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

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The Outline of This Talk

- Modeling challenges for GNEP
- The ASC program and its modeling challenges
- The evolution of the ASC program
- What ASC has done wrong
  - Focal points, Code user relationships
- What ASC has done right
  - Paradigms that work
- Suggestions for GNEP modeling to incorporate
- The persistent challenge of V&V and UQ

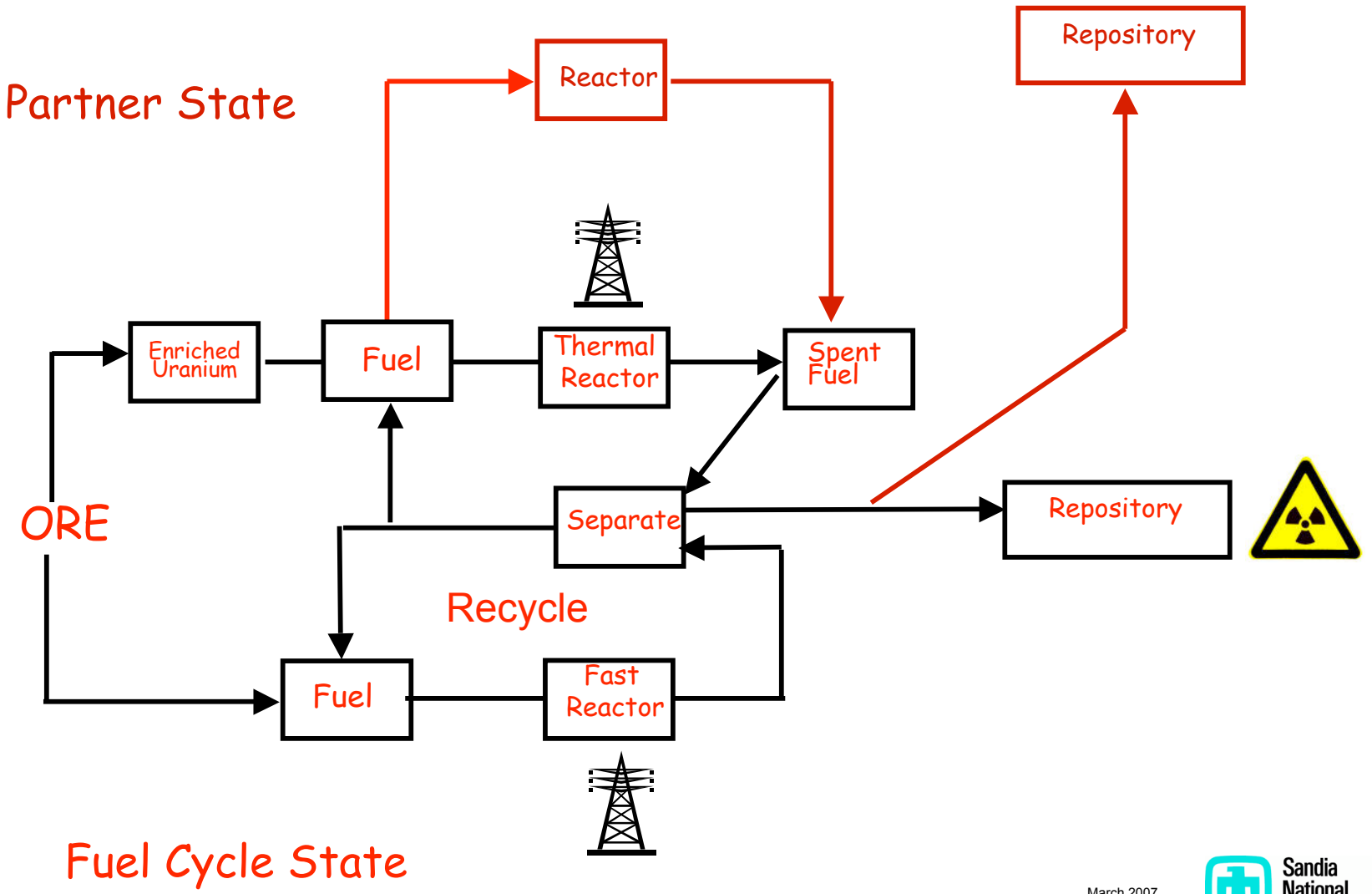
"A computer lets you make more mistakes faster than any invention in human history — with the possible exceptions of handguns and tequila."

