Advanced Simulation and Computing:

Ushering in a New Decade of Predictive Capability & the Role of the Predictive Science Academic Alliance Program

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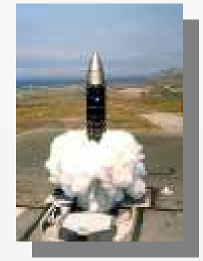
Once upon a time…

Central Problem: *Replacement of underground testing with a rigorous scientific methodology with which to assess and maintain our confidence in our nuclear stockpile.*

Time Urgencies: *Supporting national policy with respect to the maintenance of our nuclear stockpile requires that we be able to certify annually to the Secretaries of the Departments of Energy and Defense that the stockpile is safe, reliable and secure.*



National Program: *Planned and coordinated across the three Defense Program Laboratories with partnerships with academic centers and industry.*

Today we have replaced the drilling and set-up of nuclear testing, with the meshing, computer and computational science of simulation using new tools…

Advanced Simulation & Computing (ASC)
Our mission and motivation

Provide the science-based capability to assess and certify the safety, performance and reliability of nuclear weapons and their components without nuclear testing

- Create tools for annual certification & assessment
- Maintain a credible deterrent with a "zero-yield" nuclear test ban
- Support the President's Comprehensive Test Ban policy
- Ensure the effectiveness of science-based stockpile stewardship

Types of Issues:

- *As-built issues*
- *Aging issues*
- *Replacement of materials*

ASC computational science is at the intersection of leading-edge science and national policy, on a schedule to meet national nuclear security needs

The Evolving role of simulation supporting the nuclear deterrent

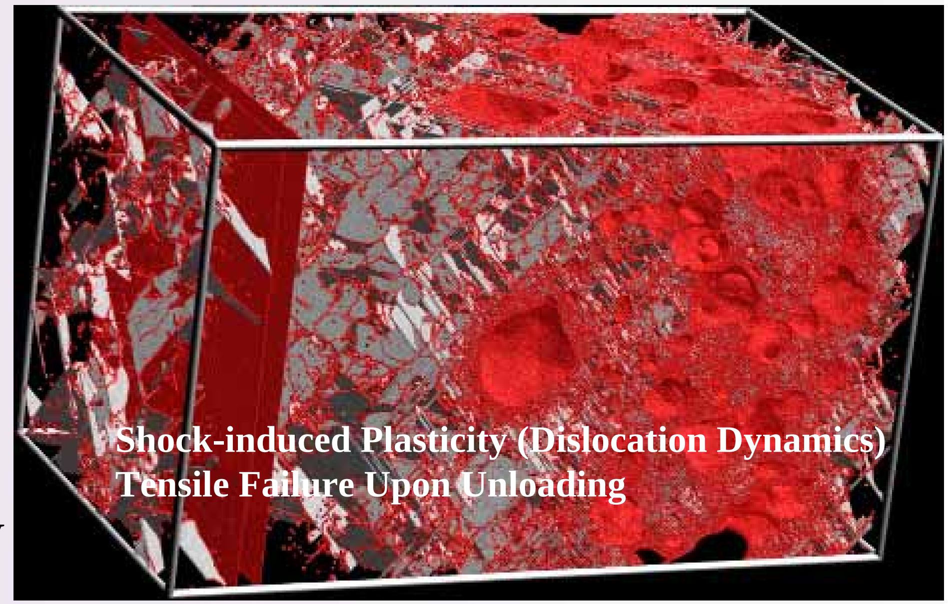
1943-1992	1992-2005	2006^{++}
Historically • Simulation supports design and test-based certification • Largely empirical physics treatments	*Early Stewardship Era* • Capability demos and selected studies show the potential of ASC Technology • Continued reliance on Legacy tools for interpolation • 100 Teraflop goal	*Stewardship Matures* • ASC technology becomes the dominant means for Stewardship • Validation methodologies for multi-scale computational science • Multi-petascale routine

Ten years of accomplishment, 100 TF goal met… next challenge is predictivity

Computational Science Critical to Scientific Discovery

One can begin to address problems that involve competing complex physical processes including:

