Can Complex Material Behavior be Predicted?

Michael Ortiz

DoE NNSA Stockpile Stewardship Graduate Fellowship Program Meeting

Washington DC, July 14, 2009

ASC/PSAAP Centers

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STANFORD UNIVERSITY PSAAP

CALIFORNIA INSTITUTE OF TECHNOLOGY 1891

PRISM NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PURDUE UNIVERSITY

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MICHIGAN

ICES The Institute for Computational Engineering and Sciences

THE UNIVERSITY OF TEXAS AT AUSTIN

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ASC Program – The early days…

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- In 1993 President Clinton committed the United States to a global ban on underground nuclear testing, and on September 24, 1996, he signed the Comprehensive Test Ban Treaty at the United Nations
- In the absence of underground testing: use modeling and simulation—requiring unprecedented levels of computing power—to certify the safety and reliability of a reduced US nuclear weapons stockpile
- ASCI is DOE's 10-year, $2 billion program, that was formed to develop the high-resolution, three-dimensional physics modeling needed to evaluate the aging nuclear stockpile

ASC Program – The early days…

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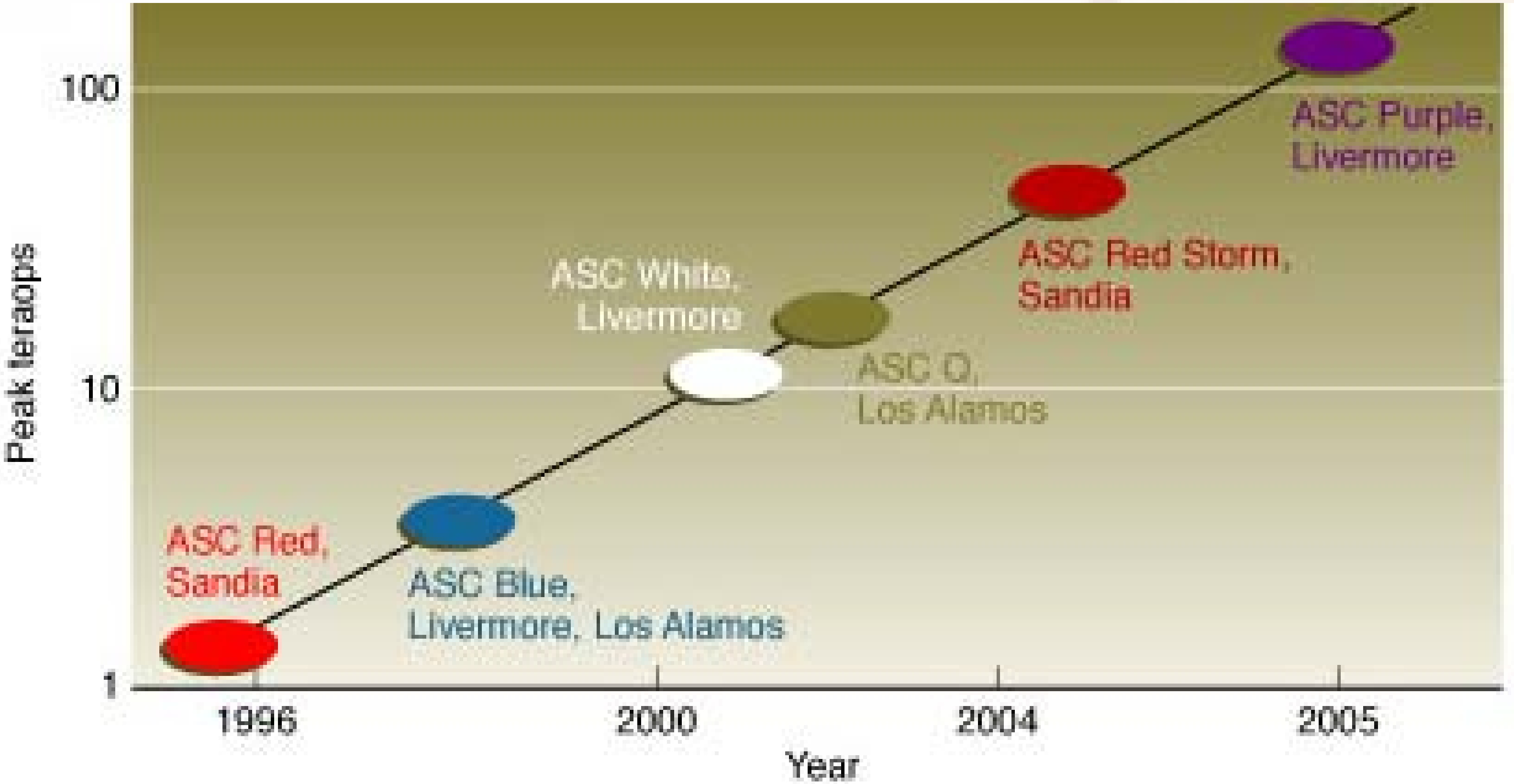

ASCI platform roadmap

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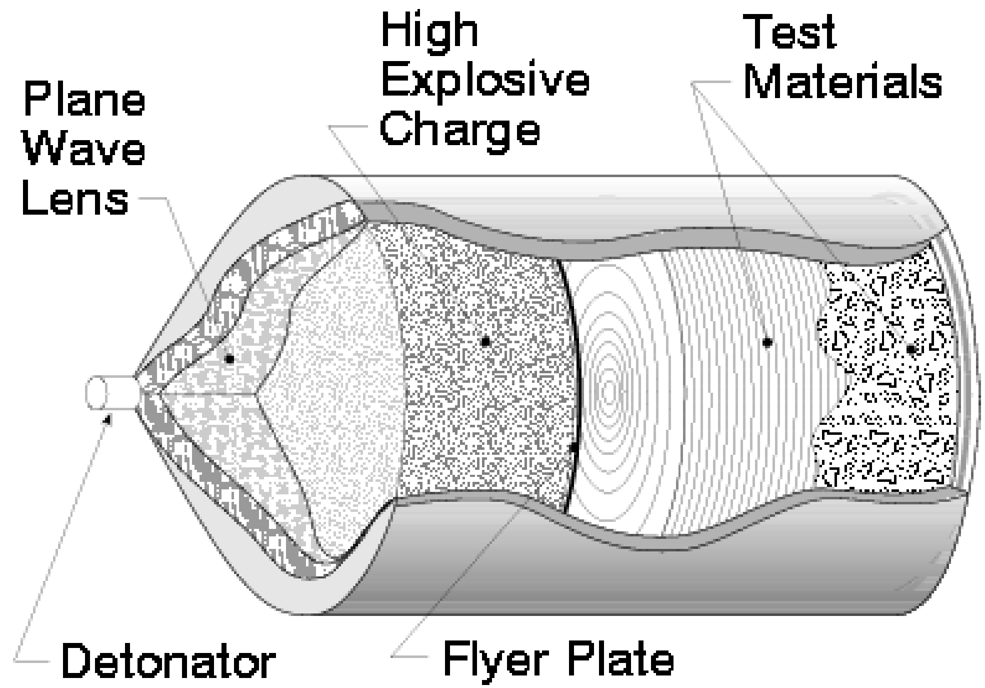
Original aims (1997):

- Develop improved models for dynamic response
  - high explosive detonation
  - material response from first principles
  - compressible mixing
- Explore the role of material imperfections
  - Simulation of 3-D response is essential
- Integrate improved models into present-day algorithms
- Explore effects of three dimensionality
- Implement on ASCI-class computers
- Provide problem solving environment
- Validate against experiment



Caltech's ASCI/ASAP Center's original overarching application

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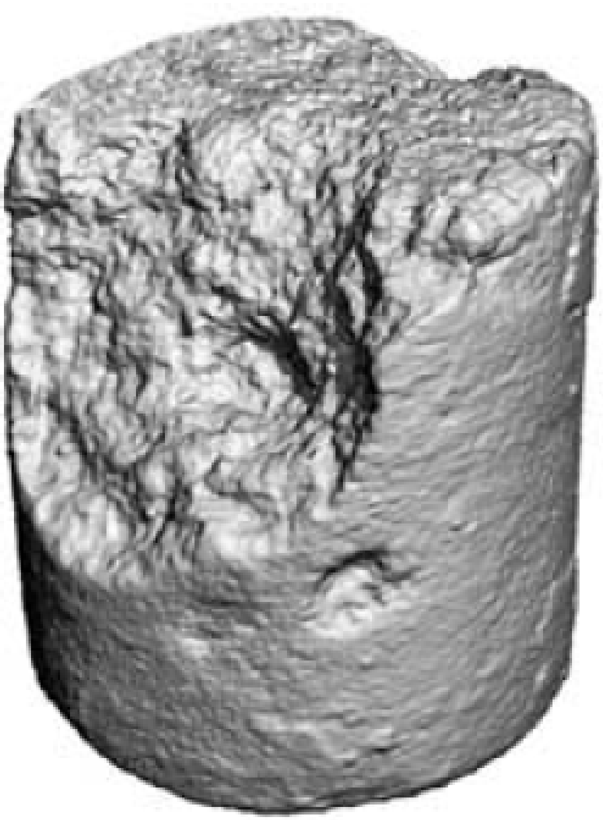
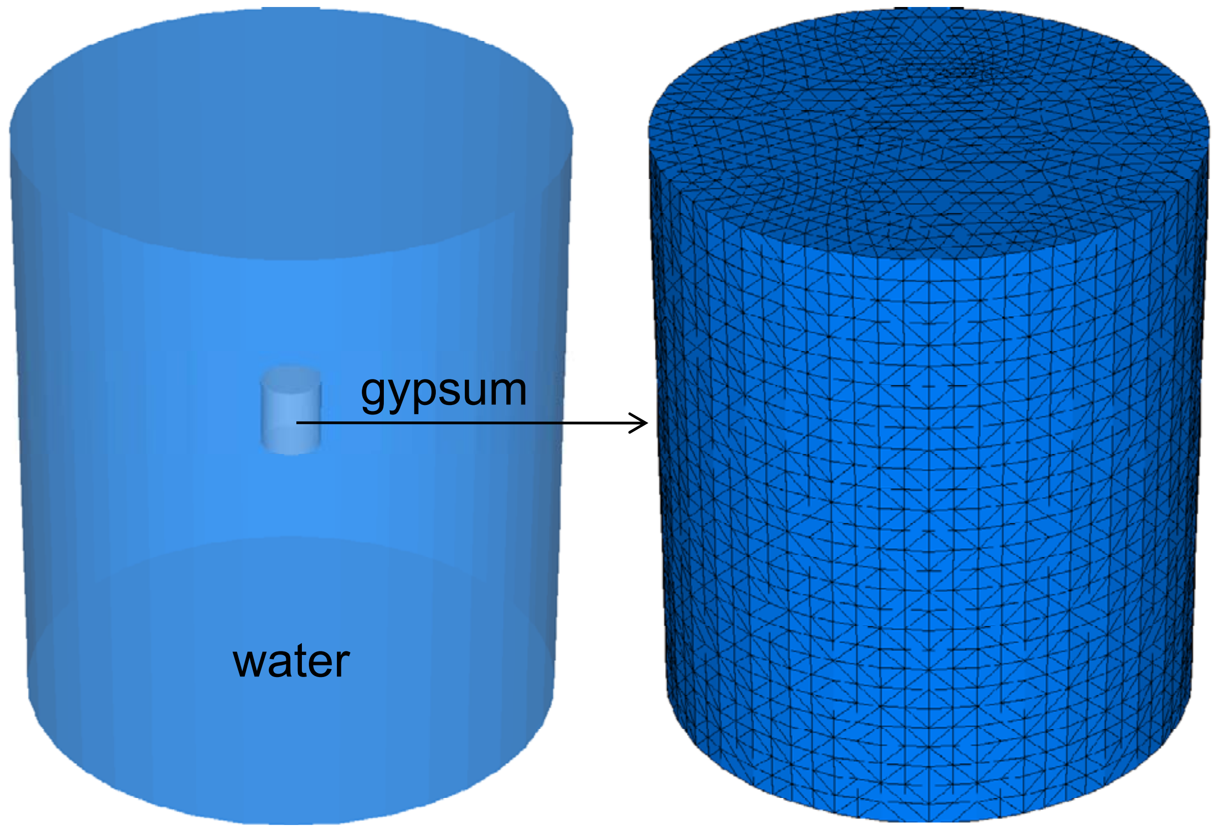


