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Title: New Horizons in Uncertainty Quantification

(View-graph Presentation)

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New Horizons in Uncertainty Quantification

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Non-Deterministic Approaches Forum

5 April 2011

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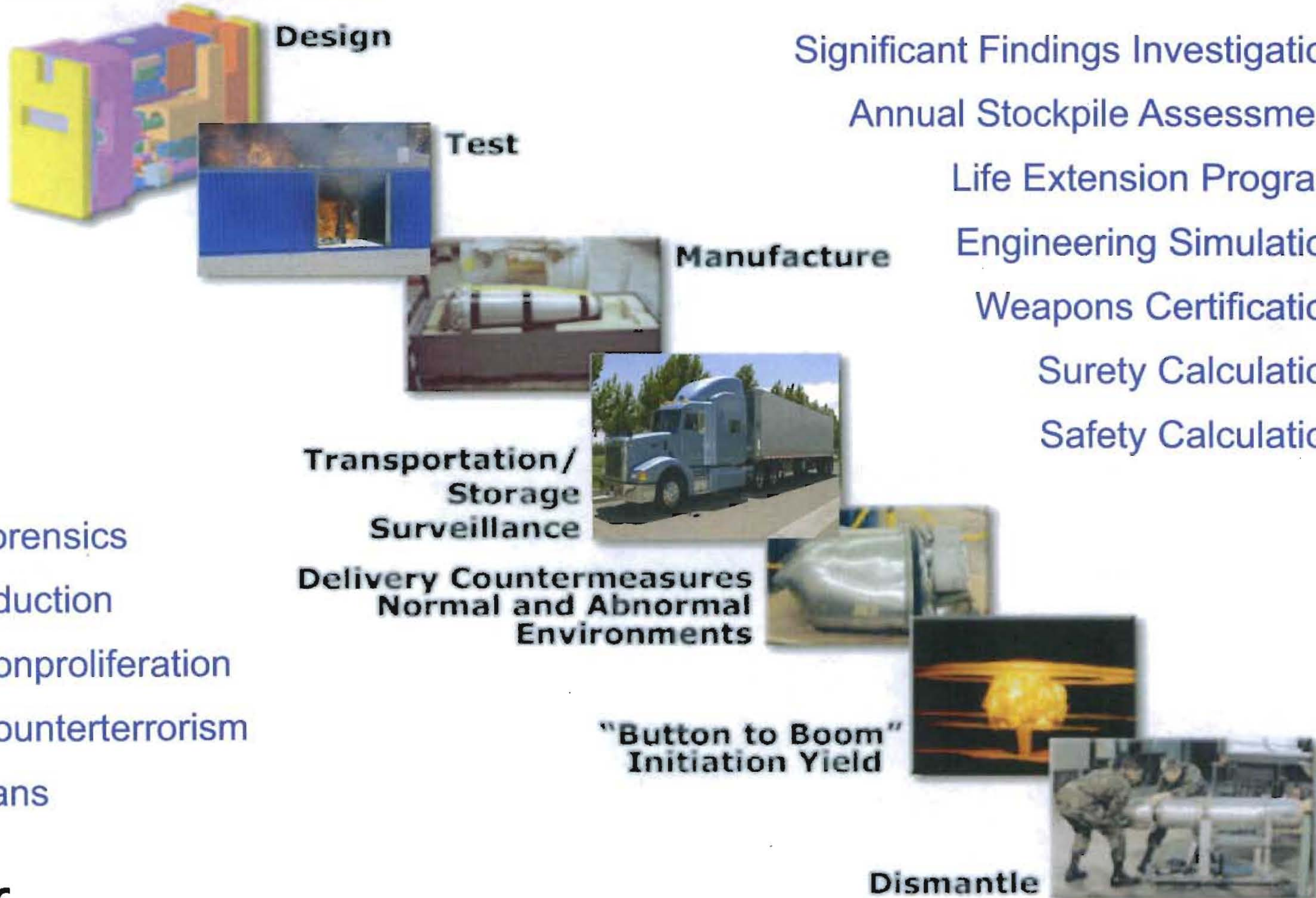
Overview

- The NNSA mission
  - The pervasiveness of simulation
  - The need for uncertainty quantification (UQ)
- A survey of the landscape
  - Verification and validation (V&V) as a framework for UQ
  - The state-of-the-art
  - Other areas that need attention
- How NNSA is investing in the future
- Supercomputers: the next generation…of challenges

NNSA is a key element in the nuclear security enterprise.

- Maintain a safe, secure, and reliable US nuclear stockpile
- Develop scientific understanding necessary to assess and certify weapons without underground nuclear testing
- Support a variety of threat reduction activities that rely on the capabilities and skills developed in the nuclear weapons program.

Today, every aspect of the the nuclear security enterprise uses simulation.



Significant Findings Investigations

Annual Stockpile Assessments

Life Extension Programs

Engineering Simulations

Weapons Certifications

Surety Calculations

Safety Calculations

Nuclear Forensics

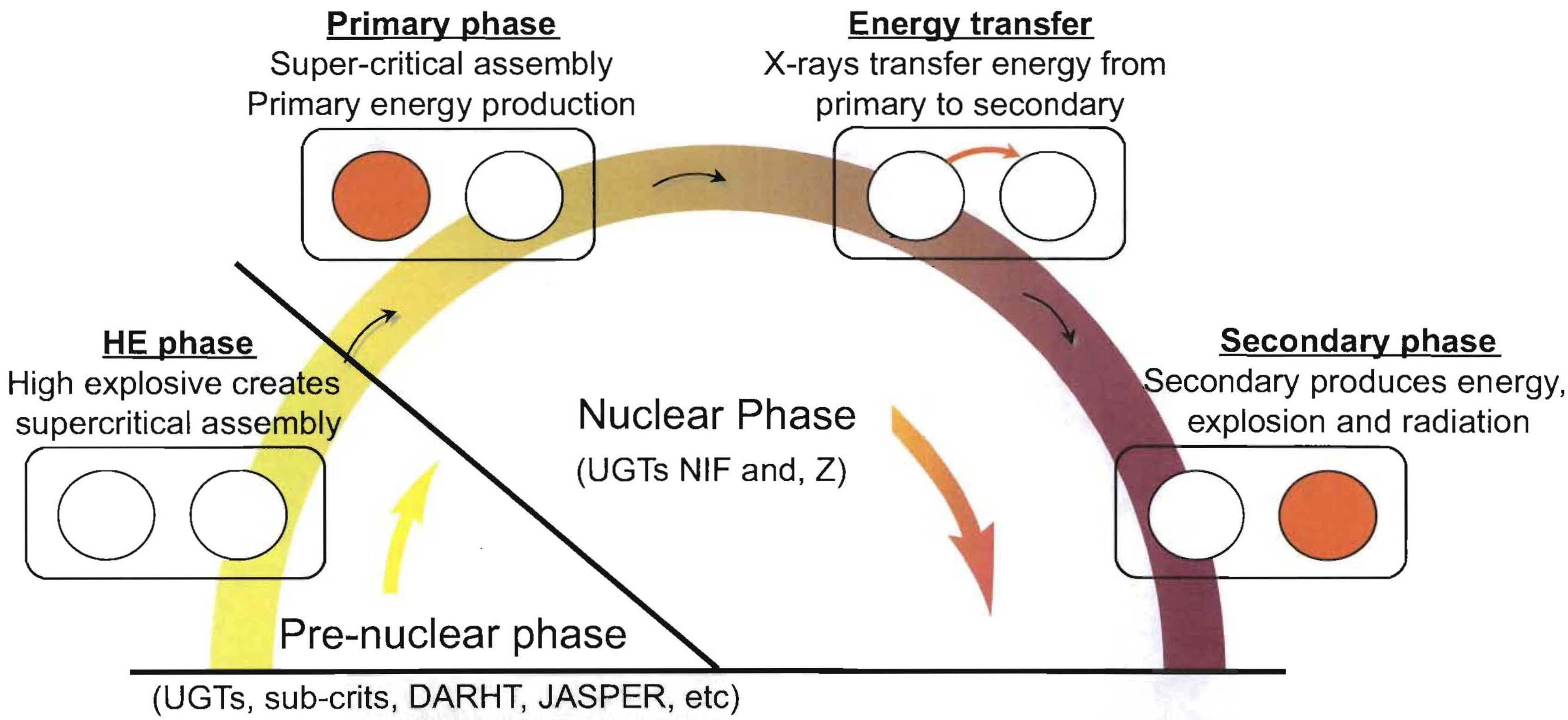
Threat Reduction

Nuclear Nonproliferation

Nuclear Counterterrorism

Secure Trans

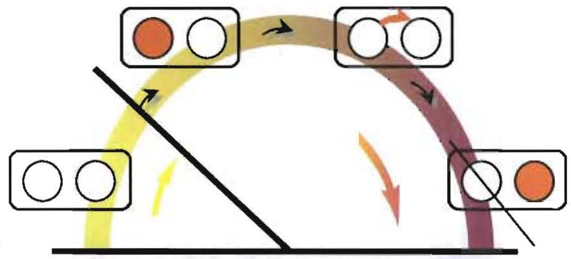
Nuclear weapons span an enormous physical range from condensed matter to plasma.

