

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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A photograph of a large, multi-story building with a curved facade, possibly a school or institutional building. The building is light-colored and has several windows. The foreground is a dark, textured surface, possibly asphalt or concrete, with some faint white lines. The text "Once upon a time..." is overlaid in the center in a yellow, serif font.

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

Historically

- Simulation supports design and test-based certification
- Largely empirical physics treatments

1992-2005

Early Stewardship Era

- Capability demos and selected studies show the potential of ASC Technology
- Continued reliance on Legacy tools for interpolation
- 100 Teraflop goal

2006⁺⁺

Stewardship Matures

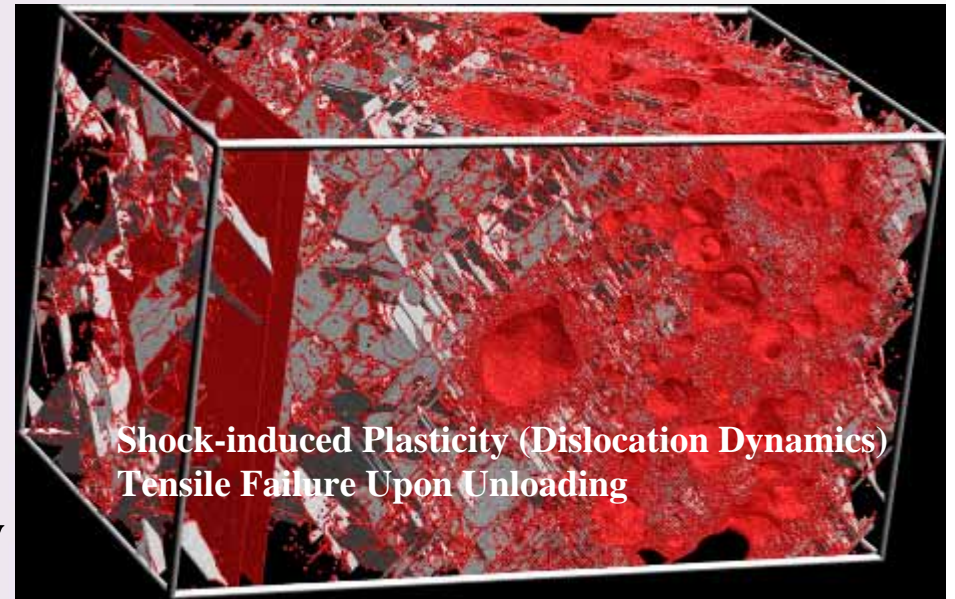
- ASC technology becomes the dominant means for Stewardship
- Validation methodologies for multi-scale computational science
- Multi-petascale routine

