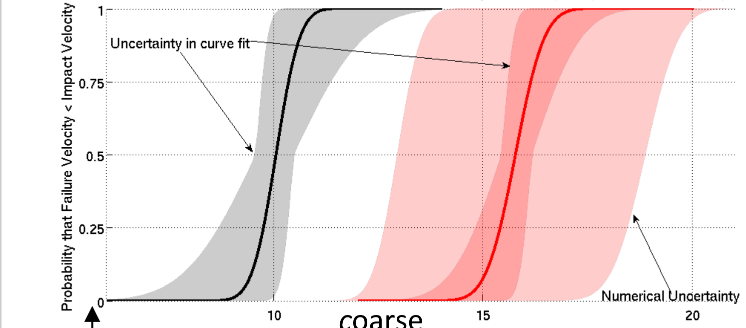
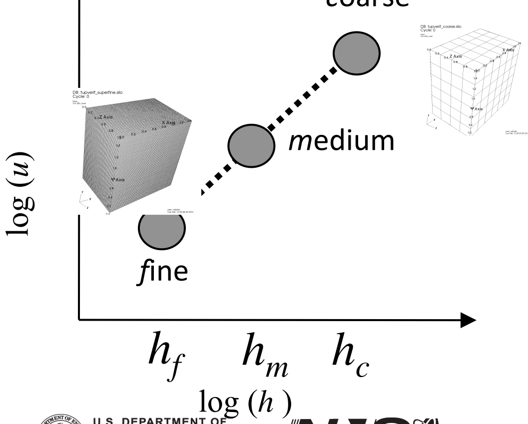
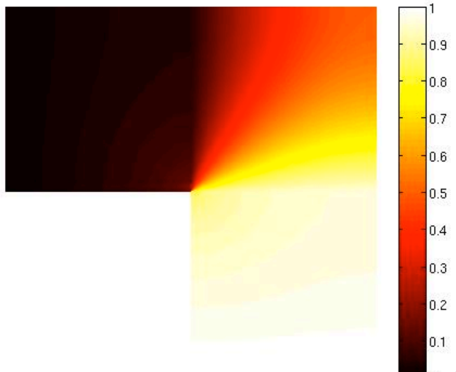
Exceptional service in the national interest

Sandia National Laboratories


Cumulative Distribution Functions of Critical Failure Velocity from Test (black) and Simulation (red)





WHAT IS NECESSARY TO SUCCEED? LESSONS FROM THE ASC PROGRAM

Bill Rider,

GEC, Rayleigh NC, Nov. 3, 2014

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

“V&V takes the fun out of computational simulation”

– Tim Trucano

Definitions: Verification and Validation

- ASC(I): Advanced Simulation and Computing Program
  - **Verification** → Verification is the process of determining that a computational software implementation correctly represents a model of a physical process.
  - **Validation** → Validation is the process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model applications.
- Close to the DMSO, ASME and AIAA definitions.

- Alternative for computational science and engineering:
  - **Verification** = Accumulating evidence that the equations are solved correctly.
  - **Validation** = Accumulating evidence that the equations are correct *for the intended application*

Definitions Continued:

- **Calibration** = "The process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with experimental data." (AIAA Guide)
- **Code** = everything that goes into producing the final numbers, unless I'm speaking about "Code Verification," in which case I mean the particular software.
- Comments:
  - **Calibration** *is not* **validation**, especially for predictive applications.
  - **Validation** is defined to be be dependent on the intended application.
  - In the sense of "solution accuracy," **verification** is dependent on the intended application.

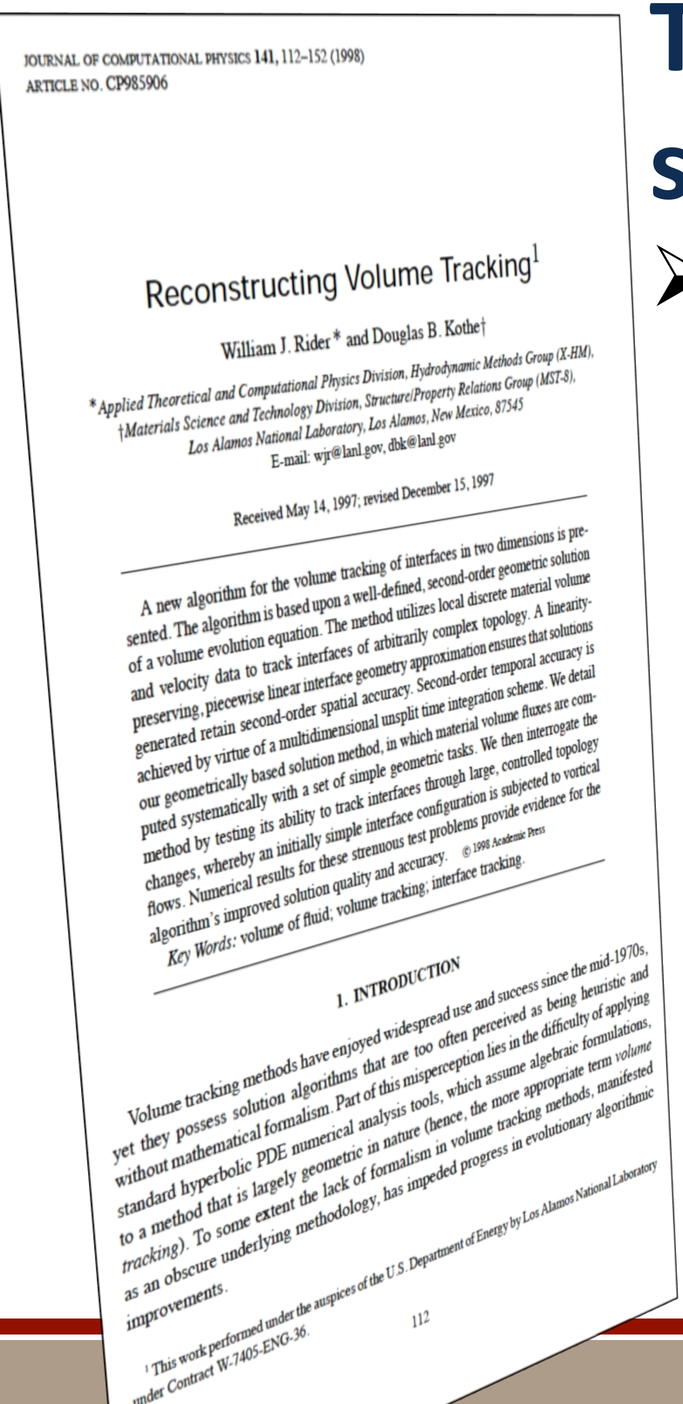
Definitions Continued:

- **Calibration** = "The process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with experimental data." (AIAA Guide)
- Comments:
  - **Calibration** *is not* **validation**, especially for predictive applications.
  - **Validation** is defined to be be dependent on the intended application.

“Change almost never fails because it's too early. It almost always fails because it's too late.” — Seth Godin

This is where V&V started for me

- The volume tracking paper is highly cited – 979 via Google Scholar
  - ✓ It was not cited for the main reason we wrote the paper, the methods…
  - ✓ It was because of the tests it introduced.



JOURNAL OF COMPUTATIONAL PHYSICS **141**, 112–152 (1998)
ARTICLE NO. CP985906

Reconstructing Volume Tracking[1]

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Received May 14, 1997; revised December 15, 1997

A new algorithm for the volume tracking of interfaces in two dimensions is presented. The algorithm is based upon a well-defined, second-order geometric solution of a volume evolution equation. The method utilizes local discrete material volume and velocity data to track interfaces of arbitrarily complex topology. A linearity-preserving, piecewise linear interface geometry approximation ensures that solutions generated retain second-order spatial accuracy. Second-order temporal accuracy is achieved by virtue of a multidimensional unsplit time integration scheme. We detail our geometrically based solution method, in which material volume fluxes are computed systematically with a set of simple geometric tasks. We then interrogate the method by testing its ability to track interfaces through large, controlled topology changes, whereby an initially simple interface configuration is subjected to vortical flows. Numerical results for these strenuous test problems provide evidence for the algorithm's improved solution quality and accuracy.

Key Words: volume of fluid; volume tracking; interface tracking.

1. INTRODUCTION

Volume tracking methods have enjoyed widespread use and success since the mid-1970s, yet they possess solution algorithms that are too often perceived as being heuristic and without mathematical formalism. Part of this misperception lies in the difficulty of applying standard hyperbolic PDE numerical analysis tools, which assume algebraic formulations, to a method that is largely geometric in nature (hence, the more appropriate term *volume tracking*). To some extent the lack of formalism in volume tracking methods, manifested as an obscure underlying methodology, has impeded progress in evolutionary algorithmic improvements.

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[1] This work performed under the auspices of the U.S. Department of Energy by Los Alamos National Laboratory under Contract W-7405-ENG-36.

Rider & Kothe, *J. Comp. Phys.*, **141**, 1998 (RK1998).

Why did we write “Reconstructing Volume Tracking” ?

- Volume tracking is an important methodology at LANL for computing multimaterial flows in the Eulerian frame.
- We wrote the paper because the standard way of coding up a volume of fluid method was so hard to debug.
    - We thought we had a better way to put the method together using computational geometry (i.e., a “toolbox”)

Why did “Reconstructing Volume Tracking” get cited so much ?

Super test problems!

Once the method was coded it needed to be tested:

- Existing methods for testing these methods were poor
- We came up with some new tests borrowed from the high-resolution methods community (combining the work of several researchers
  - Dukowicz’s vortex,
  - Smolarkiewicz’s deformation field and
  - Leveque’s time reversal)

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.

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”

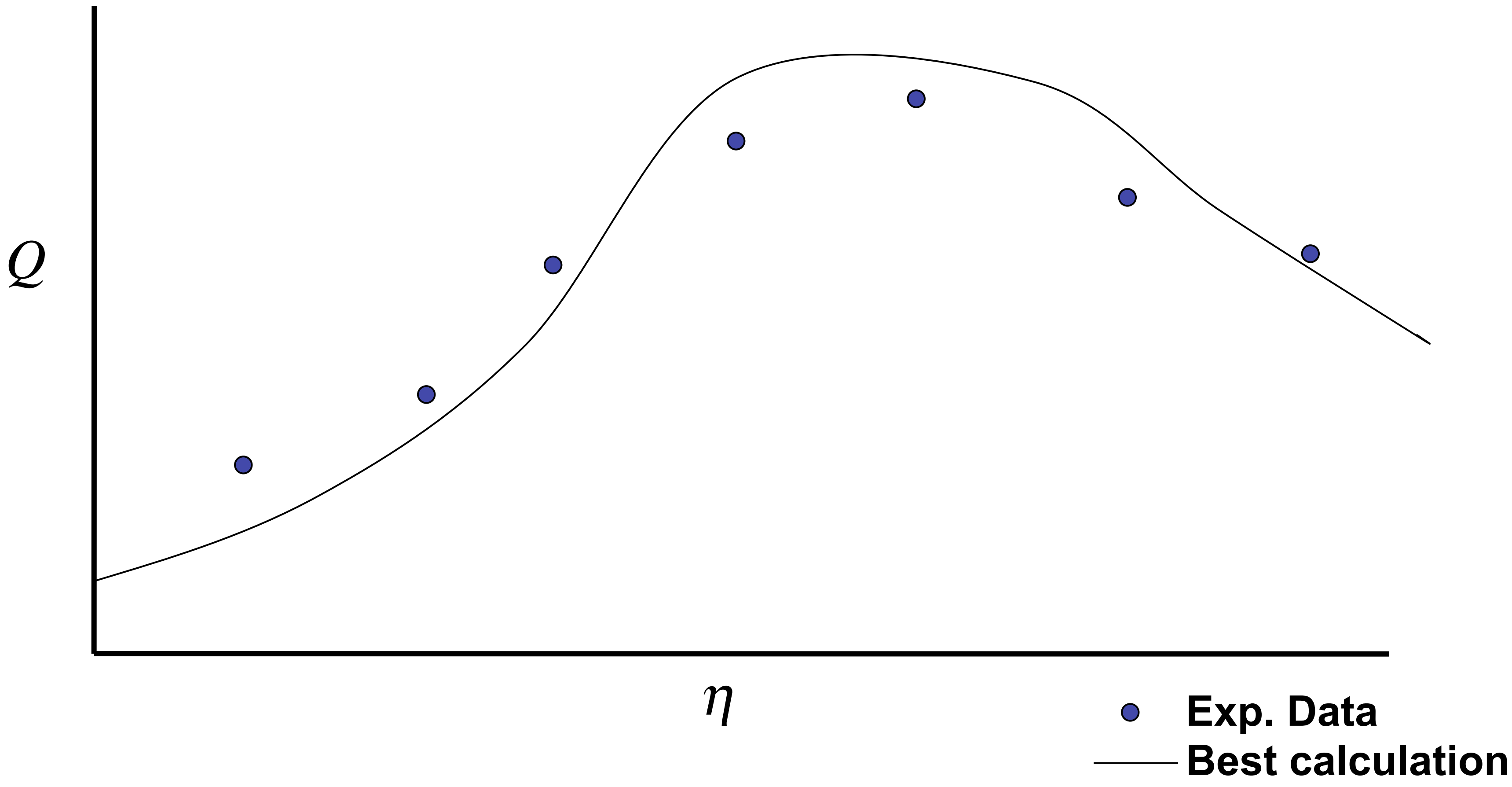
*these three slides were shown at the first tri-Lab V&V workshop in 2001.

