



# What Can Computational Modeling for GNEP Learn from the ASC Program?



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***“Progress, far from consisting in change, depends on retentiveness. Those who cannot remember the past are condemned to repeat it.”***

**–George Santayana**



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# The Outline of This Talk

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- The ASC program and its modeling challenges
- The evolution of the ASC program
- What ASC could have done better
  - Initial focus, Code-user relationships
- What ASC has done right
  - Program evolution, projects that succeed
- The persistent challenge of V&V and UQ



## In a nutshell, what are the modeling challenges for GNEP?

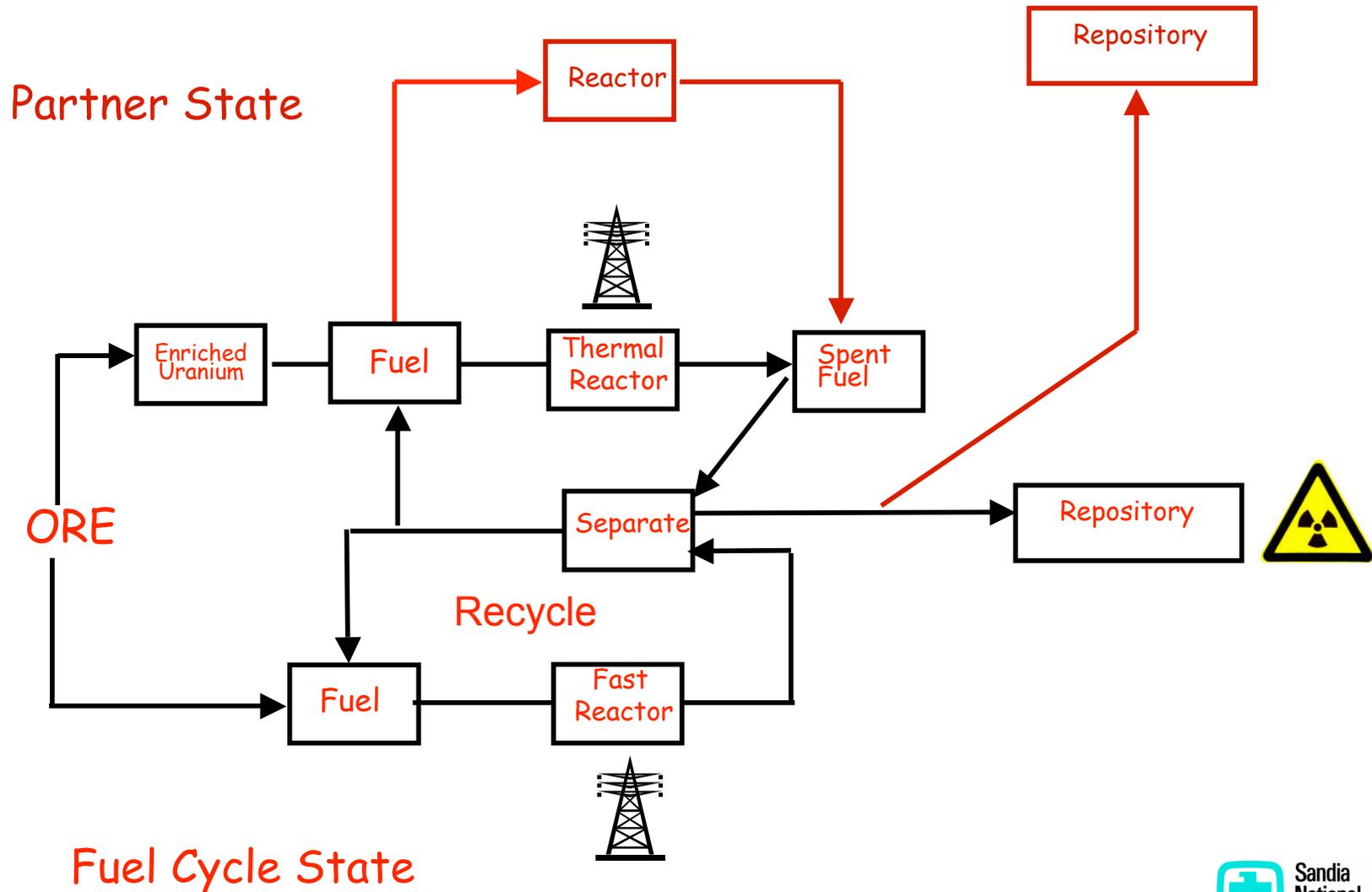
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- Essentially the challenges can be seen by looking at the fuel cycle:
  - Fuel design
  - Fuel use in reactors
    - ◆ Detailed reactor design
    - ◆ System design and analysis
  - Storage
  - Reprocessing
  - Waste stream
  - Modeling the cycle itself





# Figure from Vic Reis's talk on GNEP



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## The ASC program has challenges that parallel some of the GNEP ones.