Mitch Ratliffe, Technology Review, April, 1992

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

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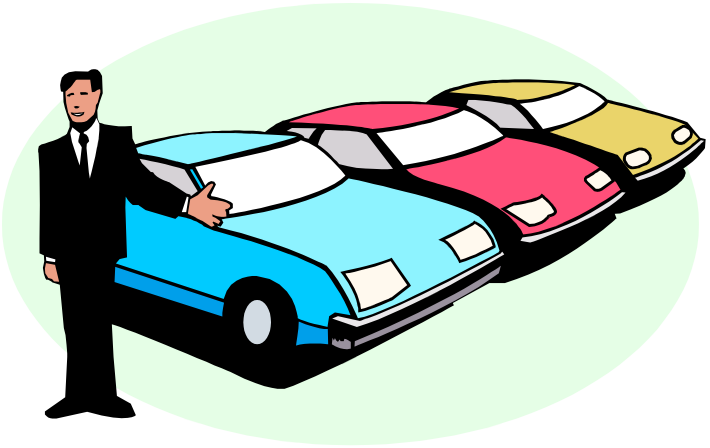
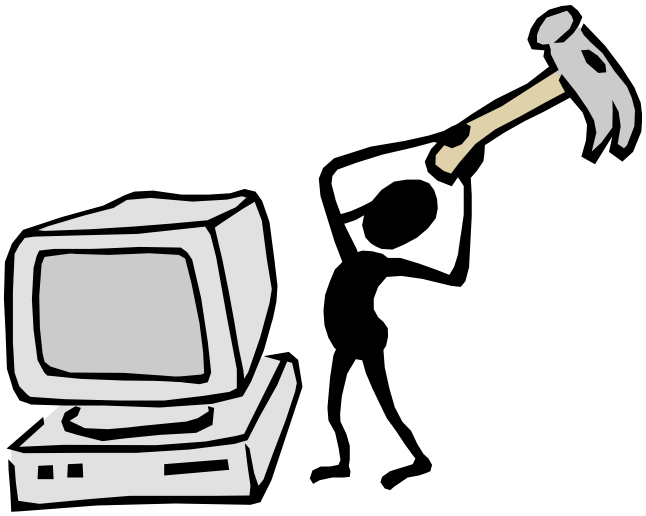
The ASC program has challenges that parallel some of the GNEP ones.

- The challenge is to use computational modeling to provide a sufficient mean to maintain the US nuclear stockpile without full scale testing.
- This provides a multitude of areas to focus on:
  - Numerical algorithms (esp. hydro & radiation)
  - Code development
  - Physical model development
  - Computer hardware and science
  - Data analysis associated with experiments.
  - Verification and validation, uncertainty quantification

Is the computational program pushing or being pulled?

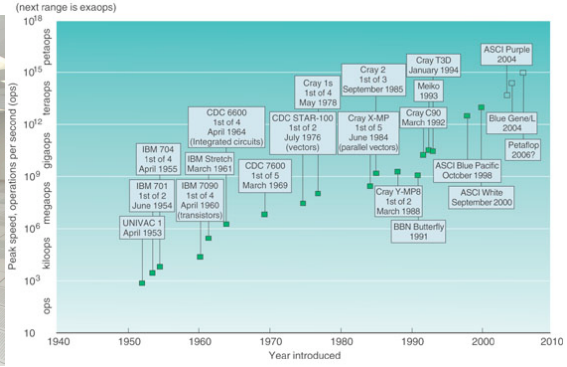
- Generally, the computational capabilities are being pushed (down the throat?) of users.
- The opposite should be true, the users of computational methods should be pulling for better methods.
- If the computational programs are too “pushy” then the users of computations become enemies.