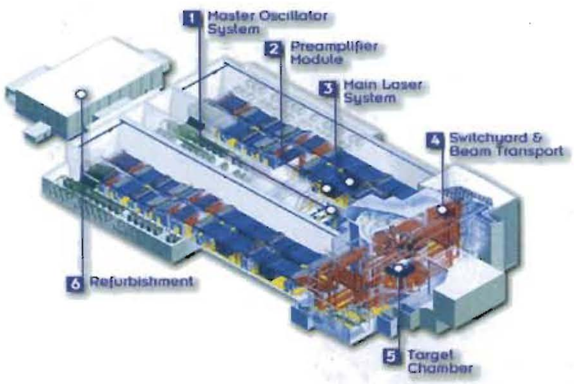


Weapons operation proceeds through the conditions of the Earth's surface to that of stellar interiors

Stockpile stewardship has evolved from nuclear testing toward predictive simulation.

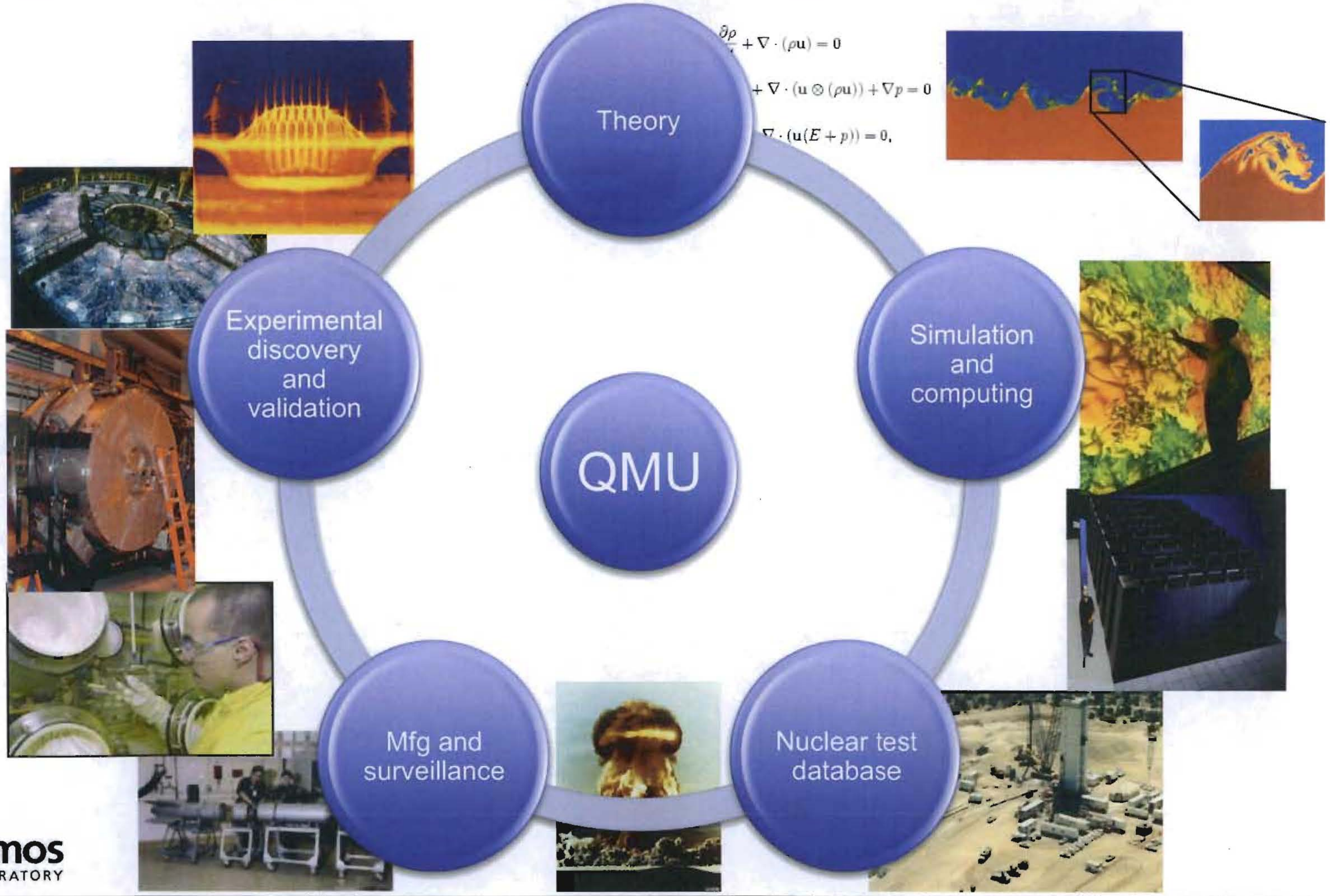
In the nuclear test era incomplete physical models were calibrated to integrated test



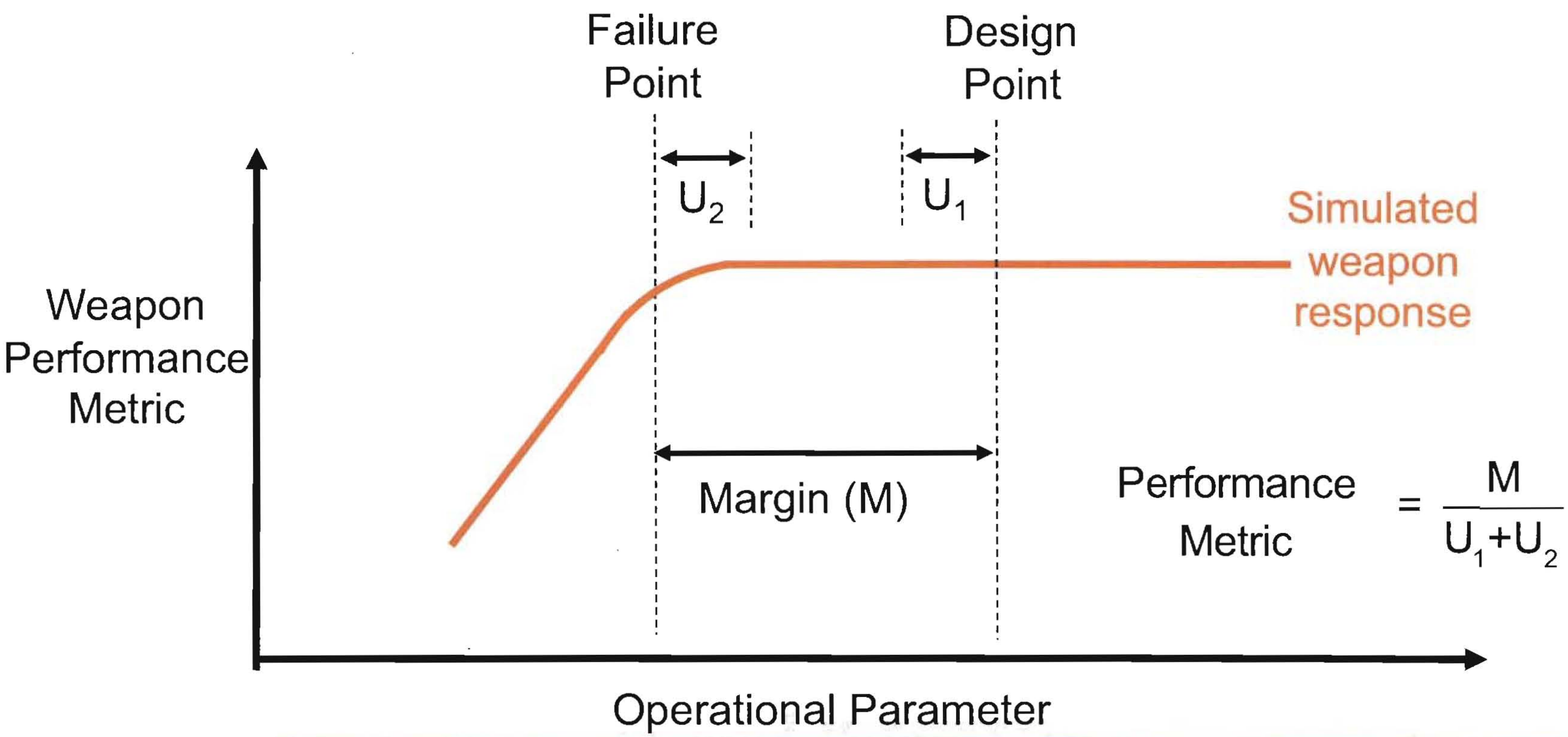


Predictive capability requires science-based simulation codes and sophisticated, challenging experiments

Uncertainties arise in all areas of the NNSA science and engineering programs.



