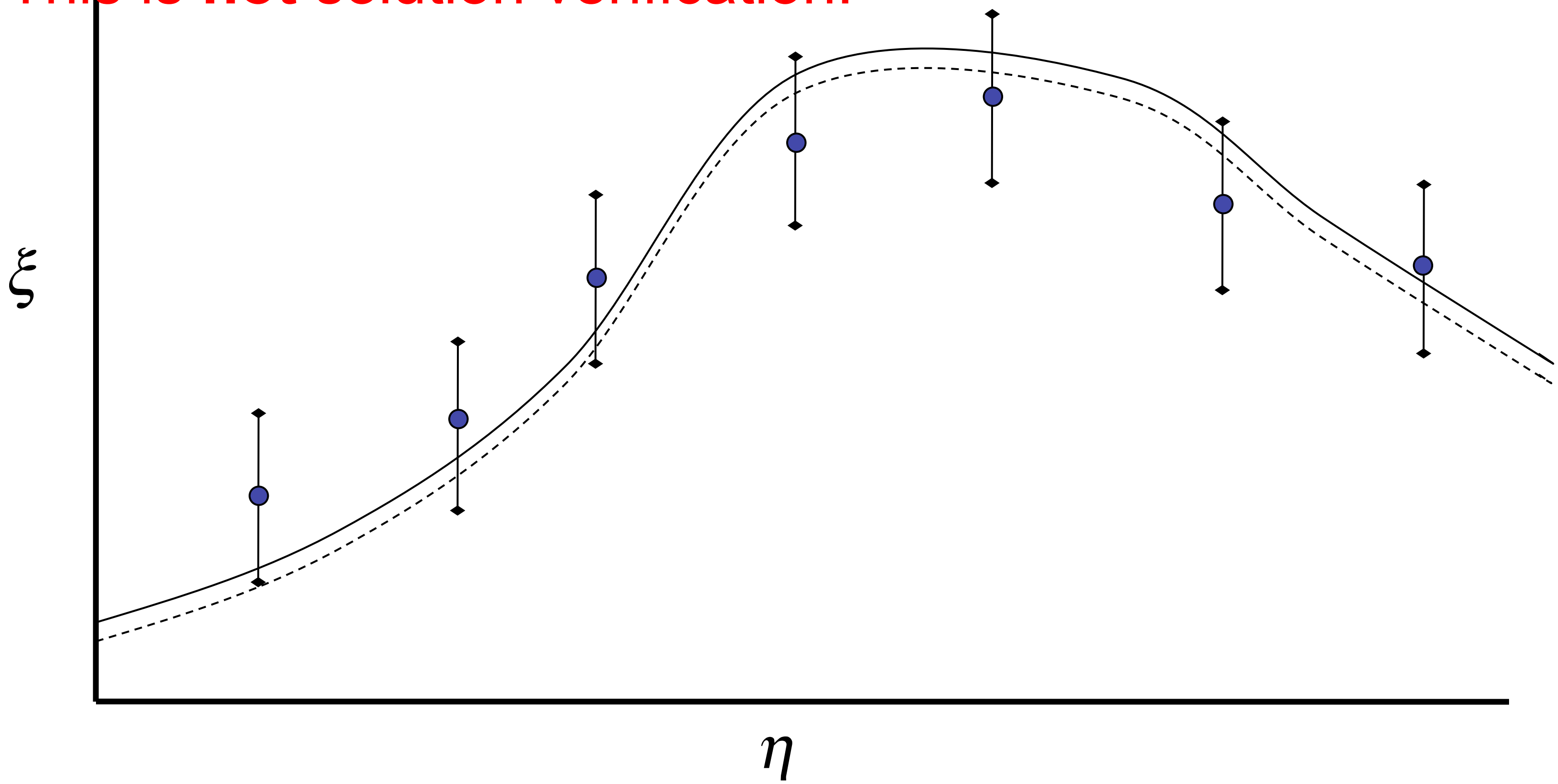
Here is a notion of how a "converged" solution might be described.

You might see this although rarely depicted in this manner.
This is **not** solution verification!



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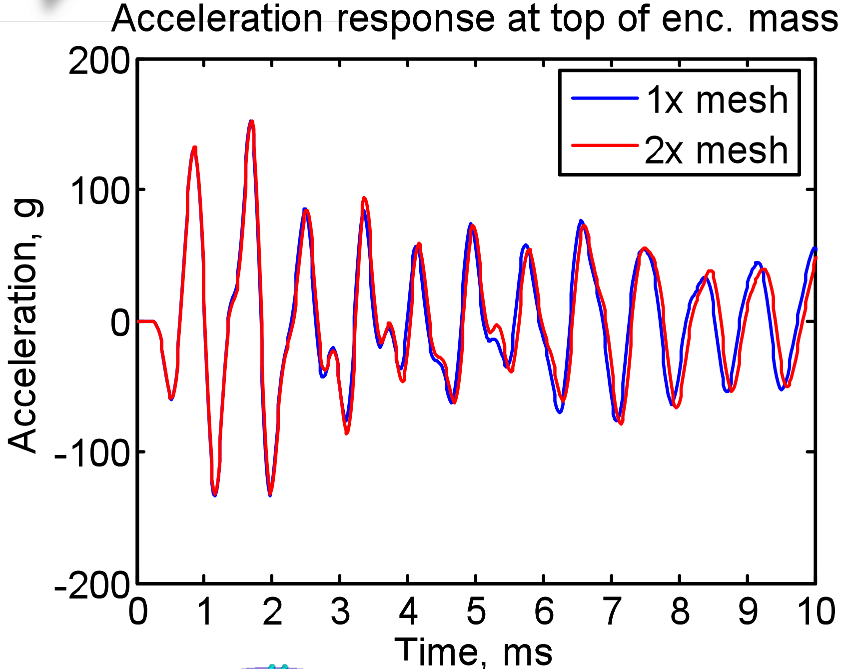
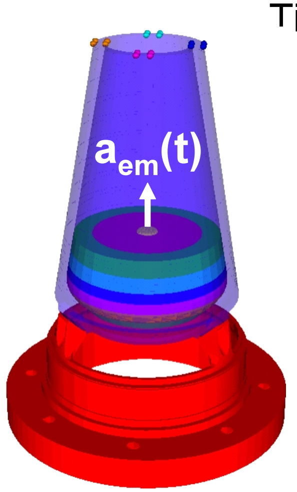
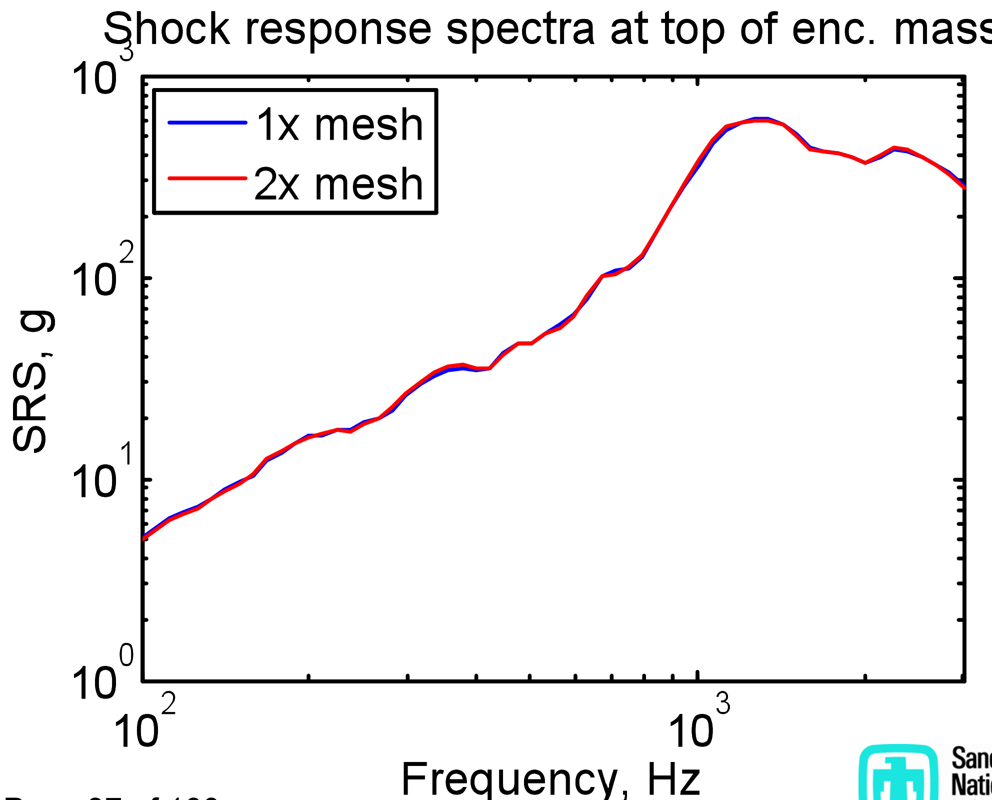
It's Common to Explore Sensitivity to Mesh Parameters



Max. relative error between SRS: +/- 5%



Structural Dynamics



Slide from Marty Pilch's PCMM overview talk

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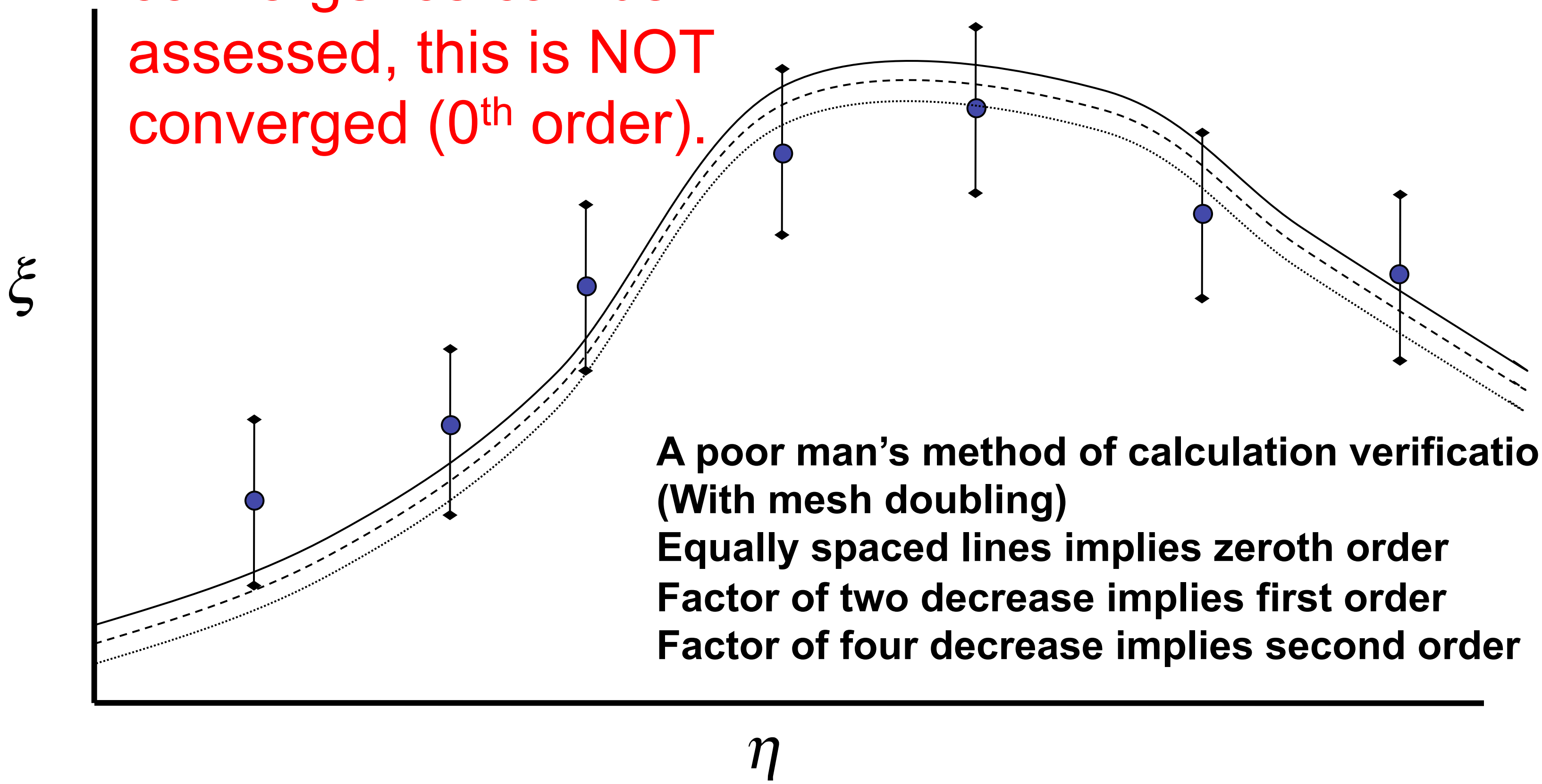
Here is a notion of how a "converged" solution might be described.