McAteer et al. (2005)



299457 nodes, 223030 element

Gypsum fragmentation experiment

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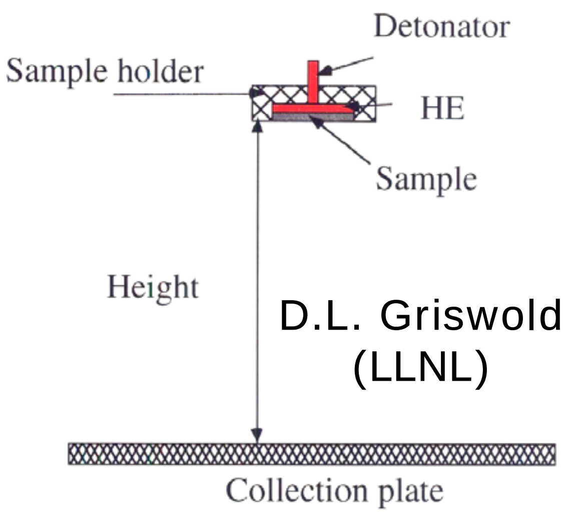
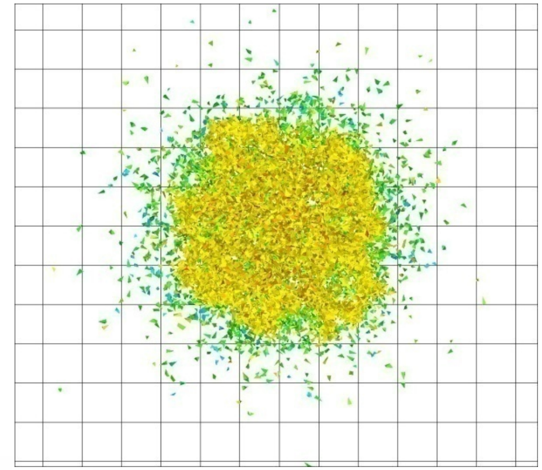


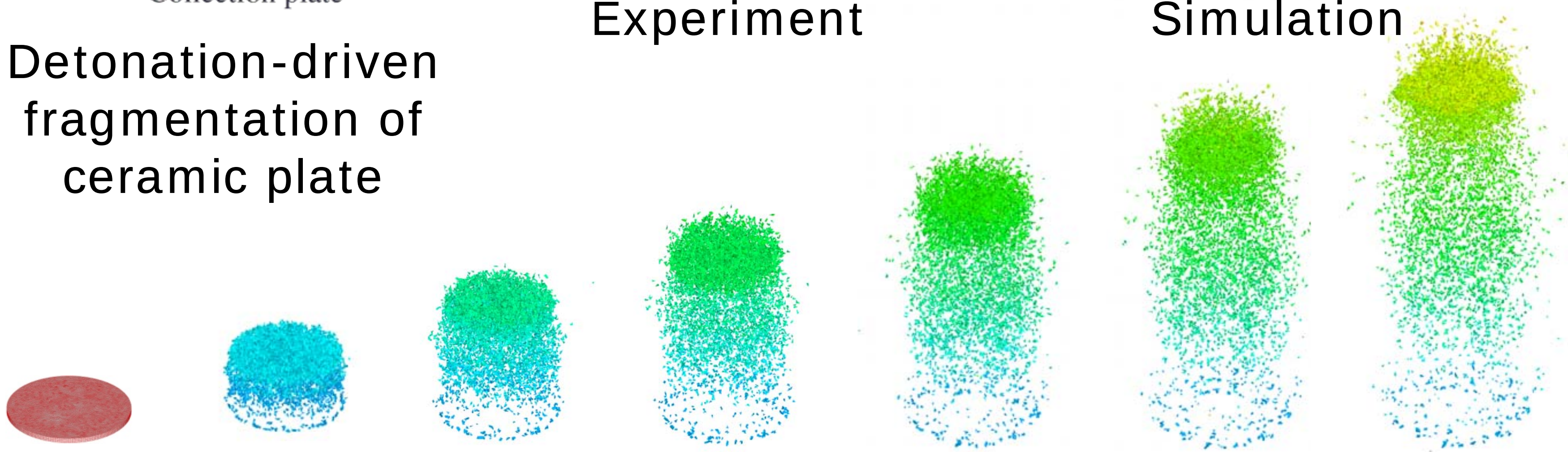
D.L. Griswold (LLNL)

Experiment



Simulation

Detonation-driven fragmentation of ceramic plate



0 μs 100 μs 200 μs 300 μs 400 μs 500 μs 600 μs

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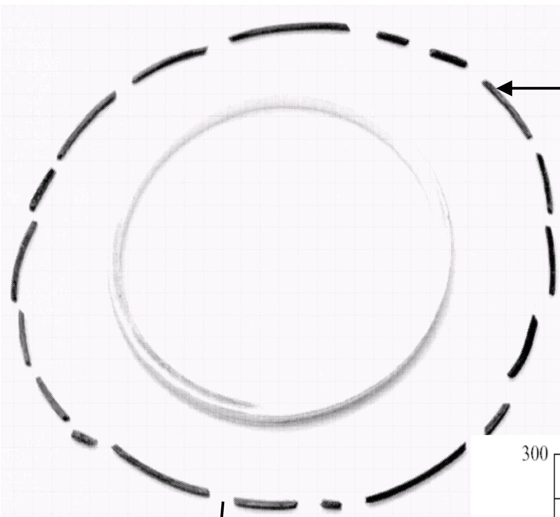
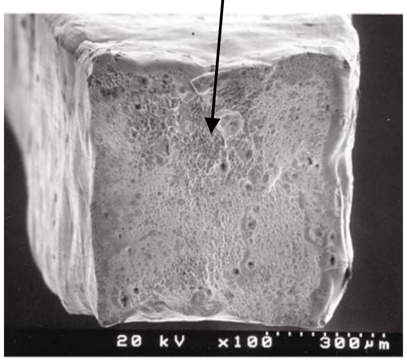
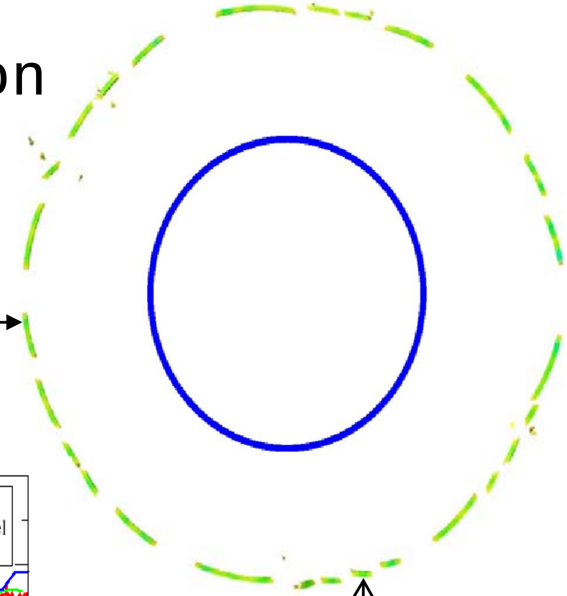


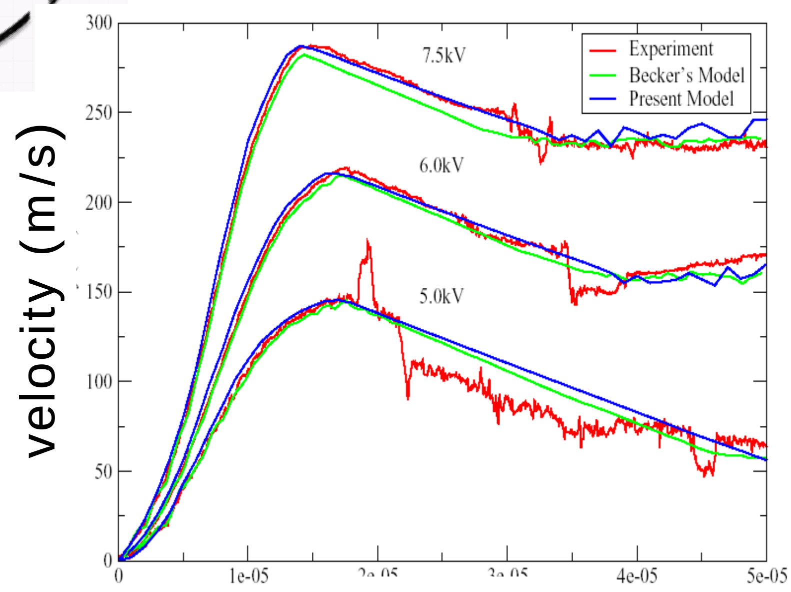
U6Nb ring expansion (Becker LLNL ‘02)

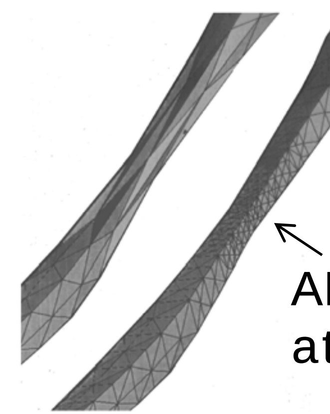


(Rich Becker, LLNL)

