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2015 NEW MEXICO JUDGES SCIENCE SCHOOL

CONFIDENCE IN NUMERICAL SIMULATIONS

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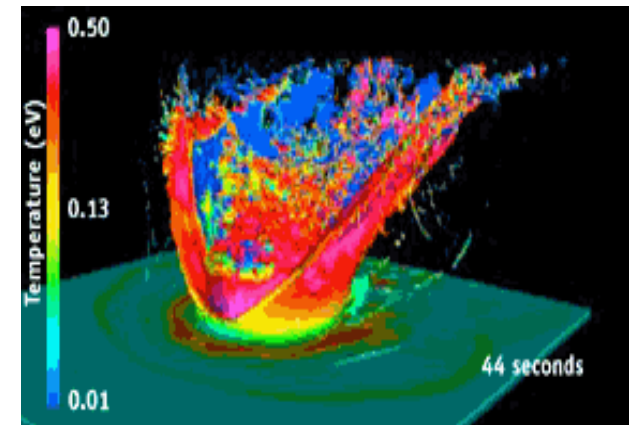


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Confidence in Numerical Simulations

François Hemez, Los Alamos National Laboratory (XTD-IDA)

2015 New Mexico Judicial Science School, LANL/UCSD Engineering Institute
Los Alamos National Laboratory, Los Alamos, New Mexico, March 2015

Abstract

This presentation offers a high-level discussion of uncertainty, confidence and credibility in scientific Modeling and Simulation (M&S). It begins by briefly evoking M&S trends in computational physics and engineering. The first thrust of the discussion is to emphasize that the role of M&S in decision-making is either to support reasoning by similarity or to “forecast,” that is, make predictions about the future or extrapolate to settings or environments that cannot be tested experimentally. The second thrust is to explain that M&S-aided decision-making is an exercise in uncertainty management. The three broad classes of uncertainty in computational physics and engineering are variability and randomness, numerical uncertainty and model-form uncertainty. The last part of the discussion addresses how scientists “think.” This thought process parallels the scientific method whereby a hypothesis is formulated, often accompanied by simplifying assumptions, then, physical experiments and numerical simulations are performed to confirm or reject the hypothesis. “Confidence” derives, not just from the levels of training and experience of analysts, but also from the rigor with which these assessments are performed, documented and peer-reviewed.

Who am I?

- I have been a Technical Staff Member at Los Alamos since 1997; I worked in the Engineering Division for seven years and I am currently with “X” Division.
- Over the past 15 years, I have worked on the validation of models applied to structural health monitoring, material modeling, weapon engineering and physics.



François Hemez, LANL

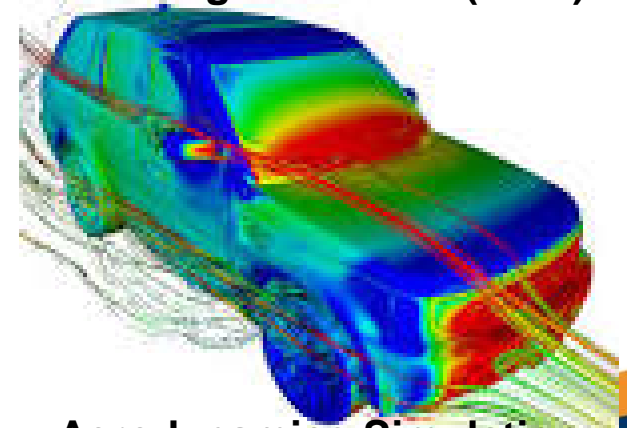
- Engineering degree in France.
- Ph.D. in Aerospace Engineering, University of Colorado, Boulder.
- Lead the ASC Verification Project and ASC Predictive Capability Assessment Project, for three years each, at LANL.
- Adjunct professor at the University of California San Diego, where I have been teaching since 2005.

In the past 15 years, the role of modeling and simulation in computational physics and engineering has radically changed ...

- Old paradigm: Experiments are qualification tests; simulations are used *a posteriori* to understand the observed behavior.
- New paradigm: Simulations predict the performance; experiments provide the data necessary to validate the models.
- Challenge: How to quantify **confidence** in this new paradigm?