- *The challenge is to use computational modeling to assist in providing a the means to maintain the US nuclear stockpile without full scale testing.*
- This provides a multitude of areas to focus on:
  - **Code development**
  - Physical model development
  - **Numerical algorithms**
  - Computer science and hardware
  - **Verification and validation, uncertainty quantification**
  - Data analysis associated with experiments.



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## Some observations on some lessons learned from the ASC program



### ■ What ASC did right.

- Broad multi-disciplinary program, lots of \$\$\$
- *Integrated V&V (eventually)*
- *SQA (eventually)*

### ■ What ASC could have done better.

- *Originally driven too much by high-end computing. Computer science focus was not application driven enough.*
- *Did not get sufficient code user community (i.e. designer) buy-in to the program's emphasis.*
- Insufficiently integrated experimental program (with a negative impact on Validation).

$$\frac{d\$}{dt} > 0$$

$$\frac{d\$}{dt} \gg 0$$

$$\frac{d\$}{dt} \ll 0$$

“Begin with the end in mind” - Steven Covey,  
7 Principles of Highly Effective People.

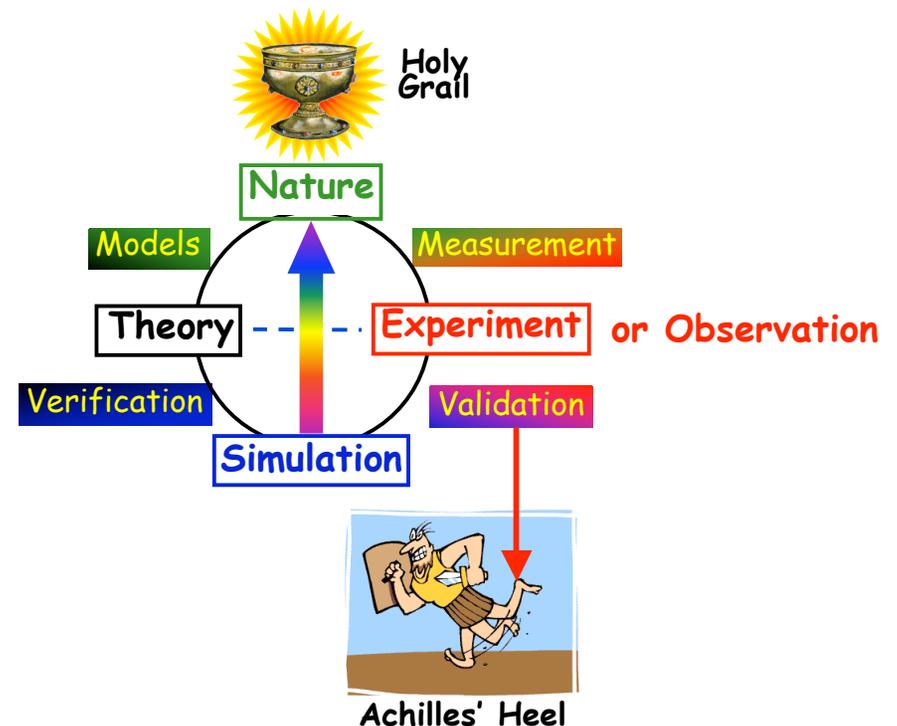
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# The issues with experimental connections are essential to avoid!

- Validation depends on experiment and measurement.
- The failure to develop a unified experimental & computational program has been a *key limiting factor in the effectiveness of ASC.*
- It's a mistake to definitely not repeat.

