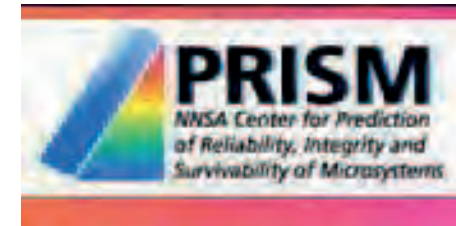# Can Complex Material Behavior be Predicted?

Michael Ortiz

DoE NNSA Stockpile Stewardship Graduate Fellowship Program Meeting

Washington DC, July 14, 2009

ASC/PSAAP Centers

STANFORD UNIVERSITY

PSAAP

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

CALIFORNIA INSTITUTE OF TECHNOLOGY 1891

CALTECH
PSAAP

PURDUE UNIVERSITY

ICES
The Institute for Computational Engineering and Sciences

MICHIGAN

CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS

THE UNIVERSITY OF TEXAS AT AUSTIN

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PSAAP: Predictive Science Academic Alliance Program

ASC Program – The early days…

- 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…

ASCI platform roadmap

Caltech ASC/ASAP Center (97-07)
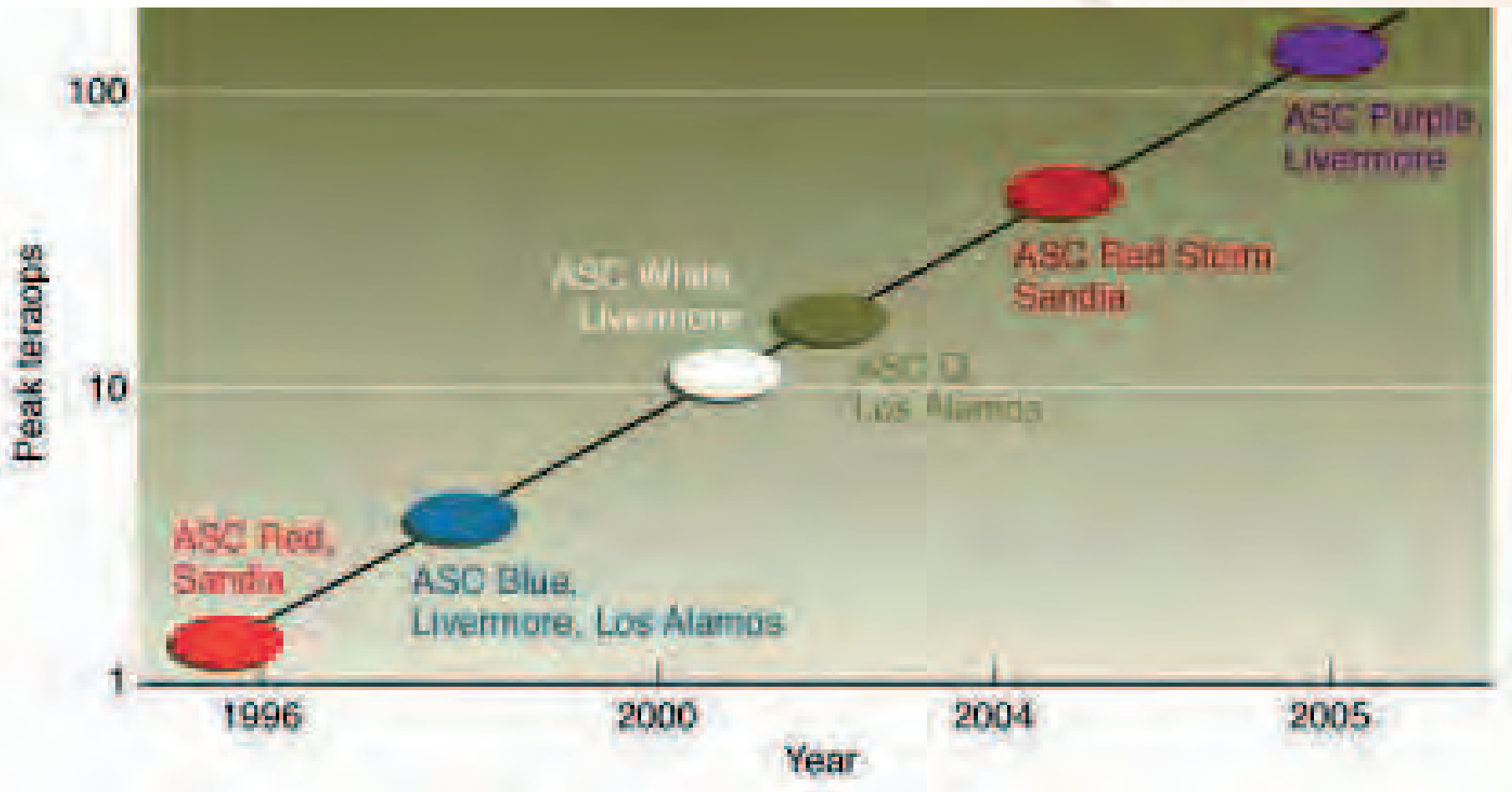
Original aims (1997):