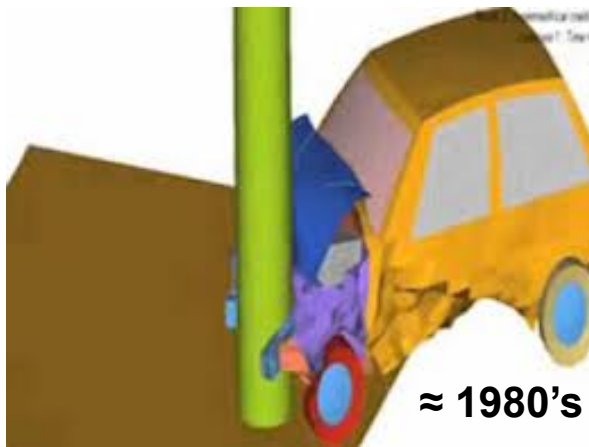
Challenger Disaster (1986)



Aerodynamics Simulation

Computing power, and the accompanying evolution of analysis codes, has brought an unprecedented fidelity in simulations.

- Better mechanics or physics
- Better coupling of phenomena
- More resolution in the calculations
- More accurate numerical solvers

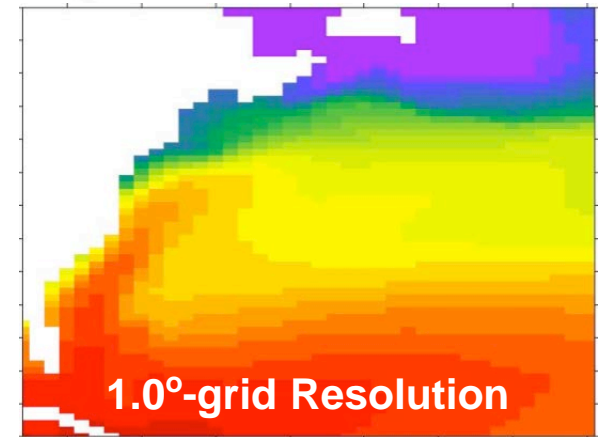


≈ 1980's

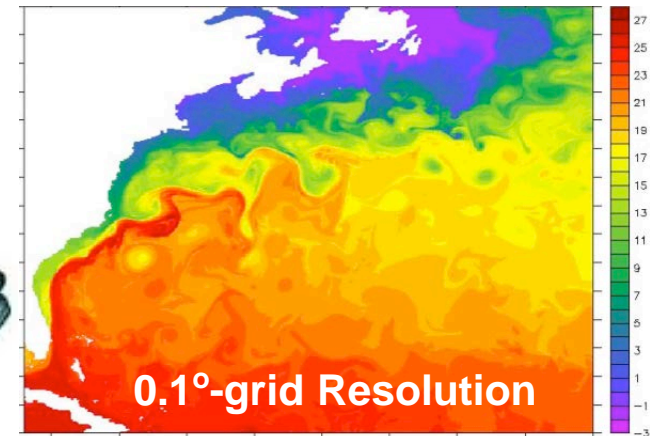


≈ 2000's

Car Crash Simulations



1.0°-grid Resolution

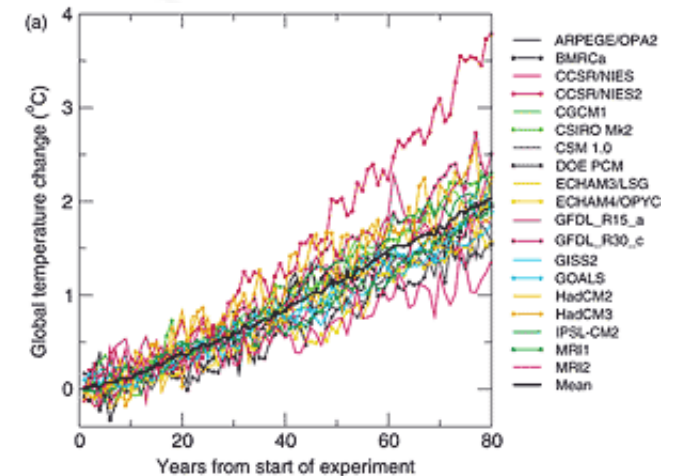


0.1°-grid Resolution

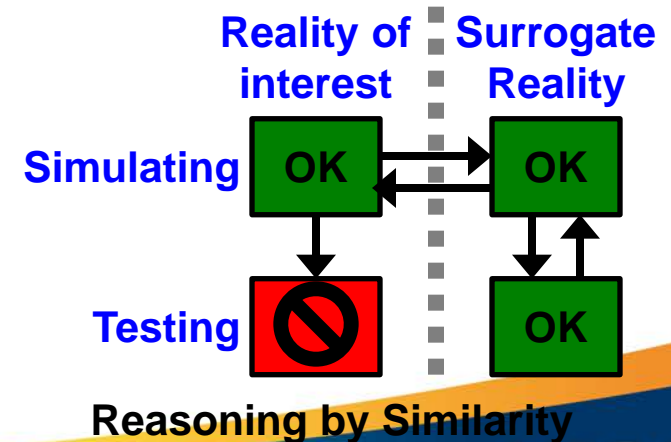
Global Circulation Models