Decisions based on simulation results must be accompanied by an estimates of the accuracy.



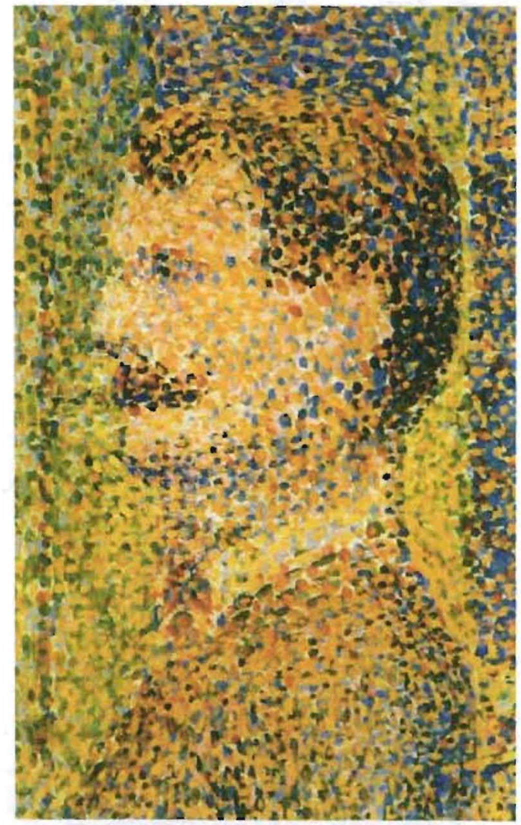
Accurate determination of both Margins and Uncertainties is heavily dependent upon a robust multi-physics simulation capability

Quantification of simulation accuracy is not solely deterministic.

- Simulations are not reality, but rather *potentially useful representations* of reality

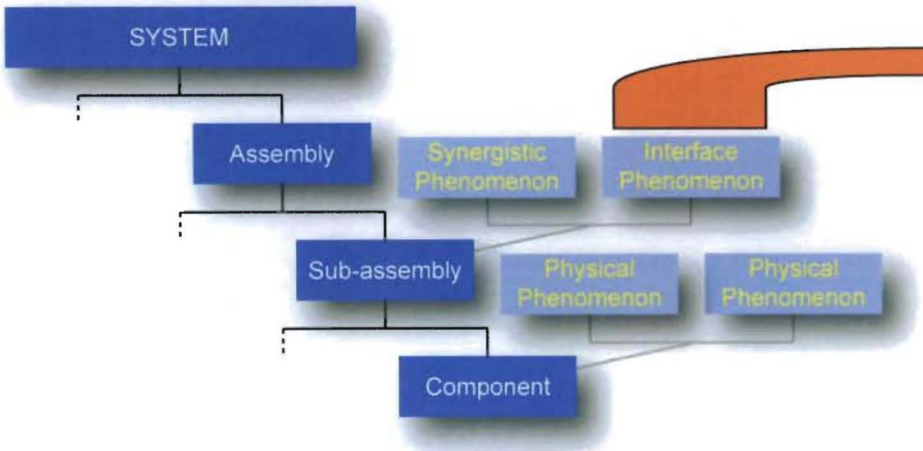
$$\frac{BEM}{BAC} \notin \mathbb{R} \qquad \frac{BEM}{BAC} \sim \mathbb{R}$$

- Verification & validation assessment provides evidence for the scientific integrity of "~"
- Uncertainty is the lingua franca of "~"

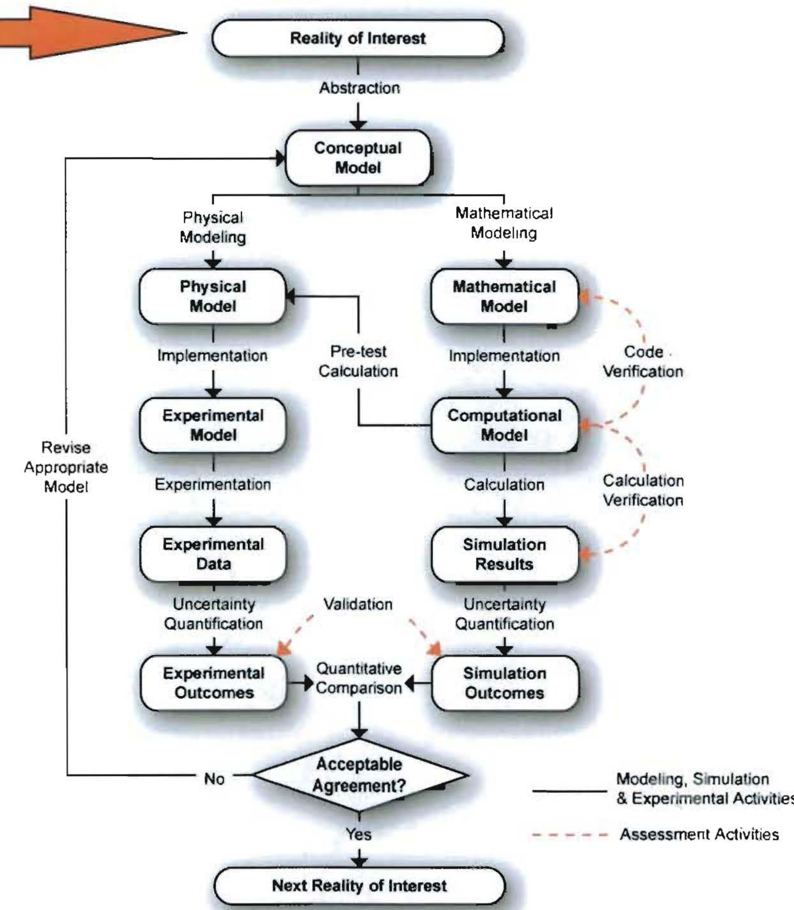


Detail from *The Parade*, Georges Seurat, 1889

Verification and Validation provides a logical framework for uncertainty quantification.



- Hierarchical decomposition
- Both top-down and bottom-up assessments
- Uncertainty-based
- Complexity ➔ prioritization



There are serious technical challenges associated with every step of the V&V process.

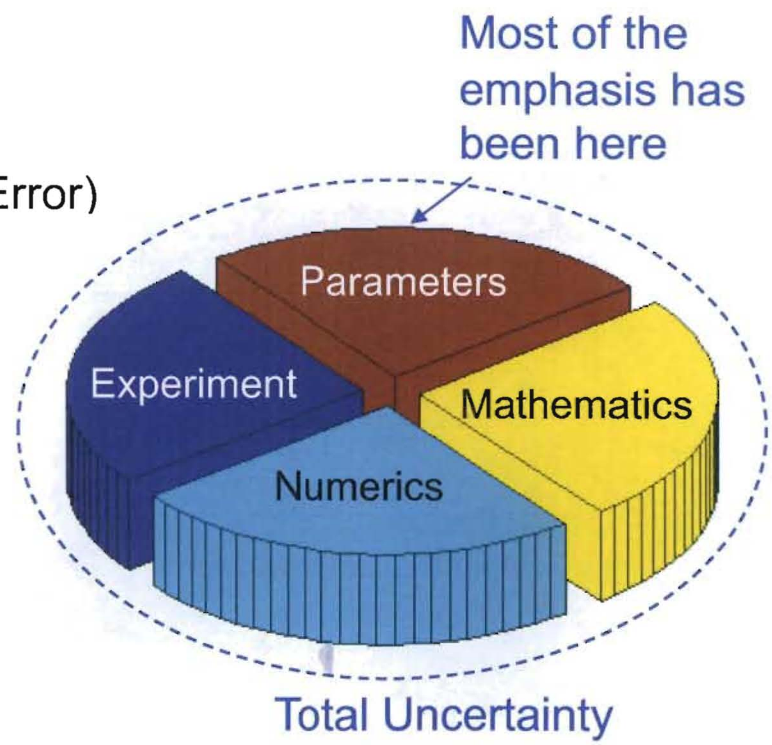
- General challenges
  - Hierarchical decomposition
  - Features & metrics
  - Dealing with calibration
- Verification challenges
  - Numerical approximations
  - Convergence analyses
- Validation challenges
  - Experimental characterization
  - Diagnostic simulation
  - Incomplete data
  - Etc.

How do we communicate the risks of our assumptions and prognostications?

Should we consider the consequences of our actions?

Perhaps the most perplexing challenges are associated with uncertainty quantification.