- Ranges of length scales
- Ranges of time scales
- Extreme conditions and complexity not experimentally accessible

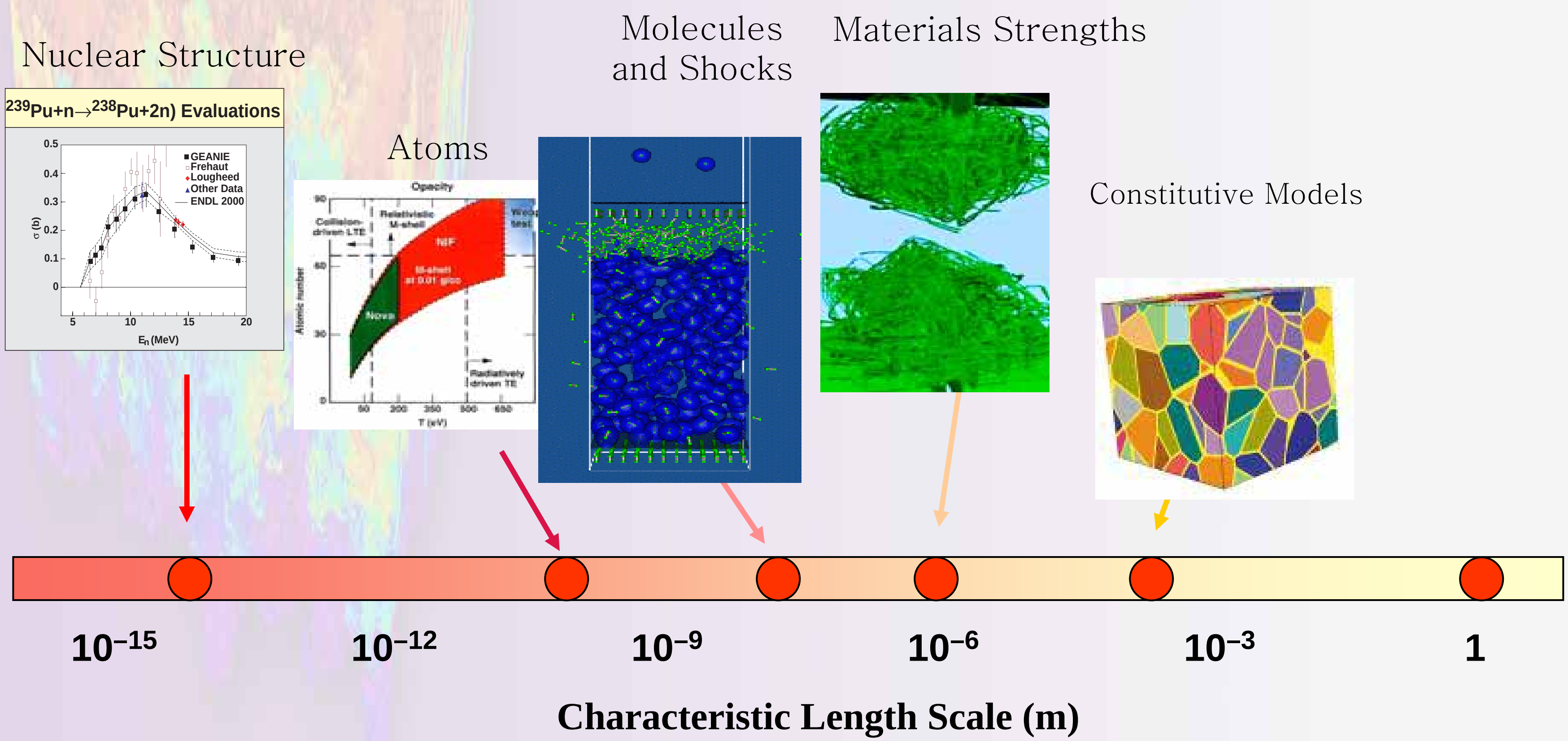


- Competing, complex physical processes and dynamics

  Non-equilibrium systems, phase transitions,…

- Informs decisions, allows virtual testing/prototyping. Virtual testing increasingly replacing experimentation (wind-tunnel evaluations of airfoils, crash tests)