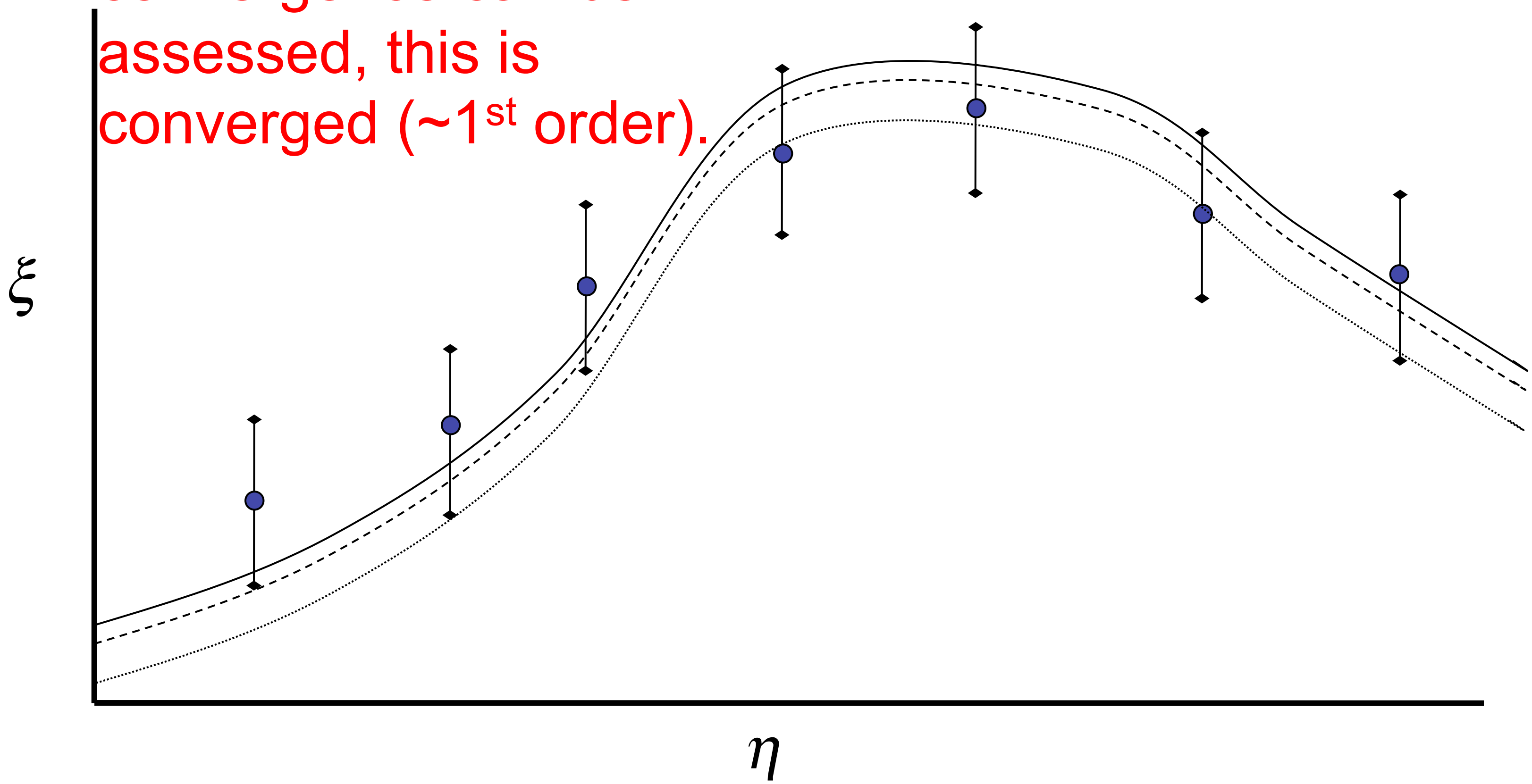
With a third resolution convergence can be assessed, this is NOT converged (0^{th} order).



This **is** solution verification despite the bad results

Here is a notion of how a "converged" solution might be described.

With a third resolution convergence can be assessed, this is converged (~1st order).



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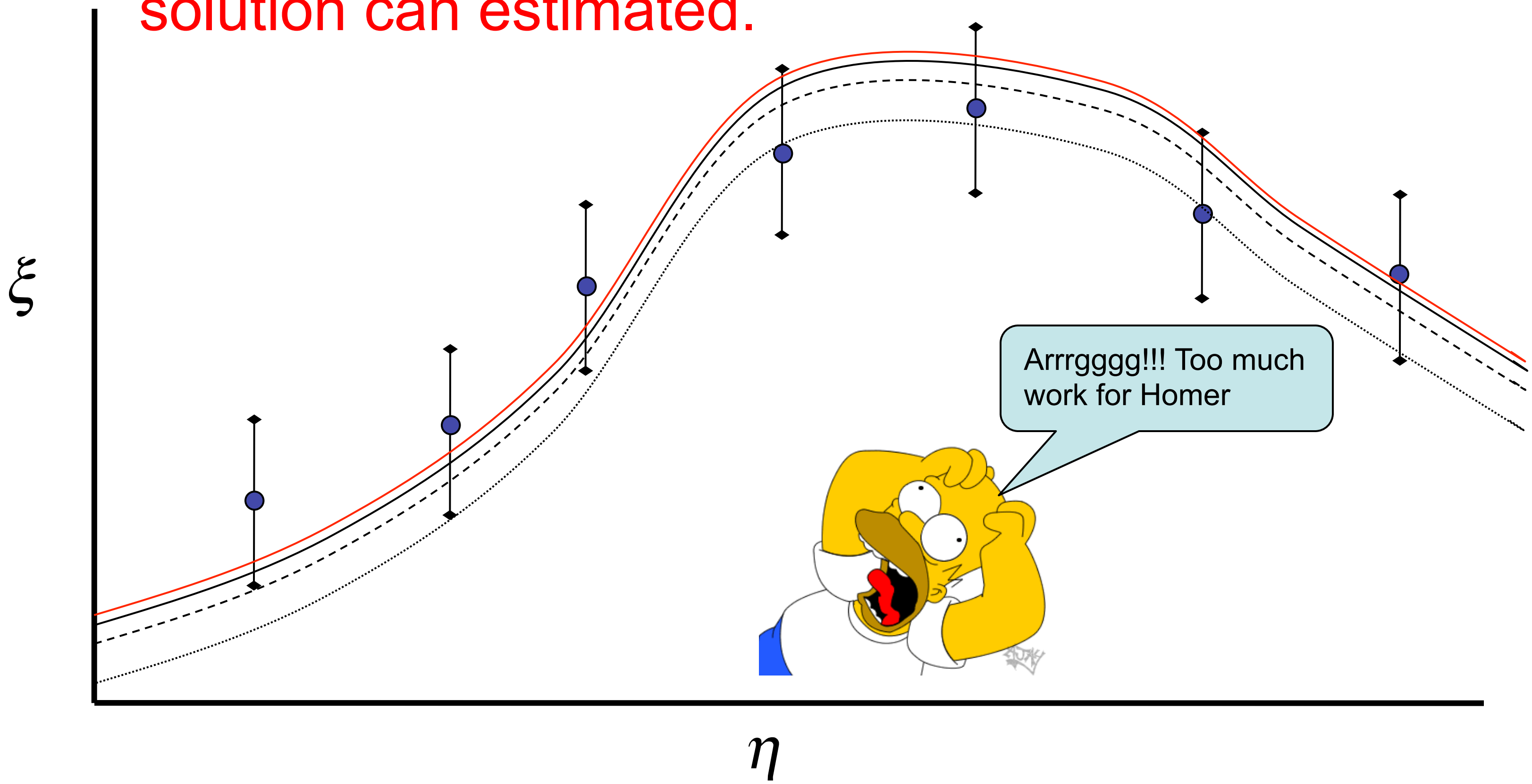
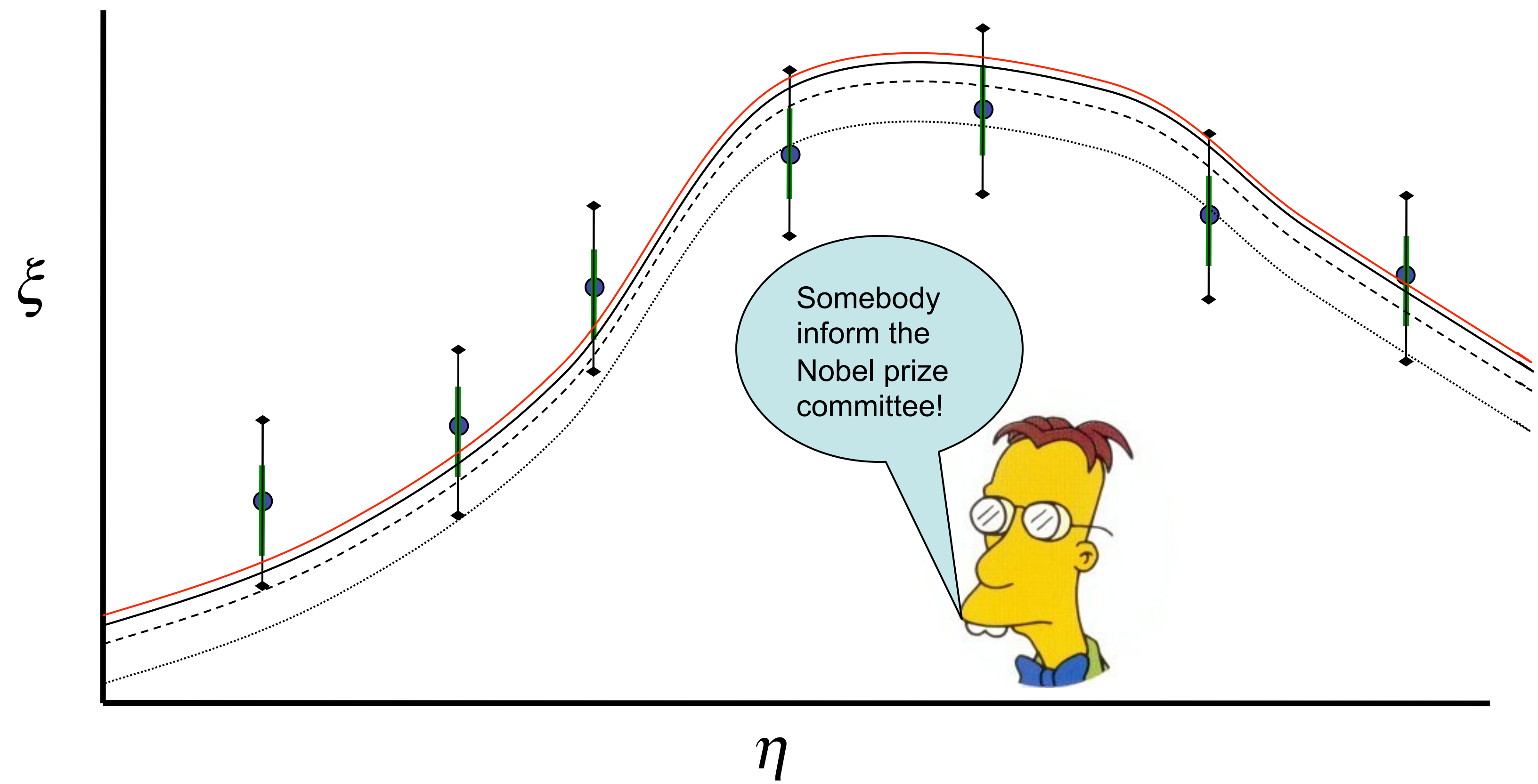
This sequence of meshes can be used to extrapolate the solution.

With three grids plus a convergence rate a converged solution can estimated.



Now we're talking!

The experimental "error" has two components (observation & variability).



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"Most daily activity in science can only be described as tedious and boring, not to mention expensive and frustrating."

Stephen J. Gould, Science, Jan 14, 2000.

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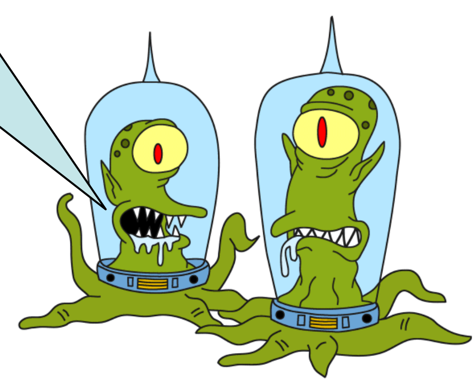
The Necessity and Role of Mathematical Theory

Theory is essential to the successful conduct and interpretation of verification results



A thought to start us off.

"An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them."

- Werner Heisenberg

For verification it is important to understand theoretical expectations.

- Truncation or approximation error
- Stability
- Lax (Richtmyer) Equivalence Theorem
- FEM: Strang&Fix, Ciarlet, Brezzi, Babuska

In hyperbolic PDEs

- The Lax-Wendroff theorem
- Godunov's theorem
- Entropy conditions
- The LeFloch-Hou theorem

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Types of CFD solver: hyperbolic, elliptic and parabolic PDEs

- The starting point for methods is usually a hyperbolic system of PDEs.
  - Methods are often explicit and have a severe time step constraint.
  - Viscous terms are parabolic.
- Incompressible flow involves an elliptic PDE along with both hyperbolic terms, and parabolic viscous terms.
  - The time step is determined by explicit terms.
- Many methods utilize some implicit methods to remove time step restrictions.

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Each type of PDE brings substantial, but different numerical challenges.

$$\boxed{\nabla \cdot u = 0} \quad \rightarrow \nabla^2 p = -\nabla \cdot \left(u \cdot \nabla u - \nu \nabla^2 u \right)$$

elliptic

$$\frac{\partial u}{\partial t} + u \cdot \nabla u + \boxed{\nabla p} = \nu \nabla^2 u$$

hyperbolic parabolic

- **Hyperbolic PDEs can support spontaneously developing discontinuous solutions.**
- **Explicit methods for hyperbolic or parabolic PDEs can carry restrictive stability conditions.**
- **Implicit methods for hyperbolic PDEs are expensive and often lack robustness.**
- **Elliptic PDEs are expensive to solve, but generally robust.**
- **Parabolic PDEs are generally easier to solve.**

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There are a lot of different numerical methods, but they all depend on the same fundamentals.