“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

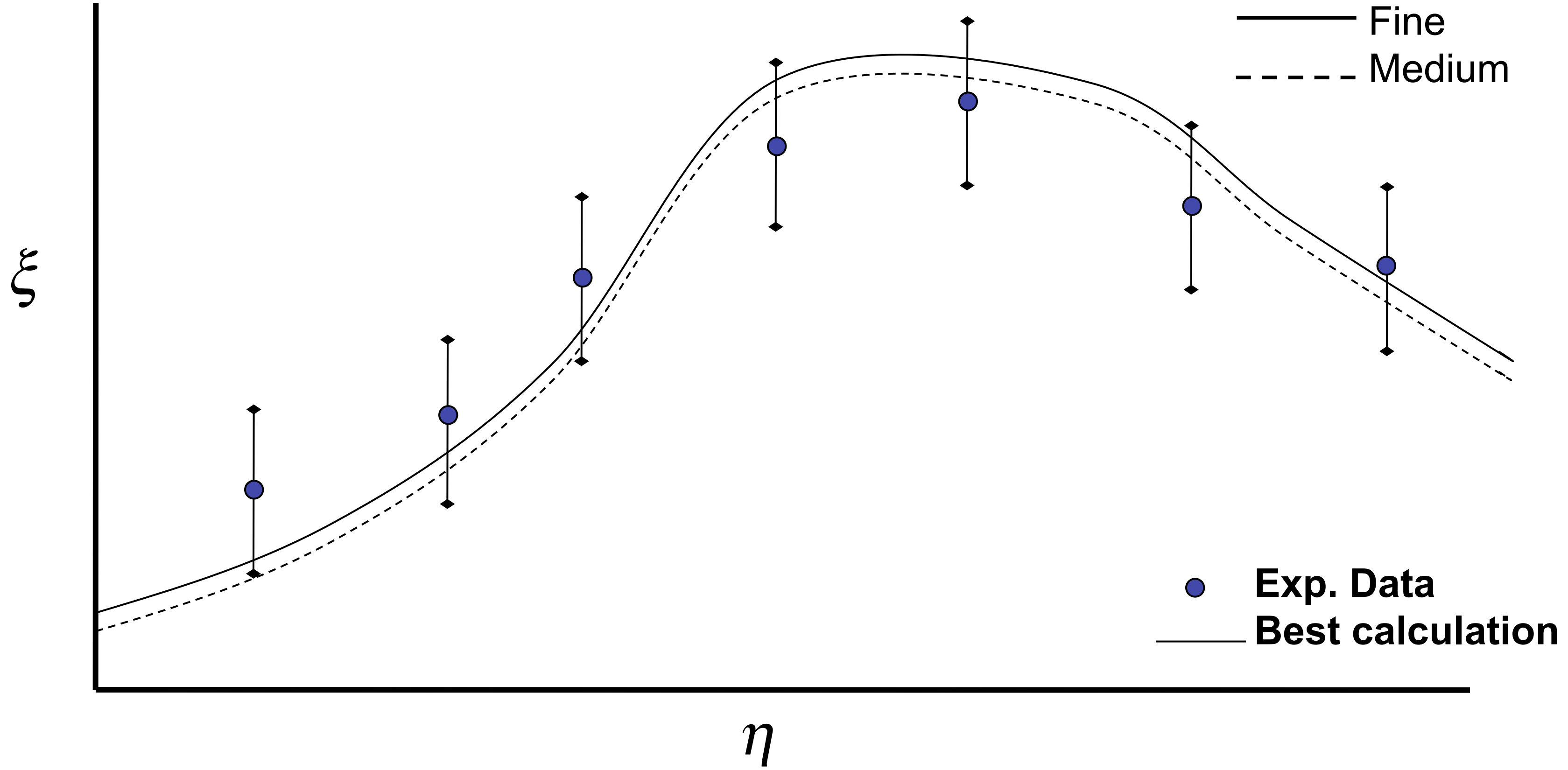
Quite often comparisons are done using the infamous "viewgraph" norm.

These plots are merely notional "cartoons" that illustrate where we want to go.



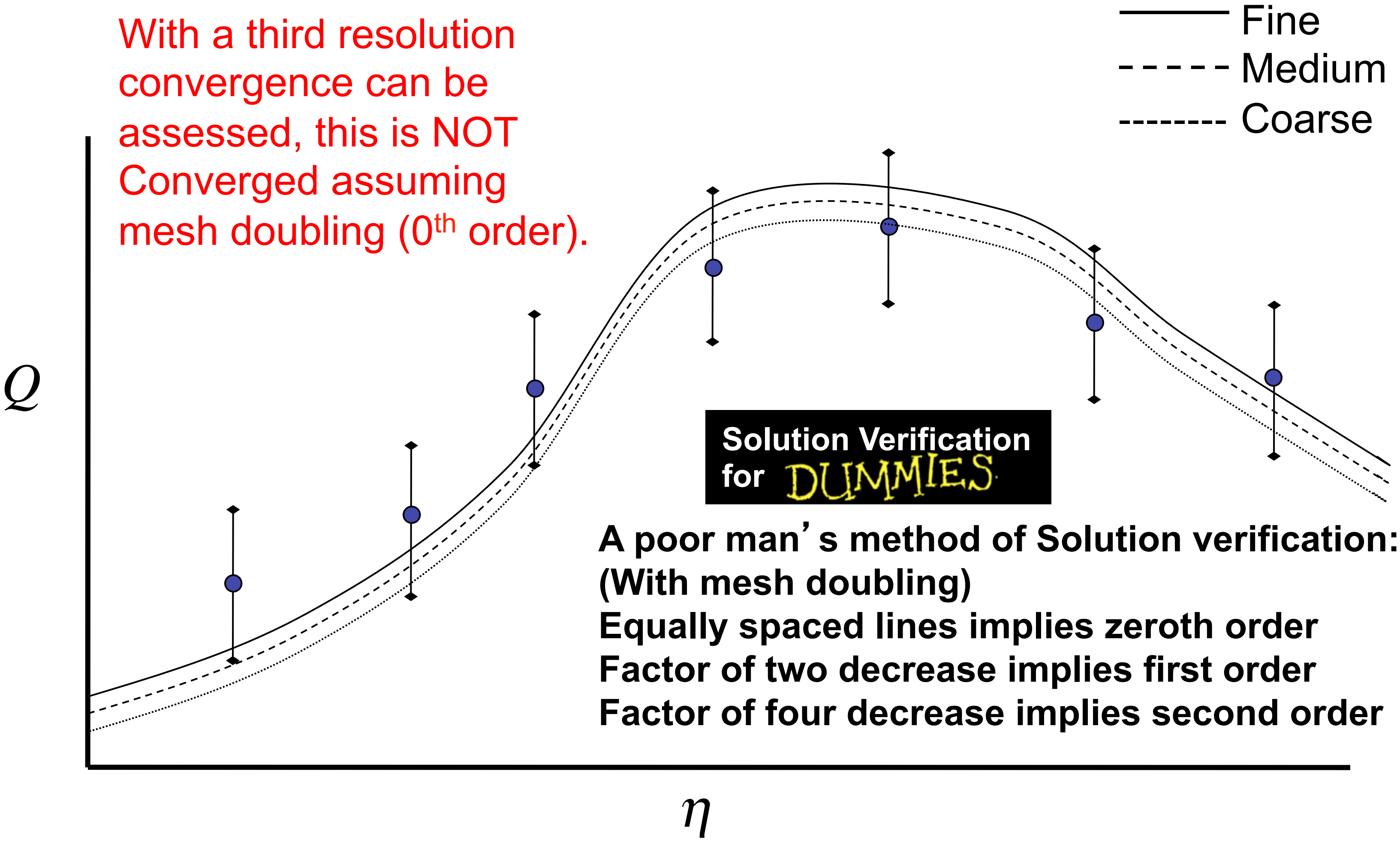
Here is a notion of how a “converged” solution is often described.

This is “mesh sensitivity”. This is **not** solution verification!



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

With a third resolution convergence can be assessed, this is NOT Converged assuming mesh doubling (0th order).



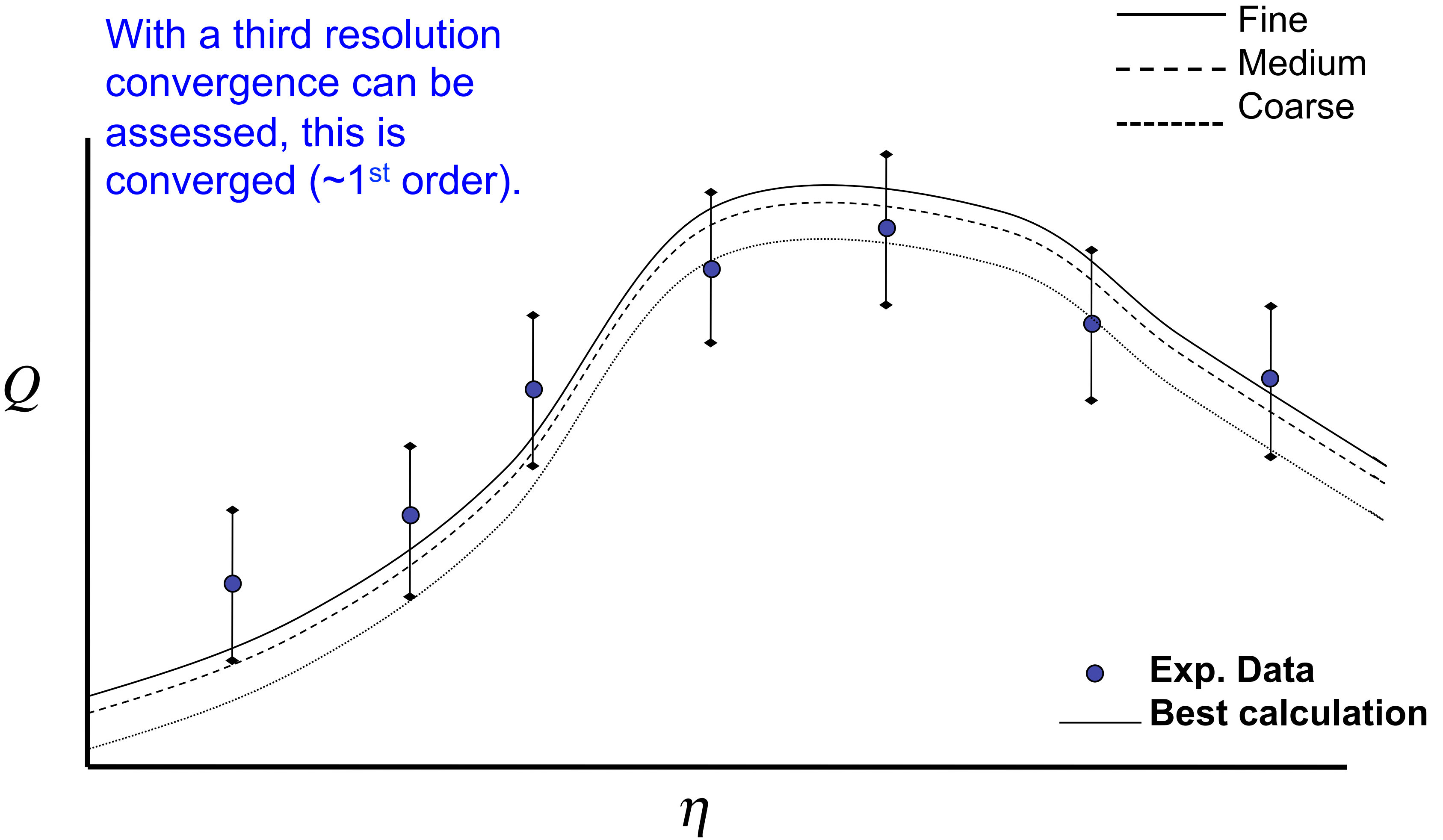
Solution Verification for DUMMIES

A poor man's method of Solution verification:
(With mesh doubling)
Equally spaced lines implies zeroth order
Factor of two decrease implies first order
Factor of four decrease implies second order

