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What Makes A Calculation Good? Or Bad?

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Sandia National Laboratories

Acknowledgements

- Tim Trucano, Marty Pilch, Jim Kamm, Randy Summers, Allen Robinson, Erik Strack, Greg Weirs, Jim Stewart, and Tony Guinta (SNL)
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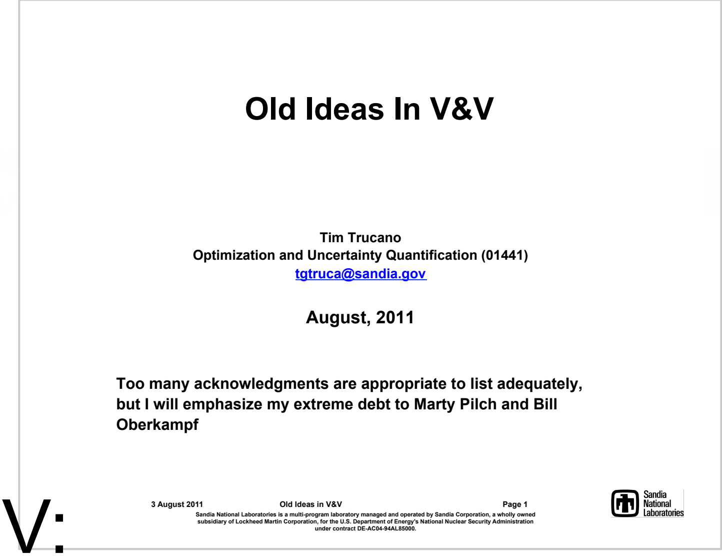
- Jim Fort (PNNL)
- Bill Oberkamf (SNL retired)
- Bart Smith (Utah State Univ.)
- Chris Roy (VTU)

Outline

- A cartoon picture of quality
- The impact of simulation on programs, the impact of programs on quality expectations
- A couple of examples from my own experience
- Where do we go from here?

Tim Trucano’s 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

Tim Trucano
Optimization and Uncertainty Quantification (01441)
tgtruca@sandia.gov

August, 2011

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

3 August 2011 Old Ideas in V&V Page 1

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- 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.”

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

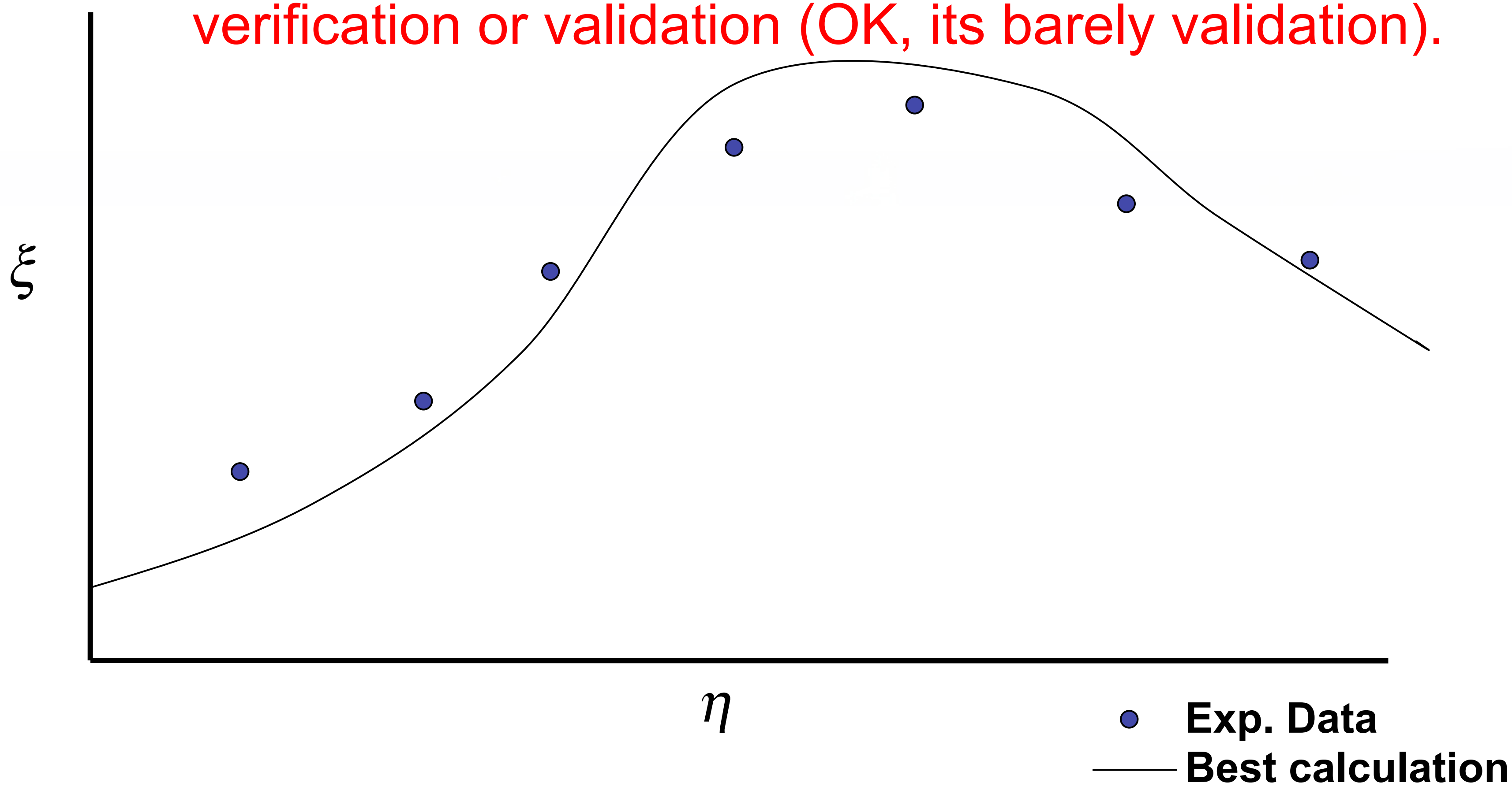
- Prudence
- Temperance
- Faith
- Hope
- Fortitude
- Justice
- Charity

Traditional “7 Cardinal Virtues”

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

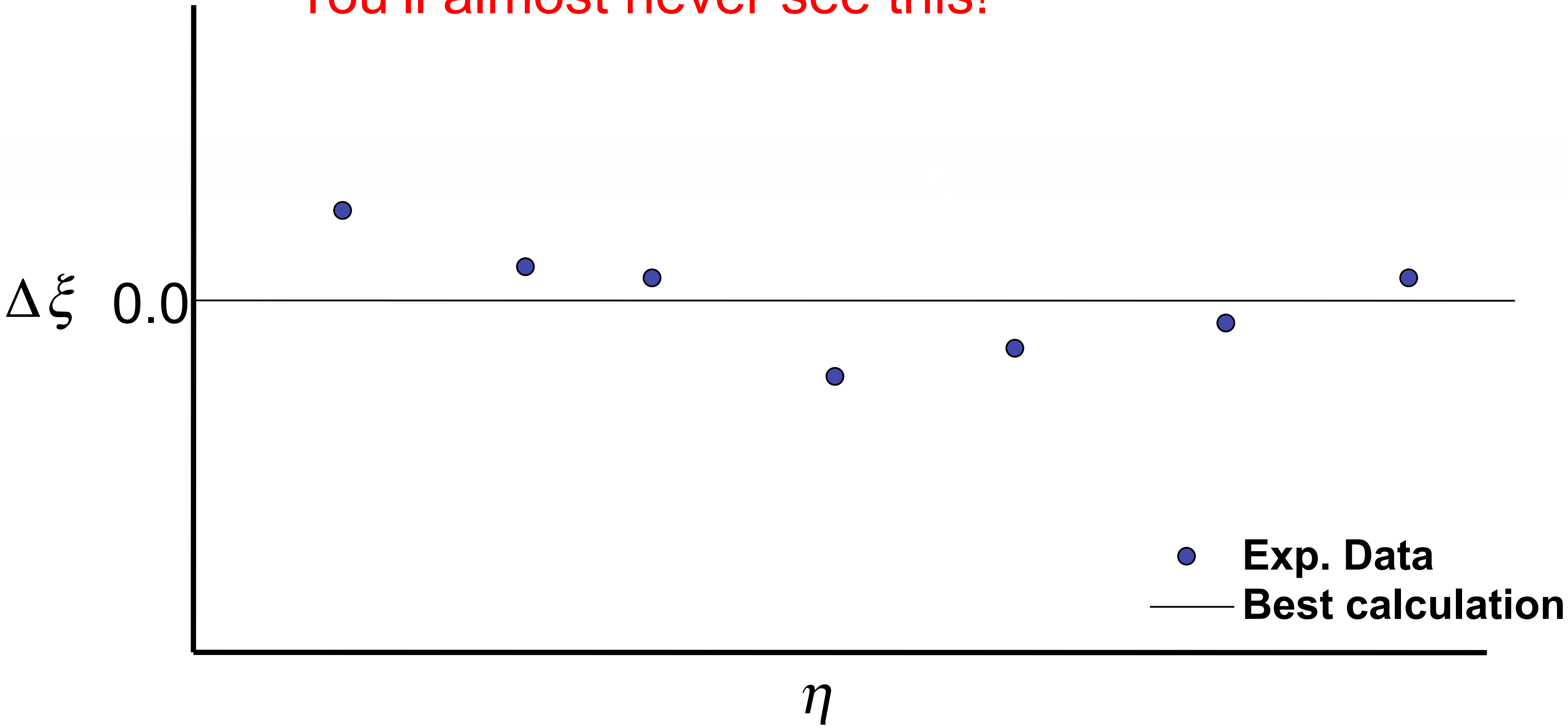
This is the way validation is usually presented in the literature.

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



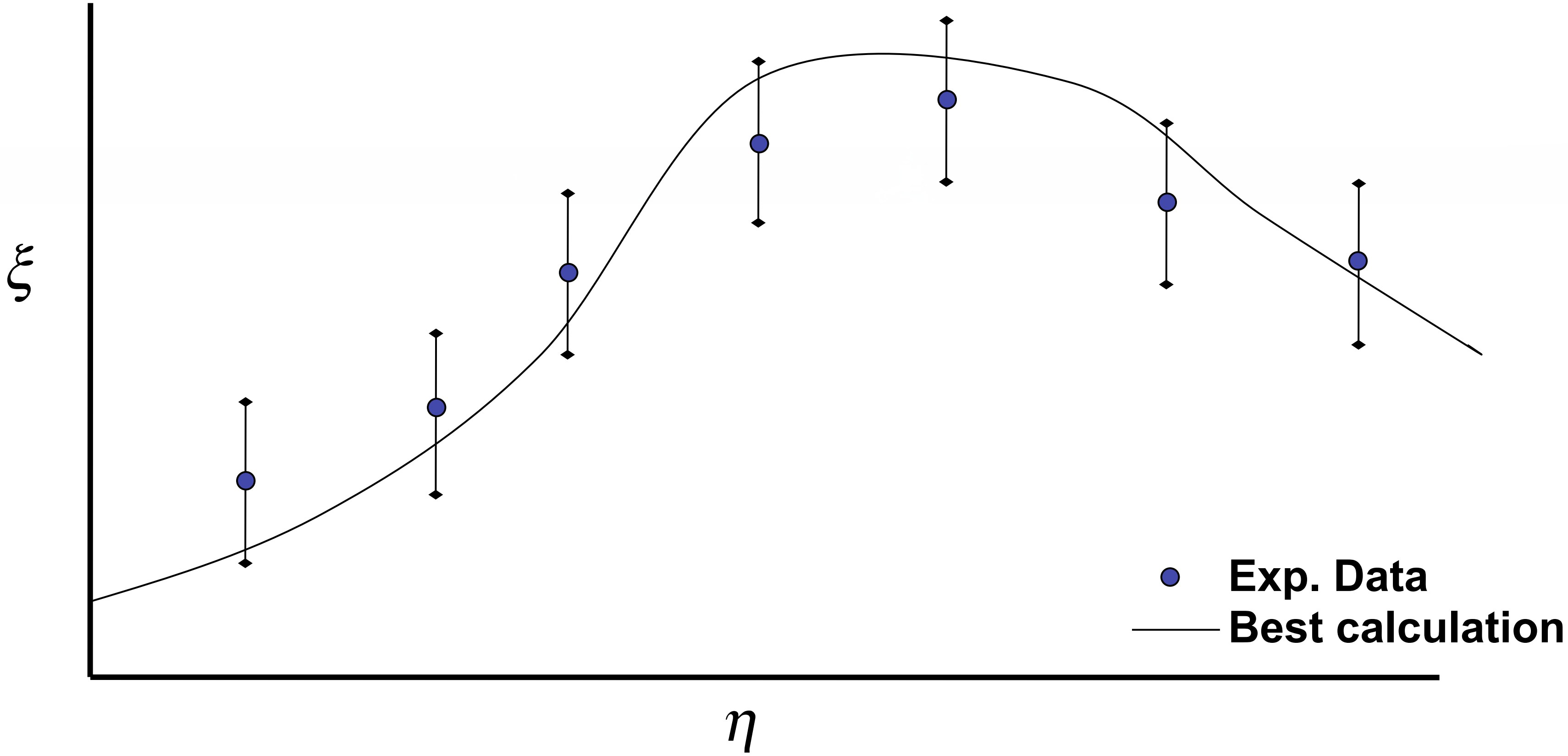
It might be even better if the figure was presented in terms of error too.

You’ll almost never see this!



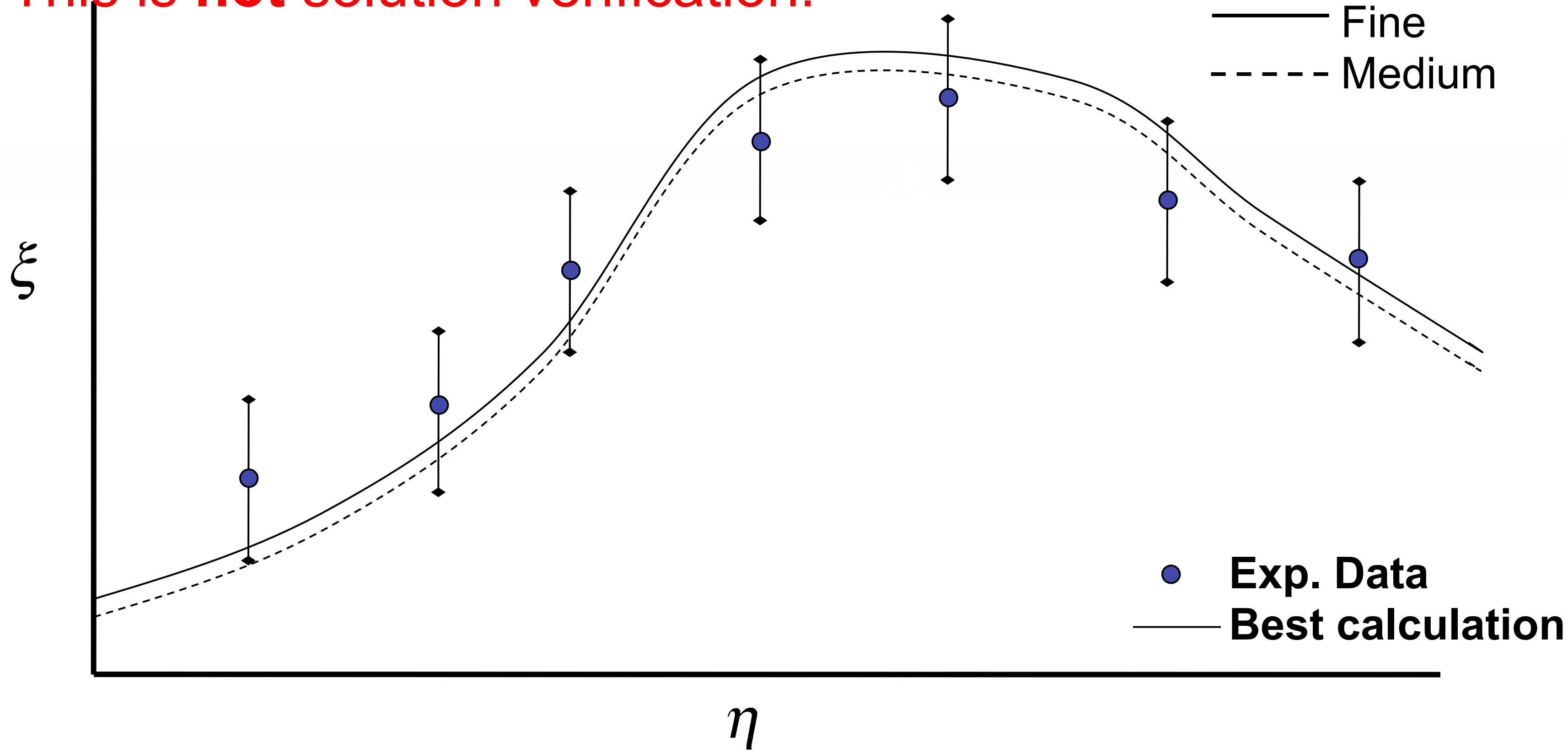
This presentation is an improvement because experimental error is shown.

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



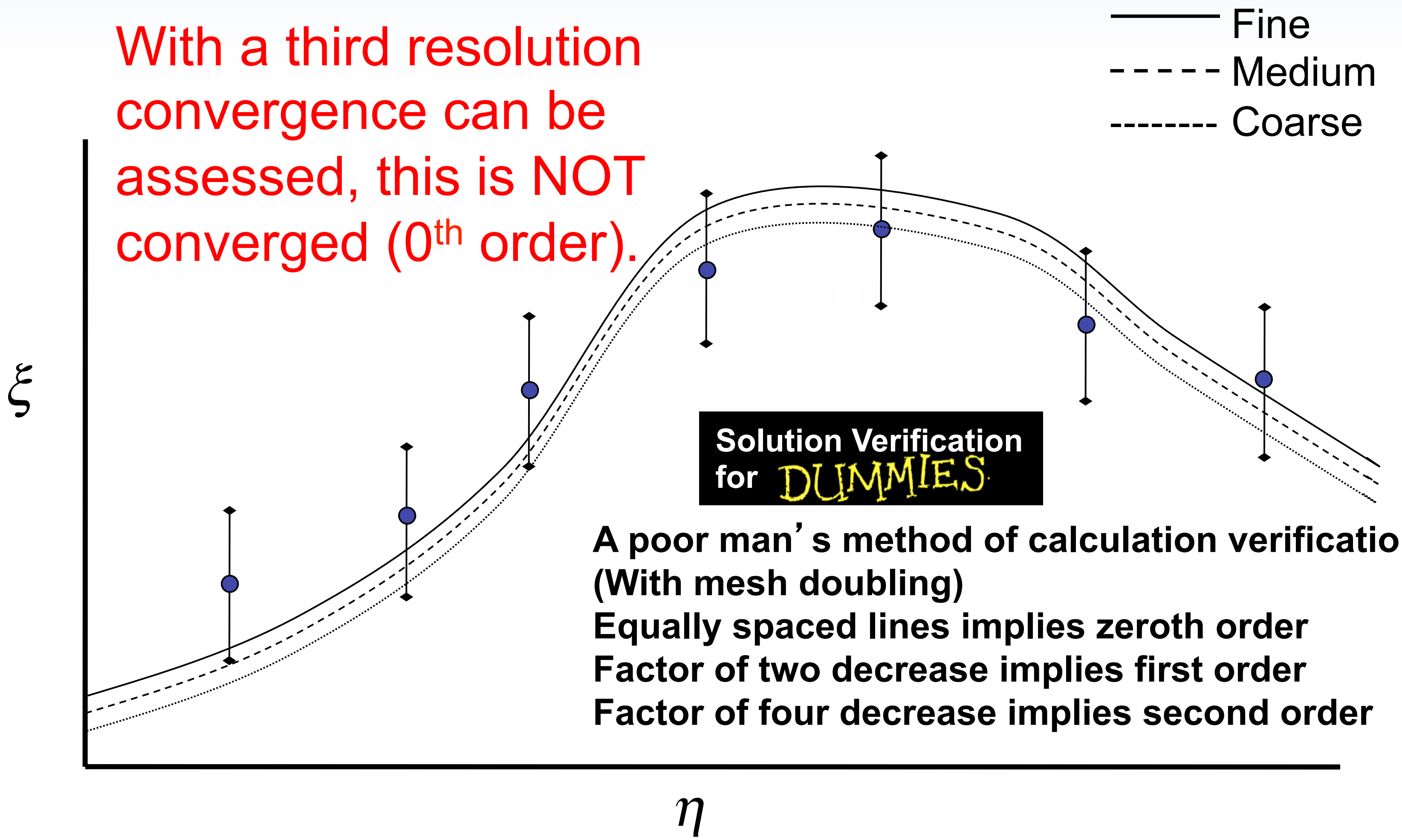
Here is a notion of how a “converged” solution might be described.