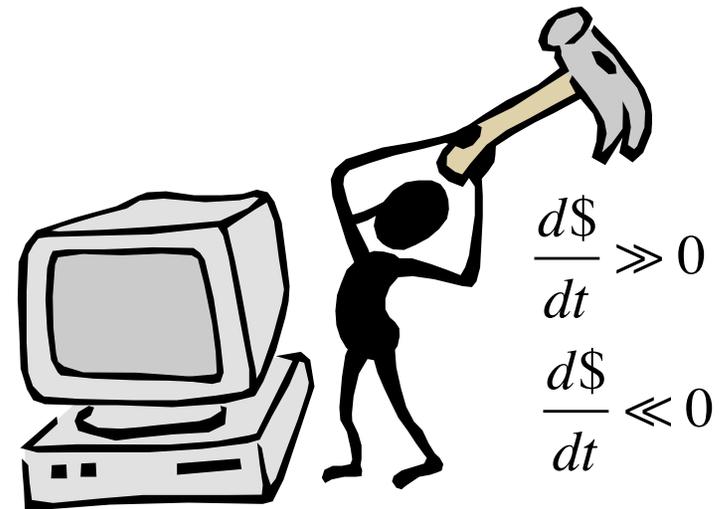
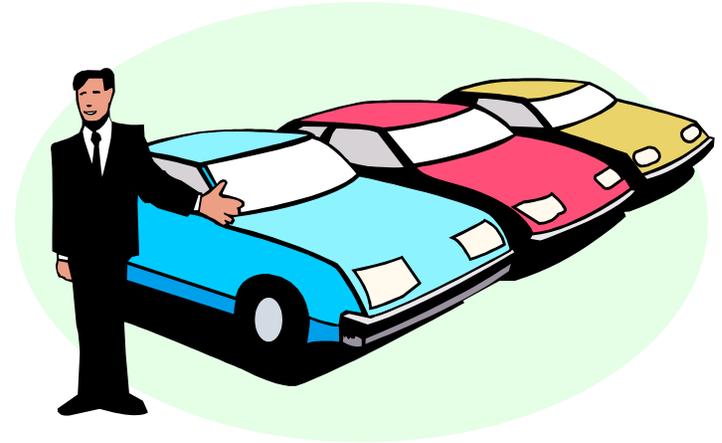
A conceptual picture of V&V within the context of science





## Is the computational program pushing or being pulled?

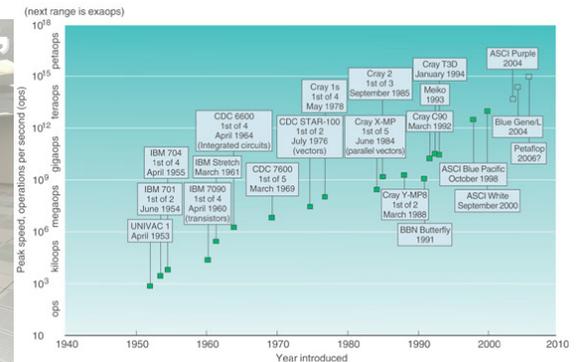
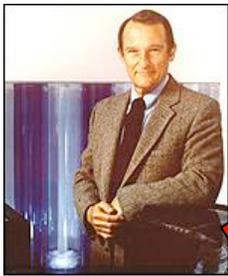
- Often, the computational capabilities seem to be pushed at users (down their throat?) .
- The opposite should be true, the users of computational methods should be pulling for better models, methods & computers.
- **If the computational programs are too “pushy” then the users of computations can become enemies.**





# The ASC program had somewhat different foci in the past.

- Providing extensive computational resources has been an enduring aspect of the program.



- The mix of code, algorithm, modeling and V&V has changed as well as the user interaction.
- Recent changes have diminished the emphasis on algorithms and modeling, with increased emphasis on quality (SQE, V&V) with hardware & code development remaining “a constant focus”.

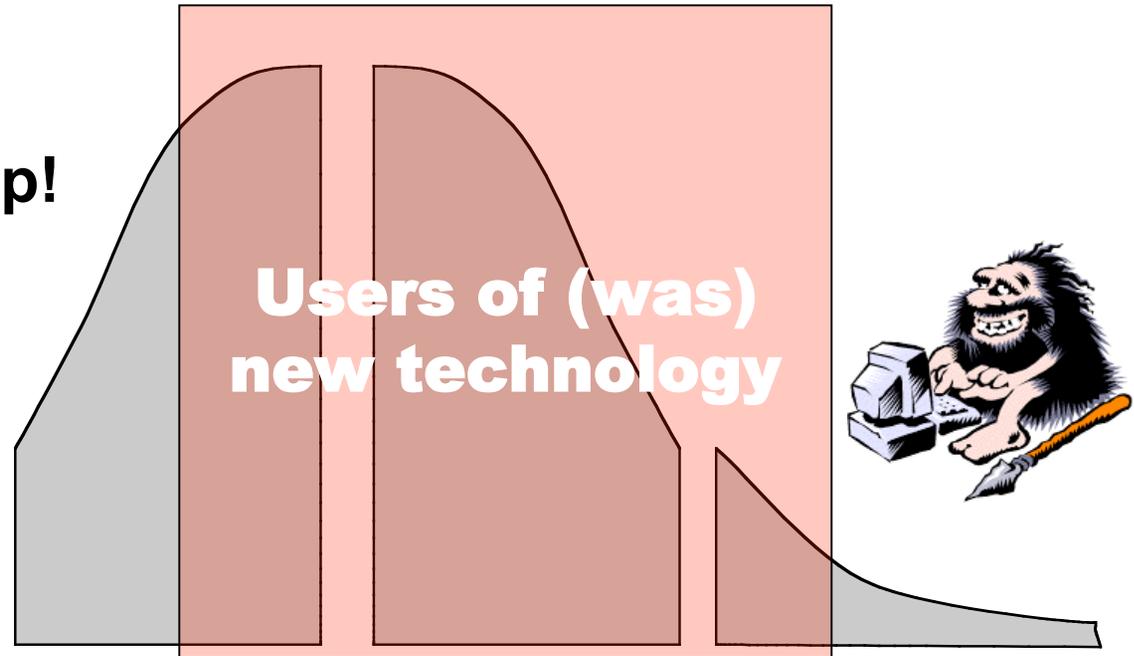
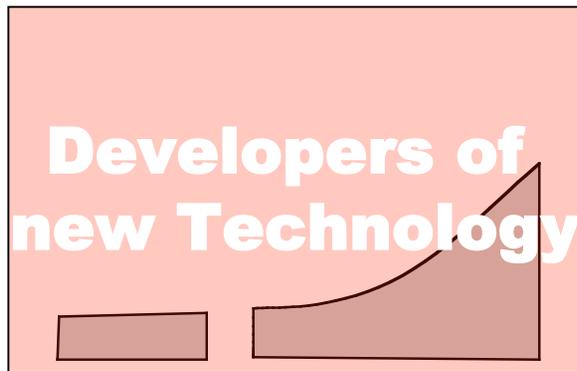
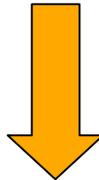


