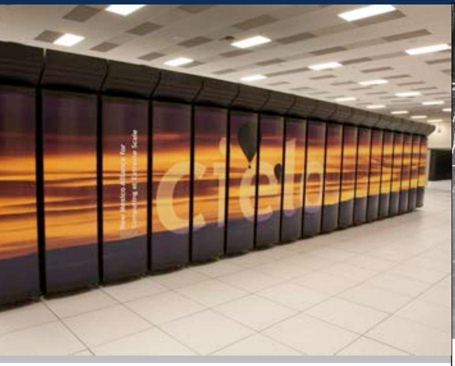
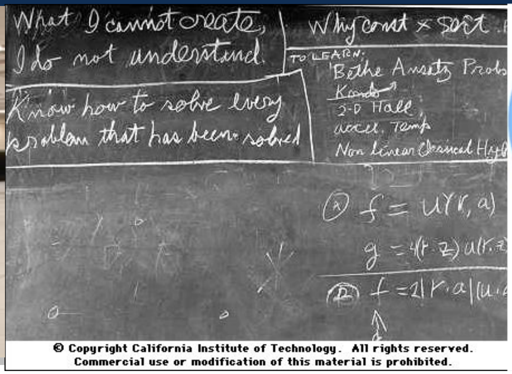
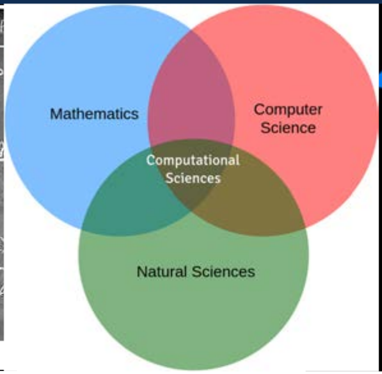
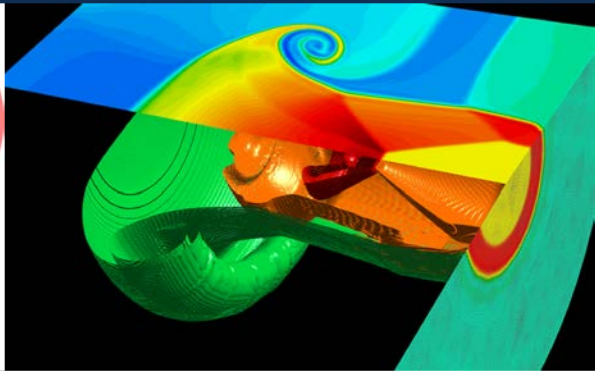
Exceptional service in the national interest

Sandia National Laboratories









The Scientific Method and Computational Science: A happy marriage? or in need of therapy?

Bill Rider, Sandia National Labs (SAND-19-2299PE)

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2018-????

“Computers are incredibly fast, accurate, and stupid: humans are incredibly slow, inaccurate and brilliant; together they are powerful beyond imagination.”
— Albert Einstein

The Three Goals for this Talk

Sandia National Laboratories

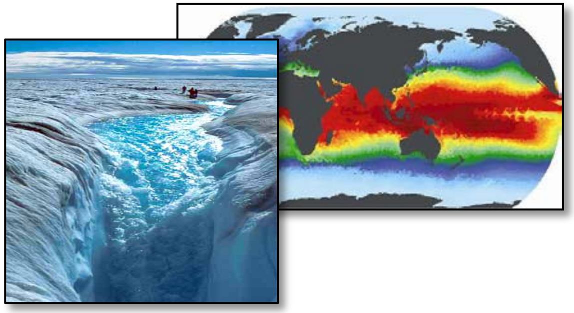
Brief introduction to Sandia and National Security Labs

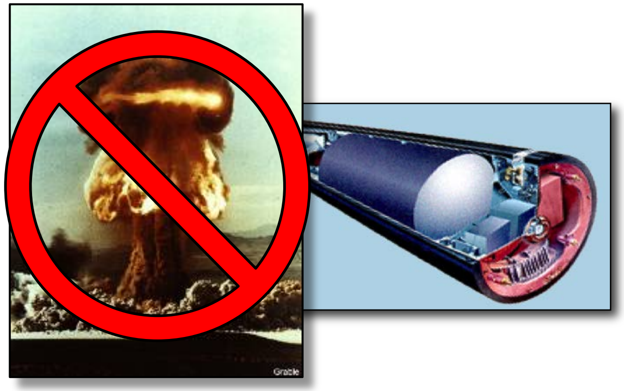
- **Goal 1:** Understand the fundamental tensions of the scientific method and computational science
  - Explore some basic themes in modern computational science, by looking at its origins
- **Goal 2:** Provide some background on the issues associated with the scientific method and the crisis of reproducibility
  - Software and computed results are distinct challenges to standard science
- **Goal 3:** Discuss how verification and validation is actually the way to apply the standard scientific method to computational science
  - **Verification is determining that the computer has the right model**
  - **Validation is comparing the model results to experiment/observation**

Computational Science should seamlessly align with the classical Scientific Method.

SNL's national security mission

- Demands risk-informed decision making; analyzing complex engineering and science phenomena
- Representative high-consequence problem areas:
  - National nuclear security: maintain safe, secure, reliable nuclear stockpile with limited tests; qualify NW (in part) with modeling and simulation
  - Energy: Reduce reliance on foreign energy, reduce energy production carbon footprint energy production
  - Climate change: Understand, mitigate, adapt to effects of global warming
  - Nuclear safety: reactor operations, underground radioactive waste storage : Yucca Mountain, WIPP
  - Security: Cyber, information, infrastructure, homeland
- Limited experimentation and/or data (safety, laws/ethics, practicality, cost/availability)





Exascale Applications Respond to DOE/NNSA Missions in Discovery, Design, and National Security

Scientific Discovery

- **Mesoscale materials and chemical sciences**
- **Improved climate models with reduced uncertainty**

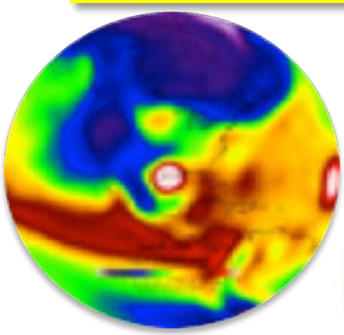
Engineering Design

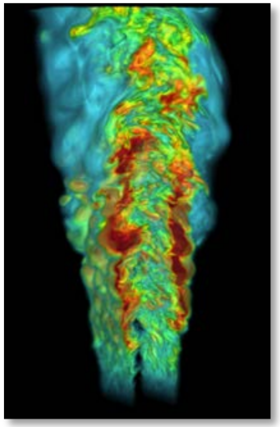
- **Nuclear power reactors**
- Advanced energy technologies
- Resilient power grid

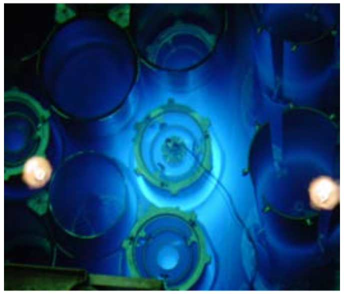
National Security

- **Stockpile stewardship**
- Real-time cybersecurity and incident response
- Advanced manufacturing

Grey Bold Text indicates planned or existing exascale application projects





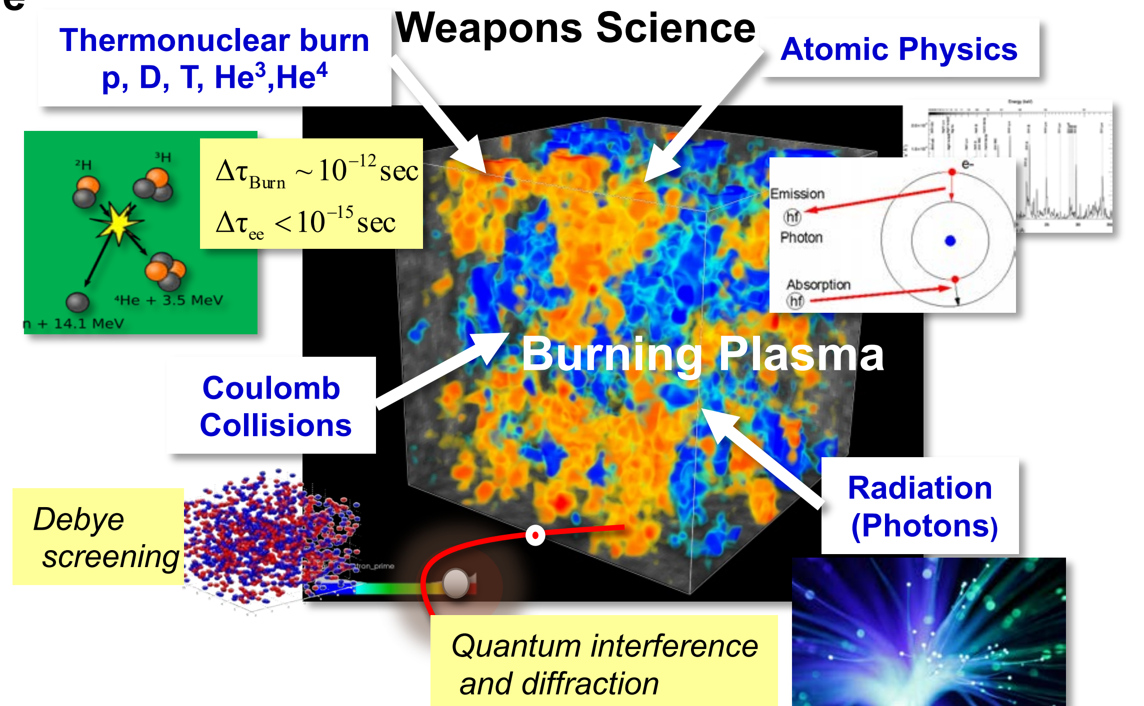


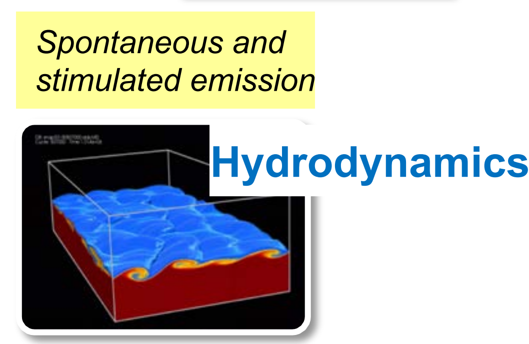
Stockpile Stewardship Challenges

Sandia National Laboratories

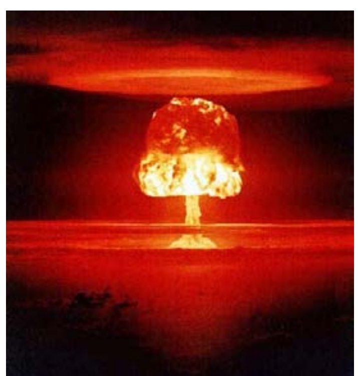
Nuclear Stockpile

- Safety
- Surety
- Reliability
- Robustness



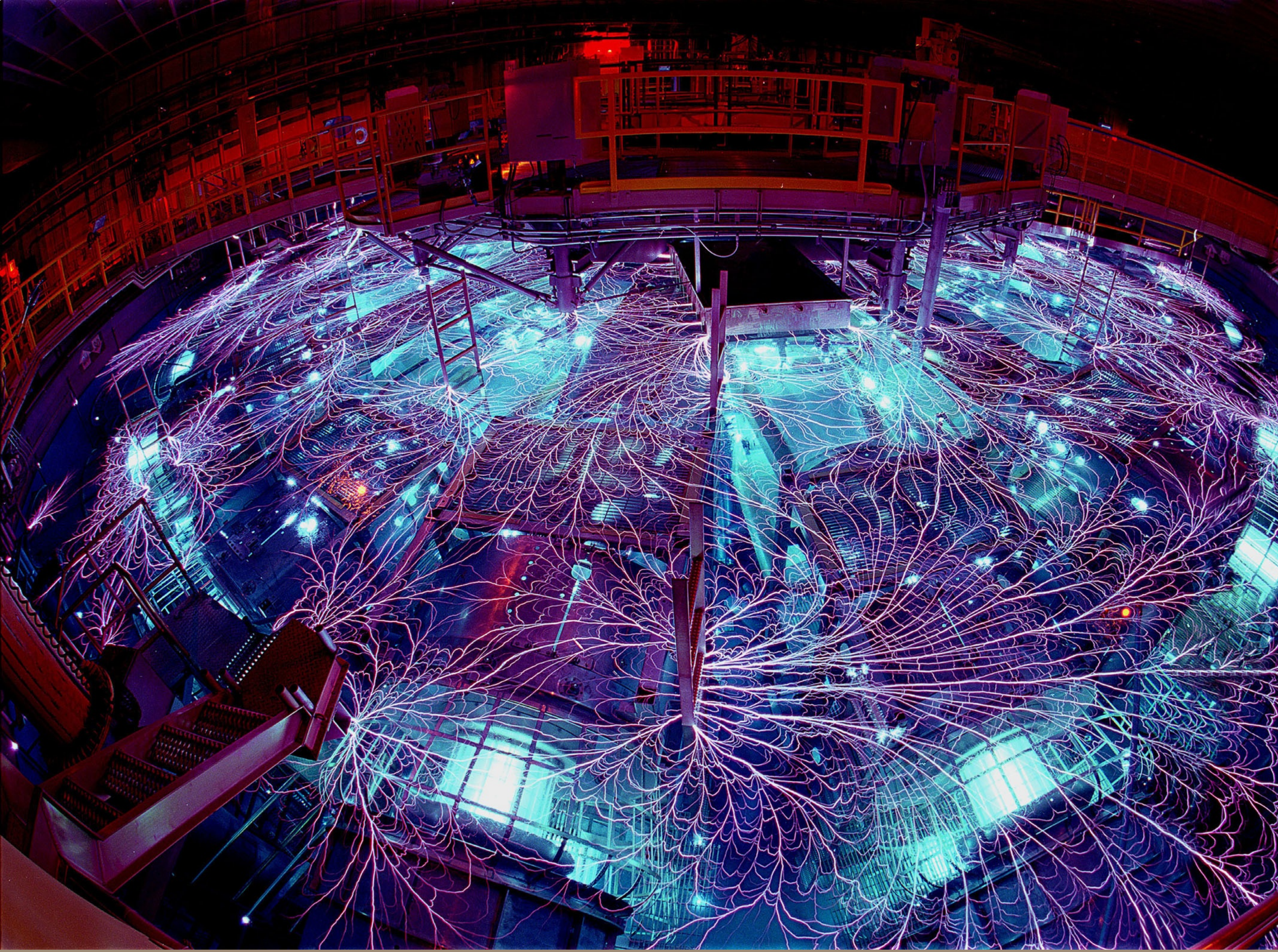


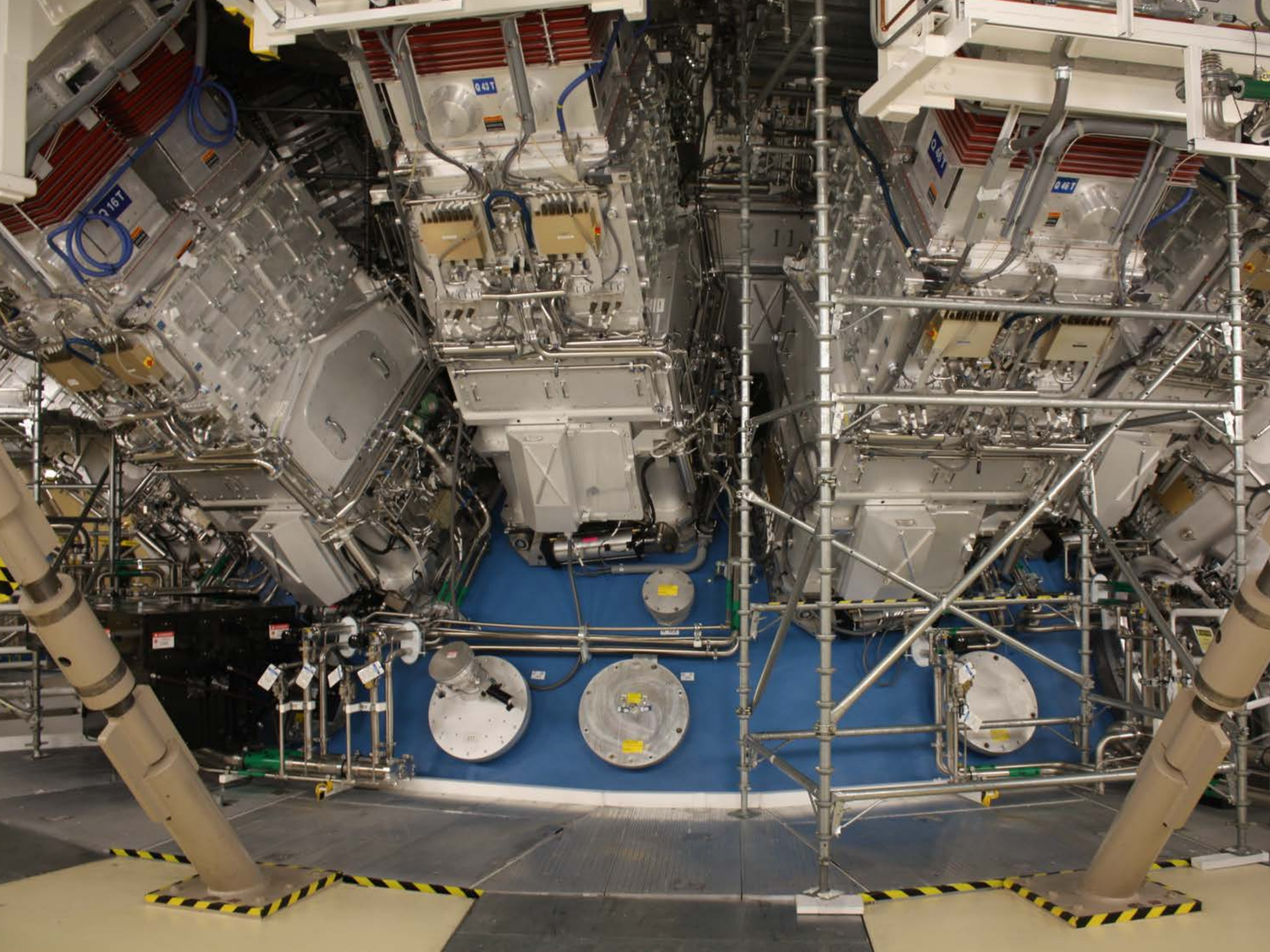
Non-Proliferation and Nuclear Counter Terrorism