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



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

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



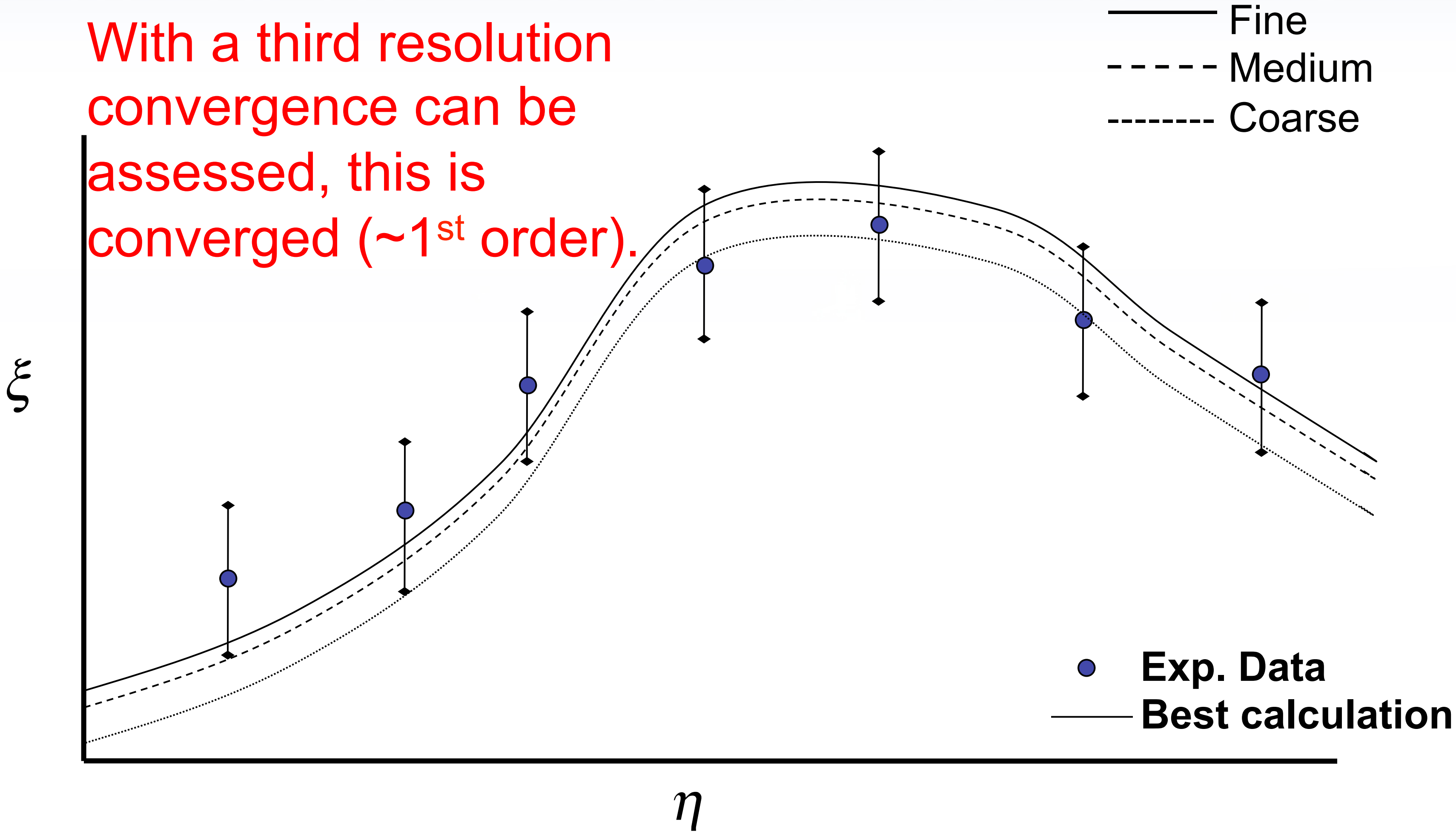
Solution Verification for DUMMIES

A poor man’s method of calculation 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

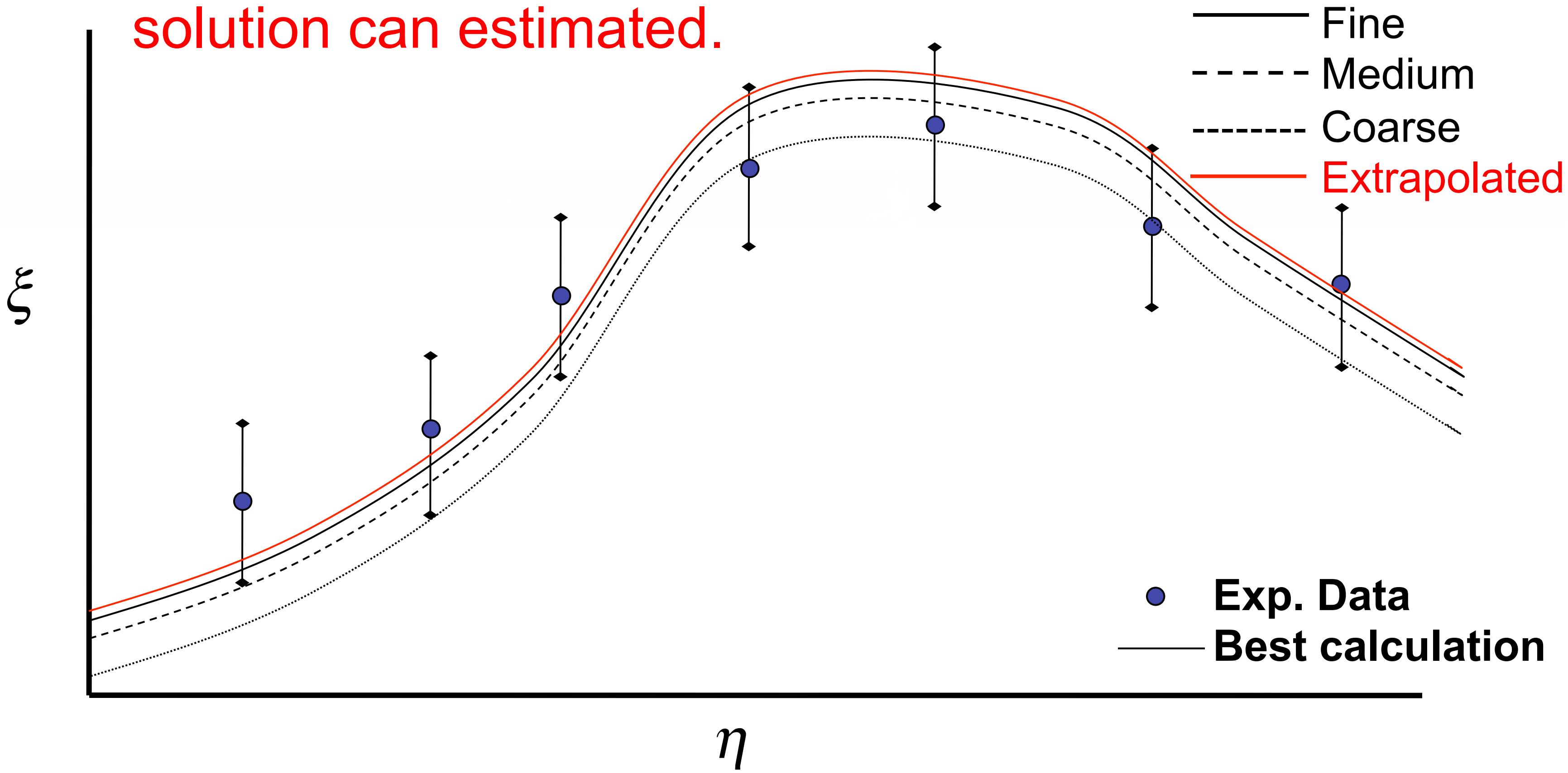
Here is a notion of how a “converged” solution might be described.

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

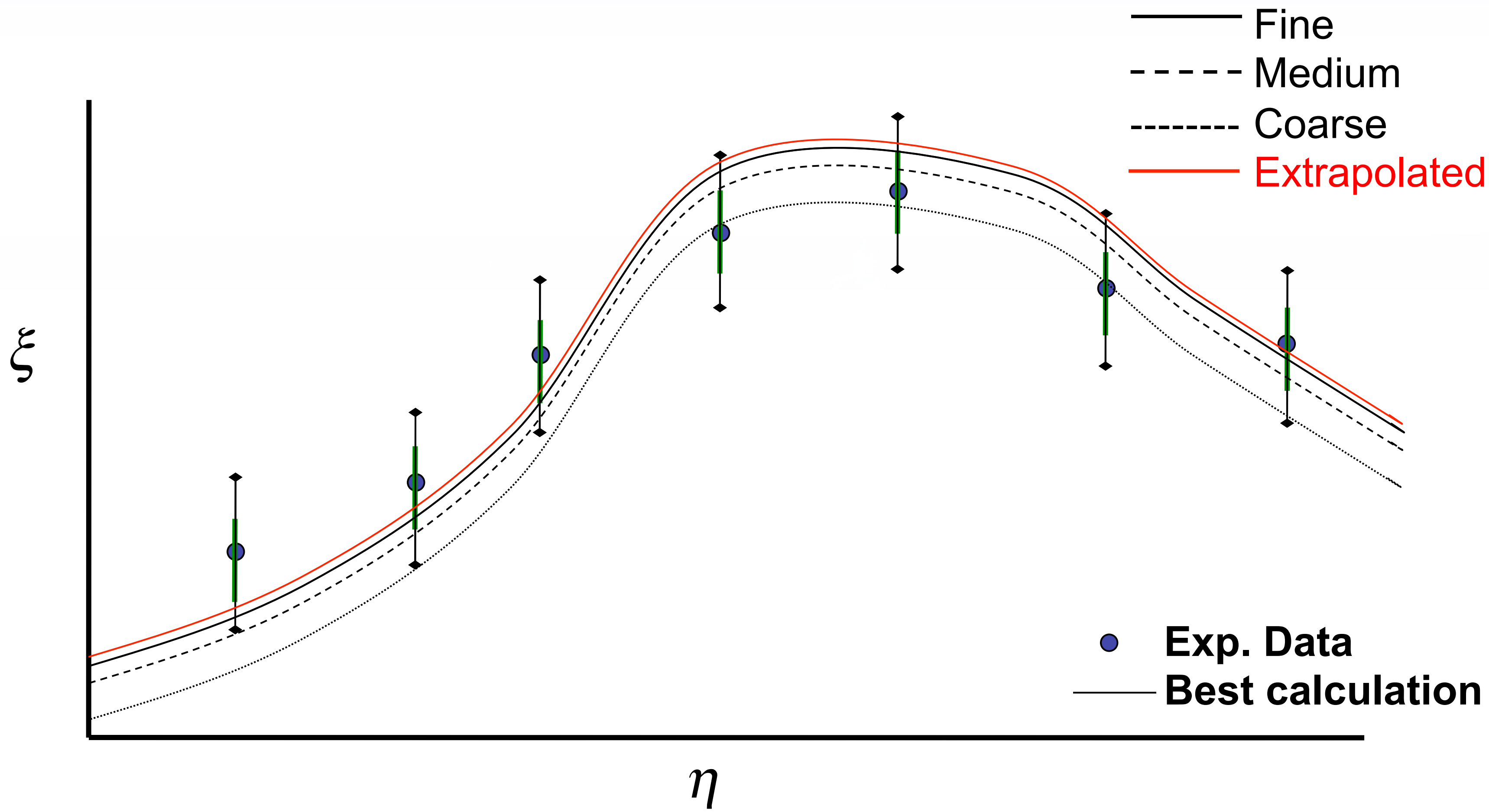


This sequence of meshes can be used to extrapolate the solution.

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



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



The origin of hydrodynamic calculations at Los Alamos in WWII

- **The first hydro calculation was reported in a Los Alamos report on June 20, 1944 – lead author Hans Bethe**
  - Feynmann was the calculational lead
- **The first codes were 1-D and Lagrangian, shocks were tracked (no viscosity, finite differences failed completely as of 1945).**
- **The first calculations were done to check for nonlinear corrections to the theory.**
  - This continued for the next 15 years
  - It was about understanding, not detail
  - Not until the 60's was quantitative accuracy an essential element.
  - Quality was still an expert judgement.

"This type of design process focuses heavily upon physics understanding of non-linear relationships and less upon brute force computational power. We used less than 1% of the computing power of the lab to design the RRW weapon. This low computer usage infuriated NNSA who personally berated me for placing understanding ahead of computer usage."

– John Pedicini, LANL Lead RRW Designer, March 7, 2007, From "LANL - the Corporate Story Blog"

Experiments are an inherent element of *any* validation analysis.

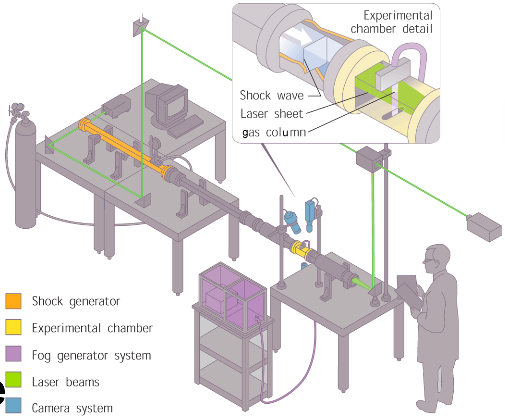
- **There are different types of experiments:**

NTS

Legacy vs. **“Live”**

Performed in the past	Currently undertaken
Often unrepeatable	Hopefully repeatable
Limited error information	More error information

LANL shock tube lab



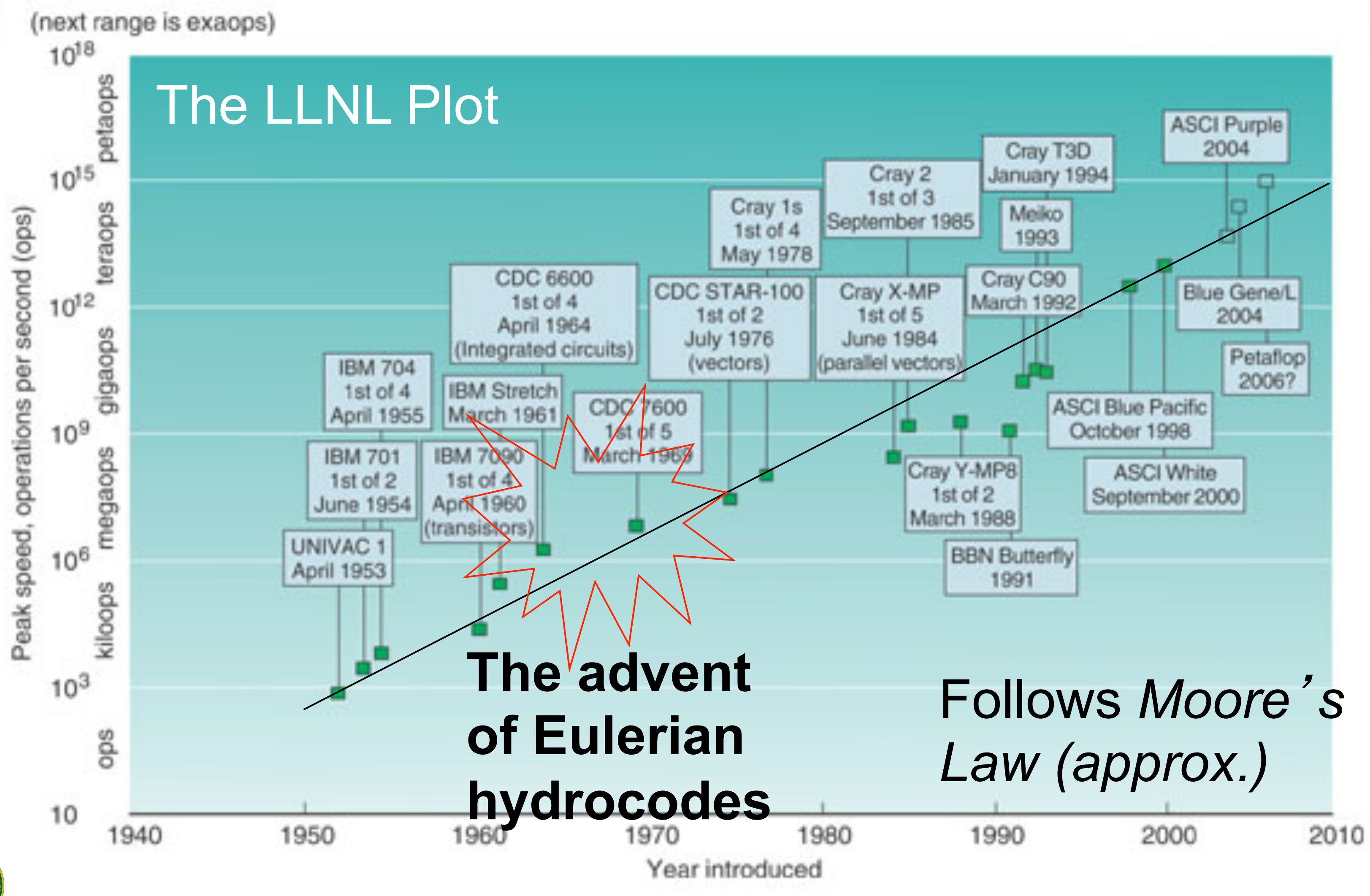
Discovery vs. **Validation**

Maybe repeatable	Necessarily repeatable
Usual experimental controls	Careful experimental controls
Usual error information	Extensive error information

- Analysts and experimentalists need to interact!
  - The whole *really is* greater than the sum of the parts.
  - You *really do* learn from each other.

See: W. Oberkampf, “What are Validation Experiments?” *Experimental* Techniques, **25**, pp. 35–40 (2001).

The most obvious aspect is the raw performance of the machines.

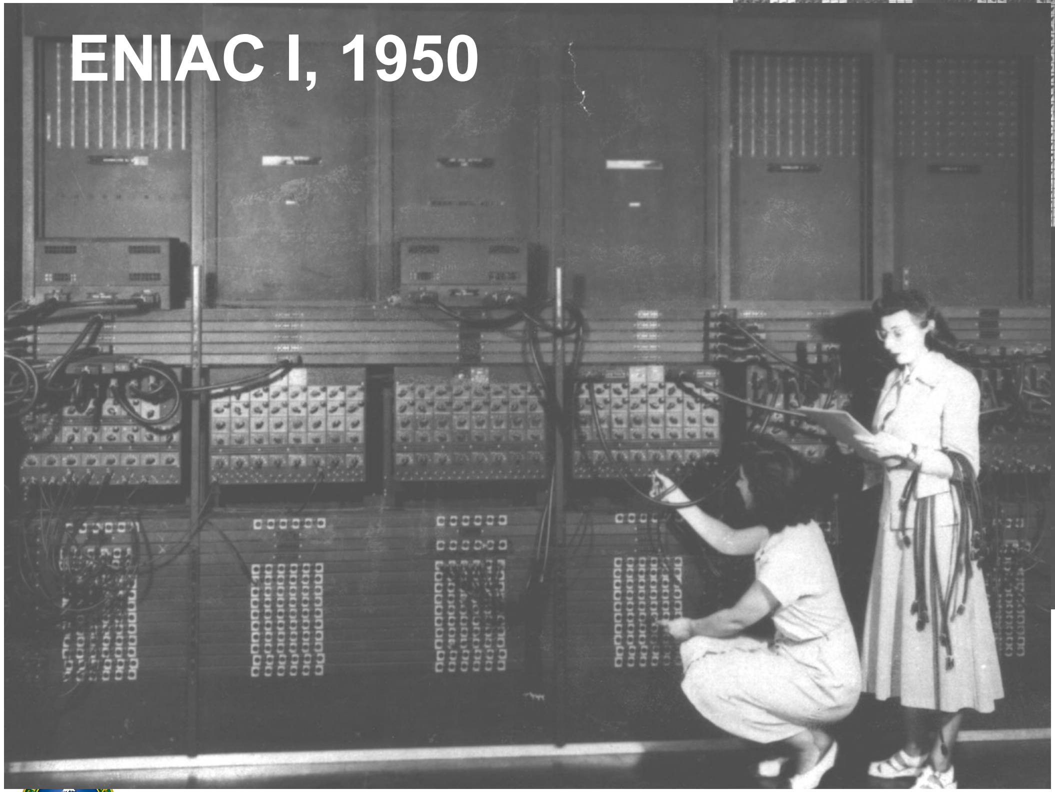


The LLNL Plot

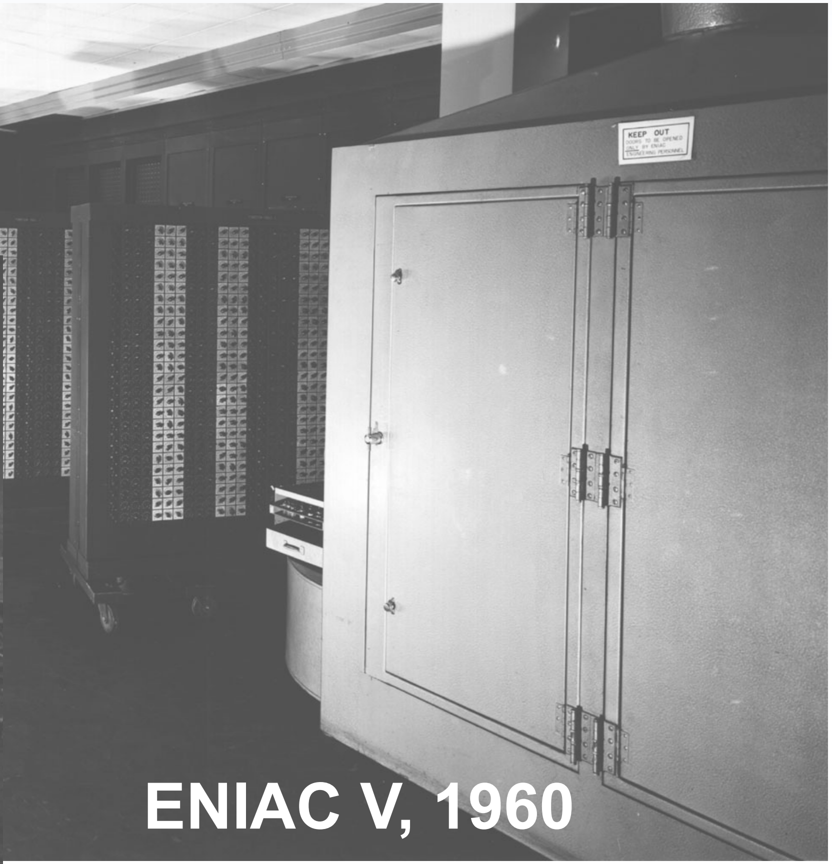
The advent of Eulerian hydrocodes

Follows *Moore's Law (approx.)*

The evolution of computers is hard to separate from the history of codes



ENIAC I, 1950

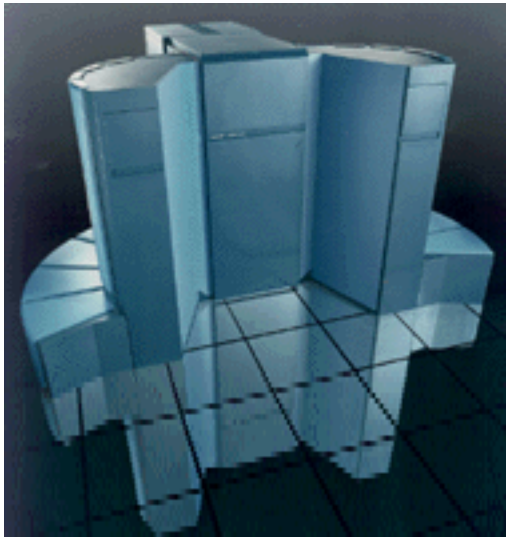


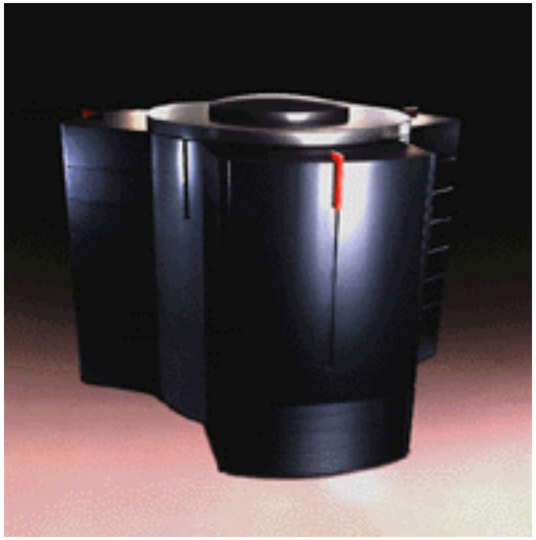
ENIAC V, 1960

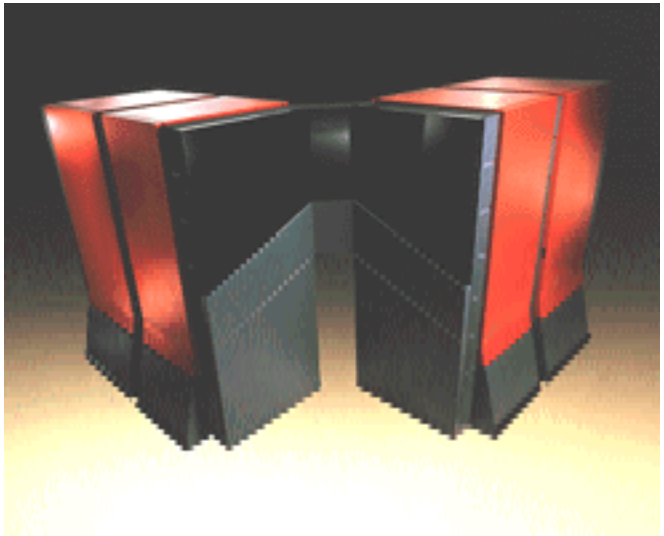
The Mid 60’s saw the rise of the CDC machines and their “father” Seymour Cray