- 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
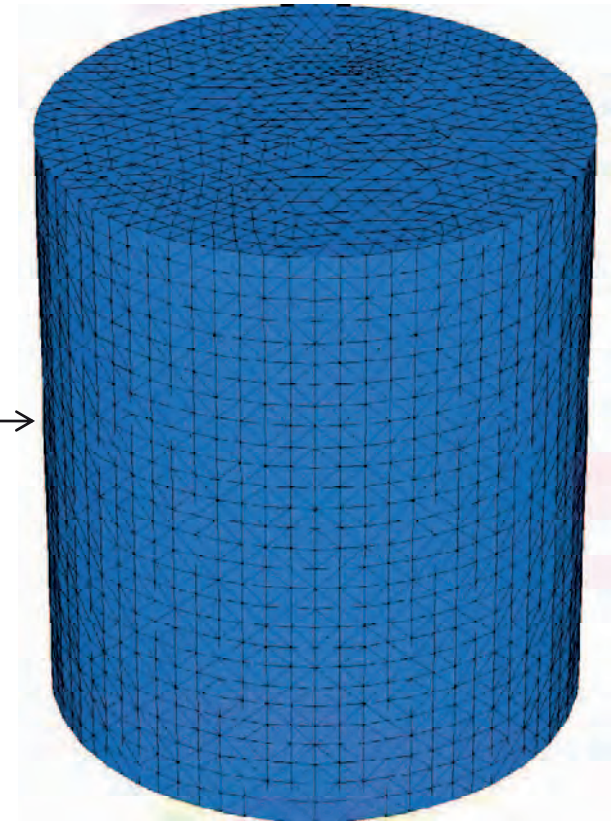- Provide problem solving environment
- Validate against experiment
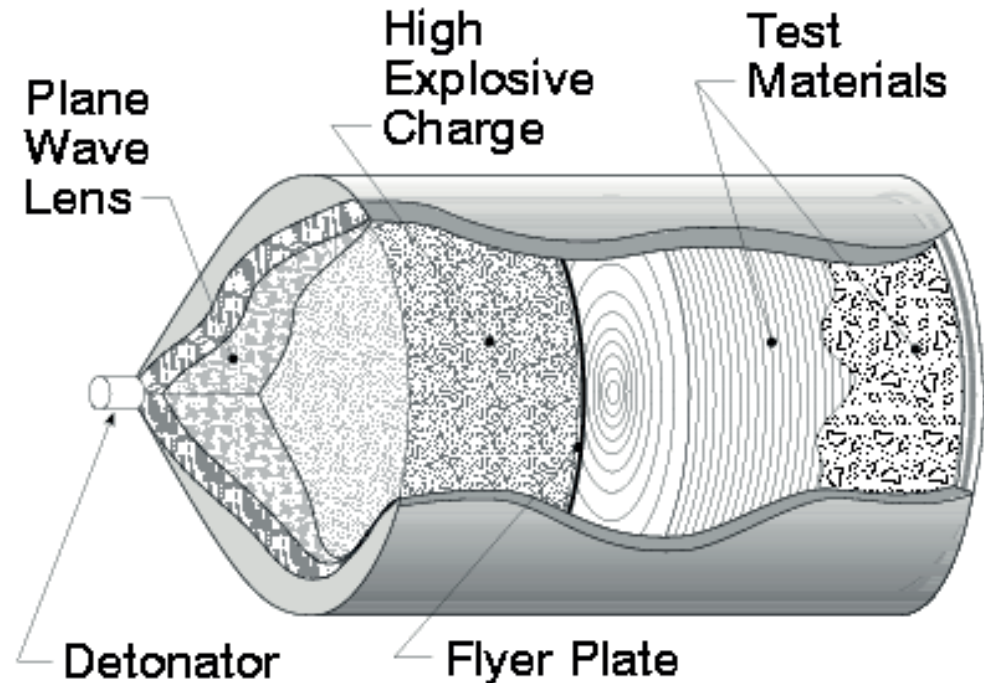
Caltech's ASCI/ASAP Center's original overarching application