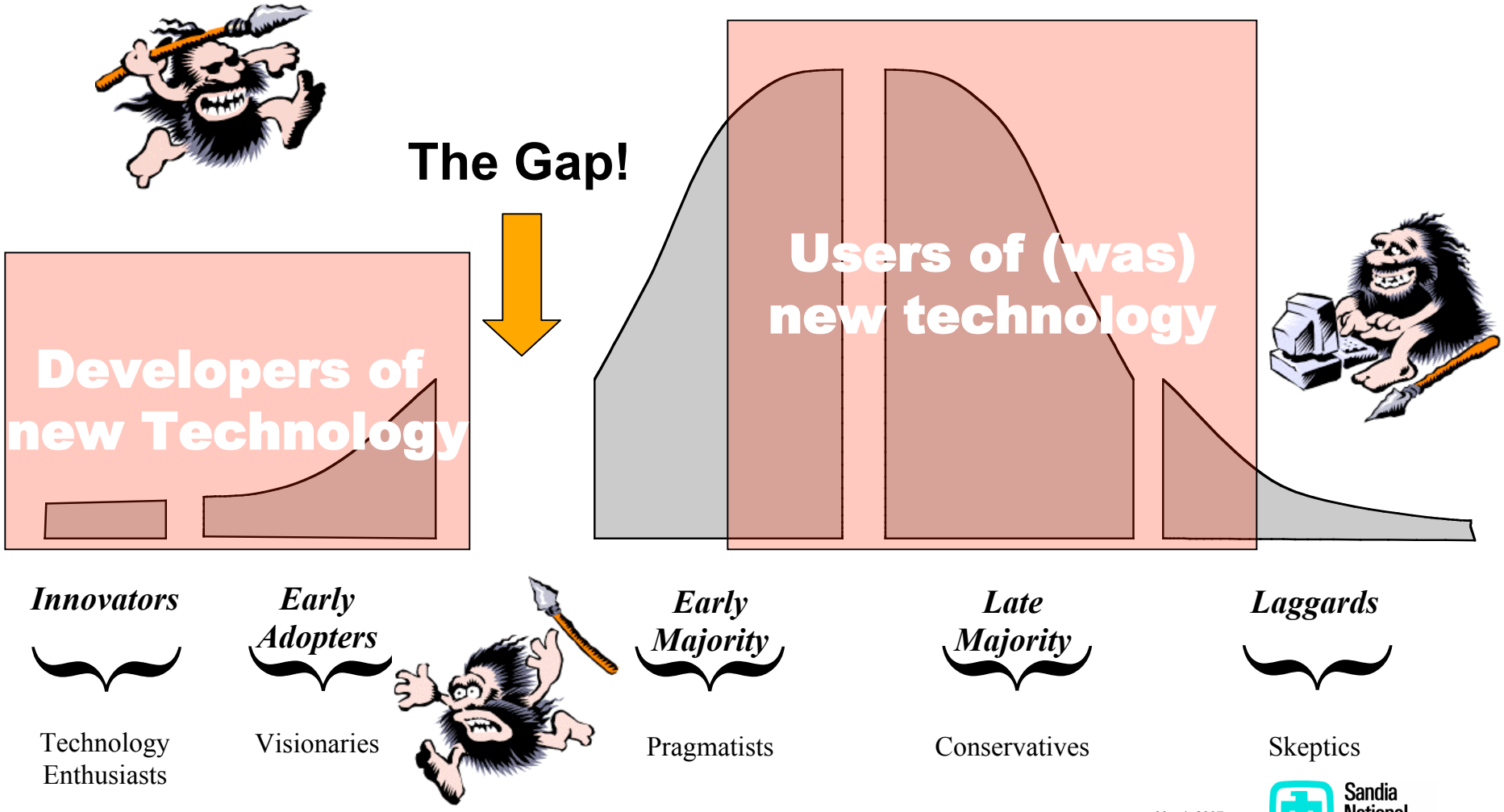
Historically, the ASC program had somewhat different foci in the past.

- Its obvious that providing extensive computational resources has been an enduring aspect of the program.



- The mix of code, algorithm, modeling and quality 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) and code.

Diffusion of innovation is useful to understand how ideas advance.