The dawn of the “supercomputer era”

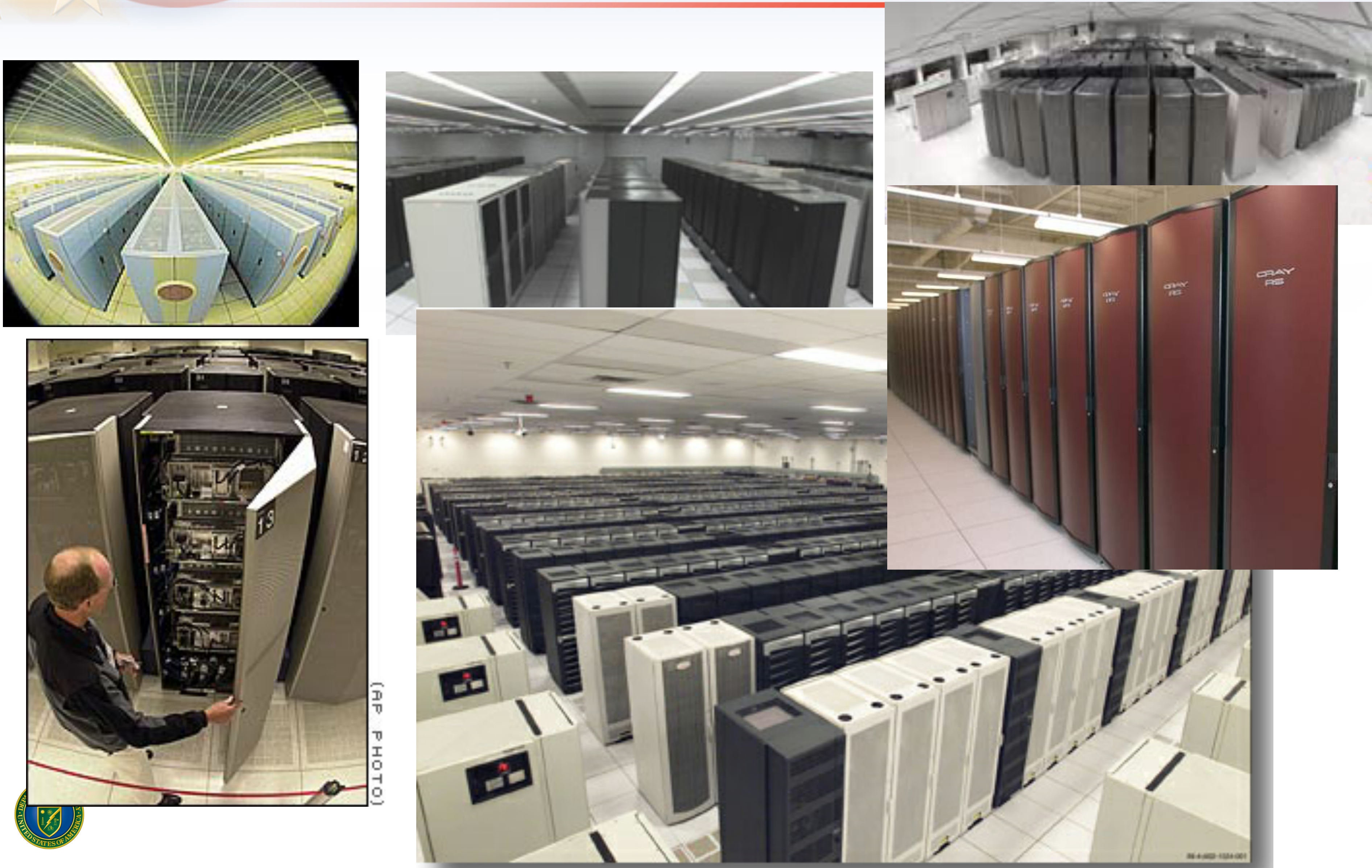
Of course there are Crays from the 70's-90's







…and the modern (ASCI) era with room filling machines again!



(AP PHOTO)

The next generation of supercomputers may be more challenging, but no "smaller"

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

– Nick Trefethen

The importance of V&V is increasing.

What’s different now?

- **Computational simulation is different now than 10-20-30 years ago (e.g., auto industry, aircraft industry, nuclear weapons industry, climate!)**
  - We’re making million/billion $ decisions that are heavily influenced by comp. sim.
- **Definition of “correct codes/models” (see previous) is now changing.**
- **“Before I spend $M/$B on a decision, I want evidence of the correctness of your simulation model and results.”**

V&V Is a Tough Sell.

V&V is expected, but not well understood, by decision makers.

- **V&V is, in a nutshell, all about putting "correct" math methods and physics models in our codes.**
- **We're <u>expected</u> to produce "correct" codes.**
- **"If you haven't been doing V&V all along, then what have you been doing with my ______ money?"**

Expectation of Quality is scope dependent

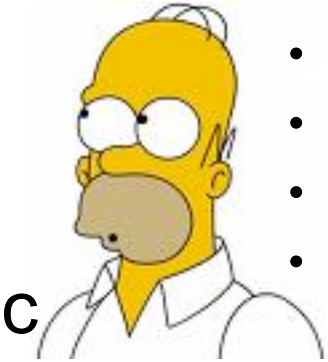
Expectations of the accuracy of scientific simulations vary. Who are you trying to convince?

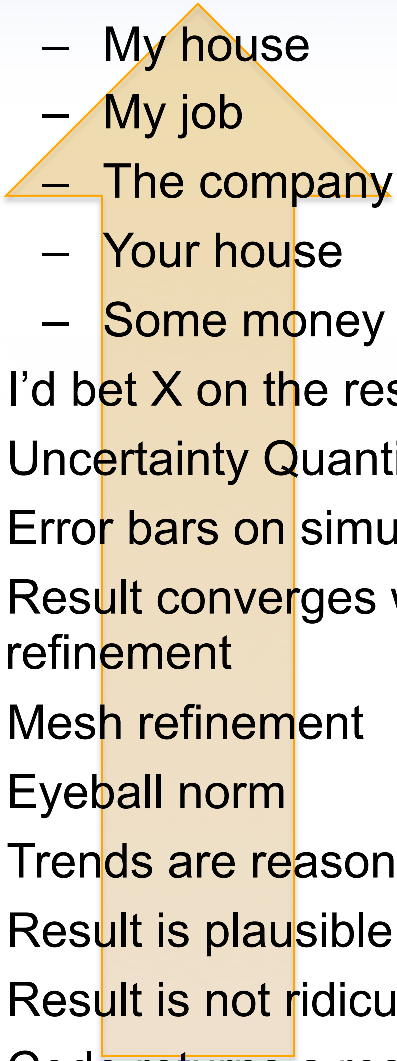
Code developers

Analysts

The customer

The public





  - My house
  - My job
  - The company
  - Your house
  - Some money
- I'd bet X on the result; X=
- Uncertainty Quantification
- Error bars on simulation results
- Result converges with refinement
- Mesh refinement
- Eyeball norm
- Trends are reasonable
- Result is plausible
- Result is not ridiculous
- Code returns a result

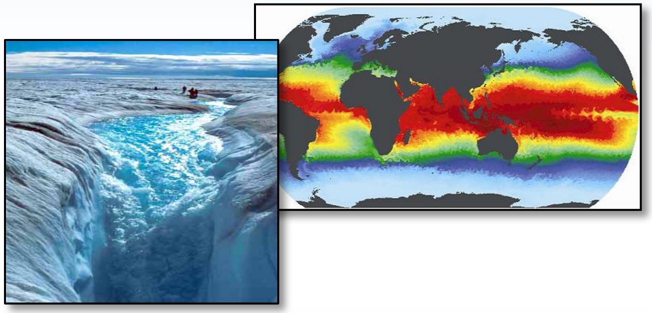
In M&S, you don’t know how good (or bad) you are if you don’t ask.

- “Due diligence” means asking all the questions, even if you don’t think you’ll like the answers.

Credit: M. Pilch.

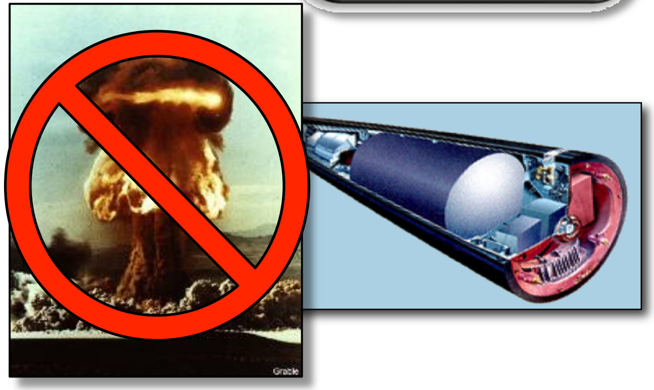
DOE mission imperatives require simulation and analysis for policy and decision making.

- ***Climate Change*: Understanding, mitigating and adapting to the effects of global warming**
  - Sea level rise
  - Severe weather
  - Regional climate change
  - Geologic carbon sequestration



- ***Energy*: Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production**
  - Reducing time and cost of reactor design and deployment
  - Improving the efficiency of combustion energy systems

- ***National Nuclear Security*: Maintaining a safe, secure and reliable nuclear stockpile**
  - Stockpile certification
  - Predictive scientific challenges
  - Real-time evaluation of urban nuclear



The ASCI Challenge

The President's Vision:

"...we can meet the challenge of maintaining our nuclear deterrent under a [comprehensive test ban] through a stockpile stewardship program without nuclear testing."

The DOE/ASCI Program Vision:

Create leading-edge computational modeling and simulation capabilities critically needed to

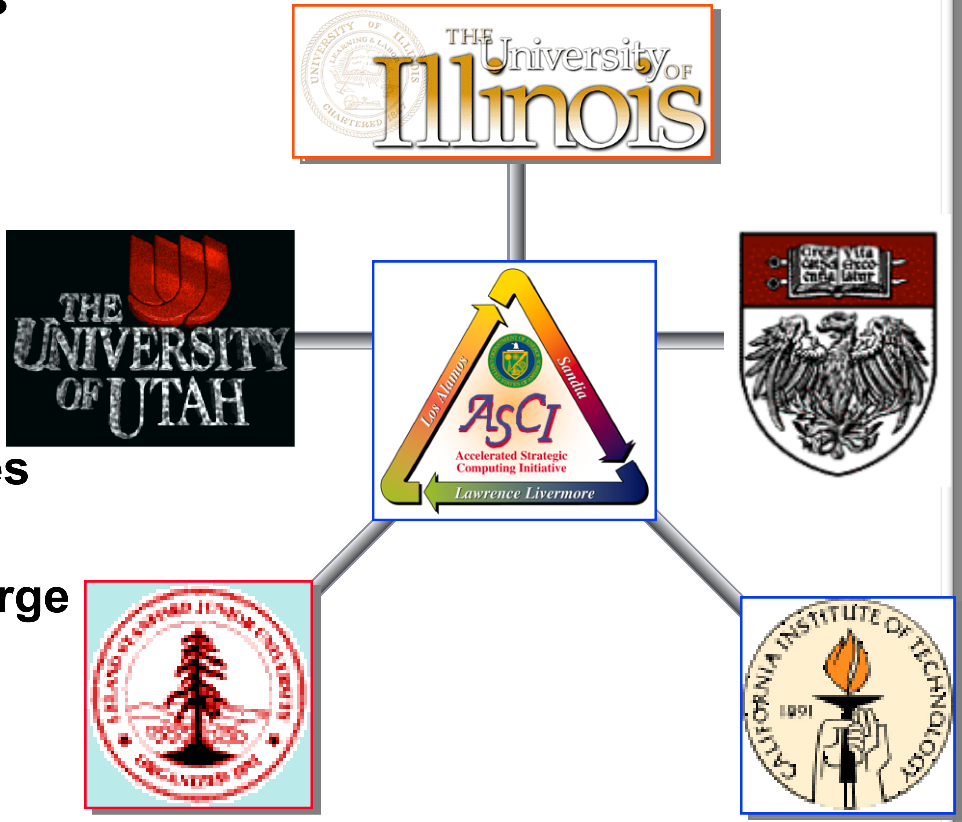
promptly shift from nuclear test-based methods to computational-based methods,

to integrate stockpile stewardship elements and thus reduce the nuclear danger.

From Paul Messina: **Ushering in the Era of Terascale Scientific Simulations (1999)**

The University Alliance program

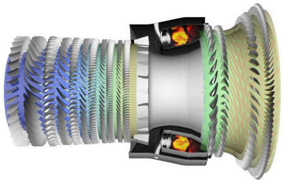
- **The five large Level I Alliance Centers have been established**
    - University of Illinois
    - California Institute of Technology
    - University of Utah
    - Stanford University
    - University of Chicago
- **More than a dozen Level Two alliances have been funded - focused groups**
- **Level 3 - Individual Collaborations; large number in place**

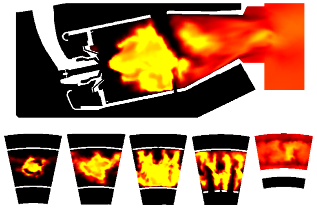


From Paul Messina: **Ushering in the Era of Terascale Scientific Simulations (1999)**

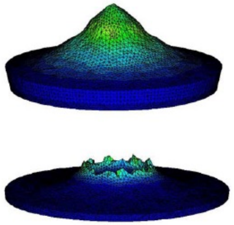
New Predictive Science Academic Alliance Program (PSAAP)

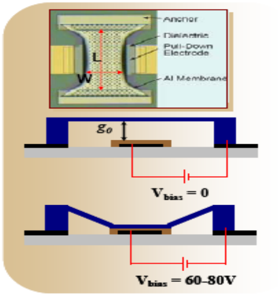
- **Focus on a multi-scale, multi-disciplinary, unclassified application of NNSA interest**
- **Demonstrate validated simulation capability for prediction**
- **Produce new methodologies on:**
  - Verification
  - Validation
  - Uncertainty quantification
  - Tight integration of experiment and simulation

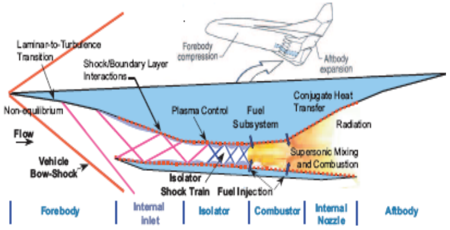


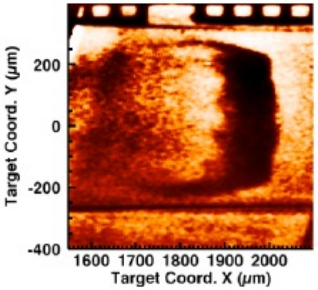


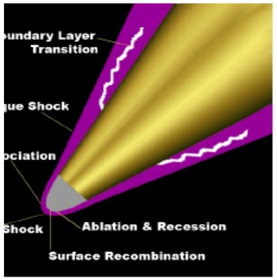
- **Projected Selection Announcement –** March 1, 2008



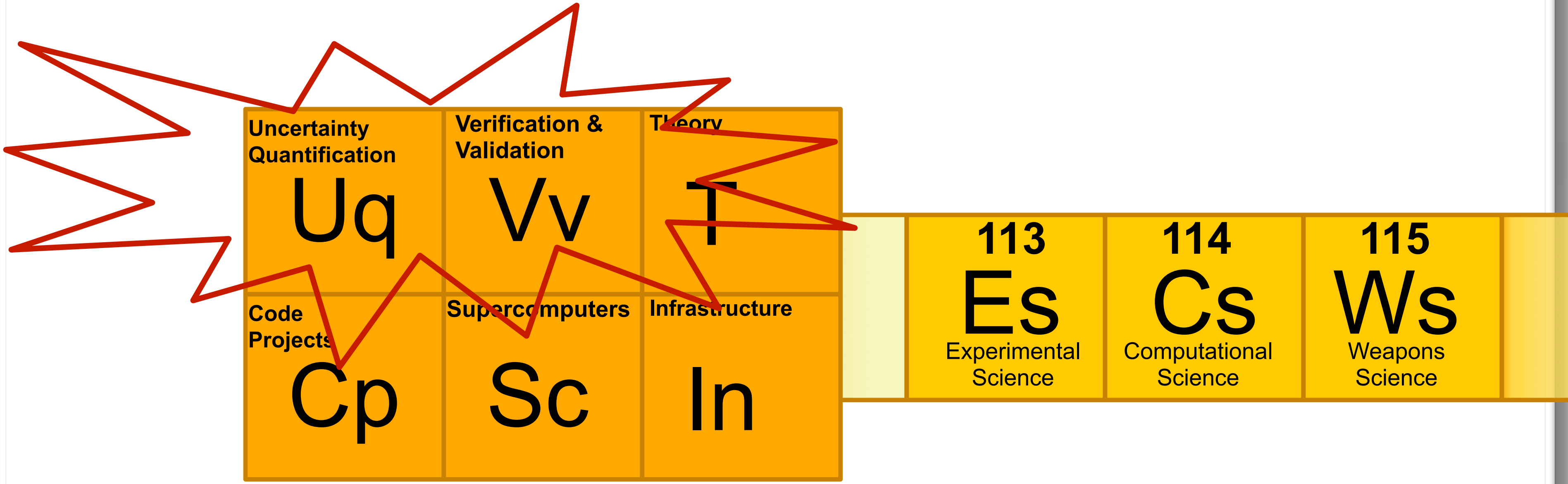








Leadership in National Security Computational Science


Uncertainty Quantification
Uq

Verification & Validation
Vv

Theory
T

Code Projects
Cp

Supercomputers
Sc

Infrastructure
In

113
Es
Experimental Science

114
Cs
Computational Science

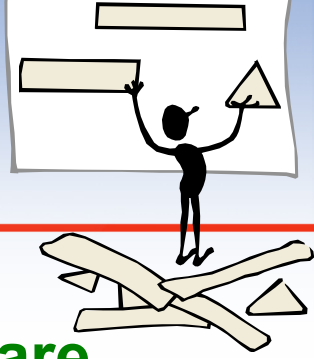
115
Ws
Weapons Science

Advanced Simulation & Computing

Address to the 2008 Principal Investigator Meeting

Dimitri Kusnezov

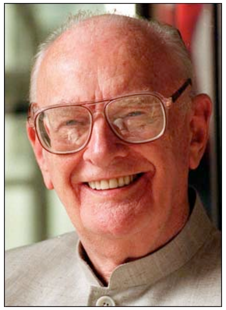
An emphasis on V&V, UQ and SQE was not part of the original program.



- ASC did not have V&V, UQ (QMU) or SQE (software quality engineering) in spelled out explicitly in its original program.
  - These activities usually did not get done without it!
- These areas of activity were added as the need for focused activity was recognized.
- V&V was added because the standard practices of the code development and user communities did not include sufficient rigor <u>without testing</u>.
- SQE was added for a similar reason.
- UQ was added because the decision makers realized that the information they needed was not present in the “standard” computational analysis.

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.



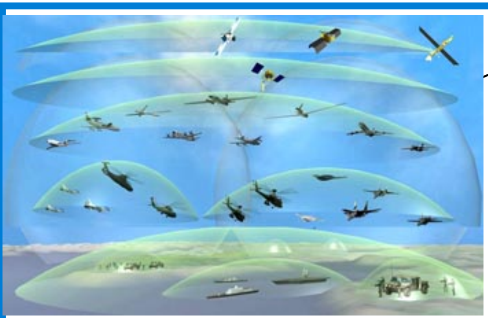
"One of the reasons why physicists need code developers is that they cannot communicate directly with a computer at their own level. In a religious context this kind of person is a shaman or a priest…" – Jack Worlton, LANL, 1982

CREATE

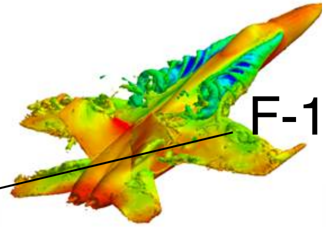
CREATE
Computational Research and Engineering Acquisition Tools and Environments

Description

- Quadrennial Defense Review calls for an agile and effective acquisition process with reduced costs and schedules.
- CREATE: Develop and deploy computational engineering tools to the acquisition programs to use with the next generation of supercomputers to design:
    1. Military Aircraft,
    2. Naval Ships, and
    3. RF antennae for military platforms.
- CREATE tools: Enable rapid development of optimized designs with fewer flaws and better performance.