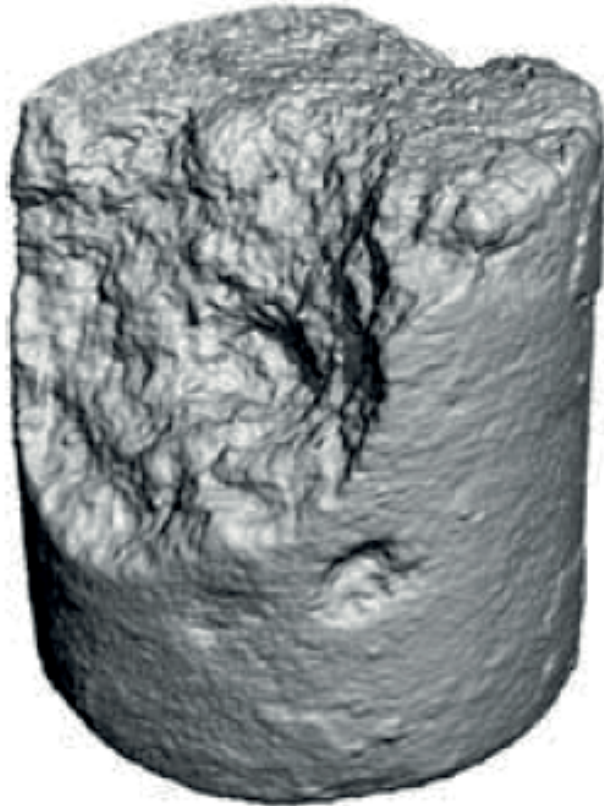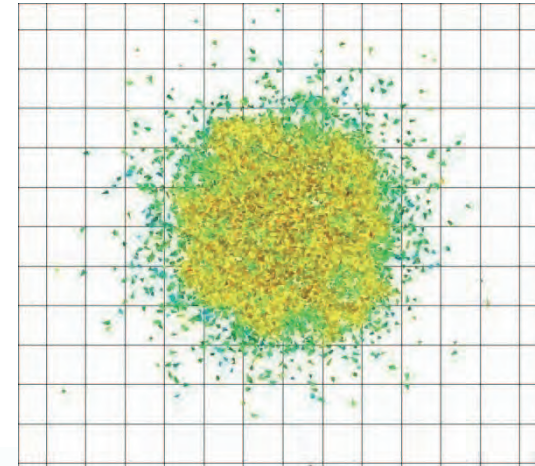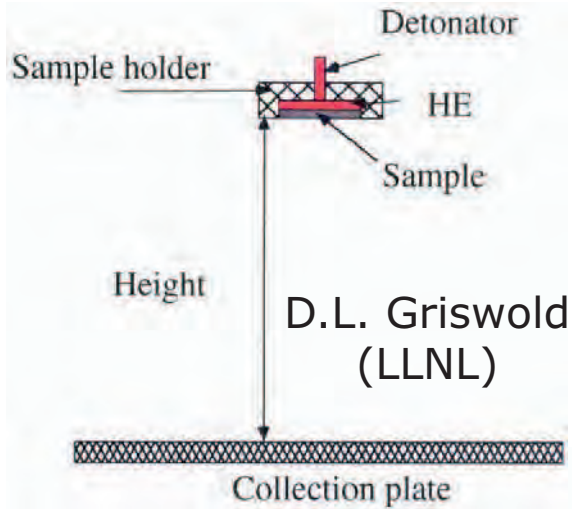
Michael Ortiz
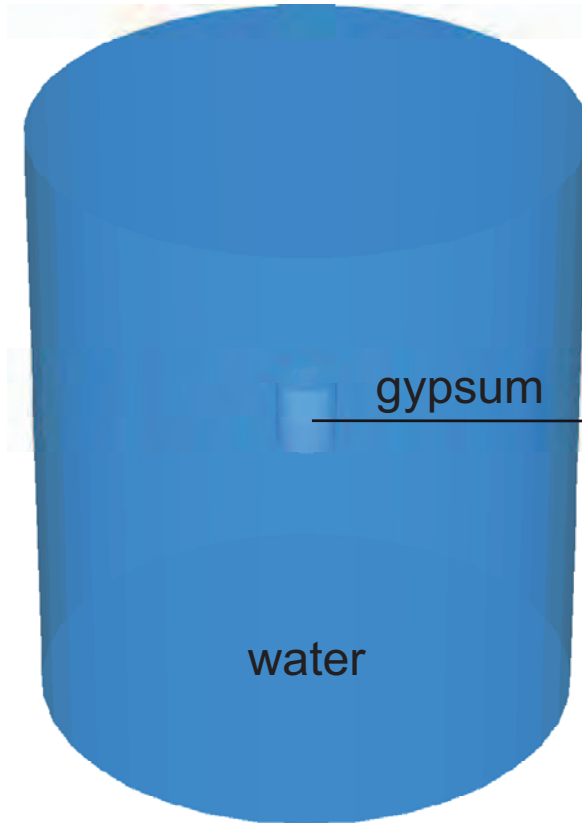
McAteer et al. (2005)   299457 nodes, 223030 element