FE simulation







AMR at necks

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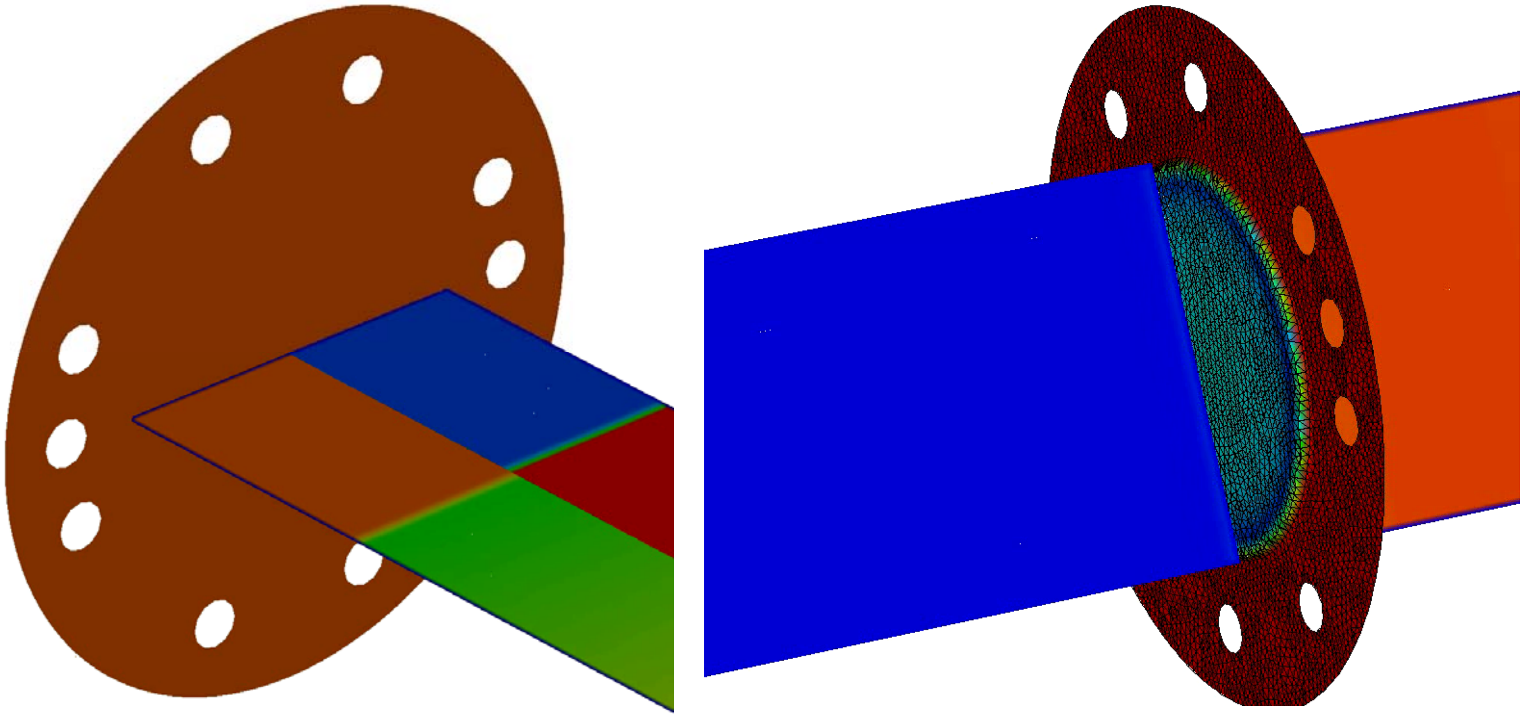
• Multiphysics, software integration: Integrating CFD and Lagrangian solid mechanics...



Water hammer impacting on fracturing shell

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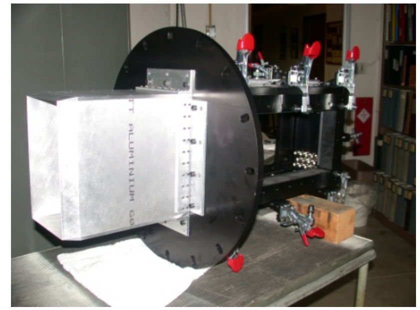
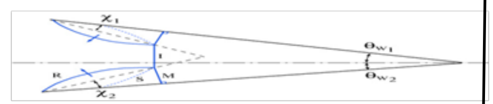
Aims for second five years:

- Establish linkage with Caltech validation efforts
- Establish close linkage with DP validation efforts
- Obtain funding (either within ASCI or externally) for validation efforts tied to simulation milestones
  - Detonation
  - Mixing
  - Dynamic response of materials
  - High pressure EOS and constitutive relations

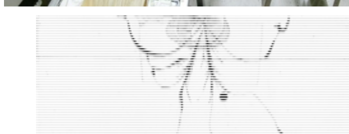




Shock focusing

Detonation-driven fracture

Dynamic deformation



Dynamic fracture

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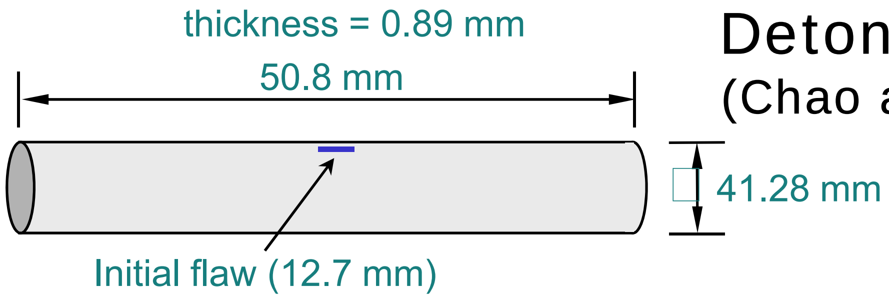
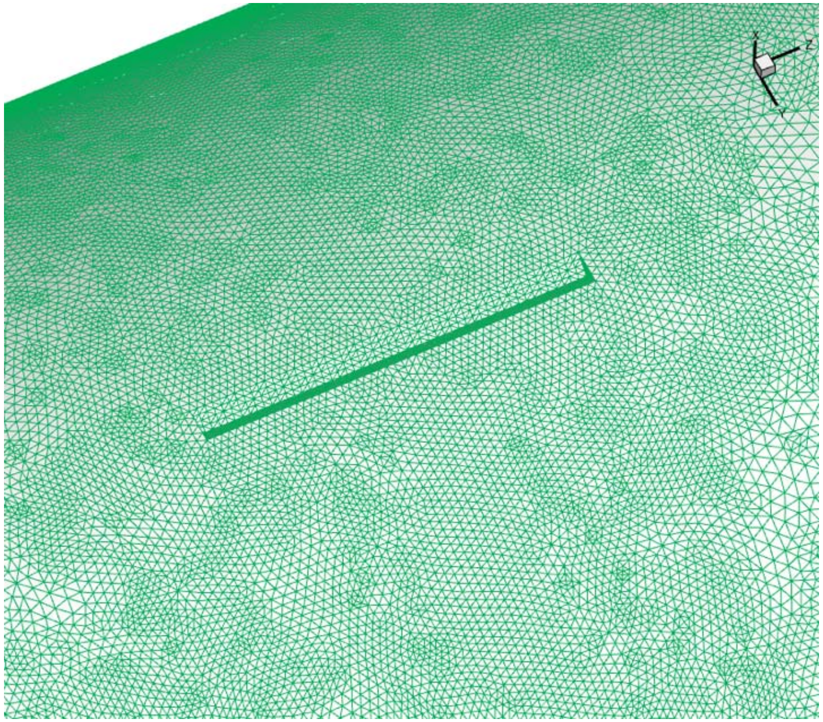
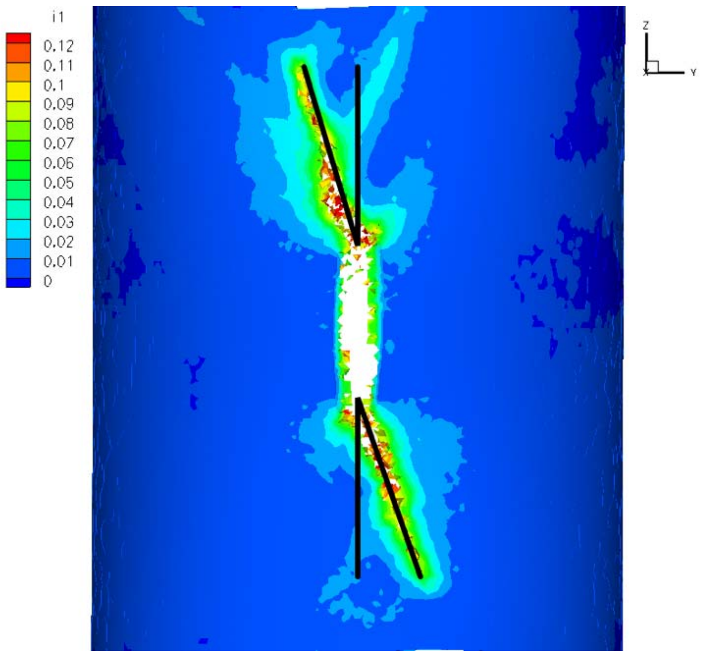




Detonation fracture, Al tubes
(Chao and Shepherd, 2004)



220945 elements, 399998 nodes
LLNL ALC, 400 processors, 8 hours run time

Parallel simulation
Crack kink angle ~ 16 degrees
Peak pressure: 6.1 MPa

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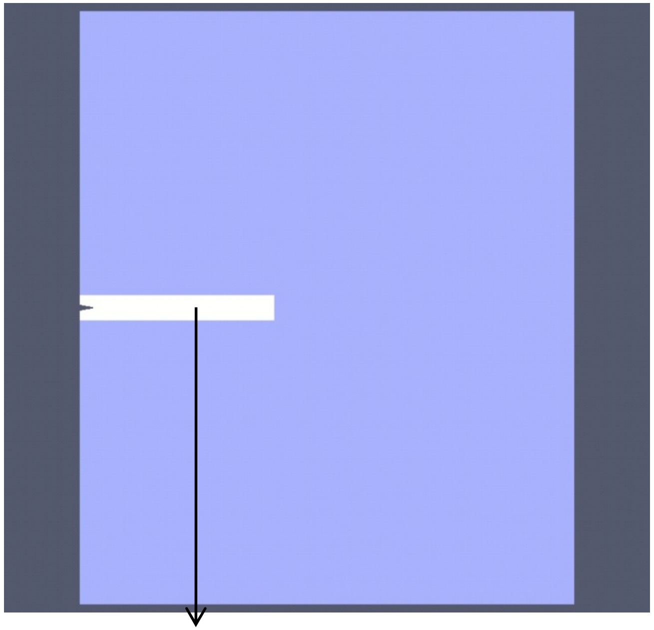