- **Methods fall into a variety of categories: finite difference, finite volume, finite element, discontinuous Galerkin, spectral, spectral element, spectral volume, semi-Lagrangian, balance etc,…**
- **For time dependent methods there are explicit, semi-implicit, implicit, linearized, nonlinearly consistent,…**
- **Different methods are advantageous for different circumstances, applications and other considerations.**
- **All methods have the same objective solve the governing equations in an accurate, stable and efficient manner,**
- ***They ultimately have to abide by the same fundamental requirements.***

Quote by Peter Lax: The American Mathematical Monthly, February 1965:

"…*who may regard using finite differences as the last resort of a scoundrel that the theory of difference equations is a rather sophisticated affair, more sophisticated than the corresponding theory of partial differential equations*."

He goes on to make two points:

1. **The proofs that an approximation converges is analogous to the estimates of the soln's to the PDEs (points to the CFL paper in 1928)***
2. **These proofs are harder to construct than for the PDEs!**

*CFL=Courant, Friedrichs, Lewy which used numerics to prove the existence of soln's to PDE and gives us the term CFL condition.

Local truncation error is the most basic concept in numerical approximation

- This can be estimated with the aid of a Taylor series expansion.

$$\exp(at) \underset{t\to 0}{\approx} 1 + at + \frac{a^2t^2}{2} + \frac{a^3t^3}{6} + \frac{a^4t^4}{24} + \cdots \frac{a^nt^n}{n!}$$

- This measures the difference between the discrete and continuous versions of the equations.

$$\textbf{truncation error} \underset{h\to 0}{=} \textbf{exact - numerical}$$

- When combined with stability it forms the foundation of numerical analysis.

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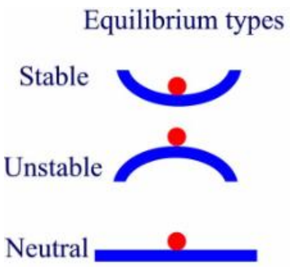
Numerical stability is central to successful methods.

- **A stable approximation is a pre-requisite for the use of that approximation.**
- **We introduce the basic concept with the analysis of a simple ODE integrator.**
- **An amplification factor is used to describe the stability of a method (greater than one is bad! Although less than one implies damping.)**
- ***Basically, one desires that the amplification of errors will be bounded, which usually means they will be damped!***



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We can examine the basic stability concepts with ODEs.

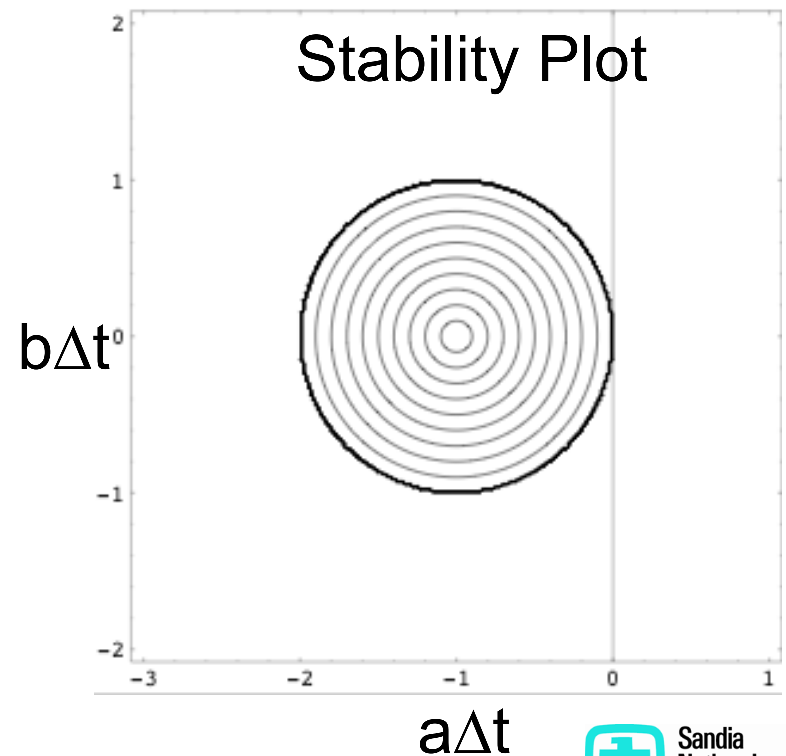
- **The forward Euler example.**

$$\frac{U^{n+1}-U^n}{\Delta t}=L\left(U^n\right)\rightarrow U^{n+1}=U^n+\Delta t L\left(U^n\right)$$

$$L=a+bi$$

- **Truncation error**

$$\frac{\Delta t^2}{2}\frac{\partial^2 L(U)}{\partial t^2}+\frac{\Delta t^3}{6}\frac{\partial^3 L(U)}{\partial t^3}+\mathrm{H.O.T.}$$



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Analysis of upwind differencing

- **Substitute the Fourier series for the grid function**

$$u_j^n = \exp(ij\theta) \Rightarrow u_j^{n+1} = u_j^n - c\left(u_j^n - u_{j-1}^n\right) \Rightarrow$$

$$A\exp(ij\theta) = \exp(ij\theta) - C\left(\exp(ij\theta) - \exp\left(i(j-1)\theta\right)\right)$$

- **Expand into trigonometric functions and collect real and imaginary parts** $A = 1 - C\left(1 - \exp(-i\theta)\right)$

$$A = 1 - C\left(1 - \cos(\theta) + i\sin(\theta)\right)$$

- **Define the amplification and phase error**

$$\mathbf{amp} = \sqrt{\left[1 - C\left(1 + \cos(\theta)\right)\right]^2 + \left(-C\sin(\theta)\right)^2}$$

$$\mathbf{phase} = \arctan\left(\frac{-C\sin(\theta)}{\left[1 - C\left(1 + \cos(\theta)\right)\right]}\right) \Big/ \left(-c\theta\right)$$

Analysis of upwind differencing (continued)

- **Perform an asymptotic expansion in small angles**
  - **Amplitude error even order errors**

$$\mathbf{amp} \approx 1 + \left(-\frac{c}{2} + \frac{c^2}{2}\right)\theta^2 + O\left(\theta^4\right)$$

  - **Phase error odd order (divide by the angle!)**

$$\mathbf{phase} \approx 1 + \left(-\frac{1}{6} + \frac{c}{2} - \frac{c^2}{3}\right)\theta^2 + O\left(\theta^4\right)$$

- **Bound the function for all angles and find the CFL limit (error goes to zero at CFL=1, then unstable).**

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The technique for modified equation analysis was introduced by Hirt.

- **Hirt (1968) introduced the technique and examined the truncation errors in physical terms.**
- **Warming and Hyett (1974) discussed the method in great detail and provided an analysis framework for fullv discrete**

JOURNAL OF COMPUTATIONAL PHYSICS 2, 339–355 (1968)

Heuristic Stability Theory for Finite-Difference Equations*

C. W. HIRT

Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87544

JOURNAL OF COMPUTATIONAL PHYSICS 14, 159–179 (1974)

The Modified Equation Approach to the Stability and Accuracy Analysis of Finite-Difference Methods

R. F. WARMING AND B. J. HYETT

Computational Fluid Dynamics Branch, Ames Research Center, NASA, Moffett Field, California 94035

Received June 11, 1973

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The modified equation technique is an important augmentation to Fourier analysis.

- The key to modified equation analysis (MEA) is the ability to..
  - …see the errors in differential form,...
  - …and extend the analysis to include nonlinearity.
- This gives us several advantages:
  - The truncation errors can be studied in terms of differential equations and directly compared with physical or modeled terms,
  - and directly treat nonlinear physics or numerics.

The Lax-Richtmyer equivalence theorem provides the barest requirements on methods.

- **Putting numerical stability and truncation error together gets us to the basic requirement for linear methods for differential equations.**

<u>Theorem (Lax Equivalence):</u> A numerical method for a linear differential equation will converge if that method is consistent and stable. Comm. Pure. Appl. Math. 1954

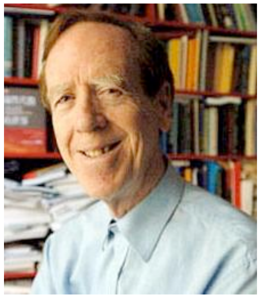
Consistency - means that the method is at least 1st order accurate – means it approximates the correct PDE.

Stable - the method produces bounded approximations

Important to recognize for its relation to verification.

Let's state this differently (Gil Strang, Introduction to Applied Mathematics)

- The fundamental theorem of numerical analysis, The combination of consistency and stability is equivalent to convergence.



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Lax-Wendroff Theorem is an essential motivator for many numerical methods for hyperbolic equations.

- **Most methods for hyperbolic PDEs are based on the discrete conservation form following the continuous conservation form because of this theorem.**

<u>Theorem (Lax and Wendroff):</u> If a numerical method is in discrete conservation form, if a solution converges, it will converge to a weak solution of the PDE. A weak solution is not <u>the</u> weak solution. There are infinitely many weak solutions.

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=0 \Rightarrow u_j^{n+1}=u_j^n-\frac{\Delta t}{\Delta x}\left(f_{j+1/2}-f_{j-1/2}\right)$$

Conservation form: the flux out of one cell is into another

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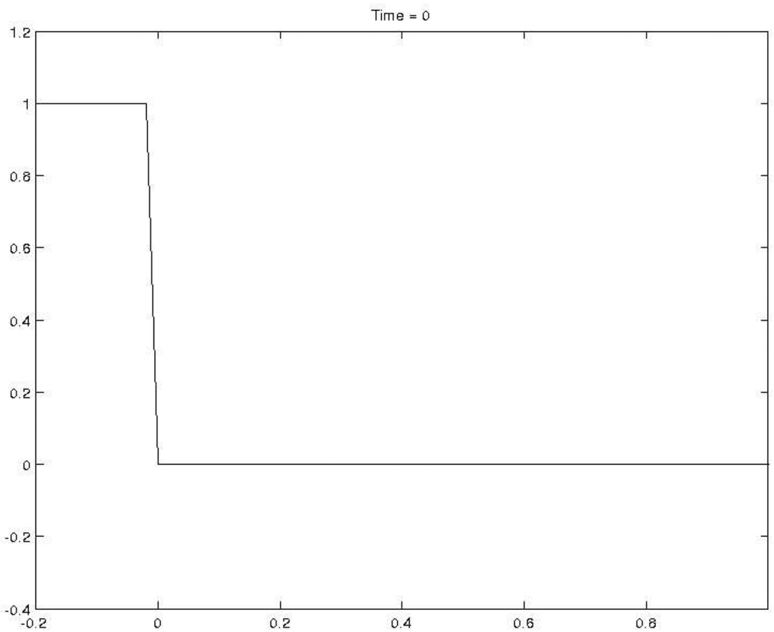
Here is an example of what happens without conservation form. Burgers' equation.

Nonconservation form

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

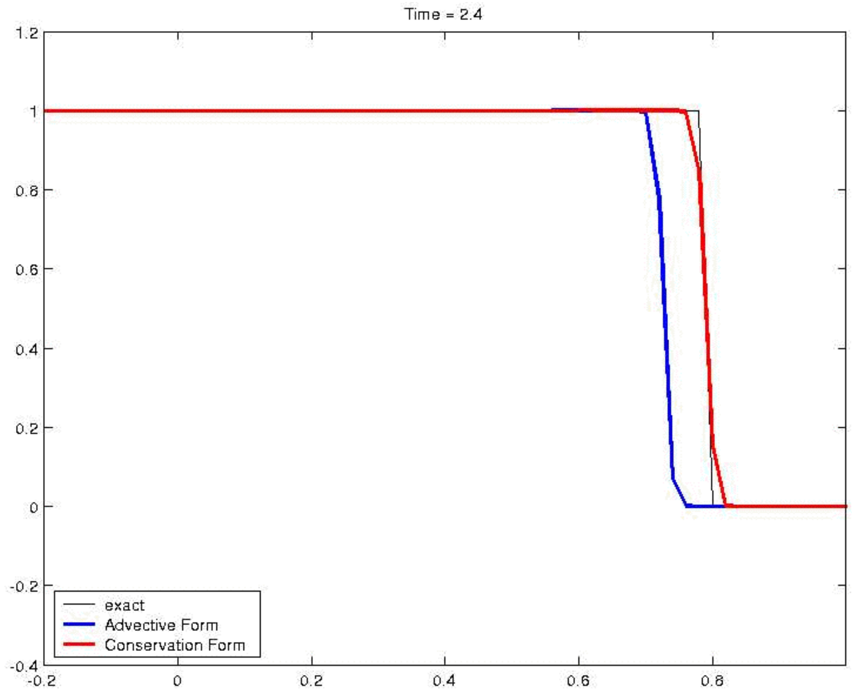
$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} u_j^n \left(u_j^n - u_{j-1}^n \right)$$



Conservation form

$$\frac{\partial u}{\partial t} + \frac{\partial\left(\tfrac{1}{2}u^2\right)}{\partial x} = 0$$

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(\tfrac{1}{2}\left(u_j^n\right)^2 - \tfrac{1}{2}\left(u_{j-1}^n\right)^2 \right)$$



Example from Randy Leveque

Entropy conditions are critical in determining physically meaningful results.