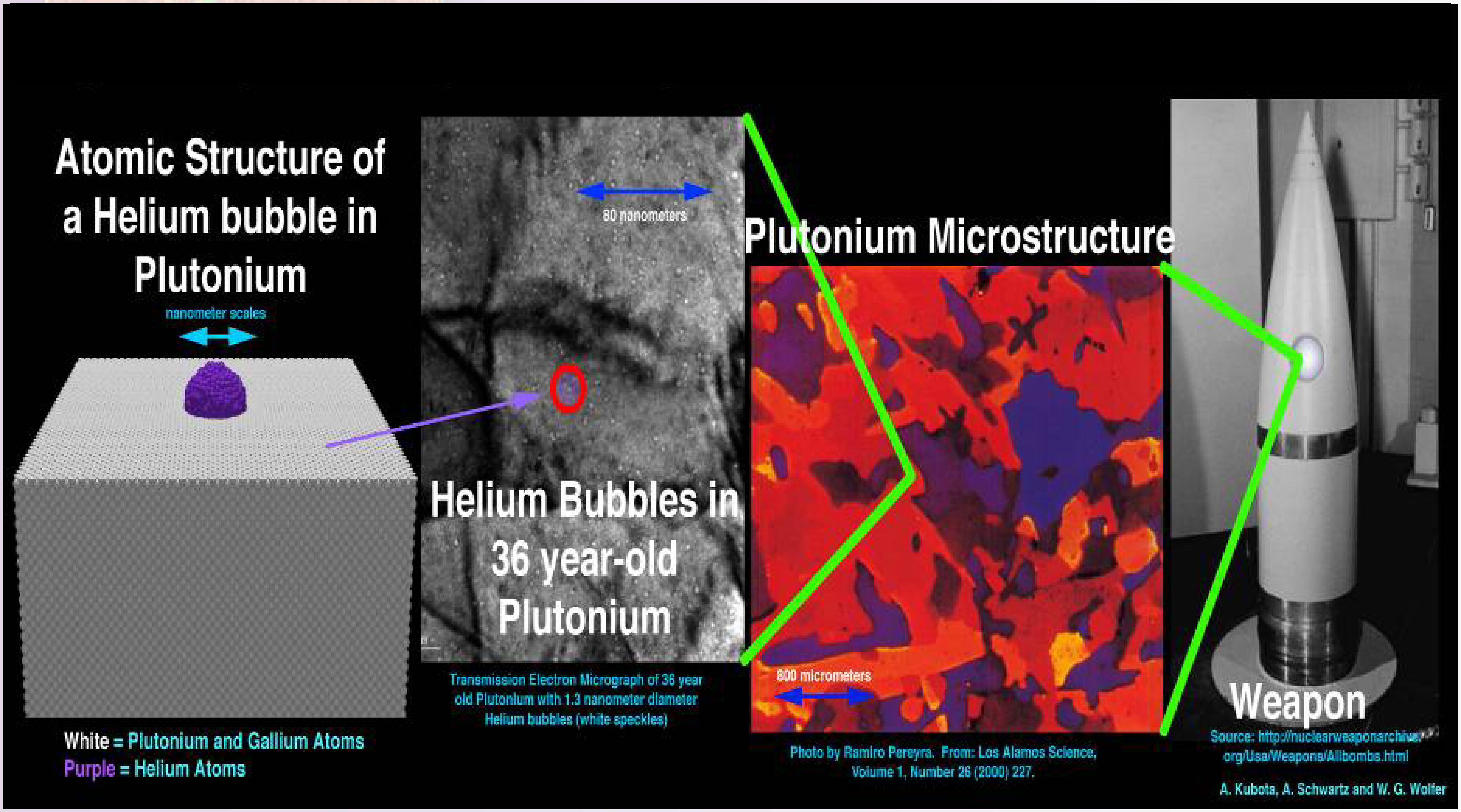
Range of Length Scales



Simulation across many length scales requires a balance of fundamental science and phenomenology.

