Verification, Validation, and Scientific Computing: Successes, Failures, and Challenges

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An Old American Journey

I am inspired by the classic American novel, Herman Melville's *Moby Dick*, 1851, for a tale of an American who travels far to see and learn about the world and nature.

Man vs. Nature is more interesting than Man vs. Man!

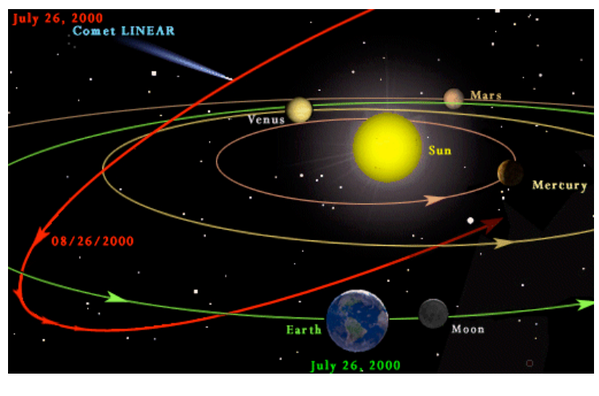
“Call me Ishmael. Some years ago- never mind how long precisely- having little or no money in my purse, and nothing particular to interest me on shore, I thought I would sail about a little and see the watery part of the world. It is a way I have of driving off the spleen and regulating the circulation....Now, when I say that I am in the habit of going to sea whenever I begin to grow hazy about the eyes, and begin to be over conscious of my lungs, I do not mean to have it inferred that I ever go to sea as a passenger. For to go as a passenger you must needs have a purse, and a purse is but a rag unless you have something in it...No, when I go to sea, I go as a simple sailor, right before the mast, plumb down into the fore-castle, aloft there to the royal mast-head.”

Herman Melville, *Moby Dick*, 1851, from Chapter 1.

A Classical Science/Engineering Paradigm

Mathematical theory and experiment are combined for prediction.

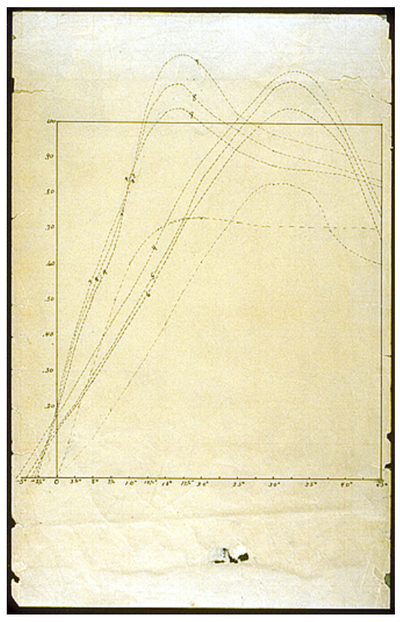
$$Theory \leftrightharpoons Experiment, \qquad m\frac{d^2\mathbf{x}}{dt^2} = \sum_{i=1}^{N} \mathbf{F}_i$$



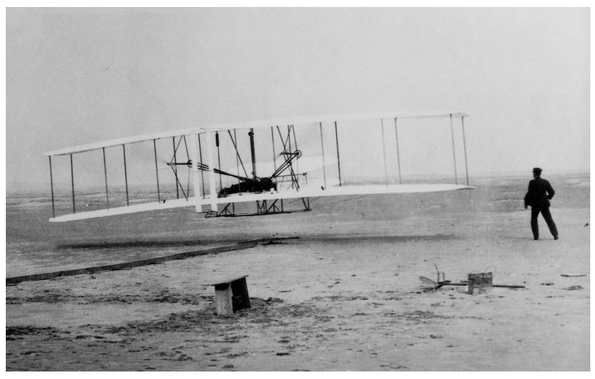
Sir Isaac Newton, 1643-1727, predicted the motions of the stars!

The Classical Paradigm Can Work!

The Wright brothers used experiment and theory for design.