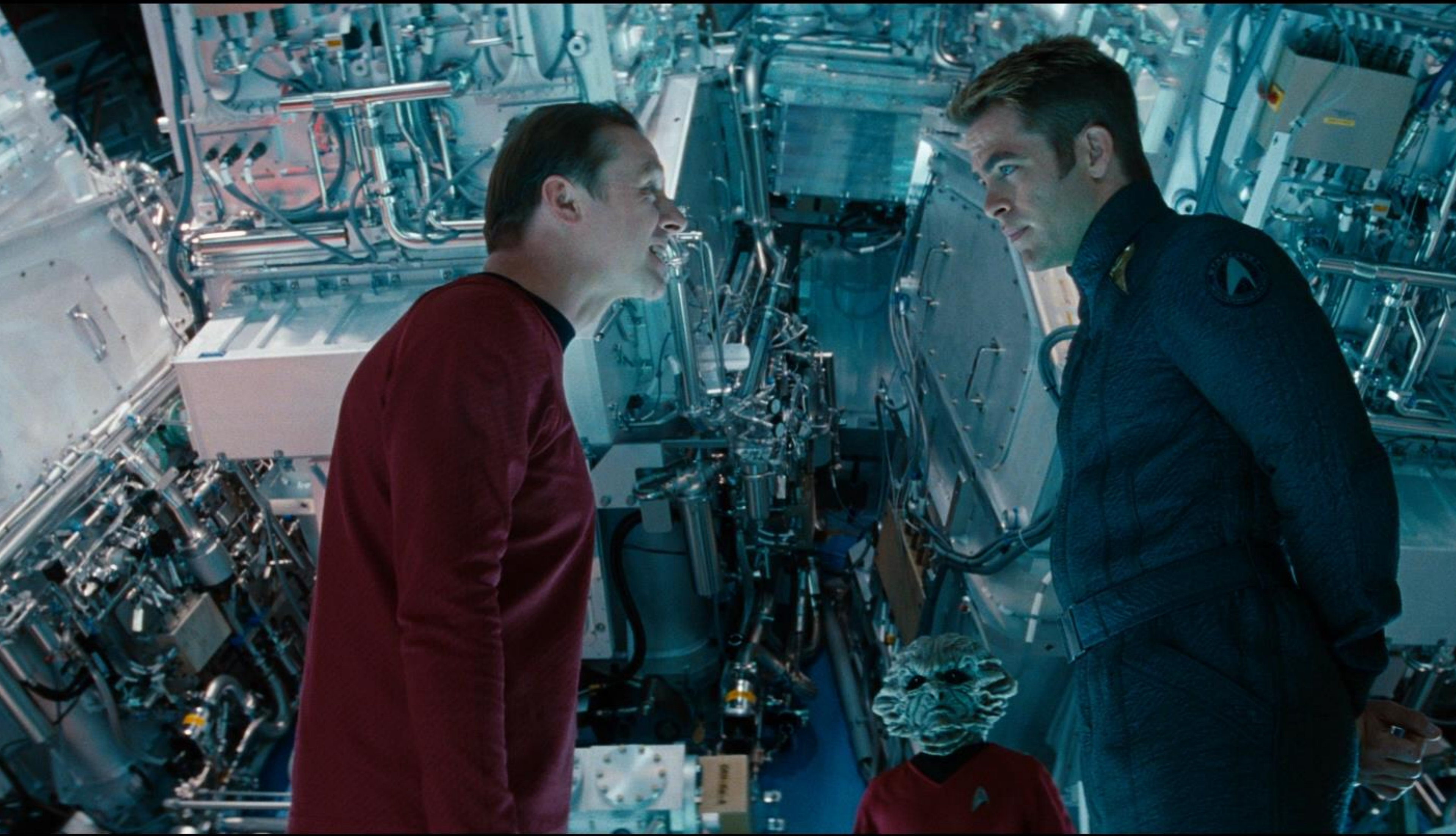



New Mexico Alliance for
Computing at Extreme Scale
NNSA
cielo


IBM
Blue Gene supercomputer
IBM
Blue Gene supercomputer




Q 16T
Q 43 T



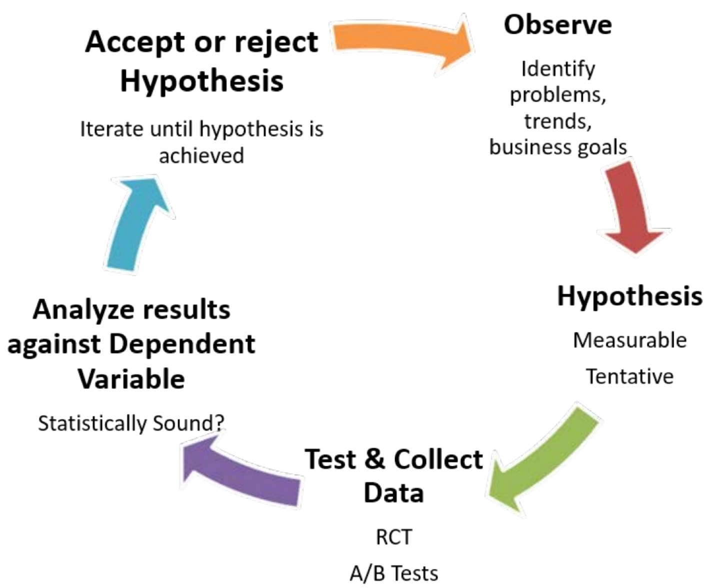

DANGER
NO
STEP
Q 44 T
Q 35 T

“People don’t want to buy a quarter-inch drill. They want a quarter-inch hole.”
— Clayton M. Christensen

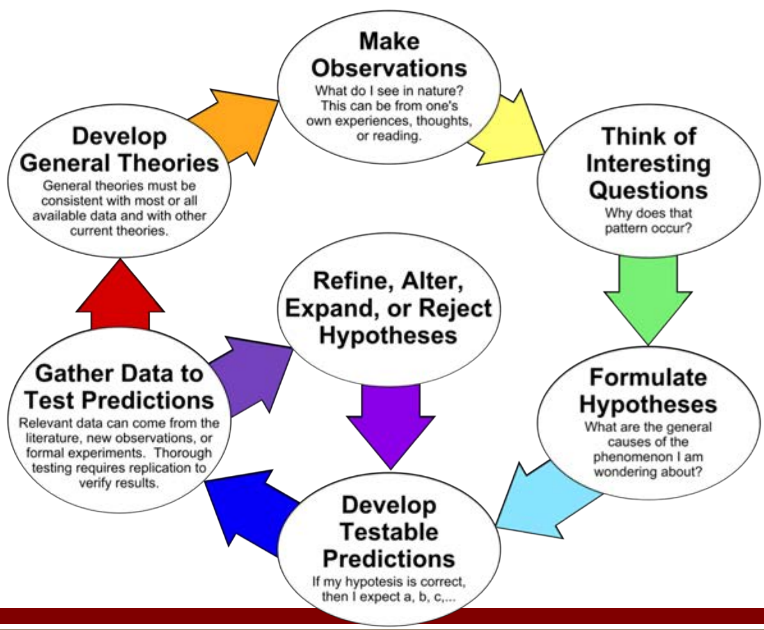
The basics of the scientific method

Sandia National Laboratories

- Ask really good questions about what makes the universe tick.
- **Experiment** or Observe the real world and measure what happens. These measurements are invariably imprecise.
- **Model** and theory the processes in the universe. These models are invariably complex and not generally amenable to exact solution.



The Scientific Method as an Ongoing Process



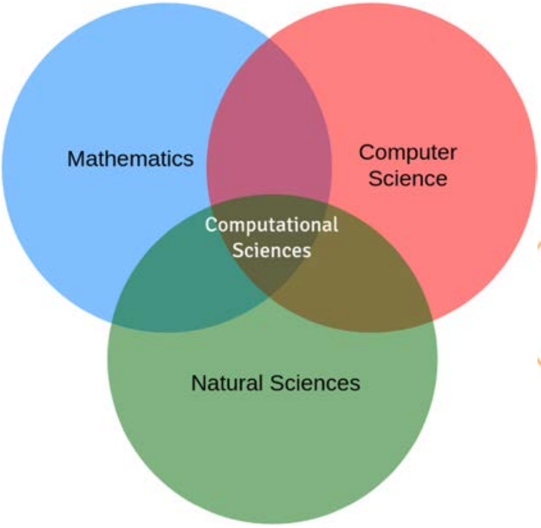
“It doesn't matter how beautiful your theory is ... If it doesn't agree with experiment, it's wrong.”

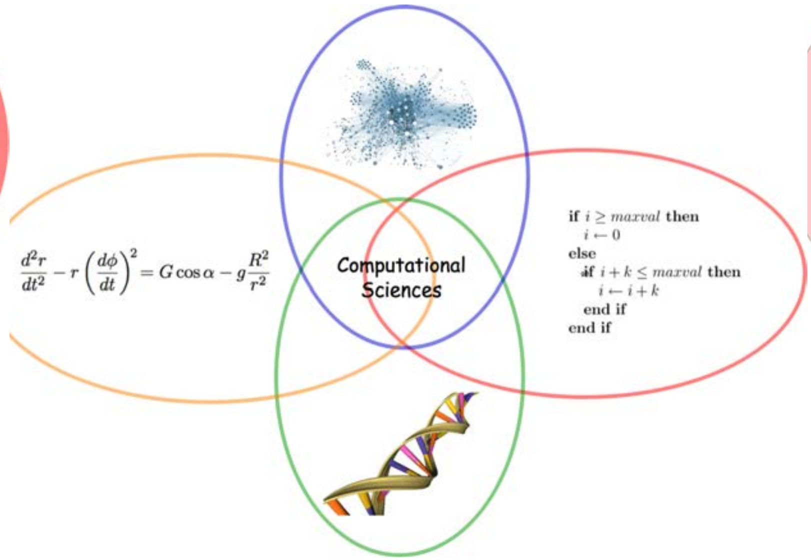
— Richard Feynman

All models are wrong,
but some are useful.
— George Box

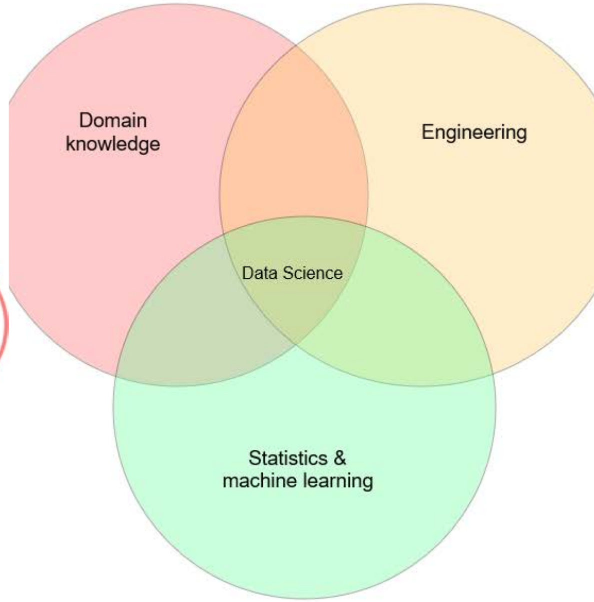
The basics of computational science

- At the center of computational science are **computers**.
- How do we use computers to do science (all the stuff on the previous slides)
- How to use computers more generally for the good of society
- A big part is solving complex models of the universe
- This includes collecting and analyzing data





Data Science



Computation as a pillar of scientific discovery and engineering design

- Theory, experiment, and computation partner to:
  - Predict, analyze scenarios
  - Generate ideas, identify gaps

This premise is worth deeper thought and consideration

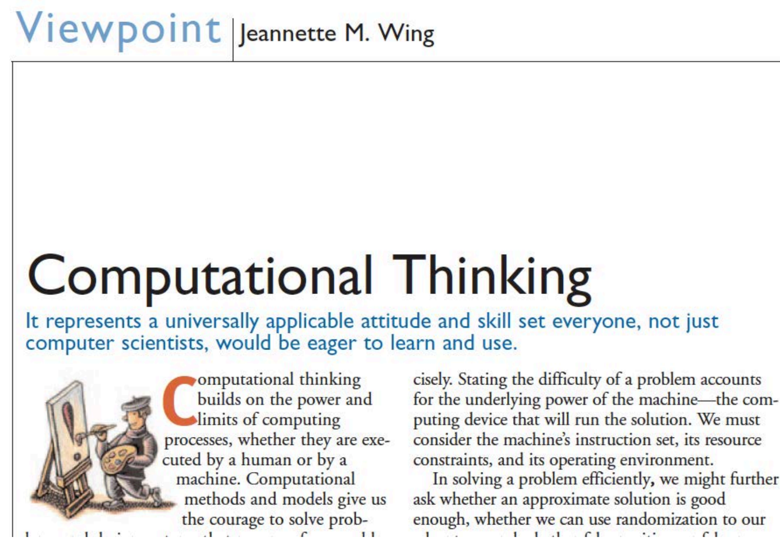
Reflect: is computation intrinsically different than what came before computers?

"Experiment is the sole source of truth. It alone can teach us something new; it alone can give us certainty."

— Henri Poincaré

Arguments that Computation and Data are new pillars of science abound

- **"Computational thinking"** has been proposed as paradigm shift, a fundamentally different approach to science
  - Wolfram among others has chimed in support
  - My colleague Kolda has also thrown support
- Rhett Alain wrote an article in Wired refuting the idea
- Data science is now a proposed fourth pillar of science
- **Is science broken? Or in need of revision?**



Viewpoint | Jeannette M. Wing

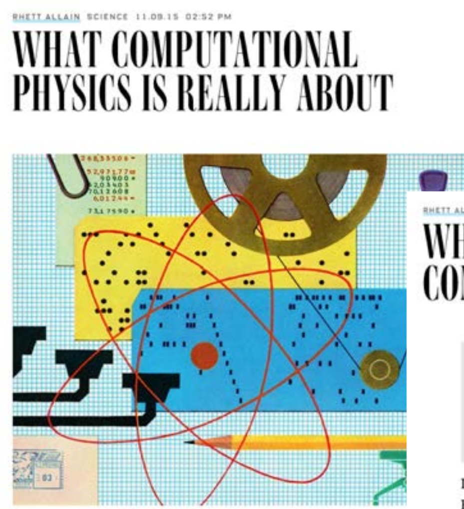
Computational Thinking

It represents a universally applicable attitude and skill set everyone, not just computer scientists, would be eager to learn and use.

Computational thinking builds on the power and limits of computing processes, whether they are executed by a human or by a machine. Computational methods and models give us the courage to solve prob-

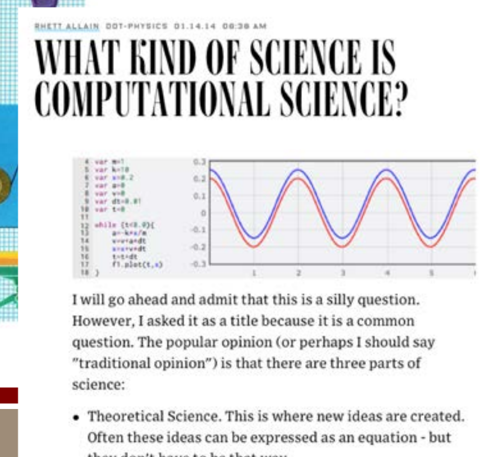
cisely. Stating the difficulty of a problem accounts for the underlying power of the machine—the computing device that will run the solution. We must consider the machine's instruction set, its resource constraints, and its operating environment.

In solving a problem efficiently, we might further ask whether an approximate solution is good enough, whether we can use randomization to our



RHETT ALLAIN SCIENCE 11.09.15 02:52 PM

WHAT COMPUTATIONAL PHYSICS IS REALLY ABOUT



RHETT ALLAIN DOT-PHYSICS 01.14.14 08:38 AM

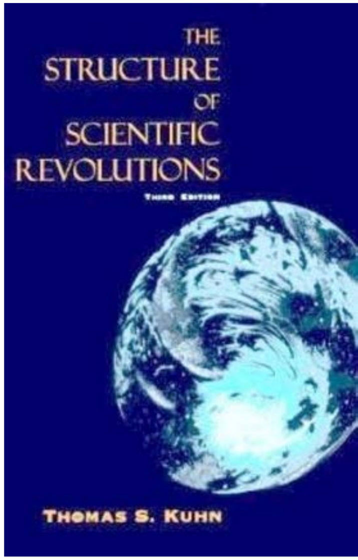
WHAT KIND OF SCIENCE IS COMPUTATIONAL SCIENCE?

I will go ahead and admit that this is a silly question. However, I asked it as a title because it is a common question. The popular opinion (or perhaps I should say "traditional opinion") is that there are three parts of science:

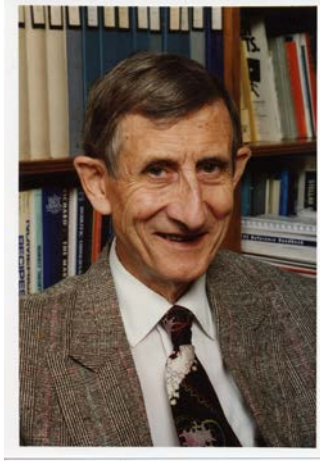
- Theoretical Science. This is where new ideas are created. Often these ideas can be expressed as an equation - but they don't have to be that way.

Thomas Kuhn and the structure of scientific revolutions

- The origin of the (now) ubiquitous term “paradigm” shift.
- Discusses fundamental changes in science as the change in conceptual viewpoints.
  - Examples: quantum physics, Galileo
  - Closely related to the concept of disruptive innovation in business
- This contrasted the view that science was a steady march forward with the slow buildup of knowledge over time.



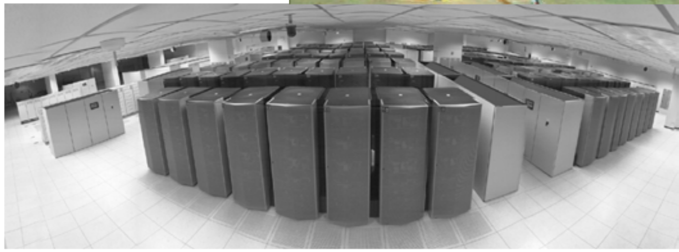
Freeman Dyson has suggested that there are two types of revolutions



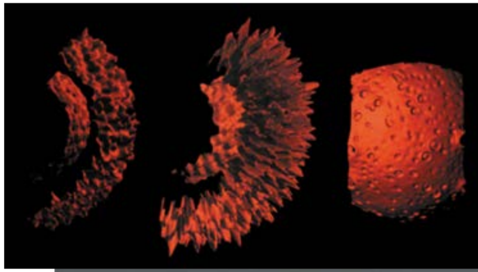
- Conceptual – the type Kuhn wrote about
  - Think quantum physics
- Tool-based – based on changes in how we look at the world/universe
  - Think the Hubble space telescope
- Computational science is a little of both
  - Von Neumann conceptualized computational science before any “real” computers existed
  - Computers as tools allow or open new doors – Computational Thinking
  - Fundamentally a computer is a tool for extending human ability
  - Do we need new concepts today or just better tools?

Where are we today in this revolution – conceptual or tool-based?

- ASCI – advanced scientific computing initiative replacing nuclear testing with stockpile stewardship including modeling & simulation.
- Is this a conceptual change? Hmmmm?
  - Are we still invested in engaging with this at a conceptual level? Not so clear, to not so much.
  - We don't know if it has worked.



