Is the Role of Science-Based Prediction Sustainable in the Nuclear Security Mission?

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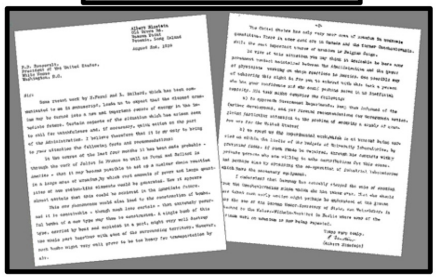
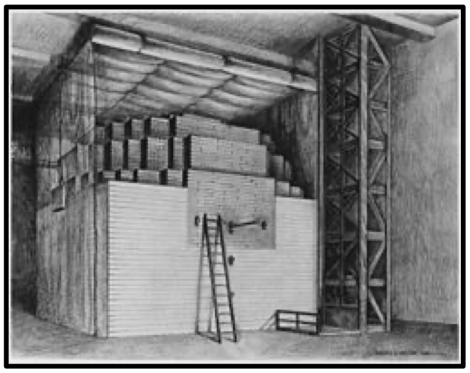
40TH ANNIVERSARY LECTURE SERIES

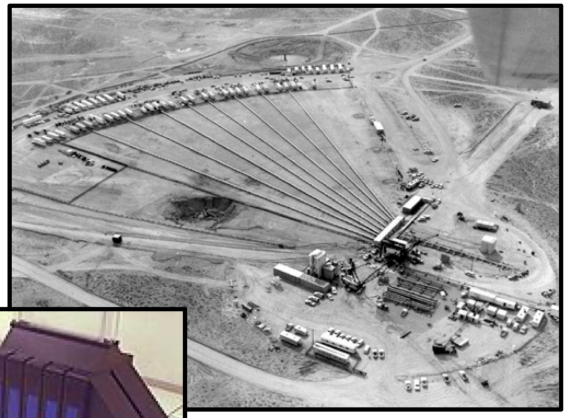
Scientific discovery can change global policy

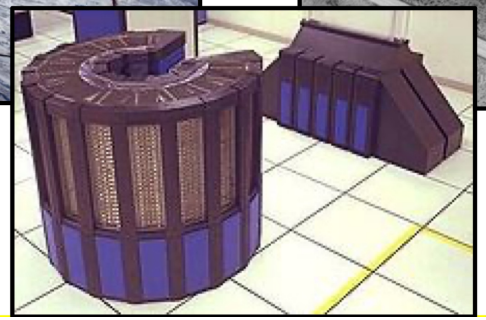




A major scientific discovery and a letter from a scientist to a President changed the landscape for the last seventy years

…but policy can also change science and technology: "*Maintain a nuclear deterrent without nuclear testing*." (1995)



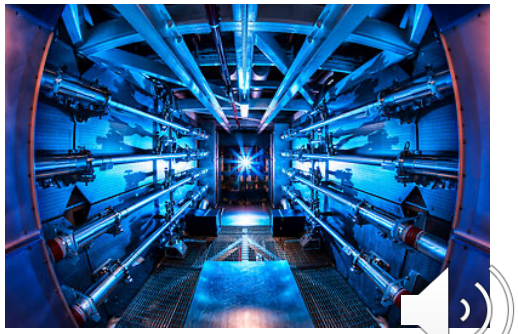


1985 **1.9 GigaFlop**
Cray 2

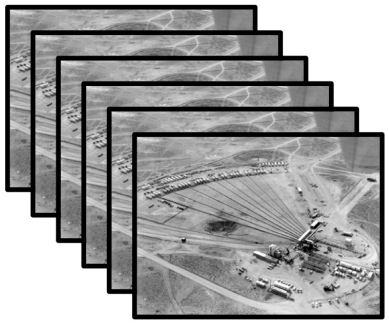
- From 1945 to 1992, the US nuclear testing program provided the essential "Ground Truth" and "Discovery" that undergirded nuclear weapon design and development.

Stockpile Stewardship was initiated as a transformational means to maintain the US nuclear deterrent without UGTs AND to preserve the science base for nuclear weapon technology

- Drive to Teraflop computing and beyond
- Develop advanced radiography at Los Alamos (DARHT)
- Develop new capabilities to produce extreme states of matter on the millimeter scale → Factor of 1E9 in energy (NIF at LLNL, Z at SNL)
- Perform treaty-compliant subcritical experiments at the NNSS (nee NTS)



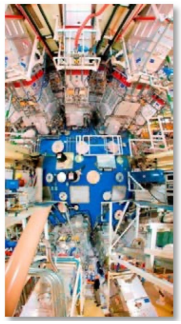
The new nuclear weapon design paradigm placed a premium on developing a certification methodology founded on ***science-based prediction***

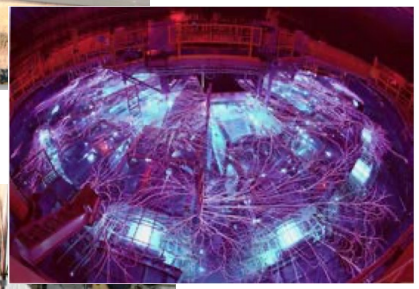


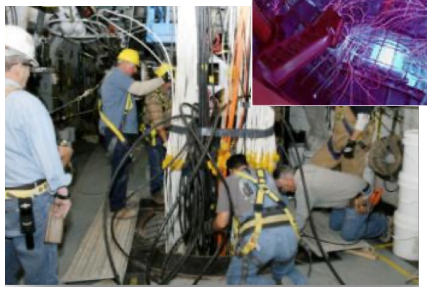
Many UGT results from testing archive.