Better Antennas for the Network Centric Warfare Battlespace



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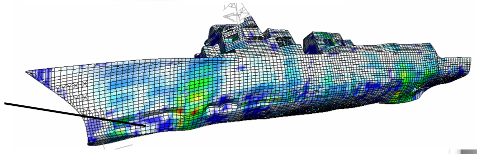
Separated Flow



Damage from Full Ship Shock Test

Benefits/Metrics

- Reduce acquisition program cost and schedule overruns by minimizing design defects that lead to schedule delays and budget over-runs.
- Enable early integration of major vehicle subsystems further reducing schedule and costs
- Optimize Test and Evaluation program through a merged modeling and test approach
- Improve flexibility and agility by enabling rapid assessment of design options and evaluation of the impact of candidate requirements
- Enable and facilitate technical oversight of prime contractors by government SPOs

Funding Requirements

~ 35 professionals/project for ~ 10 years

- Endorsed by Acquisition Program, S&T and T&E organizations
- Participation and support by Air Force, Army and Navy
- Injects technology into the early stages of the acquisition process
- Builds on present, smaller-scale computational engineering projects

From Doug Post's"**The Promise and Challenges of Large-Scale Computational Science and Engineering" 2008**

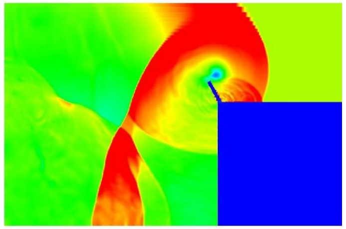
CREATE

CREATE Computational Environment
–Enabling Computational Engineering to Succeed–

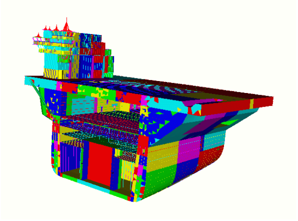
DEPARTMENT OF DEFENSE · UNITED STATES OF AMERICA

Description

- Provide the computational environment and infrastructure necessary for each CREATE project to succeed:
- Problem (Mesh) Generation Algorithms
- Software Engineering
- Computational Mathematics and Algorithms
- Analysis and Assessment Tools (e.g. visualization)
- Software Development and Collaboration Infrastructure



Visualization: Shield to protect Stryker from shock waves from IHEs



Computational Mesh for Aircraft Carrier

Benefits/Metrics

- Minimize duplication of common resources needed for development and deployment
- Provide resources to develop new solution techniques, and enable use of the best existing solution algorithms
- Ensure common and successful approaches to risk management and mitigation
- More resources available for essential data analysis and assessment tools
- Improved sharing of experiences and lessons learned

Funding Requirements
About ½ of one project

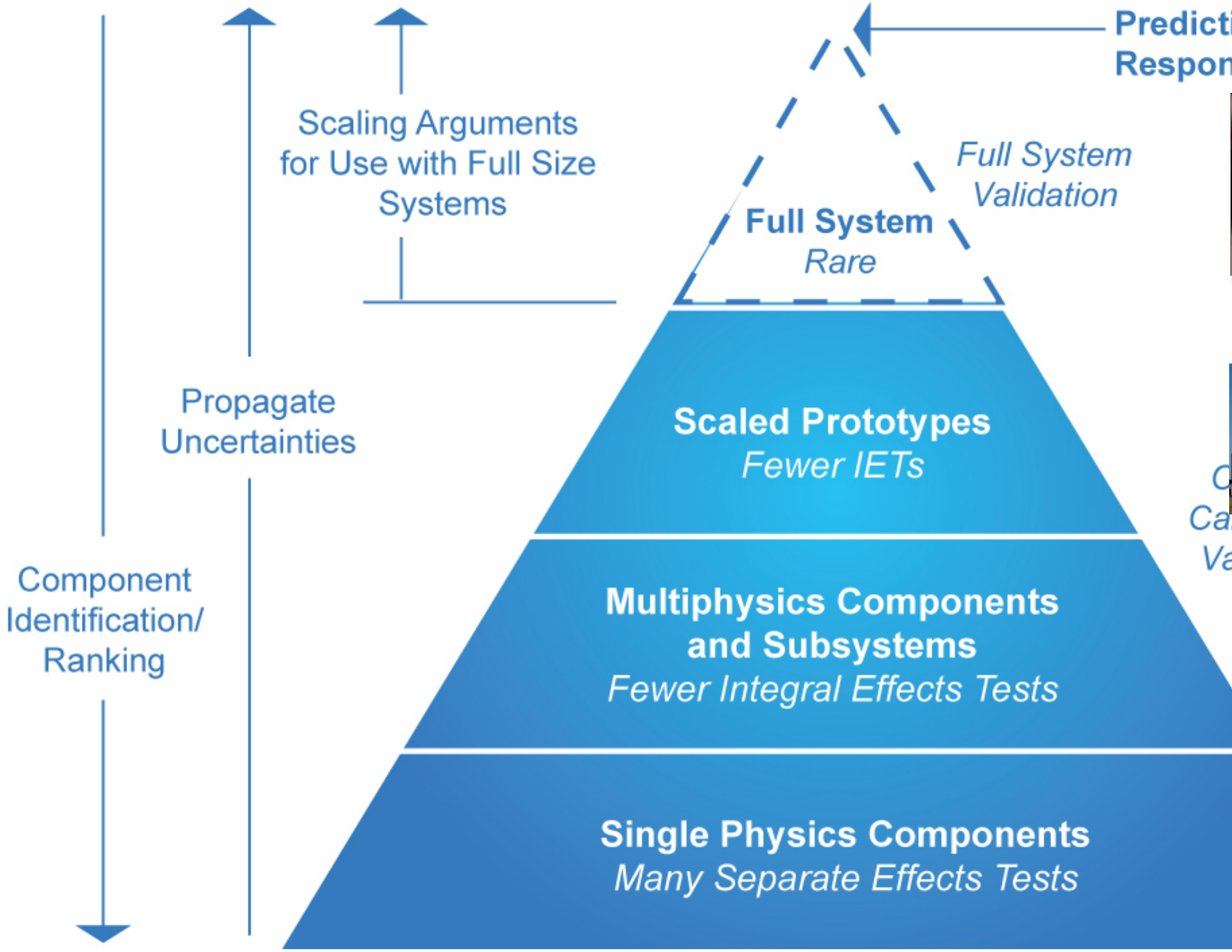
- ASCI (DOE NNSA), DOE SC, NSF, etc. computational programs find the proposed level of computational environment support essential for success
- Provides technical support to the three projects
- Encourages sharing of “lessons learned” and common experiences among the CREATE projects and with similar projects and programs in other agencies and industry

From Doug Post’s”**The Promise and Challenges of Large-Scale Computational Science and Engineering**”

“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.

Validation and Uncertainty Quantification Achieving credible, science-based predictive M&S capabilities



Prediction of Full-System Response Quantity of Interest

Scaling Arguments for Use with Full Size Systems

Full System
Rare

Full System Validation

Scaled Prototypes
Fewer IETs

C
Calibration/ Validation

Multiphysics Components and Subsystems
Fewer Integral Effects Tests

Single Physics Components
Many Separate Effects Tests

Component Calibration/ Validation

Component Identification/ Ranking

Propagate Uncertainties

CASL = Consortium for Advanced Simulation of Light Water Reactors

Validation and Uncertainty Quantification (VUQ) Achieving credible, science-based predictive M&S capabilities

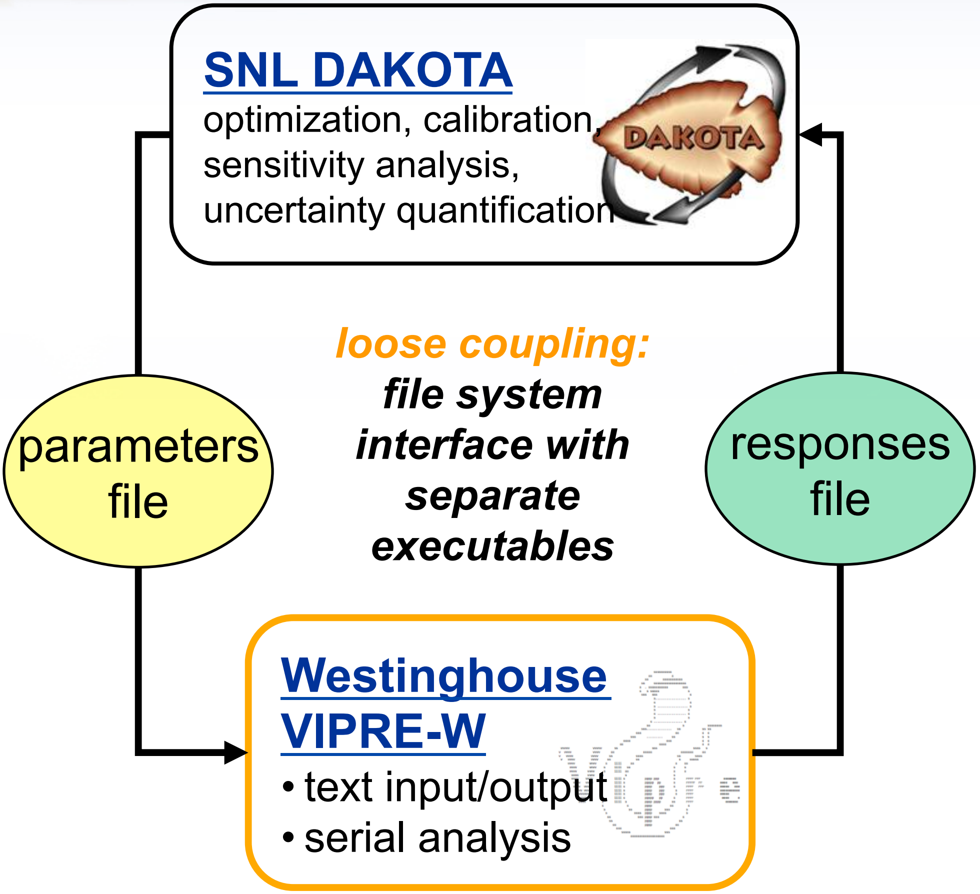
Requirements Drivers

- V&V and UQ methodologies and tools are needed by **every Focus Area.**
- VUQ is the CASL "**integrator**;" we need:
  - ✓**Partnerships** with other Focus Areas to implement uniform VUQ practices.
  - ✓Validation **data** (at all physical scales)
  - ✓**Access** to software and underlying math models

Outcomes and Impact

- **Continuous evolution** towards transformational, predictive M&S.
- Capability to **quantify** and reduce **uncertainties** for the CASL challenge problems.
- Ability **to predict *with defined confidence*** scenarios for which experimental data is not (directly) available.

Deliver Integrated Tools in VERA Simplify Interfaces/ Operation; Reduce Scripting Errors/Maintenance



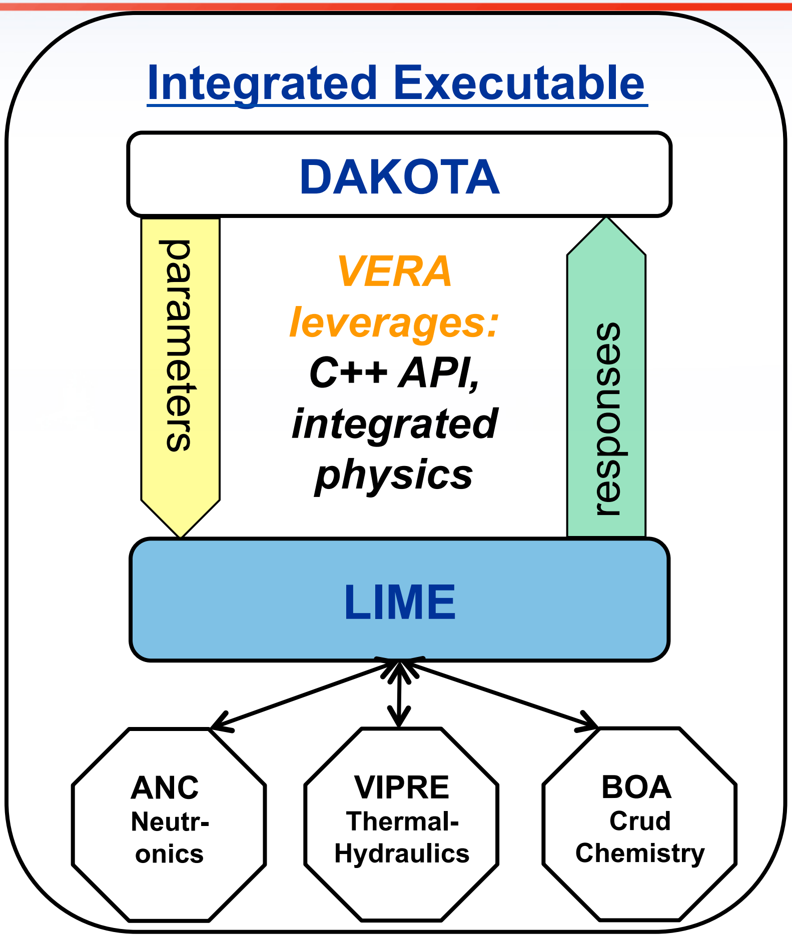
SNL DAKOTA
optimization, calibration, sensitivity analysis, uncertainty quantification

parameters file

loose coupling:
file system interface with separate executables

responses file

Westinghouse VIPRE-W
- text input/output
- serial analysis



Integrated Executable

DAKOTA

parameters

VERA leverages:
C++ API, integrated physics

responses

LIME

ANC
Neutr-onics

VIPRE
Thermal-Hydraulics

BOA
Crud Chemistry

Current

Move from potentially fragile, study-specific script interfaces to a unified, user-friendly capability

Future

NE-KAMS= Nuclear Energy – Knowledge base for Advanced Modeling and Simulation

- ✓ Multiple institutions participating in the development, i.e., Bettis, INL, Sandia, ANL, PNNL, Utah State University...
- ✓ Establish a comprehensive and web-accessible knowledge base to provide V&V-UQ resources for M&S
- ✓ Provide ability to share CFD data and models with M&S community
- ✓ Incorporate standards and procedures that allow scientists and engineers to assess the quality of their CFD models and simulations
- ✓ Developed Code Verification and Validation Data Standards Requirements

PCMM is a tool for managing risk in the use of modeling and simulation.

- **PCMM = Predictive Capability Maturity Model**
- **PCMM helps avoid four types of errors in M&S:**
  1. Believing that the model is *incorrect* when it is, in fact, *correct* (a "false negative" or "Type 1 error")
  2. Believing that the model is *correct* when it is, in fact, *incorrect* (a "false positive" or "Type 2 error")
  3. Solving the wrong problem!
  4. Using computational information *incorrectly*.

Credit: M. Pilch.

PCMM: 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

NE-KAMS verification completeness table

COMPLETENESS ATTRIBUTES	Completeness Level 0	Completeness Level 1	Completeness Level 2	Completeness Level 3
Conceptual Description	✓ Little or no description of all aspects	✓ Some description of the physical and modeling aspects tested	✓ Detailed description of the physical and modeling aspects tested ✓ Some discussion of the mathematical and numerical aspects tested	✓ Detailed discussion of the mathematical and numerical aspects tested
Mathematical Description	✓ Little or no description of all aspects	✓ Some description of the mathematical and solution aspects	✓ Detailed description of the mathematical and solution aspects ✓ Some description of the existence and uniqueness/non-uniqueness of the solution ✓ Some description of the chaotic and/or random nature of the solution, if applicable	✓ Detailed description of the existence and uniqueness/non-uniqueness of the solution ✓ Detailed description of the chaotic and/or random nature of the solution, if applicable
Boundary and/or Initial Conditions	✓ Little or no description of all aspects	✓ Detailed description of all boundary and initial conditions	✓ Some description of discontinuities and/or singularities in the boundary and initial conditions, if applicable ✓ Some description of coordinate singularities, if applicable ✓ Some discussion of discrete implementation details of initial and boundary conditions	✓ Detailed description of discontinuities and/or singularities in the boundary and initial conditions, if applicable ✓ Detailed description of coordinate singularities, if applicable ✓ Detailed discussion of discrete implementation details of initial and boundary conditions
Computer Hardware and System Software	✓ Little or no description of all aspects	✓ Some description of the hardware and system software used ✓ Some description of the compiler and effect of the options used	✓ Detailed description of the hardware and system software used ✓ Detailed description of the compiler and the effect of the options used	✓ Detailed description of results obtained on alternate hardware and system software ✓ Detailed description of results obtained on alternate compilers
SQA and Code Verification	✓ Little or no description of all aspects	✓ Some description of the software and its history ✓ Some SQA practices are documented and followed ✓ Some code verification conducted and documented	✓ Detailed description of the software and its history ✓ Detailed SQA practices are documented and followed ✓ Detailed code verification conducted and documented ✓ Observed order of numerical convergence evaluated, if applicable	✓ Detailed description of results obtained using alternate symbolic manipulators, if applicable ✓ Observed order of numerical convergence evaluated, including discontinuities, singularities, chaos, and randomness, if applicable
Solution Accuracy Assessment	✓ Little or no description of all aspects	✓ Some description of the effect of iterative error is provided, if applicable ✓ Some description of the effect of discretization error is provided, if applicable	✓ Detailed description of the effect of iterative error on all quantities of interest is provided, if applicable ✓ Detailed description of the effect of discretization error on all quantities of interest is provided, if applicable ✓ Observed order of numerical convergence estimated on all quantities of interest using multiple solutions, if applicable	✓ Detailed description of the effect of numerical algorithm parameters, if applicable ✓ Detailed description of the effect of round-off error ✓ Statistical convergence error estimated, if applicable ✓ Detailed description of the effect of discontinuities, singularities, chaos, and randomness, if applicable

NE-KAMS verification problem classification takes a graded approach on evidence.

- ✓ Closed Form Analytical problems
  - ○ The best case, includes MMS
- ✓ Significant Numerical evaluation of analytical solution
  - ○ The details are difficult, and prone to errors
- ✓ Numerical solution of ODEs
  - ○ The accuracy of the evaluation is important
- ✓ Numerical Approximations of PDEs
  - ○ Raises a number of thorny issues: code-to-code comparison, direct numerical simulation,…
  - ○ What is the error bar? Why should I trust this calculation

It is important to look at what is at stake, taking DNS as an example.

- ✓ DNS has been suggested as a means of validating lower level models, e.g., RANS, LES
  - ○ Full field data is available to compare against, and the comparison can be quantitative and precise
- ✓ Examples of important applications where turbulence is key are easy to find:
  - ○ Automobile design and performance
  - ○ Aircraft design and performance
  - ○ The America’s Cup (sailboat racing)
  - ○ Nuclear reactor design and analysis

In each case the economic impacts are potentially huge.

Xing and Stern have studied and suggested estimation procedure

“safety factor”

$$U_{num} = FS\left|\delta_\alpha\right| = \begin{cases} (2.45 - 0.85P)\left|\delta_\alpha\right|, \text{if } 0 < P \le 1 \\ (16.4P - 14.8)\left|\delta_\alpha\right|, \text{if } P > 1 \end{cases}$$

$$\delta_\alpha = \frac{\left|G^f - G^c\right|}{\sigma^\alpha - 1}$$

nic

ied (95% confidence)

$$P = \frac{\alpha_{\text{observed}}}{\alpha_{\text{theoretical}}}$$

- The same relations can apply to nonmontonically convergent sequences.
- For non-convergent sequences we suggest an approaches.

- Finally, we have to examine other discrete

$$U_{num} = 3(\max G - \min G)$$

$$U_{tol} = 1.25\left|\delta_\beta\right|$$

$$U_{approx} = \sqrt{U_{num}^2 + U_{tol}^2}$$

$$\frac{\|r\|_k}{\|r_0\|} < \text{tol}$$

$$\|\tilde{x} - x_k\| \sim \kappa(A)\frac{\|r\|_k}{\|r_0\|}$$

Turbulence DNS calculations and results from Donzis, Yeung & Sreenivasan 2008.

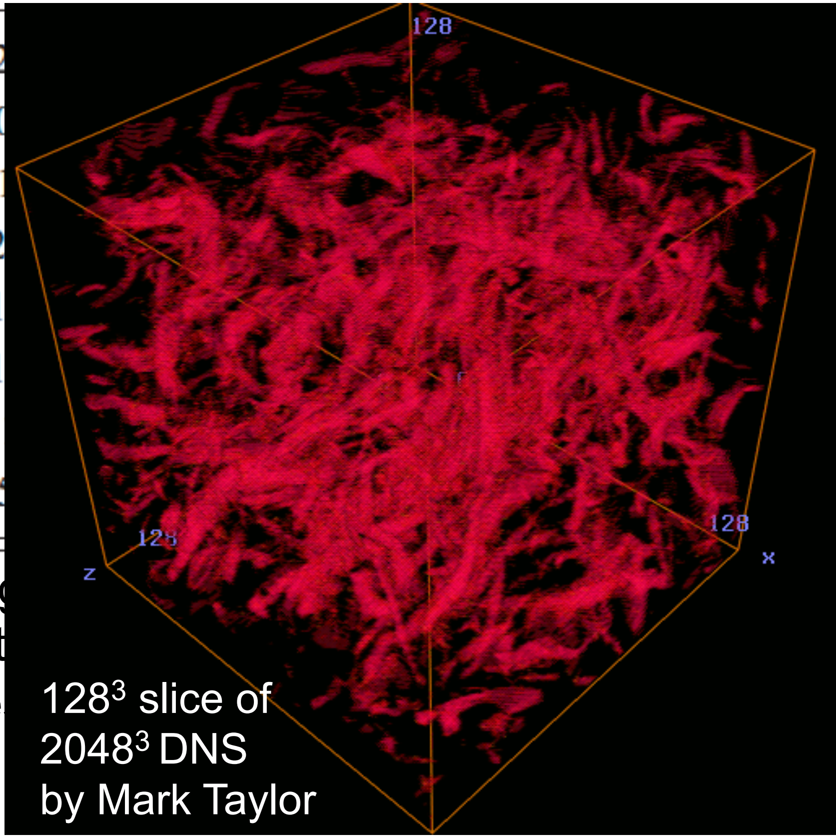
DNS should be a "slam-dunk" for verification with small numerical errors? Right?