Gypsum fragmentation experiment

Experiment

Simulation
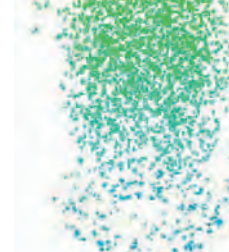
Detonation-driven fragmentation of ceramic plate
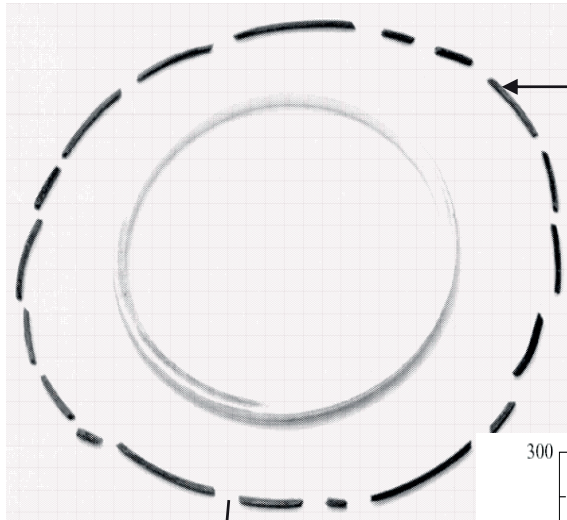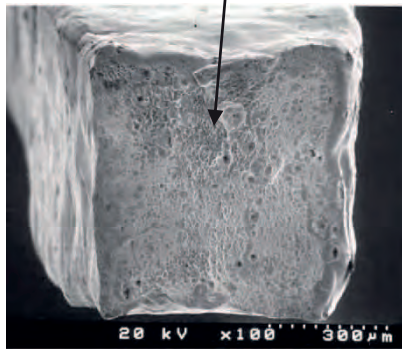
| 0 μs | 100 μs | 200 μs | 300 μs | 400 μs | 500 μs | 600 μs |

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U6Nb ring expansion
(Becker LLNL '02)

FE simulation

(Rich Becker, LLNL)