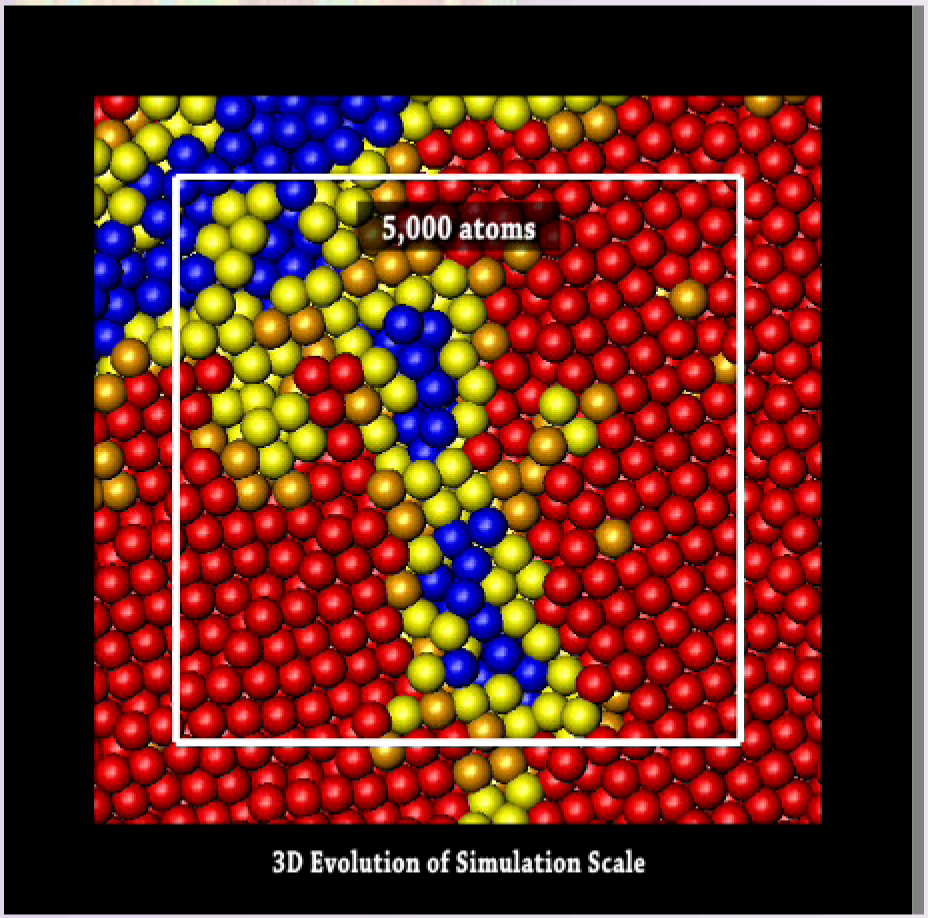
Simulation Science: Microscale to Mesoscale