Numerical simulations are used either to **extrapolate** to conditions that cannot be tested experimentally, or forecast the future.

- The model most appropriate to simulate “tomorrow” might not be known “today.”
- Forecasting and extrapolating require the analysis of many models, not a single one.
- “Reasoning by similarity” is another type of extrapolation, used to address the lack of availability of physical testing.



19 Global Warming Predictions

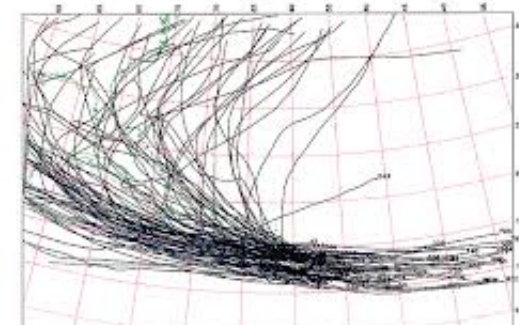
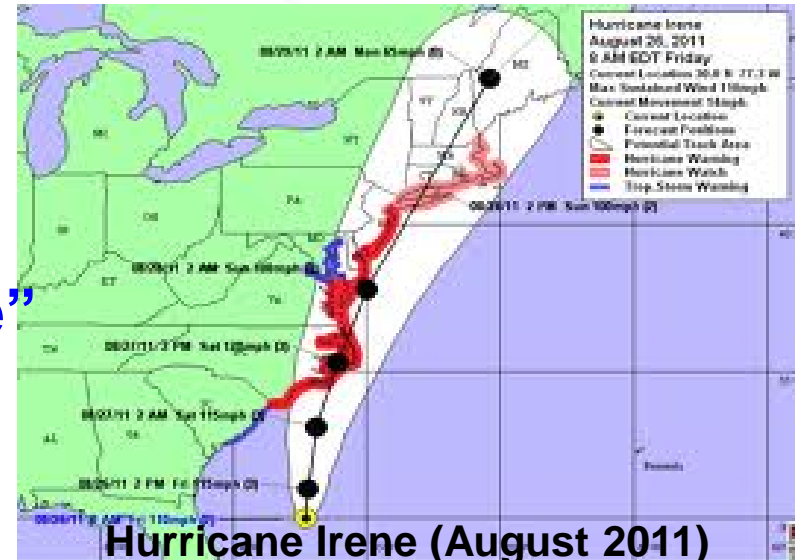


Credit: Top, D. Higdon, CCS-6, Los Alamos;
Bottom: J. Langenbrunner, XCP-8, Los Alamos.

Despite the availability of “big computers,” decision-making ultimately remains an exercise in the management of ***uncertainty***.