# Diffusion of innovation is useful to understand how ideas advance.



"So easy, even a caveman could do it" - Geico

### The Gap!



*Innovators*



Technology Enthusiasts

*Early Adopters*



Visionaries



*Early Majority*



Pragmatists

*Late Majority*



Conservatives

*Laggards*



Skeptics

Figure adapted from "After the Goal Rush: Creating a True Profession of Software Engineering" by Steve McConnell, Microsoft Press 1999

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## The ASC program has evolved over time, mostly in a positive direction.

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- One way to view these changes is the need to bridge the “gap”. The original program could not overcome **barriers that are natural to innovation.**
- Some of these differences were a relative decrease in algorithm development and computer science emphasis coupled with...
- ... **an increase in V&V, UQ and user support.**
- *The V&V has been added to provide a basis for believing the simulations (i.e. their relative quality)*
- *UQ to assist decision makers in knowing how good their simulations are.*



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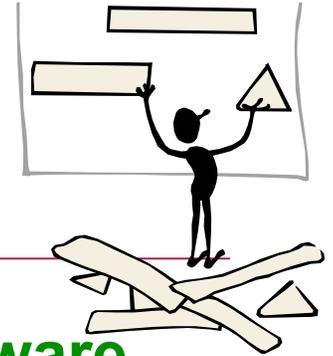
***“The plural of 'anecdote' is not 'evidence'.”***  
**Alan Leshner, publisher of Science**

***“...what can be asserted without evidence can  
also be dismissed without evidence.”***

**by Christopher Hitchens**



## 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 without testing.**
- **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.**





## Some scientific areas have also been downgraded during the evolution of ASC.

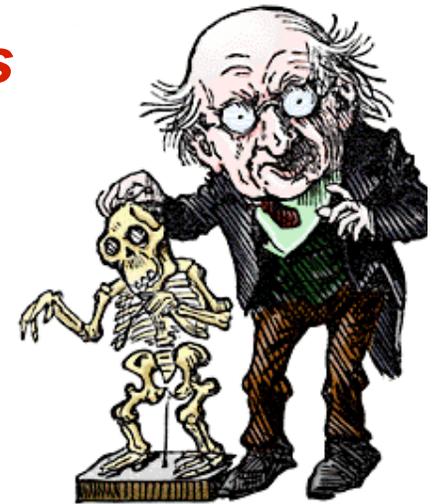


- In a relative sense the activities of V&V, UQ and SQE have been traded against other activities.  $\frac{d\$}{dt} > 0$
- Among the losers has been algorithm development:
  - *This is somewhat tragic since V&V done properly should be a big motivator for developing better methods!*  $\frac{d\$}{dt} < 0$
  - In carrying out the UQ process, one may come to the conclusion that codes are not acceptable and change (i.e. new methods) might be necessary.
  - Another key issue is that most code structures have not been able to readily accept new methods (i.e. software).



## Improving codes and methods has been a constant problem with ASC.

- The issue is complicated by software complexity.
  - We have not found a silver bullet.
- *The standards for accepting calculations is ad hoc and strongly favors existing methodologies.*
  - This is centered on an expert-based acceptance culture (more later)
  - Empirical means of calibrating calculations favor older methods (new methods need different tuning parameters or different tuning methods).
- It is much simpler to get existing methods (and codes) to produce useful results.