Thousands of sensitivity calculations….

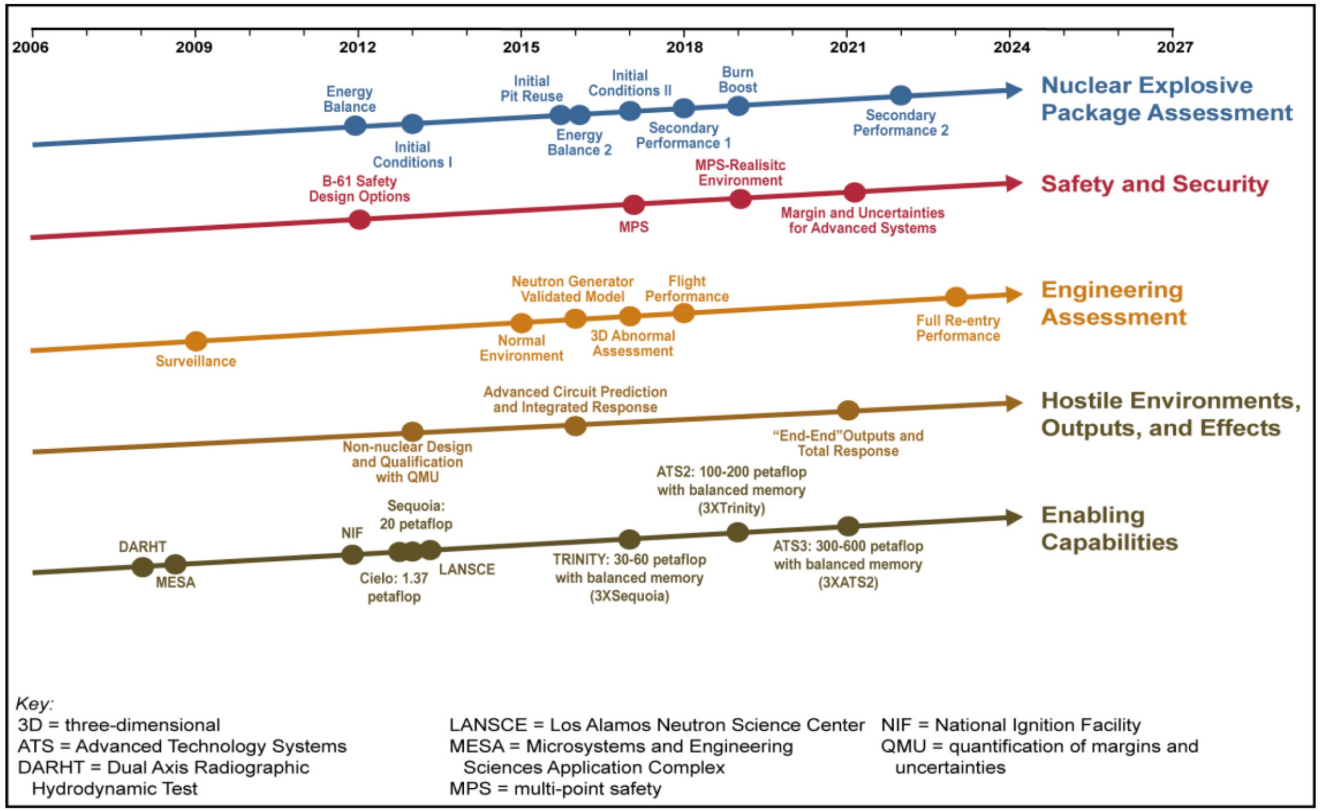
Theory and focused, smaller-scale experiments enable more predictive models to support US stockpile decisions.