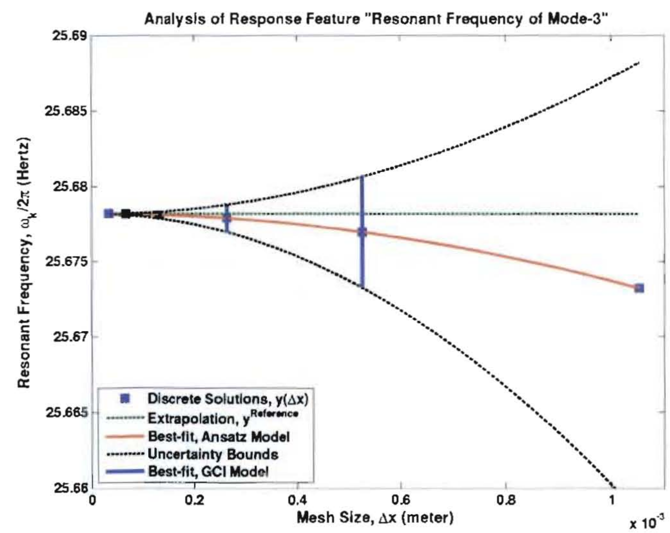
- Aleatoric uncertainty (also called Variability)
  - Inherent variation
  - Irreducible
- Epistemic uncertainty (also called simply Uncertainty)
  - Potential deficiency
  - Lack of knowledge
  - Reducible?
- Prejudicial uncertainty (also called Error)
  - Recognizable deficiency
  - Bias
  - Reducible
- Contributors to uncertainty
  - Experiment characterization & data
  - Mathematical model form
  - Numerical approx's & algorithms
  - Parameters



Verification "uncertainties" are hard to estimate and categorize.

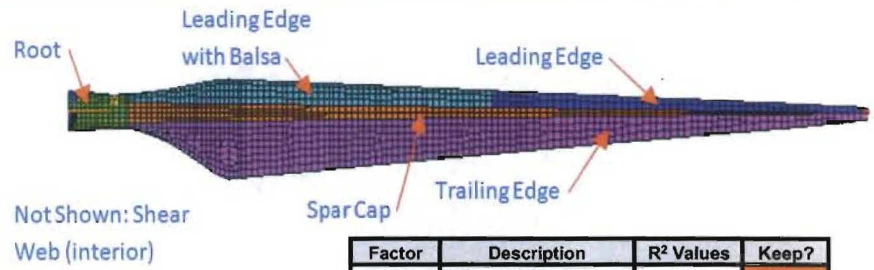
- Are they uncertainties?
- How should they be treated?
  - Deterministic error
  - Non-probabilistic uncertainty
  - Probabilistic uncertainty
- It is not just about spatio-temporal convergence analysis
- Other solution "uncertainties" exist
- This is one place a "white box" approach is needed

Chris Stull (LANL)



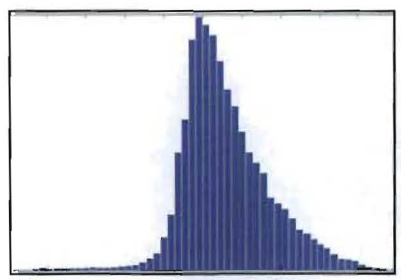
For obvious reasons, parametric uncertainty has received the most attention.

- Strong logical foundation
  - Assumes correct model
  - Mathematically “rigorous”
- Forward propagation
  - Sampling
  - Surrogate models
  - Bayesian methods
  - Non-probabilistic methods
- Stochastic fields
  - Stochastic Galerkin
  - Polynomial chaos
  - Stochastic collocation

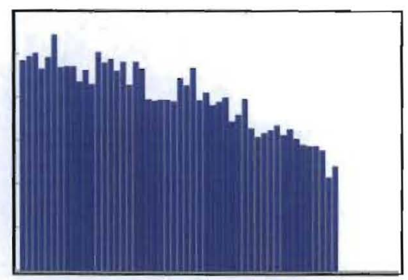


Factor	Description	R^2 Values	Keep?
A	Shear web, ρ	0.29%	No
B	Root, ρ	0.37%	No
C	Lower-edge balsa, ρ	0.32%	No
D	Spar cap, ρ	1.11%	No
E	Trailing edge, ρ	9.35%	Yes
F	Leading edge, ρ	3.03%	Yes
G	Shear web, E	1.74%	No
H	Root, E	0.00%	No
I	Lower-edge balsa, E	1.74%	No
J	Spar cap, E	65.95%	Yes
K	Trailing edge, E	9.85%	Yes
L	Leading edge, E	6.25%	Yes

Mark Mollineaux (Stanford)
Kendra Van Buren (Clemson)



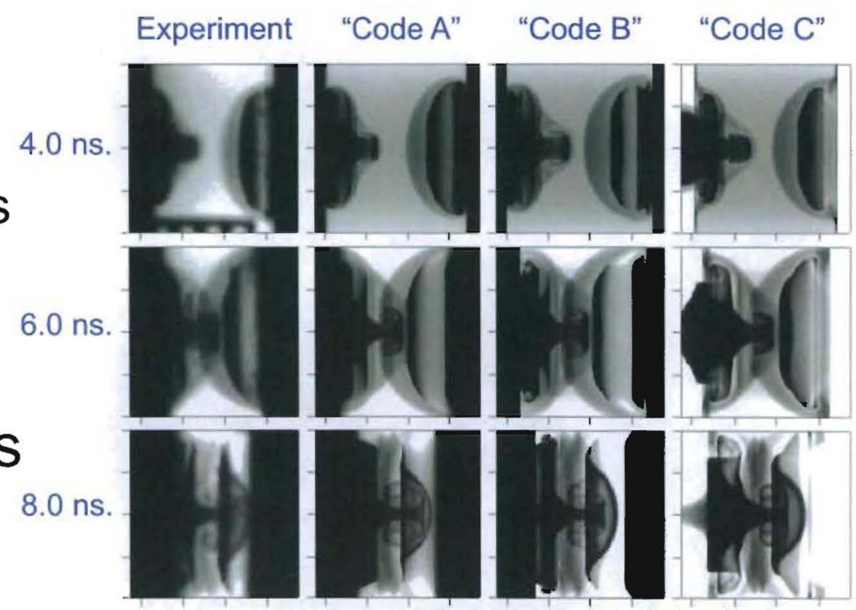
K: Trailing edge modulus



L: Leading edge modulus

Again, for obvious reasons, model form uncertainty is less amenable to estimation.

- Not a lot that can be done without some idea of the "right" model
- Anecdotal comparisons
  - Compare two or more models
  - Compare two or more codes
  - SWAG variability
- Space of admissible models
  - Limited to mathematical form comparisons
  - Assumes correct model in the set

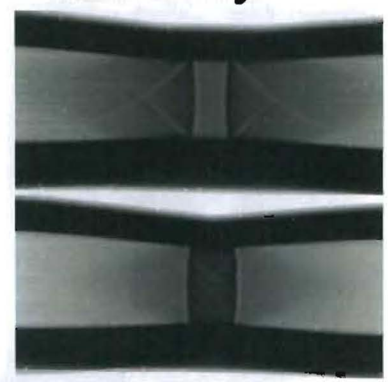


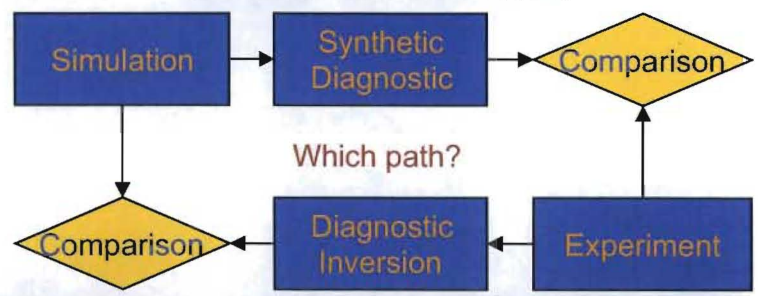
Radiation-driven Interacting Jet-shock

Kamm, J.R., et al., "Image Quantification of Experiments and Simulations of Laser-driven Jets," LA-UR-05-1441, March 2005

Experimental uncertainties also have received less attention than they deserve.