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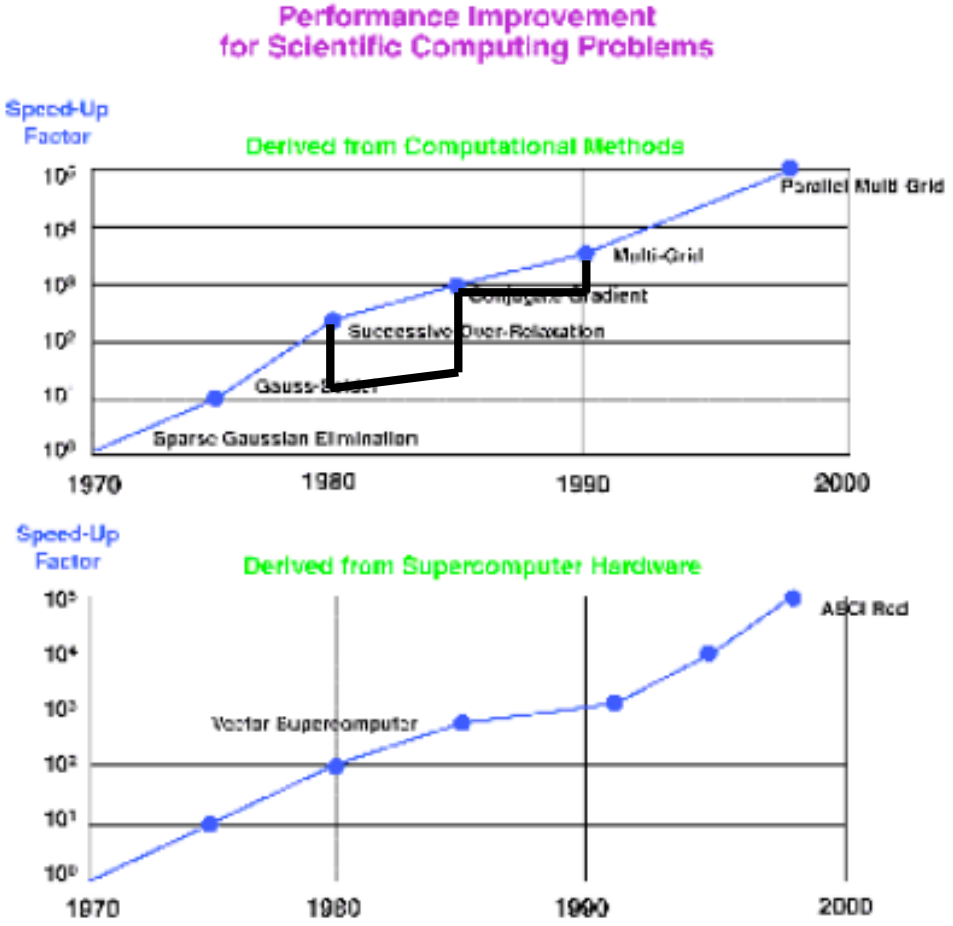
"The fundamental law of computer science: As machines become more powerful, the efficiency of algorithms grows more important, not less."

– 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 @LNLL
Originally in SIAM Review, Petzold et al., 2001

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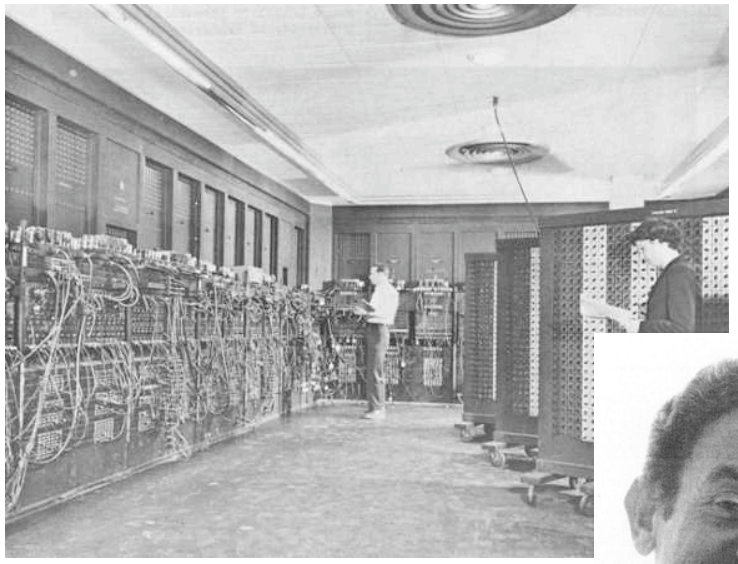
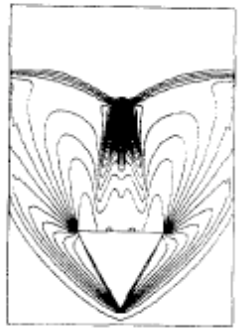
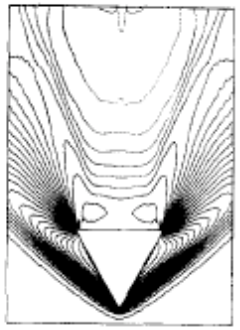
It is important to realize a couple of facts about the history of computational science.

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



Jules Charney, and ENIAC





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The History of ASC is still being written.

What has ASC level computing enabled?