- Defining hierarchical decompositions with tightly coupled phenomena

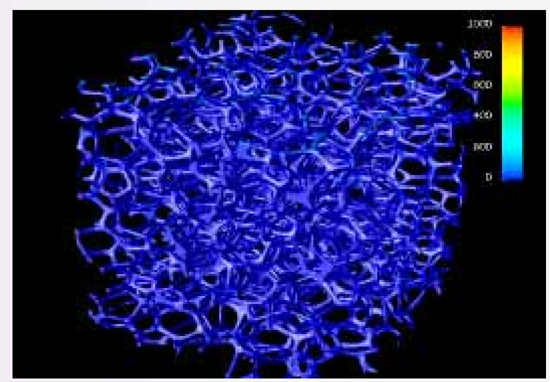


Simulation today is an integral activity

New insights into solidification of molten metals

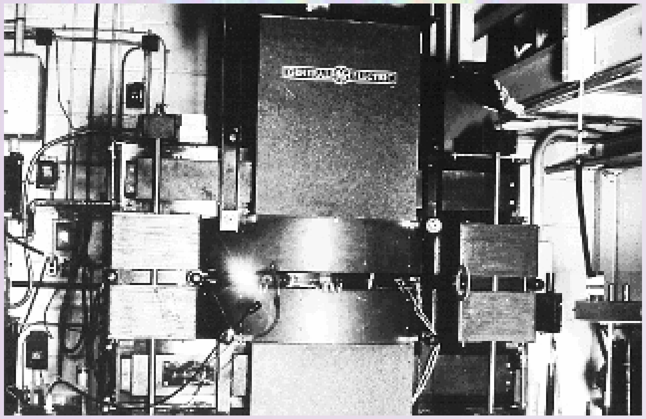


Simulation of Large Deformations in Urethane Foan



Changing paradigm for large-scale simulation

- Computers are enabling us to attack previously intractable problems
- Multi-scale simulations of complex systems are becoming more common but require collaboration of researchers from many disciplines.



The community has adjusted to the change …

VOLUME 93, NUMBER 14 PHYSICAL REVIEW LETTERS week ending 1 OCTOBER 2004

Inclusive Double-Pomeron Exchange at the Fermilab Tevatron $\bar{p}p$ Collider

141601-1 0031-9007/04/93(14)/141601(7)$22.50 © 2004 The American Physical Society 141601-1

VOLUME 93, NUMBER 14 PHYSICAL REVIEW LETTERS week ending 1 OCTOBER 2004

(CDF Collaboration)

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VOLUME 93, NUMBER 14 PHYSICAL REVIEW LETTERS week ending 1 OCTOBER 2004

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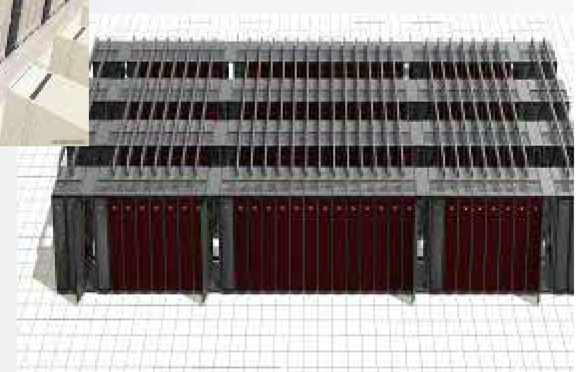
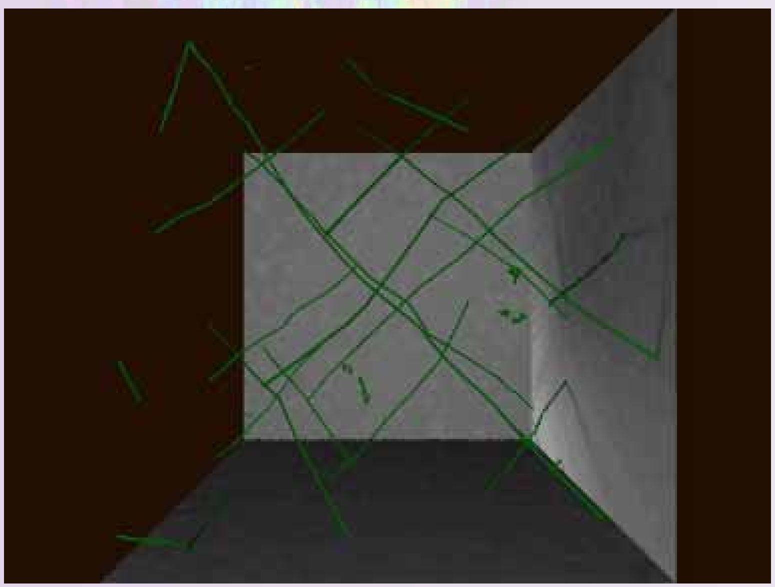
What would you compute if computing power is no longer a factor?

- Petascale computing will be available during this next solicitation period.
- Scaled up single-physics applications is not sufficient – big progress will arise through integrated efforts.