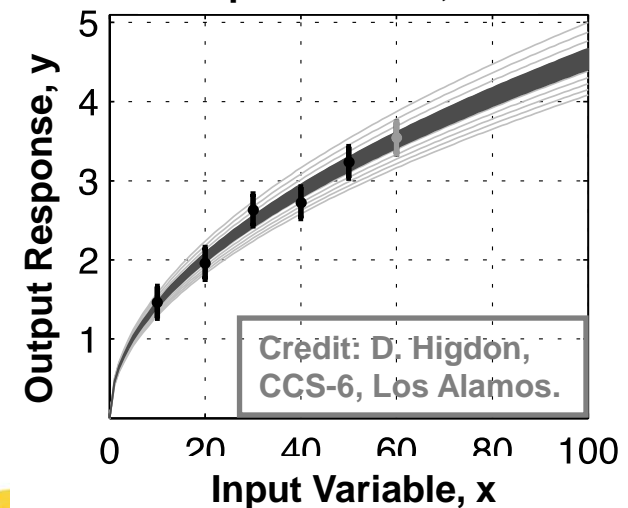
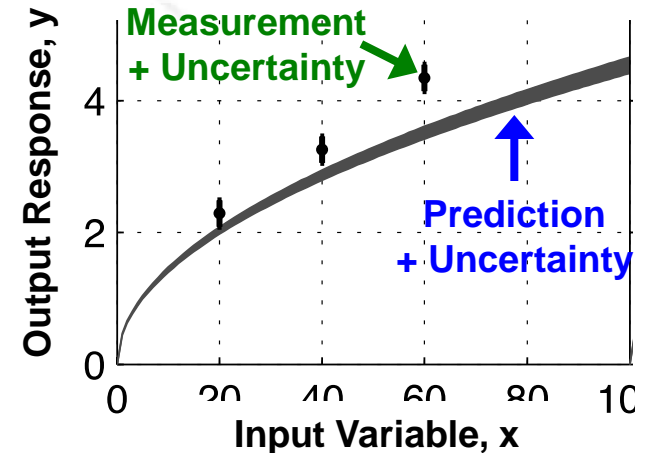
- Coupling of phenomena
- Variability, “randomness”
- Lack-of-knowledge, “ignorance”
- Truncation errors of solutions
- Measurement uncertainty
- Inference of observations
- Extrapolation of predictions

“Computers do not make decisions, people do!”



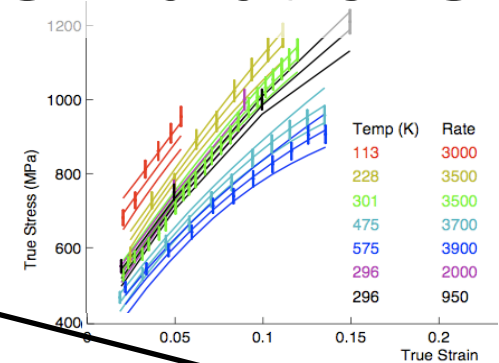
Uncertainty Quantification (UQ) develops the theory and tools to assess the uncertainty, and “quality,” of model-aided inferences.

- Sensitivity analysis, “which input variables change the response?”
- Construction of fast emulators
- Propagation of uncertainty through statistical sampling
- Statistical inference, estimation of input parameter uncertainty
- Aggregation of several sources of uncertainty in the predictions
- Informing about steps to take to reduce the prediction uncertainty