This is solution verification despite the "bad" results

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

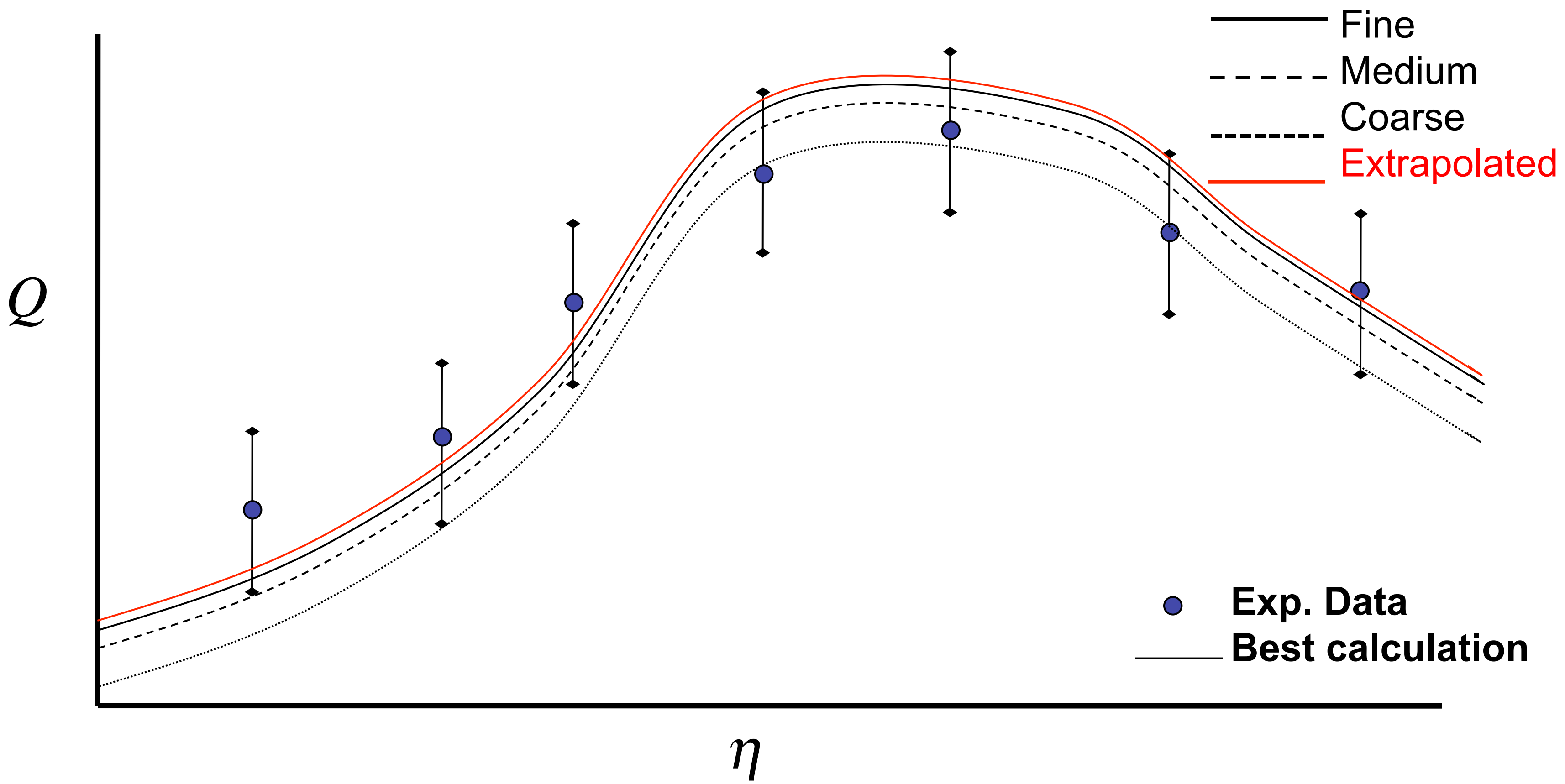
With a third resolution convergence can be assessed, this is converged (~1st order).



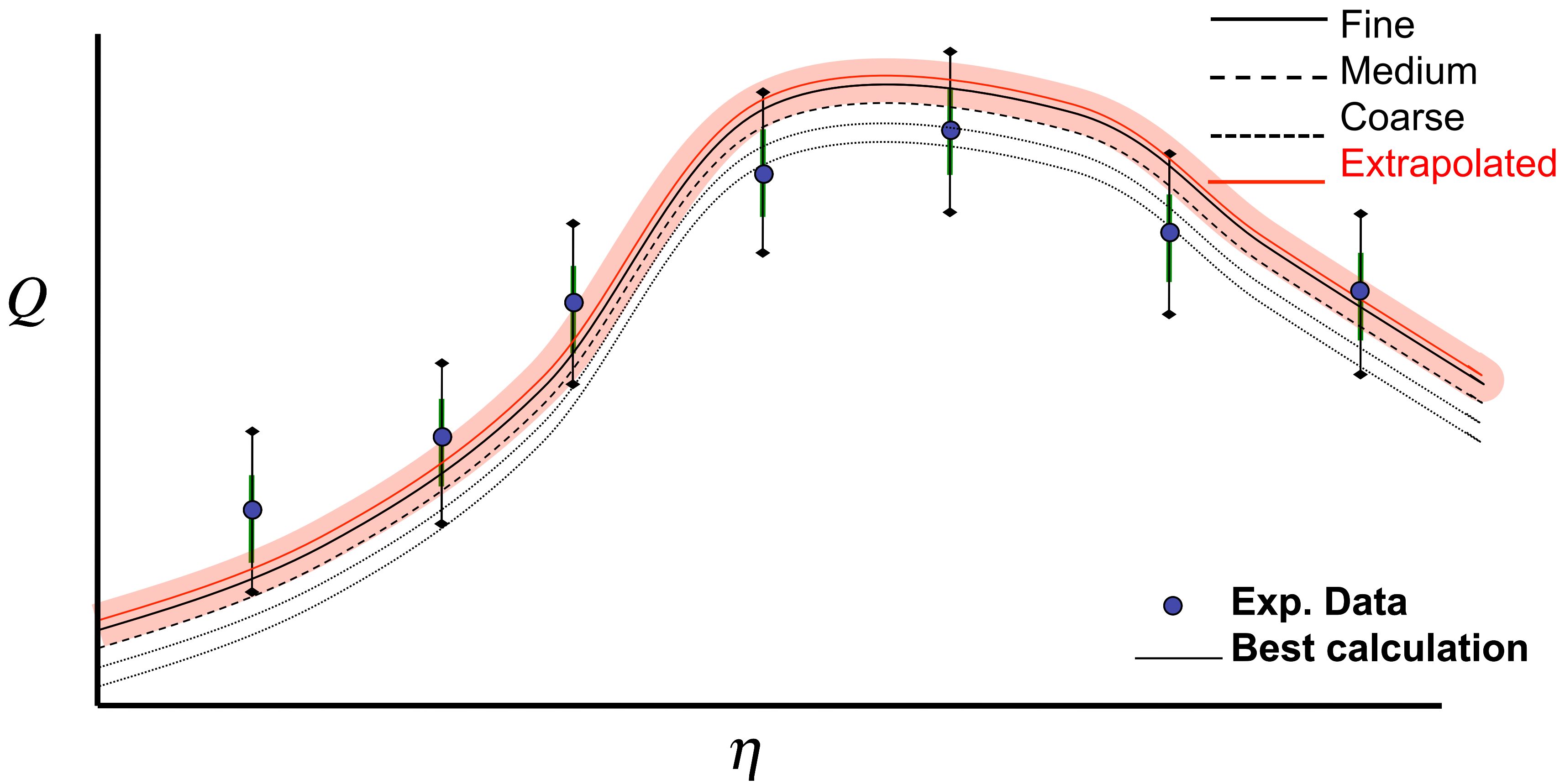
It is absolutely essential that the quantity "Q"be something that can reasonably be expected to converge numerically.

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

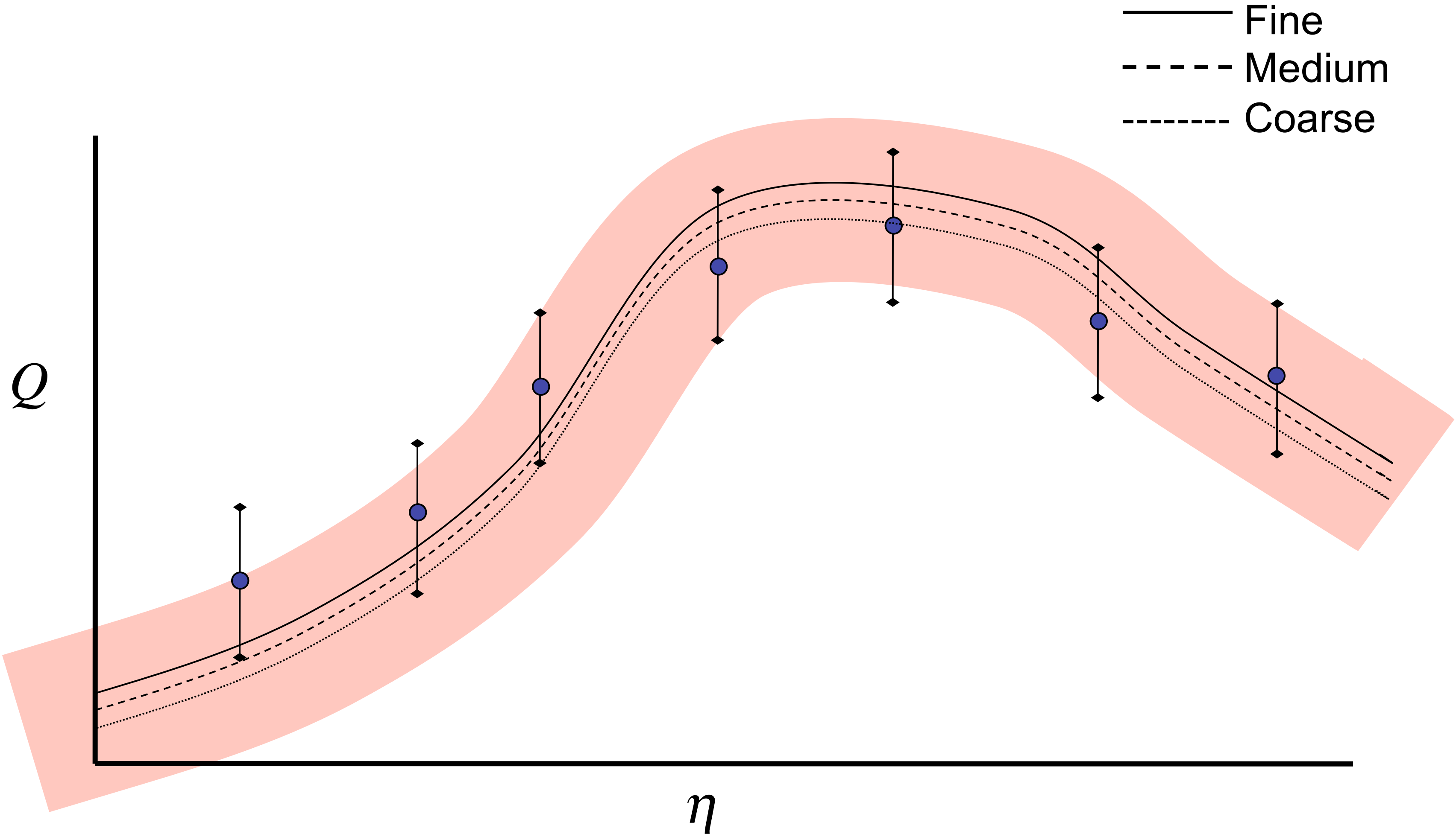
With three grids plus a convergence rate a converged solution can estimated.