**This quote is instructive in highlighting this matter in the light of current events.**

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***“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**



## There are important lessons on what sort of projects have worked under ASC.

- In one case, the ASC project “evolved” from an older code (2-D to 3-D).
  - The 3-D code was *benchmarked* in by the older 2-D code yielding substantial continuity.
  - The utility of the code was maintained.
  - The new code did provide access to the enhanced computational resources.
  - The code kept the same name.
- The code retained a user base throughout.
- This is arguably the most successful project in ASC.





## There are important lessons on what sort of projects have worked under ASC.

- Another successful case is associated with a huge change in the sort of simulation used by a community of users
- The code involved the direct support and utility by several extremely influential and capable users.
  - The code demonstrated useful and unique capabilities (solved some old & new problems)
  - The code developers were extremely devoted to V&V feedback and fixed problems promptly.
- The code had a very user-responsive development team along with some intrinsic advantages (and disadvantages) compared with earlier codes.





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

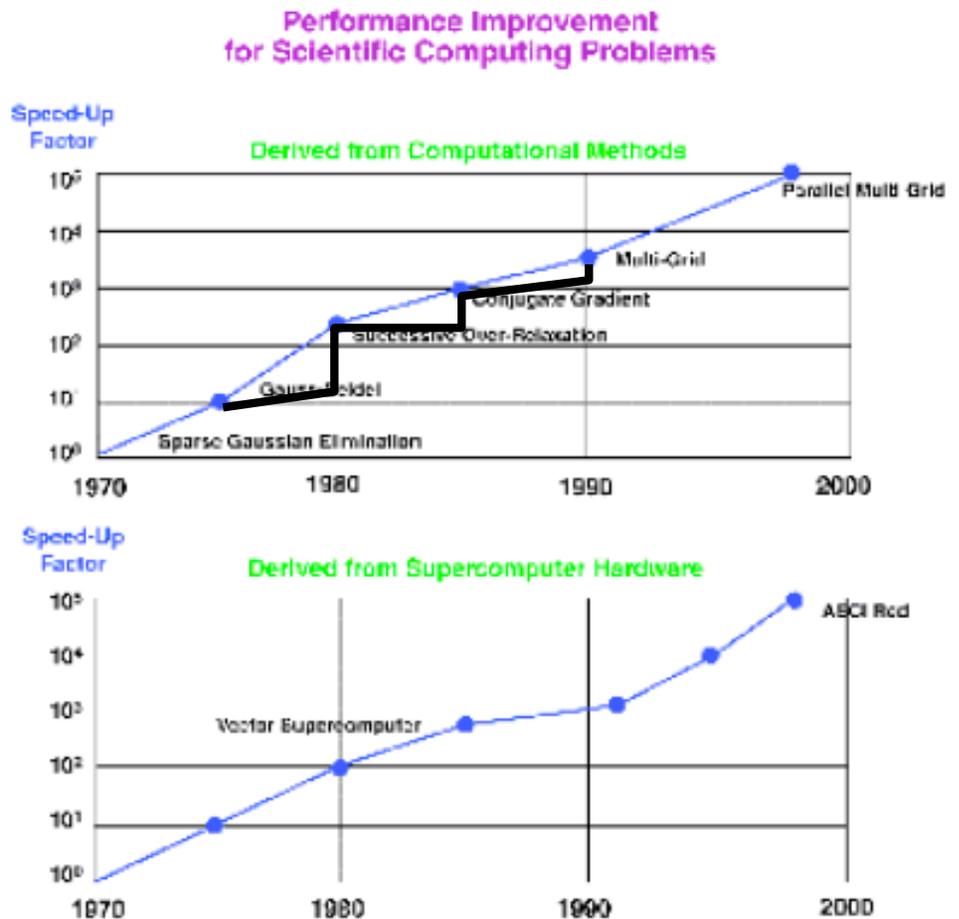
**– Nick Trefethen**





# It is important to realize a couple of facts about the history of computational science.

- **Fact 1: Algorithms have provided as much bang as the computers.**
  - **Algorithm advances are mostly quantum rather than continuous (limiters, conjugate gradient).**

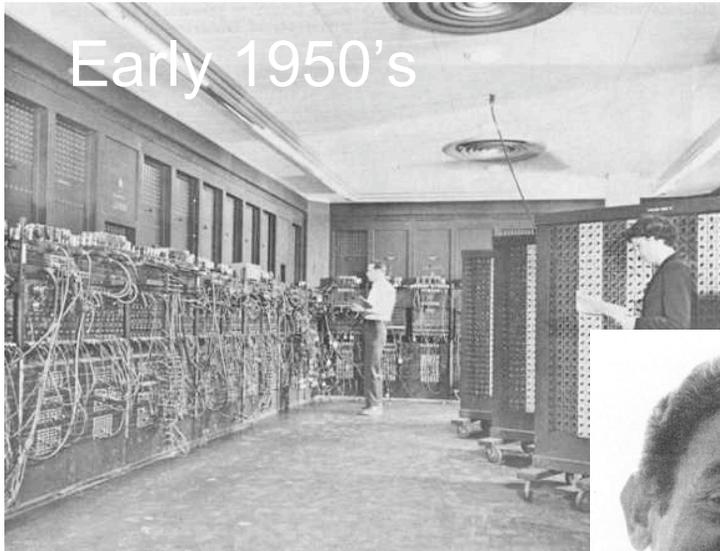


Presented by Donna Crawford 2002 @LNL  
Originally in SIAM Review, Petzold et al., 2001