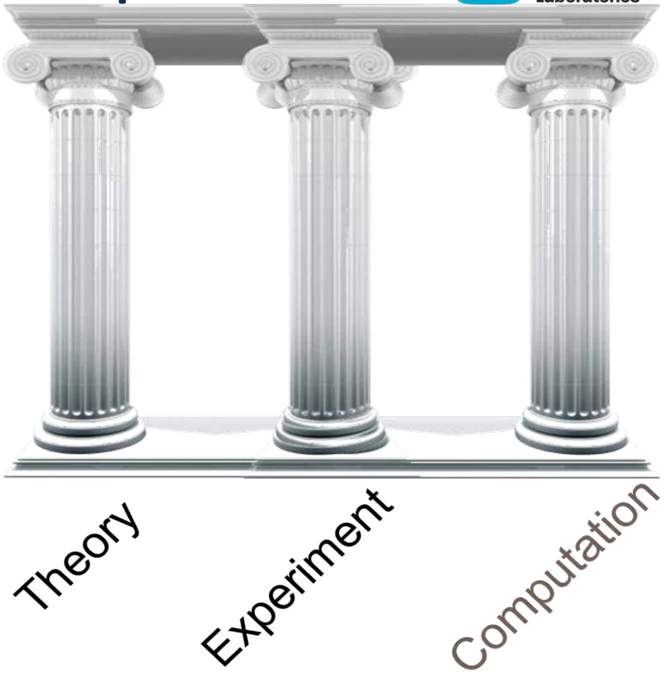
- Is it tool-based? Yes
  - Exciting experiments and lots of data
  - The focus on high-end computing is predicated on the belief that the concept is correct.
- Is it really revolutionary? Maybe



What does computational science represent?

Is it a stunning new "third way" to conduct science augmenting theory and experiment?

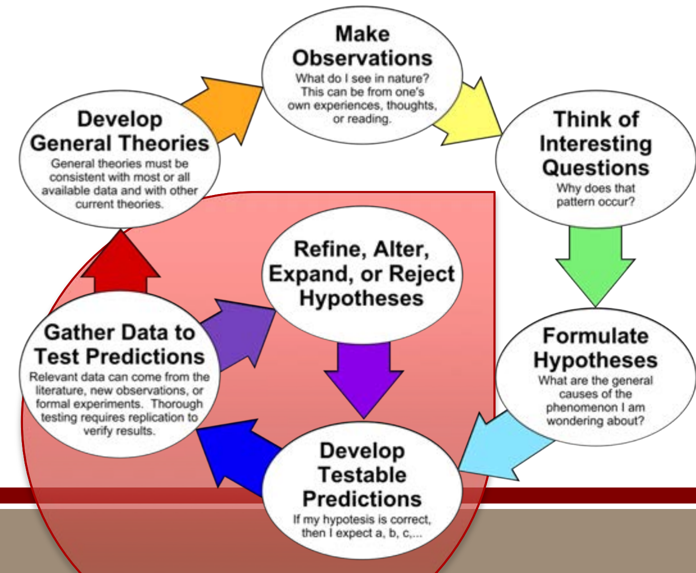
Is data science a fourth?



or

Is it a stunning new set of tools to augment the standard scientific method?

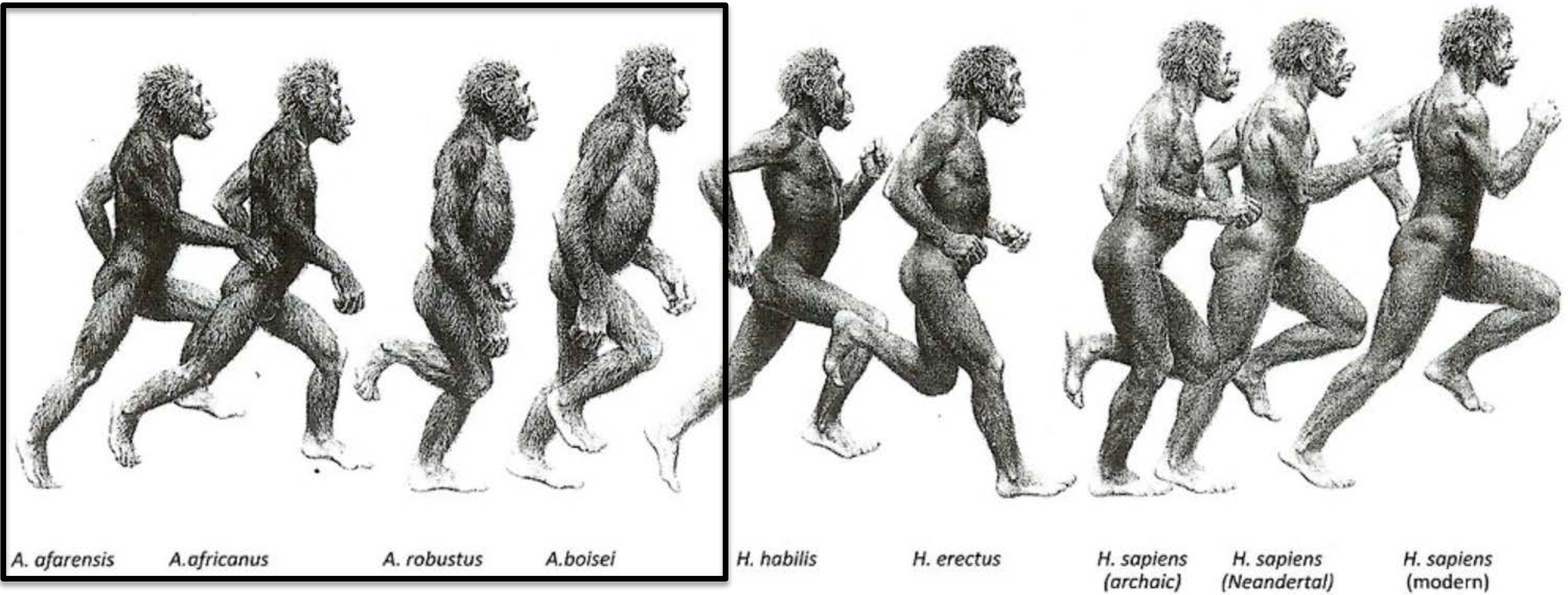
The Scientific Method as an Ongoing Process



"A generation which ignores history has no past — and no future."

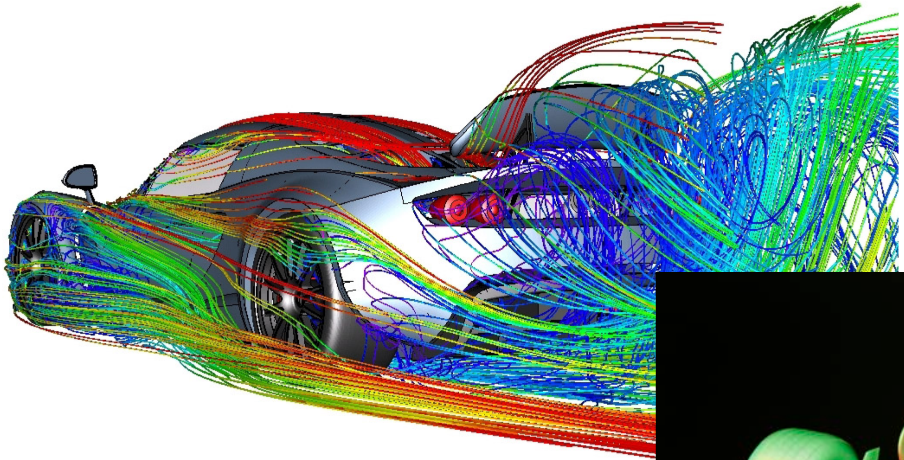
— Robert A. Heinlein

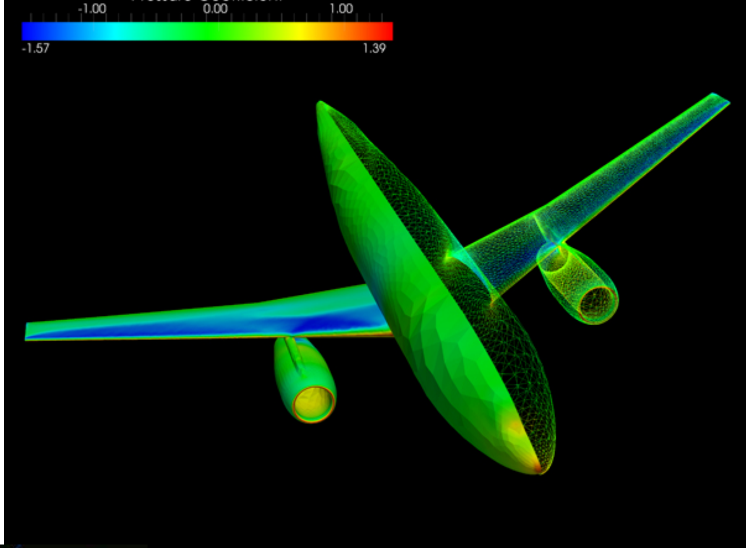
Lessons from the beginnings of computational science

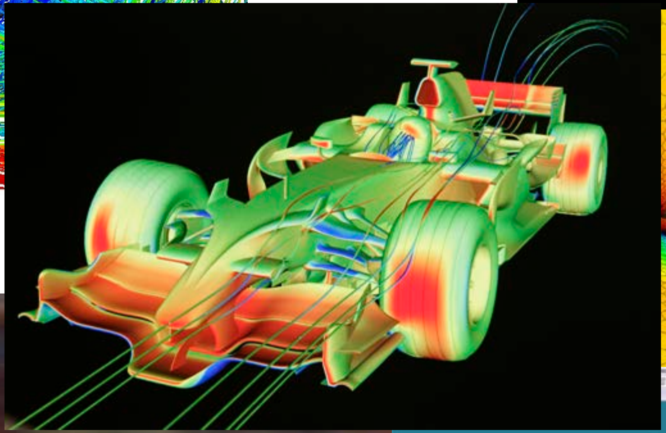


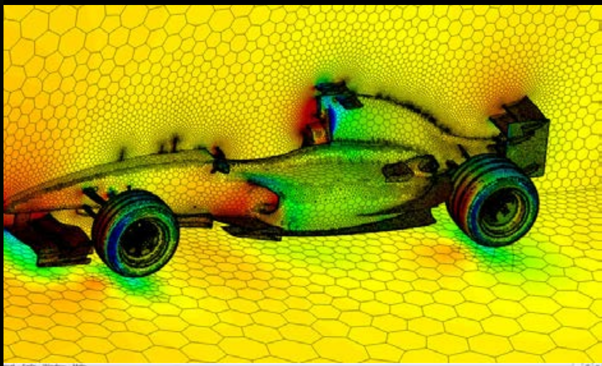
What is CFD?

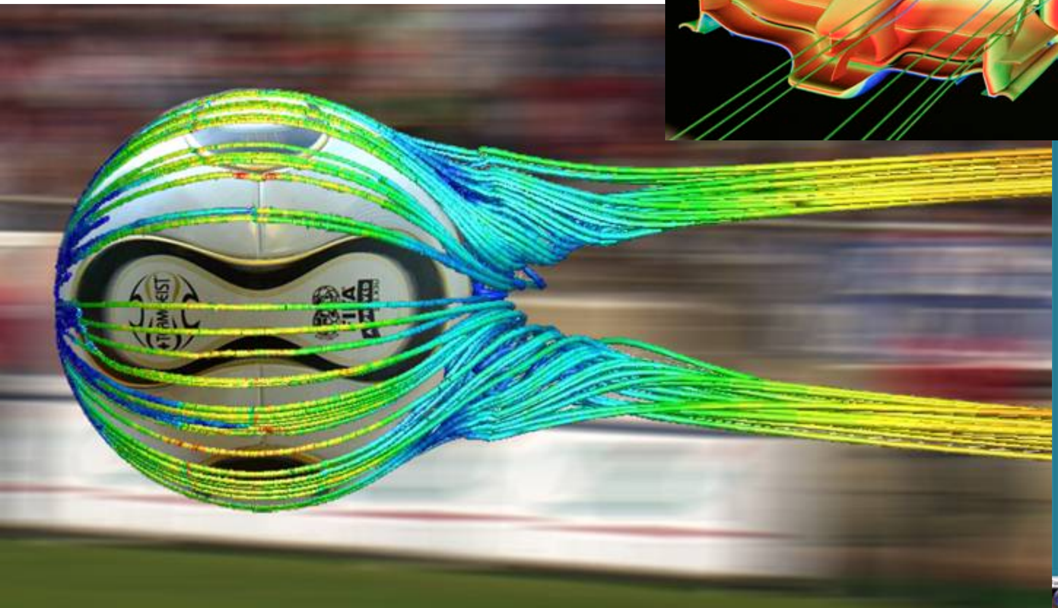
Colorful fluid dynamics

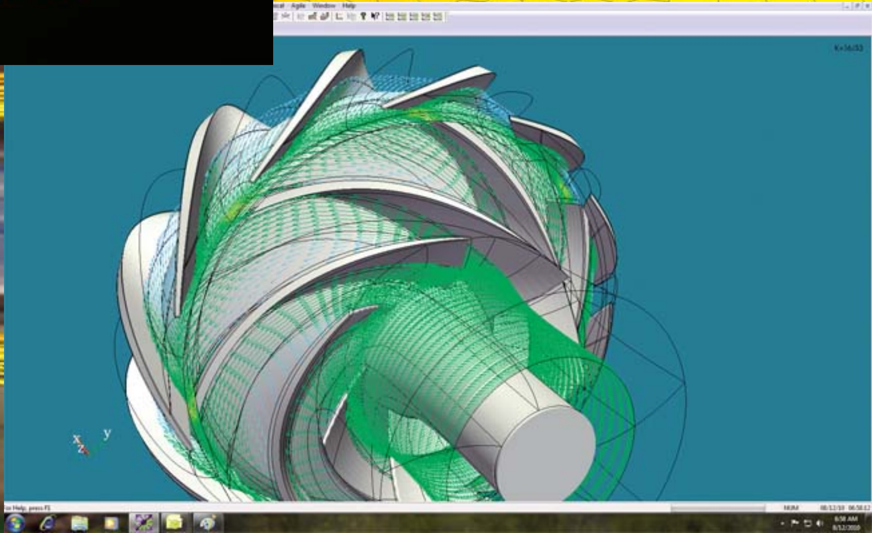






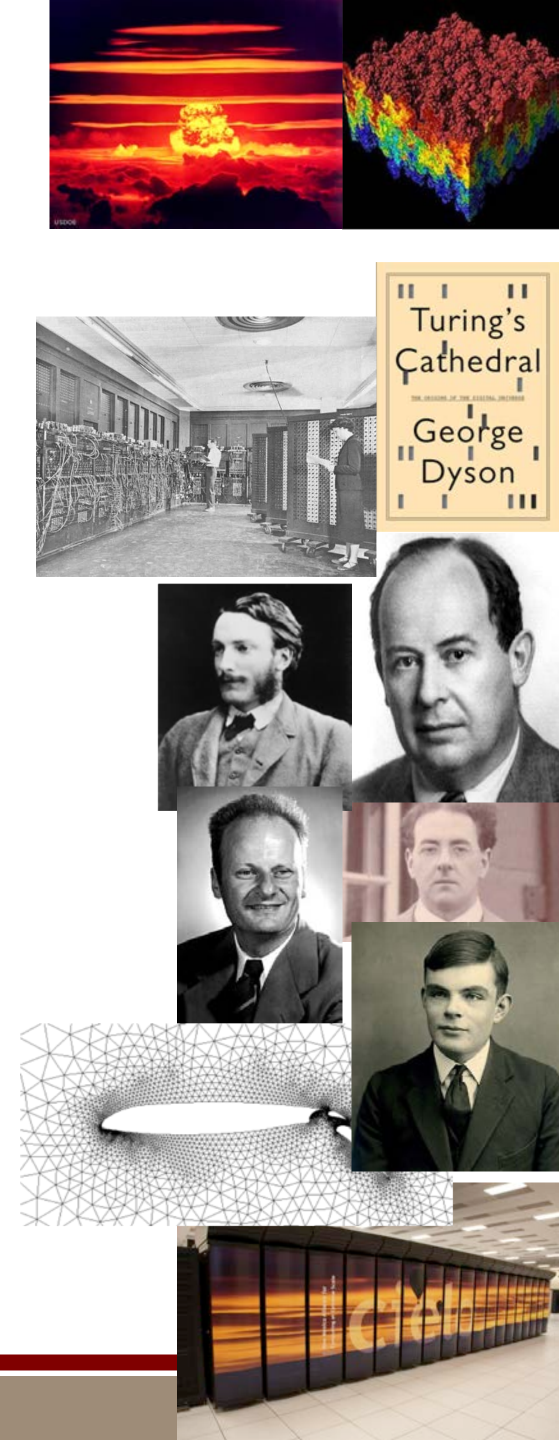






Key points

- The origin of CFD is murky and poorly known or understood.
  - Scientists are terrible historians (especially mathematicians)
  - The history available online is incomplete and/or incorrect (wikipedia)
- The people are essential to how things develop
  - Their personal views and biases are key
- Computational Science was a revolutionary idea
  - CFD is an archetype of computational science



Conceptual approach to computational simulation through physics-based modeling

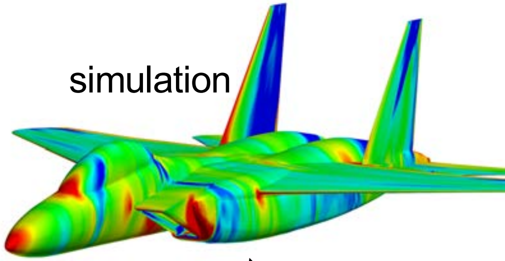
model

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}+\ldots=S$$

numerics

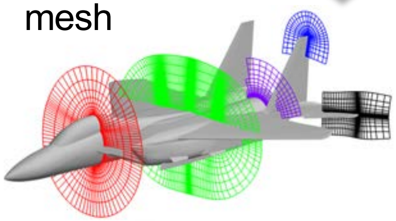
$$\frac{dU}{dt}=-\frac{\Delta_{i,j,k}F}{\Delta_{i,j,k}x}-\frac{\Delta_{i,j,k}G}{\Delta_{i,j,k}y}-\frac{\Delta_{i,j,k}H}{\Delta_{i,j,k}z}-\ldots S_{i,j,k}$$

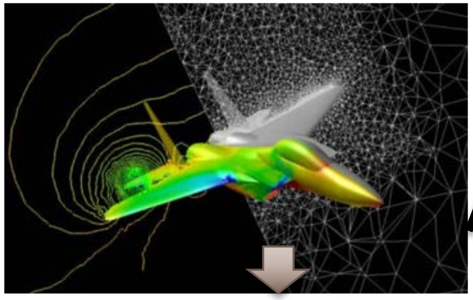
simulation



Reality

mesh

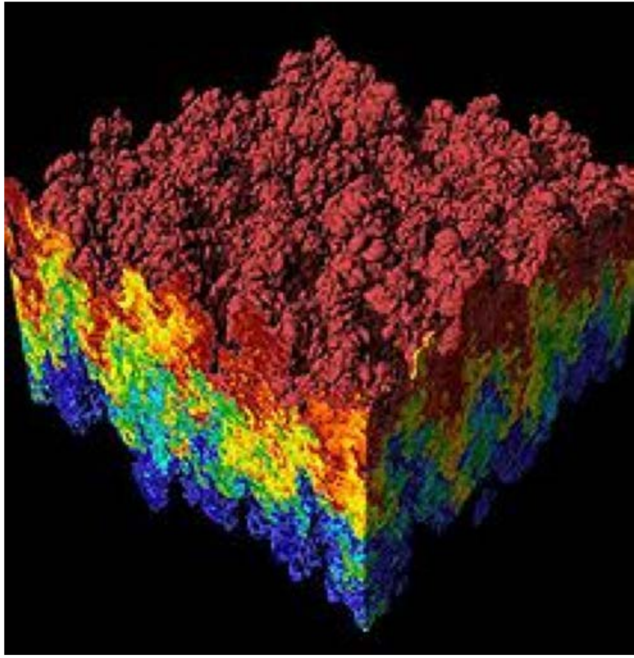




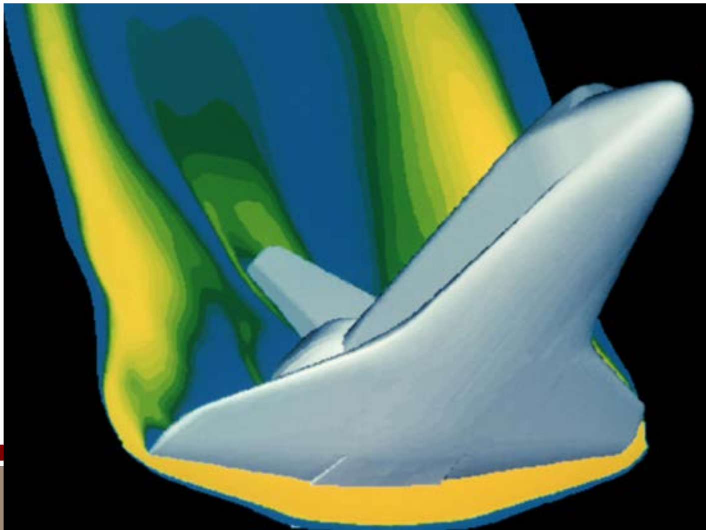
computer

experiment

Wikipedia is a bit dicey



Computational fluid dynamics, usually abbreviated as **CFD**, is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows… With high-speed supercomputers, better solutions can be achieved. Ongoing research yields software that improves the accuracy and speed of complex simulation scenarios…



Here is its history, not wrong, but certainly not right either..