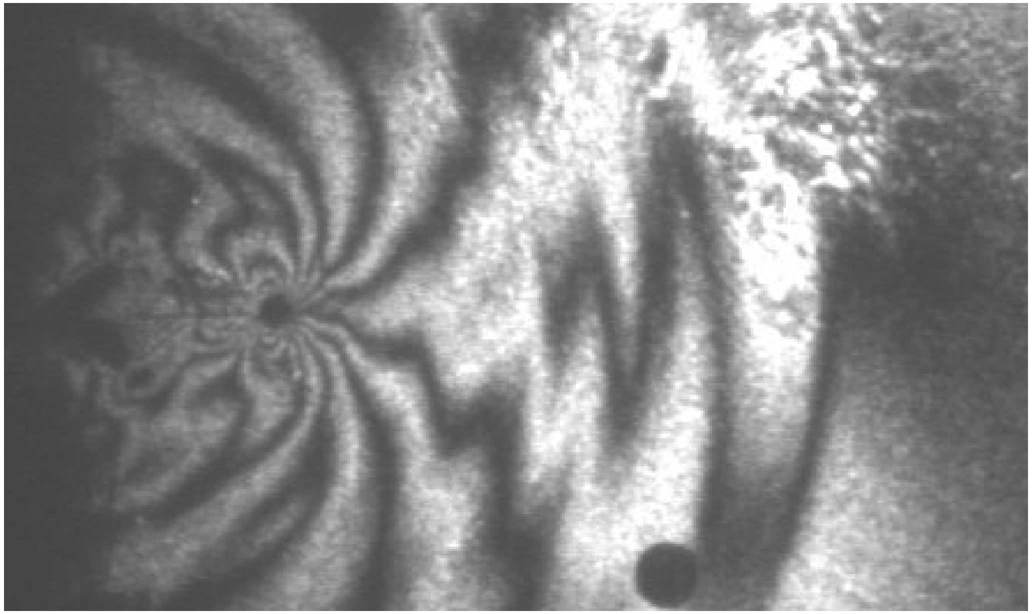

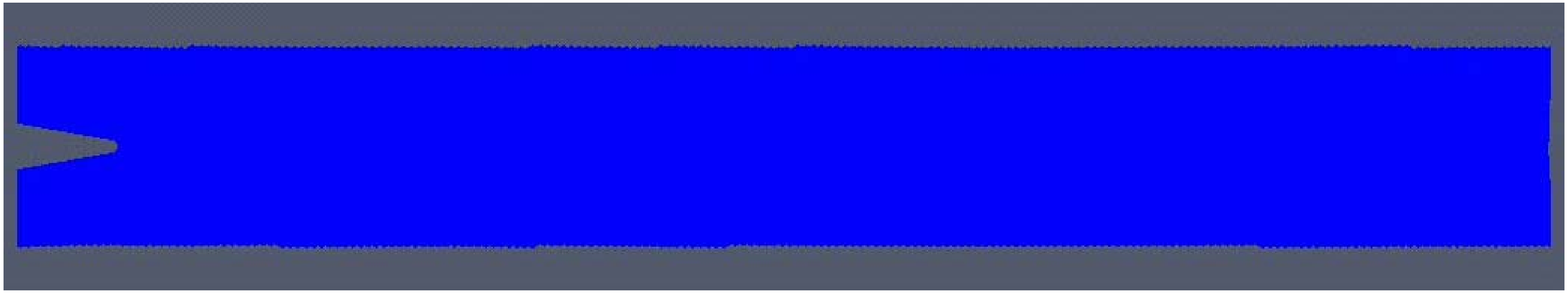

Validation run: ALC, 900 processors, 133 million elements

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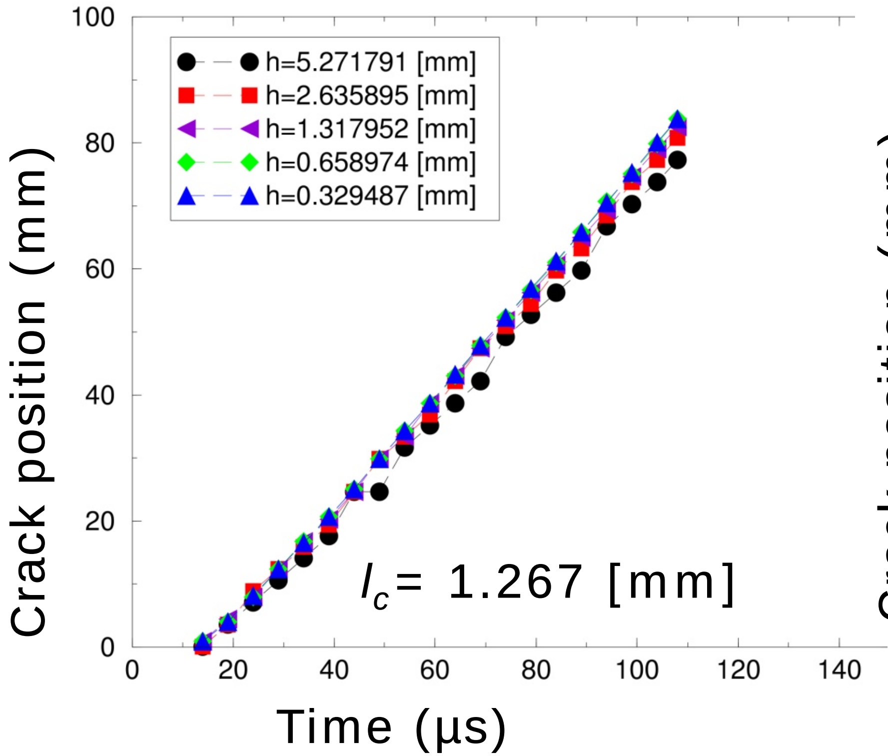
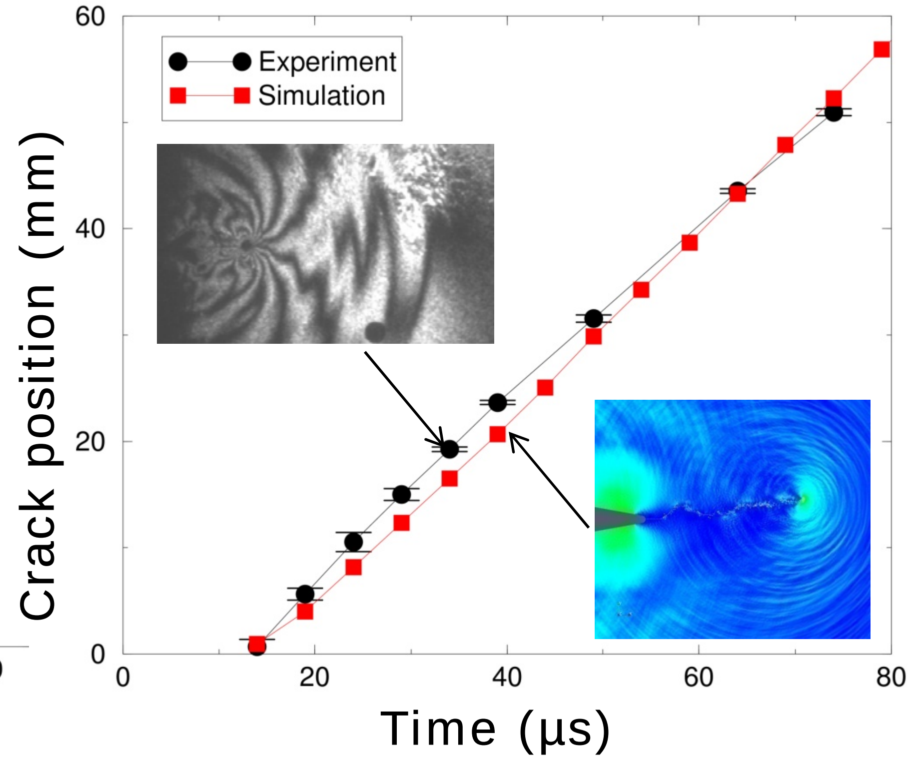


Mesh convergence



Comparison with experiment

Validation run: ALC, 900 processors, 133 million elements

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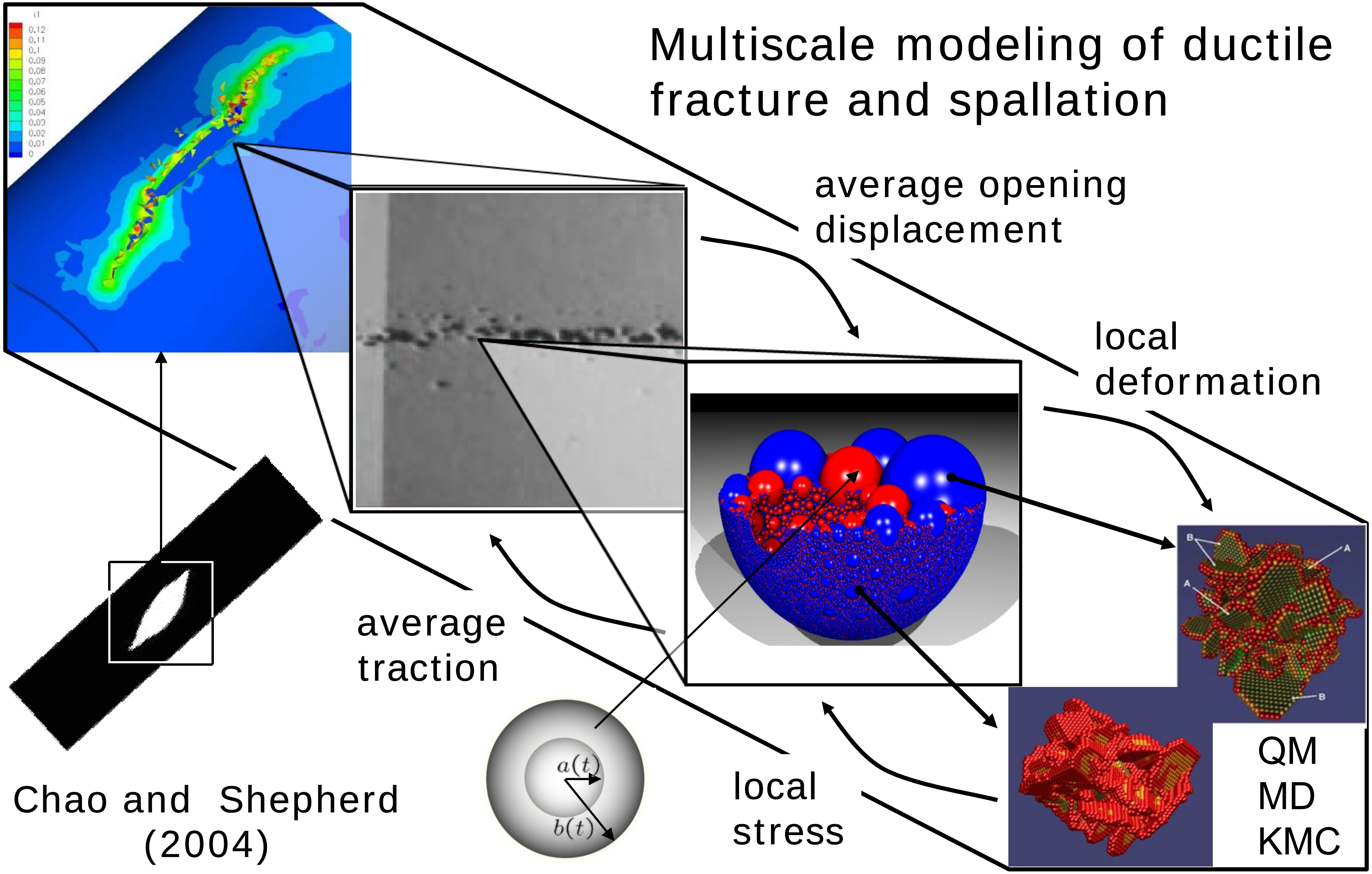
Multiscale modeling of ductile fracture and spallation