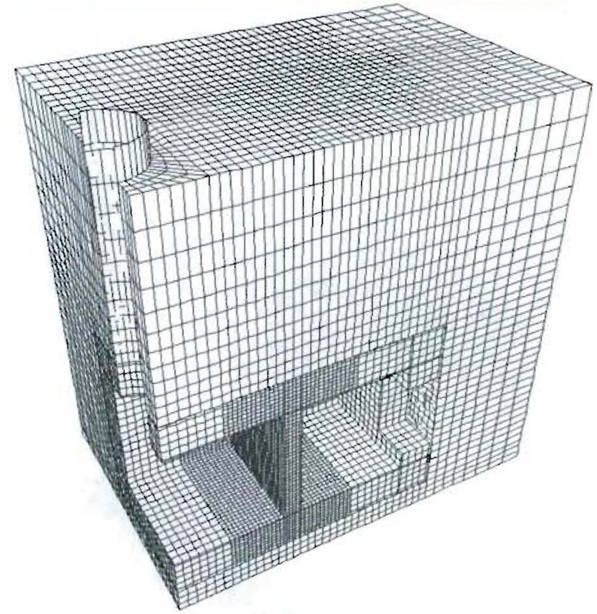
- Usually only estimate measurement uncertainty
  - Measurement noise
  - Calibration error
- There is so much more
  - "As built" test article characterization
  - "As fielded" experimental conditions
  - Diagnostic interpretation
- Who is responsible?
  - Experimenters
  - Analysts

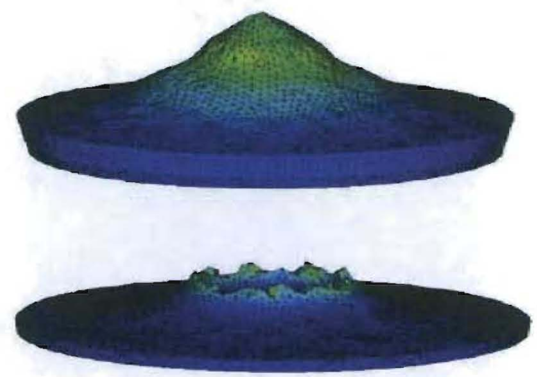




There are a couple of approaches for looking at combined uncertainties.

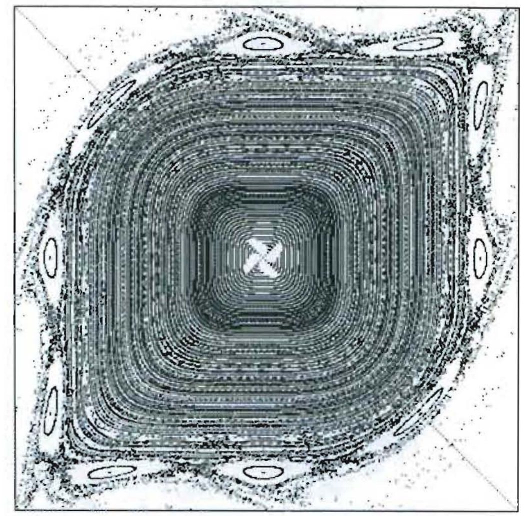
- Total (or generic) uncertainty is a measure of the difference between experimental and simulation
- Practical considerations
  - Enough samples rarely exist
  - Must consider "generic classes" of test-analysis comparisons
  - Simple differencing leads to "small differences of large numbers"
  - Normalize information so that differences are "perturbations"
- Another approach is based on the concentration of measure (COM) phenomenon [More later]

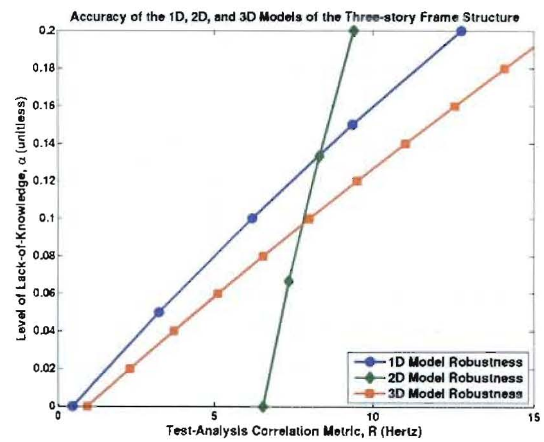




There are some areas that warrant attention for our applications.

- Metrics and completeness
  - We are throwing away a lot of information
  - Can we use information theory?
- Dynamical systems methods
  - Liapunov exponents (FTLE)
  - Lagrangian coherent structures (LCS)
- Decision support
  - Optimal communication
  - Meta-UQ: confidence in our assessments
- Robustness ideas
- Limitations of our assessments

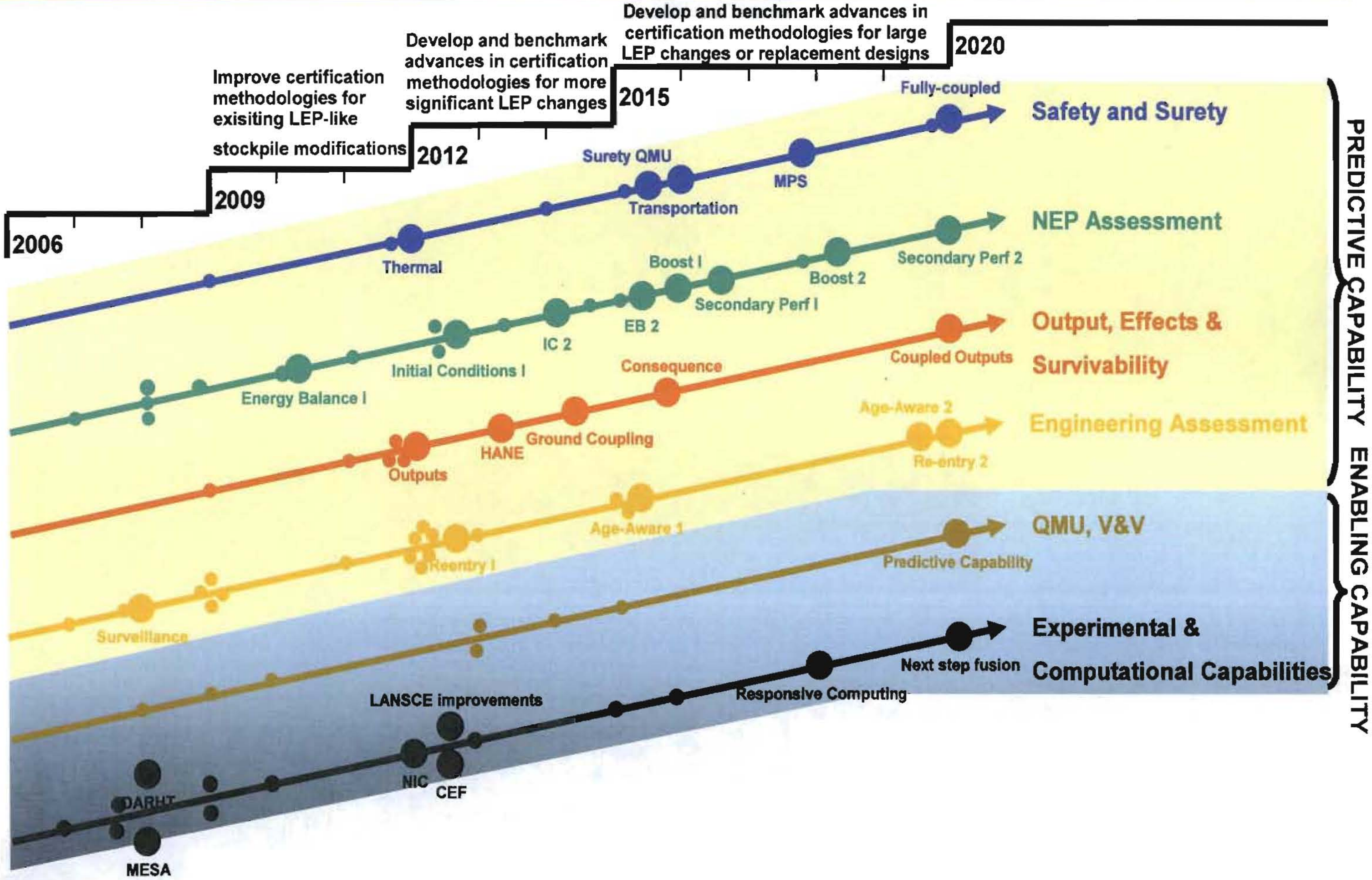




How are we exploring these horizons?

- Major programmatic efforts
  - V&V program element of Advanced Simulation and Computing
  - Advanced Certification Campaign
- Predictive Capability Assessment Project
- Predictive Science Academic Alliance Program
  - Five university teams
  - V&V and UQ are requirements
- Enhanced computing
  - Capability
  - Capacity

The Predictive Capability Framework is used to coordinate science and simulation.



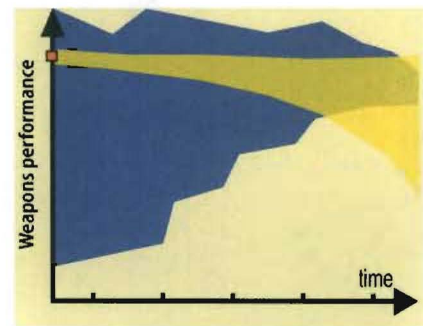
UQ is an integral part of our investment in simulation assessment for certification.