One of the earliest type of calculations resembling modern CFD are those by Lewis Fry Richardson, in the sense that these calculations used finite differences and divided the physical space in cells. Although they failed dramatically, these calculations, together with Richardson's book "Weather prediction by numerical process",[2] set the basis for modern CFD and numerical meteorology. *In fact, early CFD calculations during the 1940s* using ENIAC used methods close to those in Richardson's 1922 book.[3]

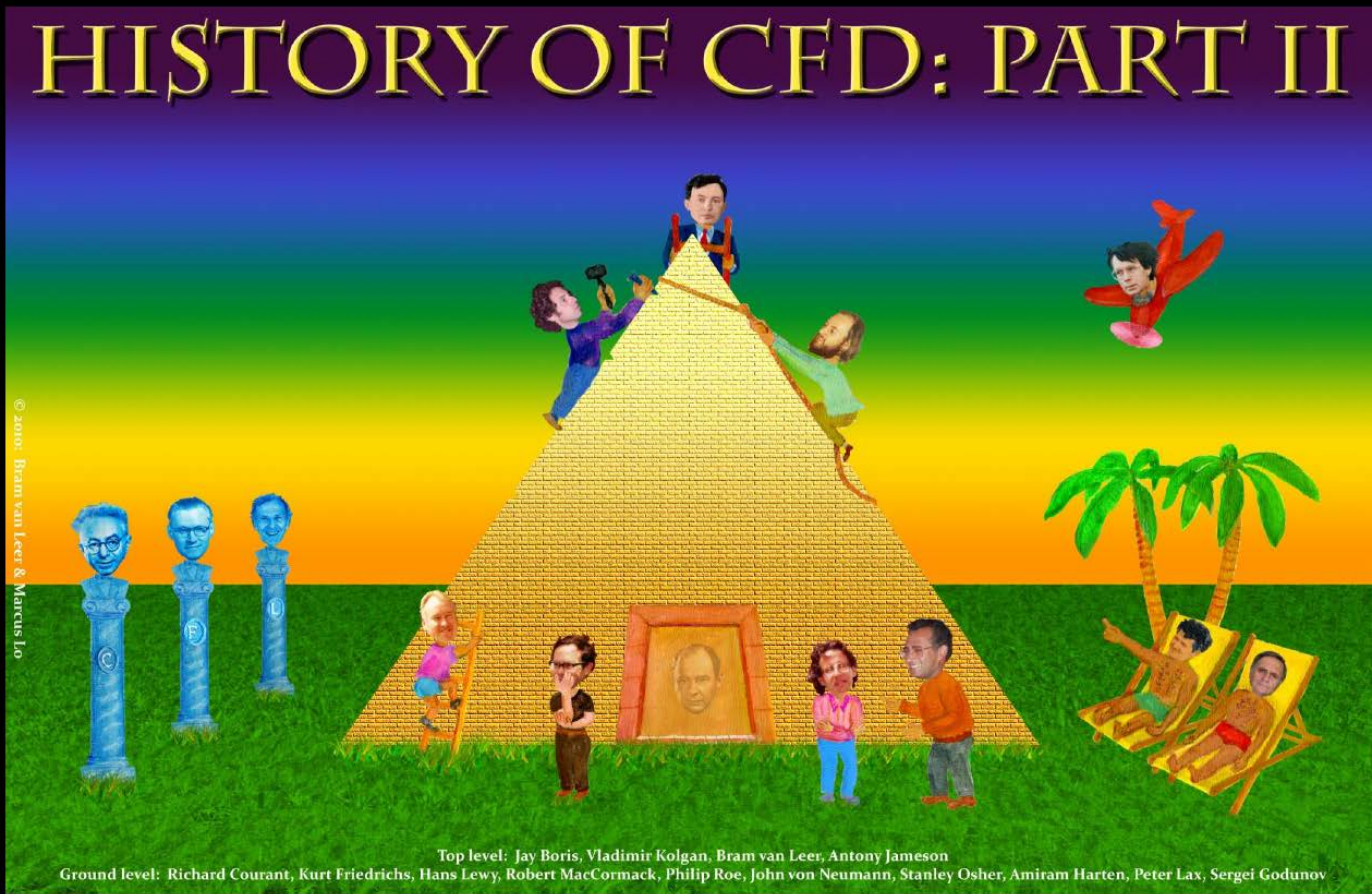
An artist's impression of Richardson's Forecast Factory (© François Schuiten).

This account misses almost everything that should be here!

The computer power available paced development of three-dimensional methods. Probably the first work using computers to model fluid flow, as governed by the Navier-Stokes equations, was performed at Los Alamos National Lab, in the T3 group.[4][5] This group was led by Francis H. Harlow, who is widely considered as one of the pioneers of CFD. From 1957 to late 1960s, this group developed a variety of numerical methods to simulate transient two-dimensional fluid flows, such as Particle-in-cell method (Harlow, 1957),[6] Fluid-in-cell method (Gentry, Martin and Daly, 1966),[7] Vorticity stream function method (Jake Fromm, 1963),[8] and Marker-and-cell method (Harlow and Welch, 1965).[9] Fromm's vorticity-stream-function method for 2D, transient, incompressible flow was the first treatment of strongly contorting incompressible flows in the world.

The next part of the history on panel methods and aero engineering is closer to the mark, but I know much less about that.

A Presentation by Bram Van Leer in 2010 and part of my inspiration for the talk.



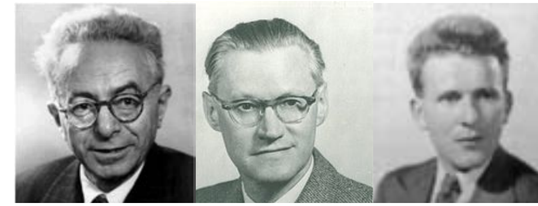

LOS ALAMOS
PROJECT
MAIN GATE
PASSES MUST BE
PRESENTED TO
GUARDS
POST
No. 1

IM-9: LAT-465

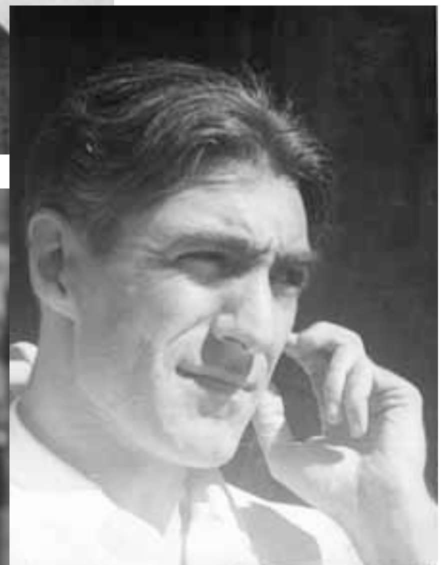
CFD was developed by many great minds

John Von Neumann

Lord Rayleigh & G. I. Taylor

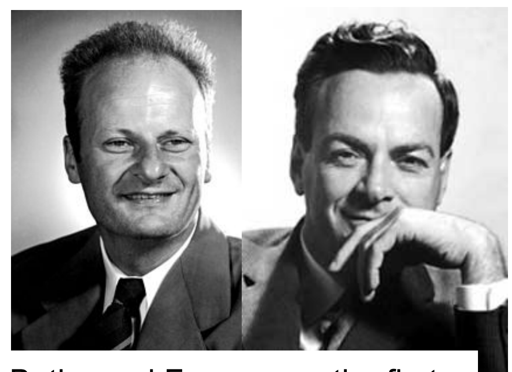


Courant, Friedrichs, Lewy – 1928 paper



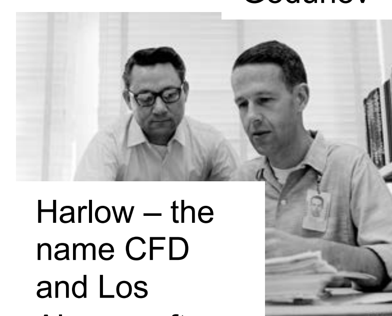
Robert Richtmyer

Peter Lax



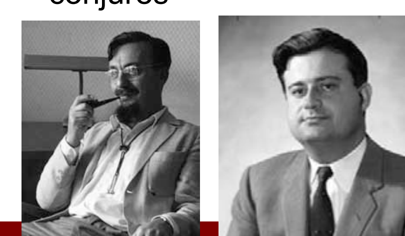
Bethe and Feynman – the first calculations using Von Neumann's method at Los Alamos in 1944

Godunov



Harlow – the name CFD and Los Alamos often conjures

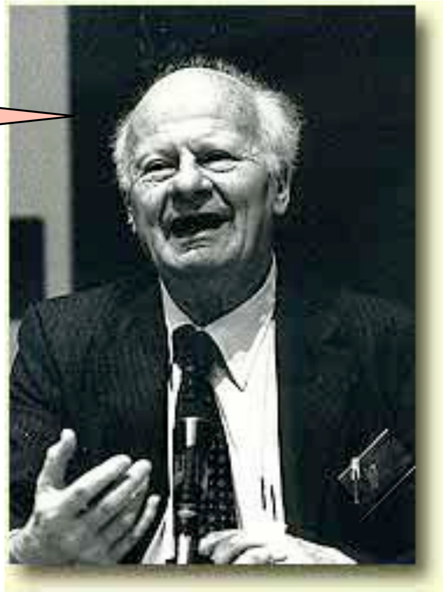
Teller, Metropolis, Ulam – Monte Carlo Methods and the H-Bomb

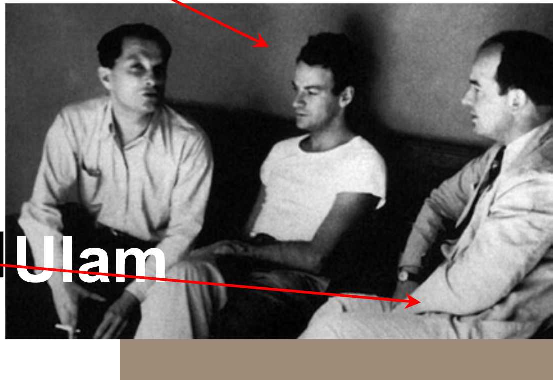


Landshoff & Rosenbluth

The first "CFD" calculations

- The first hydrodynamic calculation was described in a Los Alamos report (LA-94) on June 20, 1944 – lead author Hans Bethe
  - Feynmann was the calculational lead and marked the transition from human computers to IBM machines (done in April/May '44).
  - They used two methods to compute shocks, but only one of them worked well (the shock fitting by Peierls). The other finite difference method produced severe post-shock "wiggles" explained as thermal excitation.
- The first calculations were 1-D and Lagrangian, shocks were tracked (no viscosity, finite differences failed completely till 1948).
- Von Neumann developed a "simple" finite difference method at Aberdeen and published report on March 20, 1944.





The artificial viscosity paper by Von Neumann and Richtmyer, J. Appl. Phys. 1950

Sandia National Laboratories

A Method for the Numerical Calculation of Hydrodynamic Shocks

J. VonNeumann and R. D. Richtmyer
Institute for Advanced Study, Princeton, New Jersey
(Received September 26, 1949)

The equations of hydrodynamics are modified by the inclusion of additional terms which greatly simplify the procedures needed for stepwise numerical solution of the equations in problems involving shocks. The quantitative influence of these terms can be made as small as one wishes by choice of a sufficiently fine mesh for the numerical integrations. A set of difference equations suitable for the numerical work is given, and the condition that must be satisfied to insure their stabilty is derived.

I. INTRODUCTION

In the investigation of phenomena arising in the flow of a compressible fluid, it is frequently desirable to solve the equations of fluid motion by stepwise numerical procedures, but the work is usually severely complicated by the presence of shocks. The shocks manifest themselves mathematically as surfaces on which density, fluid velocity, temperature, entropy and the like have discontinuities; and clearly the partial differential equations governing the motion require boundary conditions connecting the values of these quantities on the two sides of each such surface. The necessary boundary

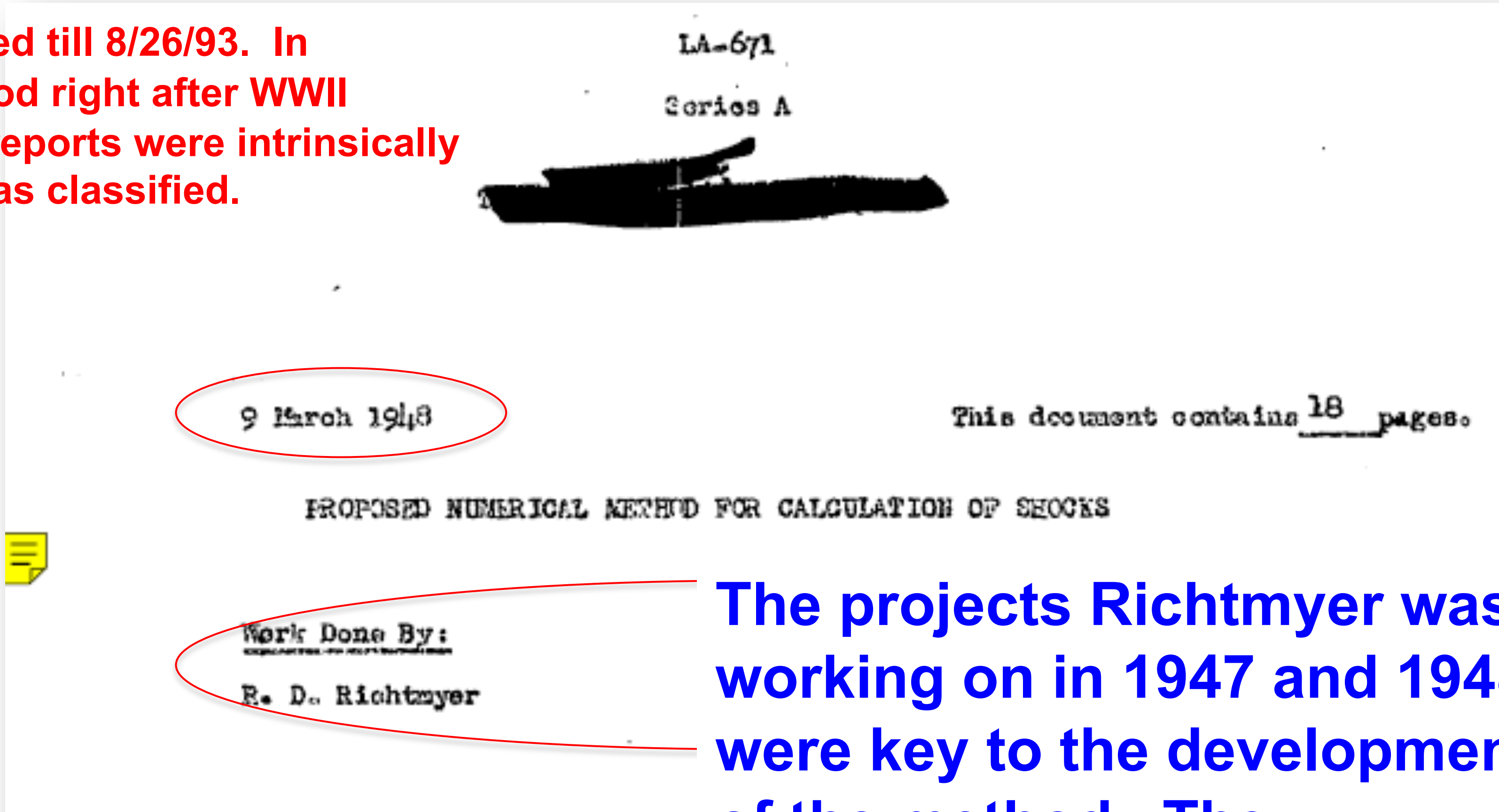
(but preferably somewhat larger than) the spacing of the points of the network. Then the differential equations (more accurately, the corresponding difference equations) may be used for the entire calculation, just as though there were no shocks at all. In the numerical results obtained, the shocks are immediately evident as near-discontinuities that move through the fluid with very nearly the correct speed and across which pressure, temperature, etc. have very nearly the correct jumps.

It will be seen that for the assumed form of dissipation (and, indeed, for many others as well), the Rankine-Hugoniot equations are satisfied, provided the thick-

Sandia National Laboratories

LA-671, The first description of artificial viscosity written by Richtmyer (only!)

Classified till 8/26/93. In the period right after WWII all Lab reports were intrinsically treated as classified.



LA-671

Series A

[redacted]

9 March 1948

This document contains 18 pages.