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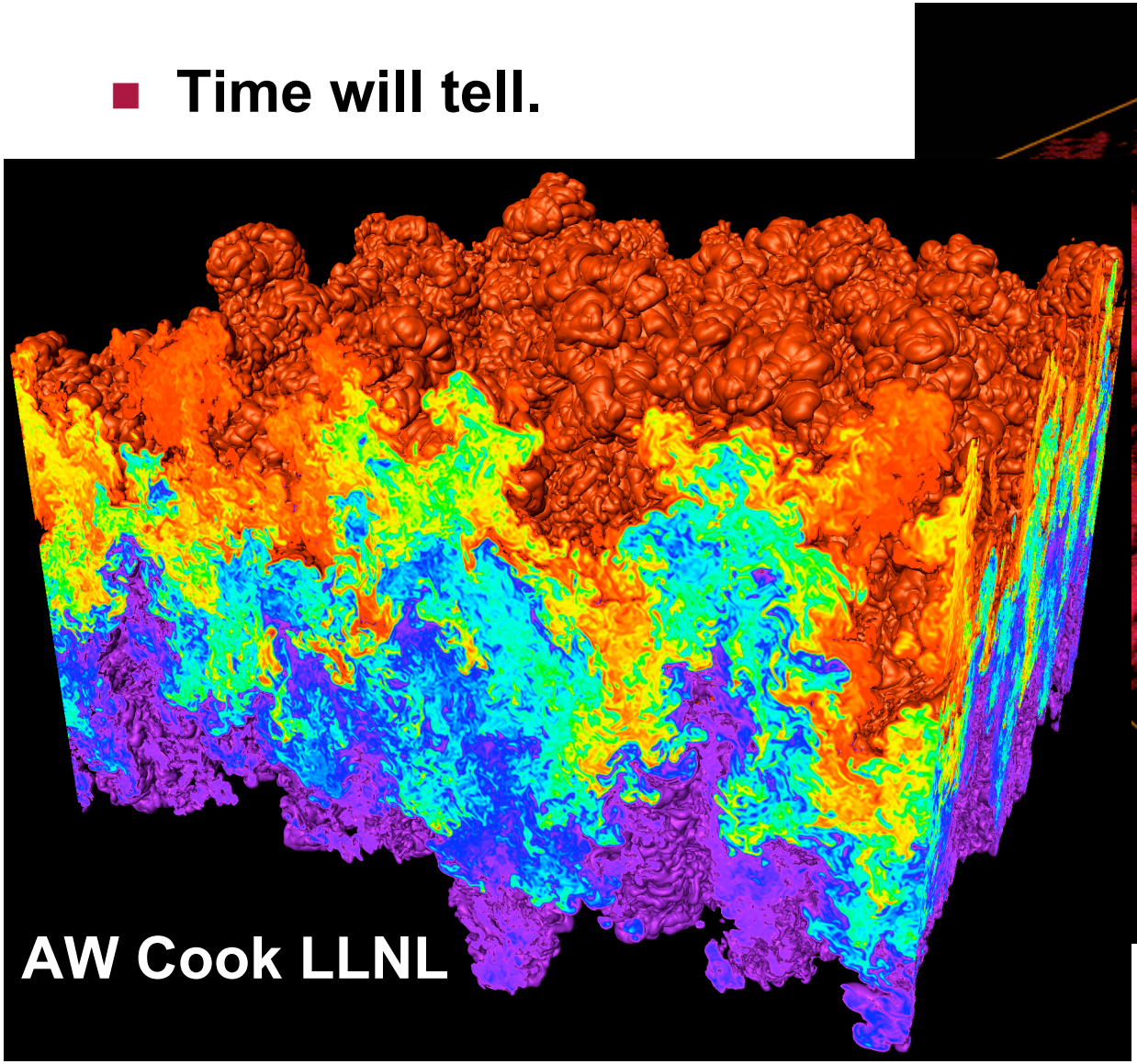
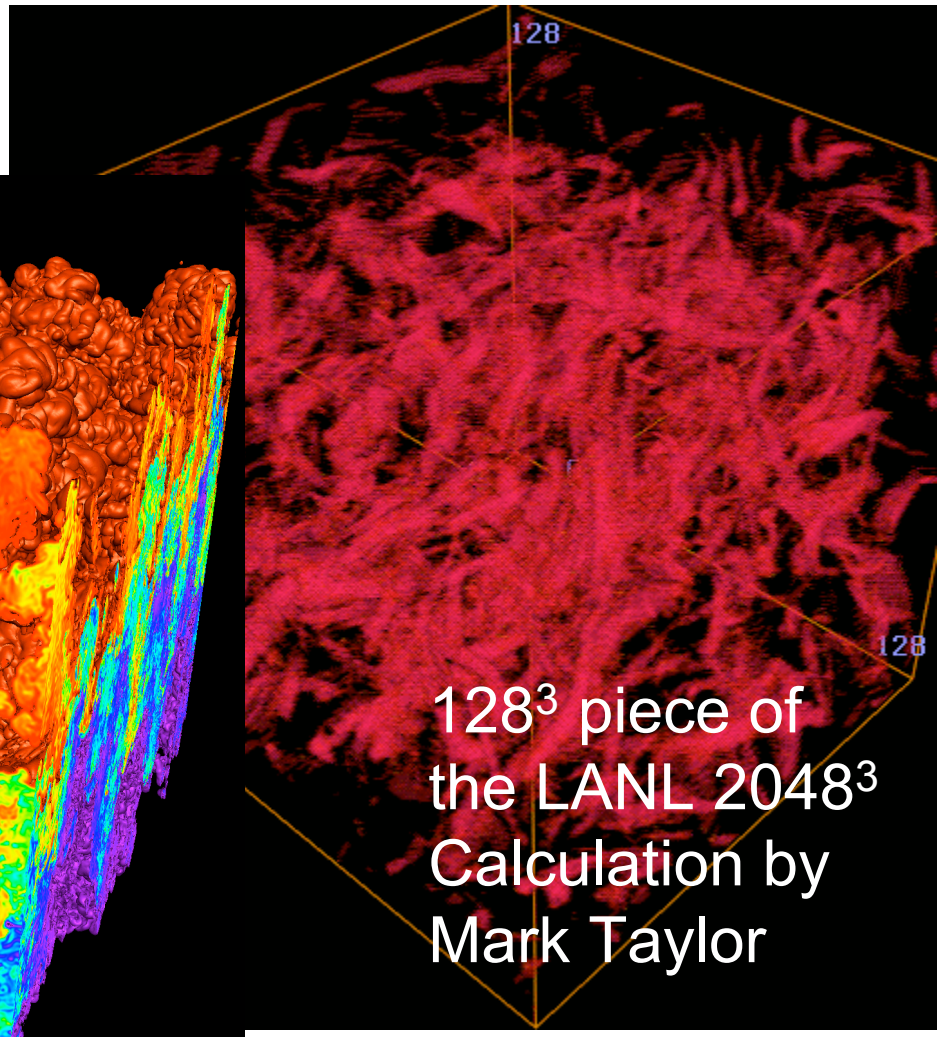
Some candidates exist, but may not be the really important developments