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

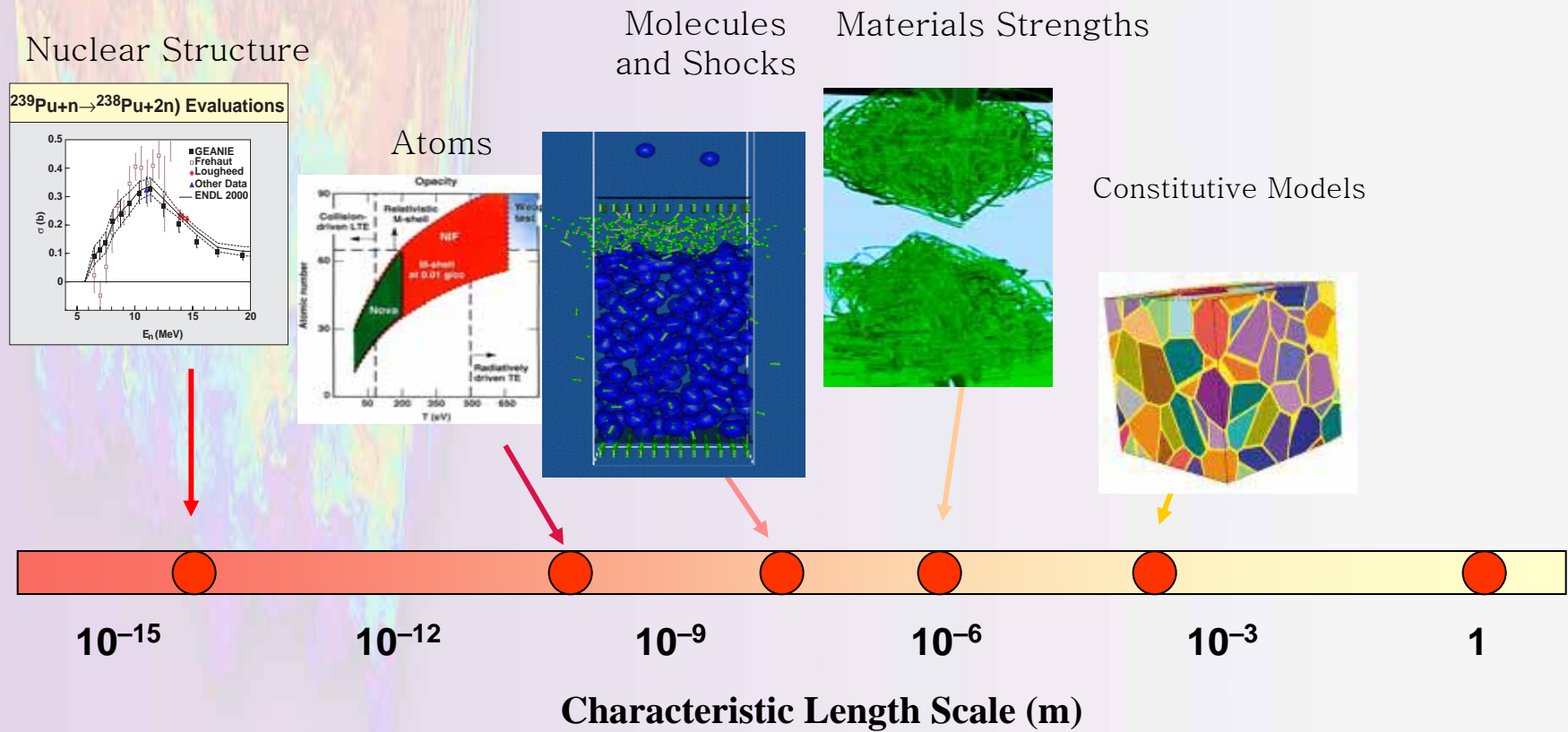
Computational Science Critical to Scientific Discovery

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)