PROPOSED NUMERICAL METHOD FOR CALCULATION OF SHOCKS

Work Done By:

R. D. Richtmyer

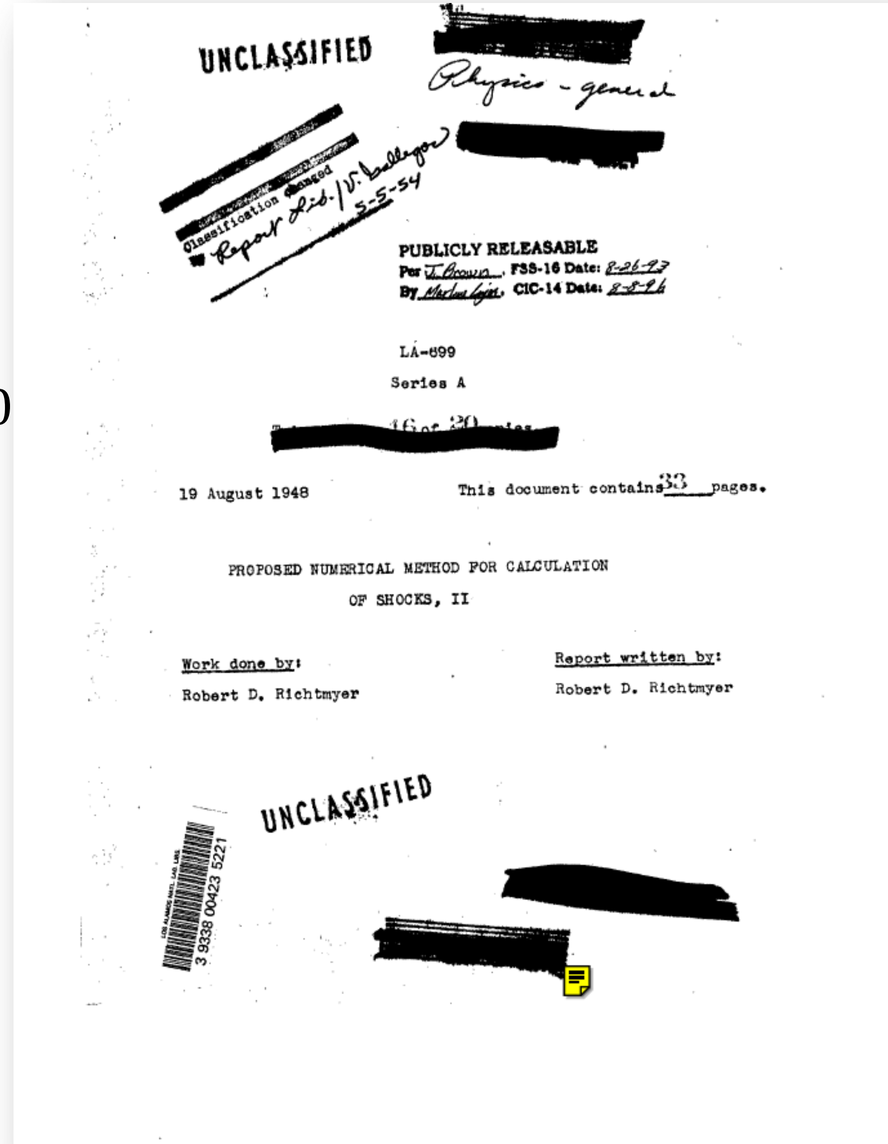
The projects Richtmyer was working on in 1947 and 1948 were key to the development of the method. The application was too complex for shock fitting.

Richtmyer published a second report five months later in 1948 (March to August) reporting on numerical experiments.

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial m}\left(p+q\right)=0 \rightarrow \frac{\partial u}{\partial t}+\frac{\partial}{\partial m}\left(p+\mu\frac{\partial u}{\partial x}\right)=0$$

$$T\Delta S=-\tfrac{1}{6}G\frac{1}{c^2}\left(\frac{\Delta V}{V}\right)^3 \rightarrow$$

$$T\Delta S=\mu\left(\frac{\partial u}{\partial x}\right)^2 \rightarrow \mu\propto\left(\Delta x\right)^2\left|\frac{\partial u}{\partial x}\right|$$


UNCLASSIFIED [redacted]

Physics - general

[redacted]

[redacted]

Classification changed Report Lib./V. Gallegos 5-5-54

PUBLICLY RELEASABLE
Per , FSS-16 Date: 8-26-93
By , CIC-14 Date: 8-8-96

LA-699

Series A

[redacted]

19 August 1948 This document contains 33 pages.

PROPOSED NUMERICAL METHOD FOR CALCULATION OF SHOCKS, II

Work done by:
Robert D. Richtmyer

Report written by:
Robert D. Richtmyer

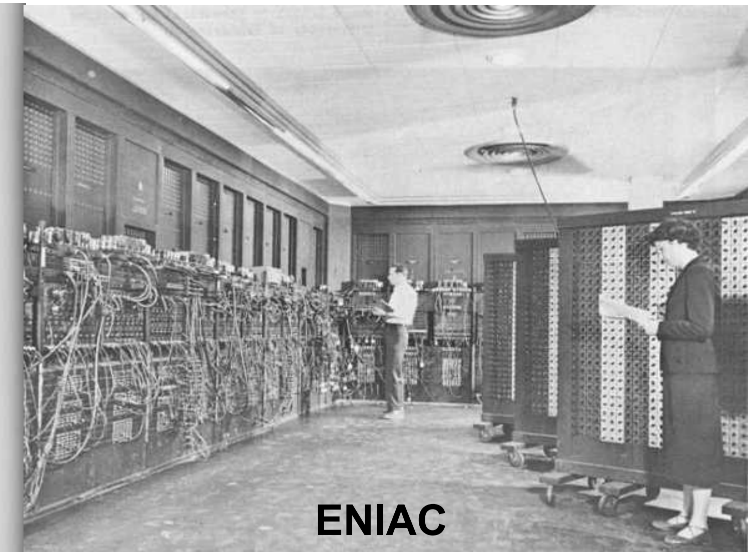
UNCLASSIFIED

[redacted]

He uses both the term “fictitious” and “mock” to describe the term, But not “artificial”. All of these are unfortunate in their connotation.

The beginning of weather/climate/turbulence modeling is connected to all of this too, through Von Neumann

In front of the Eniac, Aberdeen Proving Ground, April 4, 1950, on the occasion of the first numerical weather computations carried out with the aid of a high-speed computer. Left to right: H. Wexler, J. von Neumann, M. H. Frankel, J. Namias, J. C. Freeman, R. Fjortoft, F. W. Reichelderfer, and J. G. Charney.



First calculation
16x16x(3) mesh
Δx=300 km
48 time steps
Δt=30minutes

Norm Phillips

Joe Smagorinsky

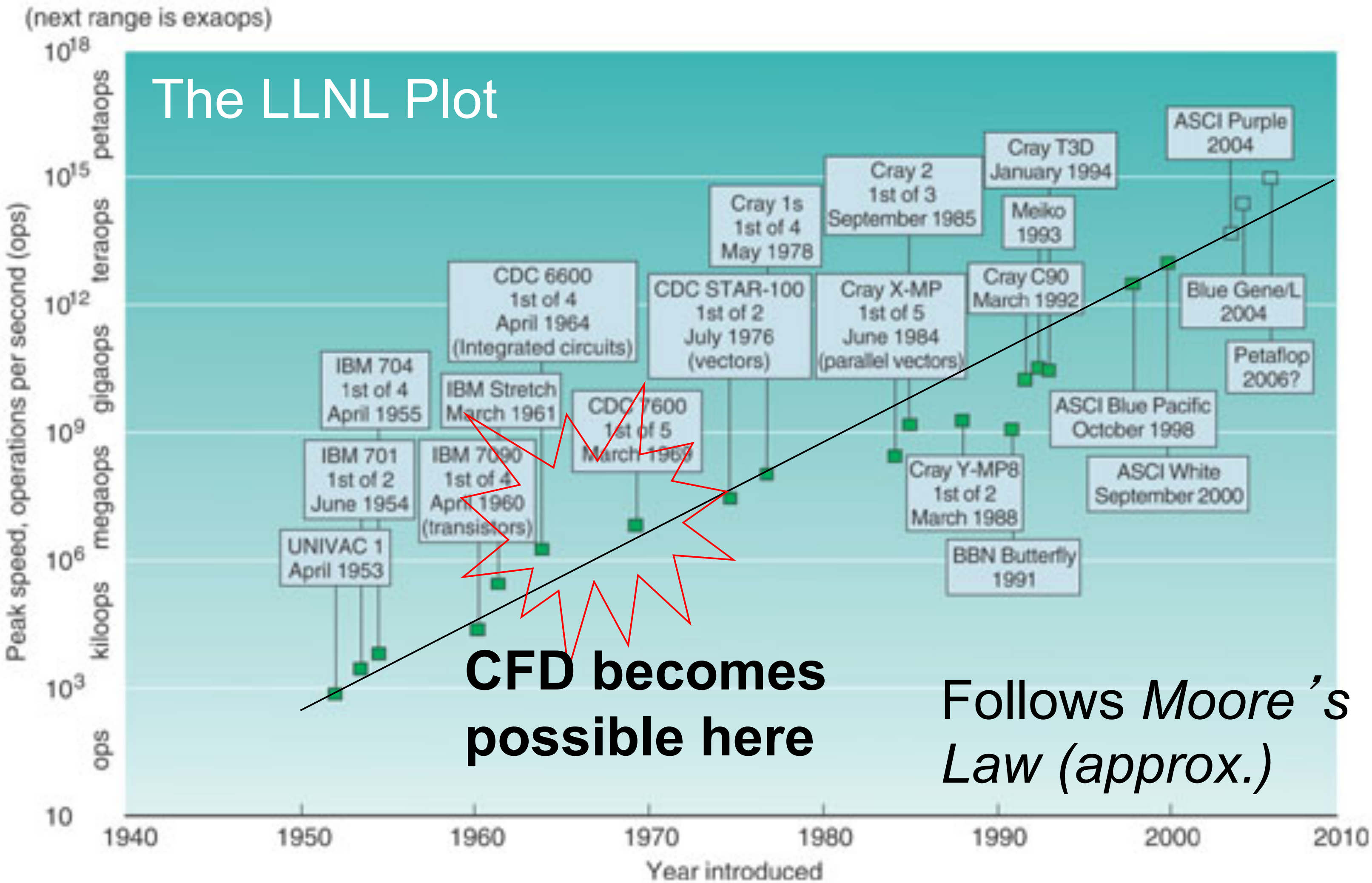
Staggered Grid

	(a)	(b)	(c)	
k	ϕ, ψ, u, v	ϕ, ψ, ρ, u, v	ρ, u, v	$p \downarrow$
$k + ½$	ρ, ω	ω	ϕ, ψ, ω	

Lax's contributions have received a great honor - the 2005 Abel Prize

- Some of the work he was honored for started at Los Alamos and continued while at NYU's Courant Institute.
  - The work on conservation laws begins in the wake of knowing shock capturing is a workable concept via Von Neumann-Richtmyer's viscosity.
  - Lax's efforts form much of the theoretical foundation for CFD today.
  - Basic theory for the analytical and numerical solution of hyperbolic conservation laws.

Computational Science has been powered by technology advances for decades…



“I suppose it is tempting, if the only tool you have is a hammer, to treat everything as if it were a nail.” — Abraham Maslow

"*In the twilight of Moore's Law, the transitions to multicore processors, GPU computing, and HaaS cloud computing are not separate trends, but aspects of a single trend – mainstream computers from desktops to 'smartphones' are being permanently transformed into heterogeneous supercomputer clusters. Henceforth, a single compute-intensive application will need to harness different kinds of cores, in immense numbers, to get its job done.*

The free lunch is over. Now welcome to the hardware jungle." — Herb Sutter 2011

Approximately a Cray 2 via linpack

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

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."

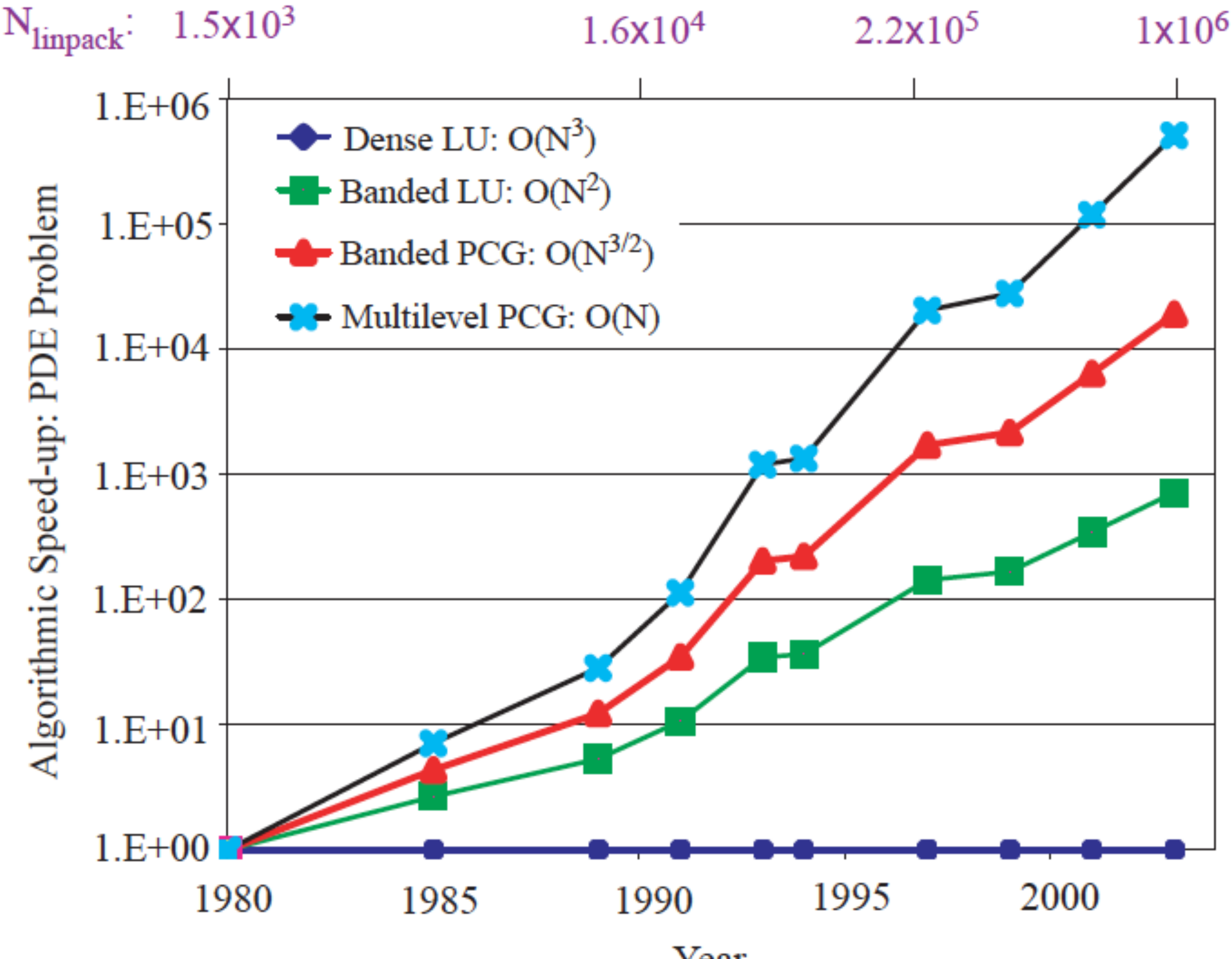
Does Moore's Law Suddenly Matter Less?
feld.com | Mar 8th 2011

A post in the New York Times this morning asserted that Software Progress Beats Moore's Law. It's a short post, but the money quote is from Ed Lazowska at the University of Washington:

"The rate of change in hardware captured by Moore's Law, experts agree, is an extraordinary achievement. "**But the ingenuity that computer scientists have put into algorithms have yielded performance improvements that make even the exponential gains of Moore's Law look trivial**," said Edward Lazowska, a professor at the University of Washington.

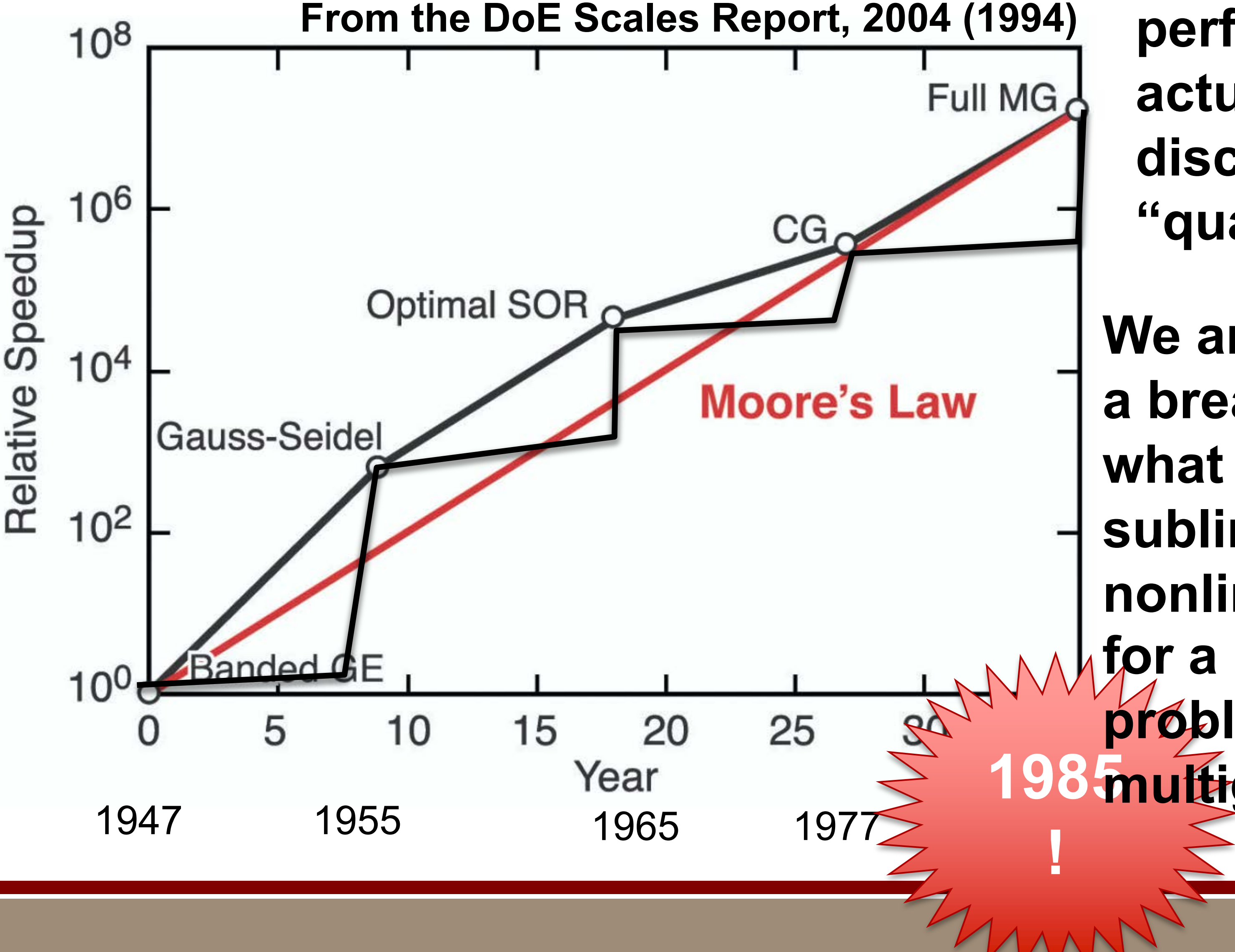
The rapid pace of software progress, Mr. Lazowska added, is harder to measure in algorithms performing nonnumerical tasks. But he points to the progress of recent years in artificial intelligence fields like language understanding, speech recognition and computer vision as evidence that the story of the algorithm's ascent holds true well beyond more easily quantified benchmark tests."