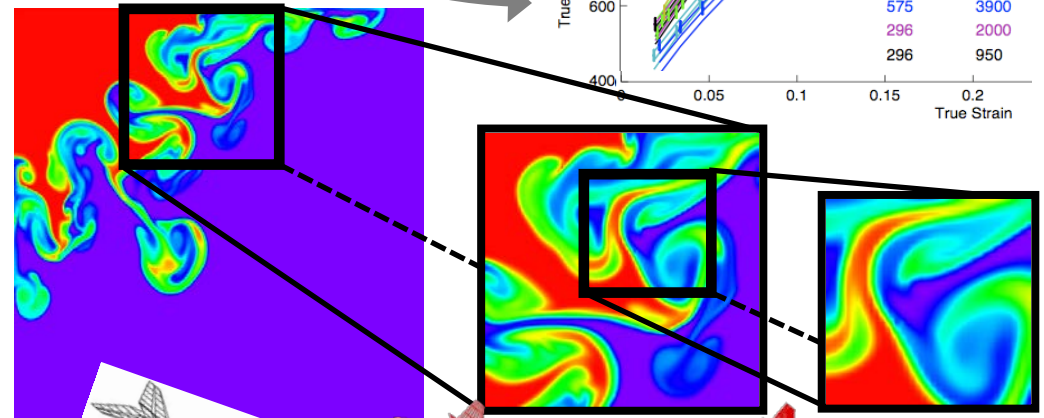


Scientists and engineers are confronted to three broad categories of uncertainty when interpreting results of numerical simulations.

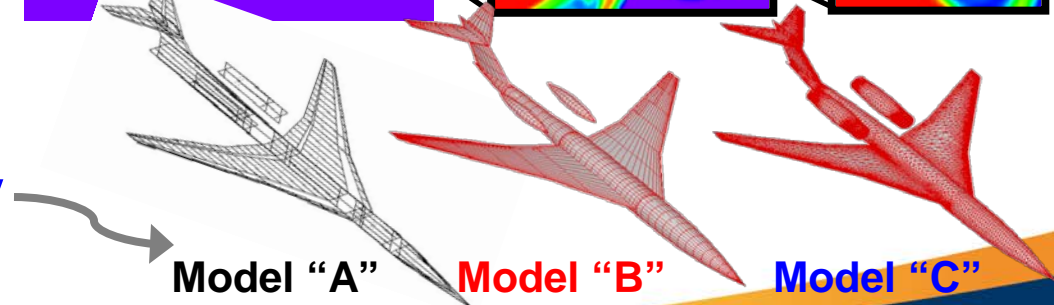
- **Variability and randomness**



- **Numerical uncertainty**



- **Model-form uncertainty**



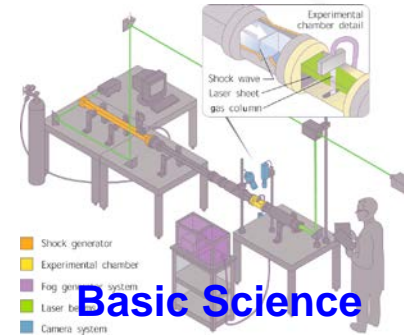
Credit: D. Higdon, CCS-6, Los Alamos; K.K. Choi, University of Iowa.

Let's try to bring everything together.



Establishing the credibility of numerical simulations is analogous to testing a hypothesis using the *scientific method*.

- What is the evidence which *confirms* the hypothesis?
- What is the evidence which *invalidates* the hypothesis?

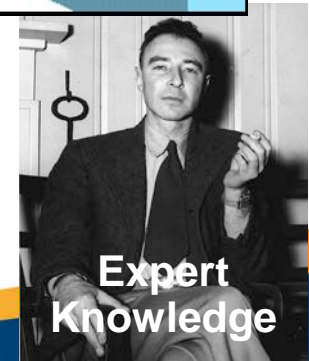
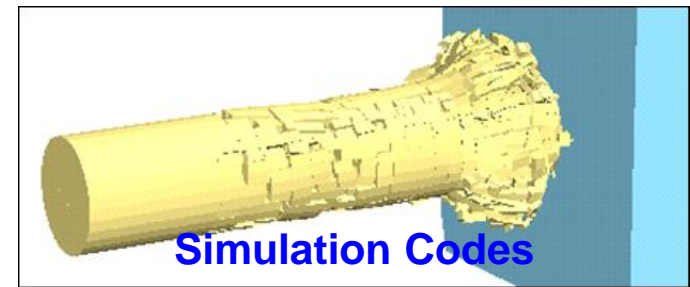
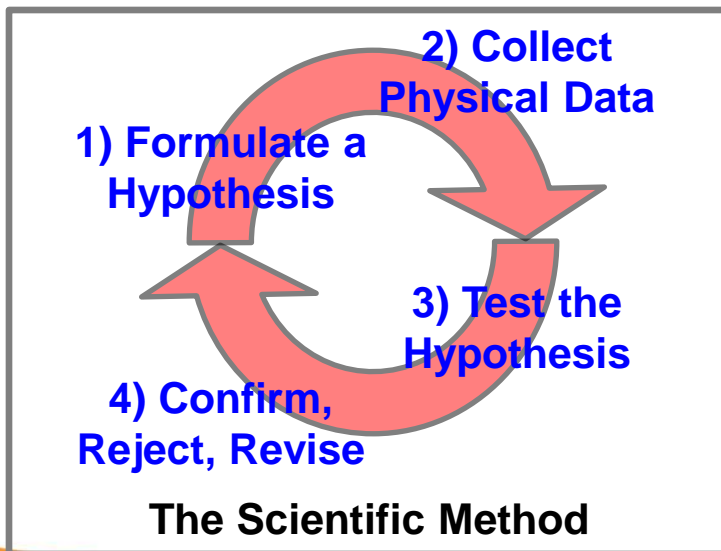