- The problem with L-W is that there are an infinity of weak solutions, we need a mechanism to pick out the correct physical one.
- The mechanism to do this entropy. The entropy created through dissipation, numerical viscosity.

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=\lambda\frac{\partial^2 u}{\partial x^2}\quad \lambda\to 0^+$$

- This is the connection to vanishing viscosity, more generally,

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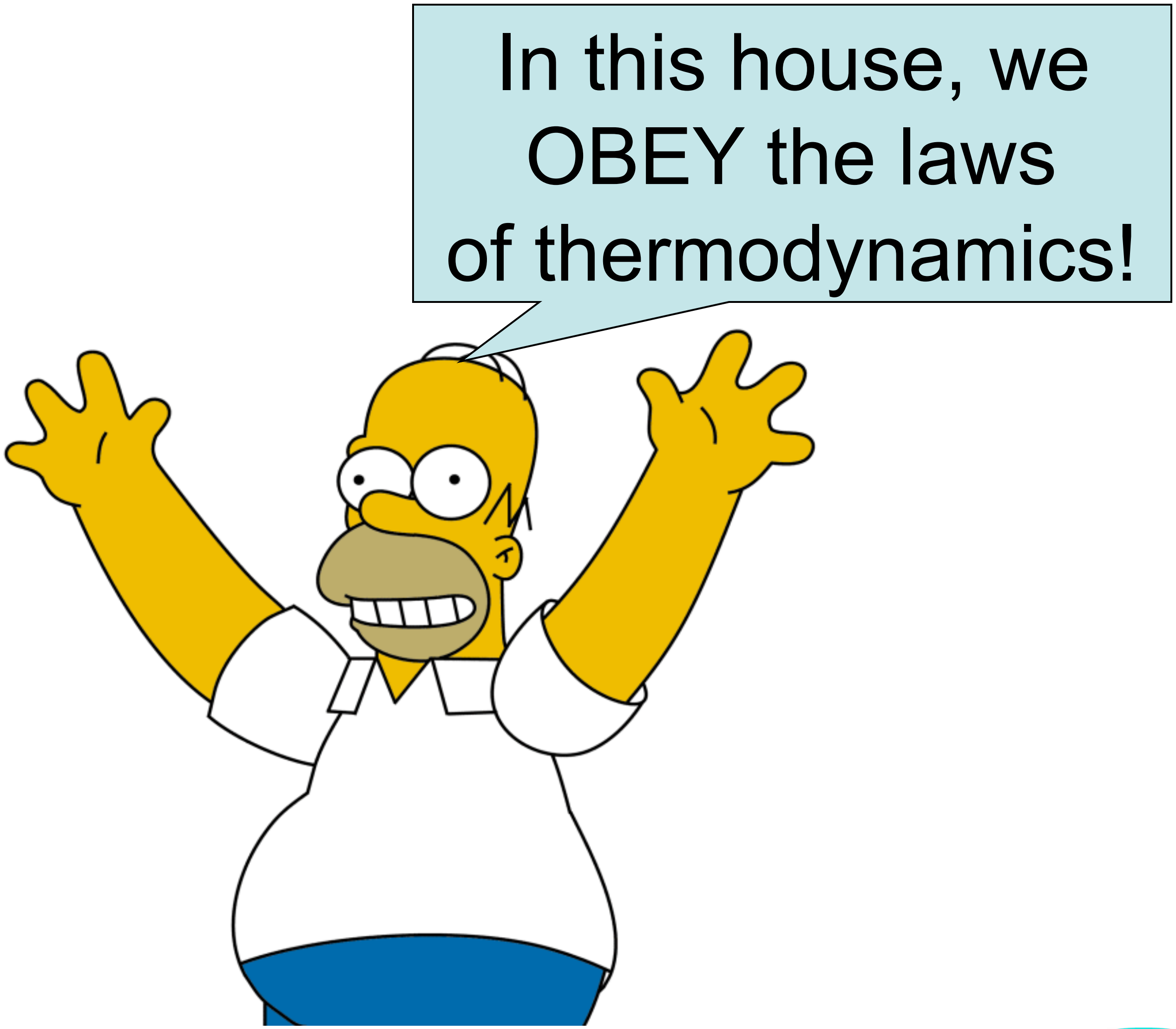
A thought about thermodynamics!



The Hou-LeFloch theorem has potentially profound consequences .

- What happens when the method is not in conservation form?
- The solution does not converge to a weak solution much less a correct one regardless of the dissipation.

<u>Theorem (Hou-LeFloch):</u> For a non-conservative method the solution differs from a weak solution by an amount proportional to the entropy produced in the solution. Math. Comp. 62, 1994

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Godunov's theorem is critical to the development of modern methods.

- It is a "barrier theorem" stating what cannot be done.
- It states that a linear second-order method cannot be monotone (i.e. non-oscillatory).
- The key word is "linear".
- Modern methods are nonlinear and monotonicity-preserving. The nonlinearity makes the difference stencil dependent on the solution.

The Majda-Osher theorem establishes accuracy expectations for discontinuous flows.

- Majda and Osher establish that the approximation of shocked or discontinuous flows will converge at be 1st order at best.

<u>Theorem (Majda and Osher):</u> A numerical solution will converge at 1st order at best for the region between any characteristics emanating from a discontinuity. Comm. Pure Appl. Math. 1977

- Nonlinear discontinuities (self-steepening like shocks) converge at 1st order.
- Linear discontinuities converge at less than 1st order (order

  m/(m+1) where *m* is the order of the method, Banks, Aslam, Rider (2009))

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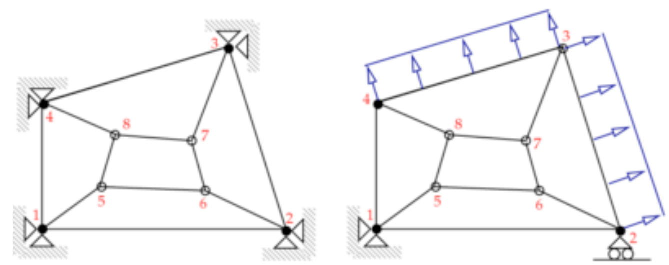
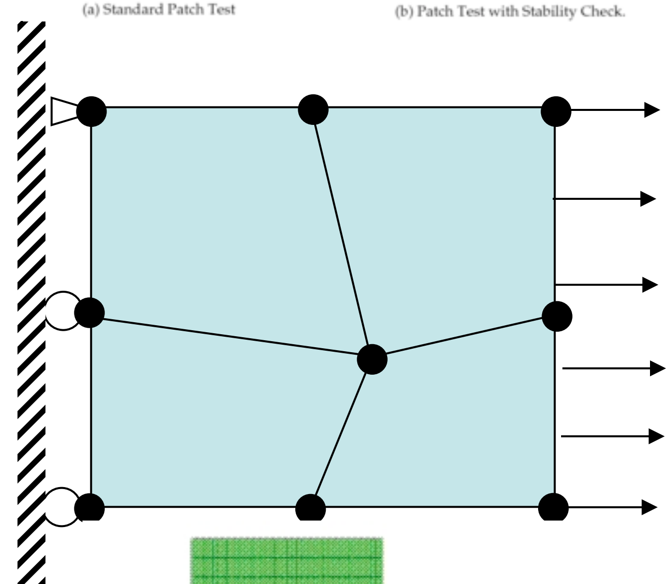
Finite element method verification

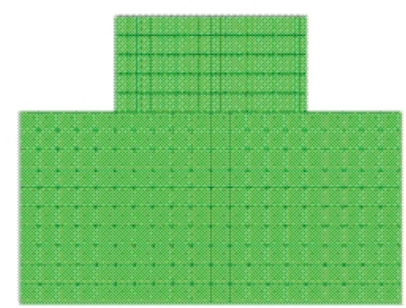
- The patch test (Irons ‘65) is usually done to check the basic implementation.
- Generally, the patch test is the “gold standard” for FEM verification, *its not*.
- It tests conditions for ***consistency*** and hence convergence (Strang ‘72).



(a) Standard Patch Test

(b) Patch Test with Stability Check.





Mathematical expectations for the numerical solution of elliptic and parabolic PDEs

- **It is generally possible to get the design order of accuracy intended for these classes of PDEs due to smoothness.**
- **For general cases with discontinuities and singularities, it is still possible to get the full order accuracy, but…**
  - **The ability of a method to achieve this is dependent on the method's utilization of special features to deal with the difficulties.**
  - **Does the testing of the method provide confidence that the special features indeed provide this?**

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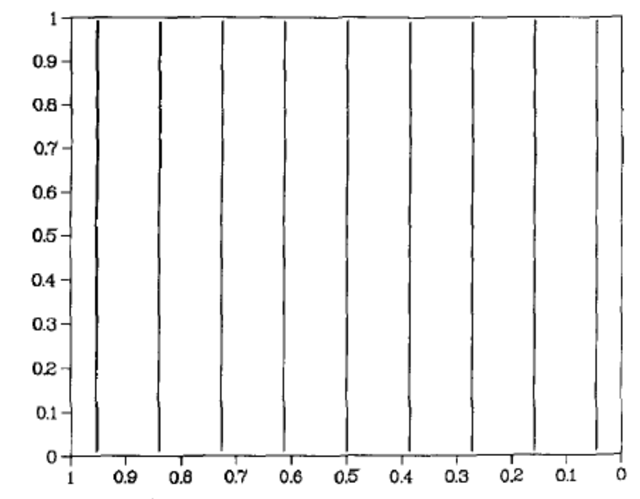
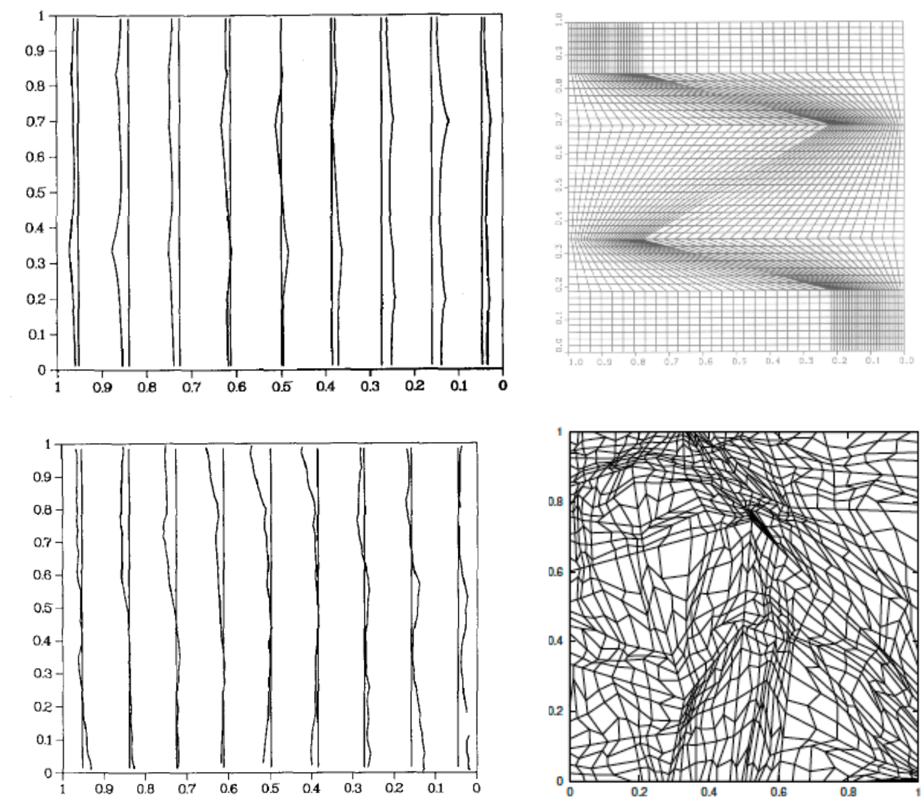
An example from radiation diffusion

- **Does the method pass the equivalent of a patch test?***



A "special" method passes the linear field test.



The classic approach fails the test!

*from Morel, Dendy, Hall, White, J. Comp. Phys. 1992.

Verification involves error estimates and computing convergence rates.

- To conduct a verification exercise one needs to compute or "rigorously" *estimate* errors.
- These errors are used to compute the convergence rates.
  - The expected rates of convergence depend on the problem solved (how smooth or regular the solution is).
- For a method to be consistent the convergence rate needs to be positive and *in line with expectations for the methods used and the problem solved*.

The Conduct of Verification Studies and Numerical Error Estimates

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Quote du jour…

- *“A computer lets you make more mistakes faster than any invention in human history—with the possible exceptions of handguns and tequila.”- Mitch Ratliffe*

“Aristotle maintained that women have fewer teeth than men; although he was twice married, it never occurred to him to verify this statement by examining his wives’ mouths.” -Bertrand Russell

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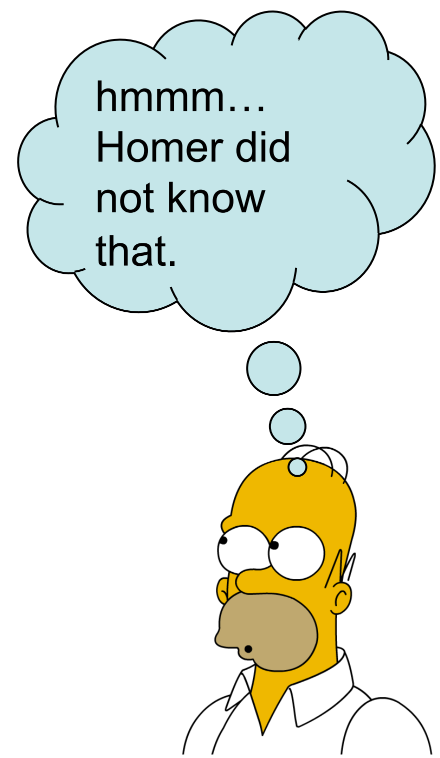
This is a very very important point!