From the DoE Scales Report, 2004 (Shadid & Plimpton)



Comparing performance improvements between hardware and algorithms.

From the DoE Scales Report, 2004 (1994)



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?

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

– Nick Trefethen

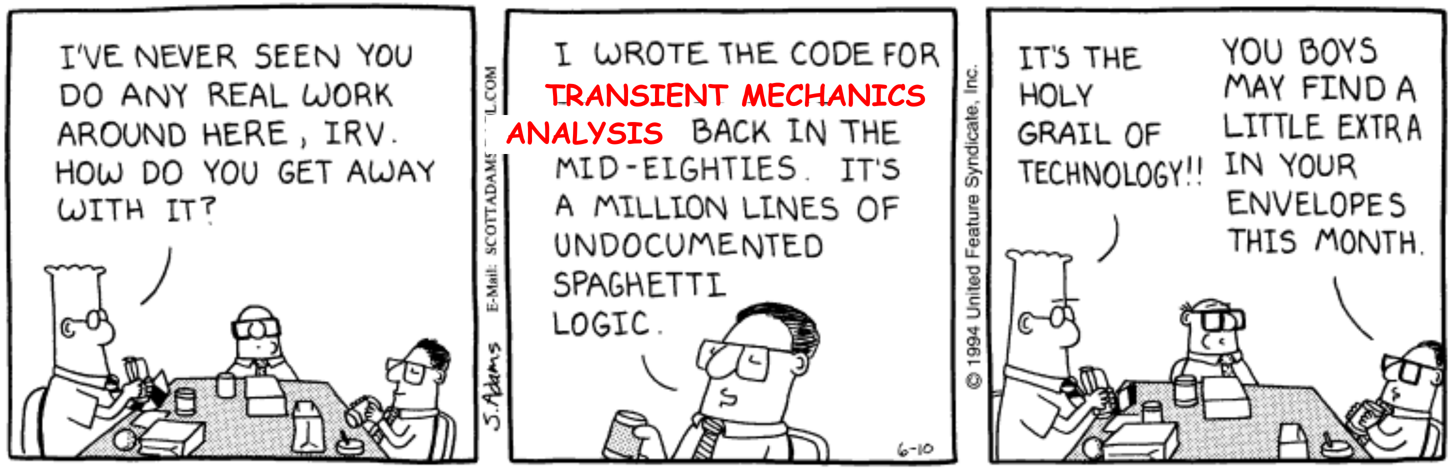
LEGACY CODE

Welcome to the project!
Here's the codebase.

seantheflexguy.com/blog

Existing technology often defines quality and correctness. ASC codes are good examples

Dilbert



From the ClariNet Electronic Newspaper <info@clarinet.com> -- Redistribution prohibited

It is essential to understand quality from this perspective if progress is to be made.

A legacy code's solutions and associated practices are the starting definition of "good."

The Threat – "Science"

Sandia National Laboratories

"… There is increasing concern that in modern research, false findings may be the majority or even the vast majority of published research claims ... However, this should not be surprising. It can be proven that most claimed research findings are false…"

By Tim Trucano (SNL, ret.)

Open access, freely available online

Essay

Why Most Published Research Findings Are False

John P. A. Ioannidis

Summary

There is increasing concern that most current published research findings are false. The probability that a research claim is true may depend on study power and bias, the number of other studies on the same question, and, importantly, the ratio of true to no relationships among the relationships probed in each scientific field. In this framework, a research finding is less likely to be true when the studies conducted in a field are smaller; when effect sizes are smaller; when there is a greater number and lesser preselection of tested relationships; where there is greater flexibility in designs, definitions, outcomes, and analytical modes; when there is greater financial and other interest and prejudice; and when more teams are involved in a scientific field in chase of statistical significance. Simulations show that for most study designs and settings, it is more likely for a research claim to be false than true. Moreover, for many current scientific fields, claimed research findings may often be simply accurate measures of the prevailing bias. In this essay, I discuss the implications of these problems for the conduct and interpretation of research.

Published research findings are sometimes refuted by subsequent evidence, with ensuing confusion and disappointment. Refutation and controversy is seen across the range of research designs, from clinical trials and traditional epidemiological studies [1–3] to the most modern molecular research [4,5]. There is increasing concern that in modern research, false findings may be the majority or even the vast majority of published research claims [6–8]. However, this should not be surprising. It can be proven that most claimed research findings are false. Here I will examine the key factors that influence this problem and some corollaries thereof.

The Essay section contains opinion pieces on topics of broad interest to a general medical audience.

Modeling the Framework for False Positive Findings

Several methodologists have pointed out [9–11] that the high rate of nonreplication (lack of confirmation) of research discoveries is a consequence of the convenient, yet ill-founded strategy of claiming conclusive research findings solely on the basis of a single study assessed by formal statistical significance, typically for a p-value less than 0.05. Research is not most appropriately represented and summarized by p-values, but, unfortunately, there is a widespread notion that medical research articles should be interpreted based only on p-values. Research findings are defined here as any relationship reaching formal statistical significance, e.g., effective interventions, informative predictors, risk factors, or associations. "Negative" research is also very useful. "Negative" is actually a misnomer, and the misinterpretation is widespread. However, here we will target relationships that investigators claim exist, rather than null findings.

It can be proven that most claimed research findings are false.

As has been shown previously, the probability that a research finding is indeed true depends on the prior probability of it being true (before doing the study), the statistical power of the study, and the level of statistical significance [10,11]. Consider a 2×2 table in which research findings are compared against the gold standard of true relationships in a scientific field. In a research field both true and false hypotheses can be made about the presence of relationships. Let R be the ratio of the number of "true relationships" to "no relationships" among those tested in the field. R is characteristic of the field and can vary a lot depending on whether the field targets highly likely relationships or searches for only one or a few true relationships among thousands and millions of hypotheses that may be postulated. Let us also consider, for computational simplicity, circumscribed fields where either there is only one true relationship (among many that can be hypothesized) or the power is similar to find any of the several existing true relationships. The pre-study probability of a relationship being true is $R/(R+1)$. The probability of a study finding a true relationship reflects the power $1 - \beta$ (one minus the Type II error rate). The probability of claiming a relationship when none truly exists reflects the Type I error rate, α. Assuming that c relationships are being probed in the field, the expected values of the 2×2 table are given in Table 1. After a research finding has been claimed based on achieving formal statistical significance, the post-study probability that it is true is the positive predictive value, PPV. The PPV is also the complementary probability of what Wacholder et al. have called the false positive report probability [10]. According to the 2×2 table, one gets $\text{PPV} = (1 - \beta)R/(R - \beta R + \alpha)$. A research finding is thus

Citation: Ioannidis JPA (2005) Why most published research findings are false. PLoS Med 2(8): e124.

Abbreviation: PPV, positive predictive value

John P. A. Ioannidis is in the Department of Hygiene and Epidemiology, University of Ioannina School of Medicine, Ioannina, Greece, and Institute for Clinical Research and Health Policy Studies, Department of Medicine, Tufts-New England Medical Center, Tufts University School of Medicine, Boston, Massachusetts, United States of America. E-mail: jioannid@cc.uoi.gr

Competing Interests: The author has declared that no competing interests exist.

DOI: 10.1371/journal.pmed.0020124

J. P. A. Ioannidis (2005), "Why Most Published Research Findings Are False," PLOS Medicine, V2, 696-701.

The Threat – Computational Physics

- **How am I supposed to reproduce the computational work?**
- **How was this refereed?**
- **(Ignition on NIF isn't going to happen.)**

By Tim Trucano (SNL, ret.)

PHYSICS OF PLASMAS **20**, 070501 (2013)

Progress towards ignition on the National Ignition Facility[a)]

M. J. Edwards,[1,b)] P. K. Patel,[1] J. D. Lindl,[1] L. J. Atherton,[1] S. H. Glenzer,[1] S. W. Haan,[1] J. D. Kilkenny,[2] O. L. Landen,[1] E. I. Moses,[1] A. Nikroo,[2] R. Petrasso,[3] T. C. Sangster,[4] P. T. Springer,[1] S. Batha,[5] R. Benedetti,[1] L. Bernstein,[1] R. Betti,[4] D. L. Bleuel,[1] T. R. Boehly,[4] D. K. Bradley,[1] J. A. Caggiano,[1] D. A. Callahan,[1] P. M. Celliers,[1] C. J. Cerjan,[1] K. C. Chen,[2] D. S. Clark,[1] G. W. Collins,[1] E. L. Dewald,[1] L. Divol,[1] S. Dixit,[1] T. Doeppner,[1] D. H. Edgell,[4] J. E. Fair,[1] M. Farrell,[2] R. J. Fortner,[1] J. Frenje,[3] M. G. Gatu Johnson,[3] E. Giraldez,[2] V. Yu. Glebov,[4] G. Grim,[5] B. A. Hammel,[1] A. V. Hamza,[1] D. R. Harding,[4] S. P. Hatchett,[1] N. Hein,[2] H. W. Herrmann,[5] D. Hicks,[1] D. E. Hinkel,[1] M. Hoppe,[2] W. W. Hsing,[1] N. Izumi,[1] B. Jacoby,[1] O. S. Jones,[1] D. Kalantar,[1] R. Kauffman,[1] J. L. Kline,[5] J. P. Knauer,[4] J. A. Koch,[1] B. J. Kozioziemski,[1] G. Kyrala,[5] K. N. LaFortune,[1] S. Le Pape,[1] R. J. Leeper,[6] R. Lerche,[1] T. Ma,[1] B. J. MacGowan,[1] A. J. MacKinnon,[1] A. Macphee,[1] E. R. Mapoles,[1] M. M. Marinak,[1] M. Mauldin,[2] P. W. McKenty,[4] M. Meezan,[1] P. A. Michel,[1] J. Milovich,[1] J. D. Moody,[1] M. Moran,[1] D. H. Munro,[1] C. L. Olson,[6] K. Opachich,[1] A. E. Pak,[1] T. Parham,[1] H.-S. Park,[1] J. E. Ralph,[1] S. P. Regan,[4] B. Remington,[1] H. Rinderknecht,[3] H. F. Robey,[1] M. Rosen,[1] S. Ross,[1] J. D. Salmonson,[1] J. Sater,[1] D. H. Schneider,[1] F. H. Séguin,[3] S. M. Sepke,[1] D. A. Shaughnessy,[1] V. A. Smalyuk,[1] B. K. Spears,[1] C. Stoeckl,[4] W. Stoeffl,[1] L. Suter,[1] C. A. Thomas,[1] R. Tommasini,[1] R. P. Town,[1] S. V. Weber,[1] P. J. Wegner,[1] K. Widman,[1] M. Wilke,[5] D. C. Wilson,[5] C. B. Yeamans,[1] and A. Zylstra[3]

[1]*Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, USA*
[2]*General Atomics, P.O. Box 85608, San Diego, California 92186, USA*
[3]*Plasma Fusion and Science Center, Massachusetts Institute of Science and Technology, 175 Albany Street, NW17, Cambridge, Massachusetts 02139, USA*
[4]*Laboratory for Laser Energetics, University of Rochester, 250 E. River Road, Rochester, New York 14623, USA*
[5]*Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA*
[6]*Sandia National Laboratory, P.O. Box 5800, Albuquerque, New Mexico 87185, USA*

(Received 26 March 2013; accepted 5 June 2013; published online 30 July 2013)

The National Ignition Facility (NIF) at Lawrence Livermore National Laboratory includes a precision laser system now capable of delivering 1.8 MJ at 500 TW of 0.35-μm light to a target. NIF has been operational since March 2009. A variety of experiments have been completed in support of NIF's mission areas: national security, fundamental science, and inertial fusion energy. NIF capabilities and infrastructure are in place to support its missions with nearly 60 X-ray, optical, and nuclear diagnostic systems. A primary goal of the National Ignition Campaign (NIC) on the NIF was to implode a low-Z capsule filled with ~0.2 mg of deuterium-tritium (DT) fuel via laser indirect-drive inertial confinement fusion and demonstrate fusion ignition and propagating thermonuclear burn with a net energy gain of ~5–10 (fusion yield/input laser energy). This requires assembling the DT fuel into a dense shell of ~1000 g/cm^3 with an areal density (ρR) of ~1.5 g/cm^2, surrounding a lower density hot spot with a temperature of ~10 keV and a ρR ~0.3 g/cm^2, or approximately an α-particle range. Achieving these conditions demand precise control of laser and target parameters to allow a low adiabat, high convergence implosion with low ablator fuel mix. We have demonstrated implosion and compressed fuel conditions at ~80–90% for most point design values independently, but not at the same time. The nuclear yield is a factor of ~3–10× below the simulated values and a similar factor below the alpha dominated regime. This paper will discuss the experimental trends, the possible causes of the degraded performance (the off-set from the simulations), and the plan to understand and resolve the underlying physics issues. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4816115]

I. INTRODUCTION

The National Ignition Facility (NIF) is the first laser system designed to demonstrate ignition and thermonuclear burn of deuterium-tritium-filled capsules. The NIF has been operational and conducting experiments since late in 2009.[1–11] A primary goal of the National Ignition Campaign (NIC) on the NIF was to demonstrate fusion ignition and burn via inertial confinement fusion (ICF). The NIC approach to ignition utilizes indirect drive, wherein the DT-filled capsule is placed inside a cylindrical cavity of a high-Z metal (a hohlraum), and the implosion drive (pressure) is provided by focusing laser energy onto the interior walls of

[a)]Paper MR1 1, Bull. Am. Phys. Soc. **57**, 200 (2012).
[b)]Invited speaker.

1070-664X/2013/20(7)/070501/10/$30.00

M. J. Edwards et al (2013), "Progress towards ignition on the National Ignition Facility," Phys. Plasmas, V20, 070501.

The Threat

"It's increasingly recognized that computational science is facing a credibility crisis: it's impossible to verify most of the computational results that are presented at conferences and in papers today …""

By Tim Trucano (SNL, ret.)


REPRODUCIBLE RESEARCH FOR SCIENTIFIC COMPUTING

Reproducible Research for Scientific Computing: Tools and Strategies for Changing the Culture

This article considers the obstacles involved in creating reproducible computational research as well as some efforts and approaches to overcome them.

> "An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures."
> —Jonathan Buckheit and David Donoho, paraphrasing Jon Claerbout[1]

It's increasingly recognized that computational science is facing a credibility crisis: it's impossible to verify most of the computational results presented at conferences and in papers today.[2] We believe that addressing this credibility crisis requires a change in the culture of scientific publishing. However, publishing truly reproducible research isn't a new idea. Our opening quote dates from 1995, and it paraphrases efforts dating back more than 20 years ago at the lab of Stanford University geosciences professor Jon Claerbout (see http://sepwww.stanford.edu/sep/jon/reproducible.html). Here we give a brief overview of some of the issues concerning reproducibility in this field, and summarize a workshop and community forum held in Vancouver in July 2011 on this topic. Other articles in this special issue grew out of talks from that workshop, as summarized in the guest editor's introduction.

The Need for Reproducibility

The notion of reproducibility as a scientific standard began with Robert Boyle and discussions within the Invisible College in the 1660s. The extensive use of computation in scientific discovery affects the implementation of these standards: Parameter values, function invocation sequences, and other computational details are typically omitted from published articles but are critical for replicating results or reconciling sets of independently generated results. Consequently, researchers from fields as diverse as geoscience, neuroscience, bioinformatics, applied mathematics, psychology, and computer science are calling for data and code to be made available in such a way that published computational results can be conveniently reproduced.[3]

A number of recent workshops, conference sessions, and committee reports have been devoted to this topic. To choose just a few examples, the annual Society for Industrial and Applied Mathematics (SIAM) Computational Science and Engineering conference featured a multispeaker session on reproducible research

1521-9615/12/$31.00 © 2012 IEEE
Copublished by the IEEE CS and the AIP

Randall J. LeVeque
University of Washington
Ian M. Mitchell
University of British Columbia
Victoria Stodden
Columbia University

R. J. LeVeque et al. (2012), "Reproducibility Research for Scientific Computing: Tools and Strategies for Changing the Culture," Computing in Science and Engineering, July/August, 13-17.

The Challenge

Sandia National Laboratories

“Reproducibility is central to the progress of science, and simulation-based research is no exception.”

By Tim Trucano (SNL, ret.)

System Dynamics Review
System Dynamics Review vol 28, No 4 (October-December 2012): 396–411
Published online 11 October 2012 in Wiley Online Library
(wileyonlinelibrary.com) DOI: 10.1002/sdr.1481

NOTES AND INSIGHTS

Reporting guidelines for simulation-based research in social sciences

Hazhir Rahmandad[a]* and John D. Sterman[b]

Syst. Dyn. Rev. **28**, 396–411 (2012)

Supporting information may be found in the online version of this article.

Introduction and motivation

Reproducibility is central to the progress of science, and simulation-based research is no exception. Only when research results are independently reproducible can different scholars verify the results reported by others, build on each other’s work, and convince the public of the reliability of their results (Laine *et al*., 2007). Given the widespread use of computational methods in different branches of science, many scientists have called for more transparency in documenting computational research to allow reproducibility (Schwab *et al*., 2000; Code, 2010; Peng, 2011). Simulation-based research in the social sciences has been on the rise over the last few decades (Gilbert and Troitzsch, 2005), yet a set of reporting guidelines that ensure reproducibility and more efficient and effective communication among researchers is lacking. As a result, many research reports lack the information required to reproduce the simulation models they discuss or the specific simulation experiments they report. In this paper we provide an initial set of reporting guidelines for simulation-based research (RGSR) in the social sciences, with a focus on common scenarios in system dynamics research. We discuss these guidelines separately for reporting models, reporting simulation experiments, and reporting optimization results. The guidelines are further divided into minimum and preferred requirements, distinguishing between factors that are indispensable for reproduction of research and those that enhance transparency. We also provide guidelines to improve visualization of research to reduce the costs of reproduction. Finally we offer suggestions to enhance the adoption of these guidelines.

To illustrate the challenge of documentation and reproducibility, we reviewed all the articles published in *System Dynamics Review* in the years 2010 and 2011. Of 34 research articles, 27 reported results from a simulation model. Of these 27, the majority (16; 59%) did not include model equations, two (7%) contained partial equations, and the rest reported the complete model, either in the text (3; 11%), in an online appendix

[a] Grado Department of Industrial and Systems Engineering, Virginia Tech, Falls Church, VA 22043, U.S.A.
[b] Sloan School of Management, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.
* Correspondence to: Hazhir Rahmandad, Grado Department of Industrial and Systems Engineering, Virginia Tech, Falls Church, VA 22043, U.S.A. E-mail: Hazhir@vt.edu

H. Rahmandad and J. D. Sterman (2012), “Reporting Guidelines for Simulation-Based Research in Social Science, System Dynamics Review, V28, 396-411.