TABLE I. DNS parameters: Taylor-scale Reynolds number $R_\lambda = u'\lambda/\nu$, number of grid points N^3, viscosity ν, resolution expressed in $k_{\max}\eta$ and $\Delta x/\eta$, mean energy dissipation rate $\langle\epsilon\rangle$ (equal to $\nu\langle\Omega\rangle$), number of instantaneous snapshots (N_r) processed as independent realizations, and simulation time period T normalized by eddy-turnover time T_E ($\mathcal{L}/u'$).

R_λ	140	140	140	140	240	2
N^3	256^3	512^3	1024^3	2048^3	512^3	10
ν (10^{-3})	2.8	2.8	2.8	2.8	1.1	1
$k_{\max}\eta$	$\boxed{1.41}$	2.82	5.72	11.15	$\boxed{1.42}$	2
$\Delta x/\eta$	2.10	1.05	0.52	0.27	2.08	1
$\langle\epsilon\rangle$	1.18	1.22	1.14	1.25	1.14	1
N_r	11	16	18	11	13	
T/T_E	10.0	7.2	8.5	6.0	9.4	5

The code used is pseudo-spectral with integrating viscous terms and 2nd order Runge-Kutta time int

The coarse grid is the recommended DNS me



128^3 slice of 2048^3 DNS by Mark Taylor

Results for key quantities.

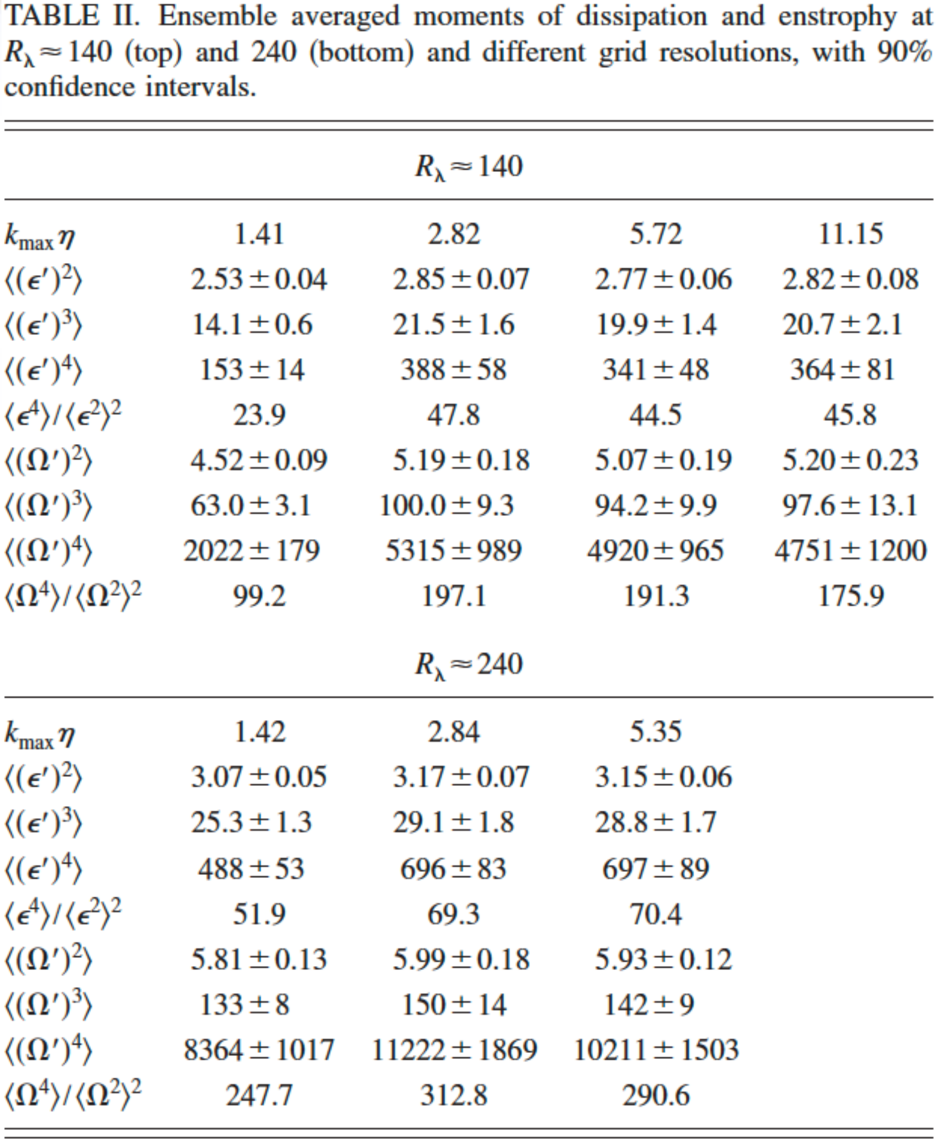


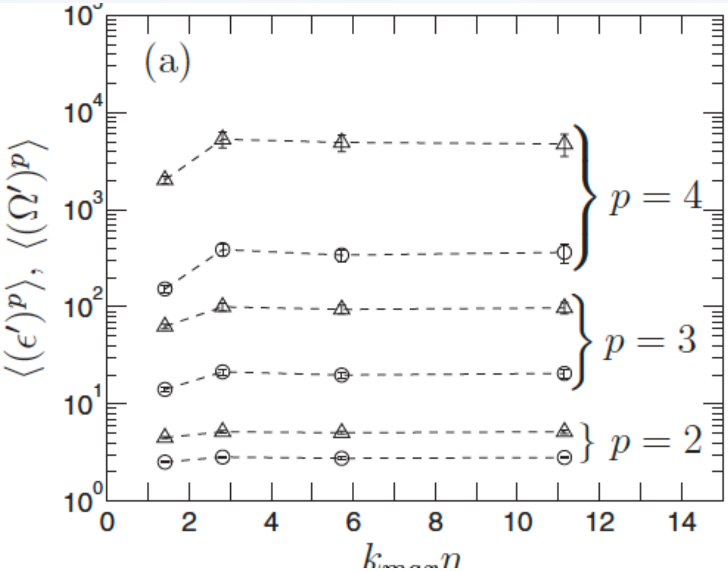
TABLE II. Ensemble averaged moments of dissipation and enstrophy at $R_\lambda \approx 140$ (top) and 240 (bottom) and different grid resolutions, with 90% confidence intervals.

$R_\lambda \approx 140$

$k_{\max}\eta$	1.41	2.82	5.72	11.15
$\langle(\epsilon')^2\rangle$	2.53 ± 0.04	2.85 ± 0.07	2.77 ± 0.06	2.82 ± 0.08
$\langle(\epsilon')^3\rangle$	14.1 ± 0.6	21.5 ± 1.6	19.9 ± 1.4	20.7 ± 2.1
$\langle(\epsilon')^4\rangle$	153 ± 14	388 ± 58	341 ± 48	364 ± 81
$\langle\epsilon^4\rangle/\langle\epsilon^2\rangle^2$	23.9	47.8	44.5	45.8
$\langle(\Omega')^2\rangle$	4.52 ± 0.09	5.19 ± 0.18	5.07 ± 0.19	5.20 ± 0.23
$\langle(\Omega')^3\rangle$	63.0 ± 3.1	100.0 ± 9.3	94.2 ± 9.9	97.6 ± 13.1
$\langle(\Omega')^4\rangle$	2022 ± 179	5315 ± 989	4920 ± 965	4751 ± 1200
$\langle\Omega^4\rangle/\langle\Omega^2\rangle^2$	99.2	197.1	191.3	175.9

$R_\lambda \approx 240$

$k_{\max}\eta$	1.42	2.84	5.35
$\langle(\epsilon')^2\rangle$	3.07 ± 0.05	3.17 ± 0.07	3.15 ± 0.06
$\langle(\epsilon')^3\rangle$	25.3 ± 1.3	29.1 ± 1.8	28.8 ± 1.7
$\langle(\epsilon')^4\rangle$	488 ± 53	696 ± 83	697 ± 89
$\langle\epsilon^4\rangle/\langle\epsilon^2\rangle^2$	51.9	69.3	70.4
$\langle(\Omega')^2\rangle$	5.81 ± 0.13	5.99 ± 0.18	5.93 ± 0.12
$\langle(\Omega')^3\rangle$	133 ± 8	150 ± 14	142 ± 9
$\langle(\Omega')^4\rangle$	8364 ± 1017	11222 ± 1869	10211 ± 1503
$\langle\Omega^4\rangle/\langle\Omega^2\rangle^2$	247.7	312.8	290.6



Donzis et al. used the plot to say the sequence was “converged” and not mesh sensitive.

Verification Analysis for DNS at Re=140

Quantity	Δ_{cm}	Δ_{mf}	Δ_{fv}	α_{cf}	α_{mv}	U_{cf}	U_{mv}	d_{cf}	d_{mv}
$\langle(\varepsilon')^2\rangle$	0.32	0.08	0.05	2.00	0.68	0.48	0.16	±0.06	±0.08
$\langle(\varepsilon')^3\rangle$	7.40	1.60	0.80	2.21	1.00	9.46	1.28	±1.4	±2.1
$\langle(\varepsilon')^4\rangle$	235.00	47.00	23.00	2.32	1.03	273.54	46.48	±48	±81
$\langle\varepsilon^4\rangle/\langle\varepsilon^2\rangle^2$	23.90	3.30	1.30	2.86	1.34	16.94	6.12	–	–
$\langle(\Omega)^2\rangle$	0.67	0.12	0.13	2.48	-0.12	0.68	0.39	±0.19	±0.23
$\langle(\Omega)^3\rangle$	37.00	5.80	3.40	2.67	0.77	31.32	8.65	±9.9	±13.1
$\langle(\Omega)^4\rangle$	3293.00	395.00	169.00	3.06	1.22	1904.57	668.18	±965	±1200
$\langle\Omega^4\rangle/\langle\Omega^2\rangle^2$	97.90	5.80	15.40	4.08	-1.41	19.02	63.60	–	–

Order of convergence

numerical uncertainty

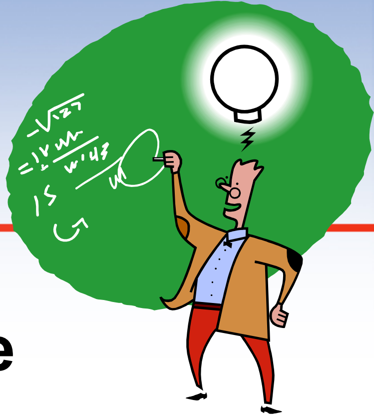
data uncertainty

The numerical uncertainty is significant at all resolutions!

NE-KAMS validation completeness table

COMPLETENESS ATTRIBUTES	Completeness Level 0	Completeness Level 1	Completeness Level 2	Completeness Level 3
1. Experimental Facility	✓ Little or no description of the facility or its operation	✓ Some information on the functional operation of the facility and its operating procedures ✓ Some information on the geometric and equipment features of the facility	✓ Detailed information on the functional operation of the facility and its operating procedures ✓ Detailed information of the geometric and equipment features of the facility ✓ Some information on the calibration procedures and reference standards for the facility ✓ Some information on the calibration results and characterization of the facility	✓ Detailed information of the fine-scale flow features/environment inside the test section ✓ Some information of the fine-scale flow features or physical processes upstream and downstream of the test section ✓ Detailed information on the calibration procedures and reference standards for the facility ✓ Detailed information on the calibration results and characterization of the facility ✓ Information on the inspection, maintenance, and repairs of the facility
2. Analog Instrumentation and Signal Processing	✓ Little or no information on sensors and calibration procedures ✓ Little or no information on instrumentation ✓ Little or no information on signal processing ✓	✓ Some information on sensors and calibration procedures ✓ Some information on transducers ✓ Some information on signal processing	✓ Detailed information on sensors and calibration procedures ✓ Detailed information on transducers ✓ Detailed information on signal processing ✓ Some assessment of instrument performance and suitability	✓ Use of independent sensors and calibration procedures ✓ Use of independent/alternative signal processing procedures ✓ Detailed assessment of instrument performance and suitability
3. Boundary and Initial Conditions	✓ Little or no information on boundary conditions ✓ Little or no information on initial conditions ✓ Little or no information on design dimensions	✓ Some inflow quantities measured ✓ Some wall quantities measured ✓ Some initial conditions measured ✓ Detailed model-design dimensions provided	✓ Most inflow quantities measured ✓ Most wall quantities measured ✓ Most initial conditions measured ✓ Detailed as-built model dimensions measured ✓ Some outflow and reverse flow quantities measured	✓ Fine-scale inflow quantities measured ✓ Fine-scale wall quantities measured ✓ Fine-scale outflow quantities measured ✓ Fine-scale initial conditions measured ✓ As-tested model dimensions measured ✓ Inflow and outflow quantities measured at multiple streamwise locations
4. Fluid and Material Properties of the Walls	✓ Little or no information on fluid and material properties ✓ Little or no information on wall properties	✓ Some thermodynamic state data of fluid (s) provided ✓ Some transport properties of fluid(s) provided	✓ Detailed information provided to determine thermodynamic state of fluid (s) ✓ Detailed information provided to determine transport properties of fluid (s) ✓ Volume fraction of additional phases is provided, plus size distribution statistics	✓ All thermodynamic, transport, and optical properties of the fluid(s) are provided, as well as how these are determined ✓ Thermal, mechanical and optical properties of the wall(s) are provided ✓ Detailed description of additional phases is provided, plus size distribution statistics
5. Test Conditions	✓ Little or no information on test conditions	✓ Some description provided of the method of control and record of the test conditions ✓ Some description provided for measuring test conditions	✓ Detailed description provided of the method of control and record of the test conditions ✓ Detailed description provided for measuring test conditions	✓ Detailed description of operational procedures for setting and controlling test conditions ✓ Detailed measurement of time and spatial variation of test conditions
	✓ Little or no information on data acquisition and sampling procedures	✓ Some information on data acquisition and sampling procedures	✓ Detailed information on data acquisition and sampling procedures	✓ Use of independent data acquisition procedures

We can see how different the user communities can be.



- If one considers that the journals characterize the leading edge of work in an area.
- For fluid mechanics, the engineering community has embraced well-defined standards (using V&V)
- While the physics community tends to embrace a standard based on expert judgment.
- These considerations tend to be reflected in practice (*albeit in very broad brush strokes*):
  - Some engineers tend to work to achieve an evidence basis for decisions
  - Most physicists tend to provide their evidence based more strongly on expertise.

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 will not consider any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation. 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.

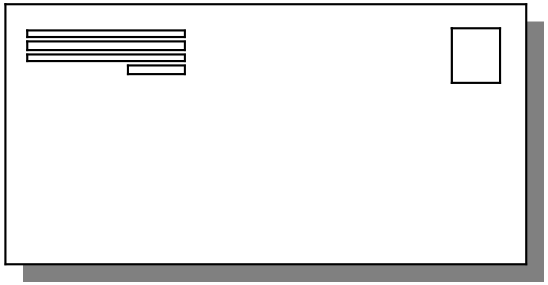
“An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them.”

- Werner Heisenberg

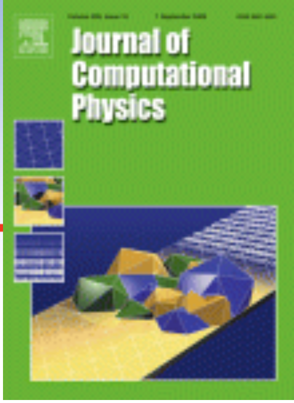
Excerpt from the editorial policy of Journal of Fluid Mechanics

“Journal of Fluid Mechanics is the leading international journal in the field and is essential reading for all those concerned with developments in fluid mechanics. It publishes authoritative articles covering theoretical, computational and experimental investigations of all aspects of the mechanics of fluids. Each issue contains papers on both the fundamental aspects of fluid mechanics, and their applications to other fields such as aeronautics, astrophysics, biology, chemical and mechanical engineering, hydraulics, meteorology, oceanography, geology, acoustics and combustion.”

- There is nothing about accuracy, validation, verification, convergence, etc…
- Everything is in the hands of the editors and reviewers, i.e. the experts.



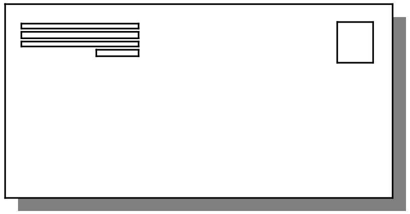
Journal of Computational Physics



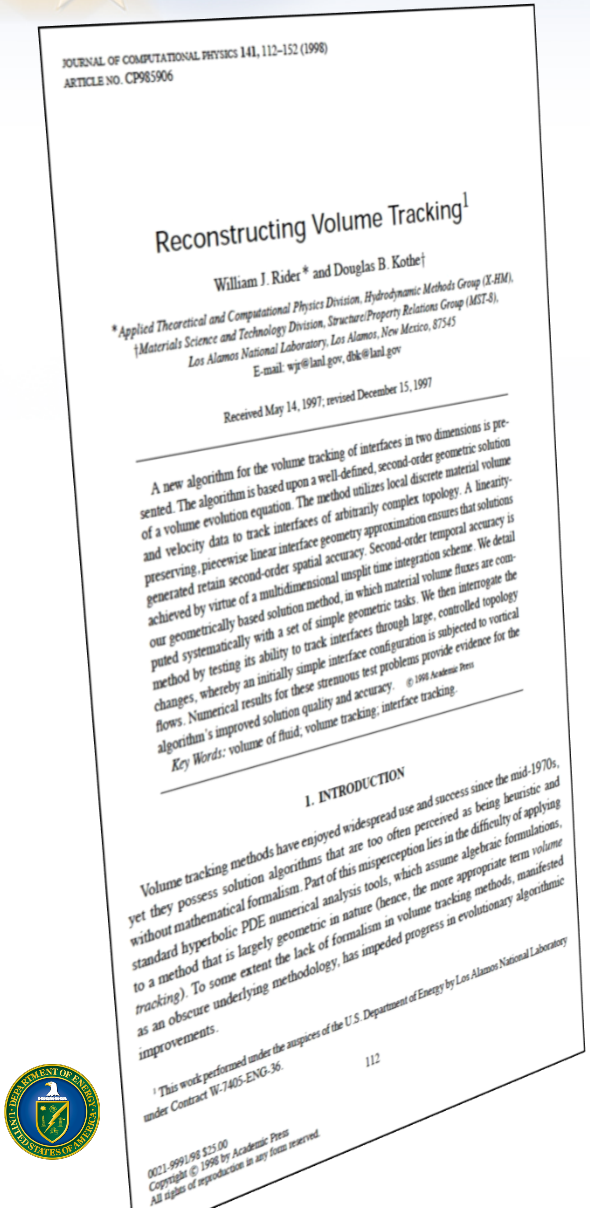
Journal of Computational Physics thoroughly treats the computational aspects of physical problems, presenting techniques for the numerical solution of mathematical equations arising in all areas of physics. The journal seeks to emphasize methods that cross disciplinary boundaries.

Elsevier’s reviewer guidance:

- Is the **methodology** appropriate? Does it accurately explain how the data was collected? Is the design suitable for answering the question posed? Is there sufficient information present for you to replicate the research? Does the article identify the procedures followed? Are these ordered in a meaningful way? If the methods are new, are they explained in detail? Was the sampling appropriate? Have the equipment and materials been adequately described? Does the article make it clear what type of data was recorded; has the author been precise in describing measurements?
- **Results:** this is where the author/s should explain in words what he/she discovered in the research, any interpretation should not be included in this section. The results should be clearly laid out and in a logical sequence. You will need to consider if the appropriate analysis been conducted. Are the statistics correct? If you are not comfortable with statistics, advise the editor when you submit your report.



As an example I’ll focus on two of my own papers, a safe approach with some pitfalls.



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

Reconstructing Volume Tracking[1]

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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. © 1998 Academic Press

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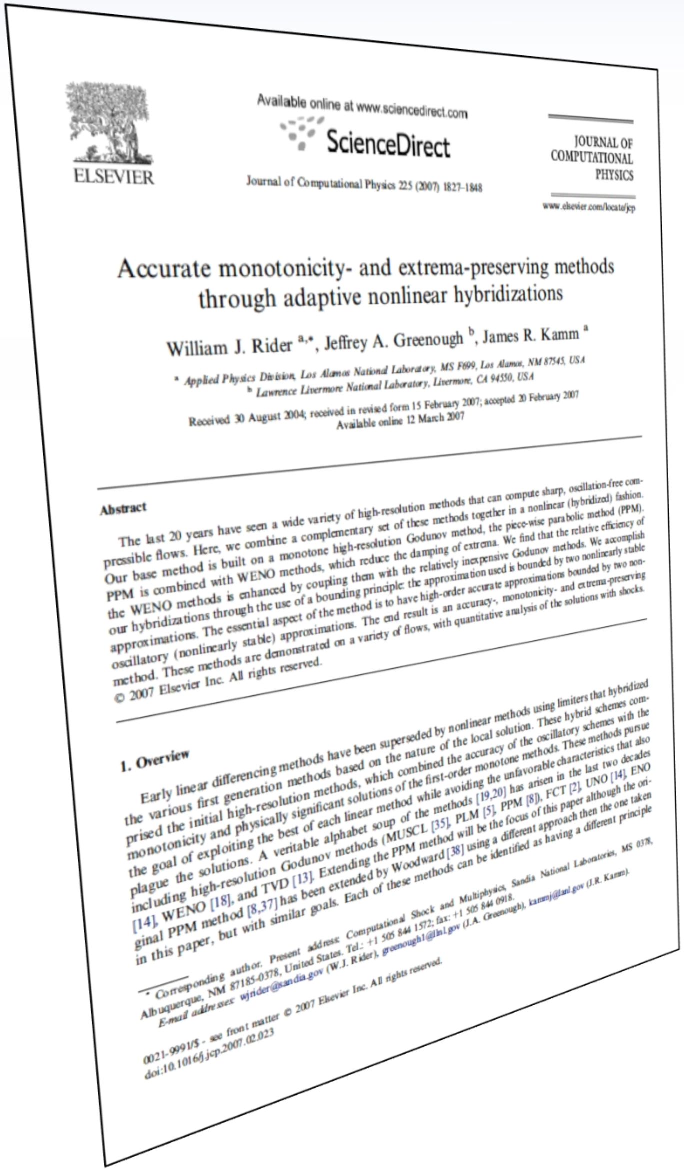
[1] This work performed under the auspices of the U.S. Department of Energy by Los Alamos National Laboratory under Contract W-7405-ENG-36.