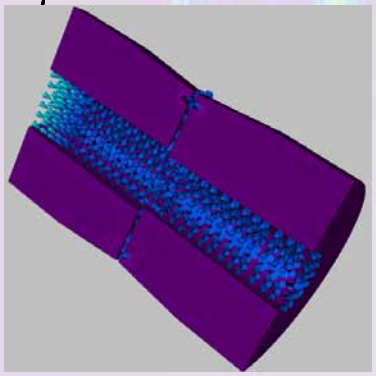
(Bulatov et al, Nature, 2006, in press)

Over 500 faculty and students are involved in ASC Alliances

California Institute of Technology
Center for Simulating Dynamic Response of Materials

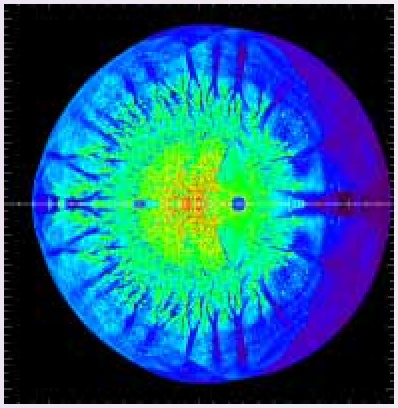
HMX detonation in a tantalum canister.

University of Illinois
Center for Simulation of Advanced Rockets



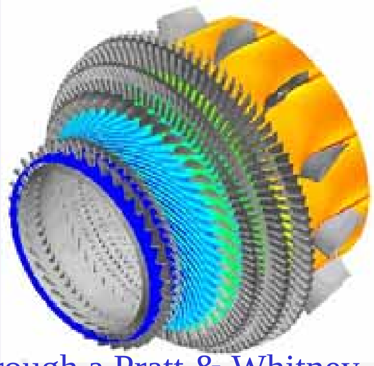
3D joint effects in Titan IV SRMU booster.

The University of Chicago
Center for Astrophysical Thermonuclear Flashes



Thermonuclear burn in a Type Ia supernova.

Stanford University
Center for Integrated Turbulence Simulations



Flow through a Pratt & Whitney 6000 engine.

University of Utah
Center for Simulation of Accidental Fires and Explosions

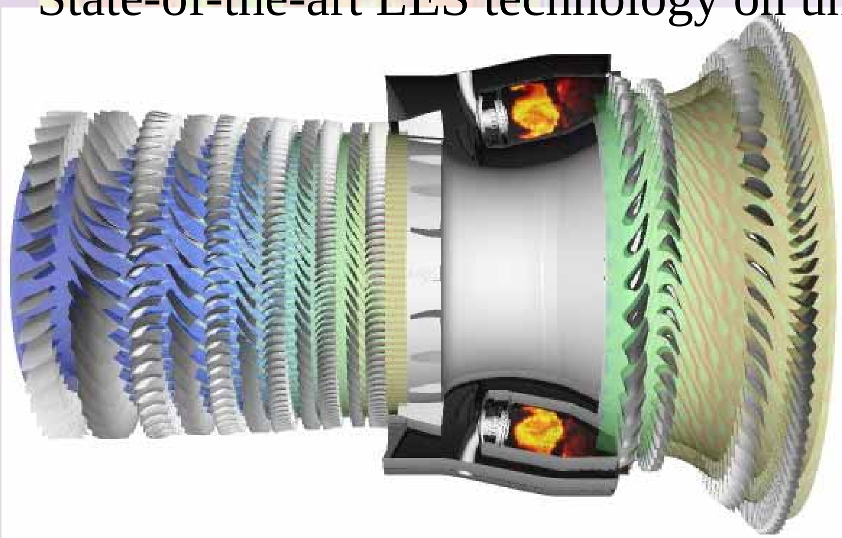
Simulation of a heptane pool fire.