The Opportunity – TOMS Replication

Sandia National Laboratories

"… We hope that the general concern for advancing the quality of computational science results will be incentive enough for authors to assent to the replicated computational results process…"

1

Editorial: ACM TOMS Replicated Computational Results Initiative

MICHAEL A. HEROUX, Sandia National Laboratories

The scientific community relies on the peer review process for assuring the quality of published material, the goal of which is to build a body of work we can trust. Computational journals such as *The ACM Transactions on Mathematical Software* (TOMS) use this process for rigorously promoting the clarity and completeness of content, and citation of prior work. At the same time, it is unusual to independently confirm computational results.

ACM TOMS has established a *Replicated Computational Results* (RCR) review process as part of the manuscript peer review process. The purpose is to provide independent confirmation that results contained in a manuscript are replicable. Successful completion of the RCR process awards a manuscript with the Replicated Computational Results Designation.

This issue of ACM TOMS contains the first [Van Zee and van de Geijn 2015] of what we anticipate to be a growing number of articles to receive the RCR designation, and the related RCR reviewer report [Willenbring 2015]. We hope that the TOMS RCR process will serve as a model for other publications and increase the confidence in and value of computational results in TOMS articles.

CCS Concepts:•**General and reference** → **Verification;** *Validation;*•**Software and its engineering** → **Formal software verification;**

General Terms: Reproducibility, Verification, Validation

Additional Key Words and Phrases: replicated computational results, reproducibility, publication

ACM Reference Format:
Michael A. Heroux, 2015. ACM TOMS Replicated Computational Results Initiative. *ACM Trans. Math. Softw.* 41, 3, Article 1 (March 2015), 5 pages.
DOI:http://dx.doi.org/10.1145/0000000.0000000

1. INTRODUCTION

The peer review process for computational journal articles rigorously checks the clarity and completeness of content, citation of prior work and logical discussion. This process also involves scrutiny of computational results in correlation to the text and conclusions. At the same time, it is unusual to independently confirm computational results. Remarkably, we seldom rigorously probe the correctness and execution times of computational results and even more rarely ask that results be replicated, either by the author or independently.

The ACM Transactions on Mathematical Software (TOMS) has established a new replicated computational results (RCR) process as part of the overall peer review process. The purpose of RCR activities is to provide independent confirmation that results contained in a manuscript are correct and replicated. Successful completion of the RCR process gives the manuscript a *Replicated Computational Results* Designation, which will be noted on the first page of the published article.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. Author's addresses: M. Heroux, Sandia National Laboratories, New Mexico P.O. Box 5800 Albuquerque, NM 87185 USA

DOI:http://dx.doi.org/10.1145/0000000.0000000

By Tim Trucano (SNL, ret.)

M. A. Heroux (2015), "Editorial: ACM TOMS Replicated Computational Results Initiative," ACM Transactions on Mathematical Software, V41, Issue 3, Article 13.

The Opportunity – Go ahead and try it

Sandia National Laboratories

“This is the story of what happened next: three years of dedicated work that encountered a dozen ways that things can go wrong, conquered one after another, to arrive finally at (approximately) the same findings and *a whole new understanding of what it means to do ‘reproducible research’ in computational fluid dynamics*.”

arXiv:1605.04339v2 [physics.comp-ph] 18 May 2016

Reproducible and replicable CFD: it’s harder than you think

Completing a full replication study of our previously published findings on bluff-body aerodynamics was harder than we thought. Despite the fact that we have good reproducible-research practices, sharing our code and data openly. Here’s what we learned from three years, four CFD codes and hundreds of runs.

Olivier Mesnard, Lorena A. Barba
Mechanical and Aerospace Engineering, George Washington University, Washington DC 20052

Our research group prides itself for having adopted Reproducible Research practices. Barba made a public pledge titled “Reproducibility PI Manifesto”[1] (PI: Principal Investigator), which at the core is a promise to make all research materials and methods open access and discoverable: releasing code, data and analysis/visualization scripts.

In 2014, we published a study on Physics of Fluids titled “Lift and wakes of flying snakes.”[2] It is a study that uses our in-house code for solving the equations of fluid motion in two dimensions (2D), with a solution approach called the “immersed boundary method.” The key of such a method for solving the equations is that it exchanges complexity in the mesh generation step for complexity in the application of boundary conditions. It makes possible to use a simple discretization mesh (structured Cartesian), but at the cost of an elaborate process that interpolates values of fluid velocity at the boundary points to ensure the no-slip boundary condition (that fluid sticks to a wall). The main finding of our study on wakes of flying snakes was that the 2D section with anatomically correct geometry for the snake’s body experiences lift enhancement at a given angle of attack. A previous experimental study had already shown that the lift coefficient of a snake cross section in a wind tunnel gets an extra oomph of lift at 35 degrees angle-of-attack. Our simulations showed the same feature in the plot of lift coefficient.[3] Many detailed observations of the wake (visualized from the fluid-flow solution in terms of the vorticity field in space and time) allowed us to give an explanation of the mechanism providing extra lift.

When a computational research group produces this kind of study with an in-house code, it can take one, two or even three years to write a full research software from scratch, and complete verification and validation. Often, one gets the question: why not use a commercial CFD package? (CFD: computational fluid dynamics.) Why not use another research group’s open-source code? Doesn’t it take much longer to write yet another CFD solver than to use existing code? Beyond reasons that have to do with inventing new methods, it’s a good question. To explore using an existing CFD solver for future research, we decided to first complete a full replication of our previous results with these alternatives. Our commitment to open-source software for research is unwavering, which rules out commercial packages. Perhaps the most well known open-source fluid-flow software is OpenFOAM, so we set out to replicate our published results with this code. A more specialist open-source code is IBAMR, a project born at New York University that has continued development for a decade. And finally, our own group developed a new code, implementing the same solution method we had before, but providing parallel computing via the renowned PETSc library. We embarked on a full replication study of our previous work, using three new fluid-flow codes.

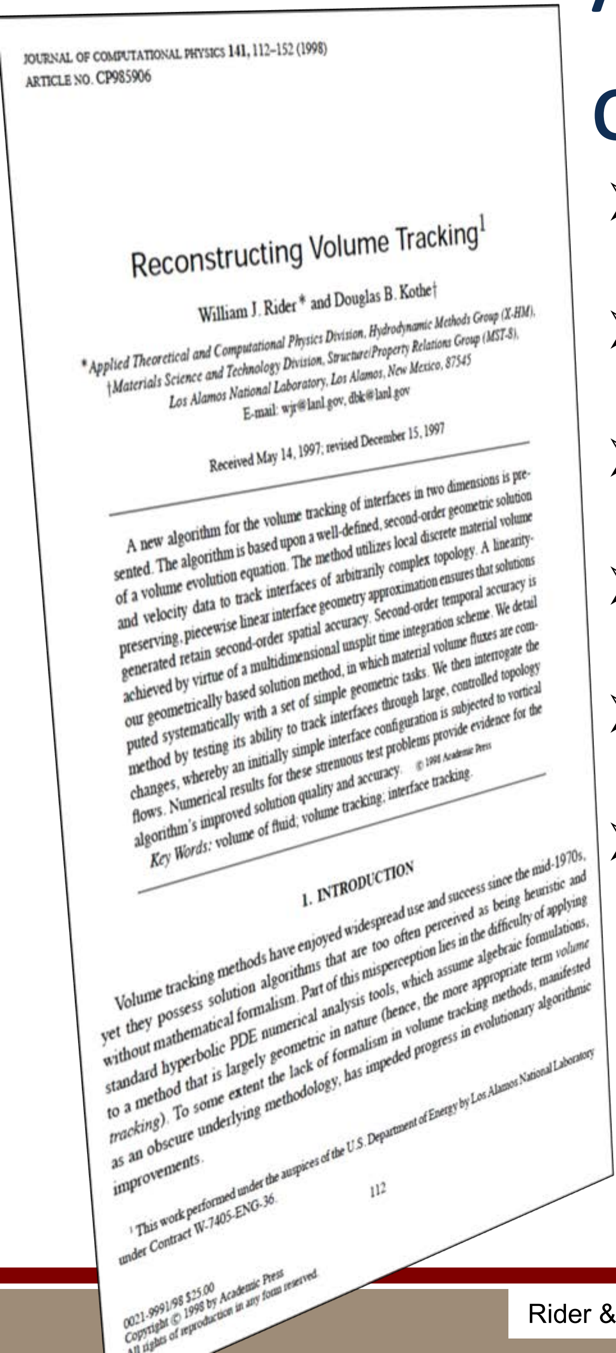
This is the story of what happened next: three years of dedicated work that encountered a dozen ways that things can go wrong, conquered one after another, to arrive finally at (approximately) the same findings and a whole new understanding of what it means to do “reproducible research” in computational fluid dynamics.

1

O. Mesnard and L. A. Barba (2016), “Reproducible and Replicable CFD: It’s harder than you think,” arXiv: 1605.04339v2

As examples, I'll focus on one of my own papers.

Sandia National Laboratories


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

Reconstructing Volume Tracking[1]

William J. Rider* and Douglas B. Kothe†
*Applied Theoretical and Computational Physics Division, Hydrodynamic Methods Group (X-HM),
†Materials Science and Technology Division, Structure/Property Relations Group (MST-8),
Los Alamos National Laboratory, Los Alamos, New Mexico, 87545
E-mail: wjr@lanl.gov, dbk@lanl.gov

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. © 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.

[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.

112

- **This paper was written 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 in other papers became a bit of a tug-of-war with the editor and reviewers.**
- **Both issues point to the process to determine quality of calculations.**
- **Releasing code was achieved in one case, but has become increasingly problematic to virtually unthinkable.**
  - ✓ **The environment at the Lab is becoming less favorable towards (full) openness although it varies with the source of your support.**

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

Why did we write “Reconstructing Volume Tracking” ?

- 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”)
- 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,
    - Smolarkiewicz’s deformation field and
    - Leveque’s time reversal)

The paper's origin actually had a lot to do with how these methods were programmed.

Horrible computer code in F77 redacted due to security and legal concerns of my current and former employers.

Notes:

1. The code has high cyclomatic complexity
2. The code is not extensible
3. The code is almost impossible to debug (see #1)

[redacted]

The logic goes on…

Continued redaction…

by the way there are two columns of 9 point Courier text, so it is a lot of code.

[redacted]

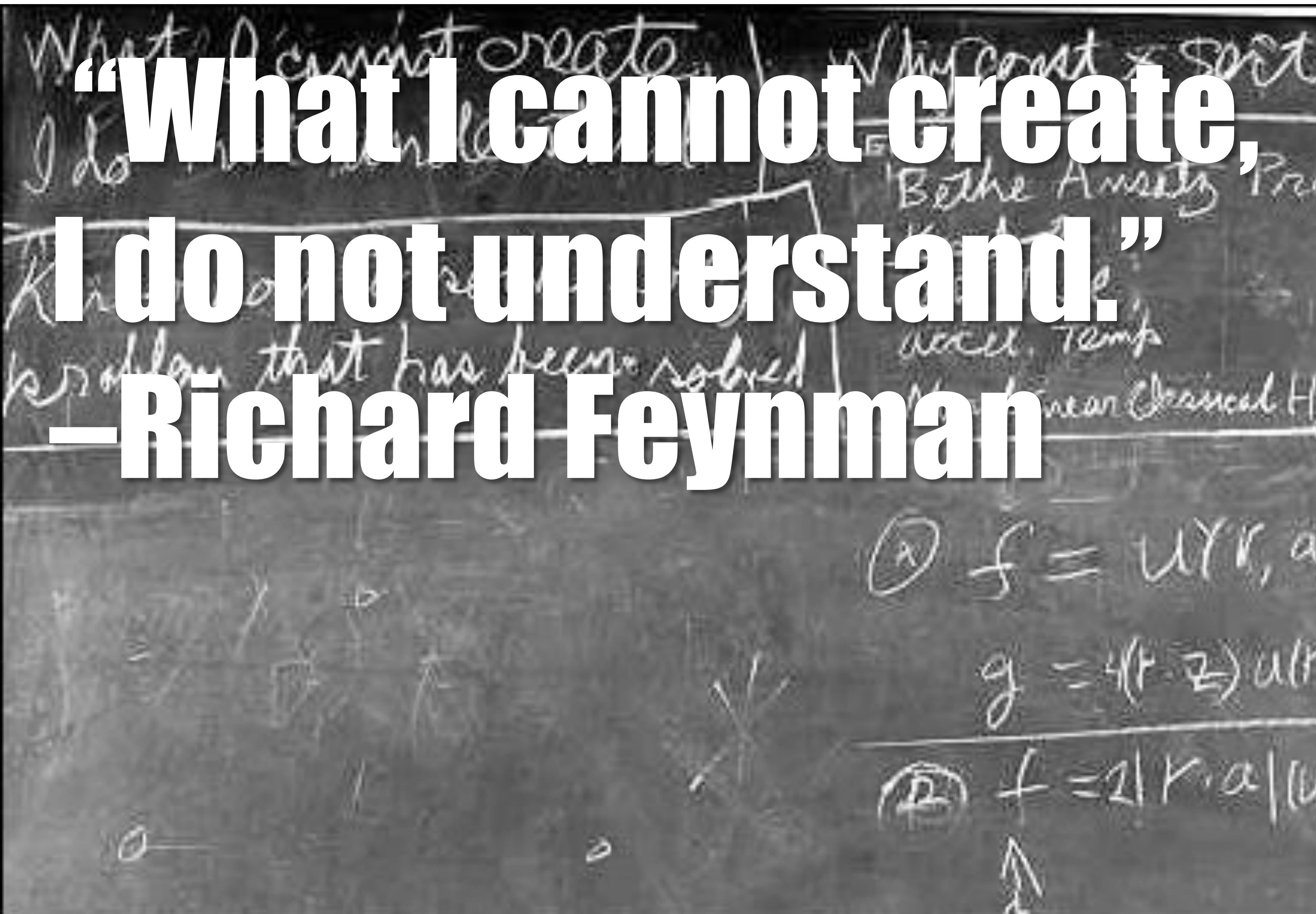
The logic goes on…

More continued redaction of code.

[redacted]

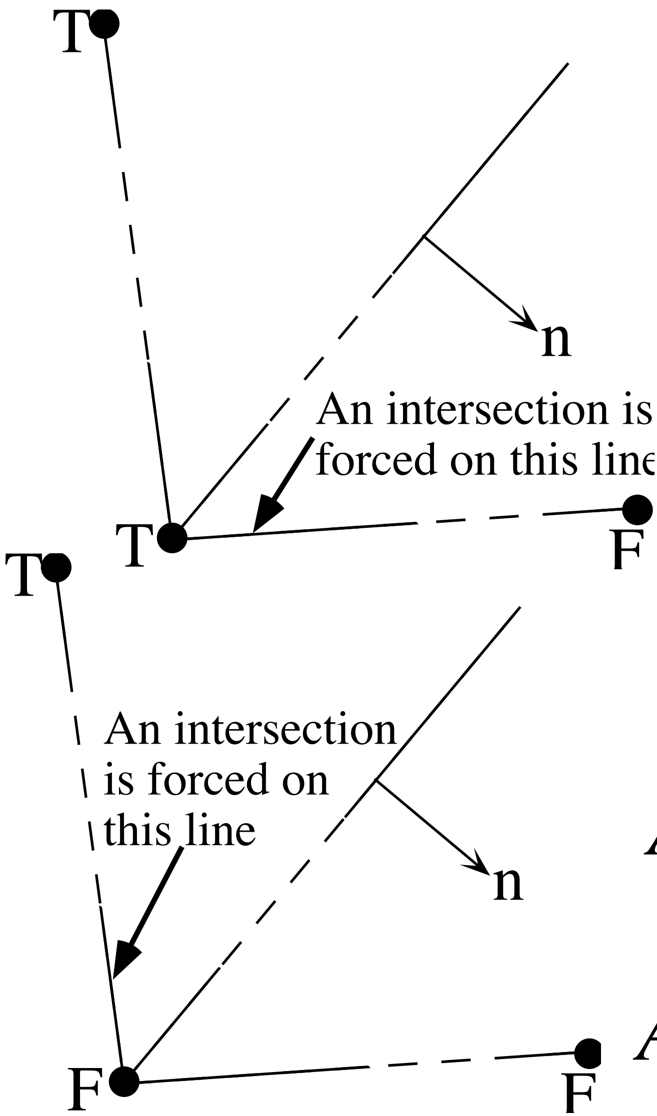
“What I cannot create, I do not understand.”

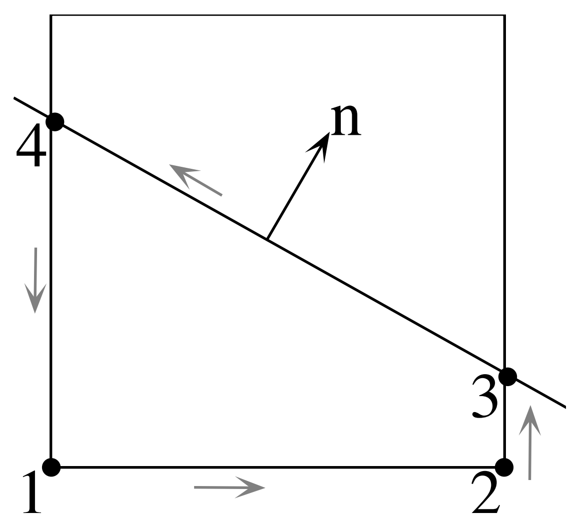
–Richard Feynman

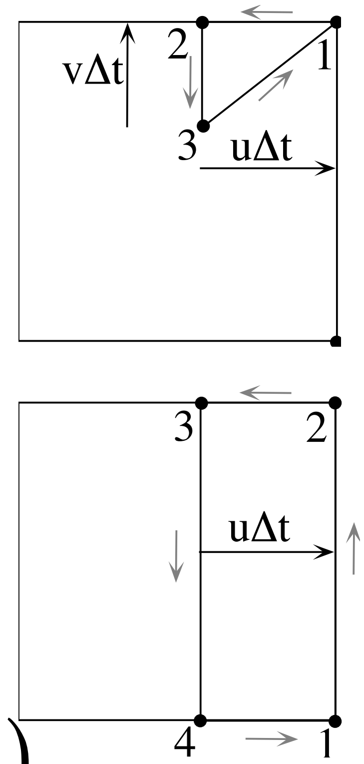


Using Computational Geometry to Construct a VOF or Volume Tracking Method

Sandia National Laboratories







Fluxes

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

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

We presented a serious rethink of the programming approach to these methods

Sandia National Laboratories

"Beautiful" F77 computer code redacted due to security and legal concerns of my current and former employers.

Notes:

1. The code has low cyclomatic complexity
2. The code is extensible
3. The code is simple to debug (see #1)

We even included the code… with serious restrictions imposed by LANL

As a condition of making the code available, I had to strip out most of the comments and formatting. this is just computational geometry!

This is just 1996, not the post-2001 World either!