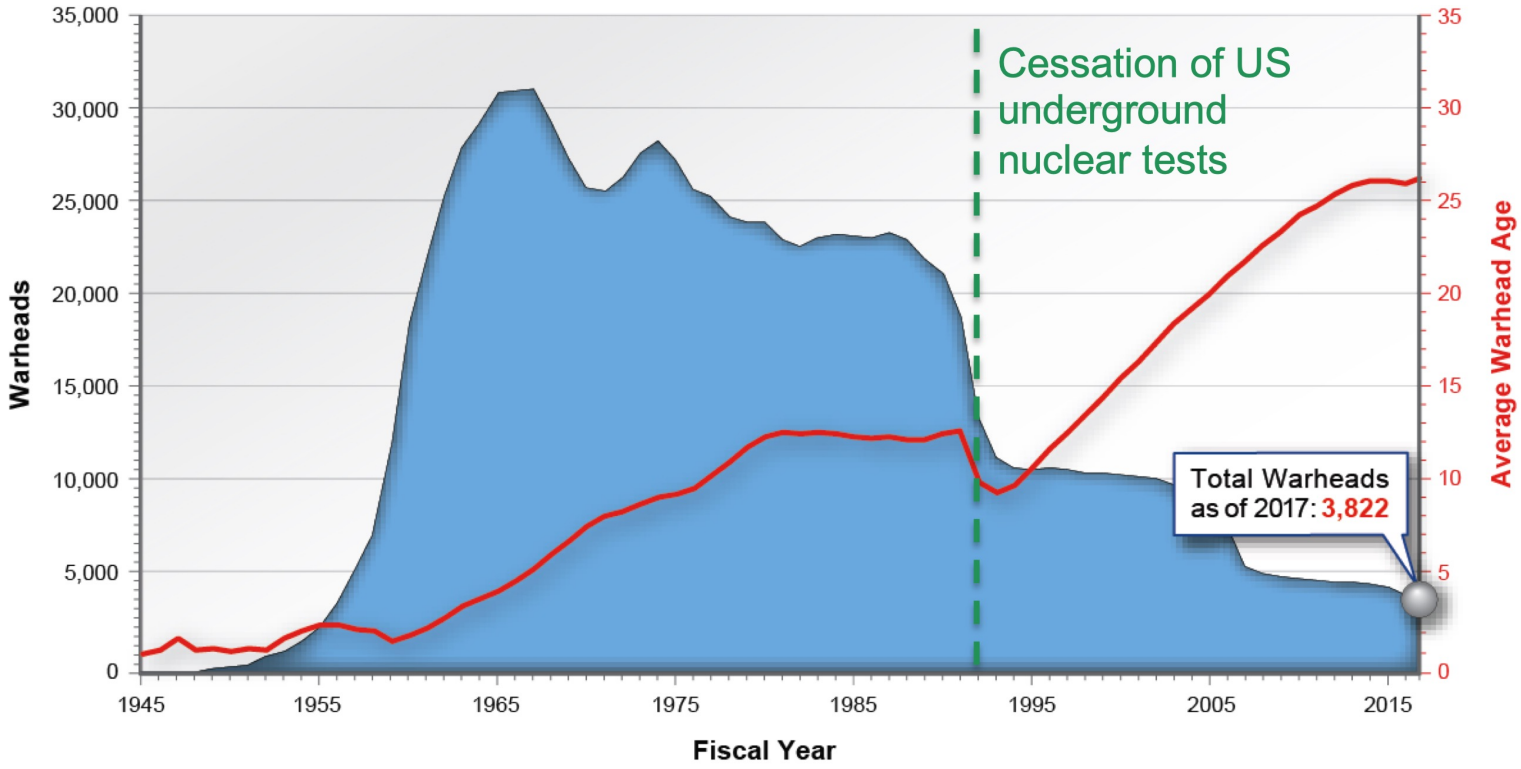




At the national level, a "Predictive Capability Framework" was instituted in order to ***integrate*** Stewardship science and simulation efforts.



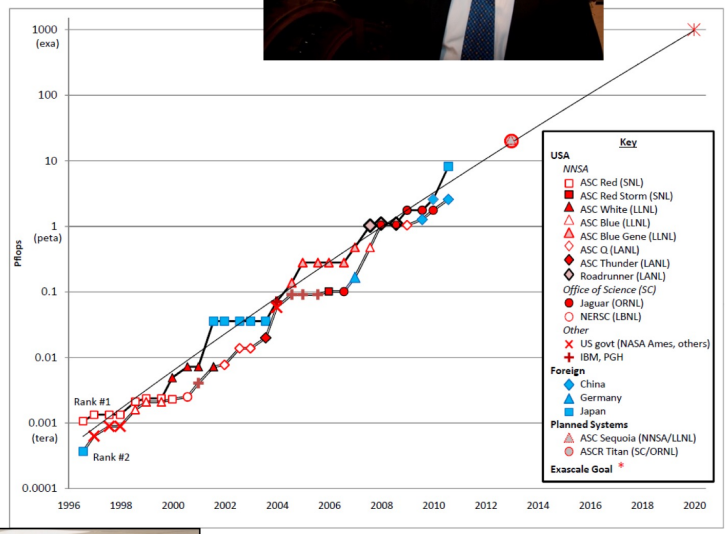
In the early days of Stewardship, most attention was given to warhead aging

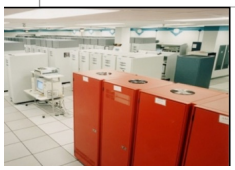


The DOE/NNSA Advanced Computing program (ASC) has transformed large-scale scientific computing

- NNSA has been a leader in increasing processing power with much needed associated memory
- Can we sustain the needed advances in computing? Can we efficiently use future computer technologies? Can we ensure we are computing on US technology?
- Computing will continue to be essential for ensuring credible nuclear deterrent into the future