Where we are going…
Using this information a numerical "error bar" can be derived with reasonable rigor.



Here is the notional non-convergent case again.



We want to be able to produce justifiable estimates even in bad cases!

“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

Code Verification vs. *Solution* Verification

Code Verification:

- You have an exact solution, so you compute exact errors
- You are testing your code (implementation, algorithm)
- Hard estimates of convergence properties
- Metrics are defined by numerical analysis
- **Convergence 1st**
- **Errors 2nd**

Solution Verification:

- You don't have an exact solution, you estimate numerical errors
- You test your solution(s)
- Soft estimates of numerical error
- **Metrics are defined by the analyst** – integrated quantities, point values, functionals of the solution
- **Error 1st**
- **Convergence 2nd**

Verification and numerical analysis are intimately and completely linked.

- The results that verification must produce are defined by the formal analysis of the methods being verified.
- The numerical analysis results are typically (always) defined in the asymptotic range of convergence for a method.
    - This range is reached as the discretization parameter (mesh, time step, angle, etc.) becomes "small" i.e., asymptotically "*close to zero*".
- Practically, the asymptotic range is rarely achieved by verification practitioners in meaningful simulations.
- Hence verification is not generally practiced where it is formally valid!

This is probably the best thing…

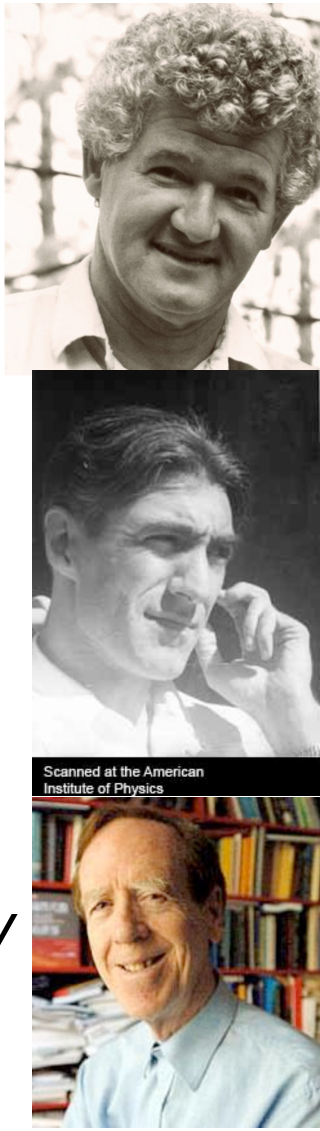
Perhaps we should just rid ourselves of some of the confusion by renaming calculation or solution verification to "**numerical error estimation**" because that is the point of it and it avoids a lot of confusion.

Theory is absolutely essential to the conduct of verification.

- The fundamental theorem of numerical analysis defined by Lax and Richtmyer (similar theorem by Dahlquist for ODEs, but it also applies to nonlinear equations!),

A numerical method for a linear differential equation will converge if that method is consistent and stable. Comm. Pure. Appl. Math. 1954

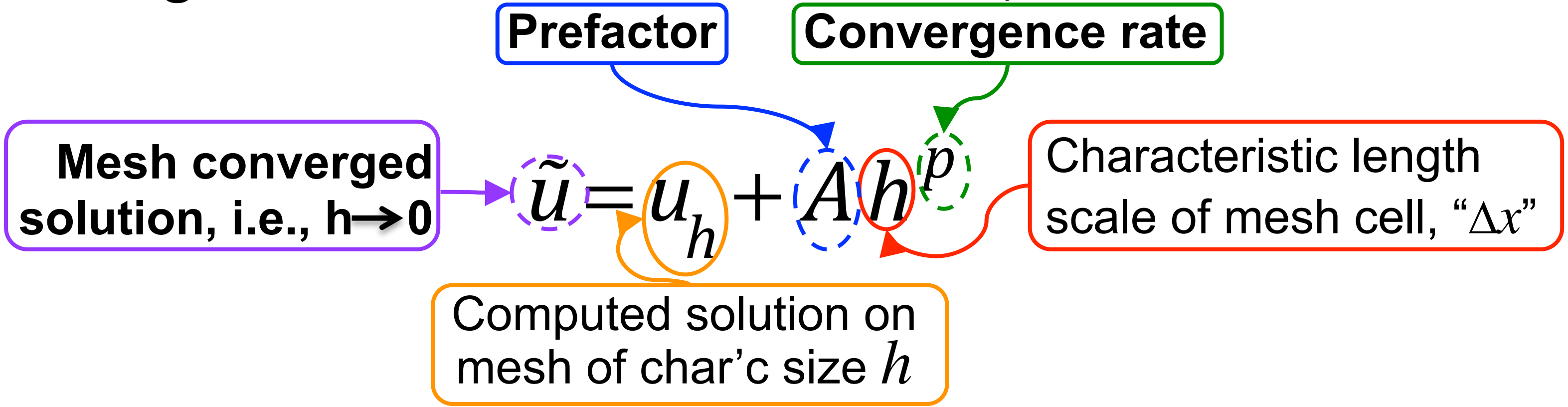
Restated by Strang - *The fundamental theorem of numerical analysis, The combination of consistency and stability is equivalent to convergence.*



Scanned at the American Institute of Physics

The Standard Setting For Calculation Verification: Richardson extrapolation for error estimation

- We begin with the standard error form,



Prefactor

Convergence rate

Mesh converged solution, i.e., h→0

$$\tilde{u} = u_h + A h^p$$

Characteristic length scale of mesh cell, “Δx”

Computed solution on mesh of char’c size h

- The standard safety factor gives an uncertainty estimate (the *GCI**):

$$\delta = \tilde{u} - u_f \qquad U_{num} = F_s \left|\delta\right|; F_s = 1.25$$

- This safety factor gives an ostensible 95% confidence interval,
  - ~2 std. dev. from CFD “experience” and computational experiments.
- Other forms will provide different estimates of F_s.
- For two grids, no estimate for δ is possible, and the uncertainty is intentionally “generous”: $U_{num} = F_s \left|u_f - u_c\right|; F_s = 3$

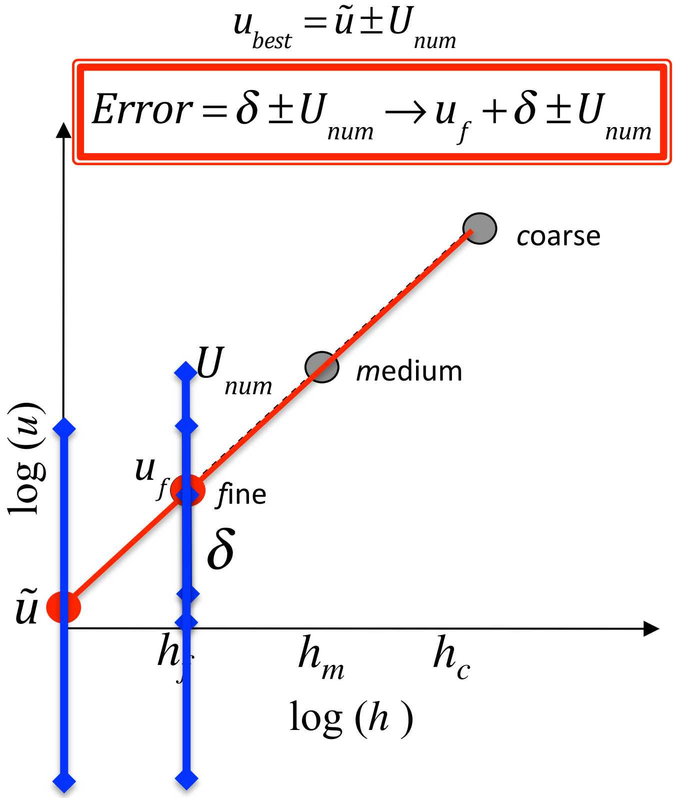
*** GCI: Grid Convergence Index, i.e., Roache’s approach**

Error bars are subject to interpretation

$$\delta = \tilde{u} - u_f \qquad U_{num} = F_s \left|\delta\right|; F_s = 1.25$$

Where should the error bar be placed (i.e., centered)?

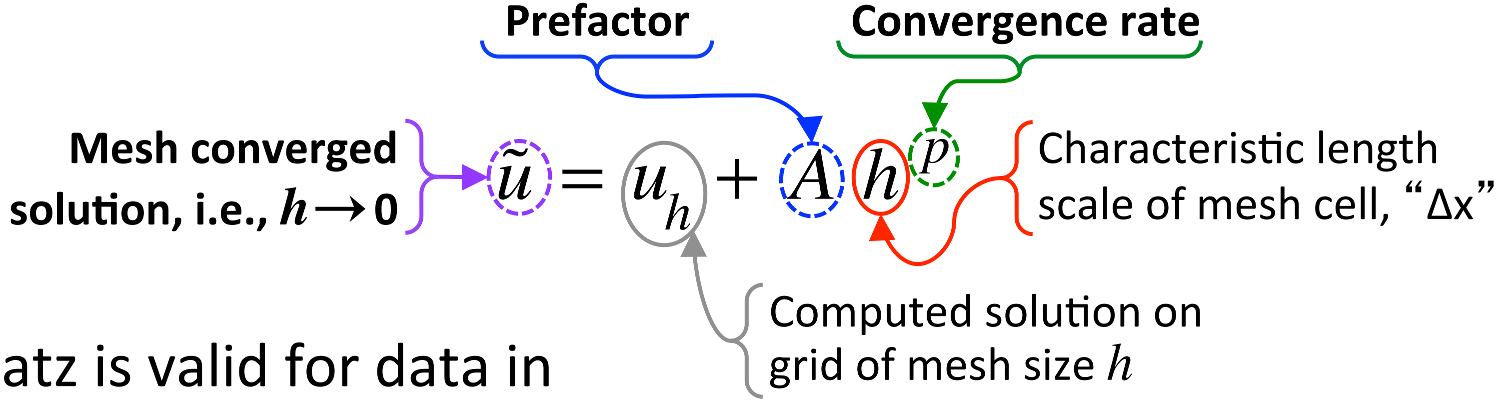
- We have choices (two examined here):
  - Around the finest grid solution
  - Around the mesh converged solution
  - **The mesh converged solution is a best estimate and should define error.**
  - Error on the fine grid “should” be asymmetric.
  - The difference is significant



$$u_{best} = \tilde{u} \pm U_{num}$$

$$\boxed{Error = \delta \pm U_{num} \rightarrow u_f + \delta \pm U_{num}}$$

There are some potential dangers to conscientiously avoid.