I fought making the code this ugly to no avail.

```
 Subroutine INTERSECT (a1, rho1, a2, rho2, xi, yi, notparallel)
      Implicit None
      Include "param.h"
      Logical notparallel
      Real a1(1:2)
      Real a2(1:2)
      Real rho1
      Real rho2
      Real xi
      Real yi
      Real smdet           ! small number for parallel line
                         ! detection
      Real det             ! determinant of the linear system
      smdet = Max (eps, smallvof * Abs(a1(1) * a2(2)),
     &                  smallvof * Abs(a2(1) * a1(2)))
c.... first compute the determinant of the linear system
      det = a1(1) * a2(2) - a2(1) * a1(2)
c.... if the determinant is approximately zero, the linear system is
c.... not solvable and we have parallel (approximately) lines.
      If (Abs(det) .gt. smdet) Then
c...... nominal (nonparallel) case
        xi = (rho1 * a2(2) - rho2 * a1(2)) / det
        yi = (rho2 * a1(1) - rho1 * a2(1)) / det
        notparallel = .true.
      Else
c...... set the flag to show that parallel lines have been found

        notparallel = .false.
      End If
      Return
      End
```

The code that took three viewgraphs to express can be shown on one slide

Sandia National Laboratories

“Beautiful” F77 computer code redacted due to security and legal concerns of my current and former employers.

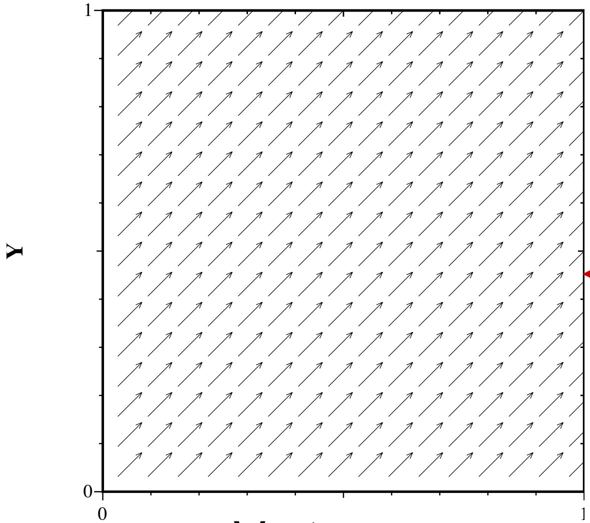
Notes:

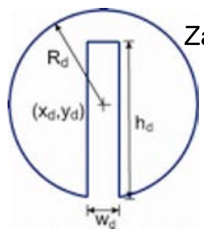
0. The code doesn’t take up the whole slide either
1. The code has low cyclomatic complexity
2. The code is extensible
3. The code is simple to debug (see #1)

Why did this paper get cited so much?

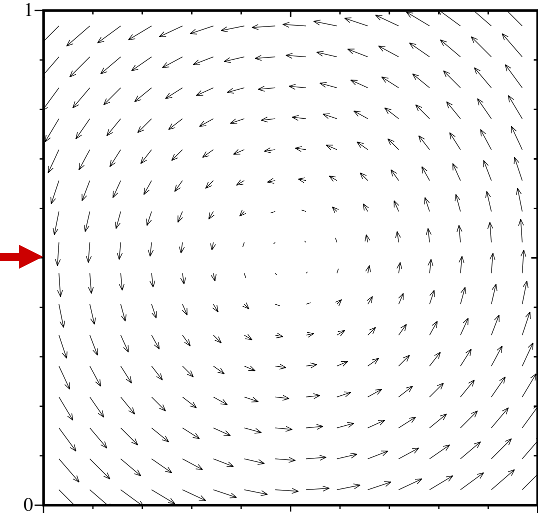
Test Problems

Body Rotation





Zalesak's disc



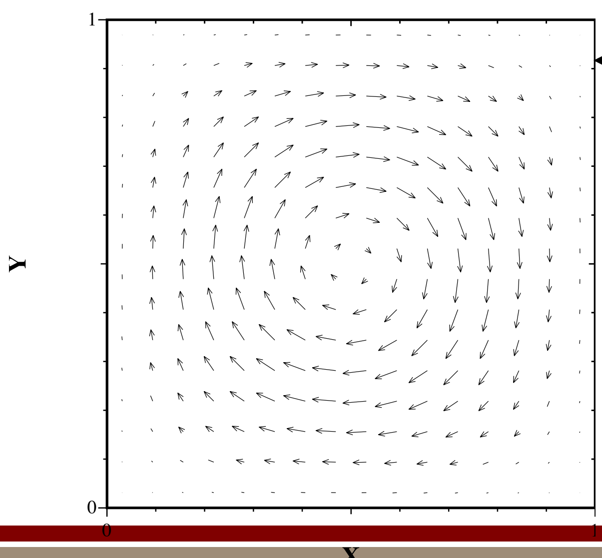
Too Easy!

For Debugging

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

Vortex

Deformation Field

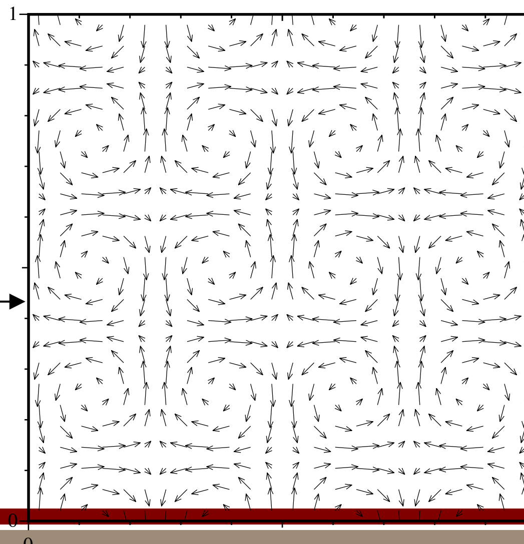


$$\Psi = \frac{1}{\pi}\sin^2(\pi x)\cos^2(\pi y)$$

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

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

$$\times\cos\left(\pi t / T\right)$$

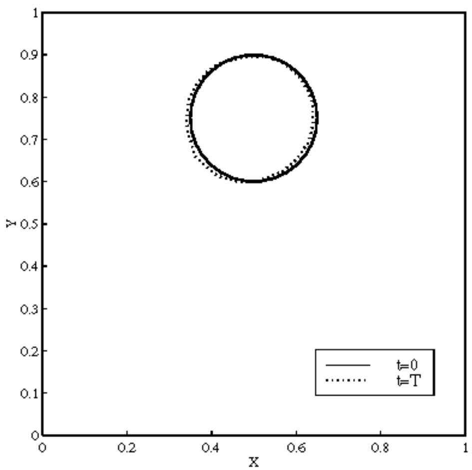


J. Dukowicz produced the earliest example I found.

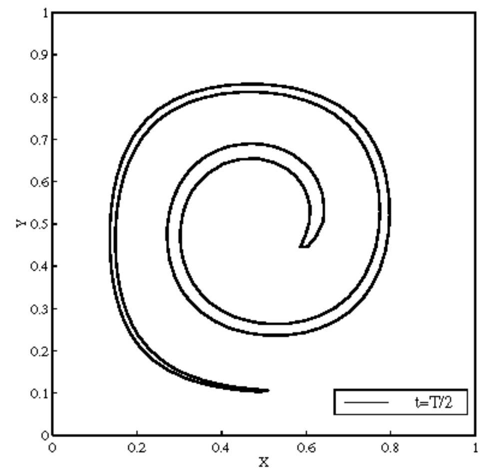
From R. Leveque

From P. Smolarkiewicz

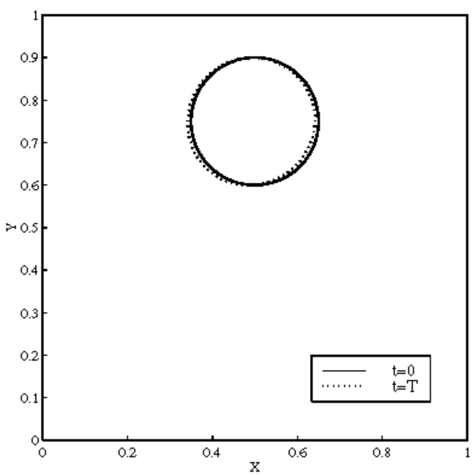
Single Vortex: Front Tracking Solutions



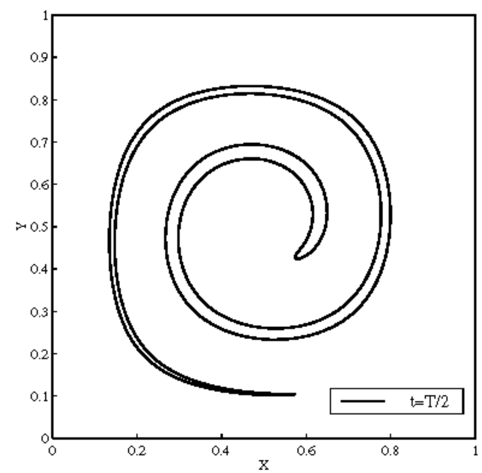
32x32 grid



solutions by
Damir Juric



128x128 grid

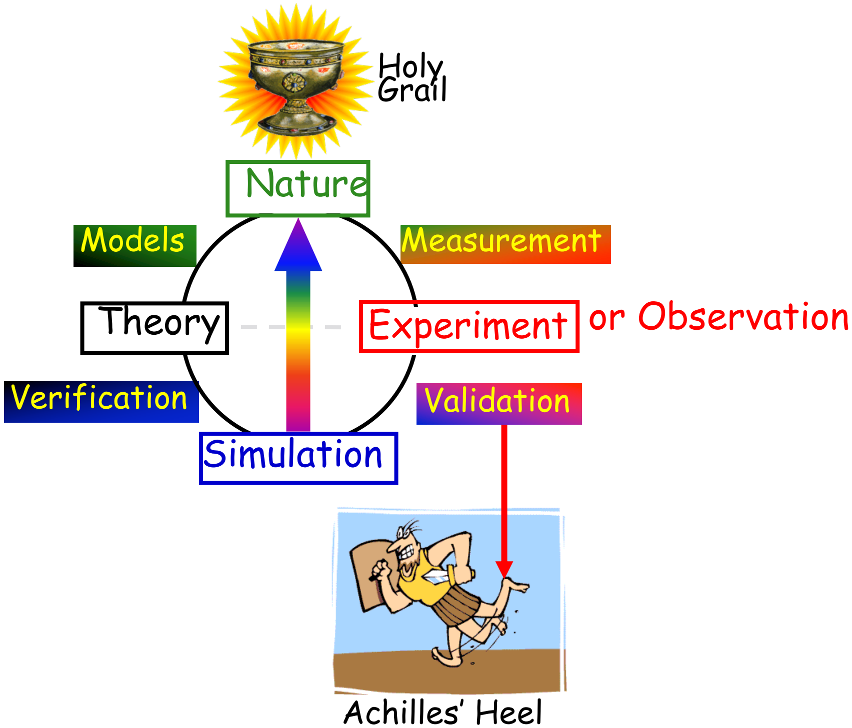


“What’s measured improves”
– Peter Drucker

We need to connect modeling & simulation with experimental design

- Science is about **understanding** and **explanation** – prediction is a quest to assist these ends
- **Validation** depends on **experiment** and measurement.
- The conduct of **experiments & computations should be conducted together** and the importance should be properly identified and focused upon – prediction & discovery.
- The assessment of modeling quality needs to consider the quality of the measurement.
  - **Bad measurements mean poor constraints for modeling.**
  - **Bad modeling should be identified by good experiments**

A conceptual picture of V&V within the context of science



Code = Theory
Simulation = Analysis

Verification and validation are essential to the quality of simulations.

Sandia National Laboratories

Complementary

- **Verification ≈ Solving the equations <u>correctly</u>**
  - Mathematics/Computer Science issue
  - Applies to both codes and calculations
- Validation ≈ Solving the <u>correct</u> <u>equations</u>
  - Physics/Engineering (i.e., modeling) issue
  - Applies to both codes and calculations
- Calibration ≈ Adjusting ("tuning") parameters
  - Parameters chosen for a specific <u>class</u> of problems
- Benchmarking ≈ Comparing with other codes
  - "There is no democracy in physics."*

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

There is a simple connection!

- Verification and Validation are the **structured application of the scientific method** to computational science. It is a means of synthesis!
- Verification is determining that an intended model is being computed properly (theory is computed right)
- Validation is the structured comparison of experiments or observations with the computed model results (computed results are reflecting reality)
- **Together these thread together computational work with the classical scientific method.**

This shows how V&V is viewed by Modeling and Simulation "customers"

Using the "FORCE" of simulation, I now understand the universe!

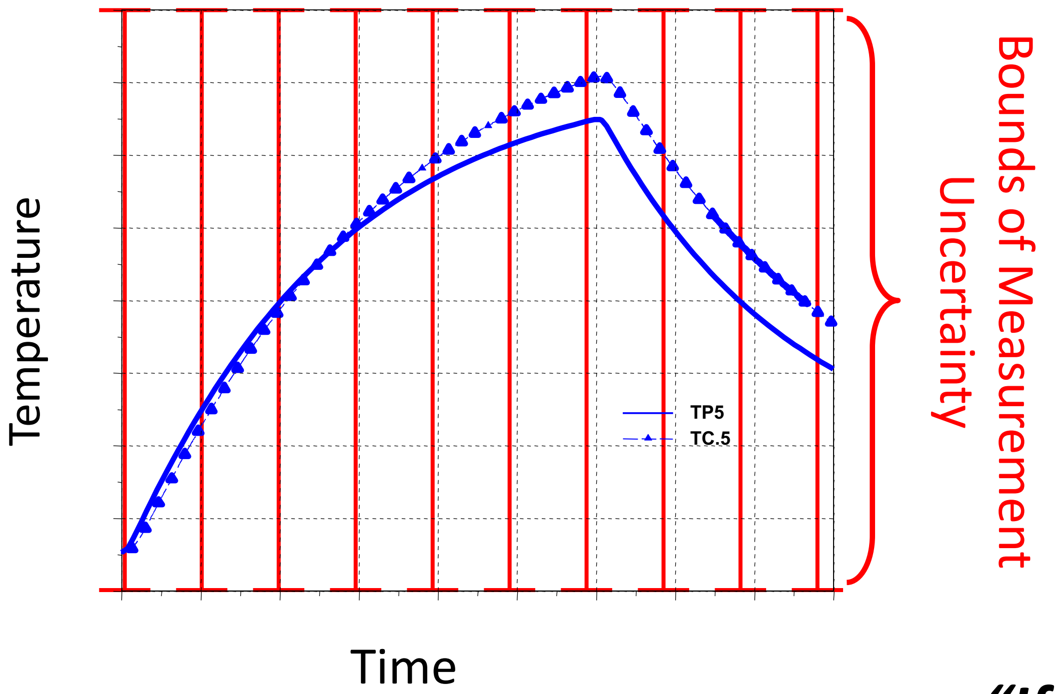
Witness the power of a fully armed and operational V&V program to call your understanding into doubt!

“V&V takes the fun out of computational simulation”
– Tim Trucano

Experimental results must have error bounds.

Measurements without error bounds are (virtually) meaningless.

Corollary: calculations without error are too!



Experiment vs. simulation of thermal physics

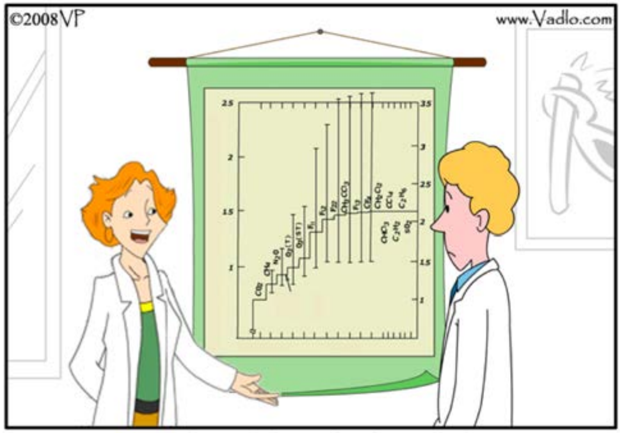
Tim Trucano (Retired)

V&V Pioneer at Sandia

"If there are no error bars, assume they're given by the limits of the plot."

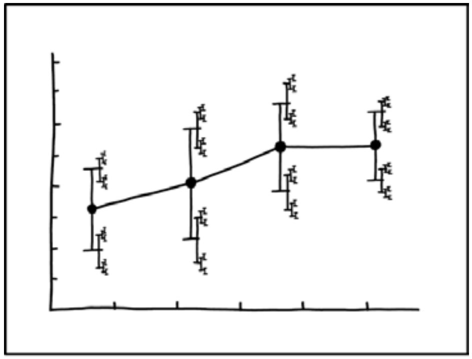
From: T. Trucano, "V&V Principles and Challenges," *2006 Nuclear Explosives Code Developers Conference (NECDC|06)*, Los Alamos National Laboratory, Los Alamos, New Mexico, 23–27 Oct. 2006.

The Default Uncertainty is Always ZERO

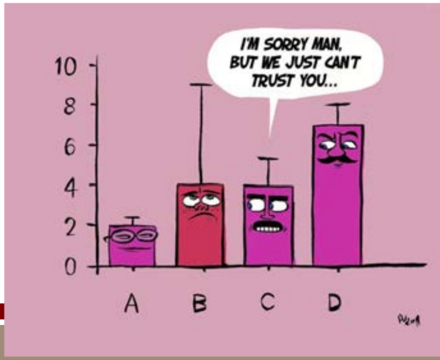


Did you really have to show the error bars?

- Actual UQ is more than what we call “UQ.”
- Uncertainty is “doubt”
- We have model form (users), numerical, model parameters, experimental uncertainty
- In some cases we don’t know what these are for a variety of reasons (e.g., a single experiment and hence no variability)
- The accepted habit is that an unknown uncertainty is assigned the very smallest value possible! ZERO
- This is critically damaging to the conduct of science
- Uncertainties must be estimated or bounded – especially the irreducible ones.



I DON'T KNOW HOW TO PROPAGATE ERROR CORRECTLY, SO I JUST PUT ERROR BARS ON ALL MY ERROR BARS.




ONE DOES NOT SIMPLY
HAVE ZERO UNCERTAINTY
imgflip.com

The default uncertainty is always ZERO!

- One of the key things to recognize is the community wide practice of not assessing key uncertainties in modeling and simulation and **the implicit assessment of that uncertainty as exactly zero**.
- This practice is widespread and pernicious.
- As a result doing any work increases uncertainty instead of decreasing it.
- This is a massive barrier to progress.
- **If someone asserts a zero uncertainty, the truth is they don't know what it is, or afraid to be truthful.**

What's the bottom line?

Sandia National Laboratories

- Computational science & computers are a stunning new set of tools to augment the standard scientific method. **The scientific method is fine as is.**
- Computers (of all sizes), programs, algorithms, methods, data, communication, analysis are all indispensable tools to conduct scientific investigation. **Computational thinking is key**.
- The origins of computational science is intertwined with solving complex models for applied scientific purposes. **History is key**.
- Improvements in the tools are focused on big iron although **algorithms have shown greater payoff**.
- **Science should be highly reproducible** and the complexity and transience of computational tools makes this a huge challenge
- **V&V is the scientific method made operational for modeling & simulation work.**

FIN

E-mail: wjrider@sandia.gov

“The scientific method’s central motivation is the ubiquity of error - the awareness that mistakes and self-delusion can creep in absolutely anywhere and that the scientist’s effort is primarily expended in recognizing and rooting out error.” David Donoho et al. (2009)

“An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.”
– David Donoho