Computational Capabilities in 2005

Integrated Simulations based on fully-featured, validated CITS codes

Multicode coupling based on general-purpose API

State-of-the-art LES technology on unstructured grids



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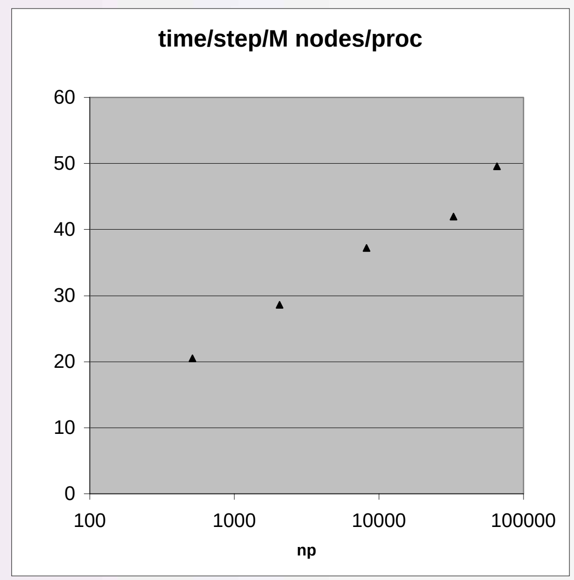
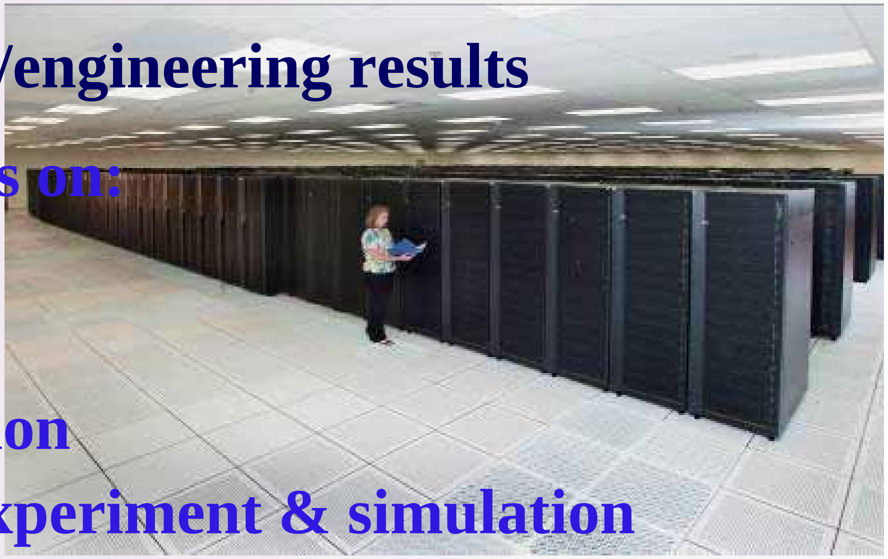


Goals of ASC Predictive Science Academic Alliance Program (PSAAP)

- **Focus on a multi-scale, multi-disciplinary, unclassified application of NNSA interest**
- new **Demonstrate validated simulation capability for prediction**
- **Demonstrate capability on available ASC computing system**
- **Produce significant science/engineering results**
- **Produce new methodologies on:**
  - **Verification**
  - **Validation**
  - **Uncertainty quantification**
  - **Tighter integration of experiment & simulation**
- **Improve quantity & quality of tools and algorithms**



Example: Uncertainty Quantification Issues

Three main issues exist:

- Characterization of uncertainties as inputs to simulations:
  - Probability density functions valid in some cases for well-behaved, stochastic, even subjective types of uncertainty
  - Unclear how to treat epistemic uncertainty where even notion of a distribution might be misleading.
- Propagation of uncertainties (aggregation/convolution) to through codes to quantify uncertainty in some integrated performance parameters.
- How calibration works within a structured, disciplined UQ methodology and for what purpose.

Development is needed in a broad area so that alternative approaches can be weighed and contrasted.