- **Time will tell.**





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

- Based on addressing the issues associated with the use of the fruits of the ASC program, and decision making with simulation change was needed.
- Some of these differences were a relative decrease in algorithm development and computer science couple 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.

“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 Chirstopher 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 its original program.
- These areas of activity were added as the need for focused activity was recognized.

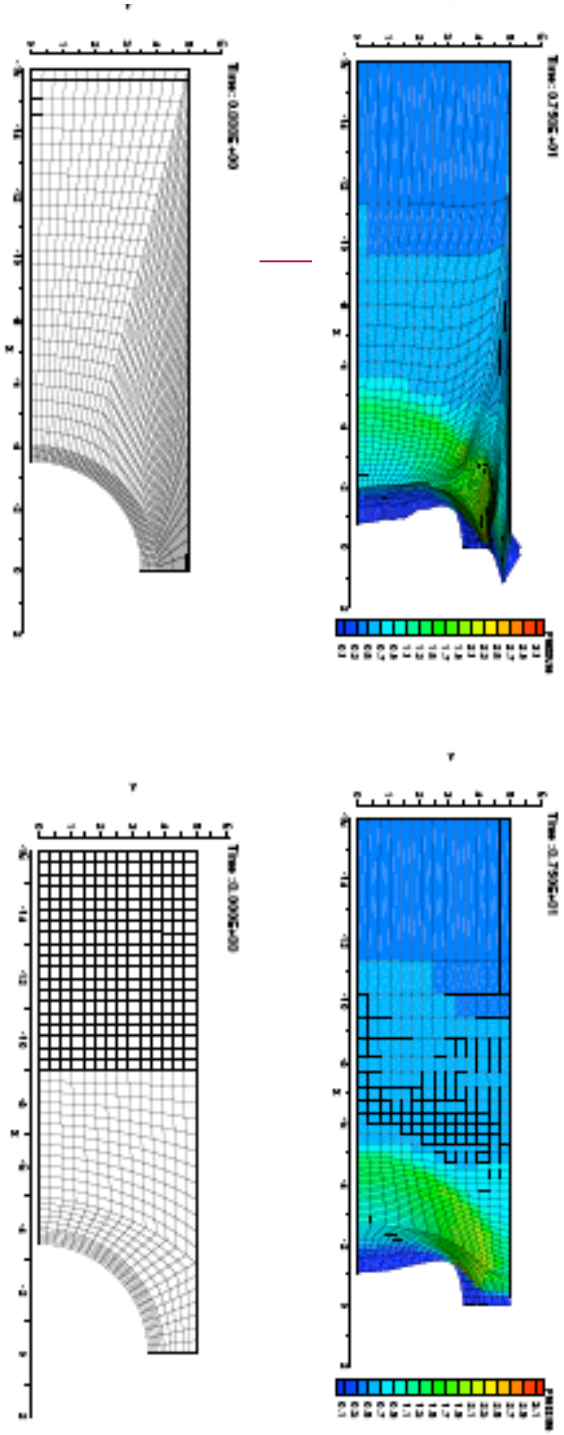
- V&V was added because the standard practices of the code development and user communities did not include much rigor.
- SQE was added for a similar reason.
- UQ was added because the decision makers realized that the information they needed was not present in the "standard" computational analysis.