0021-9991/98 $25.00

- Both papers were written for the “same” reason, to report algorithmic progress.
- Testing, i.e. verification became important although for different reasons.
- The volume tracking paper is highly cited because of the tests it introduced.
- The testing of the other paper became a bit of a tug of war with the editor and reviewers.
- Both issues point to the process to determine quality of calculations.



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Accurate monotonicity- and extrema-preserving methods through adaptive nonlinear hybridizations

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Abstract

The last 20 years have seen a wide variety of high-resolution methods that can compute sharp, oscillation-free compressible flows. Here, we combine a complementary set of these methods together in a nonlinear (hybridized) fashion. Our base method is built on a monotone high-resolution Godunov method, the piece-wise parabolic method (PPM). PPM is combined with WENO methods, which reduce the damping of extrema. We find that the relative efficiency of the WENO methods is enhanced by coupling them with the relatively inexpensive Godunov methods. We accomplish our hybridizations through the use of a bounding principle: the approximation used is bounded by two nonlinearly stable approximations. The essential aspect of the method is to have high-order accurate approximations bounded by two non-oscillatory (nonlinearly stable) approximations. The end result is an accuracy-, monotonicity- and extrema-preserving method. These methods are demonstrated on a variety of flows, with quantitative analysis of the solutions with shocks.
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1. Overview

Early linear differencing methods have been superseded by nonlinear methods using limiters that hybridized the various first generation methods based on the nature of the local solution. These hybrid schemes comprised the initial high-resolution methods, which combined the accuracy of the oscillatory schemes with the monotonicity and physically significant solutions of the first-order monotone methods. These methods pursue the goal of exploiting the best of each linear method while avoiding the unfavorable characteristics that also plague the solutions. A veritable alphabet soup of the methods [19,20] has arisen in the last two decades including high-resolution Godunov methods (MUSCL [35], PLM [5], PPM [8]), FCT [2], UNO [14], ENO [14], WENO [18], and TVD [13]. Extending the PPM method will be the focus of this paper although the original PPM method [8,37] has been extended by Woodward [38] using a different approach then the one taken in this paper, but with similar goals. Each of these methods can be identified as having a different principle

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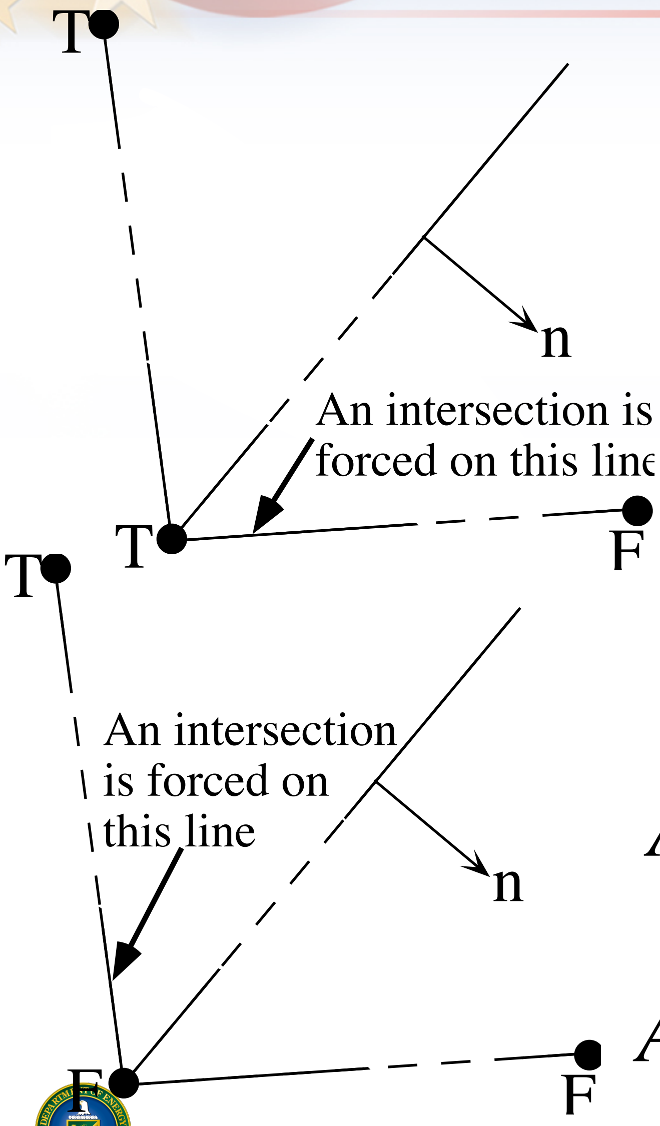
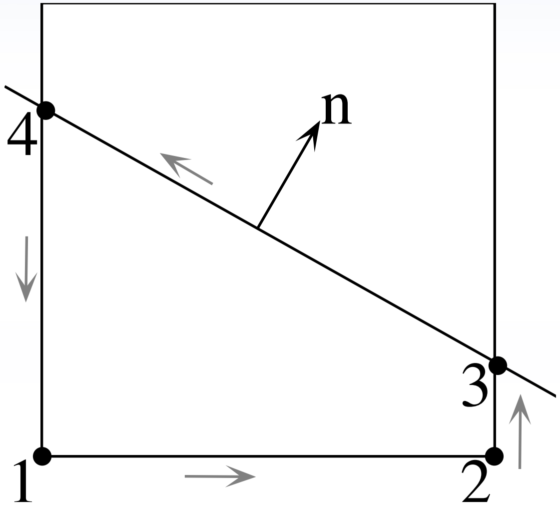
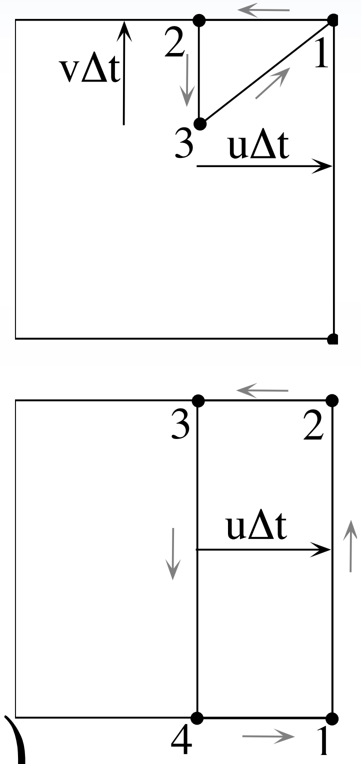
Why did I write "Reconstructing Volume Tracking" with Doug Kothe.

- **I wrote the paper because the standard way of coding up a volume of fluid method was so hard to debug.**
- **I thought we had a better way to put the method together using computational geometry (i.e., a "toolbox")**
- **Once the method was coded it needed to be tested:**
    - In addition existing methods for testing these methods were pretty lame.
    - We came up with some new tests borrowed from the high-resolution methods community (combining the work of several researchers Dukowicz's vortex, Leveque's time reversal, Smolarkiewicz's deformation field)

Using Computational Geometry to Construct a VOF or Volume Tracking Method







Fluxes

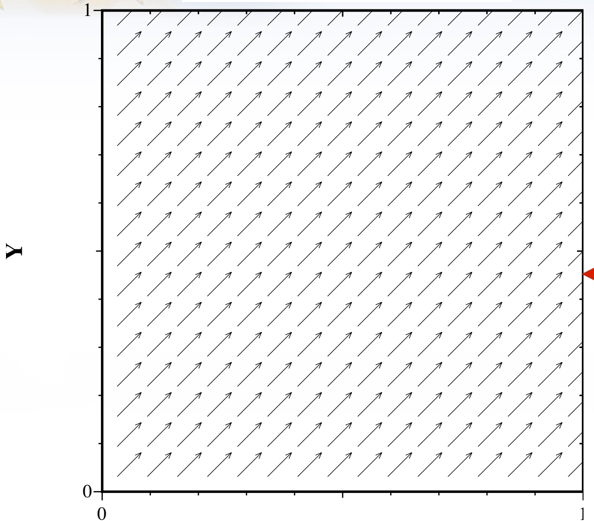
$$A = \frac{1}{2}\sum_{v=1}^{n}\left(x_v y_{v+1} - x_{v+1} y_v\right)$$

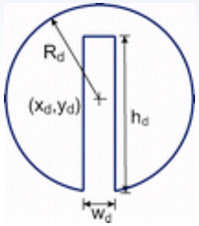
$$A = \frac{\pi}{6}\sum_{v=1}^{n}\left(r_v + r_{v+1}\right)\left(r_v z_{v+1} - r_{v+1} z_v\right)$$

Why did this paper get cited so much?

Test Problems

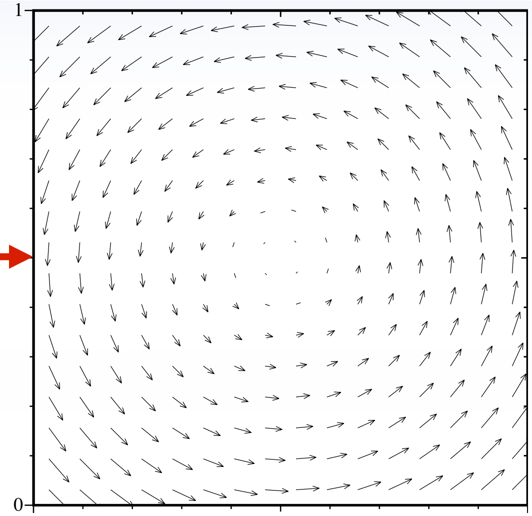
Translation





Too Easy!
For Debugging

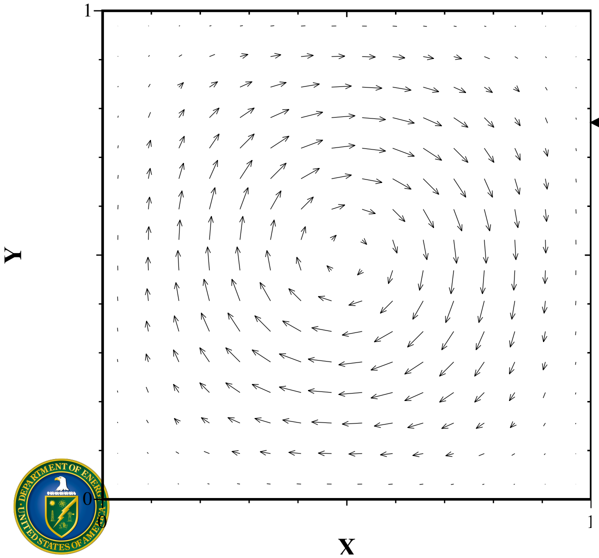
Solid Body Rotation



Vortex

$$u=-\frac{\partial\Psi}{dy},v=\frac{\partial\Psi}{dx}$$

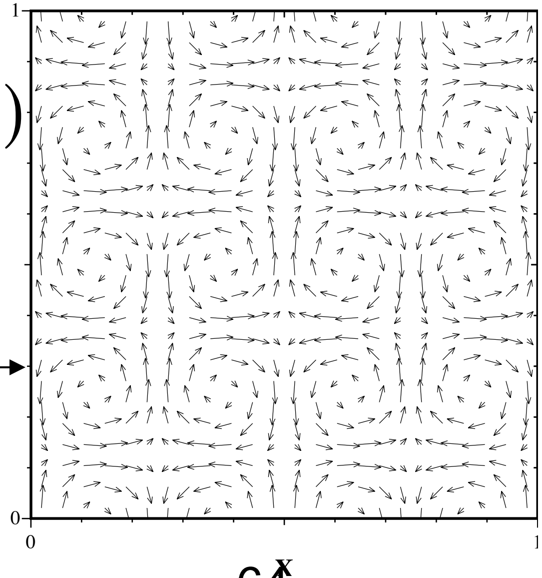
Deformation Field

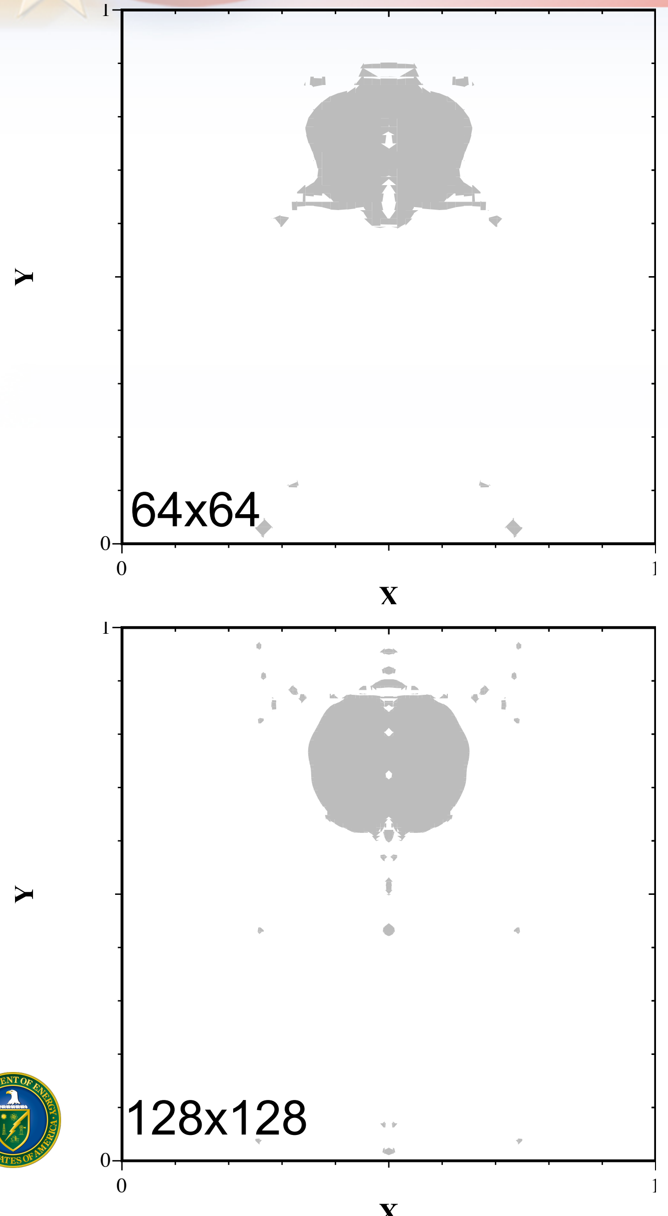


$$\Psi=\frac{1}{\pi}\sin^2(\pi x)\cos^2(\pi y)$$

$$\Psi=\frac{1}{4\pi}\sin\left(4\pi\left(x+\tfrac{1}{2}\right)\right)$$

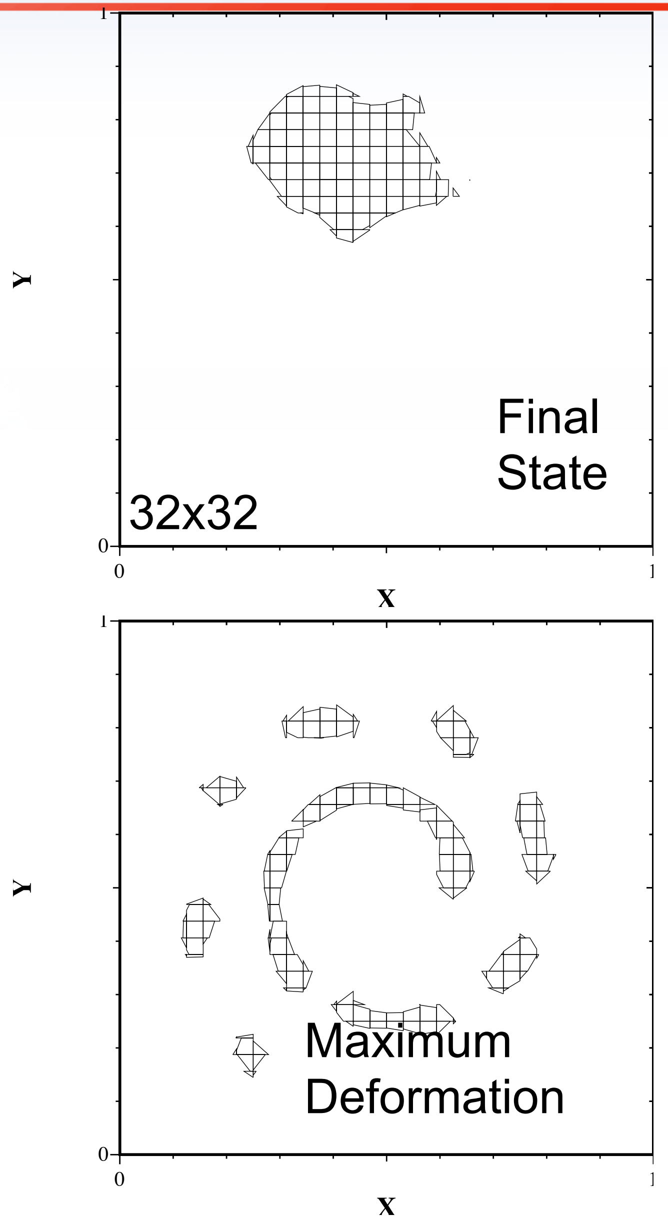
$$\times\cos\left(4\pi\left(y+\tfrac{1}{2}\right)\right)$$