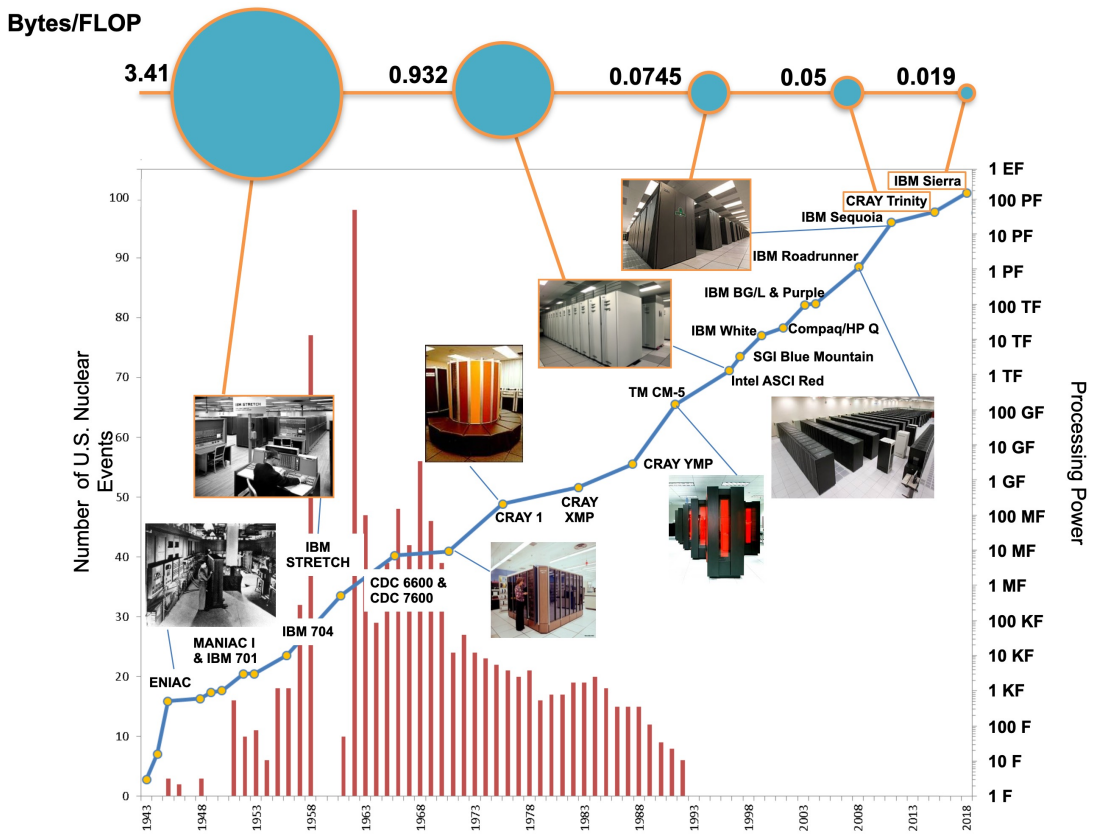
2011
1 TF on a chip
<0.25 kW





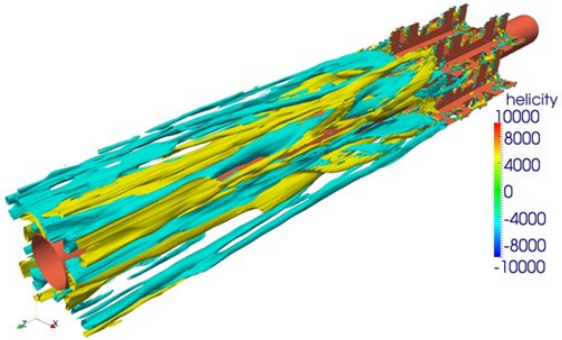
1996
1 TF in a room
500 kW

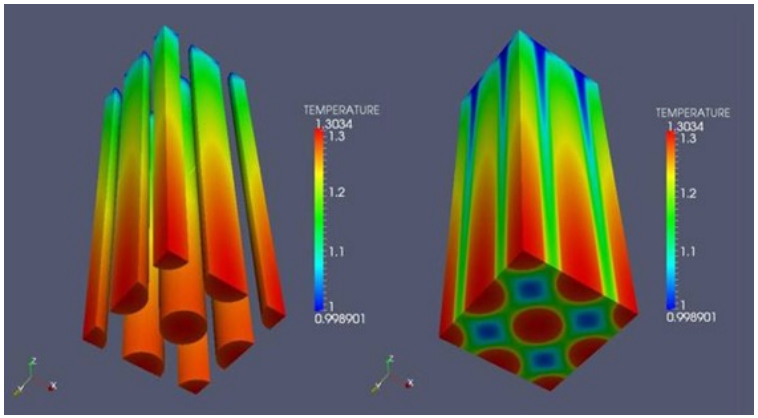
Exascale computing is now within sight…

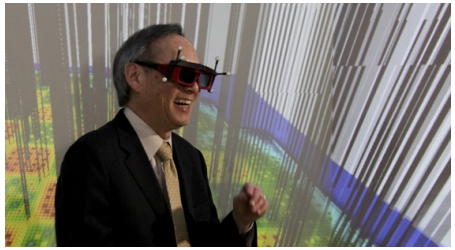


- Porting ASC simulation codes will continue to be a challenge
- Partner with system vendors to influence computing industry developments
- Adapt to new architectures: reinvent algorithms
- Balance “capacity” computing and “capability” computing

Energy Innovation Hub at ORNL: Consortium for the Advanced Simulation of Light-Water Reactors (CASL)







Predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics.

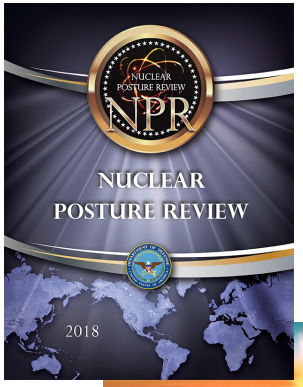
Stockpile Stewardship is NOT ”just like any other” technology development program

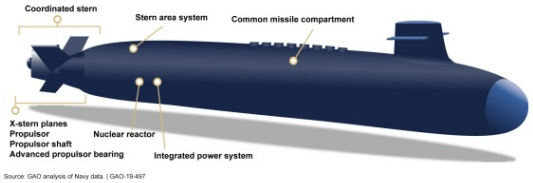
- Will demand a rigorous program balance between:
  - Experimental and modeling/simulation activities (V&V)
  - Small-scale physics experiments vs integral experiments (multi-physics integration)
  - Science-based prediction and advanced manufacturing/production (responsive)
- Will never have the benefit of a full-scale integral test of the “finished product” (CTBT observance precludes “new” nuclear weapons)
- Requires ***disciplined methodology*** for explicit understanding and communication of quantified performance margins and uncertainties (”QMU”)
- Demands that a “timely” design cycle will be supported by a validated, prediction-based methodology

World events have broadened the global security missions, but the need for Ground Truth and Discovery remains.