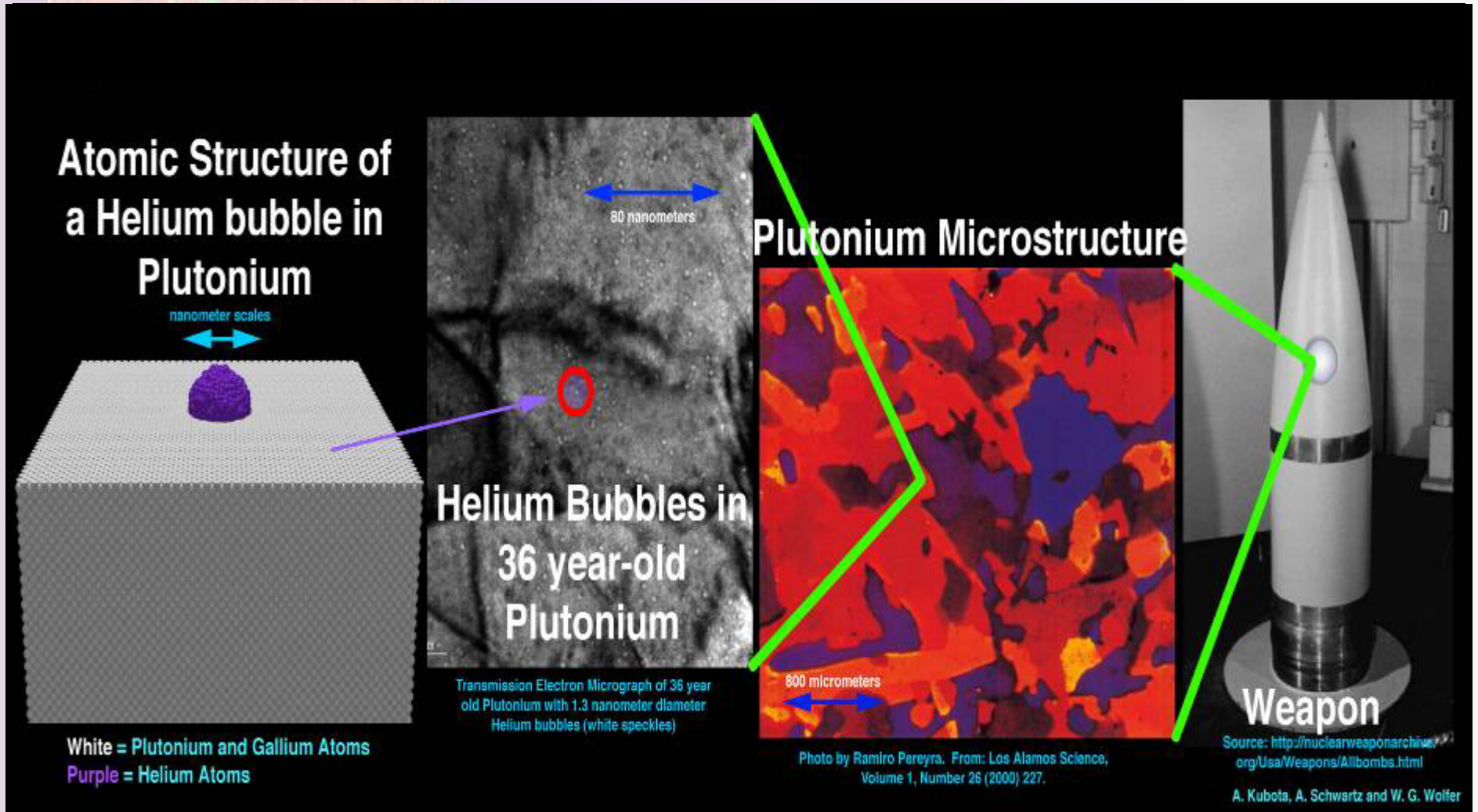
Range of Length Scales



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

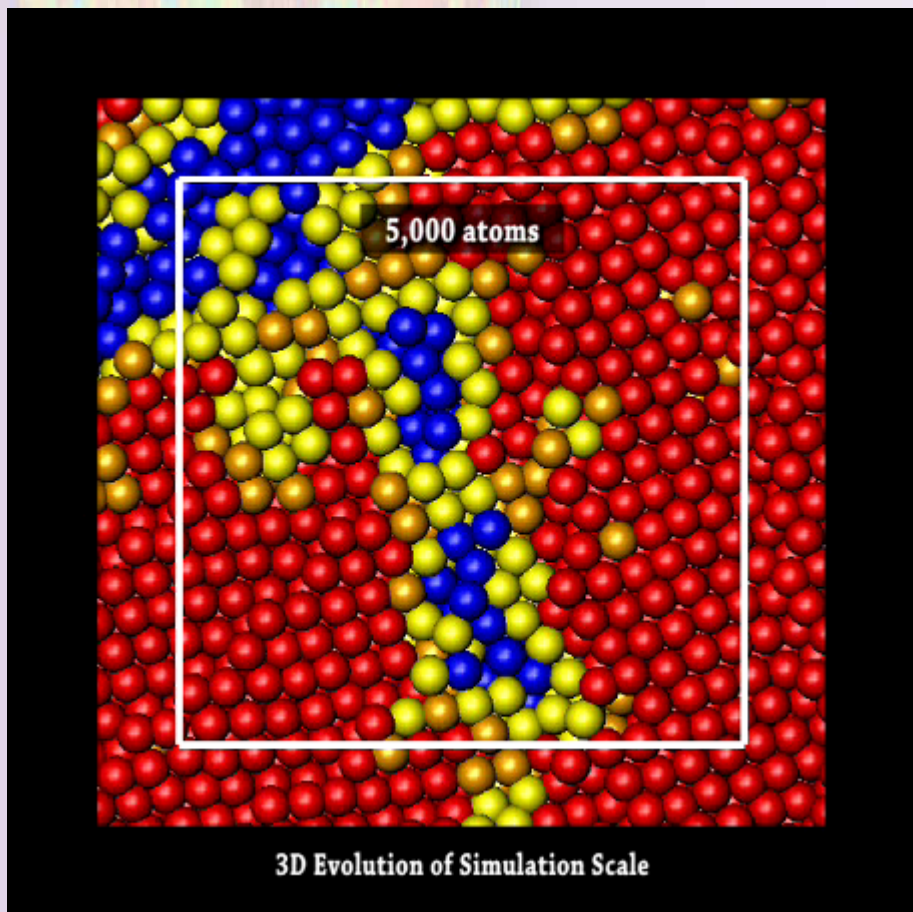
Simulation Science: Microscale to Mesoscale