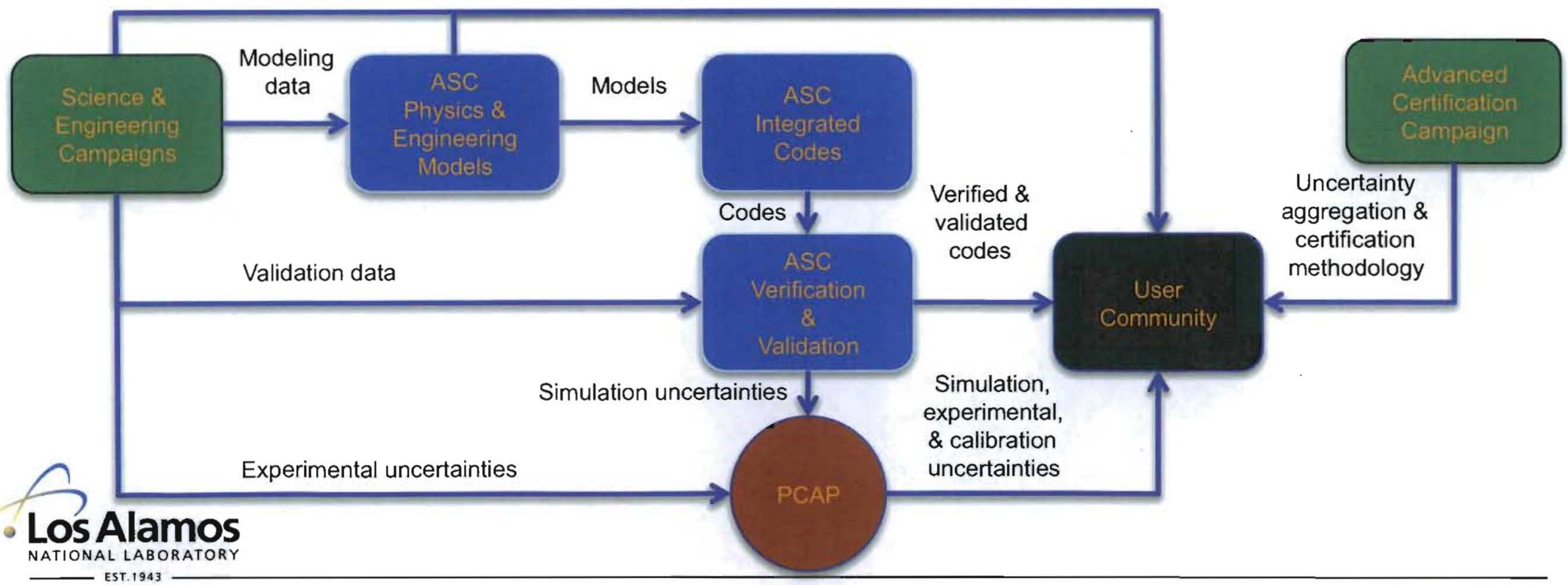
- ASC invests through two program elements
  - V&V
    - Methods and tools
    - V&V assessments
    - Predictive capability assessments
  - Physics and Engineering Models
    - Parametric uncertainties
    - Model form and parametric constraints

- The Science and Engineering Campaigns also invest
  - General: experimental uncertainties
  - Advanced Certification Campaign
    - QMU methodology
    - Certification metrics
    - Near neighbor definition

The PCAP attempts to quantify the effect of integral calibration.

- Document V&V basis for the codes
- Develop suites of small scale and integral simulations
- Compare "non-calibrated," suite-calibrated, and system-specific simulations



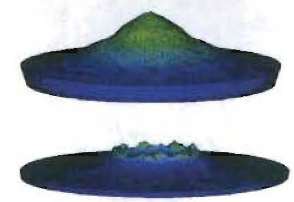


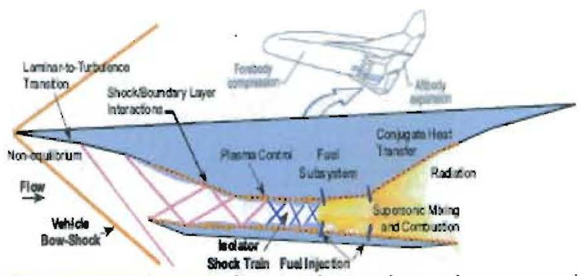
The PSAAP covers a wide range of applications and scales.

- Focus on unclassified applications of NNSA interest
- Demonstrate validated simulation capability for prediction
- New methodologies and tools for V&V/UQ

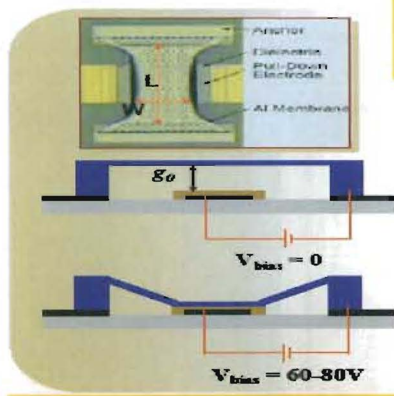
U of TEXAS, Austin - Center for Predictive Engineering and Computational Sciences (PECOS)

CALTECH - Center for the Predictive Modeling and Simulation of High-Energy Density Dynamic Response of Materials

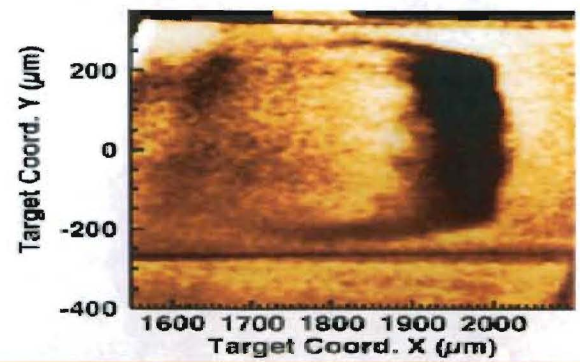




STANFORD - Center for Predictive Simulations of Multi-Physics Flow Phenomena with Application to Integrated Hypersonic Systems



PURDUE – Center for Prediction of Reliability, Integrity, Survivability of Microsystems (PRISM)



U of MICHIGAN - Center for Radiative Shock Hydrodynamics (CRASH)

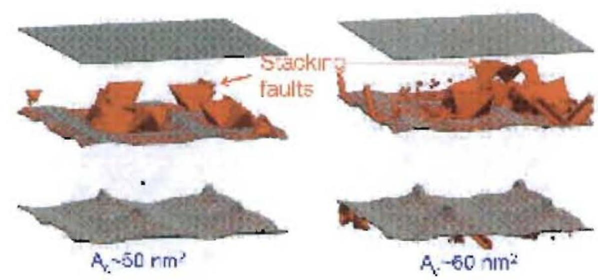
The Caltech Center is applying a rigorous concentration of measure approach to UQ.*

- Concentration of measure has few assumptions
  - Measure theoretic basis (obviously)
  - No *a priori* assumptions re distributions
- Not restricted to parametric uncertainty
  - Can include numeric uncertainties
  - Accommodates experimental uncertainties
- Must be extended for LANL application
  - Already extended to hypothesis testing
  - Epistemic uncertainty treatment unclear
  - Accommodation of calibration non-trivial
  - Only historical integral data available

*California Institute of Technology

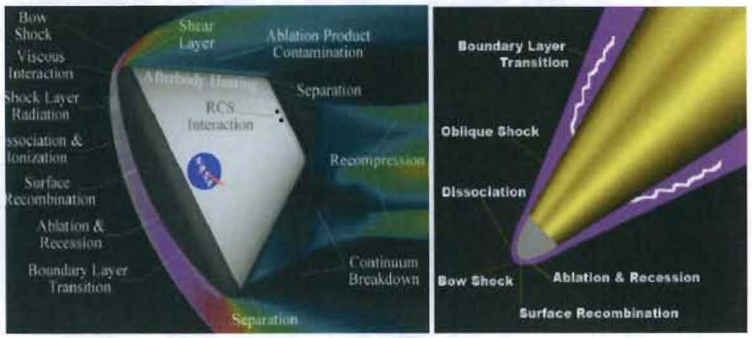
The Purdue Center is tackling the multi-scale and stochastic field UQ problems.*