Modernization of the US nuclear force structure will reflect greater ***flexibility*** and ***resilience*** (2018 NPR)

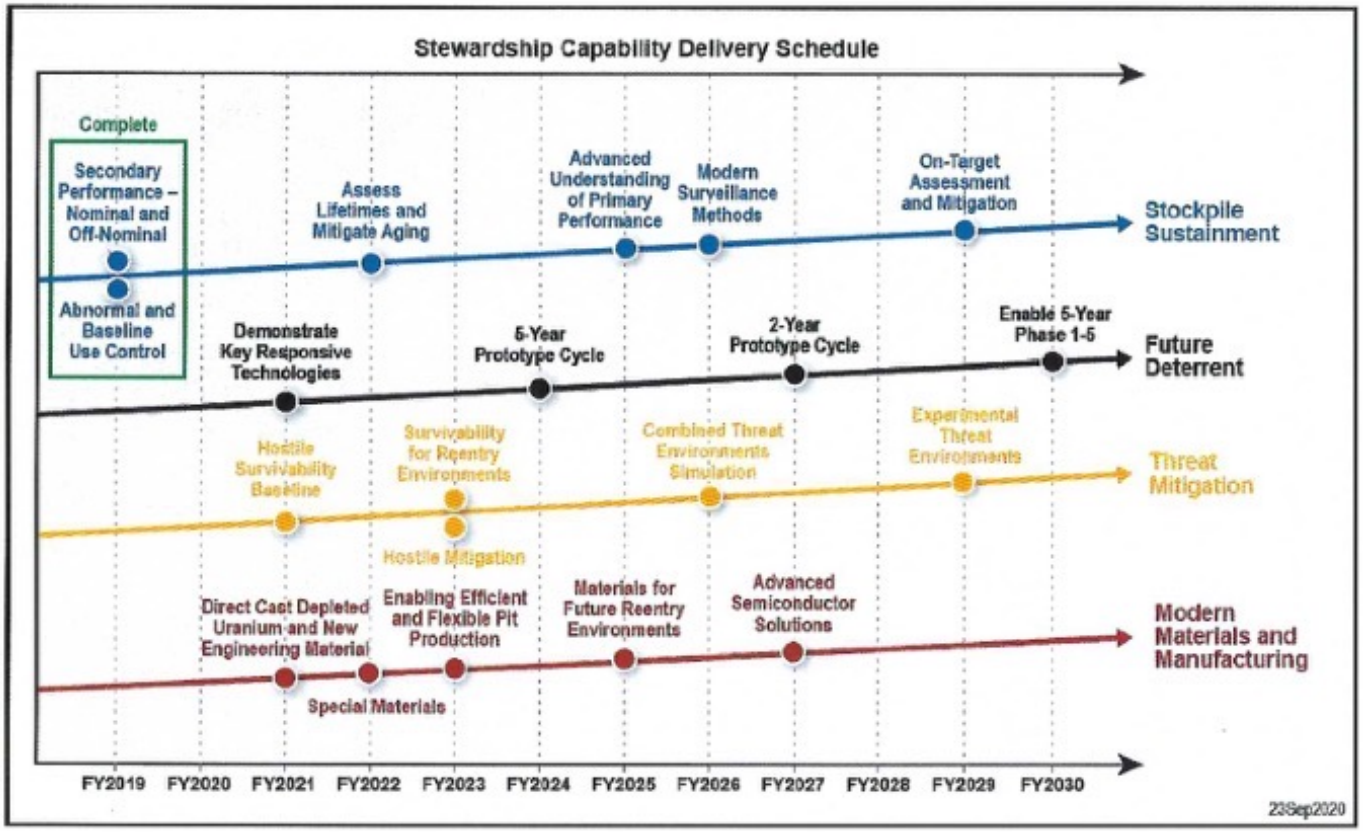
- Complete LEPs: W76-1, B61-12, W88 Alt
- Synchronize W80-4 LEP with DoD proposed LRSO (2031)
- Replacement for MM III ICBM (*GBSD*), advance W78 replacement
- Low-yield SLBM (W76-2)
- Next gen SSBN: *Columbia*-class (12)
- Next gen bomber: *B-21 Raider*
- SLBM WH to penetrate adversary defenses
- Nuclear SLCM in longer-term





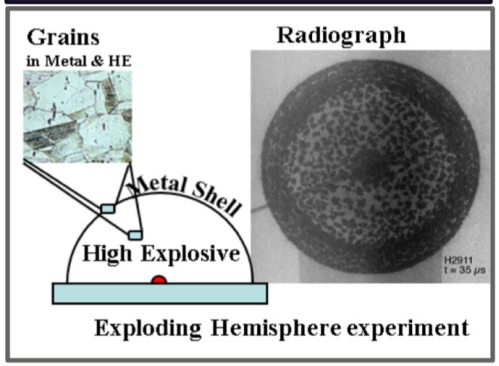
Twelve warhead types will be replaced by five nuclear warheads that have benefited from life-extension adaptations.