Prefactor

Convergence rate

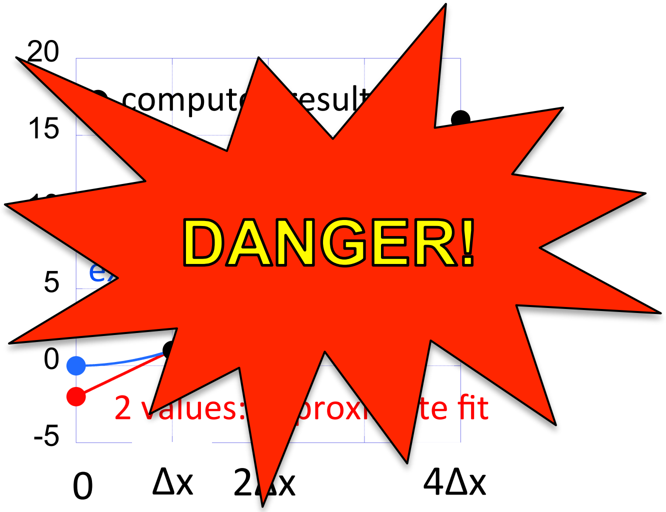
Mesh converged solution, i.e., $h \to 0$

$$\tilde{u} = u_h + A h^p$$

Characteristic length scale of mesh cell, "Δx"

Computed solution on grid of mesh size h

- This ansatz is valid for data in the asymptotic range of convergence.
  - Usually, we <u>assume</u> that the calculations are in the asymptotic range of convergence.
  - With two calculations, we have an under-determined fit through the results ( ).
  - With many calculations, the error ansatz is fully determined or over-determined; one can perform a **regression** fit.



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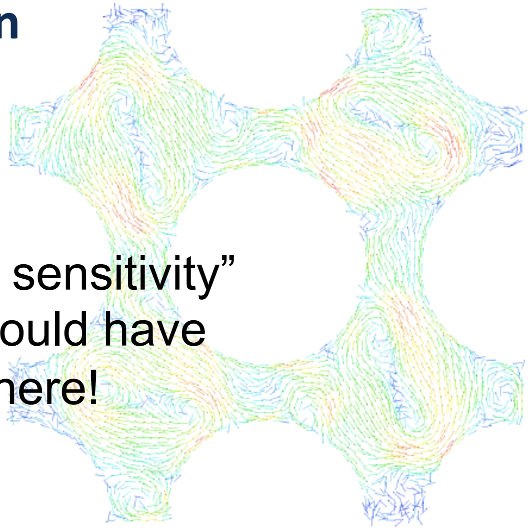
*P. Roache, *Verification and Validation in Computational Science and Engineering*, Hermosa Publishing (1996).

An example of how verification can go "off the rails"

Preliminary Verification Results for CFD* for a CASL challenge problem (GTRF) with Fuego and Drekar (Δp), just spatial resolution

# ele.	Mesh	Fuego	Drekar
664K	Coarse	31.8 kPa	26.7 kPa
1224K	Medium	24.6 kPa	23.8 kPa
1934K	Fine	24.4 kPa	22.0 kPa

A "mesh sensitivity" study would have us stop here!



Fuego

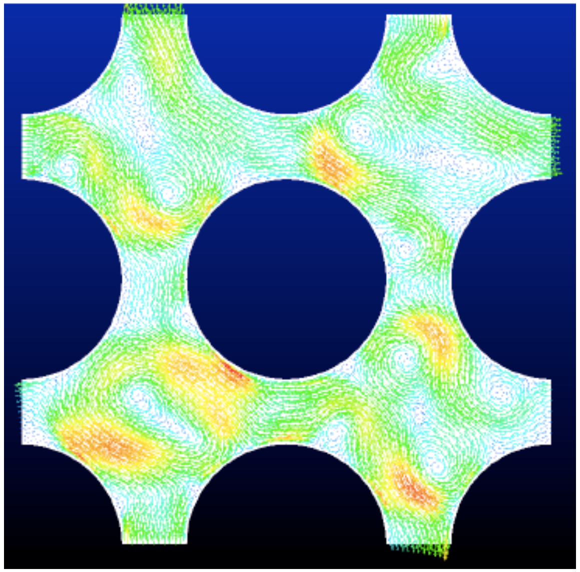
$$\Delta p(h) = 24340 + 26.6h$$

15.85!!

95 % Error Bound 80Pa (Roache, GCI) to 18.6kPa (Stern)

Drekar

$$\Delta p(h) = 17420 + 16370h^{1.234}$$



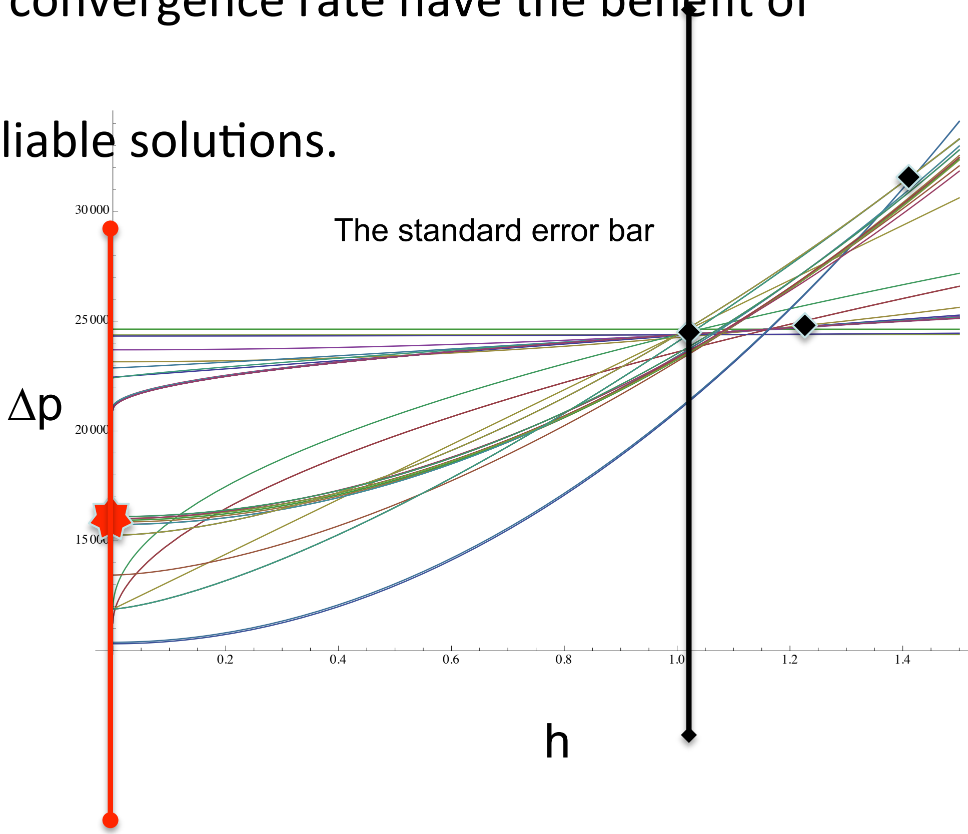
The Fuego result exemplifies one of the problems with the standard setting, 16th order convergence is absurd!

Preview: Our procedure gives *a Δp=16.1kPa ±13.5kPa.*

***CASL: Consortium for the Advanced Simulation of Light Water Reactors,** CFD: computational fluid dynamics
GTRF: Grid-to-rod-fretting

This is a good place to dig a bit deeper on why verification analyses can go so very, very wrong.

- The data in this study is poorly conditioned: the grids are too close in resolution, and far from the asymptotic range.
  - **The super-high convergence rate is not ruled out, but could be.** The use of constraints on the solution for the convergence rate have the benefit of avoiding such *absurd* outcomes.
- Such poor conditioning produces unreliable solutions.
- **Once constraints are added to the problem, the solution no longer is unique. The norm that is minimized to obtain the solution changes the solution significantly.**
- Introducing these changes across a set of norms gives a diversity of results that requires a rethink of how such analysis is conducted.



Judge a man by his questions, rather than his answers.
- Voltaire

Frameworks for discussing modeling and simulation quality are essential.

- Without a framework to guide, the entire process tends to fall to conventional emphases.
  - In T-H this becomes modeling and “validation(calibration)”
- We can look at a couple of frameworks as archetypical:
  - CSAU: Code Scaling, Applicability and Uncertainty
  - PCMM: Predictive Capability Maturity Model
- One is the template for how the nuclear reactor community views M&S, and the other came from the nuclear weapons’ community.
- Both of these are incomplete and generally inadequate for moving forward.

PCMM: Predictive Capability Maturity Model

- Developed at Sandia National Lab for the DOE Advanced Simulation and Computing (ASC) program as a means of assessing the completeness of the modeling and simulation activities
- It had a focus that was necessarily nuclear weapons and Sandia-mission focused.
  - We have begun applying it to NE applications through the CASL program
- In broad brushes the basic precepts of PCMM apply to a much broader range of M&S activities.
- It needs to be extended and improved to provide a more complete framework.

Predictive Capability Maturity Model (PCMM)