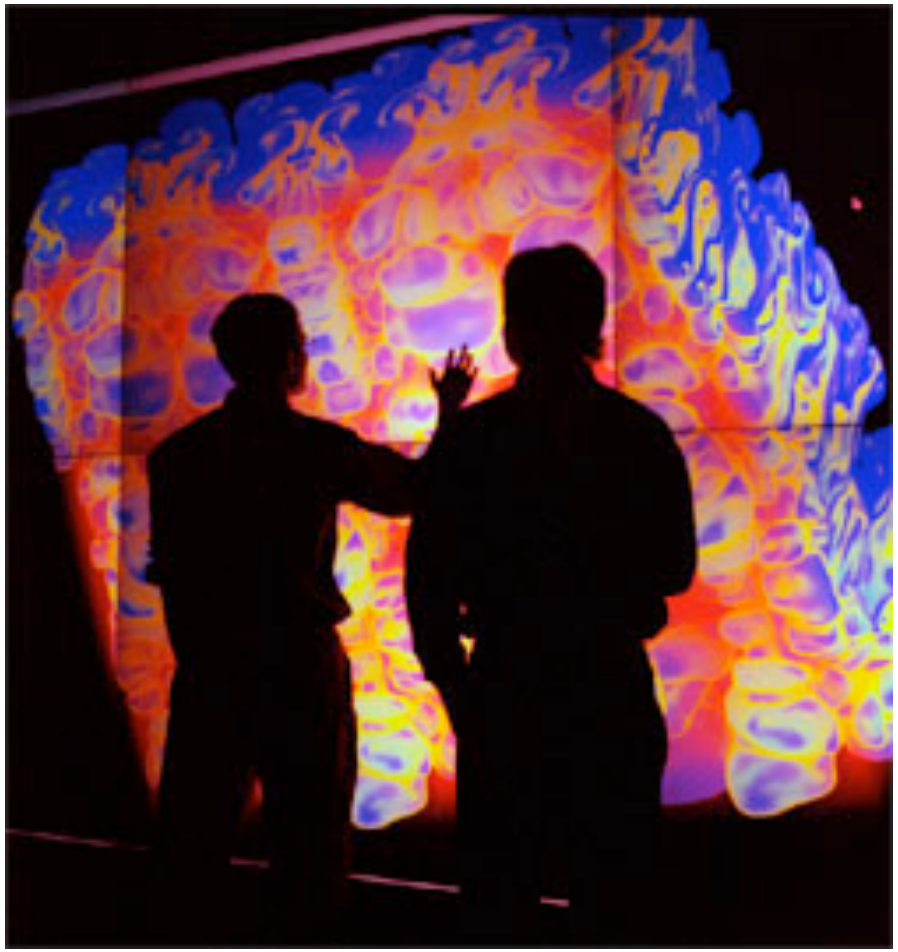
Some scientific areas have also been downgraded during the evolution of ASC.

- In a relative sense the activities of V&V, UQ and SQE have been traded against other activities.
- Among the big losers has been algorithm development:
  - This is somewhat tragic since V&V done properly should be a big motivator for algorithms
  - To do UQ properly one reasonably comes to the conclusion that the current codes can not do this correctly (need new algorithms)
  - The other issue is that code structures have not been able to readily accept new methods.

The Algorithm Development Issue under ASC.