Capability Delivery schedule has replaced the Predictive Capability Framework



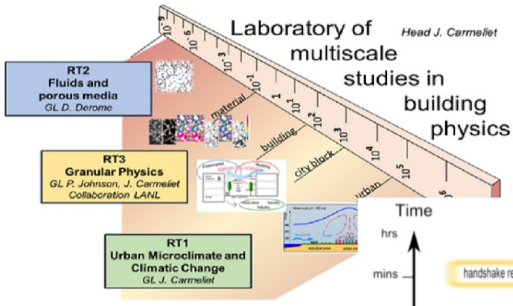
Multi-scale methods are critical for the high-fidelity, full-physics simulation of complex systems

Multi-scale methods



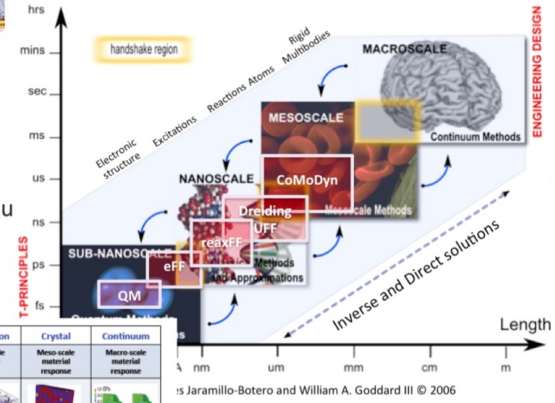
Resolving grain-level physics: improved fidelity in experiment *and* simulation (DARHT, MaRIE)

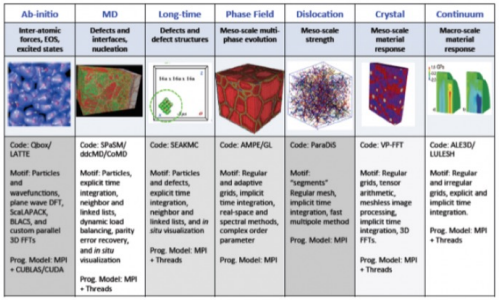
- **Models at different scales (*fine* to *coarse*) & bridging between them (*multi-scale methods*)**
- **Coarse: multi-physics coupling**
- **Fine: higher fidelity *and* asynchronous concurrency**



Climate
*http://empa.ch

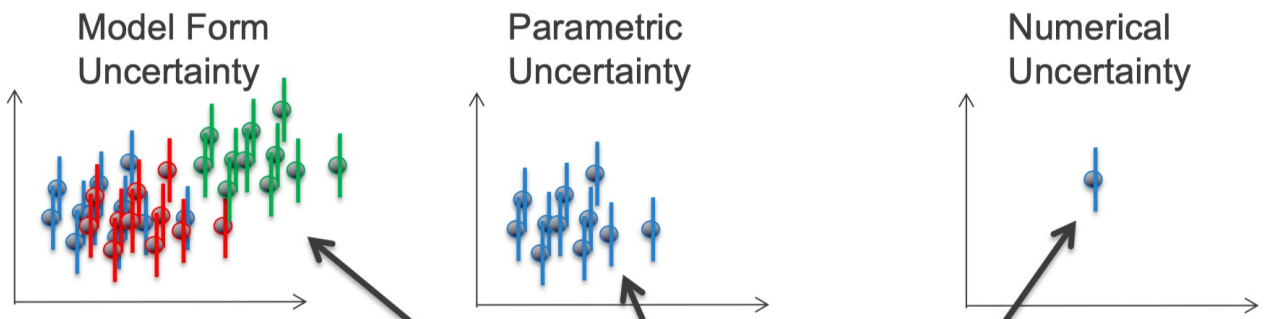
Biology
*http://wag.caltech.edu





Materials
*Ex Mat Ex

Uncertainty Quantification (UQ) must also be explicitly considered in using a hierarchy of models to bridge quantum and continuum-length scales.

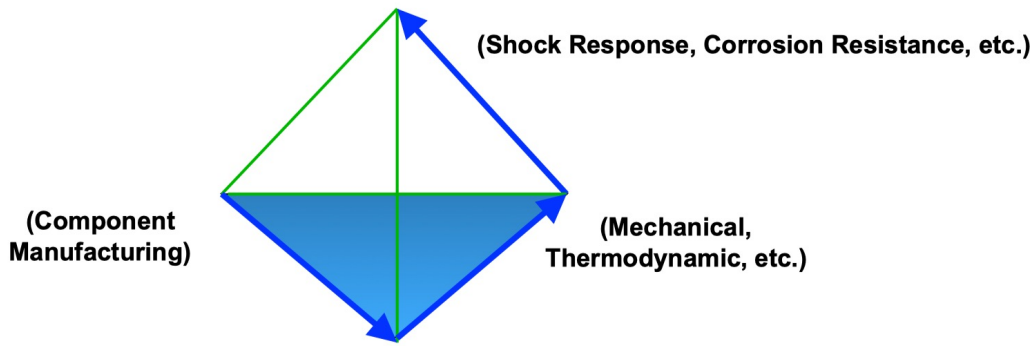


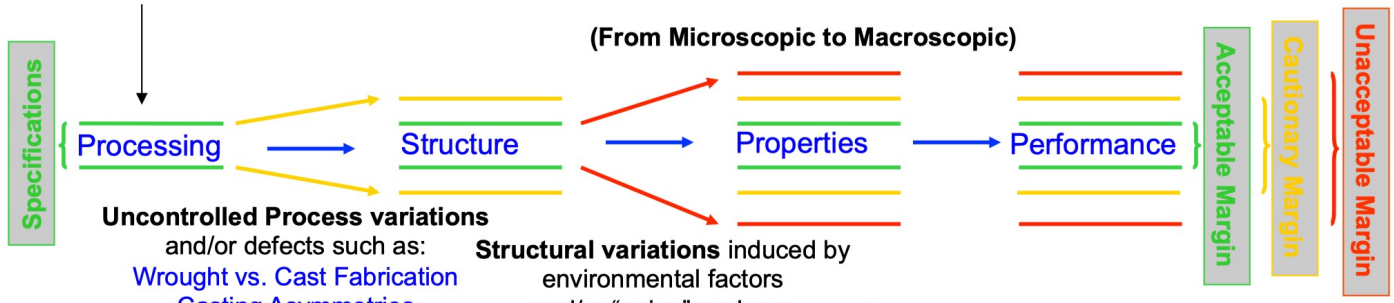
$$U = G(p) + \varepsilon$$

- **Experimental comparisons are a necessary ingredient for predictive science**
  - Experiments must quantify the errors
  - Simulations must quantify the uncertainty
- **Codes should be designed to enable straightforward fielding of a diverse set of physics algorithms**
  - Numerical and parametric uncertainty studies tend to be easier to accommodate
  - Model form uncertainty studies tend to be more invasive

Process-Aware Manufacturing (PAM) will demand an understanding of the linkage between manufacturing processes and material performance.