AMR
at necks

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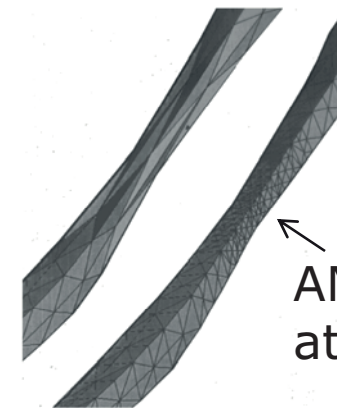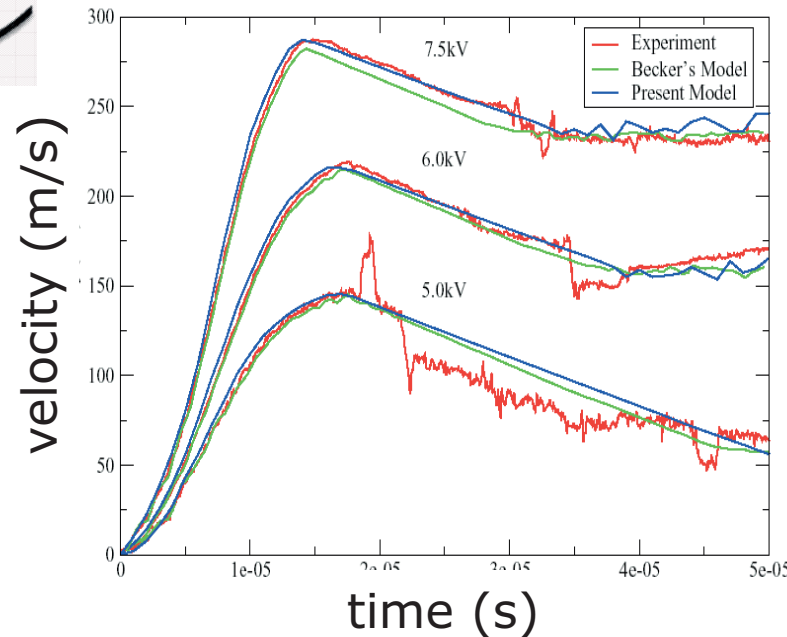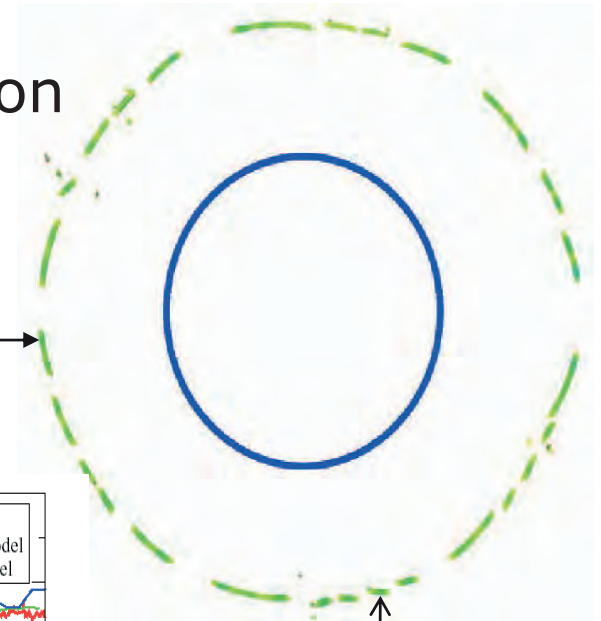
Caltech ASC/ASAP Center (97-07)

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

Water hammer impacting on fracturing shell

Caltech ASC/ASAP Center (97-07)

Aims for second five years:

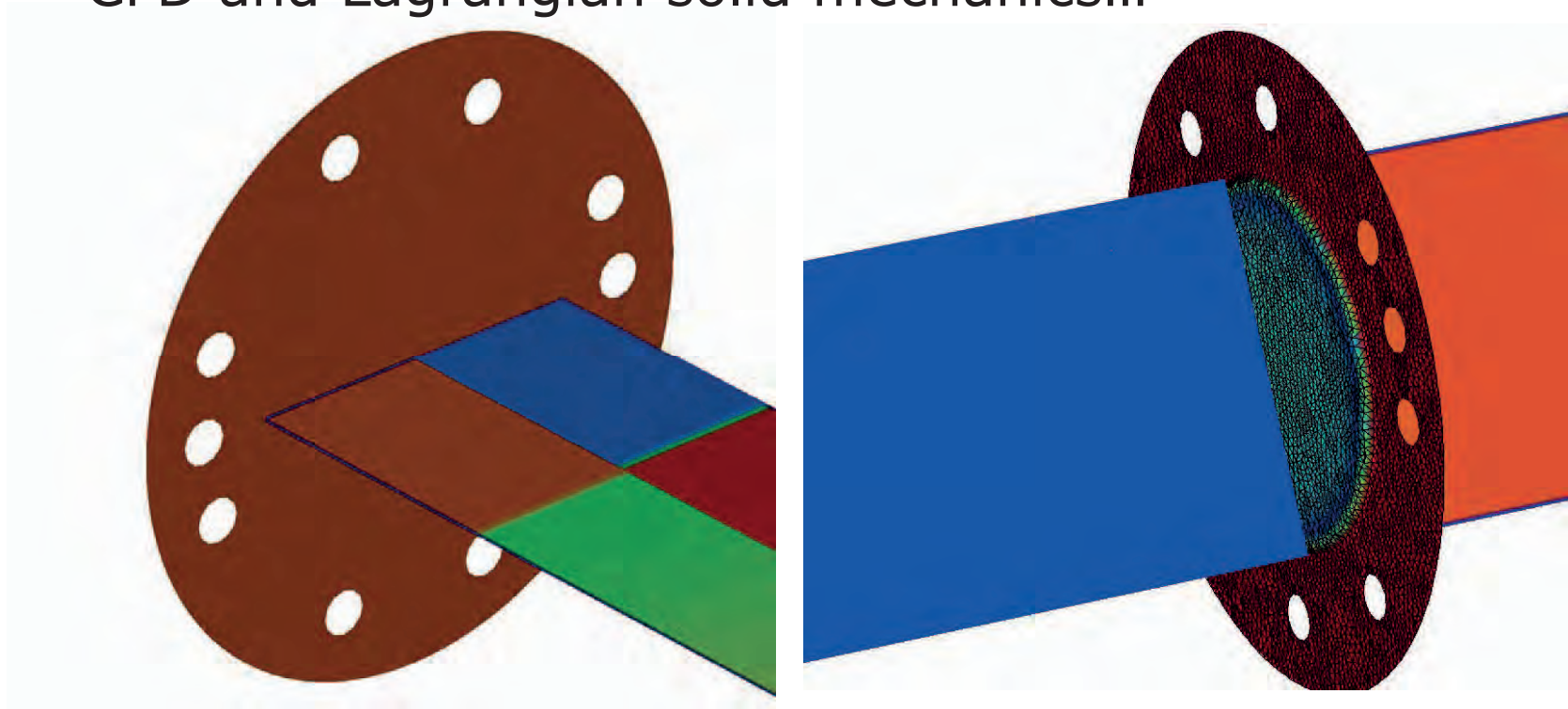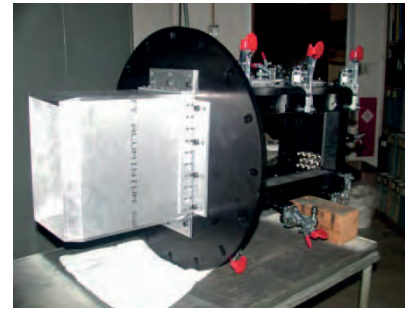- Establish linkage with Caltech validation efforts

- 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
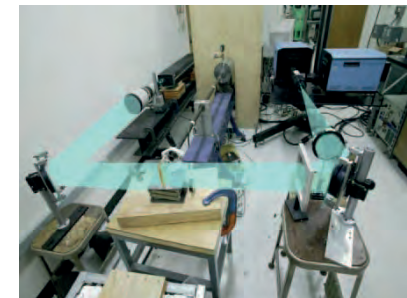 - High pressure EOS and constitutive relations

Shock focusing

Detonation-driven fracture

Dynamic deformation

Dynamic fracture

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Caltech ASC/ASAP Center (97-07)