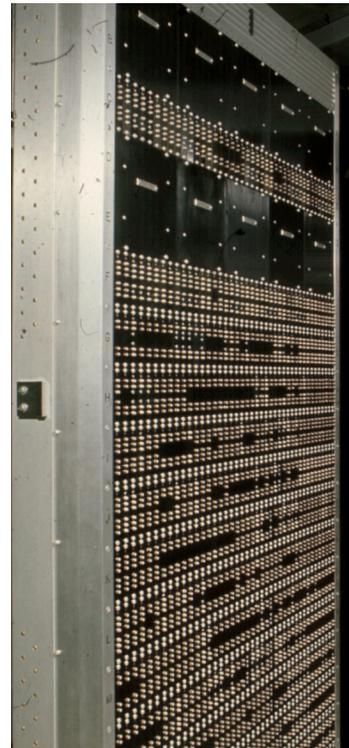


## It is important to realize a couple of facts about the history of computational science.

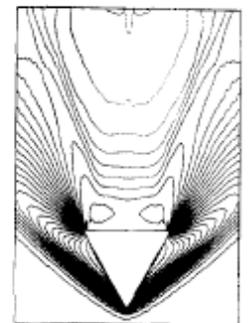
- **Fact 2: Computational resources are enabling.**
  - **Certain calculations cannot be attempted without having computers of a certain class (climate modeling, external aerodynamics,...).**