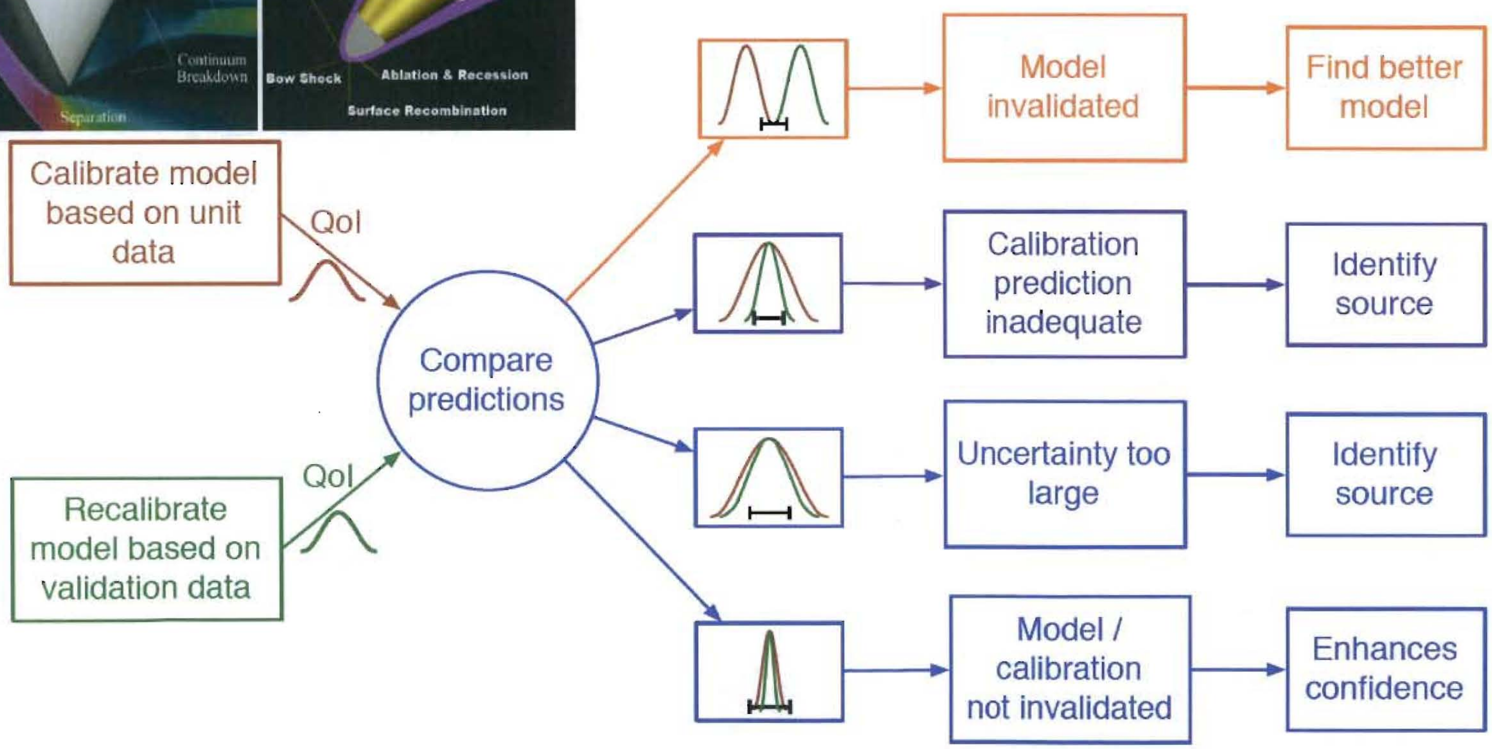
- Coupled physics across multiple scales
  - Electrostatics coupled with solid mechanics and gas dynamics
  - Atomistic simulations of contact
  - Meso scale models informed by atomistic models
  - Macro scale continuum models informed by meso scale models
- Stochastic field approach to UQ is required
  - Reduce computational requirements via collocation
  - Propagate uncertainties from smaller to larger scales



*Purdue University

The Texas Center extends the Bayesian UQ approach to support a certification framework.*

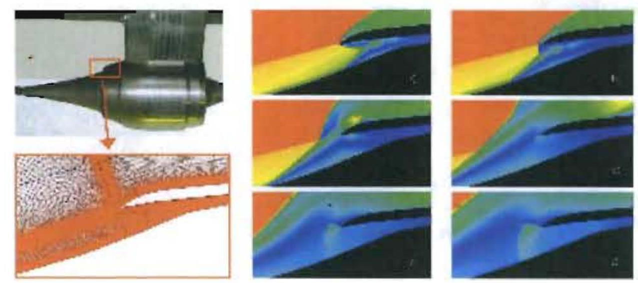




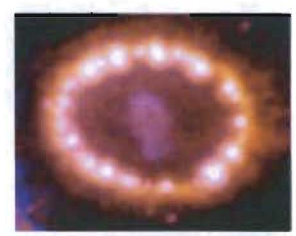
*University of Texas

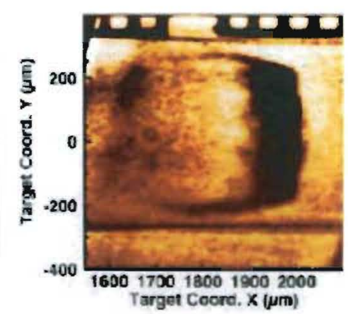
Stanford and Michigan are also pursuing novel approaches to UQ.*

- Stanford extends the Bayesian approach in one way
  - Reduced order models
  - Likelihood averaging (LAPS)
  - Adjoint-based polynomial chaos



- Michigan extends the approach in another way
  - Adjoint-based error estimation
  - Bayesian Hierarchical System (BHS)

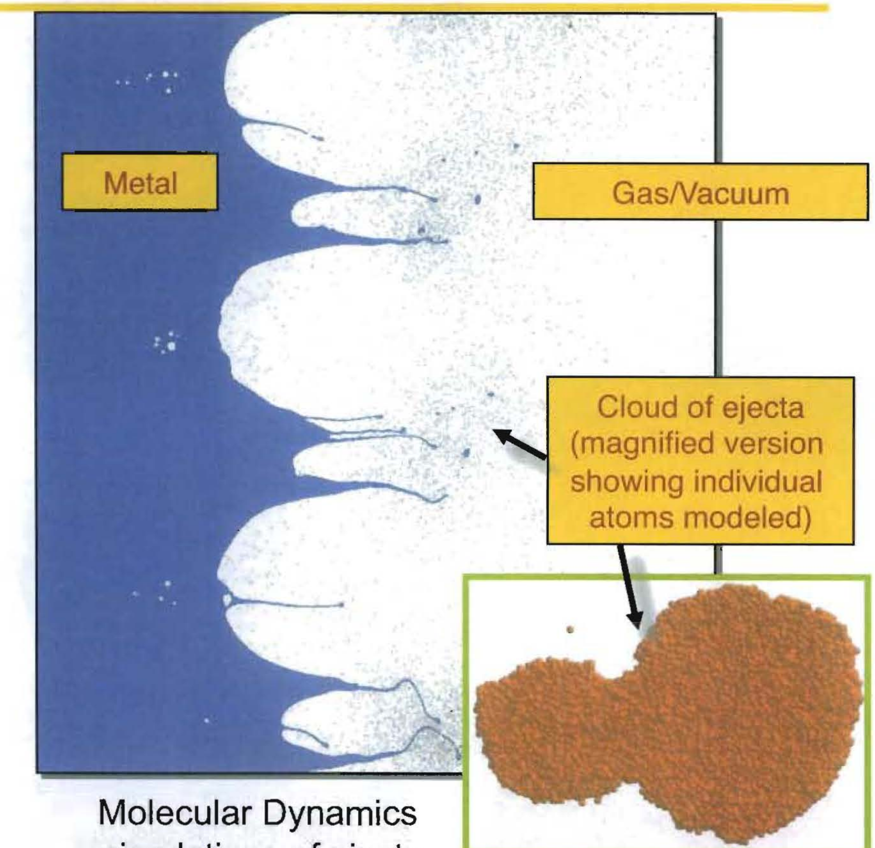




*Stanford University and University of Michigan

Enhanced computing is necessary to resolve physics issues and reduce uncertainty.