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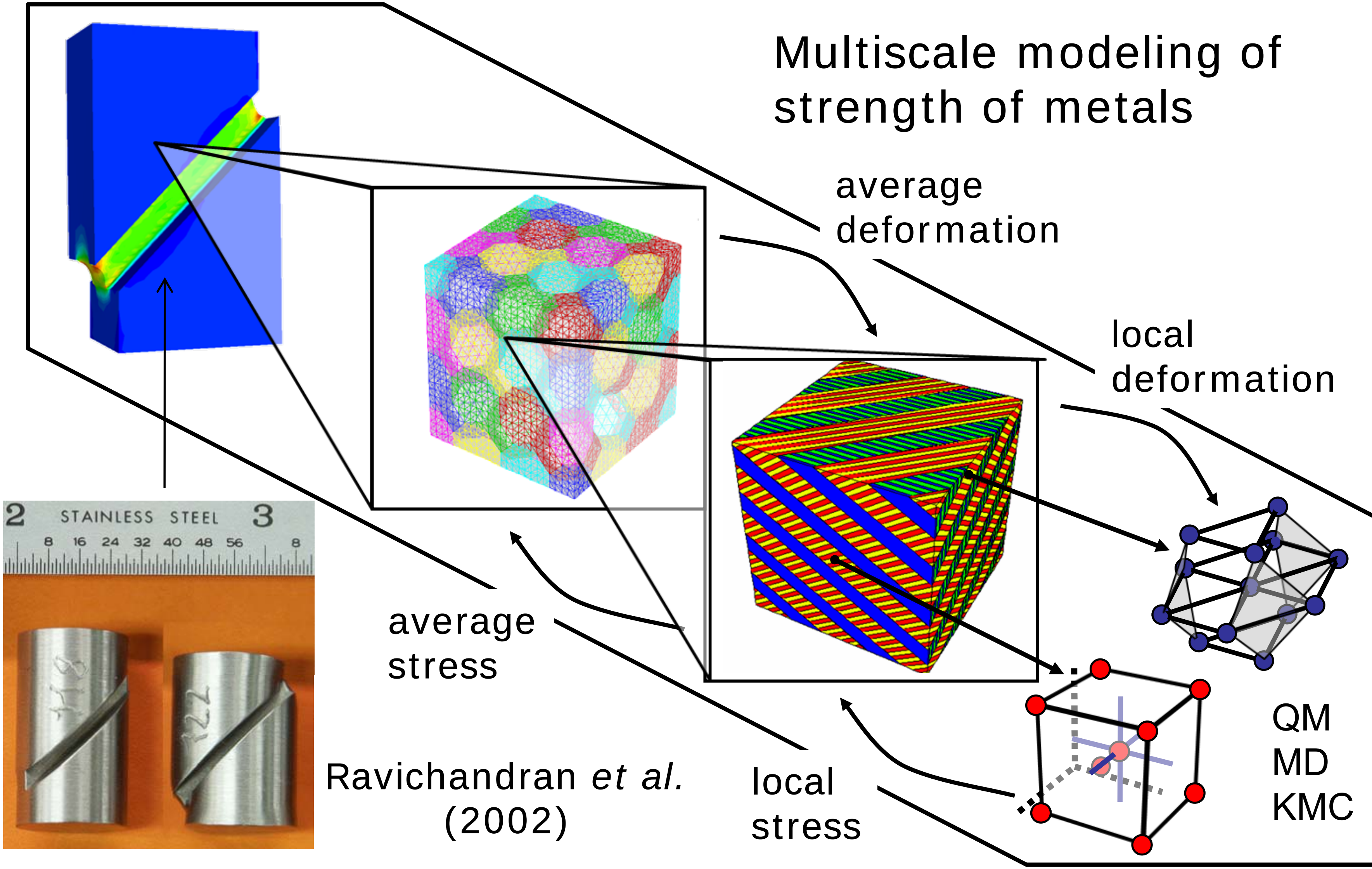

The ASAP→PSAAP phase transition

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Caltech's ASC/ASAP accomplishments:

- Software integration (Lagrangian/Eulerian)
- Algorithmic development
- Efficiency and scalability in complex simulations
- Rigorous multiscale material models under 'normal' conditions
- 'Conventional' V&V

Caltech's ASC/ASAP unfinished business:

- Real objective: rigorous certification of complex systems operating under extreme conditions
- 'Conventional' V&V falls short in important ways:
  - What experiments?
  - What metrics?
  - What is enough?
  - How to guarantee performance?

Caltech's ASC/PSAAP Center

- Overarching objectives:
  - Develop a multidisciplinary Predictive Science methodology focusing on *high-energy-density dynamic response of materials*
  - Demonstrate Predictive Science by means of a concerted and highly integrated experimental, computational, and analytical effort that focuses on an overarching ASC-class problem: *Hypervelocity normal and oblique impact at velocities up to 10 km/s*
- Overarching approach: A *rigorous and novel QMU methodology* will drive and closely coordinate the experimental, computational, modeling, software development, verification and validation efforts within a *Yearly Assessment* format

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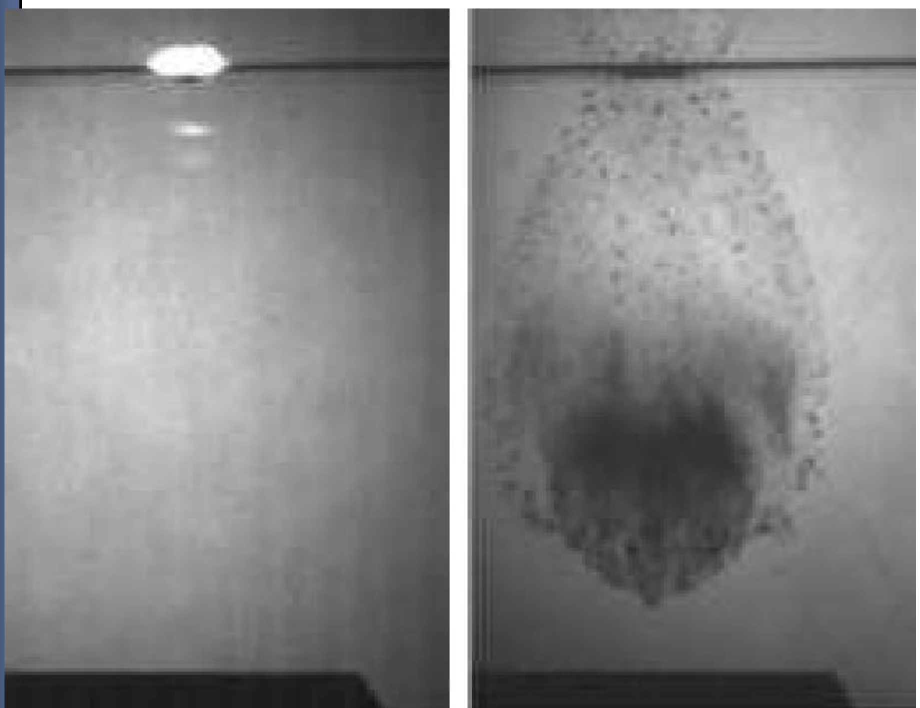
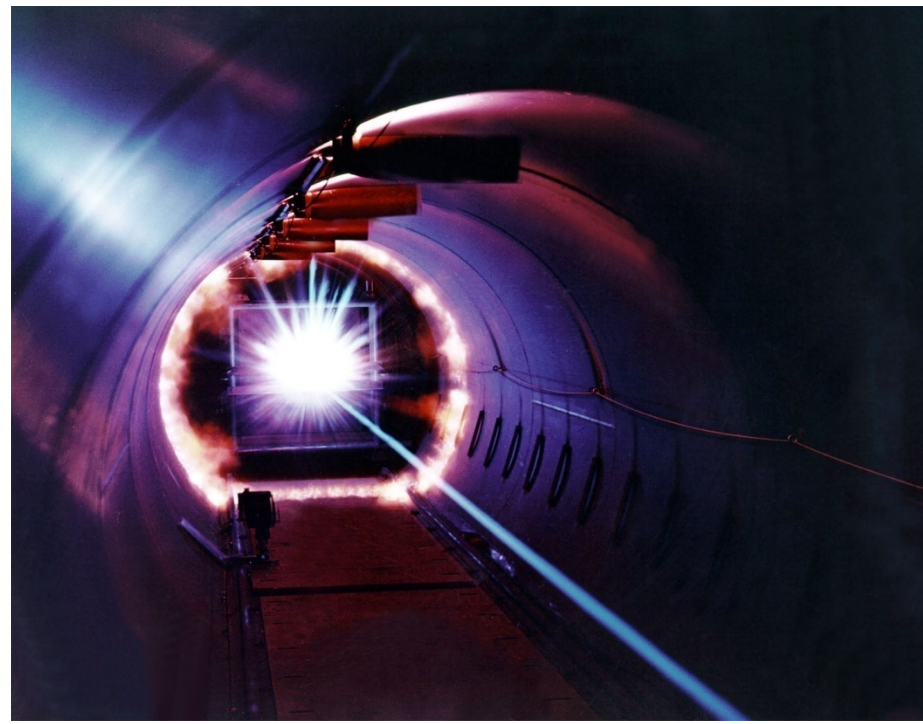
- Hypervelocity normal and oblique impact of projectiles/targets at impact velocities of up to 10 km/s



Hypervelocity impact of bumper shield.
a) Initial impact flash. b) Debris cloud
(Ernst-Mach Institut, Freiburg Germany).



NASA Ames Research Center
Energy flash from hypervelocity test
at 7.9 Km/s

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- Grand-challenge problem in Predictive Science, well-matched to the direct interests of the NNSA mission:
  - Pressures in Mbar range (160-800 GPa)
  - Strain-rates up to $10^{11}s^{-1}$
  - High temperatures (4,000-36,0000 K)

  } states of matter 'of interest'

- Physics that challenge modeling and simulation:
  - melting and vaporization, dissociation, ionization, plasma
  - luminescence and radiative transport
  - hydrodynamic instabilities, mixed-phase flows, mixing
  - solid-solid phase transitions, high-strain-rate deformation, thermo-mechanical coupling
  - fracture, fragmentation, spall and ejecta, deformation instabilities such as shear banding

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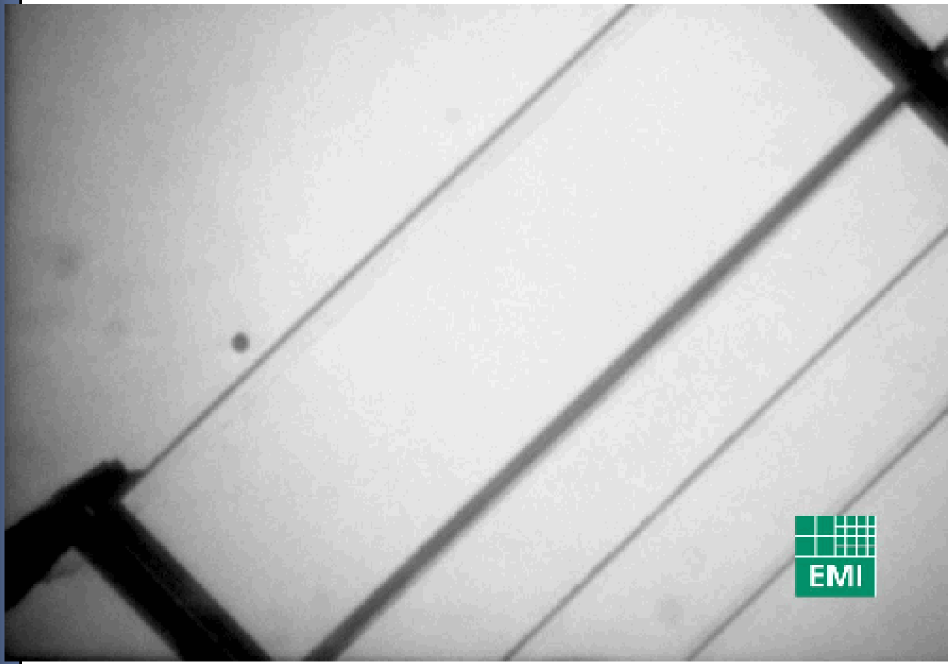
- Hypervelocity impact is of interest to a broad scientific community: Micrometeorite shields, geological impact cratering…