- Solution verifications does not require mesh refinement!
  - One can coarsen meshes as well,
  - The mesh can be refined or coarsened locally (just document what you are doing)
- It requires changes in mesh resolution done somewhat systematically
- It does not require mesh doubling!
  - Or halving
  - It just makes the math easier!



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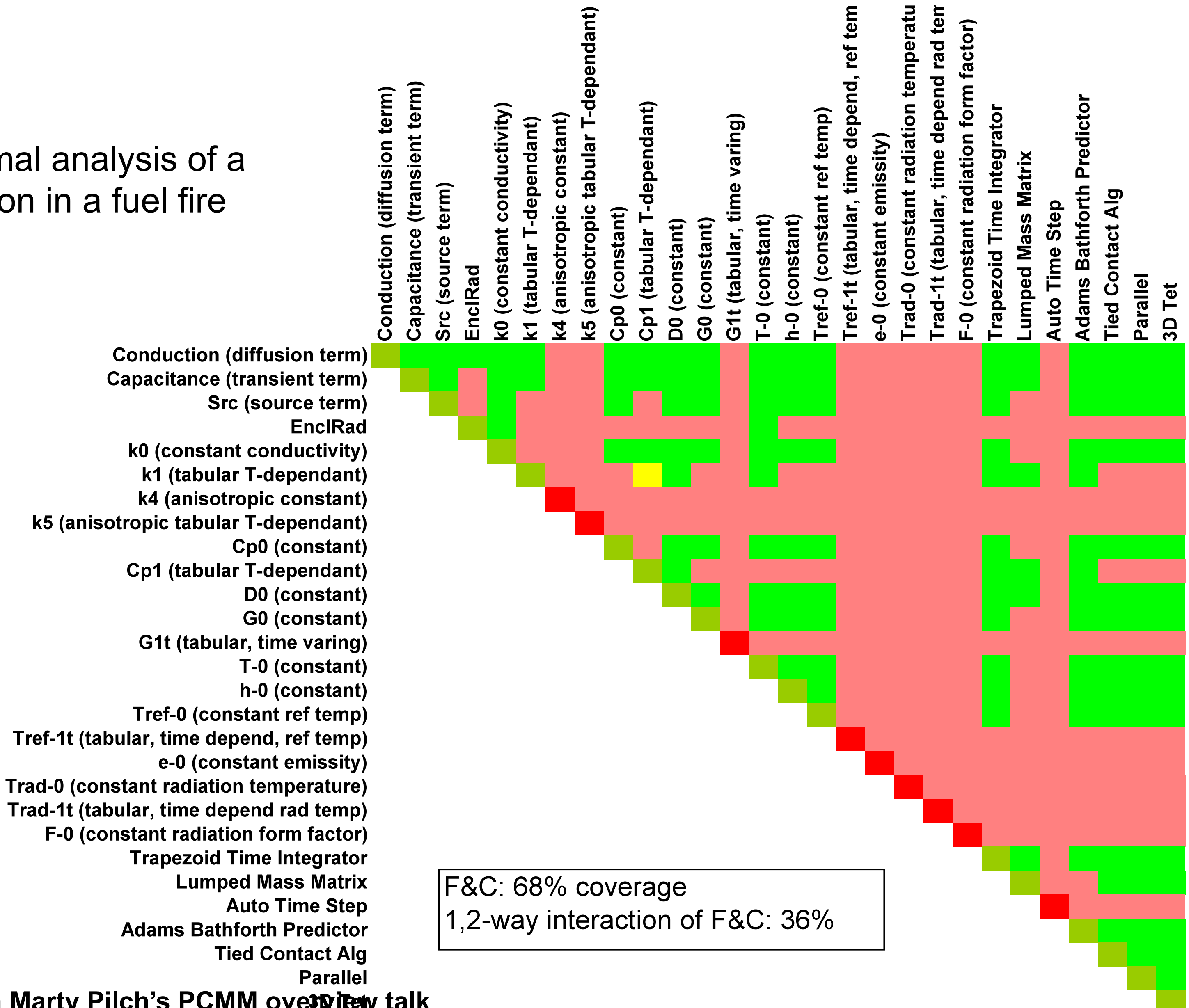
A code verification checklist: Knupp & Ober (SAND2008-4832)

- Ensure a code can be tested
  - Document mathematical model and its solution
  - Ensure support for source terms in the code (manufactured solutions)
  - Document the codes features, and input
  - The software supports refinement studies
- Ensure the test suites are well-designed, comprehensive and maintained
  - Identify specific application and its metrics
  - Create and maintain a coverage table related to the test suite.
  - Tests are added to the regular suite and run on-demand
  - Document, document, document…

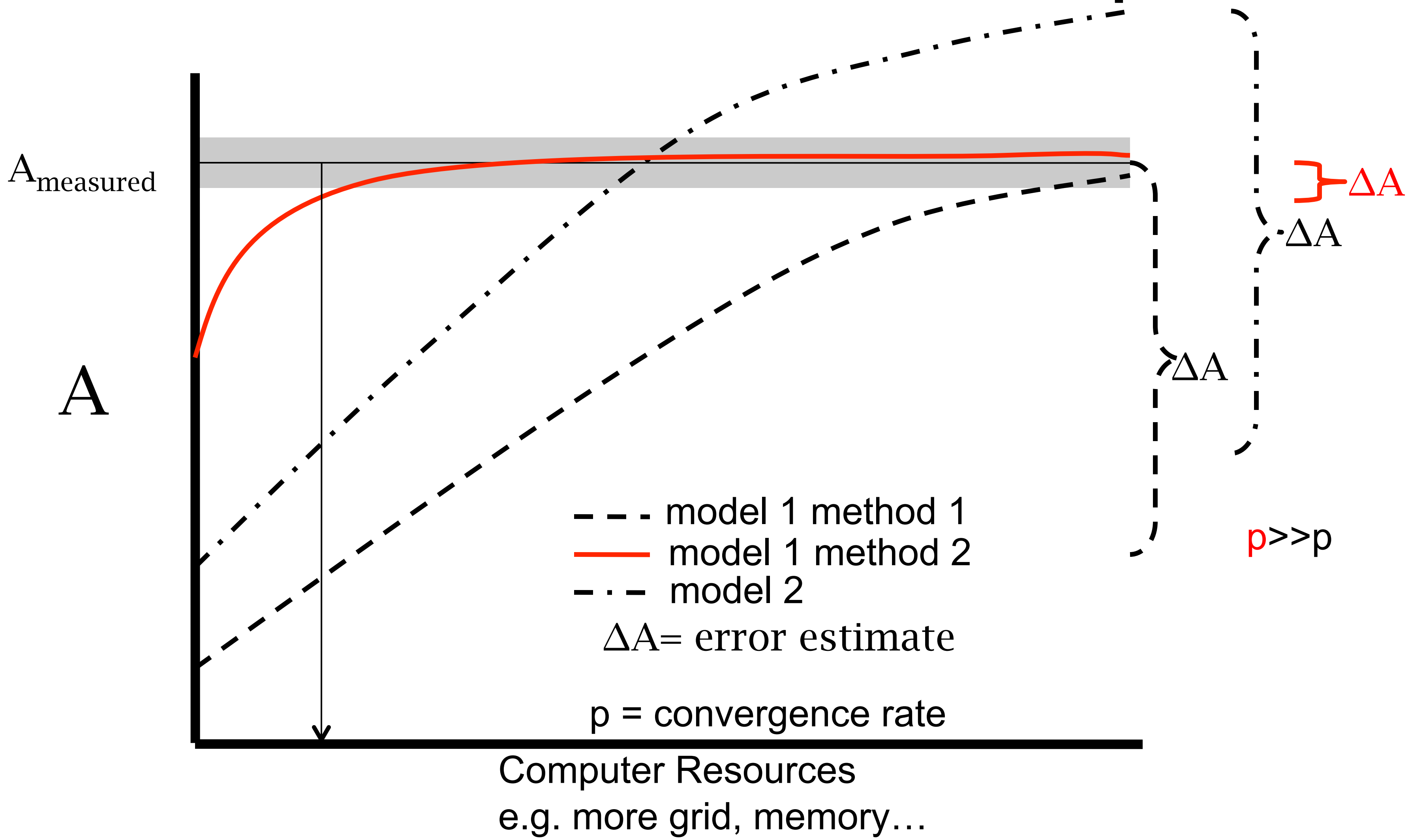
We Are Shifting Our Focus to Verification of Features and Capabilities and Their Interactions

Thermal analysis of a weapon in a fuel fire

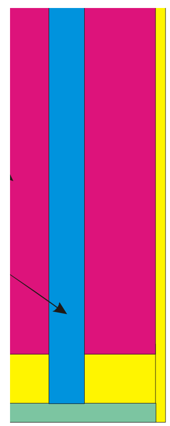


Slide from Marty Pilch's PCMM overview talk

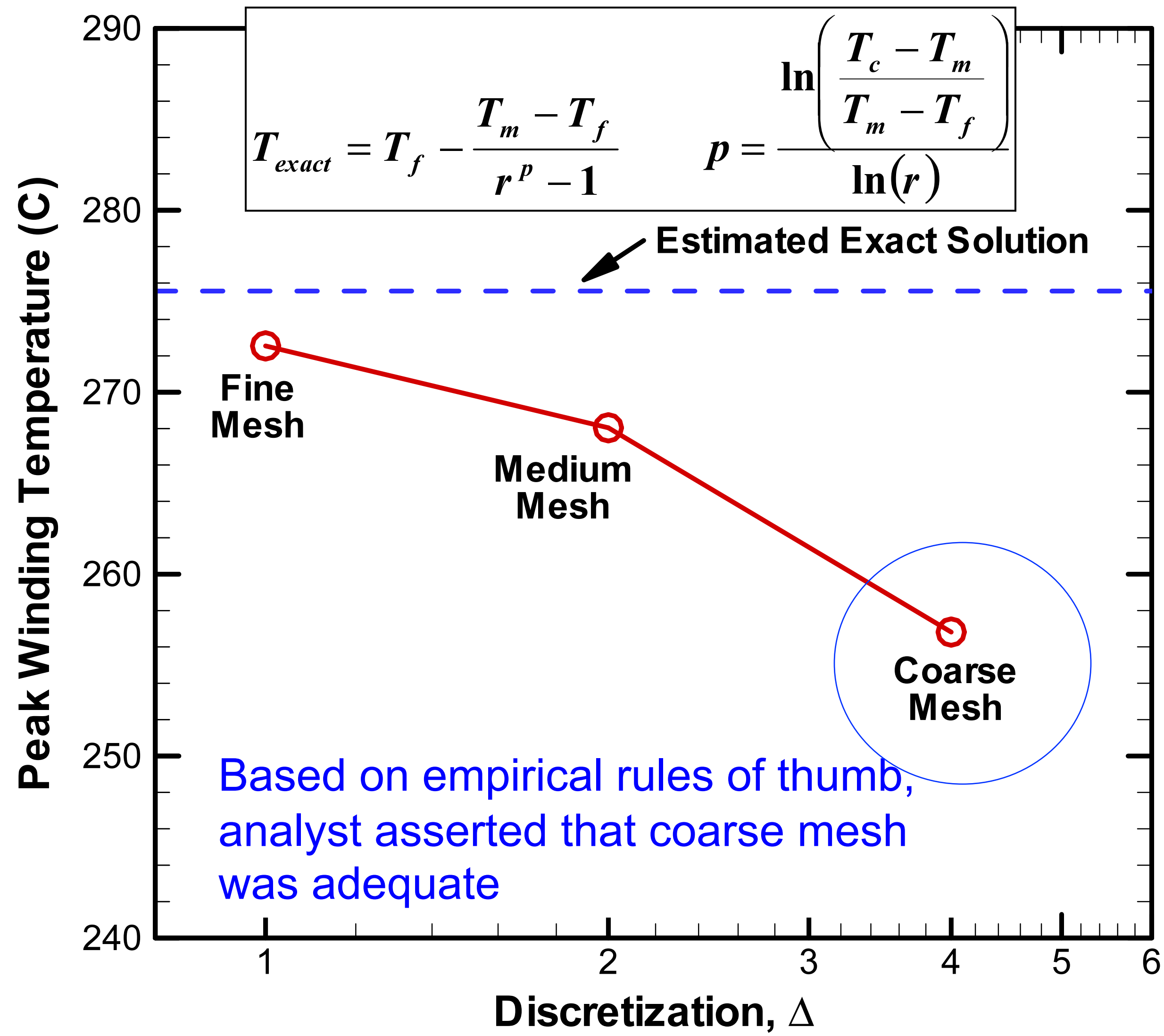
This schematic shows the sort of information that calculation verification can provide.