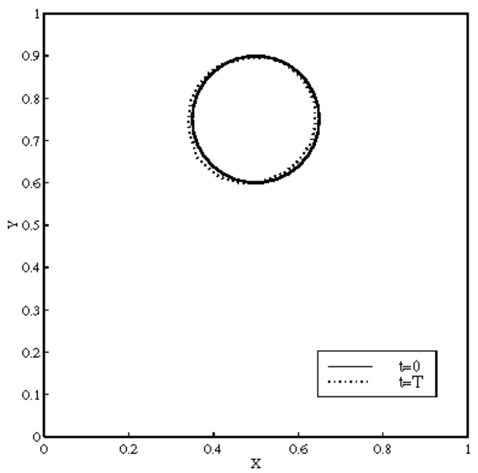


Deformation Flow with Time Reversal

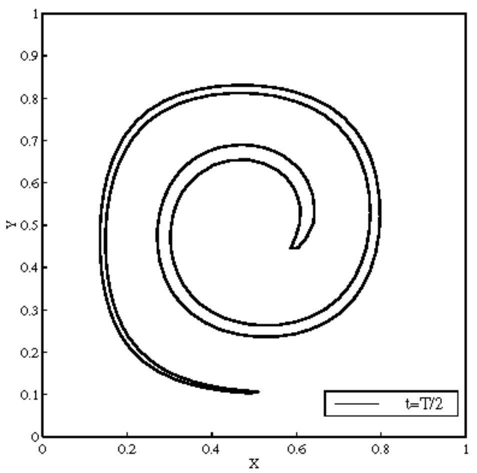
Vortex with Time Reversal

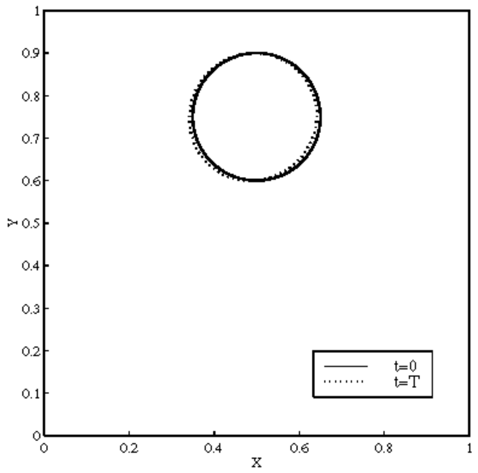


Single Vortex: Front Tracking Solutions

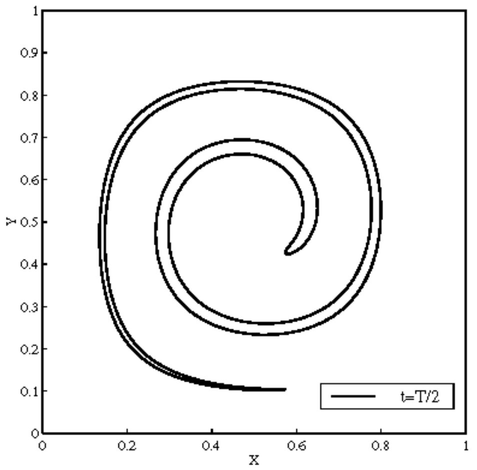


32x32 grid



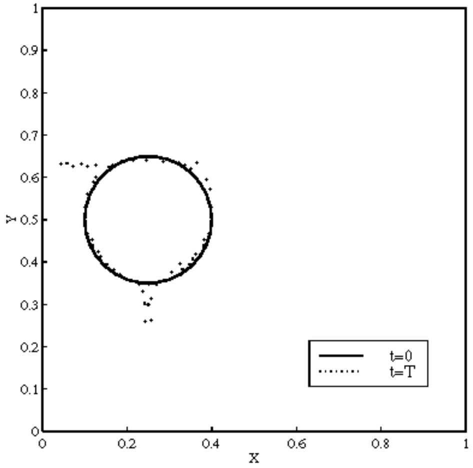


128x128 grid

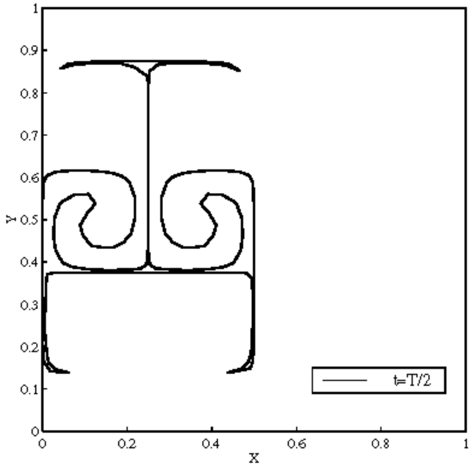


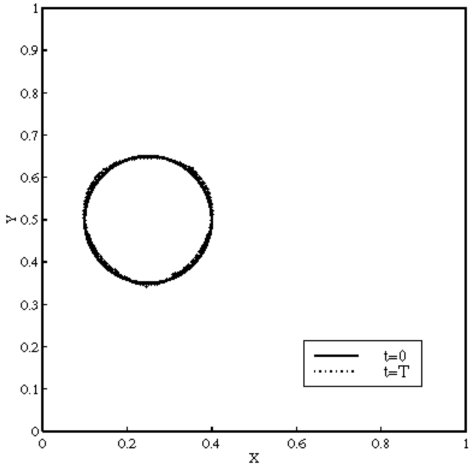
solutions by
Damir Juric

Deformation Field: Front Tracking Solutions

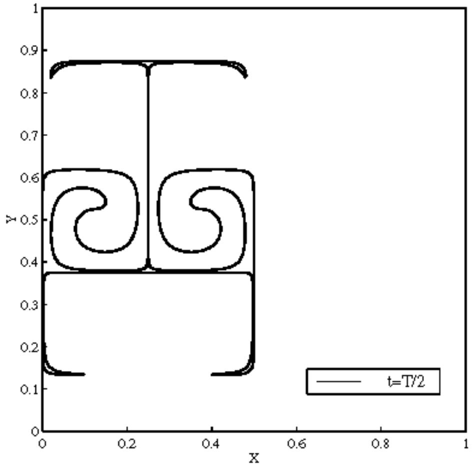


32x32 grid



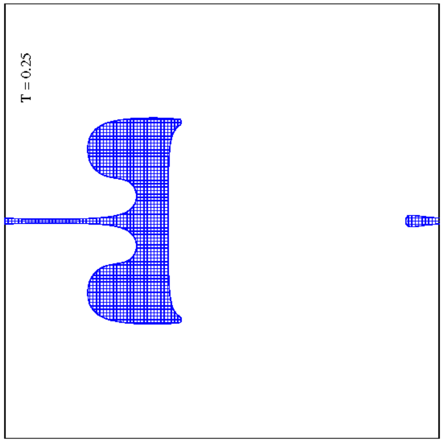


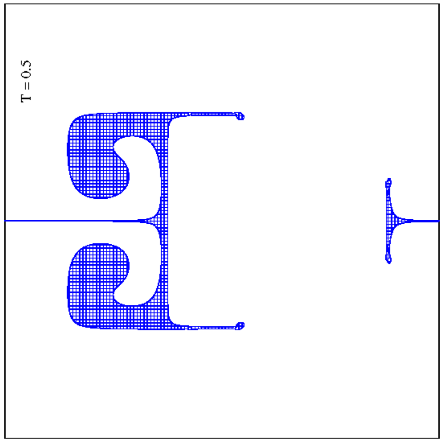
128x128 grid



solutions by
Damir Juric

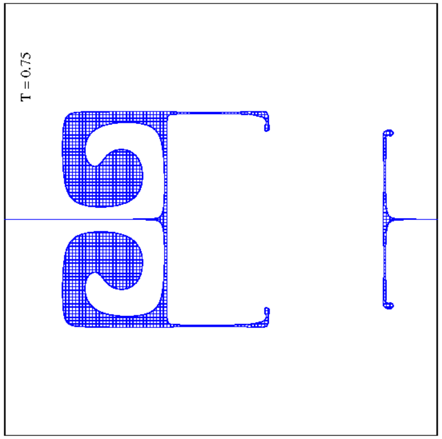
Deformation Field: PPIC Solutions

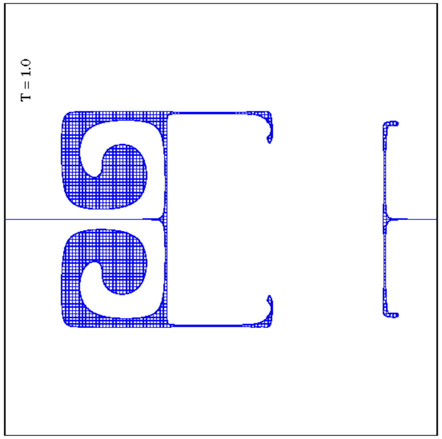




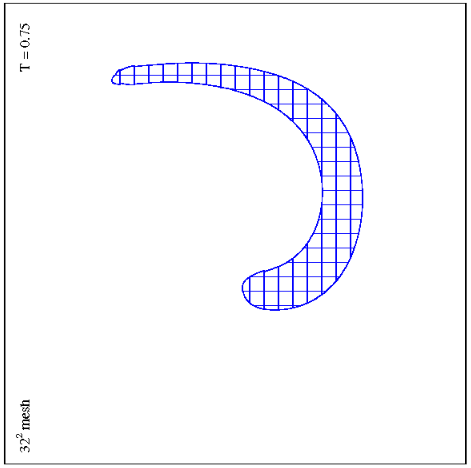
128x128 grid

solutions by
Glenn Price

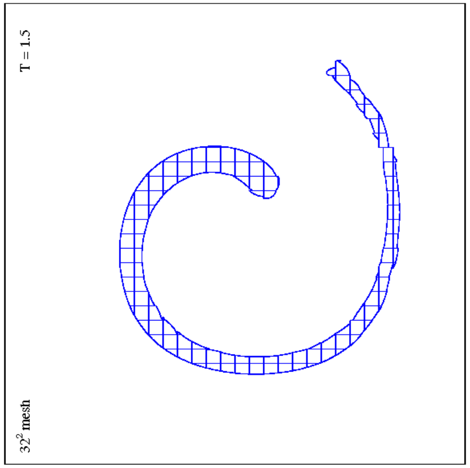




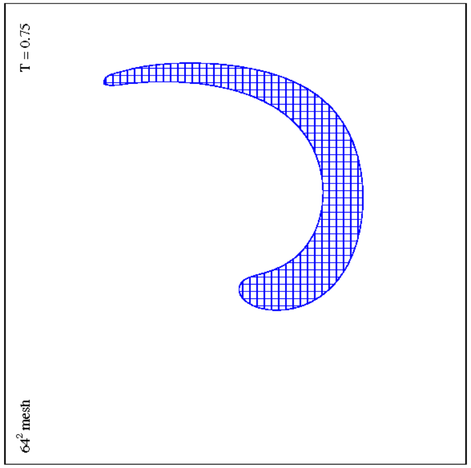
Single Vortex: PPIC Solutions



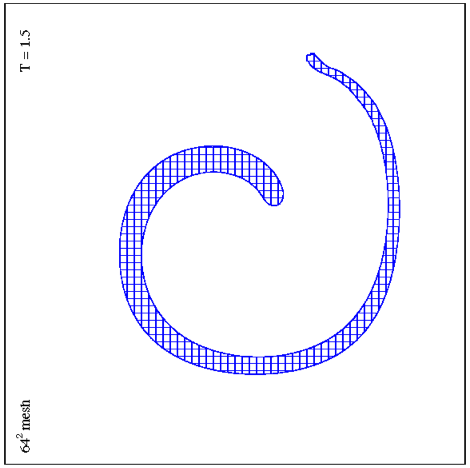
32x32 grid



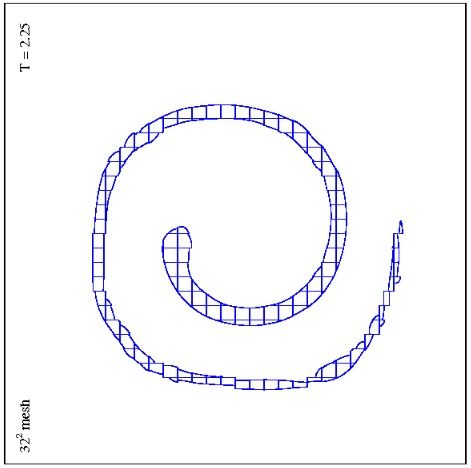
solutions by
Glenn Price

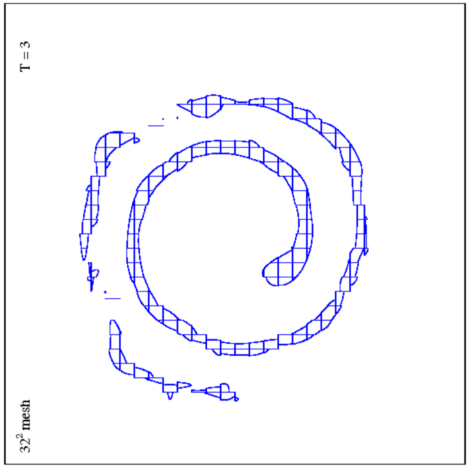


64x64 grid

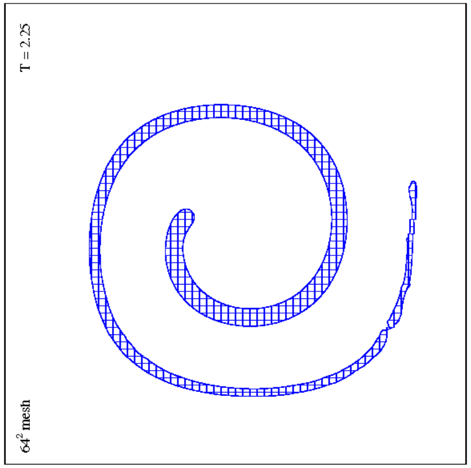


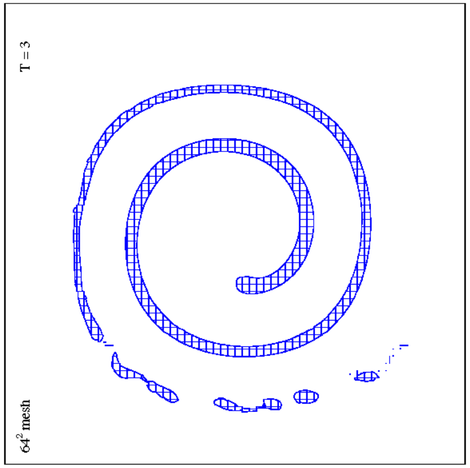
Single Vortex: PPIC Solutions





32x32 grid





64x64 grid

solutions by
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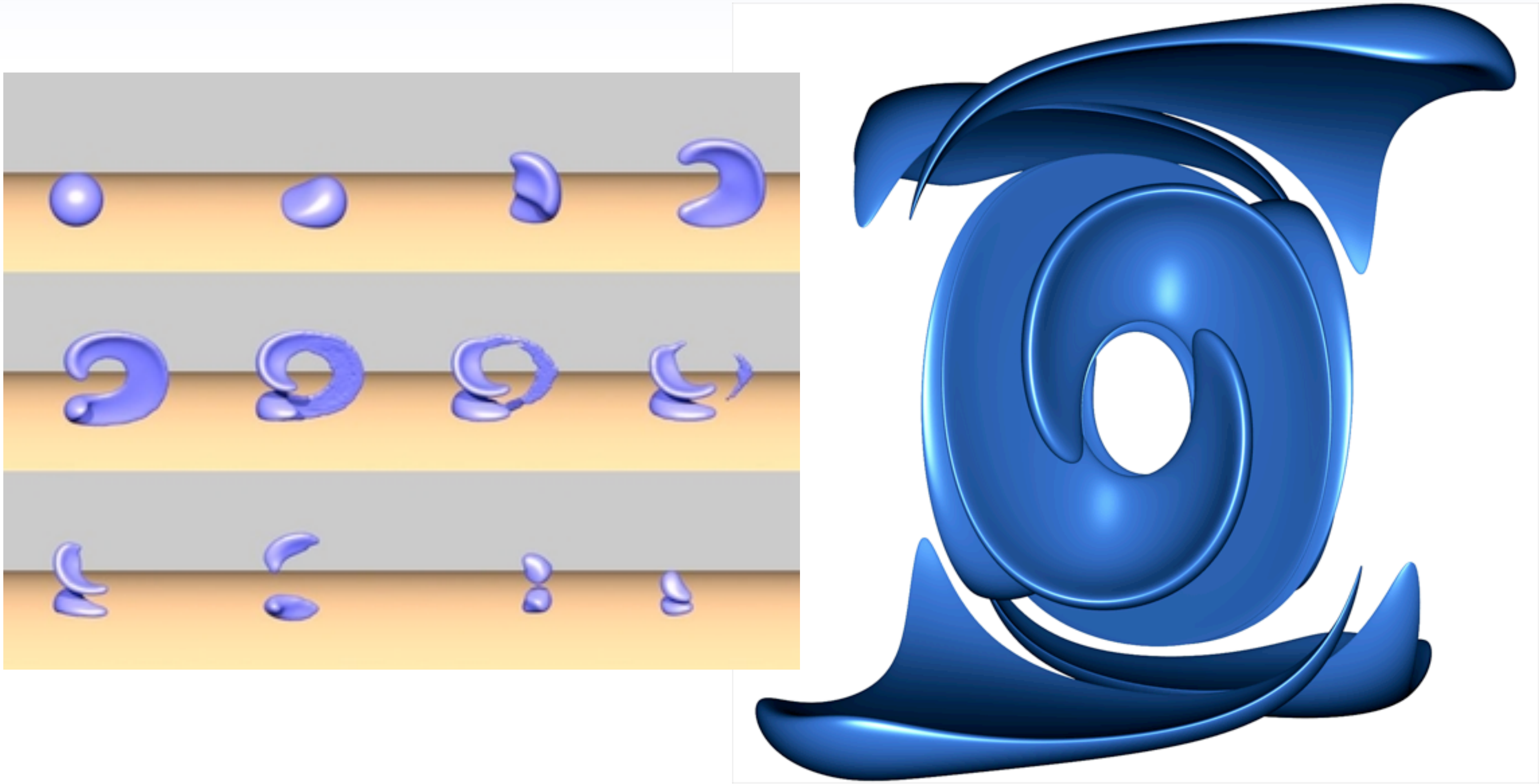
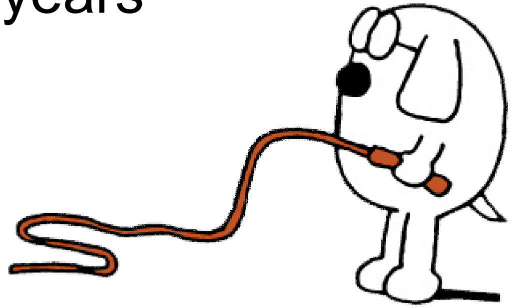
In fact 3-D Versions of these problems now exist thanks to Fedkiw, Enright, Ferzinger and Mitchell.



The new tests came from the level set community, who were originally quite resistant to these problems. In the process they have made their method a great deal better.

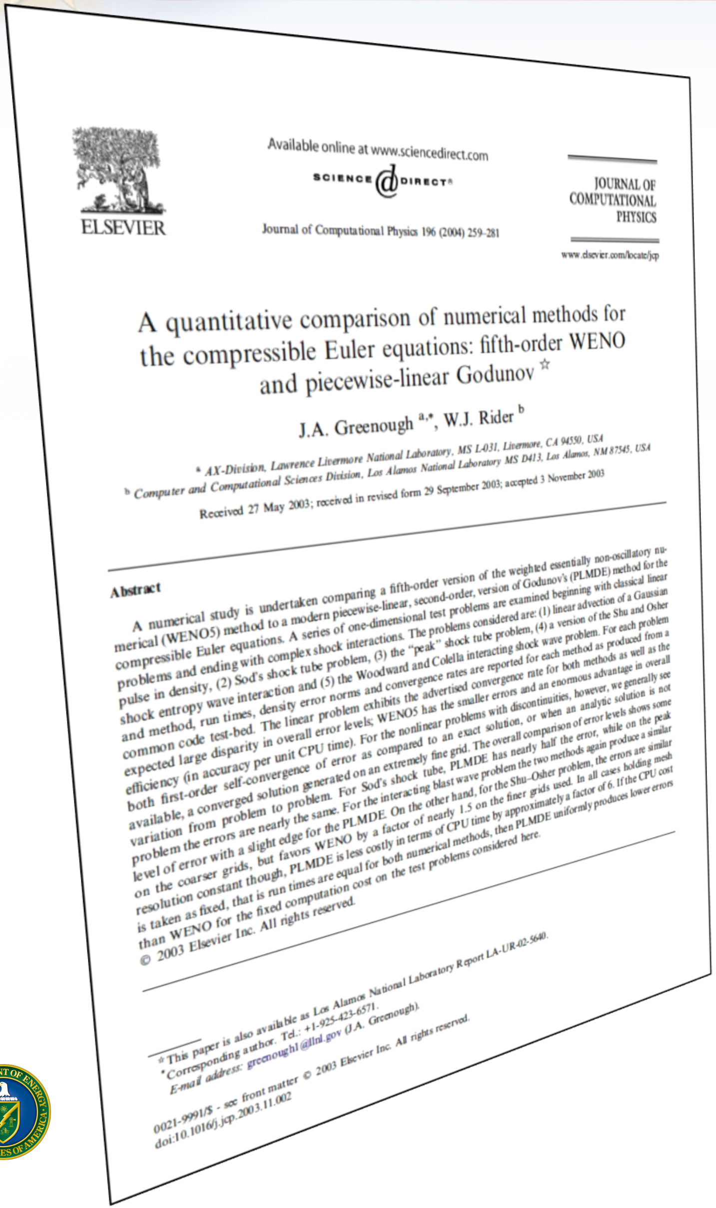
Why did I write the paper on "Accurate Monotonicity and Extrema-Preserving Methods…"

- **I had developed some new methods that extended the concepts in "high-resolution" methods**
- **To provide an introduction to *high-resolution* schemes there is a simple principle to invoke.**
  - These methods have provided an enormous upgrade in computational performance over the past 30 years



  - Dogbert: "*Logically all things are created by a combination of simpler, less capable components*" (see Laney in Computational Gasdynamics)
  - I wanted to make the simple components, the older high-resolution methods (e.g. TVD, ENO, WENO, etc…)

Summary of Greenough-Rider's paper that formed the motivation for the later paper.



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A quantitative comparison of numerical methods for the compressible Euler equations: fifth-order WENO and piecewise-linear Godunov ☆

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Abstract

A numerical study is undertaken comparing a fifth-order version of the weighted essentially non-oscillatory numerical (WENO5) method to a modern piecewise-linear, second-order, version of Godunov's (PLMDE) method for the compressible Euler equations. A series of one-dimensional test problems are examined beginning with classical linear problems and ending with complex shock interactions. The problems considered are: (1) linear advection of a Gaussian pulse in density, (2) Sod's shock tube problem, (3) the "peak" shock tube problem, (4) a version of the Shu and Osher shock entropy wave interaction and (5) the Woodward and Colella interacting shock wave problem. For each problem and method, run times, density error norms and convergence rates are reported for each method as produced from a common code test-bed. The linear problem exhibits the advertised convergence rate for both methods as well as the expected large disparity in overall error levels; WENO5 has the smaller errors and an enormous advantage in overall efficiency (in accuracy per unit CPU time). For the nonlinear problems with discontinuities, however, we generally see both first-order self-convergence of error as compared to an exact solution, or when an analytic solution is not available, a converged solution generated on an extremely fine grid. The overall comparison of error levels shows some variation from problem to problem. For Sod's shock tube, PLMDE has nearly half the error, while on the peak problem the errors are nearly the same. For the interacting blast wave problem the two methods again produce a similar level of error with a slight edge for the PLMDE. On the other hand, for the Shu–Osher problem, the errors are similar on the coarser grids, but favors WENO by a factor of nearly 1.5 on the finer grids used. In all cases holding mesh resolution constant though, PLMDE is less costly in terms of CPU time by approximately a factor of 6. If the CPU cost is taken as fixed, that is run times are equal for both numerical methods, then PLMDE uniformly produces lower errors than WENO for the fixed computation cost on the test problems considered here.

☆ This paper is also available as Los Alamos National Laboratory Report LA-UR-02-5640.