Hypervelocity impact test of multi-layer micrometeorite shield

The International Space Station uses 200 different types of shield to protect it from impacts

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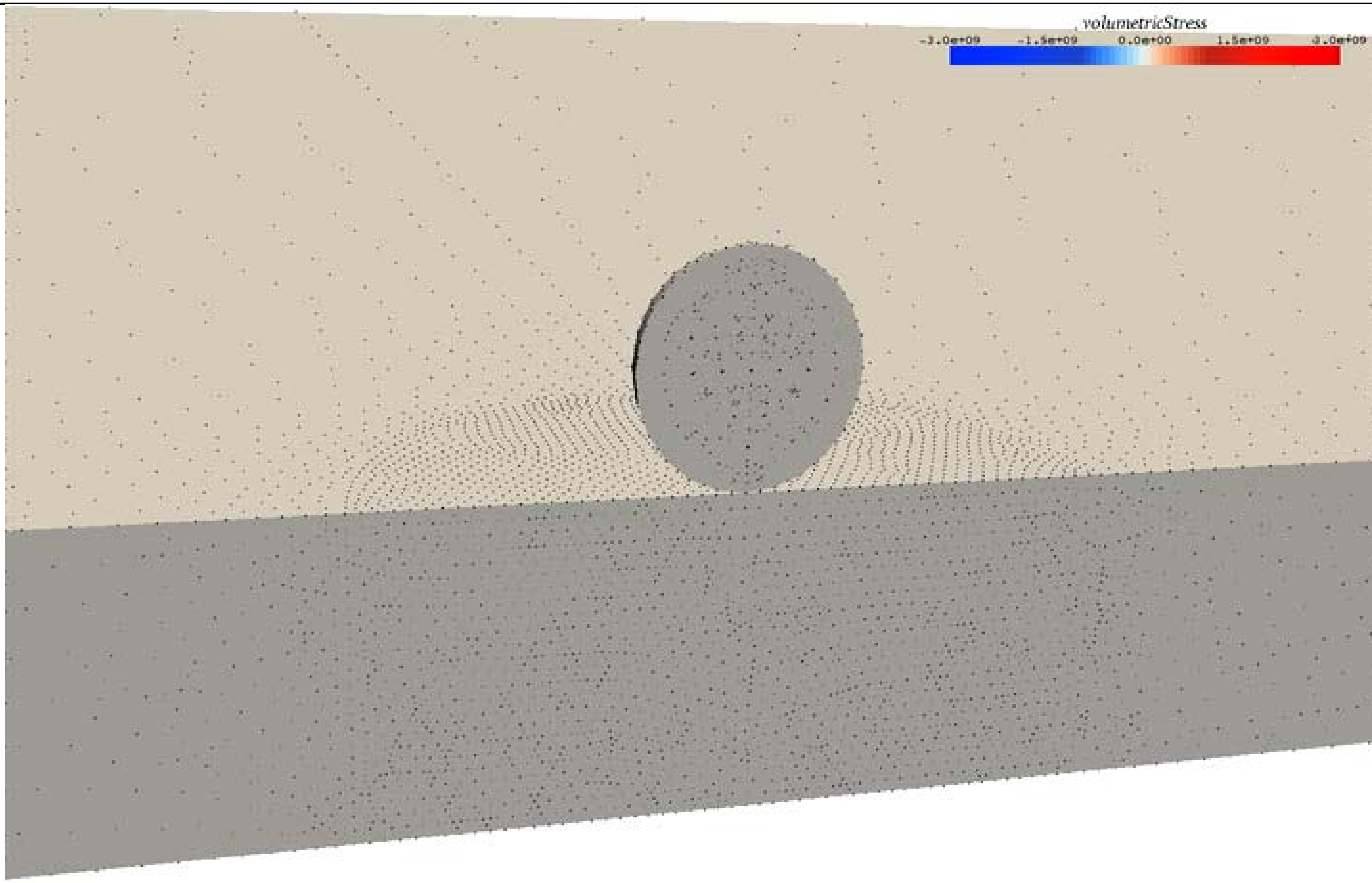

Finite-element model (VTF) of steel-steel ballistic test

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- ***Fundamental question***: How can we use physics models AND experiments to certify the performance of a complex system?
- ***Our strategy***: Formulate, evaluate, rigorous ***upper bounds on the probability of failure*** of the system $\rightarrow$ Rigorous Certification!
- From probability theory: An upper bound on the probability of failure of a system can be obtained from ***two measures***:
  - ***The model diameter***: Measures the variability of the system (e.g., due to random inputs)
  - ***The model-experiment distance***: Measures the discrepancy between model predictions and test data.

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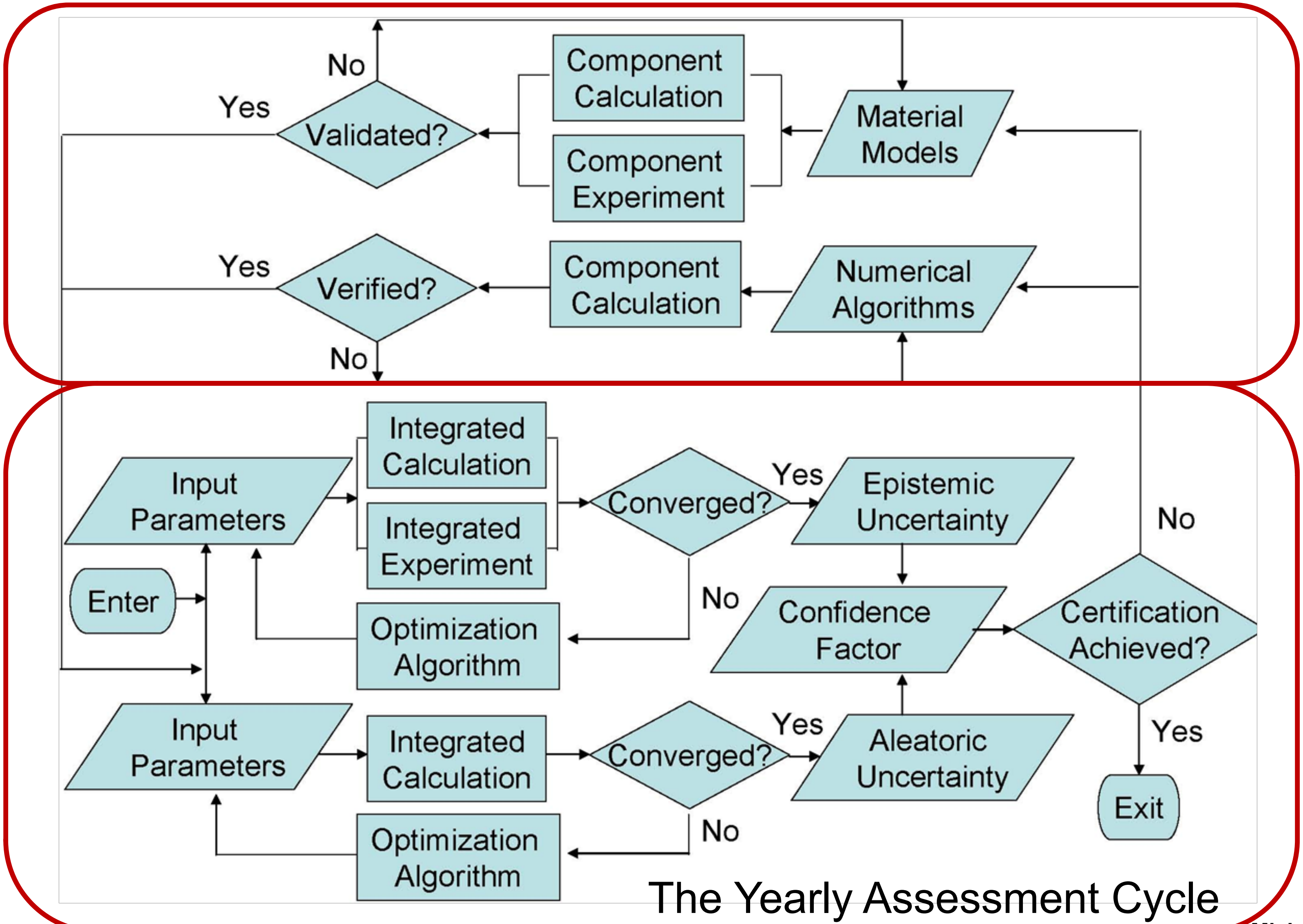

The Yearly Assessment Cycle

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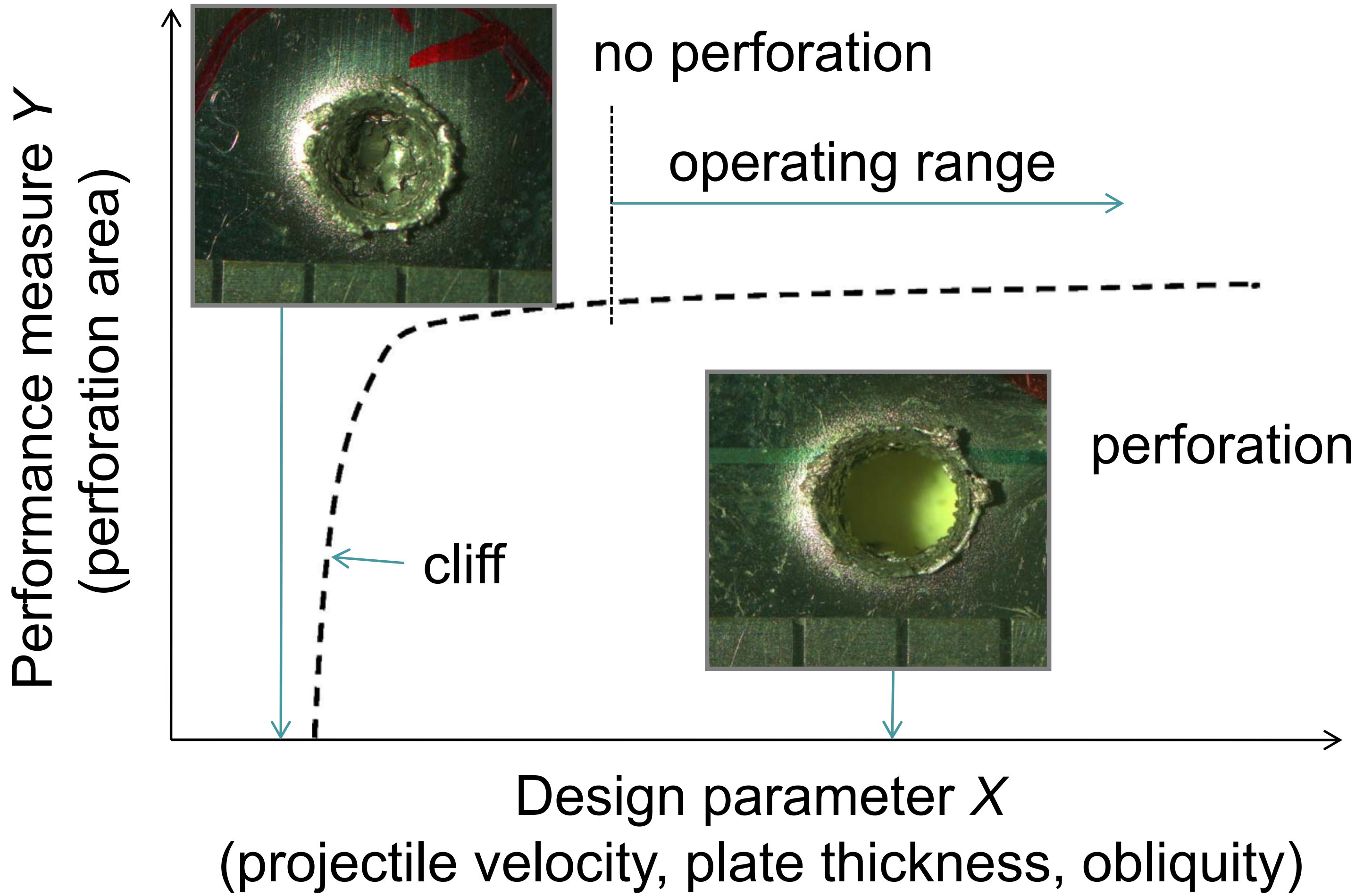