Sandia National Laboratories

Increasing completeness and rigor

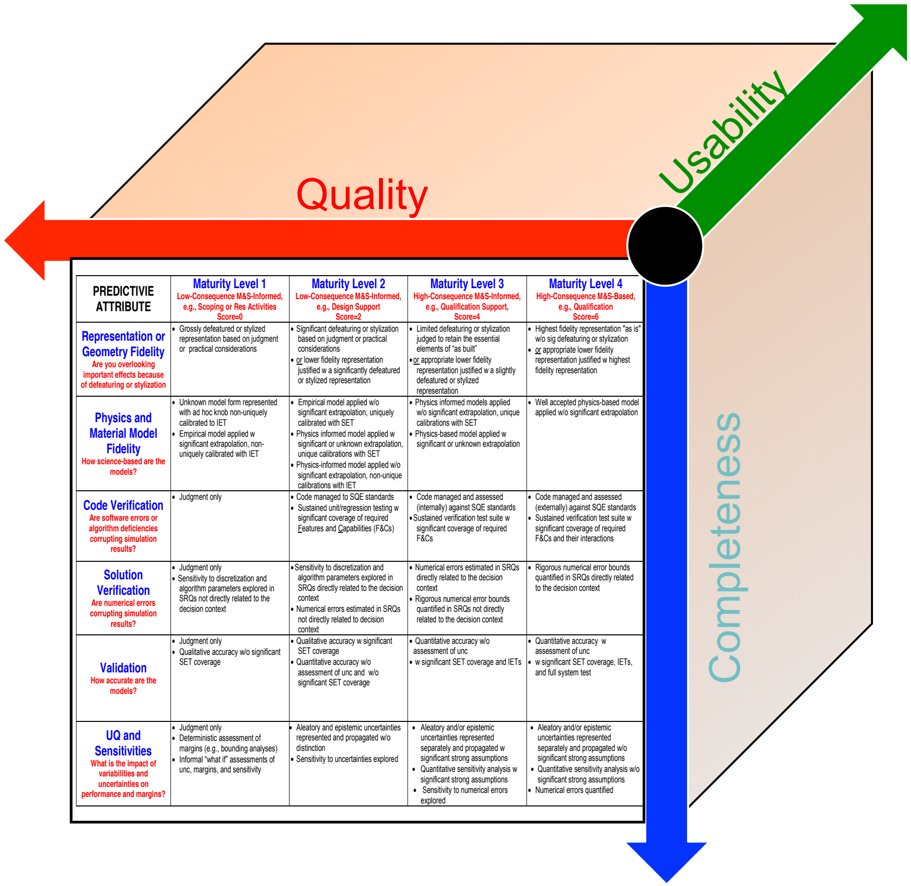
Decreasing risk

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

SAND2007-5948

Rethinking the framework*



PREDICTIVIE ATTRIBUTE	Maturity Level 1 Low-Consequence M&S-Informed, e.g., Scoping or Res Activities Score=0	Maturity Level 2 Low-Consequence M&S-Informed, e.g., Design Support Score=2	Maturity Level 3 High-Consequence M&S-Informed, e.g., Qualification Support, Score=4	Maturity Level 4 High-Consequence M&S-Based, e.g., Qualification Score=6
Representation or Geometry Fidelity Are you overlooking important effects because of defeaturing or stylization	• Grossly defeatured or stylized representation based on judgment or practical considerations	• Significant defeaturing or stylization based on judgment or practical considerations • or lower fidelity representation justified w a significantly defeatured or stylized representation	• Limited defeaturing or stylization judged to retain the essential elements of "as built" • or appropriate lower fidelity representation justified w a slightly defeatured or stylized representation	• Highest fidelity representation "as is" w/o sig defeaturing or stylization • or appropriate lower fidelity representation justified w highest fidelity representation
Physics and Material Model Fidelity How science-based are the models?	• Unknown model form represented with ad hoc knob non-uniquely calibrated to IET • Empirical model applied w significant extrapolation, non-uniquely calibrated with IET	• Empirical model applied w/o significant extrapolation, uniquely calibrated with SET • Physics informed model applied w significant or unknown extrapolation, unique calibrations with SET • Physics-informed model applied w/o significant extrapolation, non-unique calibrations with IET	• Physics informed models applied w/o significant extrapolation, unique calibrations with SET • Physics-based model applied w significant or unknown extrapolation	• Well accepted physics-based model applied w/o significant extrapolation
Code Verification Are software errors or algorithm deficiencies corrupting simulation results?	• Judgment only	• Code managed to SQE standards • Sustained unit/regression testing w significant coverage of required Features and Capabilities (F&Cs)	• Code managed and assessed (internally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs	• Code managed and assessed (externally) against SQE standards • Sustained verification test suite w significant coverage of required F&Cs and their interactions
Solution Verification Are numerical errors corrupting simulation results?	• Judgment only • Sensitivity to discretization and algorithm parameters explored in SRQs not directly related to the decision context	• Sensitivity to discretization and algorithm parameters explored in SRQs directly related to the decision context • Numerical errors estimated in SRQs not directly related to decision context	• Numerical errors estimated in SRQs directly related to the decision context • Rigorous numerical error bounds quantified in SRQs not directly related to the decision context	• Rigorous numerical error bounds quantified in SRQs directly related to the decision context
Validation How accurate are the models?	• Judgment only • Qualitative accuracy w/o significant SET coverage	• Qualitative accuracy w significant SET coverage • Quantitative accuracy w/o assessment of unc and w/o significant SET coverage	• Quantitative accuracy w/o assessment of unc • w significant SET coverage and IETs	• Quantitative accuracy w assessment of unc • w significant SET coverage, IETs, and full system test
UQ and Sensitivities What is the impact of variabilities and uncertainties on performance and margins?	• Judgment only • Deterministic assessment of margins (e.g., bounding analyses) • Informal "what if" assessments of unc, margins, and sensitivity	• Aleatory and epistemic uncertainties represented and propagated w/o distinction • Sensitivity to uncertainties explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w significant strong assumptions • Quantitative sensitivity analysis w significant strong assumptions • Sensitivity to numerical errors explored	• Aleatory and/or epistemic uncertainties represented separately and propagated w/o significant strong assumptions • Quantitative sensitivity analysis w/o significant strong assumptions • Numerical errors quantified

- Completeness (predictive) – whether all the necessary concepts & activities enter into the simulation?
- Quality (rigor) – How good the work and evidence is for each area?
- Usability (pervasive) – how useful and usable is each activity is including the impact of the user and simulation customer?

PCMM : How to make it less complex

Idea 1: Foundational/application specific

Idea 2: verification/validation

Idea 3: Completeness, Quality, Usability

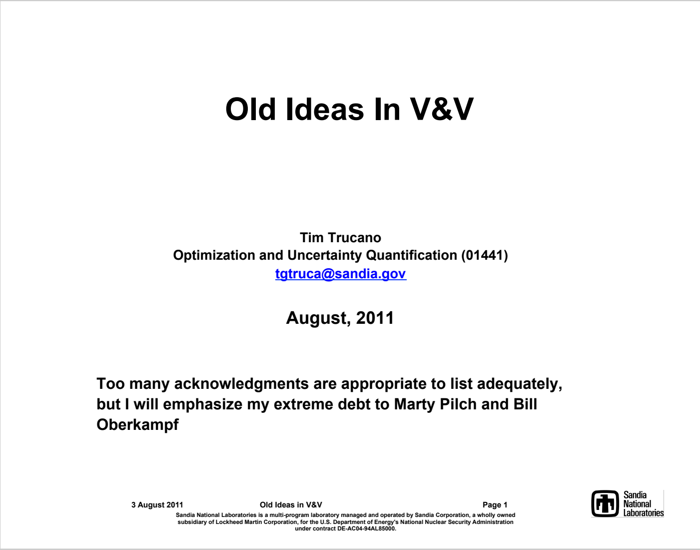
Idea 4: Rigor, Predictive, Pervasive

“Questions are infinitely Superior to answers.”

–Dan Sullivan

Tim Trucano’s (one of the father’s of V&V theory) observations on V&V…

- Key V&V themes have not changed “for decades”:
  - “Codes are not solutions, people are solutions.”
  - “Credibility of computational simulations for defined applications is evolutionary…”
  - “… at worst, credibility is non-existent in specific applications.”
  - “Single calculations will never be ‘the right answer’ for hard problems.”
  - **“Real V&V and real UQ are a lot of work.”**



Old Ideas In V&V

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August, 2011

Too many acknowledgments are appropriate to list adequately, but I will emphasize my extreme debt to Marty Pilch and Bill Oberkampf

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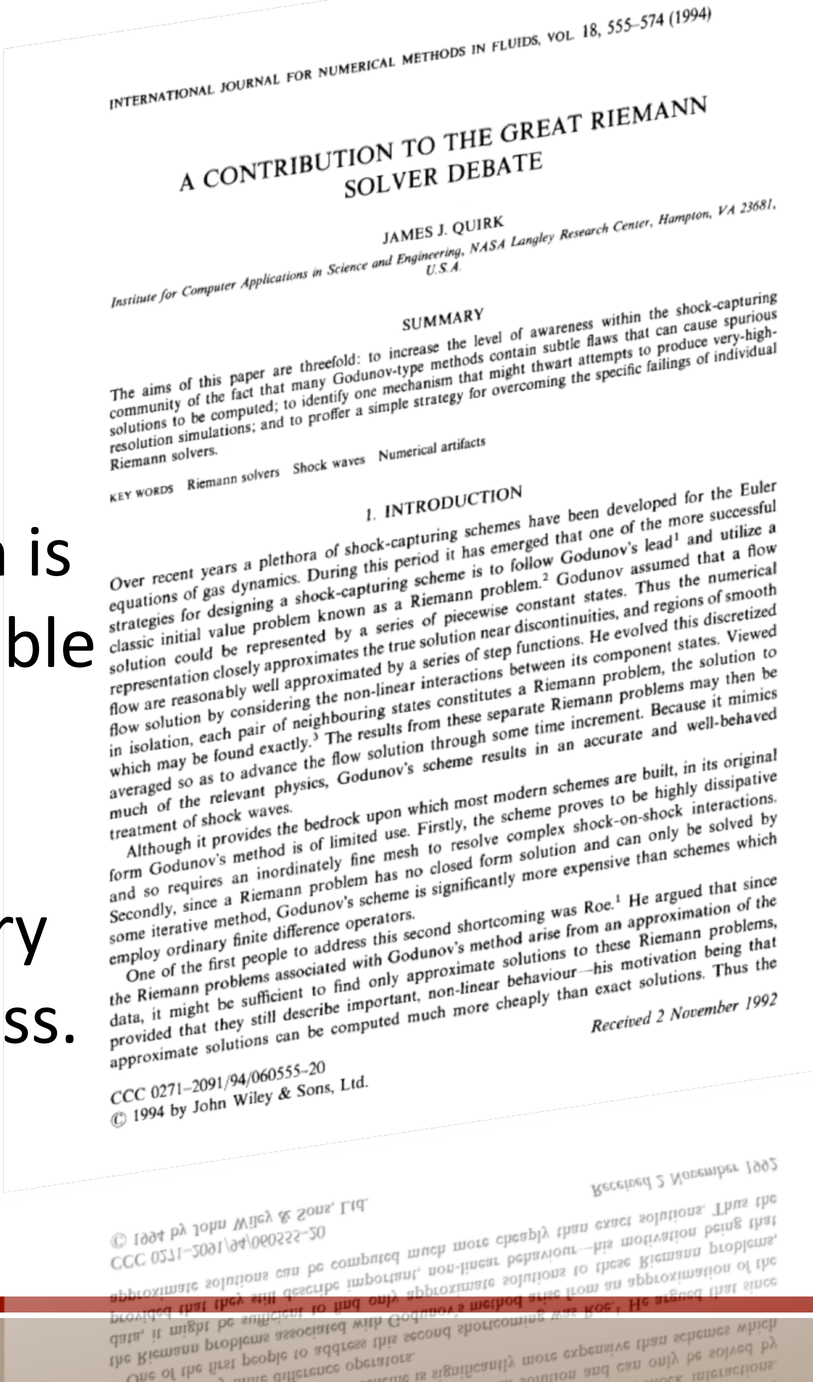
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

- Trucano’s four insights on V&V:

1. “V&V — pay me now or pay me later.”
2. **“Journal editorial policies and practices must change.”**
3. “Ask ‘What’s good enough?’”
4. **“Saying you don’t need verification is like saying you don’t need oxygen.”**

Failures and mistakes are rarely published

- This isn’t just a problem of statistically based criteria for significance.
- An important aspect of research is the failure of otherwise reasonable and seemingly good ideas.
- When reports of failures are published, the paper is often very good. These papers seed progress. We need more of these.



INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 18, 555–574 (1994)

A CONTRIBUTION TO THE GREAT RIEMANN SOLVER DEBATE

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SUMMARY

The aims of this paper are threefold: to increase the level of awareness within the shock-capturing community of the fact that many Godunov-type methods contain subtle flaws that can cause spurious solutions to be computed; to identify one mechanism that might thwart attempts to produce very-high-resolution simulations; and to proffer a simple strategy for overcoming the specific failings of individual Riemann solvers.

KEY WORDS Riemann solvers Shock waves Numerical artifacts

1. INTRODUCTION

Over recent years a plethora of shock-capturing schemes have been developed for the Euler equations of gas dynamics. During this period it has emerged that one of the more successful strategies for designing a shock-capturing scheme is to follow Godunov's lead[1] and utilize a classic initial value problem known as a Riemann problem.[2] Godunov assumed that a flow solution could be represented by a series of piecewise constant states. Thus the numerical representation closely approximates the true solution near discontinuities, and regions of smooth flow are reasonably well approximated by a series of step functions. He evolved this discretized flow solution by considering the non-linear interactions between its component states. Viewed in isolation, each pair of neighbouring states constitutes a Riemann problem, the solution to which may be found exactly.[3] The results from these separate Riemann problems may then be averaged so as to advance the flow solution through some time increment. Because it mimics much of the relevant physics, Godunov's scheme results in an accurate and well-behaved treatment of shock waves.

Although it provides the bedrock upon which most modern schemes are built, in its original form Godunov's method is of limited use. Firstly, the scheme proves to be highly dissipative and so requires an inordinately fine mesh to resolve complex shock-on-shock interactions. Secondly, since a Riemann problem has no closed form solution and can only be solved by some iterative method, Godunov's scheme is significantly more expensive than schemes which employ ordinary finite difference operators.

One of the first people to address this second shortcoming was Roe.[1] He argued that since the Riemann problems associated with Godunov's method arise from an approximation of the data, it might be sufficient to find only approximate solutions to these Riemann problems, provided that they still describe important, non-linear behaviour—his motivation being that approximate solutions can be computed much more cheaply than exact solutions. Thus the

CCC 0271–2091/94/060555–20
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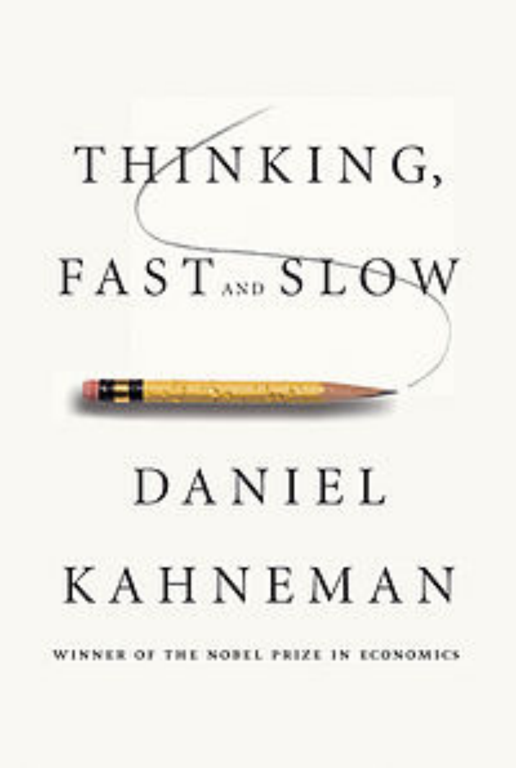
Received 2 November 1992

What Determines Quantity of Simulations (or Calculations) i.e. is it Good? Or Bad?