- Defining hierarchical decompositions with tightly coupled phenomena

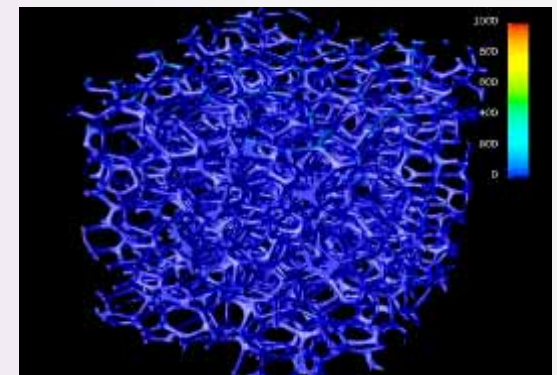


Simulation today is an integral activity

New insights into solidification of molten metals



Simulation of Large Deformations in Urethane Foam



PSAAP Bidders Meeting May 2006

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.

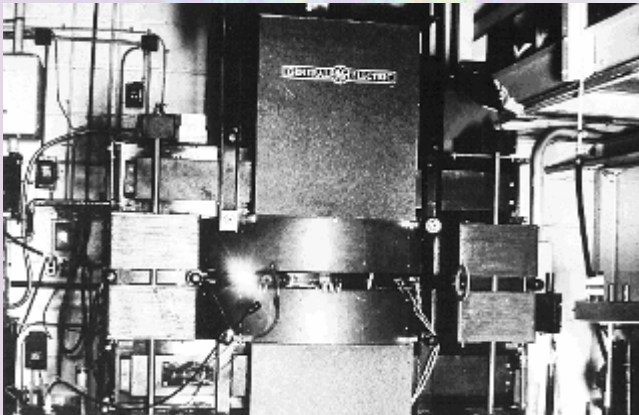


Table of contents for Volume 83, Number 14, including the title 'Inelastic Double-Pomeron Exchange of the Pomeron Production pp Collider' and a list of authors and their affiliations.

The community has adjusted to the change ...

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We report results from a study of events with inelastic Pomeron-Pomeron exchange produced in pp collisions at $\sqrt{s} = 200$ GeV. The events are identified by a leading p-pomeron and a large diffractive gap on the outgoing proton side. We find that the diffractive production cross section rises in energy with predictions based on Regge theory but disagrees with the rise of double-Pomeron exchange to single diffractive production rates in energy unaccounted for in Regge theory.