ASC Strategy: Simulation as a Predictive Tool

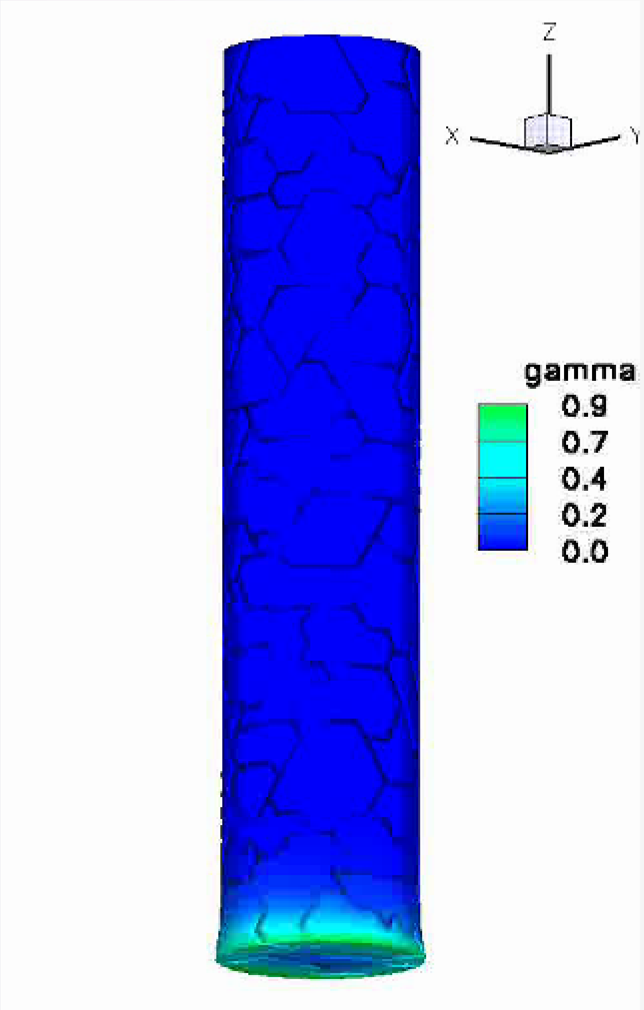
- ASC has the responsibility to develop the tools to address evolving NNSA mission requirements.
- ASC is evolving from a proof-of principle initiative to a program that is providing improved capabilities essential to maintaining technical confidence in the stockpile.
- As ASC's ability to predict weapons behavior with confidence increases, simulation will become an even more valuable component of intellectual framework supporting the annual assessment and certification plan.
  - Essential to this undertaking is the calculation, measurement, and understanding of the uncertainty in the predictions of ASC's simulation results

There are still many challenges

- Computers are becoming so powerful, they are enabling scientific progress at remarkable scales.
- Leading edge simulation is beyond that of the individual scientists or small groups. The talent base must now be diverse.
- An essential paradigm shift is needed in the way research is done at Universities. Multi-disciplinary will be essential for pushing the frontier.
- Scientific expertise is beyond a single field, techniques are broad, visualization and understanding are challenging. Like big CERN experiments where one creates terabytes of data and then spends time sifting though it.
- Similar to transition from lab experiments to centralized national and now international facilities. Costs and time between upgrades becoming so large that one has to centralize.
- Validation is tough – no well defined process although some are being worked on. One must be careful not to fool oneself – simulation is a tool but has many successes

PSAAP is a unique opportunity for scientific discovery

- Scientific discovery today is focused on the determination and enumeration of higher organization principles of nature.
- Scientific progress has often come from measurements of effects that are not believed to be important or relevant, but their evidence contradicts our understanding and leads to new areas of research *– e.g. in the Quantum Hall Effect the conductance was not supposed to be quantized.*
- Developing useable, quality codes is a multidisciplinary challenge and will require simultaneous collaboration of many subject matter experts, including physicists, chemists, mathematicians, numerical analysts, computer scientists.
- The time is right for scientific discovery



Summary: Goals of PSAAP

- Integrate science/engineering, computational math and computer science into a focused research effort
- Increase Center/Lab interactions
  - Interplay between experiment & simulation
- Broaden the academic base of expertise in large-scale, multidisciplinary, simulation-based predictability