- The answer to the question is that it is still quite subjective, but…
- … it is becoming more evidence based.
- This is largely a function of where you do your work,
  - In academic/physics settings it is dominantly expert based (i.e., more subjective), but change is happening.
  - In engineering, it has become more evidence based.
  - Is mathematics becoming more evidence based?
  - Demands on modeling & simulation from society (legal issues) are pushing the community toward a greater reliance on evidence based criteria.

What Determines Quantity of Simulations (or Calculations) i.e., is it Good? Or Bad?

- In a nutshell, the current criteria is largely subjective,
  - In other words “expert” based.
  - I think the future criteria will still be expert-based
- Various programs are helping to add evidence to the judgments regarding calculation quality.
- Professional societies and publications have an uneven role to play in moving the criteria forward
  - Engineering societies and journals (ASME) have a more evidence based determination of quality
  - Physics/hard sciences are more expert based in the determination of quality
  - What about mathematics?



How much of our strategy is based on sunk cost?
What would a clean sheet strategy be?

Rather than consider the odds that an incremental investment would produce a positive return, people tend to "throw good money after bad" and continue investing in projects with poor prospects that have already consumed significant resources. In part this is to avoid feelings of regret.[3]

“The validated and verified ASCI codes will eventually become the *production codes of the future* as such they will eventually transition to the custody of Stockpile Computing.”
–1998 **Strategic Computing & Simulation Validation & Verification Program**

“Production Codes == Legacy Codes”

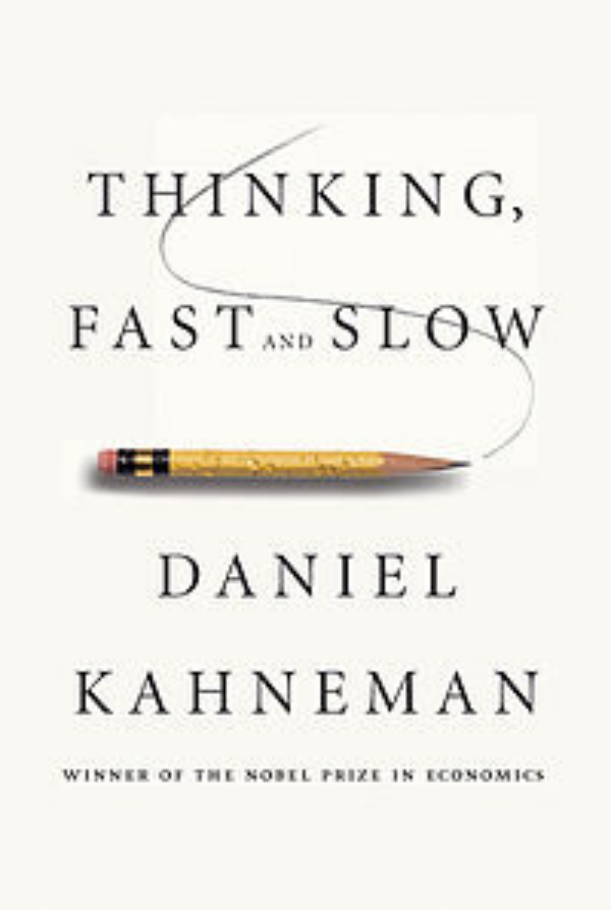
Close your eyes…

What code produced that movie in your head?

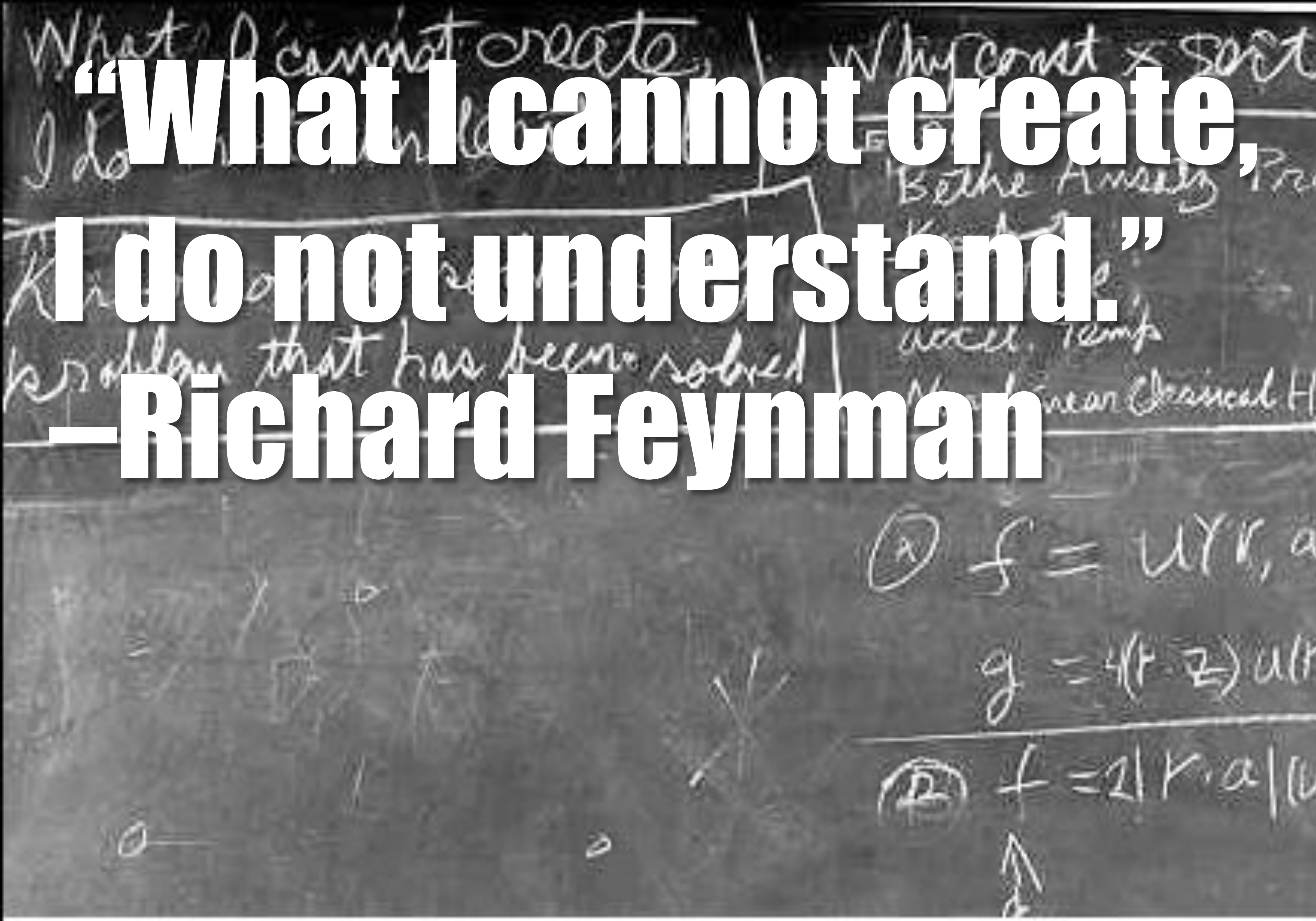
How does this bias your perceptions of what a different code might produce?

Do existing codes form an anchor bias for how solutions should look? Does this cause a resistance to change?

Anchoring or focalism is cognitive bias that describes the common human tendency to *rely* too heavily on the first piece of information offered (the "anchor") when making decisions. During decision making, anchoring occurs when individuals use an initial piece of information to make subsequent judgments.



“An important step in V&V will be detailed comparisons between various codes to ensure that the new ASCI level codes can faithfully reproduce the results of previous legacy codes in their domain of validity or trust.”–1998 **Strategic Computing & Simulation Validation & Verification Program**



“What I cannot create, I do not understand.”

–Richard Feynman

“Any sufficiently advanced technology is indistinguishable from magic.”
– Arthur C. Clarke

Technical debt a term invented by Ward Cunningham

*Our shock codes are 25 and 30 years old, the code base contains ideas that are 4 or 5 generations behind. This will become an even bigger issue with the next generation of hardware. This is **technical debt** in the classical sense.*

Scott Wood suggested "**Technical Inflation** could be viewed as the ground lost when the current level of technology surpasses that of the foundation of your product. All our codes suffer from this.

*Our production codes are the archetypes for **technical inflation** this includes CTH & ALEGRA. e.g., CTH could have used PPM, but didn't for hardware reasons that are no longer valid. As I will show you, it costs them a factor of two in mesh (probably ALEGRA too).*

The origin of numerical hydro is a relevant and keen example of technical inflation. Richtmyer and Von Neumann developed their method between 1948 and 1950.

In Los Alamos (!), Lax developed a different methodology starting in 1951 and 1952. The methodology and theory developed by Lax dominates compressible hydro world wide and has little impact on our codes today.

In two years technical inflation overtook us from our own backyard!

ASC Road Map, SAND 2006-7535 P

- Legacy code: Application codes that existed prior to the start of the ASC Program, before 1995. In many cases, Legacy codes are no longer being actively developed.

- Modern code: Application codes first developed under the ASC Program, starting after 1995. Some codes that would have been classified as Legacy codes have been significantly redesigned under the ASC Program and are therefore classified as modern codes

Are these defintions fixed and immutable?

"Code written in the 1970's is the bane of modern programming. It even has a special name: legacy code. Legacy code is feared, poorly understood, and worried over; most software professionals try to avoid making its maintenance part of their careers...”

- J. A. Whittaker and J. M. Voas (2002), "50 Years of Software: Key Principles for Quality," IT Pro, Nov/Dec issue.

"Institutions will try to preserve the problem to which they are the solution.”
– Clay Shirky