Established Manufacturing Process
Known performance and margin based on well-known causal relationship between processing specifications and resultant structure, properties, and performance.





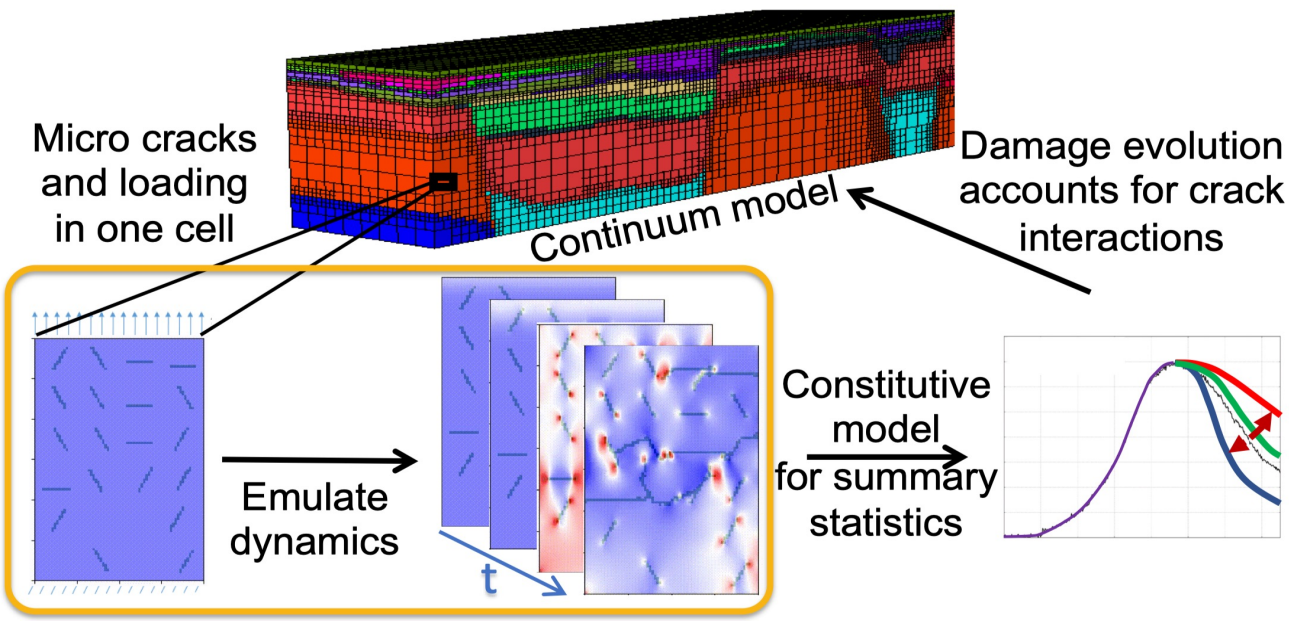
Uncontrolled Process variations and/or defects such as:
Wrought vs. Cast Fabrication
Casting Asymmetries
Impurities and Inclusions
lead to structural variations.

Structural variations induced by environmental factors and/or "aging" such as:
Oxidation and/or Corrosion
Fatigue and/or Fracture
lead to properties variations.

Variations (intentional or not) propagate through these relationships and must be well understood to effectively manage **impact** to **performance margin**.

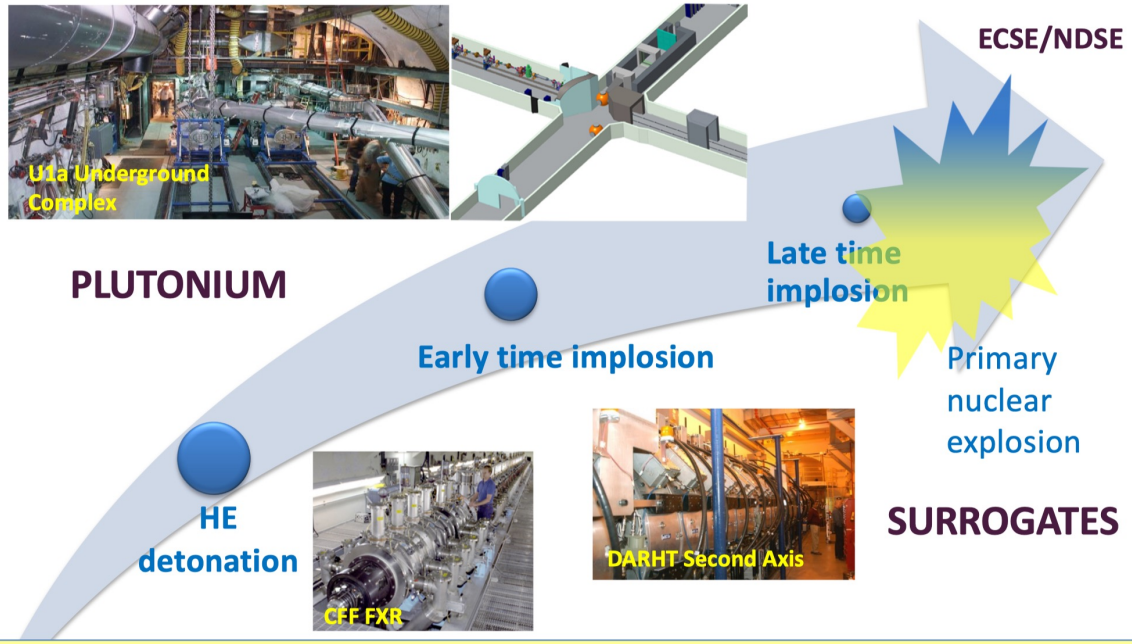
Machine Learning (ML) can be used to enable the bridging of scales through fast emulation.