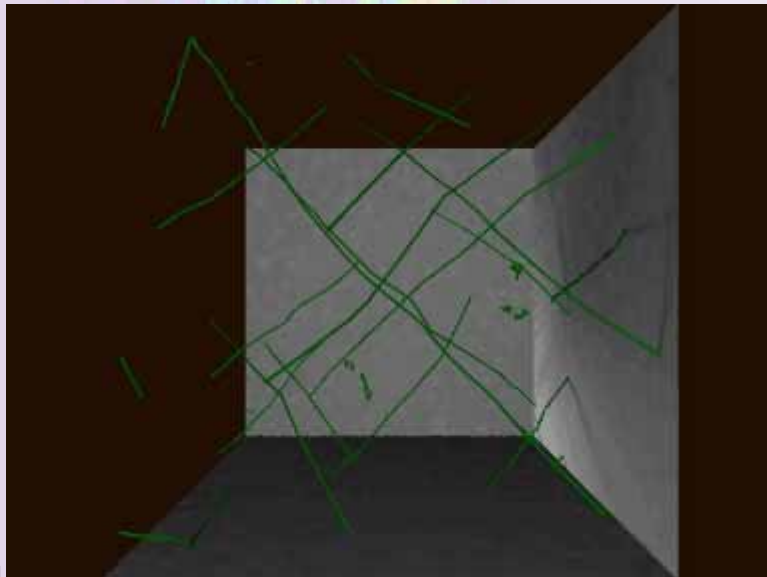
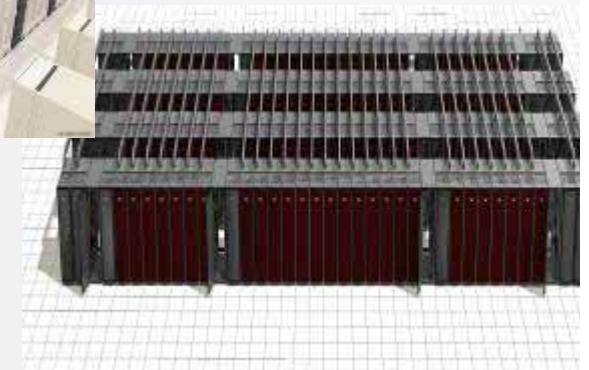
The success of perturbative quantum chromodynamics (QCD) in describing strong interactions at high transverse momentum transfers sets on the factorization theorem, which allows hadronic cross sections to be expressed in terms of parton-level cross sections hadronizing (convoluted with usually defined hadron parton distribution functions) not surprising that the breakdown of factorization was reported in a previous paper for diffractive production [1], a process containing both a hard scattering and the characteristic capillary gap production of diffraction, has attracted considerable theoretical attention. Capillary gaps, defined as regions of suppressed $0 < \Delta < 100$ GeV, are proposed to be formed in diffractive events by the exchange of Pomeron (P), which is QCD-motivated in terms of gluon exchange with the quark members of the nucleus [2] (see Fig. 1). The breakdown of factorization in diffraction is expressed as a suppression of the cross section and is generally attributed to additional partonic interactions within a diffractive event that spoil the capillary gap signature [3]. In processes with two capillary gaps, as in that with two forward gaps traditionally referred to as double-Pomeron exchange (DPE), shown in Fig. 1(b), it has been proposed that either both gaps survive or are sequentially spoiled, leading to a largely unaccounted ratio of two-gap to one-gap rates [4] which is observed to equal one [5], that the ratio of the rate of DPE to single diffractive QCD diffractive production is about 1.

FIG. 1 (color online) Schematic diagrams for event topology for (a) single diffractive, $p + p \rightarrow p + X$, and (b) double-Pomeron (DPE) diffractive, $p + p \rightarrow p + X + p$, the shaded circle represent pseudorapidity regions of gluon production.



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.

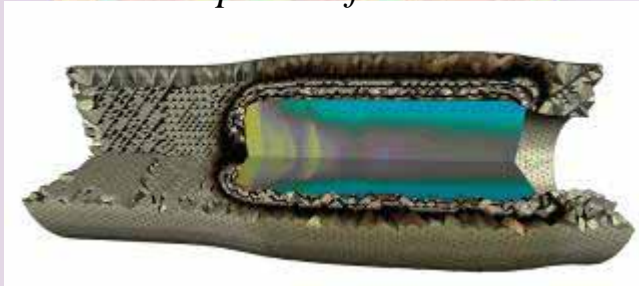


14 (Bulatov et al, Nature, 2006, in press)

PSAAP Bidders Meeting May 2006

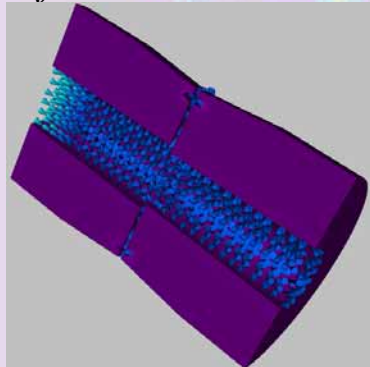
Over 500 faculty and students are involved in ASC Alliances