IBM
System x3755


NASA
sgi
sgi

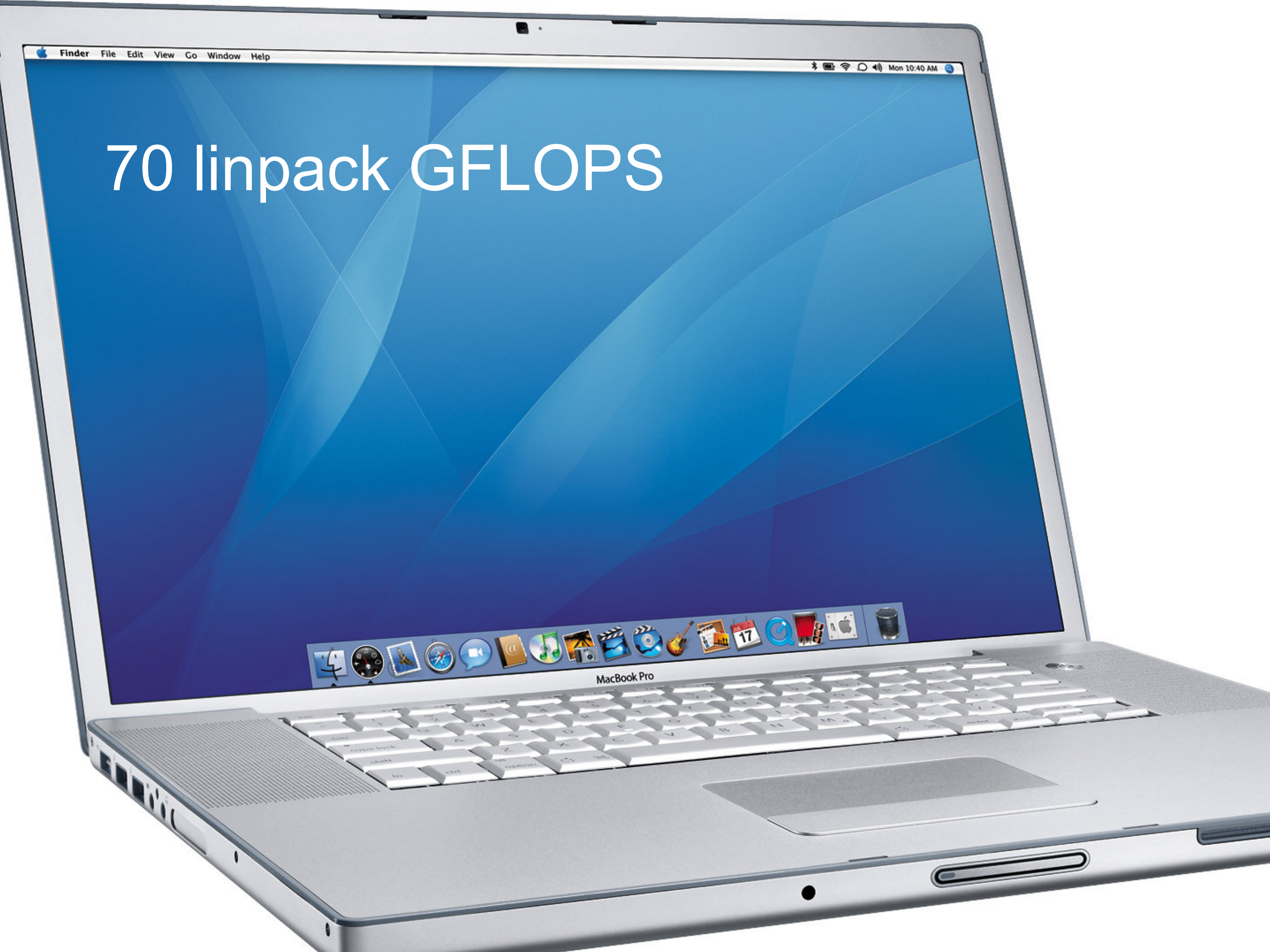

TITAN
CRAY

“There ain’t no such things as a free lunch”– Robert Heinlein

Approximately a Cray 2 via linpack

Approximately a Cray 2 via linpack

70 linpack GFLOPS



Mac Pro

The future of the pro desktop. Coming later this year.

Reputed to be ~7 TFLOPS

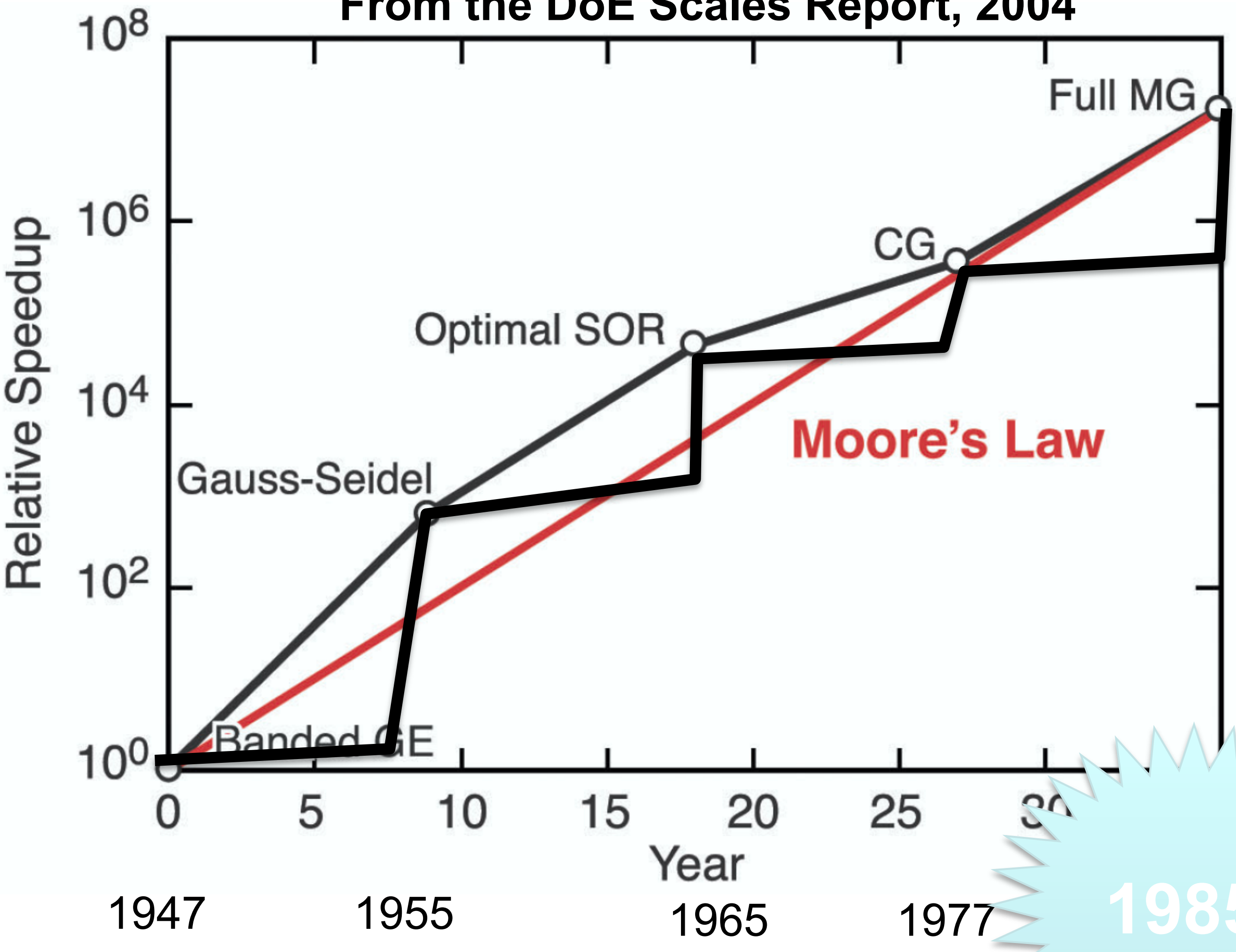
“The free lunch is over. Now welcome to the hardware jungle.”

– Herb Sutter

(http://herbsutter.com/welcome-to-the-jungle/)

Comparing performance improvements between hardware and algorithms.

From the DoE Scales Report, 2004



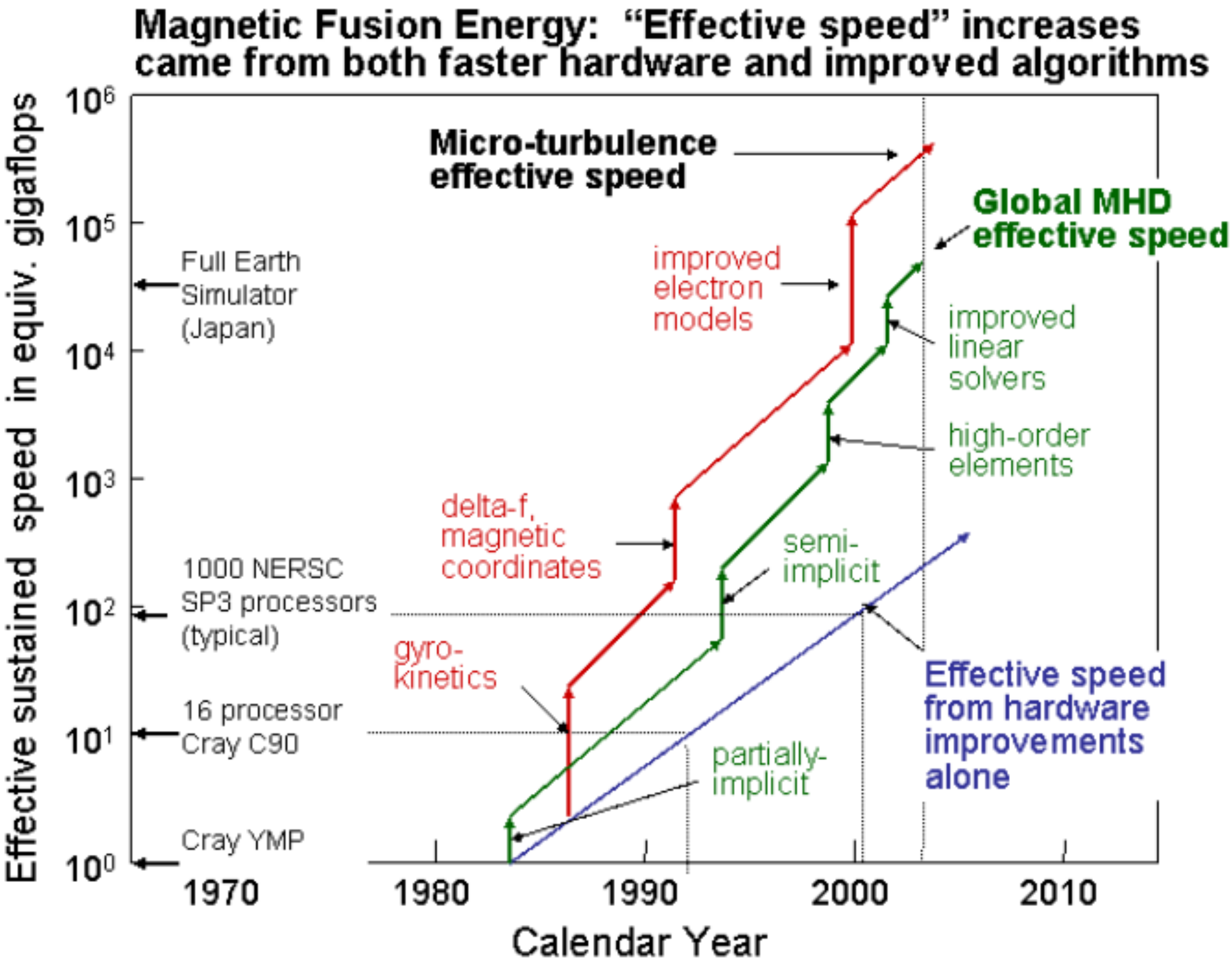
The jumps in performance are actually more discrete… “quantum”

We are *overdue* for a breakthough, but what will it be? sublinear? A nonlinear method for a linear problem, or maybe multigrid is it?

REPORT TO THE PRESIDENT AND CONGRESS DESIGNING A DIGITAL FUTURE: FEDERALLY FUNDED RESEARCH AND DEVELOPMENT IN NETWORKING AND INFORMATION TECHNOLOGY

"In the field of numerical algorithms, however, the improvement can be quantified. Here is just one example, provided by Professor Martin Grötschel of Konrad-Zuse-Zentrum für Informationstechnik Berlin. Grötschel, an expert in optimization, observes that a benchmark production planning model solved using linear programming would have taken 82 years to solve in 1988, using the computers and the linear programming algorithms of the day. Fifteen years later – in 2003 – this same model could be solved in roughly 1 minute, an improvement by a factor of roughly **43 million**. Of this, a factor of roughly **1,000 was due to increased processor speed**, whereas a factor of roughly **43,000 was due to improvements in algorithms!** Grötschel also cites an algorithmic improvement of roughly 30,000 for mixed integer programming between 1991 and 2008."

From the DoE Scales Report, 2004



“The fundamental law of computer science: As machines become more powerful, the efficiency of algorithms grows more important, not less.”

– Nick Trefethen

Algorithms and Methods (two kinds):

- Those that support the efficiency of solution, but don’t change the answer
  - linear algebra, sorting, data structures, domain decomposition,…
  - Often third party libraries

Those that change the answer: hydro, radiation, ODE solvers

Where have we invested? what is the right balance?

Discretization errors and modeling can look very much the same. In other words the error can look like (or be) a subgrid model competing with physics.

“If you are deliberately trying to create a future that feels safe, you will willfully ignore the future that is likely.”

— Seth Godin

Fin

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Twitter: @TotalFutbalNow

Blog: http://wjrider.wordpress.com
The Regularized Singularity

Who Am I ?

- I'm a staff member at Sandia, and I've been there SNL for 7 1/2 years. Prior to that I was at LANL for 18 years. I've worked in computational physics since 1992.
- 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.