thickness = 0.89 mm

50.8 mm

41.28 mm

Initial flaw (12.7 mm)
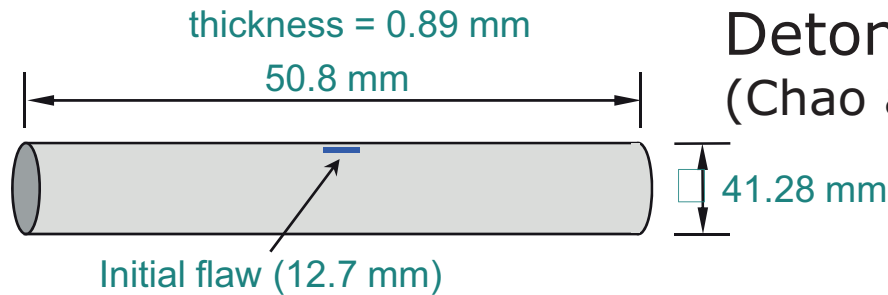
Detonation fracture, Al tubes
(Chao and Shepherd, 2004)
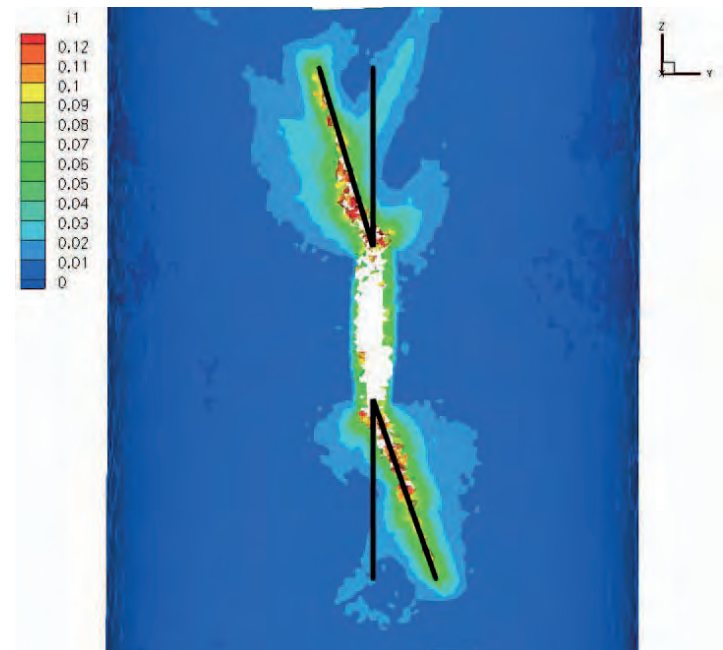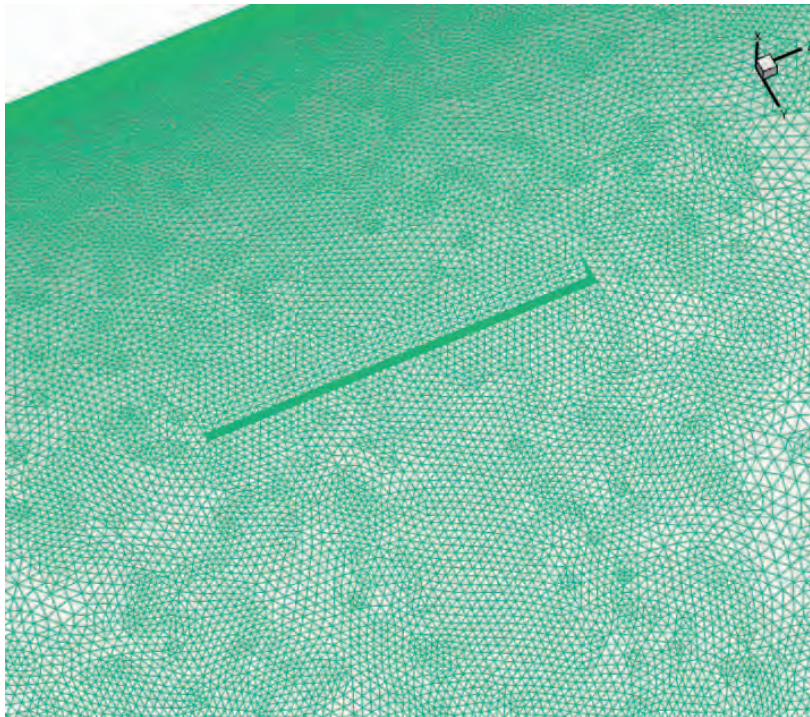
220945 elements, 399998 nodes
LLNL ALC, 400 processors, 8 hours run time

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

Caltech ASC/ASAP Center (97-07)

Validation run: ALC, 900 processors, 133 million elements

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Caltech ASC/ASAP Center (97-07)