$$\frac{\partial \mathbf{p}}{\partial t} + \frac{\partial(\mathbf{p}\mathbf{u})}{\partial \mathbf{x}} = 0$$

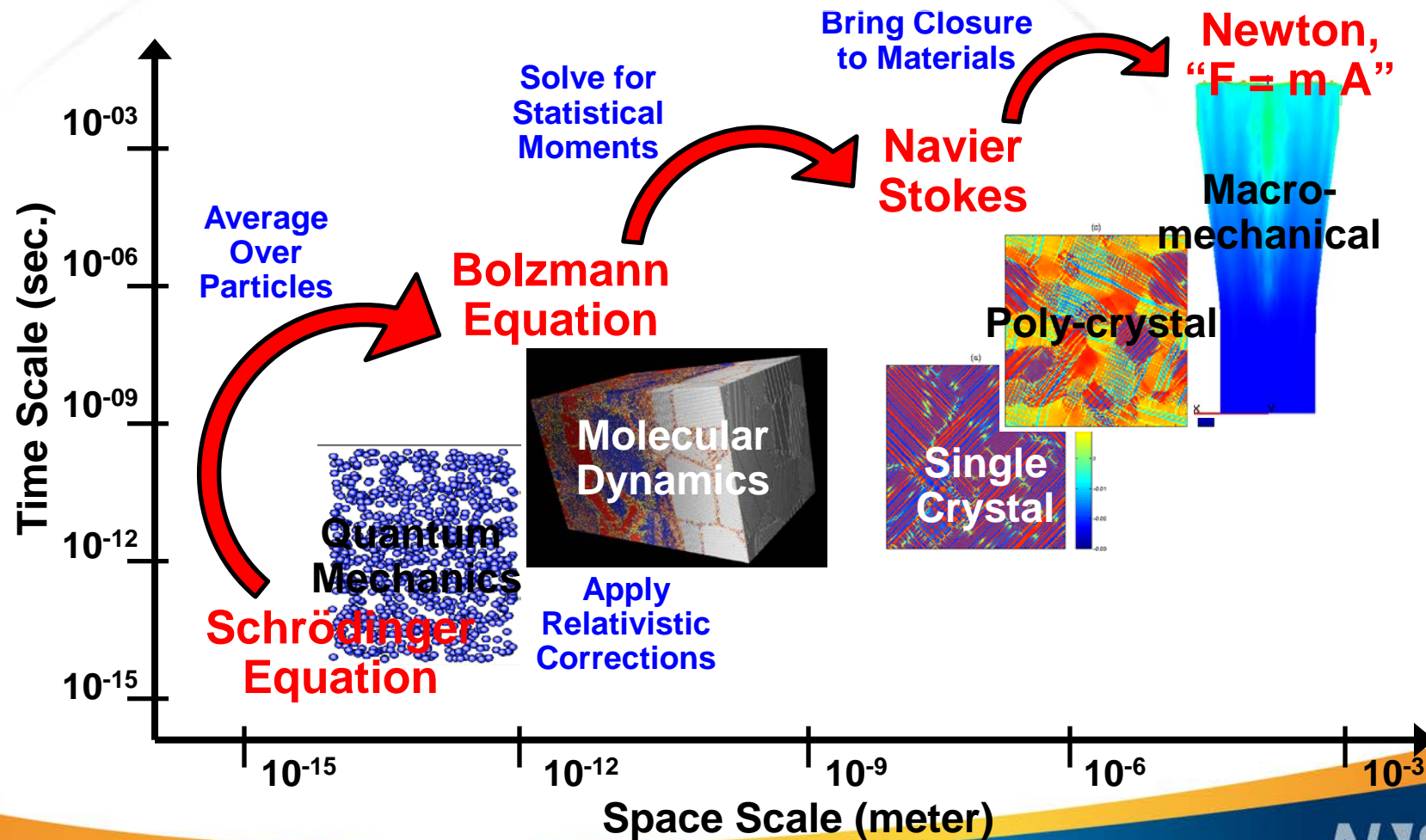
$$\frac{\partial(\mathbf{p}\mathbf{u})}{\partial t} + \frac{\partial(\mathbf{p}\mathbf{u}^2 + \mathbf{p})}{\partial \mathbf{x}} = 0$$