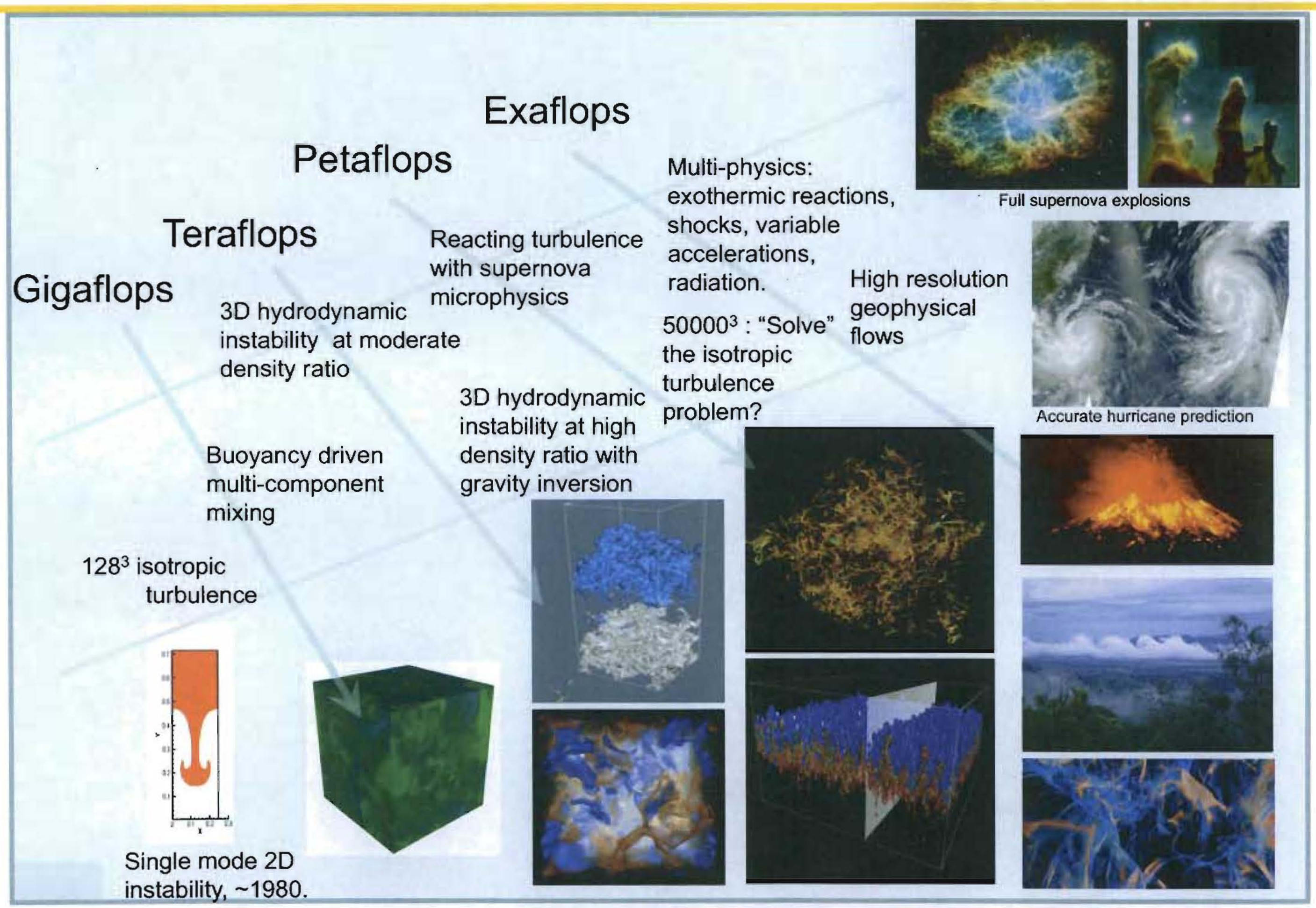
- Improved GEOMETRIC fidelity
  - Safety features
  - Design features
  - 3D phenomena, e.g., turbulence
- Improved NUMERICAL fidelity
  - Spatial convergence
  - Strongly-coupled physics
  - Better UQ sampling
- Improved PHYSICS fidelity
  - Multi-scale phenomena
  - Material damage and fracture
  - Plasma physics



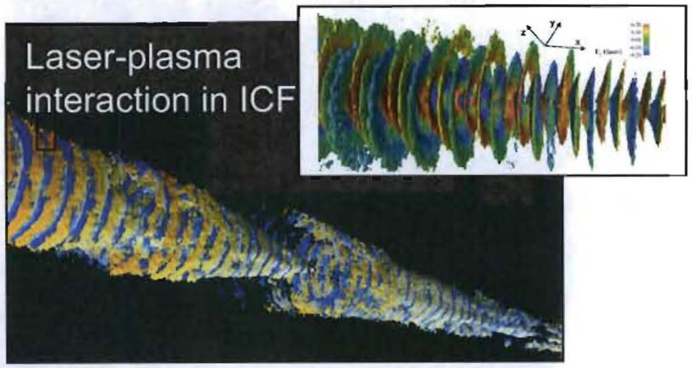
Molecular Dynamics simulations of ejecta

3D simulations of ductile spall failure and ejecta transport will require exascale resources

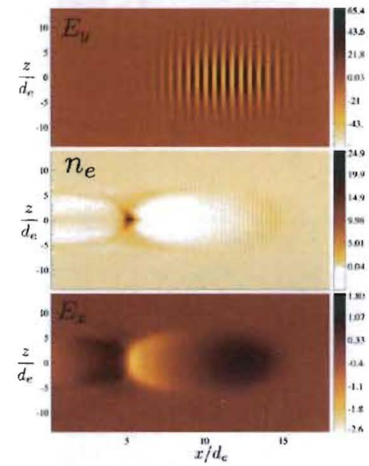
Turbulence simulation is an iconic example of this need.

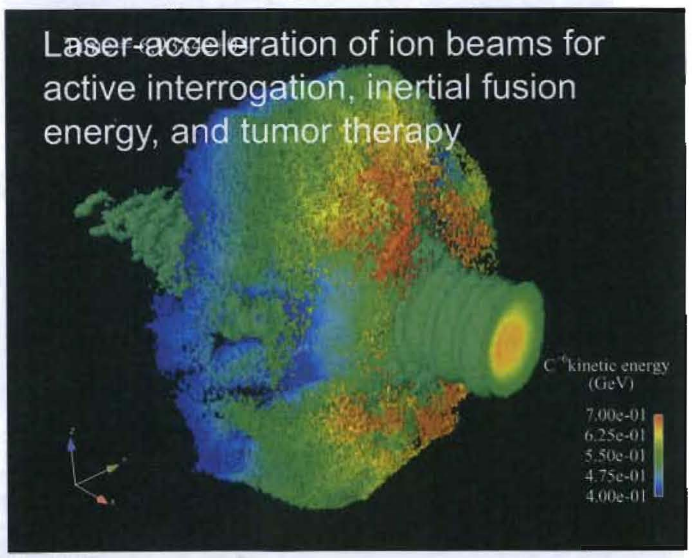


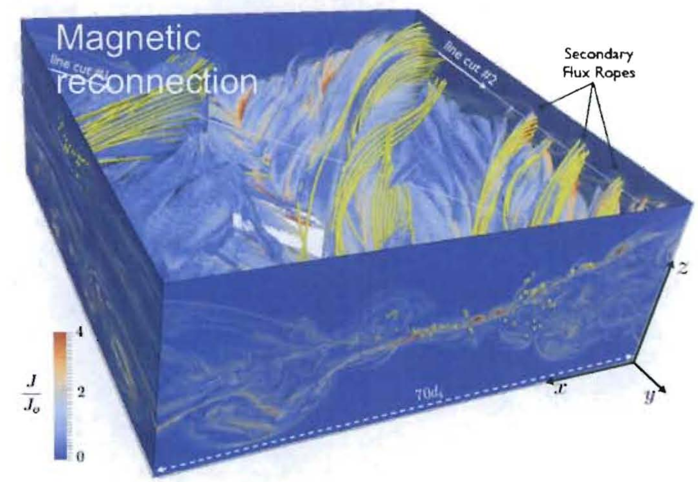
Several areas of kinetic plasma science are also drivers for enhanced computing capability.



Electron
accelerators
and XFELs







Significant advances in computing power bring new challenges in simulation and UQ.

- Exascale computing (10^{18} FLOPS) is a challenge
  - 1000x more powerful than the current computing capability
  - 100's MW power w/current technology
  - Simulation codes must evolve
    - Billions of cores (processors)
    - Multiple levels of parallelism
- Resilience and correctness
  - Current approach: "Kill the wabbit!"
  - Not practical at exascale
  - Do we need bit reproducibility?

- Non-determinism not associated with resilience
  - Loss of reproducibility :order of operations, repartition of problem

Summary

- The NNSA mission relies heavily on simulation and UQ
  - The scientific integrity of our simulations is essential
  - Quantified uncertainties are central to certification
- Much progress has been made on UQ
  - Other need more attention in the coming years
- NNSA is investing seriously in the future
  - Internal investments in simulation and science
  - External investments in academia
- A key element of the future is much larger computers
  - Capability requirements are driven by science
  - This level of computing brings new challenges for UQ

Abstract

Many concepts in uncertainty quantification have been developed for parametric uncertainty, including sampling-based and stochastic methods. Other areas have received less attention. These areas include verification uncertainty, experimental uncertainty, model form uncertainty, and the effects of calibration. New generations of supercomputers will bring additional challenges such as non-determinism in the computations themselves. All of these areas are constrained by the available information, for which there are serious limitations. Future investment is needed to map these boundaries and fill in the gaps in our capabilities.