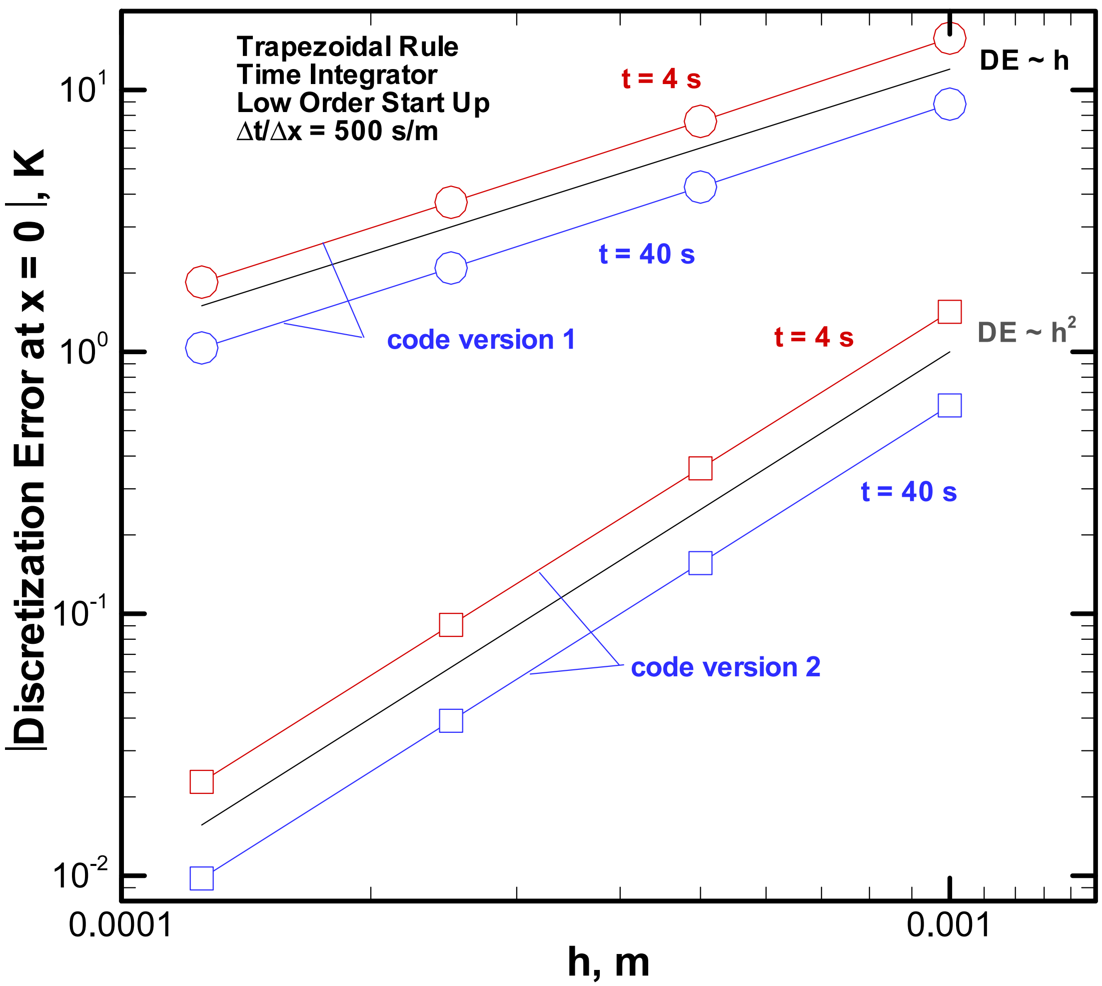
Numerical Errors Pollute Validation Assessments

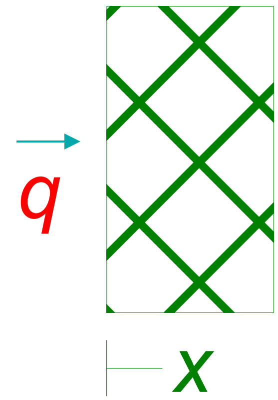


Capacitor



"Order of Convergence" is a Sensitive Metric for Detecting Algorithm Deficiencies





- Transient response of planar 1-D slab to constant flux with analytic solution as the benchmark
- Code bug discovered and fixed based on priority and resource availability. Status tracked in code issue log, which can be accessed by analysts

Modeled as full 3-D object

Slide from Marty Pilch's PCMM overview talk

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Most verification is built upon this simple error ansatz.

- Here is the simplest way to characterize the error, $\|E\|_k = \|S - A\|_k = Ch^{\alpha}$
  - E is an error measure (norm), S is the numerical solution, A is the “answer”, h is the mesh spacing
- One can get the errors in one of two ways:
  - An exact solution (2 numerical solutions needed), A is the exact solution.
  - Assuming the finer grid is more accurate (3 numerical solutions needed), A is the finer grid solution.

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There are several different ways to do a convergence analysis.

- **Code Physics Verification: convergence analysis**

Hard!

Convergence rate

Error in computed solution $= \left\| \boxed{f_{\text{exact}}} - f_{\text{comp}} \right\| \sim E_0 + A(\Delta x)^p + B(\Delta t)^q + C(\Delta x)^r (\Delta t)^s + \ldots$ = Spatial and temporal dependence

Zone size

  - Has demonstrated results with many codes

  - Alternate technology: Method of Manufactured Solutions (MMS)

Continuous: $N(f^*) = 0$ Apply $\Rightarrow$ $N(f) = g$ (Unknown, Known) Project $\Rightarrow$ $\hat{N}(\hat{f}) = \hat{g}$ (Computable) Discrete

    - Successfully used for smooth flows
    - Research: MMS for multi-D discontinuous flows

- Calculation Verification

Easy!

$$\left\| \boxed{f_{\text{fine}}} - f_{\text{coarse}} \right\| \sim E_0 + A(\Delta x)^p + B(\Delta t)^q + C(\Delta x)^r (\Delta t)^s + \ldots$$

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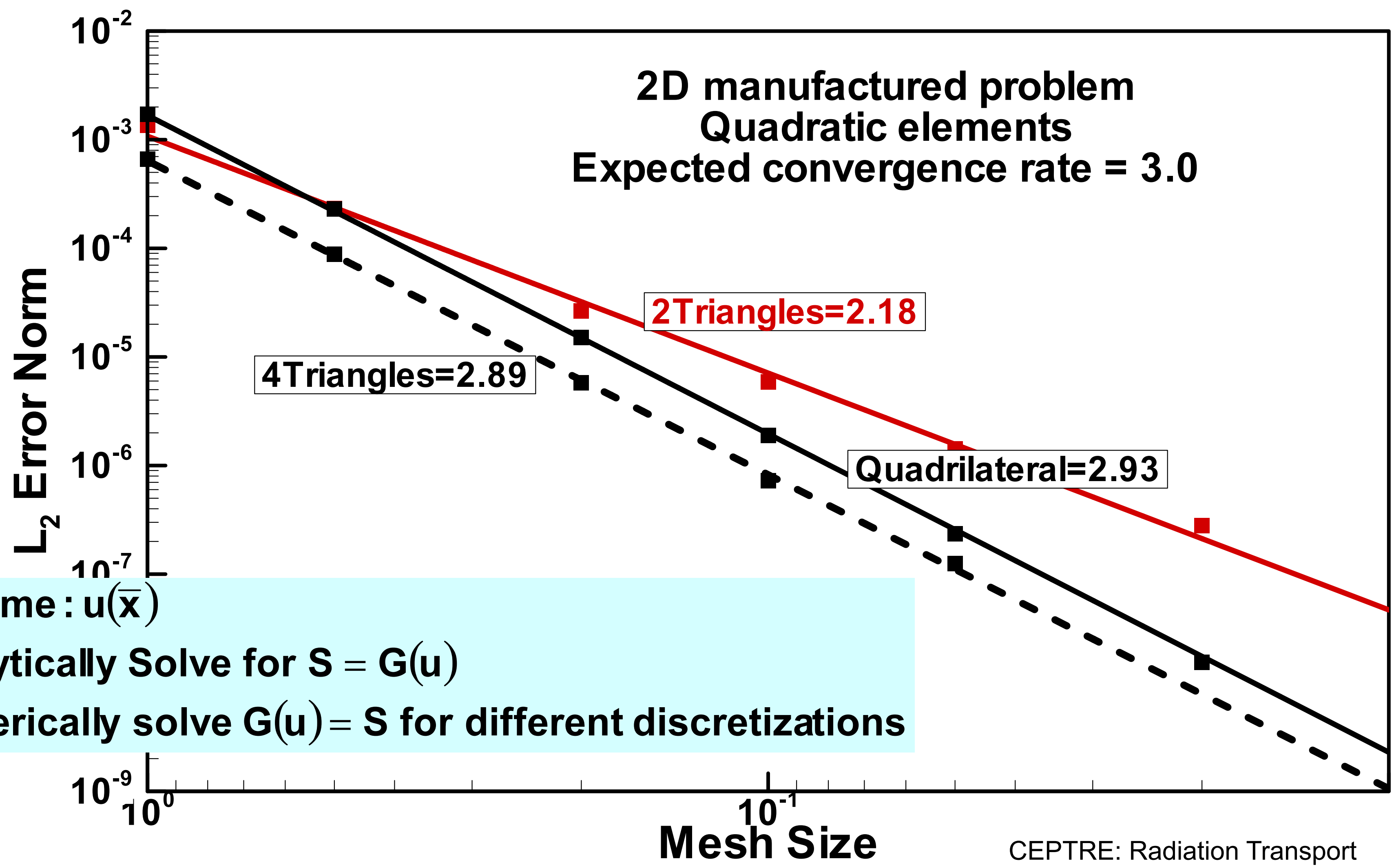
No Exact Analytic Solution?

Verification with a Manufactured Solution



Assume: $u(\bar{x})$

Analytically Solve for $S = G(u)$

Numerically solve $G(u) = S$ **for different discretizations**

CEPTRE: Radiation Transport

Slide from Marty Pilch's PCMM overview talk

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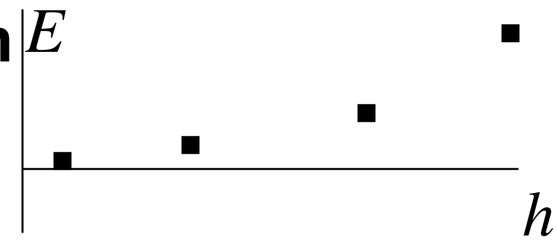
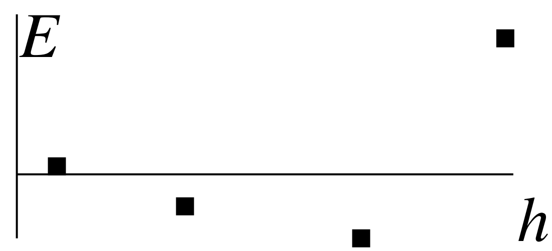
There are different basic models of how the errors will behave.

- **Monotone**: the best case, the norm for simple problems



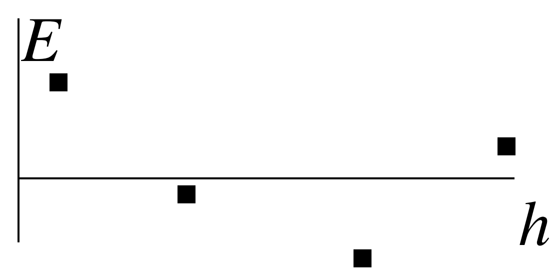
$$E = S - A = Ch^{\alpha}$$

- **Bounded**: an OK condition, often observed



$$|E| = |S - A| = Ch^{\alpha}$$

- **Statistical-Indeterminate**: ***bad news***, but often observed a problem difficulty increases. Not OK, it's a sign of problems.