- Train deep learning model to emulate micro-scale simulations
- Feed quantities of interest to macro-scale model



Use of integral experiments is at the threshold of transformational advancement: ECSE/NDSE

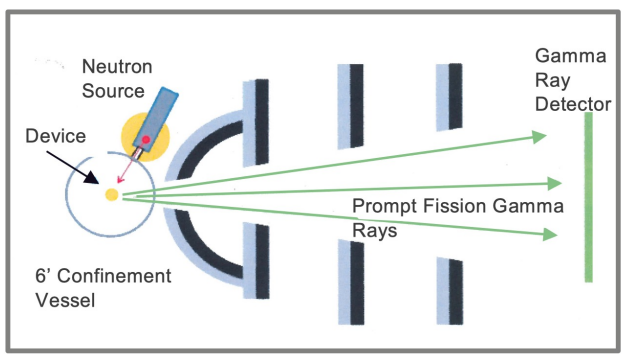
Enhanced Capabilities for Subcritical Experiment's (ECSE) Mission
Need: Nuclear performance depends on the way plutonium implodes

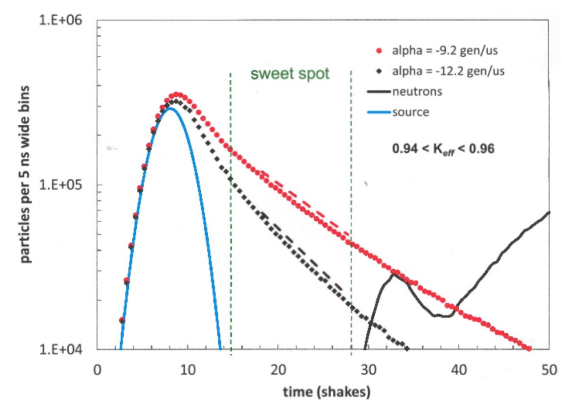


ECSE's Radiographic and Neutron Diagnosed Subcritical Experiment (NDSE) measurements will fill a critical gap in experimental capabilities: evaluating plutonium response at late times

Key elements required to make NDSE measurements on subcritical Plutonium implosion

- **Neutron source**: Initiate a short (~80ns HWTM) burst of fissions via an external neutron or photofission source at peak plutonium compression
- **Fission gamma ray detector:** Gamma ray detector minimally effected by neutrons (source, fission, and scattered) and scattered gamma rays
- **Background Reduction**: Collimation and shielding that control neutrons and gamma scattering to reduce noise levels
- **Simulations:** Computing power coupled with Monte Carlo forward modeling





What options are available if performance changes cannot be assessed with "confidence"?

- Replace aging materials; use qualified advanced manufacturing processes
- Push back on Military Characteristics (MCs) and Stockpile-to-Target Sequence (STS) requirements, delivery vehicle interfaces
- "Conditional" certification based on uncertainties, or accept the uncertainties (political pressure will be severe!)
- Require a return to nuclear testing (will probably require more than one test to complement the contemporary design methodology?)

Demonstrate the use of objective uncertainty quantification by rigorously comparing uncertainties to performance margins (i.e., QMU methodology)

Will we "know" when to say "no"?

- Although scope of deliverables may have increased, retreating from "science-based prediction" is NOT an option for Stockpile Stewardship
- MUST more rigorously pursue UQ in model development, and "up-scale" and propagate uncertainties to continuum level.
- All certification assessments must be tied to a nuclear test "pedigree" to preserve ground truth, but a "Common Model" approach may become too limiting, depending on future stockpile requirements
  - *Know where the boundaries of the "design regime" are!*
- Continue to ensure that the balance between experimental and computational programs supports ***timely stockpile decisions*** and ***prototype/phase development schedules***.
- Support a new UQ-informed design methodology whereby full-physics 3D simulation results can return to designers in reasonable cycle time.

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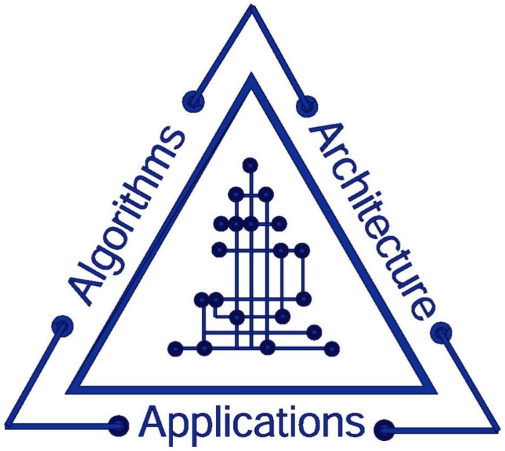
- Anishi Mehta, et al



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