Jules Charney



Mid 1960's





## The History of ASC is still being written.



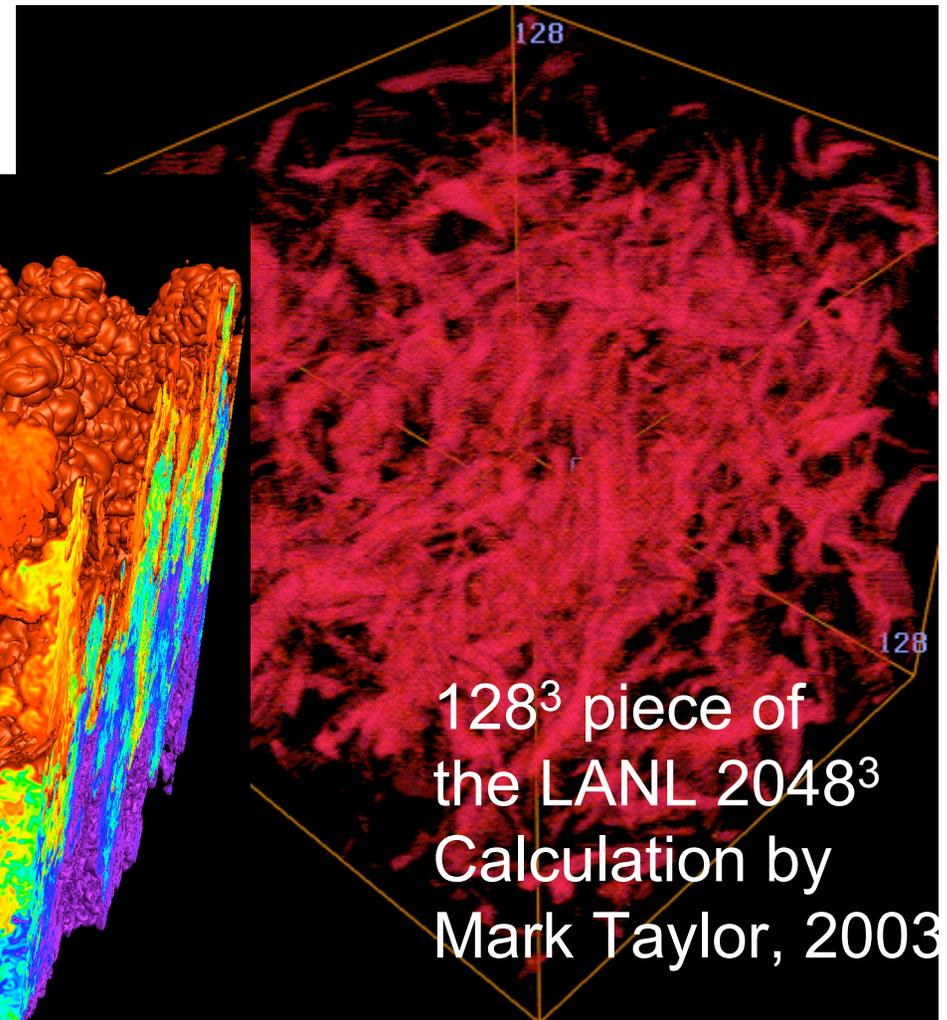
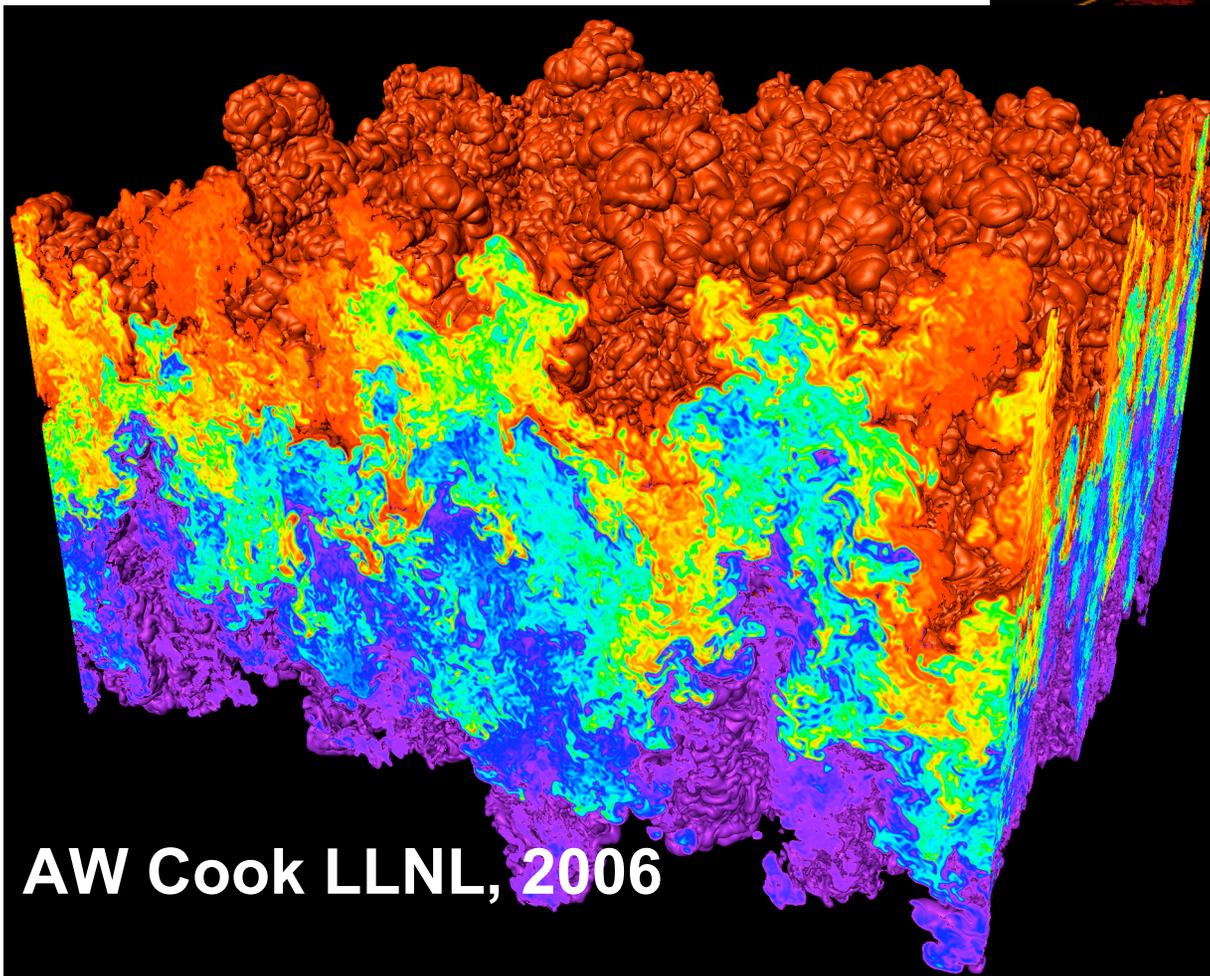
**What has ASC level computing enabled?**

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## Some candidates exist, but may not be the really important developments

- Time will tell.