Y1 UQ analysis scope

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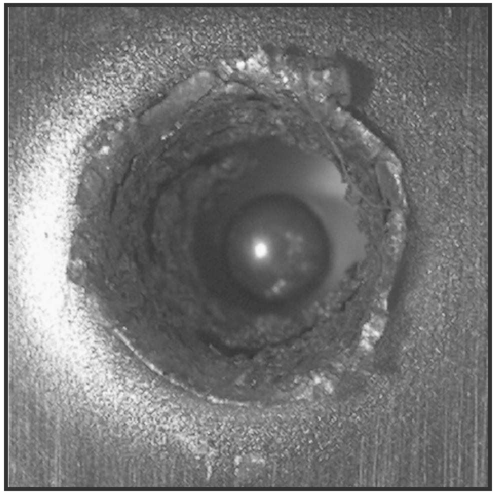
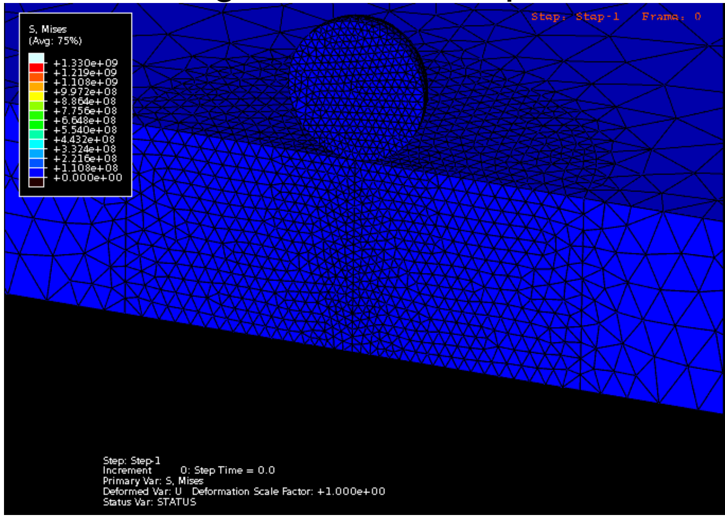
- Completed our first full year assessment (full UQ run!)
- Target/projectile materials:
  - Target: 304 Stainless Steel
  - Projectile: 440 C Steel Spheres
- Performance measure (output): Perforation area
- Model parameters (inputs): Plate thickness, obliquity, impact velocity, yield stress, time step, mesh size.
- ABAQUS model



Steel-on-steel, 2.6 km/s damage zone and impactor



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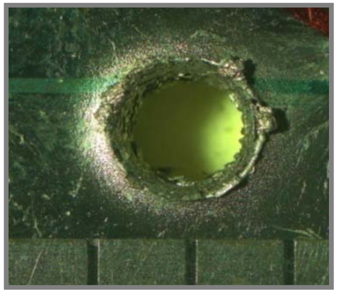

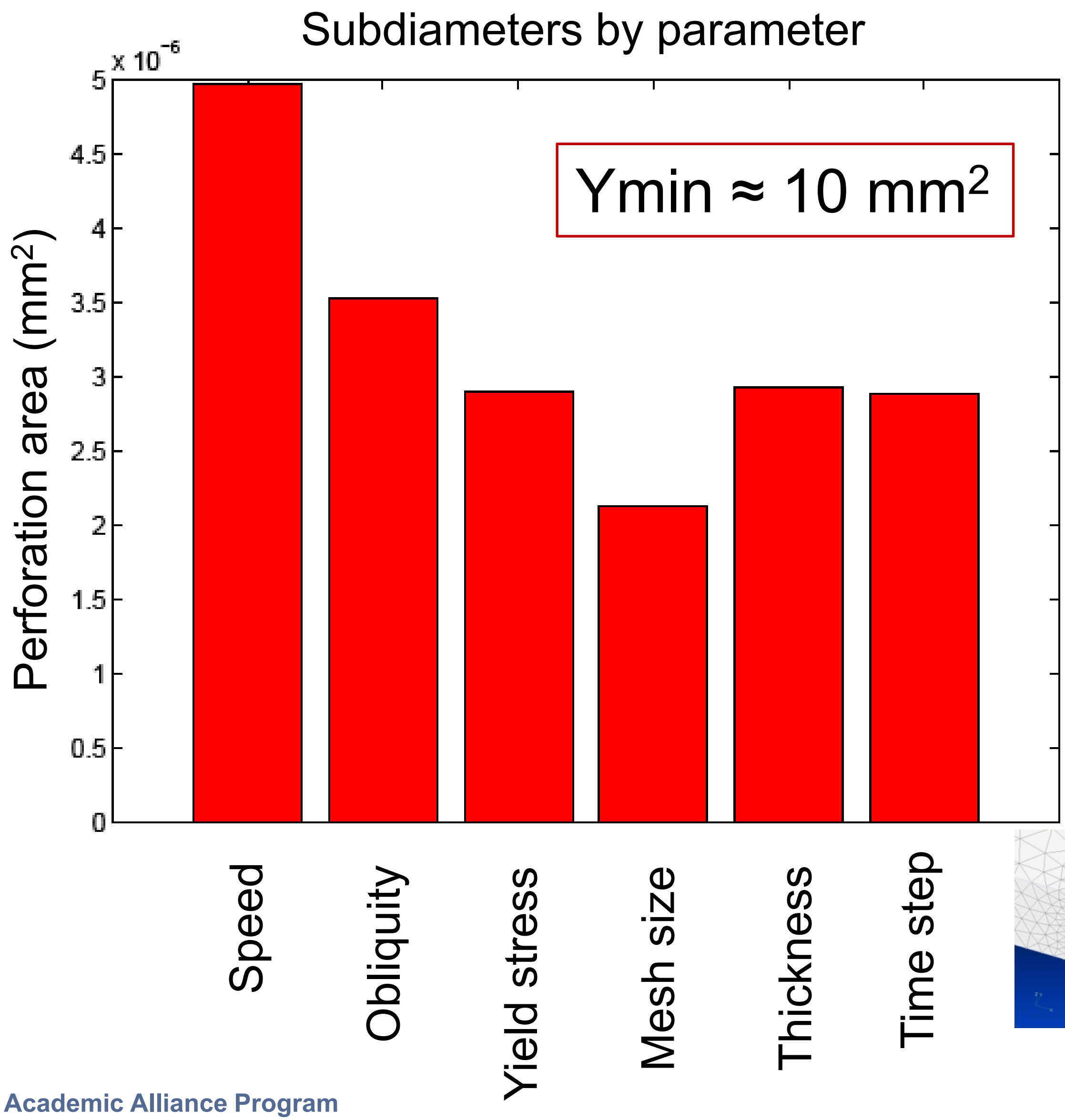

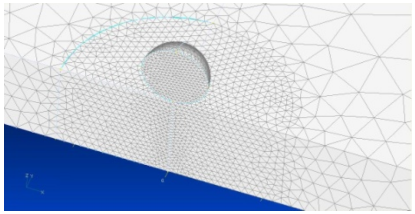

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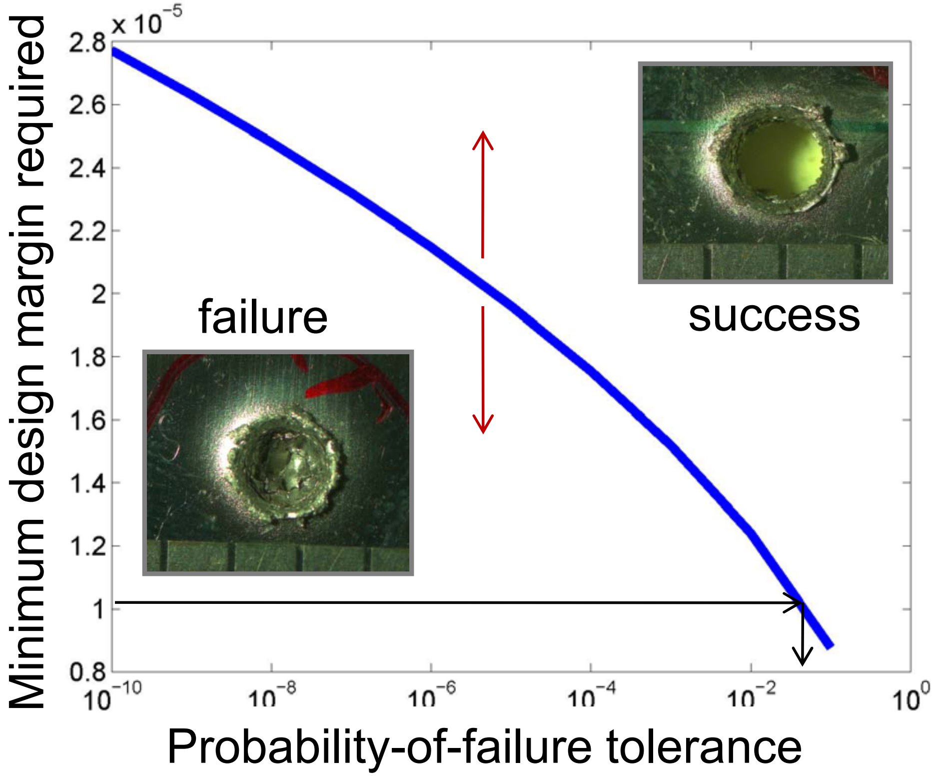
- Quantified uncertainties are too high near the cliff!
- Models not yet sufficiently predictive!
- Need improvements in:
  - Material models: Multiphase EoS, strength, energy balance, transport properties…
  - Algorithms: Erosion, fragmentation, dynamics, multiphysics
  - UQ pipeline: Spatial resolution, NNSA lab platforms…



Design margin requirements resulting from Y1 UQ analysis for impact velocities near ballistic limit of target plate

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Computational Fluid Dynamics