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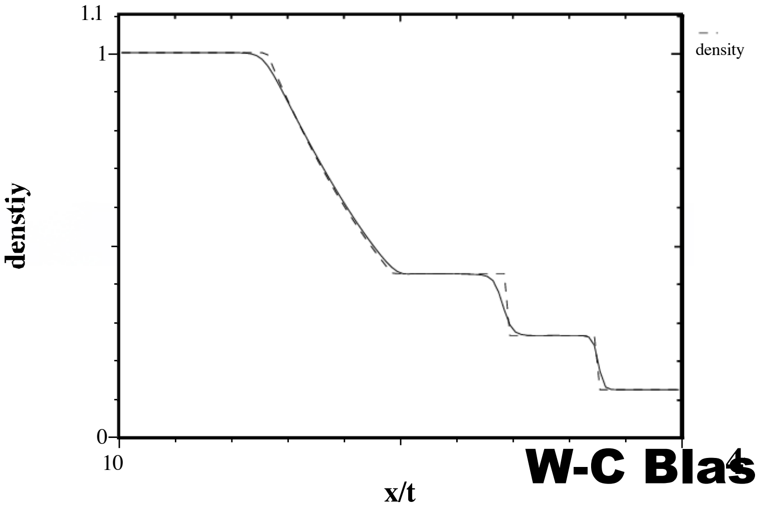
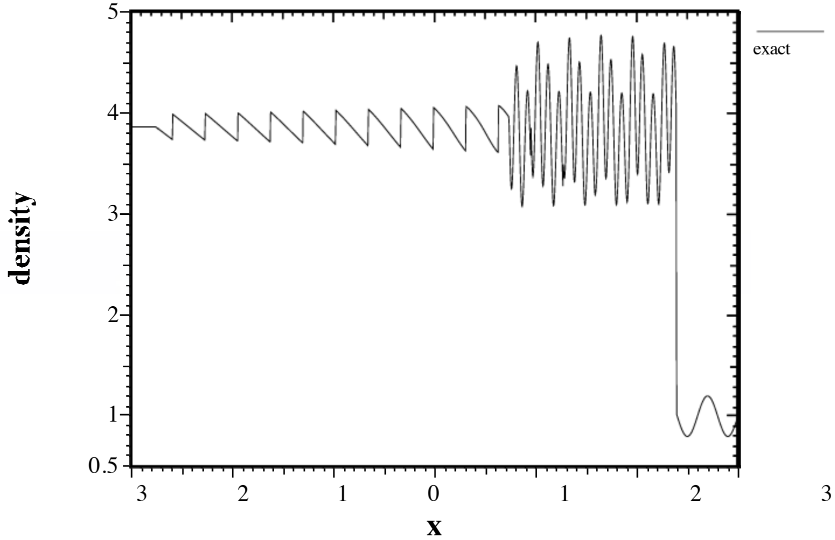
- WENO5 is much more efficient for linear problems
- PLMDE is more efficient than WENO5 on all nonlinear problems (with discontinuities)
- The advantage is unambiguous for Sod's shock tube and the Interacting Blast Waves
- The advantage is less clear-cut for the "peak" problem
- At a given mesh spacing WENO5 gives better answers for the Shu-Osher problem, but worse than PLMDE at fixed computational expense

1-D Shock Physics Problems

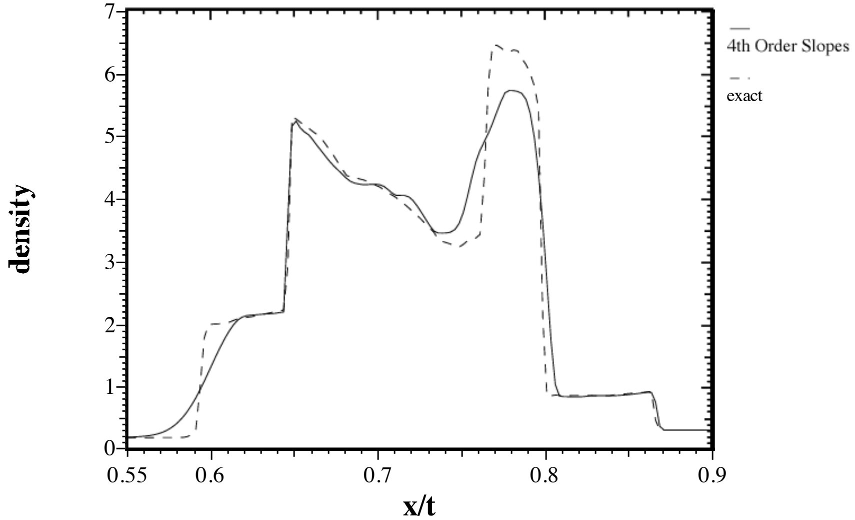
Sod’s Shock Tube



Shu-Osher Entropy Wave



W-C Blast Waves



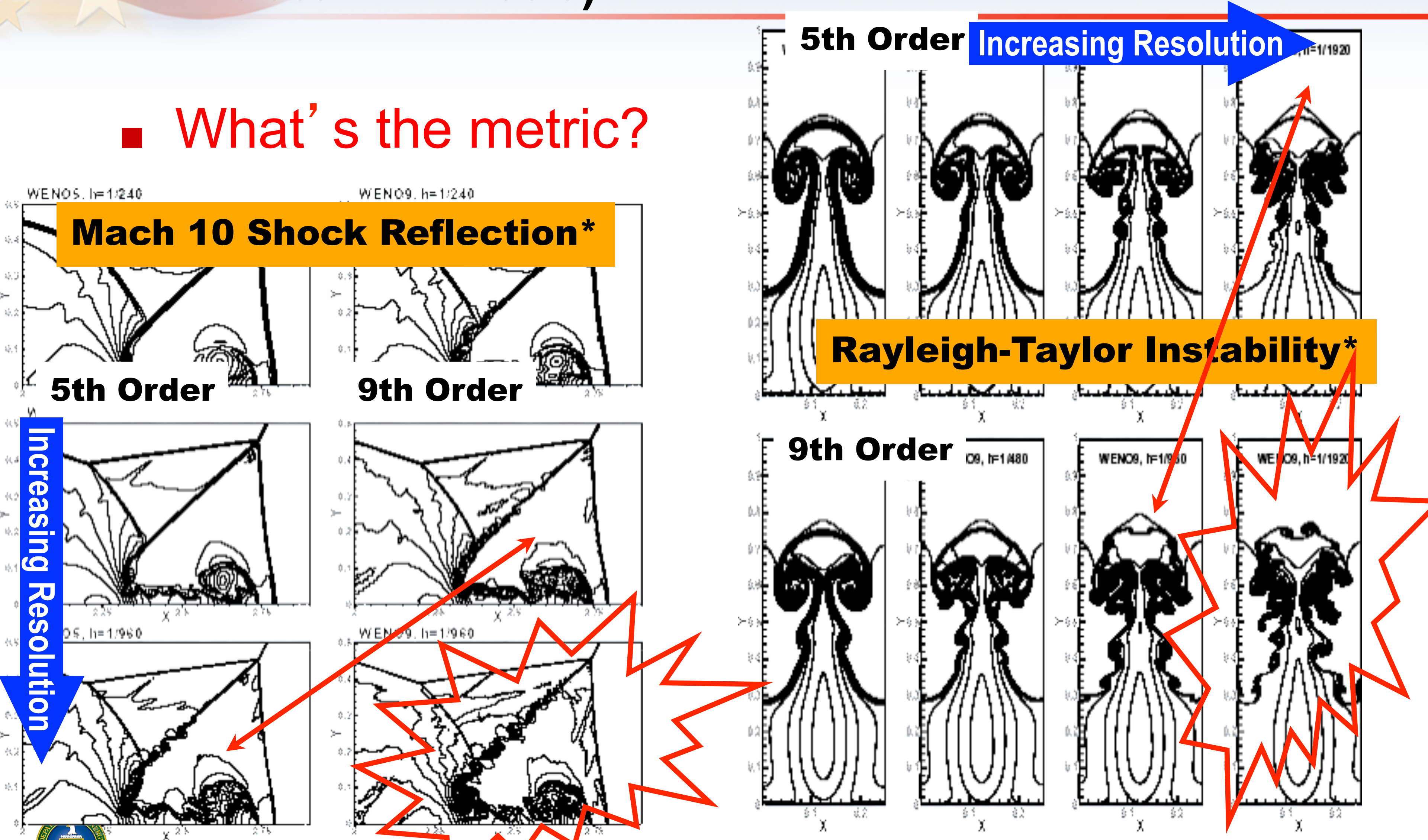
Goal: Compare results with “off-the-shelf” methods (Greenough-Rider)

Efficiency is also important!
High-Order must pay its way

- Both methods are implemented in a similar manner (by me)
- For these 1-D problems WENO5 was about 6 times the cost of PLMDE
  - Two nonlinear differences per edge through the flux-splitting (~1.5X)
  - Multistage Runge-Kutta instead of forward-in-time (~3X)
  - Smaller CFL number (~1.5 X)
- Error/CPU - provides a real measure of efficiency

Multidimensional Problems Are Difficult (non-determininstic)

- What's the metric?



Mach 10 Shock Reflection*

5th Order

9th Order

Increasing Resolution

Rayleigh-Taylor Instability*

5th Order

9th Order

Increasing Resolution

*Resolution of High Order WENO Schemes for Complicated Flow Structures
Shi, Zhang & Shu, J. Comp. Phys. **186**, 2003.

Why discontinuities are special: first order accuracy is expected for solutions containing discontinuities.

- **For *coupled systems* (even linear) with *discontinuities* high-order accuracy is lost between characteristics emanating from the discontinuity***
  - Several recent works have re-confirmed this result (Osher, Carpenter, *Greenough & Rider*)
  - Can be overcome is very restrictive special cases‡

- **Generally with smooth data and a nonlinear system of hyperbolic conservation laws a discontinuity (i.e., shock) will eventually form**
  - *Therefore the loss of accuracy is virtually inevitable!*

***Majda & Osher, *Comm. Pure Appl. Math.*, 30 1977.**

‡Siklosi & Kriess, SIAM J. Num. Anal., 41, 2003.

How did verification contribute to its difficulty in being published?

- **We thought that continuing the line of investigation from Greenough-Rider would be a good idea,…**
  - So we computed the detailed error character of both old and new methods with a focus on overall efficiency.
- **Here is a quote from our peer review:**

“I know that LLNL and LANL are currently making a big deal over verification, but in fact the issues that are discussed here in laborious detail have been part of the common culture in the CFD research community for the last 25 years (at least), and consequently don't require this level of recapitulation / justification in a JCP article.”

We capitulated, but the comment has no basis in fact.

Let's look at the presentation of shock problems in detail.

From Sod's classical 1978 paper (*J. Comp. Phys*. **27**)
(i.e., where Sod's problem comes from)

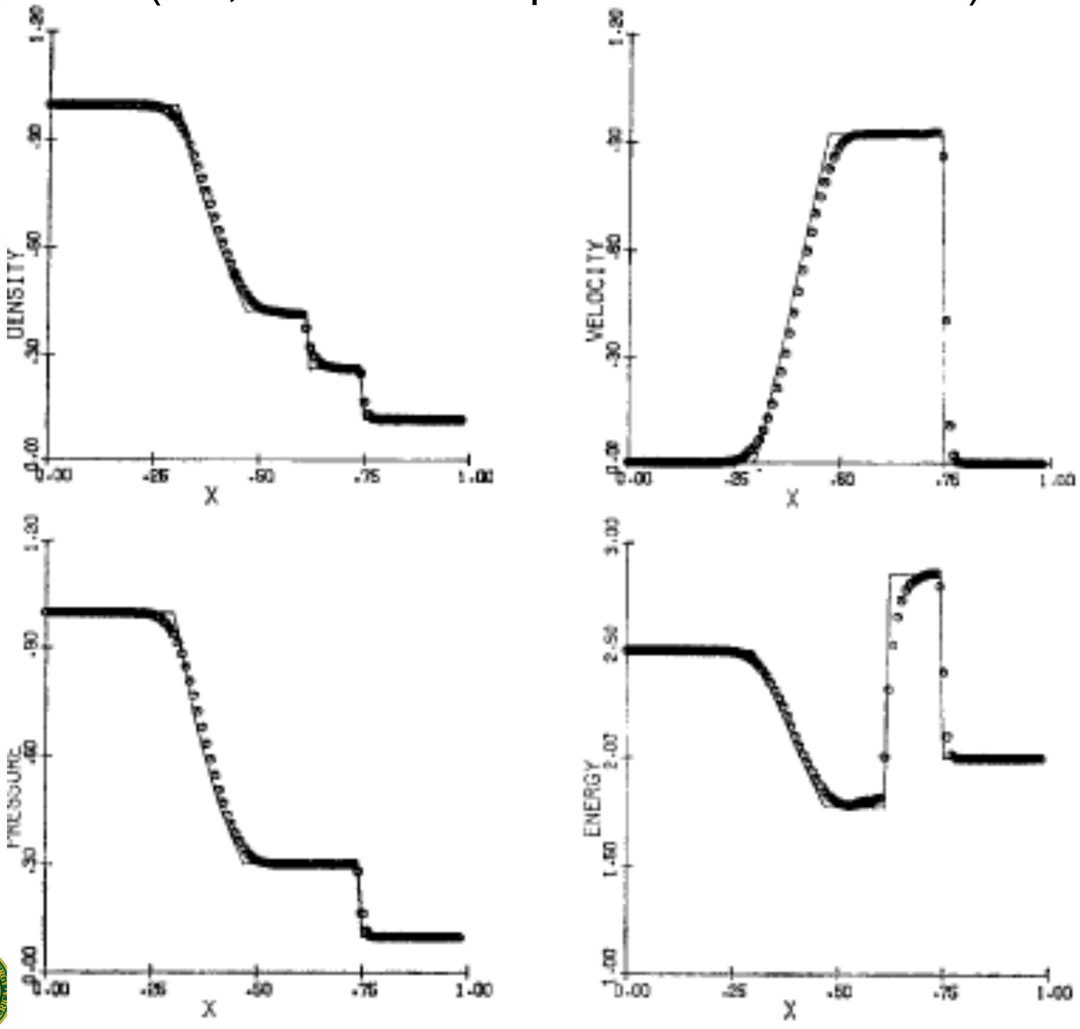
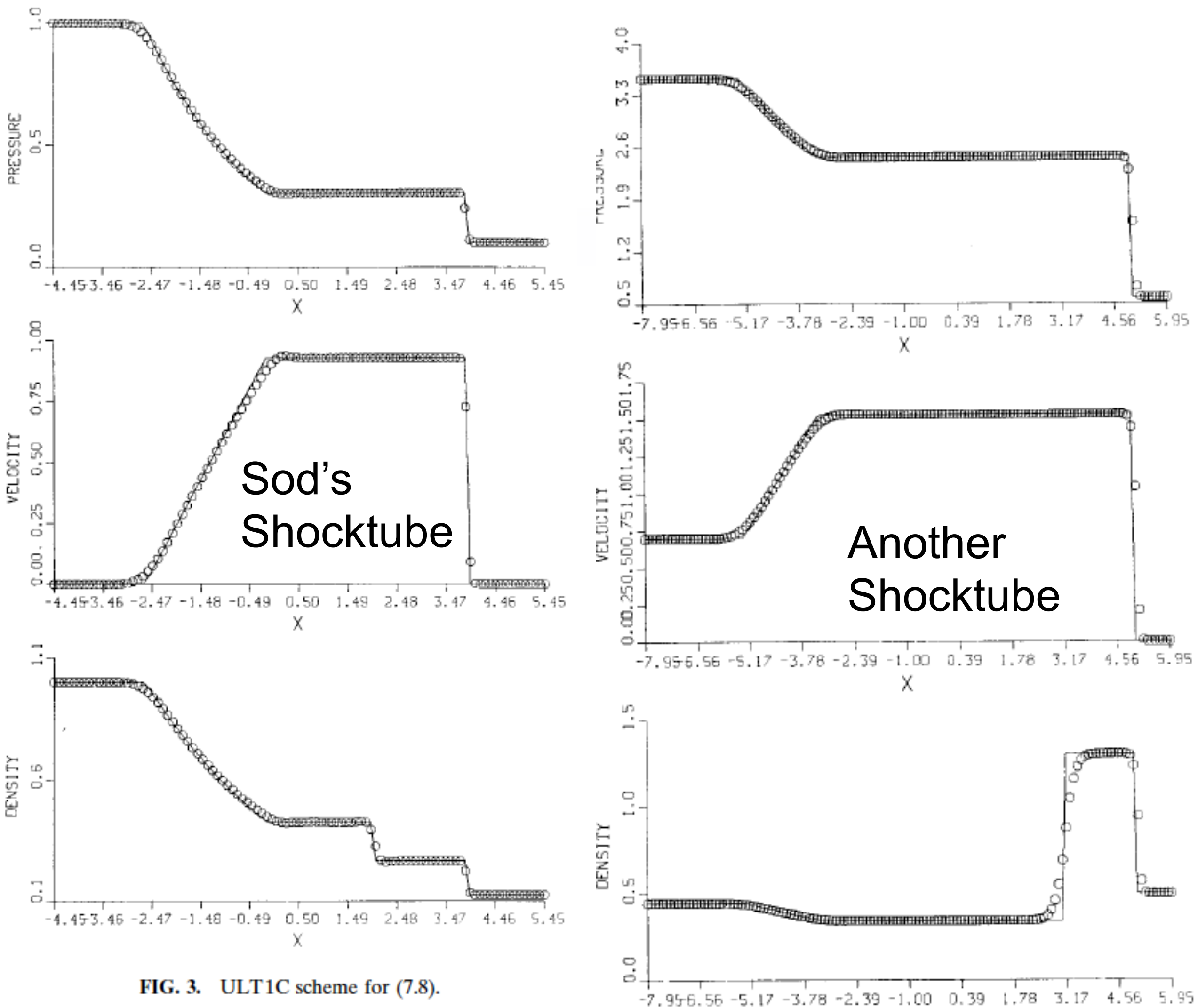


FIG. 14. Hybrid method with *ACM*.

No error or convergence rates discussed anywhere in the paper. Run time on a computer is given.

Move forward 5 years to Harten's paper introducing TVD methods

From Harten's classical 1983 paper (*J. Comp. Phys*. **49**)
(i.e., where TVD methods are introduced)



Sod's Shocktube

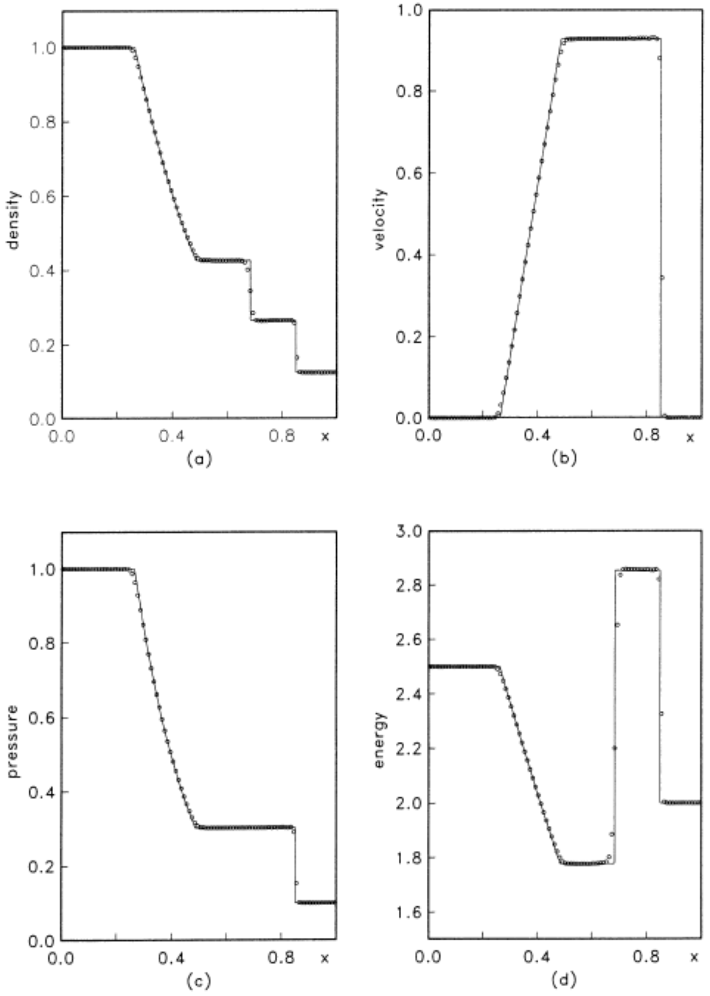
Another Shocktube

FIG. 3. ULT1C scheme for (7.8).

No error or convergence rates discussed anywhere in the paper. Run time on a computer is given.

Move forward another decade to Huynh’s excellent paper in SIAM J. Num. Anal.

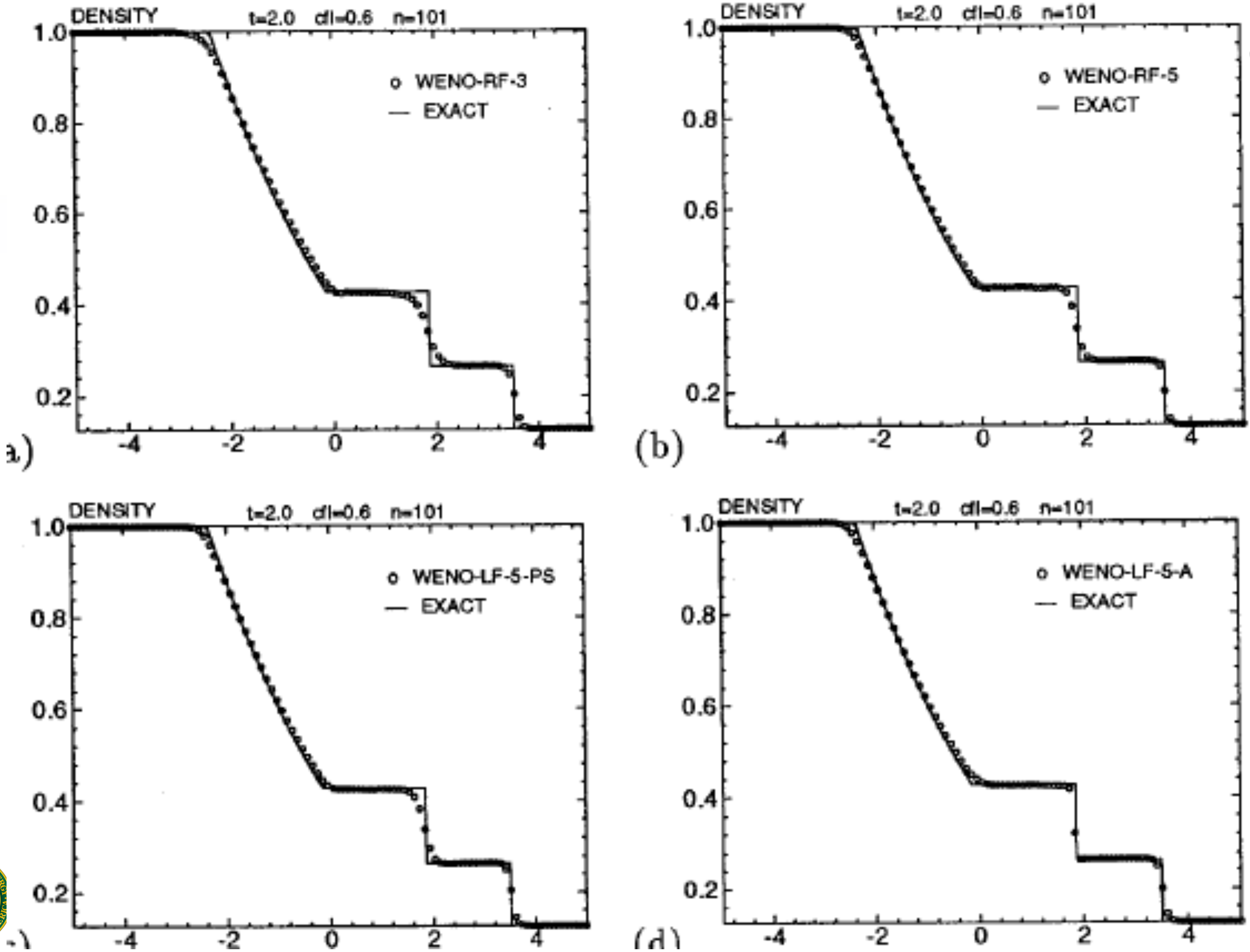
From Huynh’s 1995 paper (*SIAM J Num. Anal.* **49**)
(i.e., where a fantastic overview of methods is provided)



No error or convergence rates discussed anywhere in the paper. Run time on a computer is given.

Staying in this era, but returning to J. Comp. Phys.

From Jiang and Shu's WENO paper (*J. Comp. Phys*. **126** - introduced 5th order WENO)



No error or convergence rates discussed anywhere in the paper. Run time on a computer is given.

So…
What Makes A Calculation Good? Or Bad?

- **The answer to the question 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)
  - In engineering, it is becoming more evidence based
  - Demands on modeling & simulation from society are pushing the community toward a greater reliance on evidence based criteria.

Who Am I ?

- I’m a staff member at Sandia, and I’ve been there SNL for 5 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.