Wind Tunnel Data

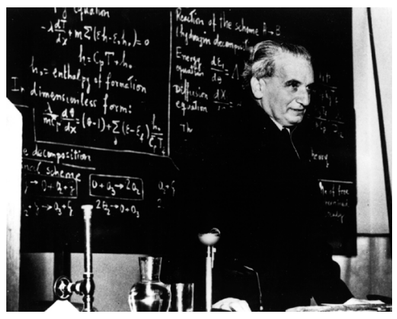


Kitty Hawk, North Carolina, 1903

A Modern Science Paradigm

Theory, computation, and experiment are used together.

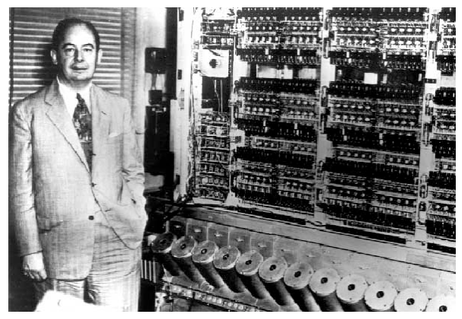
$$Theory \leftrightharpoons Computation \leftrightharpoons Experiment$$



Theodore von Kármán

1881-1963

Father of Aerothermochemisty



John von Neumann

1903-1957

Father of Scientific Computing

The Modern Paradigm Can Work!

Modern aerospace design relies on CFD, wind tunnels, and theory.

Boeing 787

NASA X43-A, Mach=9.6

November 6, 2004

The Modern Paradigm Can Fail

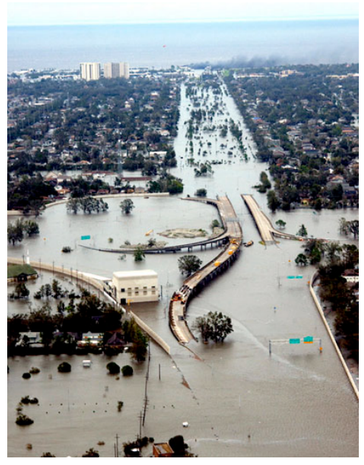
- Hurricane dynamics
- Large scale structural failures (bridges, passenger aircraft, etc.)
- Underground motion of harmful pollutants
- Global climate dynamics
- Scientific computing was used to forecast the economy (badly): Financial system collapse!
- . . .

There can be tragically large loss of human life and treasure!

But decision-makers need good predictions for humankind.

New Orleans, Louisiana August 2005

Hurricane Katrina: a natural disaster made worse by human engineering failures and human leadership failures.



Some scientific predictions of flooding were accurate! They were ignored, and the evacuation was too late for 1,836 people.

Scientific Computing of Hurricane Storm Surges

Storm surges

J. J. Westerink, a leader in Verification and Validation, argues for careful computation in *Physics Today*, 2008.

Ancient Decision-Makers Needed Verified and Validated Computation

Chinese emperors needed good astronomers to accurately predict the seasons for agriculture to feed the people.

Ancient Beijing Observatory

Longji Rice Fields

Modern Decision-Makers Now Use Verified and Validated Computation

Modern government and industry leaders have employed our best scientific/engineering predictions to “feed” today’s people.

In China and worldwide, modern manufacturing benefits from scientific computing for product development and economic forecasting.

Our Modern Predictions Have Limitations

- Finite computational resources hinder prediction of tough, multi-scale problems.
- We scientists and engineers are sometimes reluctant to fully inform decision-makers of our limitations (e.g. the US Space Shuttle Challenger and Columbia disasters).
- Many people truly do not understand the scientific limitations of easy-to-use software tools (e.g. Fluent, Abaqus, etc.).
- It is our responsibility to humanity to use these tools wisely.

The Modern Paradigm Can Fail

- Hurricane Ike, September 1-14, 2008.
- One US agency code, using a coarse computational grid, over-predicted the storm surge by a factor of two.
- A second US agency code, using a fine computation grid, predicted the storm surge accurately.
- A decision-maker had to decide whether or not to evacuate Houston, Texas, with over 2 million people!
- NASA Space Shuttle Columbia disaster, February 1, 2003.
- A bad physics model running on an Excel spreadsheet guided a decision-maker to think there was no danger to the astronauts, who all died.