California Institute of Technology
*Center for Simulating Dynamic
Response of Materials*



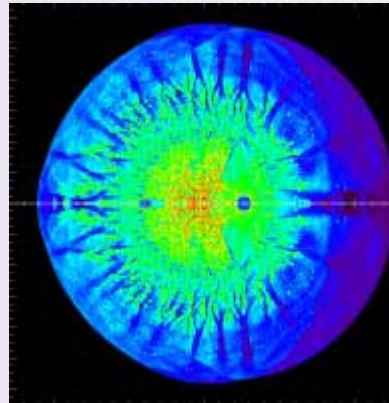
HMX detonation in a tantalum canister.

University of Illinois
*Center for Simulation
of Advanced Rockets*



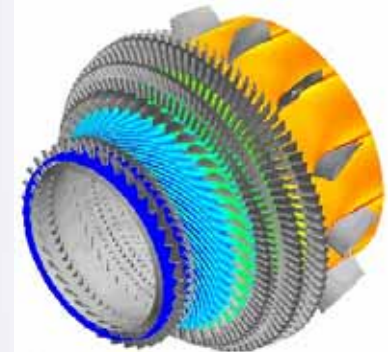
3D joint effects in Titan IV SRMU booster.

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*



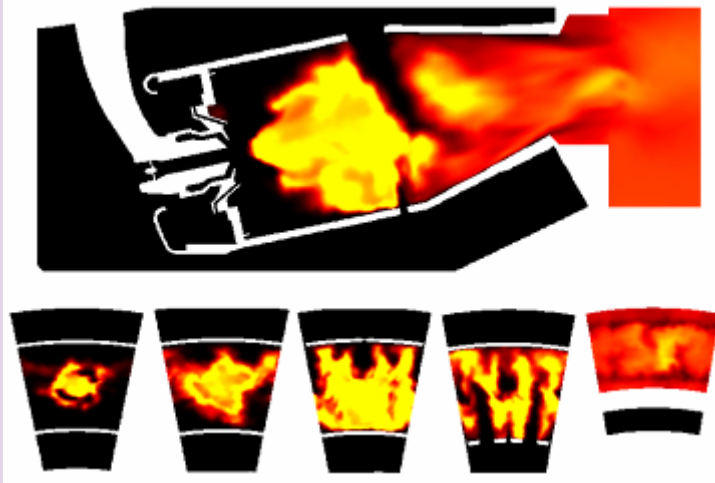
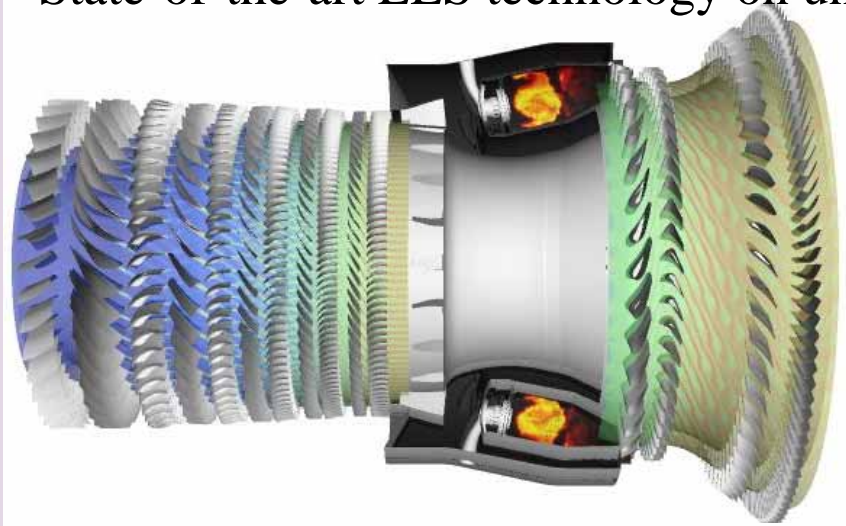
Simulation of a heptane pool fire
TSAAF Budget Meeting May 2006