$$|E| = \mathbf{PDF}$$

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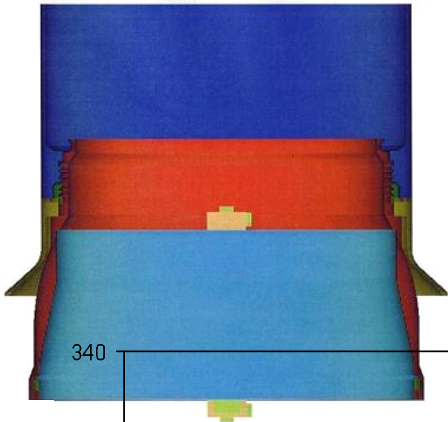
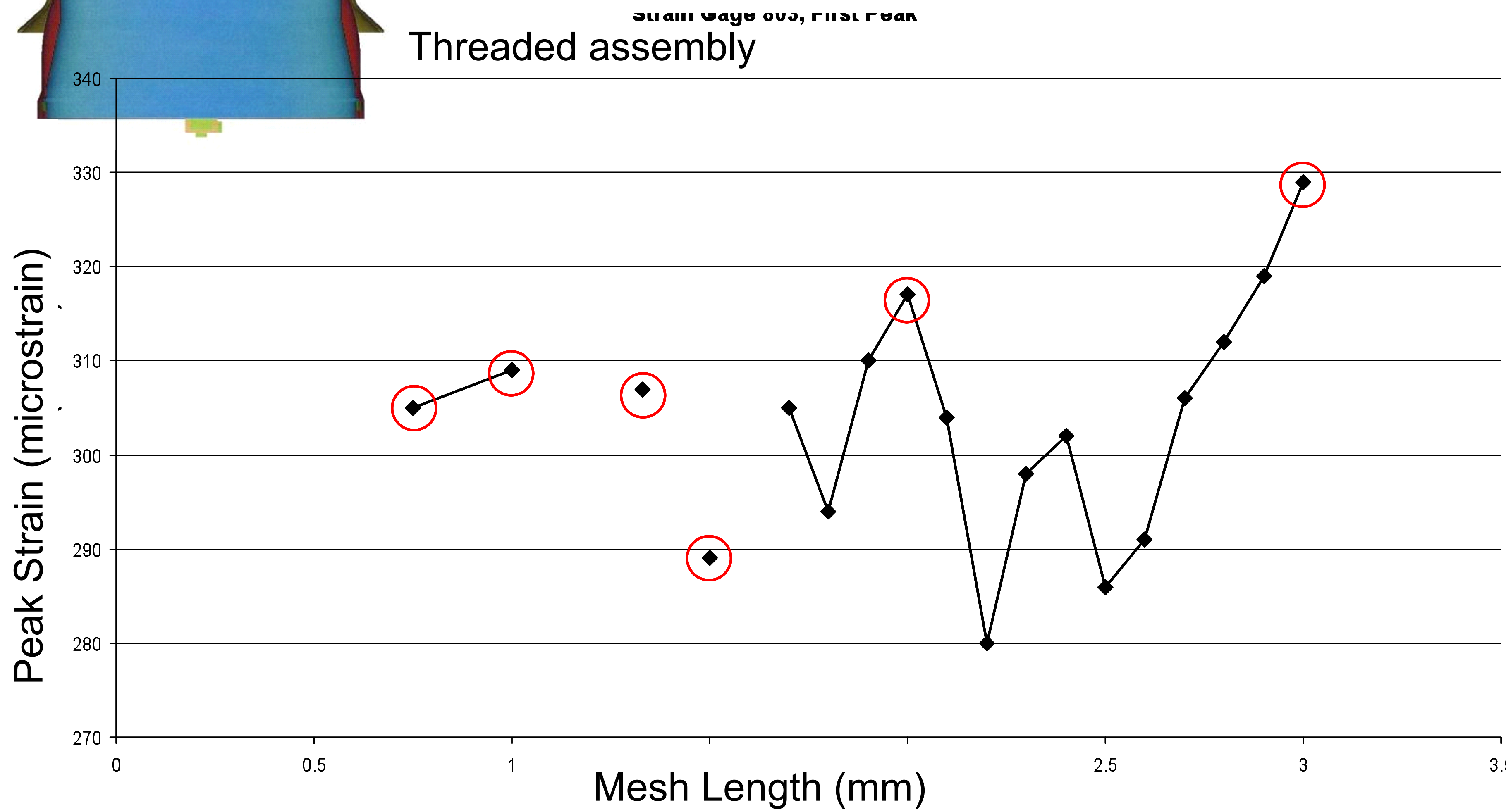
Solutions Don’t Always Converge

Ryan Maupin, ESA-WR, LANL: IMAC-XXIV 1/31/06

Threaded assembly





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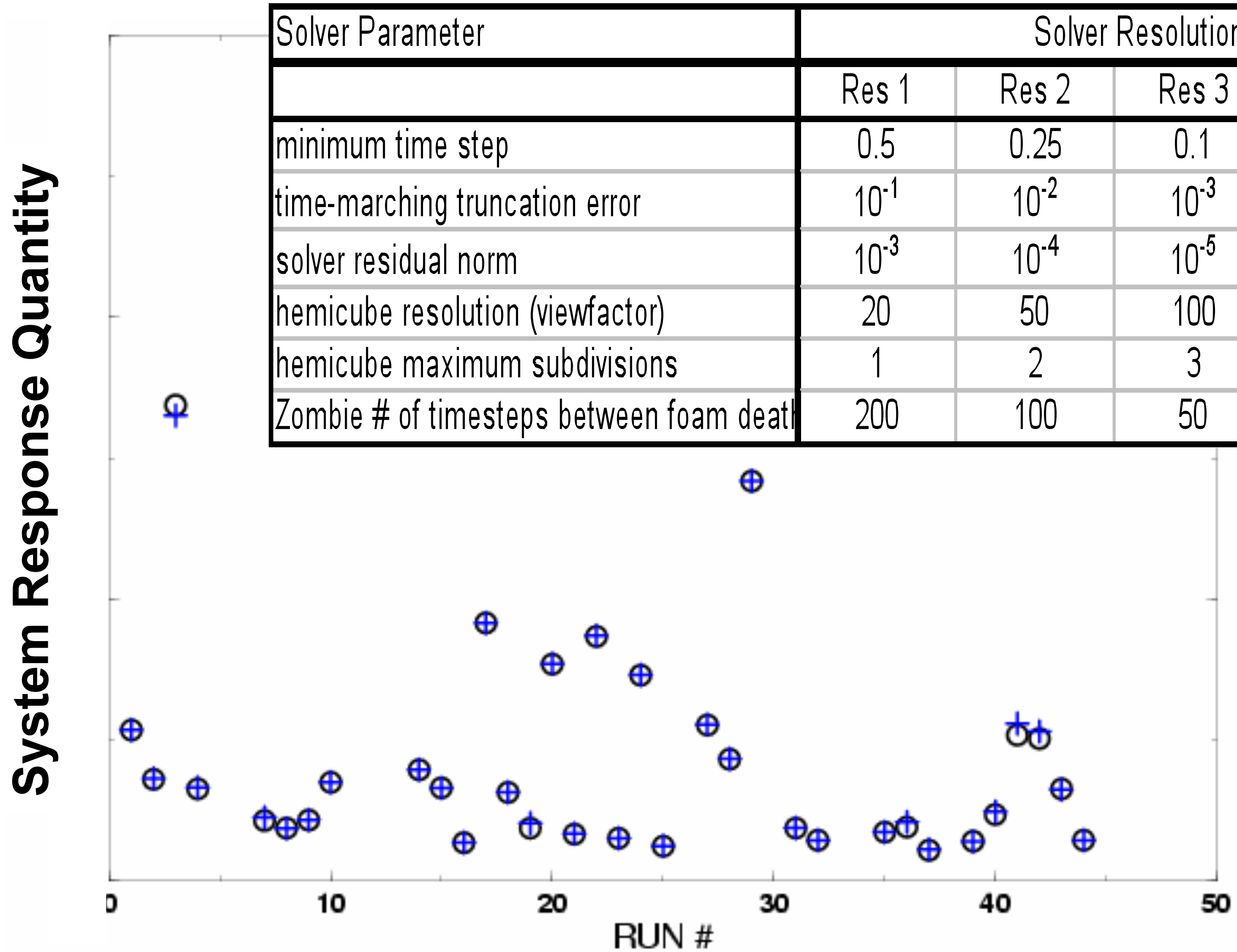
Solution Verification Must Address Solver Settings as Well as Discretization Parameters

Solver Parameter	Solver Resolution Settings				
	Res 1	Res 2	Res 3	Res 4	Res 5
minimum time step	0.5	0.25	0.1	0.05	0.01
time-marching truncation error	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
solver residual norm	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
hemicube resolution (viewfactor)	20	50	100	200	300
hemicube maximum subdivisions	1	2	3	4	5
Zombie # of timesteps between foam deat	200	100	50	20	1



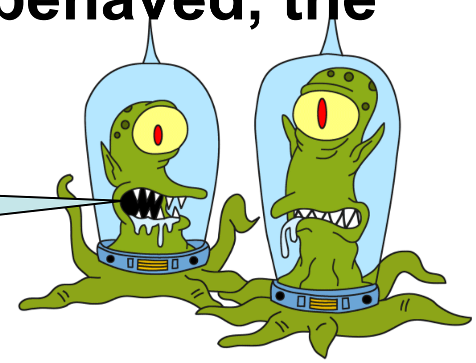
Error estimates can be computed in many norms and several ways.

- The three most common error norms are the L_1, L_2 (i.e., RMS) and $L_{infinity}$ norms.
- These are all L_p norms,

$$\|E\|_p = \left(\sum_{j=1}^{N} |E|^p \right)^{1/p}$$

- The L_1 norm is related to total variation and monotonicity.
- The L_2 norm is the energy norm and related to stability in the sense of Hilbert and Banach spaces (eeeiiiiikkkkk!!!!)
- The $L_{infinity}$ norm is really poorly behaved, the largest error in the system.

Through the systematic use of error norms we enslaved the entire galaxy!



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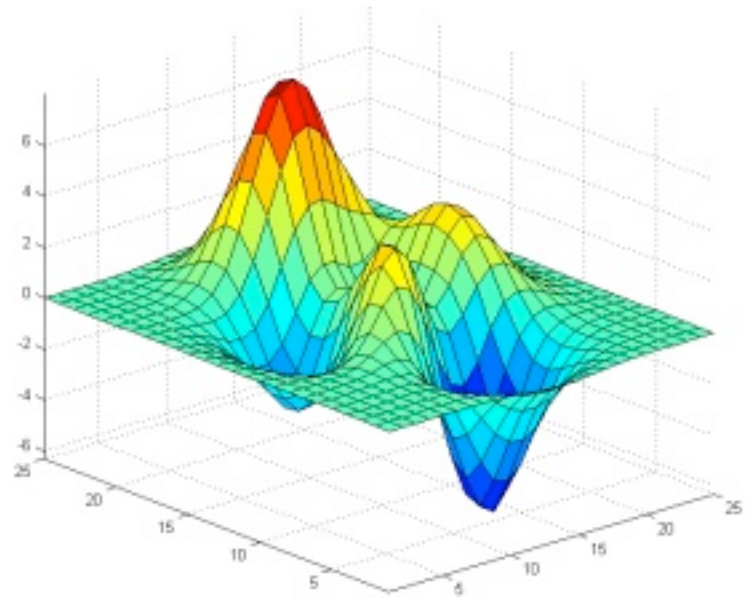
Convergence rates are based on the method and the nature of the problem.

- One can expect to get the full order of accuracy for a method for an ideal test problem where the data begins and remains smooth (continuously differentiable).
- If the problem has a discontinuity or a discontinuous derivative (say a kink), than convergence will be degraded.
- One needs to watch for spontaneously generated discontinuities.

What verification means in numerical analysis!

"For the numerical analyst there are two kinds of truth; the truth you can prove *and the truth you see when you compute*." – Ami Harten



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The numerical uncertainty can be estimated with various models.

- **One model to consider by Roache.**
  - **This is the Grid Convergence Index (GCI) methodology with a set "safety ratio."**

- Another model was proposed by Stern.
  - This model produces a safety factor that depends on both the observed and theoretical convergence rates.
- There are other models, but we believe that these two should be considered primary.
  - Our philosophy is that the focus should be in *applying* the estimates to realistic calculations.

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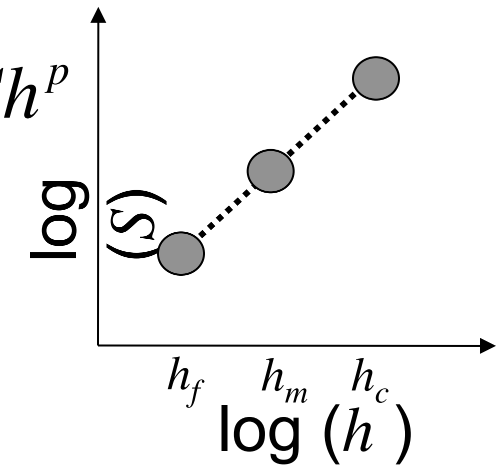
Roache's Grid Convergence Index (GCI)* uses a <u>fixed</u> safety factor.

- **The standard power error ansatz,**

$$S = A + Ch^p$$



$$S = A_k + Ch_k^p;\text{unknowns } S, C, p$$

gives an estimate of numerical error

$$\delta = \frac{\Delta_{mf}}{r_{mf}^p - 1};\Delta_{mf} = S_f - S_m, r_{mf} = \frac{h_m}{h_f}$$

- **A safety factor gives the uncertainty estimate:**

$$U_{num} = F_s\delta; F_s = 1.25$$

- **This safety factor (supposedly) gives a 95% confidence interval (the consequence of CFD "experience"). Does it apply more generally?**

*P. Roache, *Verification and Validation in Computational Science and Engineering*, Hermosa(1996).

Stern's Uncertainty Estimate has a variable "safety factor" or asymptotic correction.

- **The estimate developed by Stern uses the same basic framework, but with a key difference…**
- **The safety factor is not constant, but depends on two pieces of information,**
  - **The observed order of convergence** p_{ob}
  - **The theoretical order of convergence** p_{th}

$$F_s = \frac{r^{p_{ob}} - 1}{r^{p_{th}} - 1}$$

- **This potentially makes it attractive when the computation is not in the asymptotic range,**

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Testing the estimates against an analytical solution builds confidence.

- The errors can be estimated via calculation verification and exactly using the exact solution.
- This will enable us to examine the quality and safety of the uncertainty estimates.
- We will use three examples:
  - A simple linear ODE
  - A simple linear ODE with “bad” Δt’s
  - Sod’s shock tube

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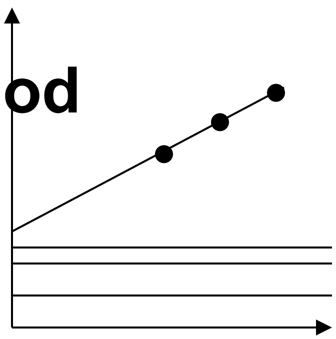
Results for linear ODE

- **We'll start with the simplest thing possible,**

$$\dot{u} = \lambda u \rightarrow u(t) = u(0)\exp(-\lambda t)$$

  - **Use a first-order forward Euler method**



$$\begin{array}{lll} p_T = 1 & \Delta_{cm} = 0.027 & F_{\text{Roache}} = 1.25 \\ p = 1.13 & \Delta_{mf} = 0.012 & F_{\text{Stern}} = 1.18 \\ & \delta = 0.015 & F_{\text{Exact}} = 1.12 \end{array}$$

  - **Compare with a second-order modified Euler**

$$\begin{array}{lll} p_T = 2 & \Delta_{cm} = 0.0036 & F_{\text{Roache}} = 1.25 \\ p = 2.16 & \Delta_{mf} = 0.0008 & F_{\text{Stern}} = 1.16 \\ & \delta = 0.0002 & F_{\text{Exact}} = 1.09 \end{array}$$

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Results for linear ODE with a bad choice for time step size.