Computational Science and Engineering

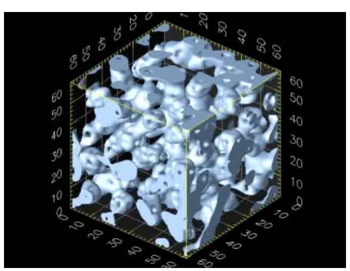
Experimental Science

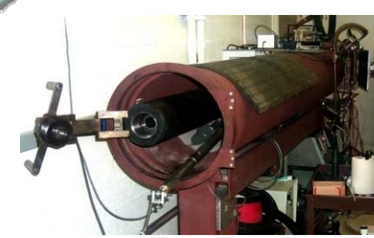
Computational Solid Dynamics

Materials Models and Properties

Uncertainty Quantification

Predictive Science





Student co-mentoring program

MS 200 Sec: 13 - Advanced Work in Materials Science **FA 2006-07**

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Hansen
Benjamin Lee
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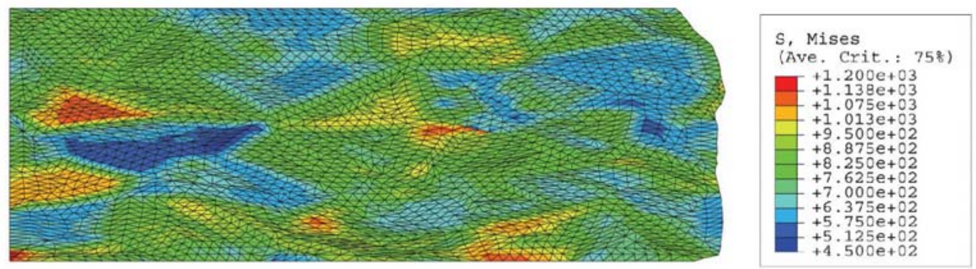

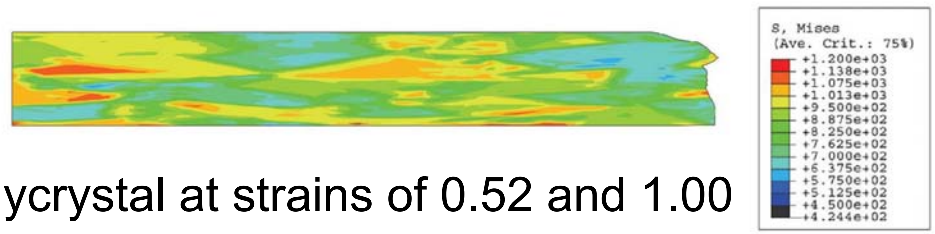

Ta polycrystal at strains of 0.52 and 1.00

CONDENSED MATTER, MATERIALS SCIENCE, and CHEMISTRY

Local Deformation Behavior of Metallic Polycrystals

Curt A. Bronkhorst and B. L. Hansen, T-3

Los Alamos NATIONAL LABORATORY EST. 1943

A U.S. Department of Energy Laboratory

Theoretical Division Nuclear Weapons Program Highlights 2005-2006

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Summer practica at NNSA labs

AE 200 Sec: 09 - Advanced Research in Aeronautics Summer 2008
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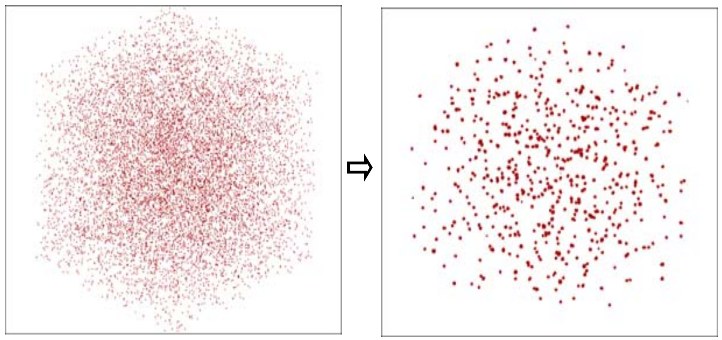
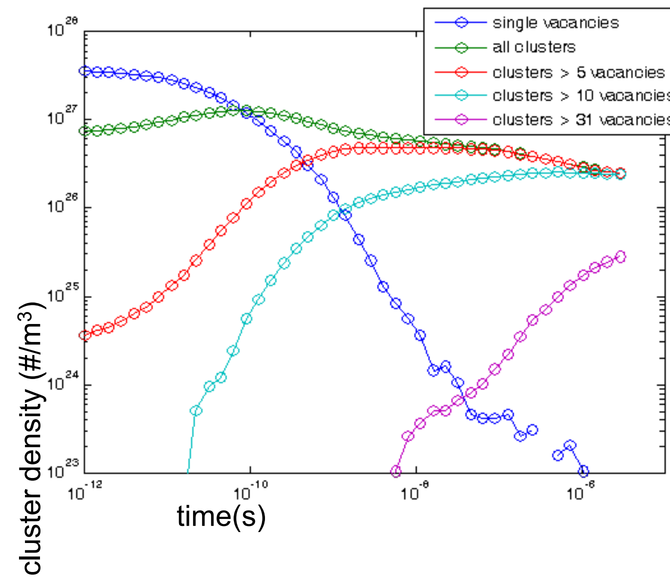


Evolution of cluster density in Al



Jaime Marian – Chemistry, Materials and Life Sciences Directorate

Lawrence Livermore National Laboratory

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Some of our graduates...

Marisol Koslowski
Assistant Professor of
Mechanical Engineering
Purdue University

Raul Radovitzky
Associate Professor of
Aeronautics & Astronautics
MIT

Adrian Lew
Assistant Professor of
Mechanical Engineering
Stanford

- Our alumni are our most enduring legacy…

ASC – Towards exascale computing

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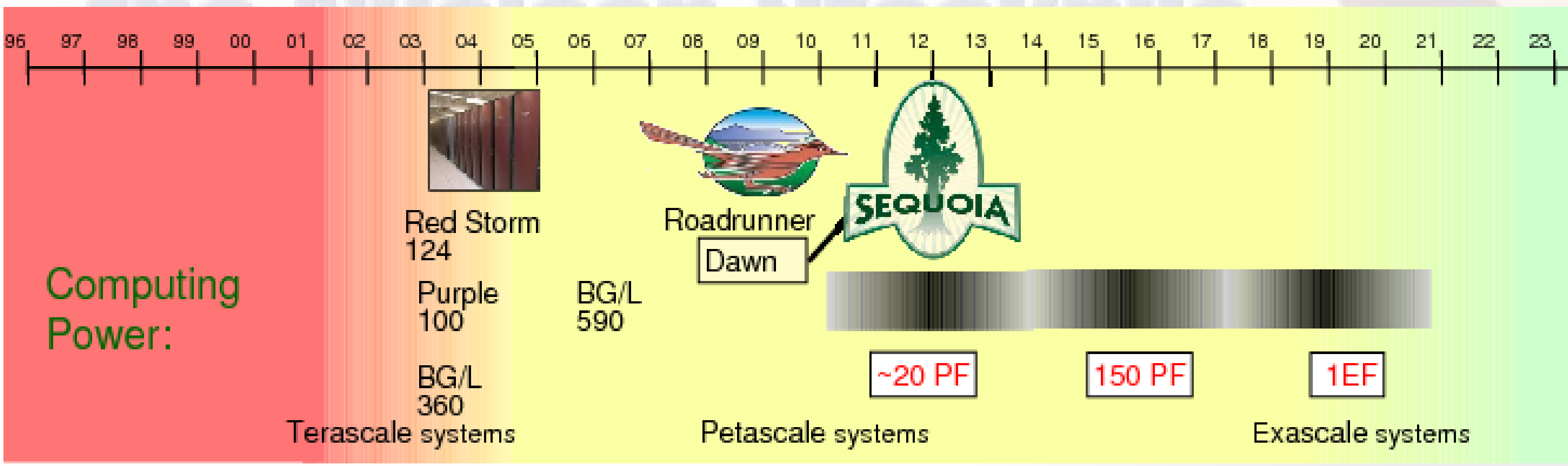
Purple – 0.1PF/s

BlueGene/L – 0.4



Our vision for predictive science…

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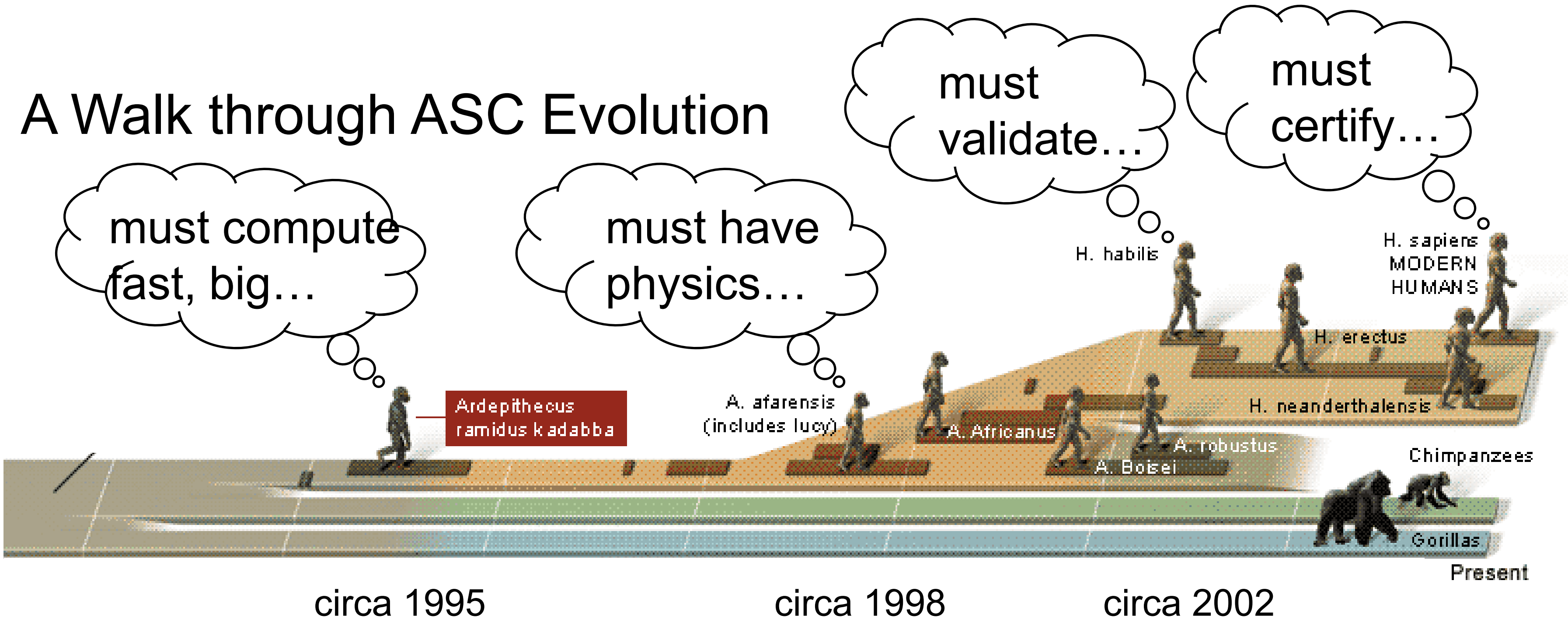
A Walk through ASC Evolution



- QMU is the next logical step in the evolution of ASC
- Articulating QMU in precise, rigorous and quantitative terms is a grand challenge of our time!

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Thank you!

Michael Ortiz