Verification and Validation (V&V)

A well-defined framework for guiding scientific computing to aid in decision-making

- Obvious to many!
- Not obvious to even more!
- *Verification*: solving the equations right (mathematics)
- *Validation*: solving the right equations (physics)
- Verification must precede validation; both must be done!
- In short: 1) resolve the grid, 2) compare to experiment. If wrong, then adjust model, and repeat 1), and 2).
- **It is easy to fool others AND yourself with bad computation!**

Verification and Validation: Present Status

- Ongoing debate at present in US government agencies and academic journals with no clear consensus.
- Why? Often lack of understanding of the mathematics problem!
- V&V is now the key element of the new DOE **P**redictive **S**cience **A**cademic **A**lliance **P**rogram (PSAAP), a major national effort: U. Texas, Stanford, Cal Tech, U. Michigan, Purdue U., DOE Laboratories, $\sim \$85$ million over five years.
- from the PSAAP homepage: *"This Predictive Science is the application of verified and validated computational simulations to predict properties and dynamics of complex systems."*

AIAA Policy Statement on Numerical Accuracy

"The AIAA journals will not accept for publication any paper reporting numerical solutions of an engineering problem that fails adequately to address the accuracy of the computed results...The accuracy of the computed results is concerned with how well the specified governing equations in the paper have been solved numerically. The appropriateness of the governing equations for modeling the physical phenomena and comparison with experimental data is not part of this evaluation. "

A separate AIAA policy exists for experimental validation...

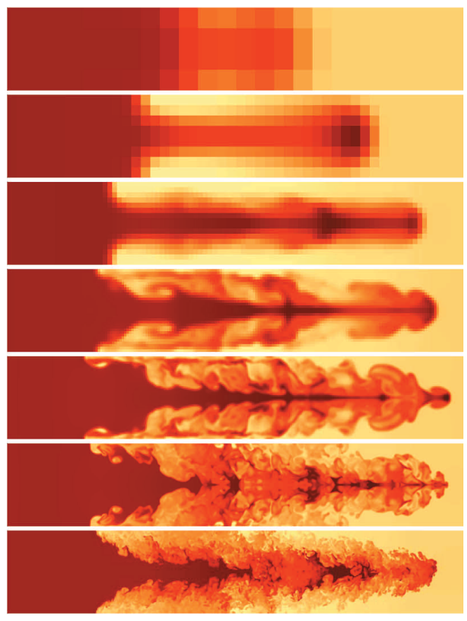
Verification and Validation: Challenges

- Bad news: Tough, non-linear multi-scale problems have a tremendous appetite for computer resources and mathematical expertise.
- Good news: We will have a job for some time!
- Existence argument: We have had great successes in the past through careful theory, experiment and now computation. There is every reason to think that better math, better algorithms, and better hardware will continue to allow us to reveal new scientific truths to better humankind. But, we must be careful!

"...the flow is extremely complex and quite sensitively dependent on the computational resolution...The take-home message is that resolution matters..."

Leo Kadanoff, University of Chicago, Dept. of Physics, on results obtained in DOE Accelerated Supercomputing Initiative (ASCI), *Computing in Science and Engineering*, 2004.

“Resolution Matters”: Kadanoff, 2004



Finer grids give different physical predictions!

The lead quotation from an **April 2009** joint report from Los Alamos, Sandia, and Livermore National Laboratories, “Enhanced Verification Test Suite for Physics Simulation Codes” LA-14379, SAND2008-7813, LLNL-TR-411291:

“In an age of spreading pseudoscience and anti-rationalism, it behooves those of us who believe in the good of science and engineering to be above reproach whenever possible. Public confidence is further eroded with every error we make As Robert Laughlin noted in this magazine, there is a serious danger of this power [of simulations] being misused, either by accident or through deliberate deception. Our intellectual and moral traditions will be served well by conscientious attention to verification of codes, verification of calculations, and validation, including the attention given to building new codes or modifying existing codes with specific features that enable these activities.”

Patrick J. Roache

(The Father of V&V)

"*One of the important lessons of the past ten years of the ASC program is the complexity and the importance of verification .... For example, in the absence of verification evidence, good agreement of calculations with experimental data may be an irrelevant observation, as the numerical solution could be completely wrong and the experimental agreement completely accidental.*"

Joint LANL, SNL, LLNL Report, April 2009.

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