Computational Capabilities in 2005

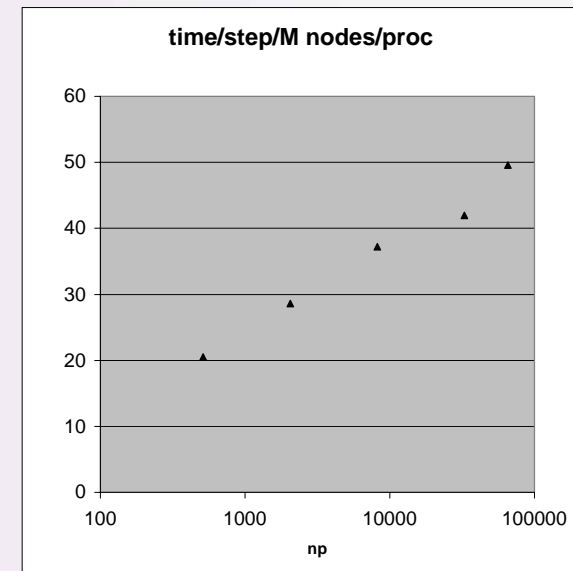
Integrated Simulations based on fully-featured, validated CITS codes

Multicode coupling based on general-purpose API

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



BG/L



Goals of ASC Predictive Science Academic Alliance Program (PSAAP)

- Focus on a multi-scale, multi-disciplinary, unclassified application of NNSA interest
- 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

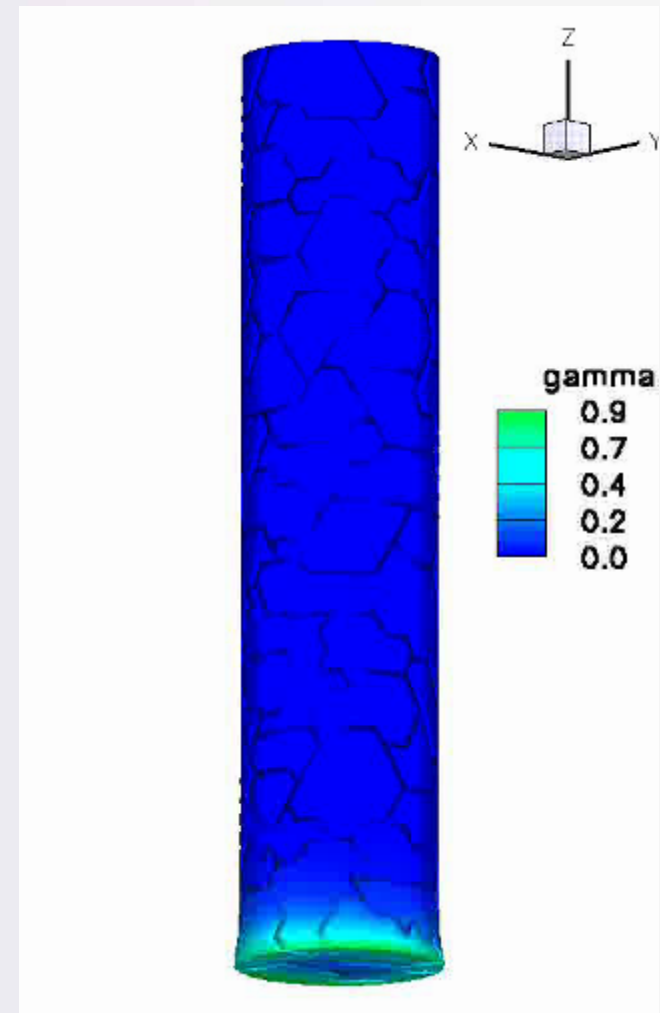
- ASC has the responsibility to develop the tools to address evolving NNSA mission requirements.
- ASC is evolving from a proof-of principle initiative to a program that is providing improved capabilities essential to maintaining technical confidence in the stockpile.
- As ASC's ability to predict weapons 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 through 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