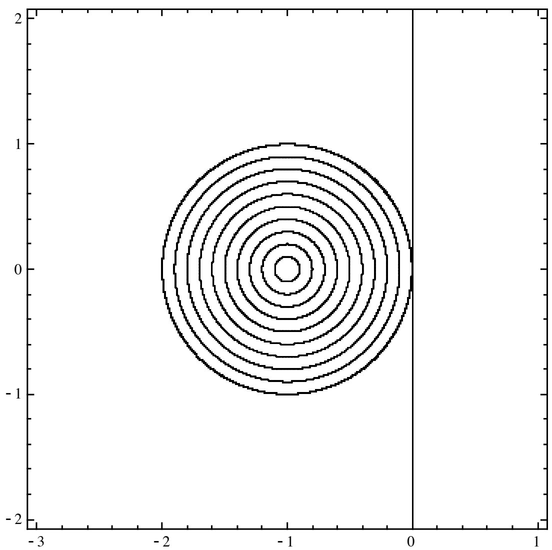
- We'll continue with the simplest thing possible and forward Euler, $\dot{u} = \lambda u \rightarrow u(t) = u(0)\exp(-\lambda t)$
- Use a too large time step, $\Delta t = 0.1$,

$$
\begin{array}{lll}
p_T = 1 & \Delta_{cm} = 0.0022 & F_{Roache} = 1.25 \\
p = 0.44 & \Delta_{cm} = 0.0016 & F_{Stern} = 2.81 \\
\lambda = 5 & \delta = 0.0045 & F_{Exact} = 2.33
\end{array}
$$

- Study a “growing” case

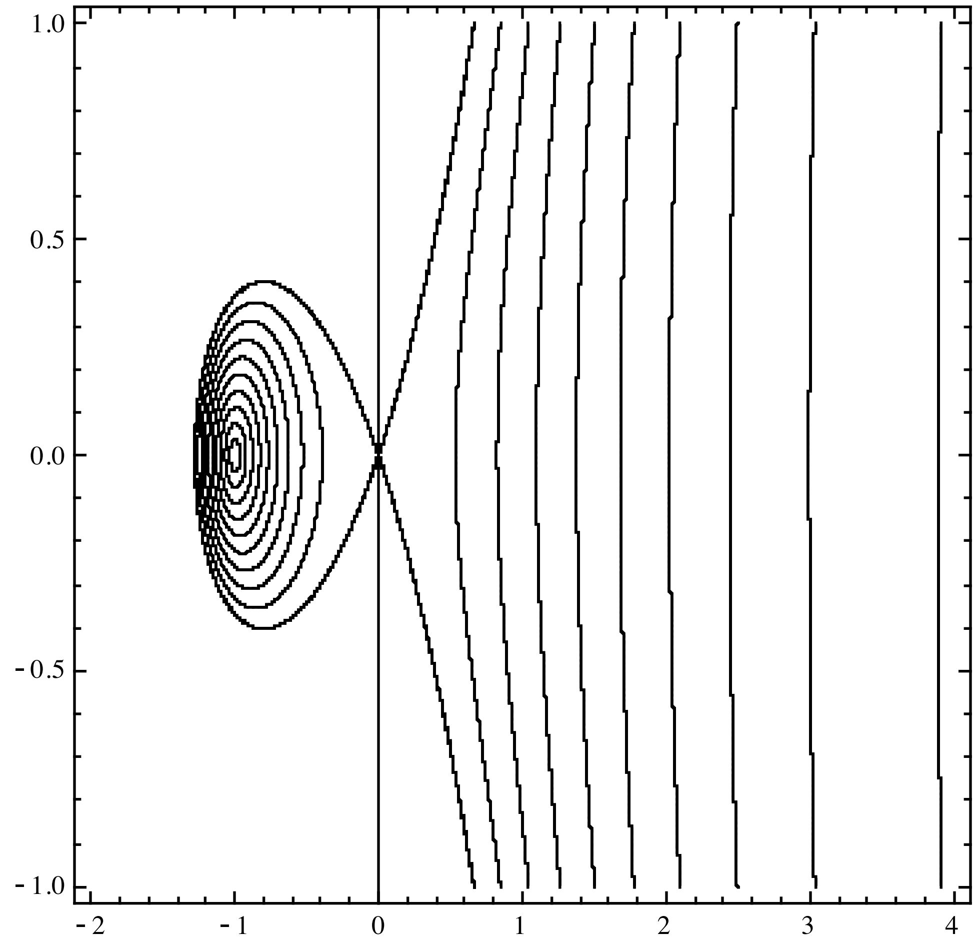
$$
\begin{array}{lll}
p_T = 1 & \Delta_{cm} = -29.07 & F_{Roache} = 1.25 \\
p = 0.25 & \Delta_{cm} = -24.46 & F_{Stern} = 5.31 \\
\lambda = -5 & \delta = -129.9 & F_{Exact} = 3.49
\end{array}
$$

This can be understood with a bit of numerical analysis



Stability plot

$$|1-\lambda\Delta tL|\leq 1$$



Order star $$\frac{|1-\lambda\Delta tL|}{\exp(-\lambda\Delta t)}\leq 1$$

Results for numerical UQ estimation with Sod's Shock Tube.

- **Sod's shock tube uses an ideal gas with a pressure ratio of 10 and a density ratio of 8**
  - **Solve this with a Godunov-type method**

$$
\begin{array}{ccc}
p_T = 4/5 & \Delta_{cm} = 1.21 \times 10^{-3} & F_{\text{Roache}} = 1.25 \\
p = 1.19 & \Delta_{mf} = 5.28 \times 10^{-4} & F_{\text{Stern}} = 1.74 \\
 & \delta = 4.09 \times 10^{-4} & F_{\text{Exact}} = 1.39
\end{array}
$$

Density

$$
\begin{array}{ccc}
p_T = 1 & \Delta_{cm} = 8.93 \times 10^{-4} & F_{\text{Roache}} = 1.25 \\
p = 1.13 & \Delta_{mf} = 4.07 \times 10^{-4} & F_{\text{Stern}} = 1.19 \\
 & \delta = 3.52 \times 10^{-4} & F_{\text{Exact}} = 0.82
\end{array}
$$

Pressure

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Example, Combined Space-Time Convergence Analysis

- **Consider the following error Ansatz:**

$$\mathrm{F}(\xi;\Delta x,\Delta t) = \left\| f_{\mathrm{exact}} - f_{\mathrm{comp}} \right\| \sim A(\Delta x)^{p} + B(\Delta t)^{q} + C(\Delta x)^{r}(\Delta t)^{s}$$

Seven unknowns ➡ Seven equations required

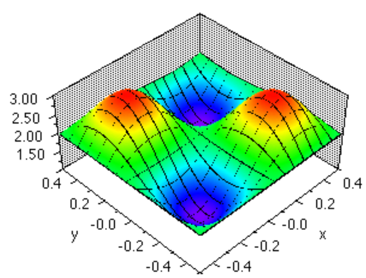
$$\mathrm{g}(\xi;\Delta x_n,\Delta t_n) = \left\| f_{\mathrm{exact}} - f_{\mathrm{comp}} \right\| - \xi_1(\Delta x_n)^{\xi_2} - \xi_3(\Delta t_n)^{\xi_4} - \xi_5(\Delta x_n)^{\xi_6}(\Delta t_n)^{\xi_7}$$

$$\mathrm{g}(\xi;\Delta x_n,\Delta t_n) = 0\ ,\ n = 1,\ldots,7 \ \Rightarrow\ \boxed{\mathrm{G}(\xi) = 0}$$

Obtain solutions with generalized Newton's method

  - Strength: Assumption regarding combined error sources
  - Weakness: Complexity, cost, uncertainty in solution
- Example: 2D linear advection

Analysis of problem involving nonlinear fields is in progress…



A	p	B	q	C	r	s	
0.010	1.90	0.0067	1.95	0.010	0.90	0.90	*Set 1*
0.010	2.00	0.0078	1.97	0.010	1.01	1.00	*Set 2*

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Summary, Advise and Closure

What happens when codes don't converge.

- **Start simplifying the problem:**
  - Weaken the jumps or magnitude of problem difficulty,
  - Take the problem to asymptotic limits (strong shock or weak shock limit, etc…)
  - Change the problem in small ways
  - Refine the grid some more (is the grid sufficient?)
- **If all else fails, admit that there is a problem that can't be fixed without going deeper.**
- **Non-convergence is not an acceptable end-point, it is indicative of a serious problem.**

Begin expecting methods to fail, don't begin expecting them to succeed.

- The best way to proceed with a testing (verification) study is to assume that something is wrong with the code and prove what the problem is.
  - If you cannot prove that the code has an error than the code is more likely to be correct.
  - The opposite point-of-view can be extremely frustrating, and prone to incorrect assertions.
- The code is only correct to the extent of the testing coverage.

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Its important to always remember the theoretical expectations.

- The Lax equivalence theorem: consistency & stability equals convergence
- What kind of equations are you solving? (elliptic, hyperbolic, parabolic, mixed,… what is dominant?)
  - Use the theory to manage your expectations…
  - and interpret your results (it tells you if its good or bad!)
  - Much of the theory is method agnostic!
- What sort of character do the methods in the code bring? Do you know?

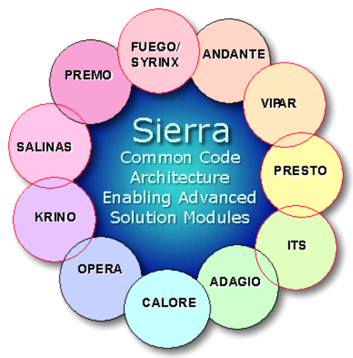
Attributes of Code and Solution Verification

Demonstrating Convergence to Correct Answer for the Intended Application

Inference → Application

Solution Verification: Convergence for intended application, *but is it the right answer?*

• *Address adequacy of spatial AND temporal AND other discretizations AND numerical knobs*



Coupled Multi-Physics Across Codes

Coupled Multi-Physics Within Code

Separate Physics

Issues: non-smooth solutions, contact, constitutive laws, internal constraints, multiscale physics, global/local norms, etc.

Inference

Regression Testing

Code Verification: Convergence to correct answer, *wrong application*

• Eliminate code bugs *AND* inadequate algorithms

SQE(A)

Slide from Marty Pilch's PCMM overview talk

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- Jeff Greenough and Jeff Banks (LLNL)
- Bill Oberkamf (SNL retired)
- Chris Roy

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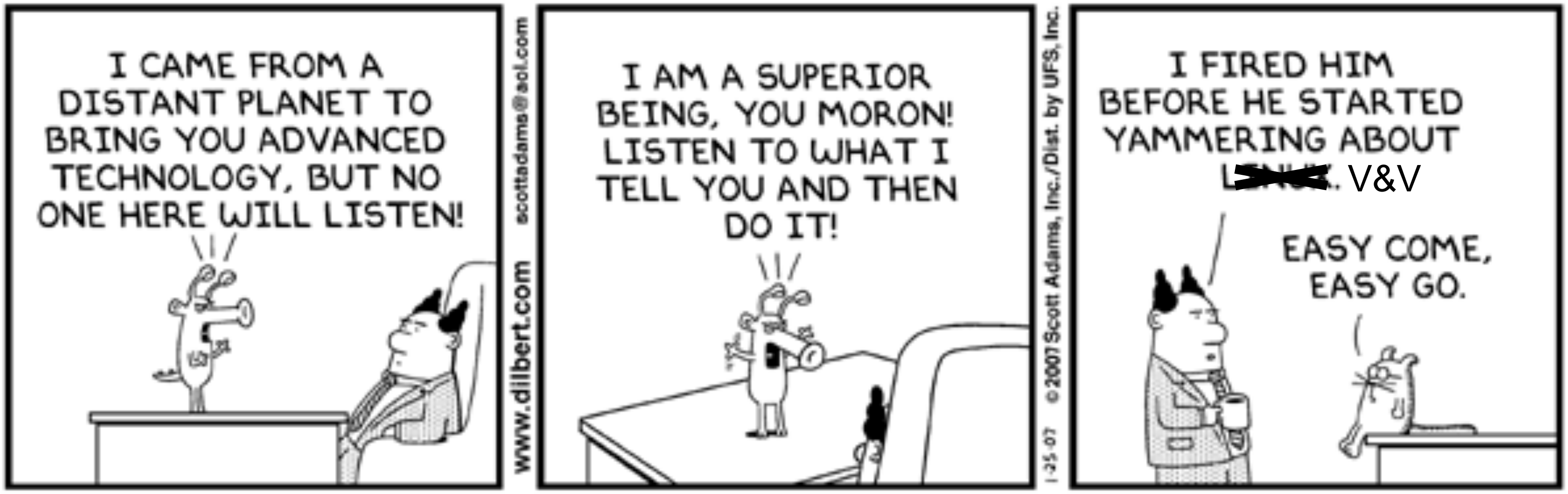
“Dilbert isn’t a comic strip, it’s a documentary” – Paul Dubois



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