- The issue is complicated by software complexity.
- General frameworks have not yielded broad based success, generally speaking they have failed.
- The standards for accepting calculations (and improved algorithms) is ad hoc and deeply favors existing methodologies.
  - This is based on an expert-based acceptance culture (more later)
  - Empirical means of tuning calculations favor older methods (new methods need different tuning parameters).
- It is much simpler to get existing methods (and codes) to produce useful results.





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

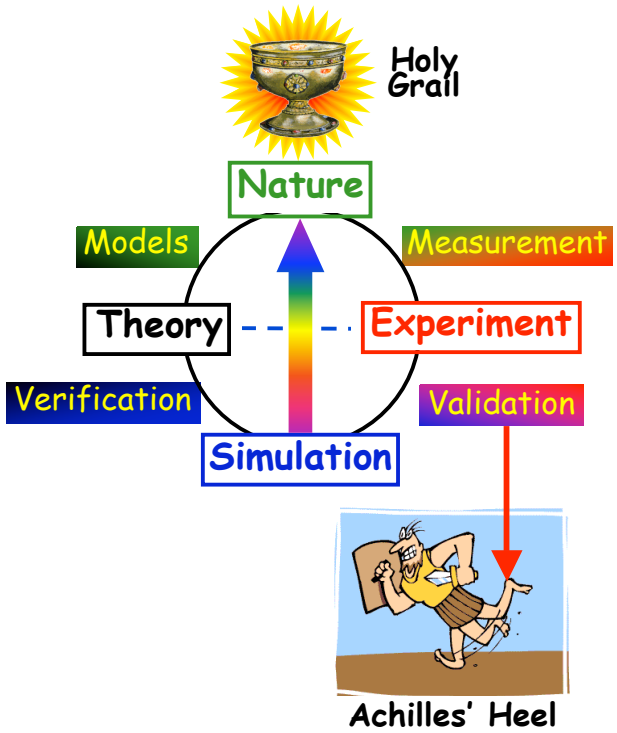
- In one case the ASC project *"evolved"* from an older code (2-D to 3-D).
  - The 3-D code was benchmarked in 2-D by the older code
  - The utility of the code was maintained.
  - The code did provide access to the enhanced computational resources.
  - The code kept the same name.
- The code retained 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 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 an extremely influential and capable user.
  - The code demonstrated useful and unique capabilities (solved 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.

Problems with how ASC was constructed.

- ***Largely driven by high-end computing, not by applications. Becomes an end unto itself, not a tool***
- **Initially did not get code user (i.e. designer) community buy-in in constructing the program.**
- **Insufficiently integrated experimental program (with a profound negative impact on Validation).**



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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!

- One issue is that V&V work is "dull" and often finds 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 for the foundation for UQ which starts to open new scientific questions:
  - What is the intrinsic variability in physical phenomena? (experimental)
  - Does the model produce the same variability as the physical system? (computational)

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 computational engineering community generally embraces V&V and has put standards into practice in their publications.
  - With that said, various parts of the community still resist V&V
- The computational physics community does not have identified standards with V&V.
  - The physics community instead embraces an "expert" based standard.

"The simulation is good because I'm a good physicist."

Excerpt from the editorial policy of JFE

"Journal of Fluids Engineering disseminates technical information in fluid mechanics of interest to researchers and designers in mechanical engineering. The majority of papers present original analytical, numerical or experimental results and physical interpretation of lasting scientific value. Other papers are devoted to the review of recent contributions to a topic, or the description of the methodology and/or the physical significance of an area that has recently matured."

Excerpt from the editorial policy of Physics of Fluids

"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.

Excerpt from the editorial policy of JFE (digging a bit deeper)

"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

"*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.* "

This is must different than *Physics of Fluids*! There nothing can be found. Other journals in each field have similar statements.

Excerpt from the editorial policy of JFE (digging a bit deeper, there's more!)

"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.

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 (and V&V)
- While the physics community embraces a standard based on expert judgement.
- These considerations tend to be reflected in practice:
  - Engineers tend to work to achieve a strong evidence basis for decisions
  - Physicists often base their evidence based on expertise.

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

- Since GNEP is much more centered around an engineering activity, the concept of V&V is more acceptable.
- Many of the problems with computation's acceptance with the user community for ASC are because 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.

Summary of comments

- Programs and their objectives evolve over time, ASC is an 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 hence a mismatch.
- The nature of the user communities should be factored into plans (engineers and physicists are different),
  - The user communities have differing views of computation and how to assess its quality.