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

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



## Getting science to accept V&V and UQ as a “way of life” is a persistent challenge!

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- One issue is that V&V work is “dull” and can find itself immersed in obscure mathematical details.
- Doing a complete V&V study is time-consuming and requires effort that is not focused directly on physics or engineering.
- It does form the foundation for UQ, which starts to open new scientific questions:
  - **What is the intrinsic variability in physical phenomena or devices? (experiment)**
  - **Does the model produce the same variability as the physical system or device? (theory & computation)**



## It is important to know your audience.



- **The engineering and physics community have reacted differently to V&V, just look at the scientific literature.**
- **The engineering community more generally embraces V&V and has put standards into practice in many of their publications.**
  - **With that said, various parts of that community still resist V&V**
- **The physics community does not have identified standards associated with V&V.**
  - **The physics community tends to embrace an “expert” based standard.**

“The simulation is good because I’m a good physicist.”



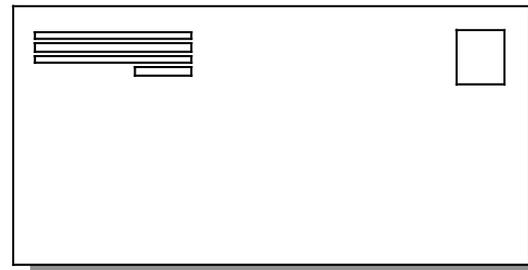
## Excerpt from the editorial policy of Physics of Fluids

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**“Physics of Fluids, published monthly by the American Institute of Physics with the cooperation of the American Physical Society, Division of Fluid Dynamics, is devoted to original theoretical, computational, and experimental contributions to the dynamics of gases, liquids, and complex or multiphase fluids.”**

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

I'm not picking on Physics of Fluids,  
there are many other examples



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## Excerpt from the editorial policy of JFE

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**“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.”**



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

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**“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!)

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**“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 gives a sense of the difference in communities.**



## Excerpt from the editorial policy of JFE

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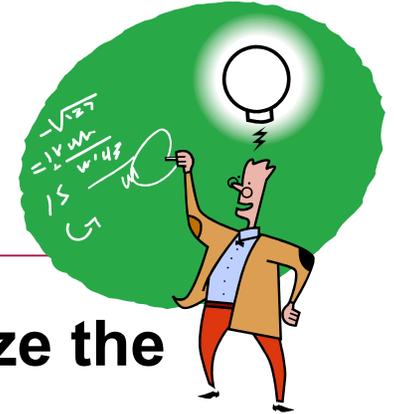
***“The Journal of Fluids Engineering will not consider any paper reporting the numerical solution of a fluids engineering problem that fails to address the task of systematic truncation error testing and accuracy estimation. Authors should address the following criteria for assessing numerical uncertainty.”***

**The differences in approach are substantial.**

**Other journals in each field have similar statements.**



## 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:
  - Engineers tend to work to achieve a strong evidence basis for decisions
  - Physicists tend to provide their evidence based more strongly on expertise.





## **There is reason to believe that V&V will be more accepted under GNEP than ASC.**

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- **Since GNEP is much more centered around engineering activities, the concept of V&V is more likely to be acceptable to the community.**
- **Many of the problems with computation's acceptance with the user community for ASC are the physicist's standard of acceptance (as reflected by the editorial statements).**
- **This difficulty is reflected by the difficulties in making a large impact that the V&V program has had in ASC.**
- **One might surmise that V&V could have a larger impact for GNEP related simulation (if done right).**



## Summary of comments

- Programs and their objectives evolve over time, ASC is a good example.
- **ASC originally did not have a strong V&V or UQ focus, but these elements have increased in importance over time.**
- ASC was essentially a technology push, but the user pull was not strong enough hence a mismatch.
- The nature of the user communities should be factored into plans (**i.e. engineers and physicists are different**),
  - The user communities have differing views of computation and how to assess its quality.

$$\frac{d\$}{dt} \gg 0$$
$$\frac{d\$}{dt} \ll 0$$



# Dilbert helps us understand that we're not alone in our struggle.



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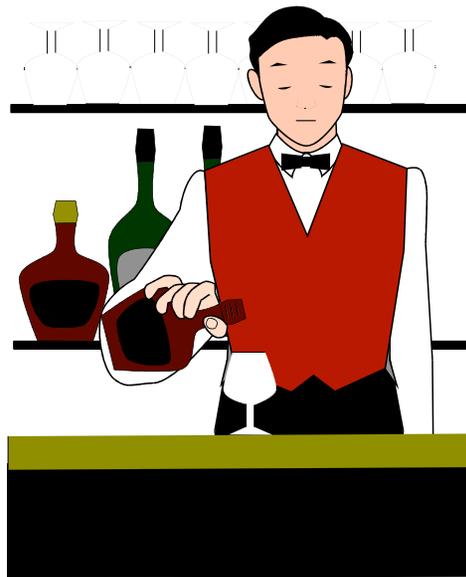


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***“A computer lets you make more mistakes faster than any invention in human history — with the possible exceptions of handguns and tequila.”***

**Mitch Ratliffe, Technology Review, April, 1992**



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