$$\frac{\partial(\mathbf{p}\mathbf{E})}{\partial t} + \frac{\partial(\mathbf{p}\mathbf{E}\mathbf{u} + \mathbf{p}\mathbf{u})}{\partial \mathbf{x}} = 0$$

Basic Science Theory

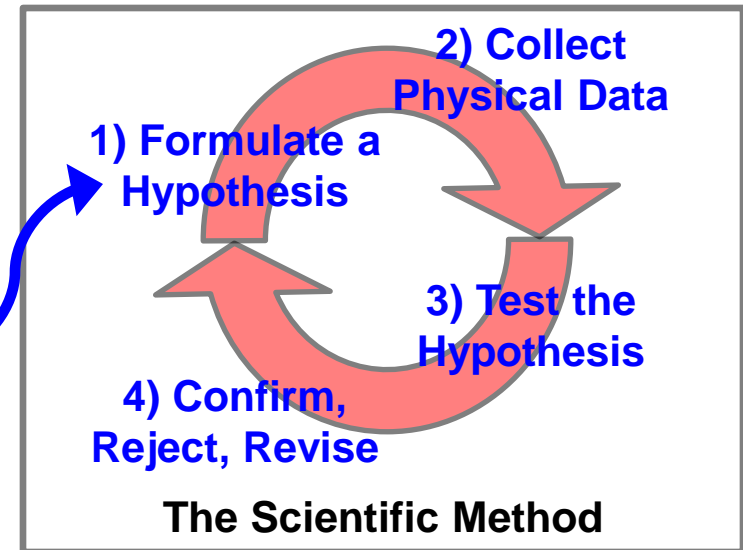


Scientific reasoning starts by understanding the space, time and energy scales that are relevant to the phenomenon being studied.



Scientific reasoning is articulated around these broad elements, which “echo” steps of the well-known scientific method.

- Understand space-time scales
- Write conservation laws
- Obtain orders-of-magnitude
- Perform numerical simulations
- Validate using physical data
- Manage the simulation uncertainty
- “Extrapolate” the predictions



Color Legend:

■ Explore a Question

■ Support a Decision

“Confidence” derives from the level of rigor with which these questions are answered.

- What are the decision, and prediction, requirements?
- What are the physical and modeling reasoning logics?
- What are the *assumptions* and *caveats* of the analysis?
- What are the sources of error and uncertainty, including variability, truncation and model-form?
- Which sources are included in the assessment, and which are not?
- What evidence, including its uncertainty, supports validation?
- What are the accuracy and uncertainty of model predictions?
- What evidence is produced by Verification and Validation (V&V) activities?
- By how much are predictions changed by what might be *unknown* or *uncontrolled*?