l_c = 1.267 [mm]
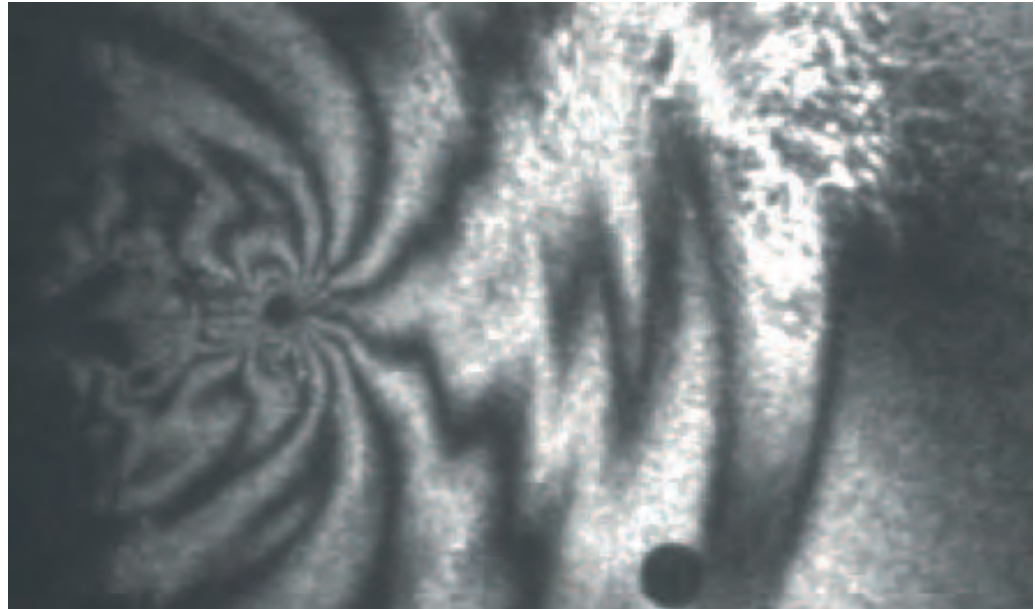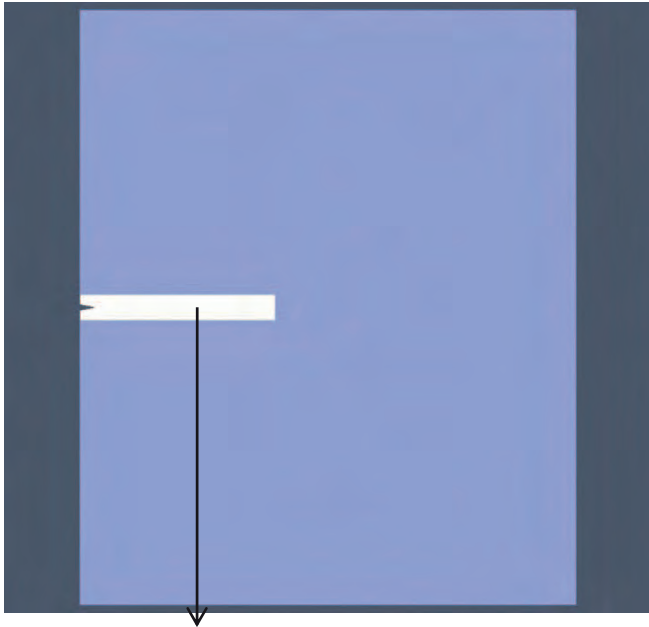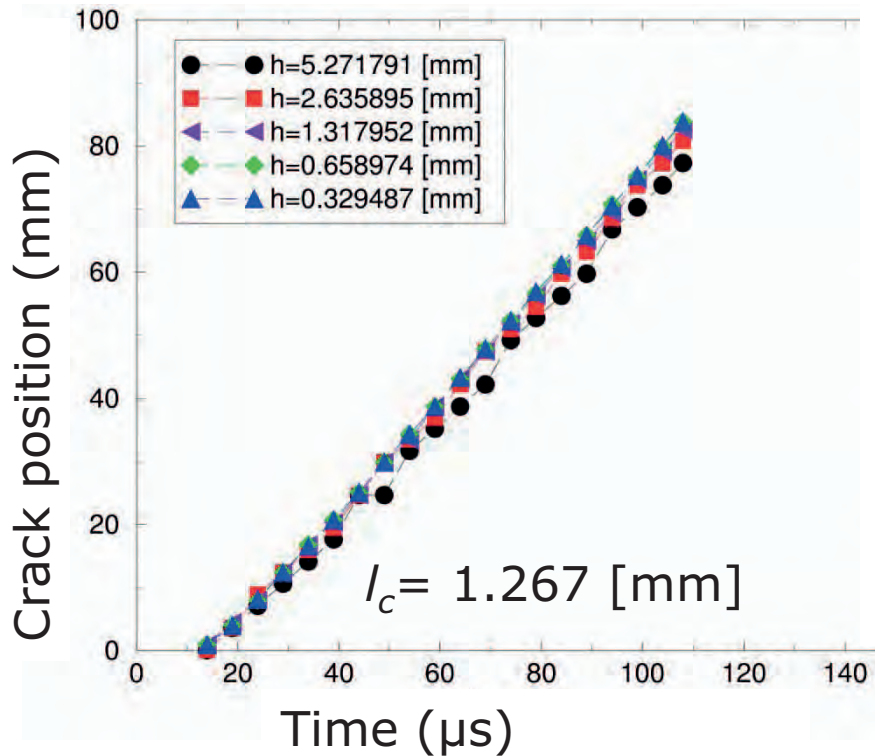
Mesh convergence
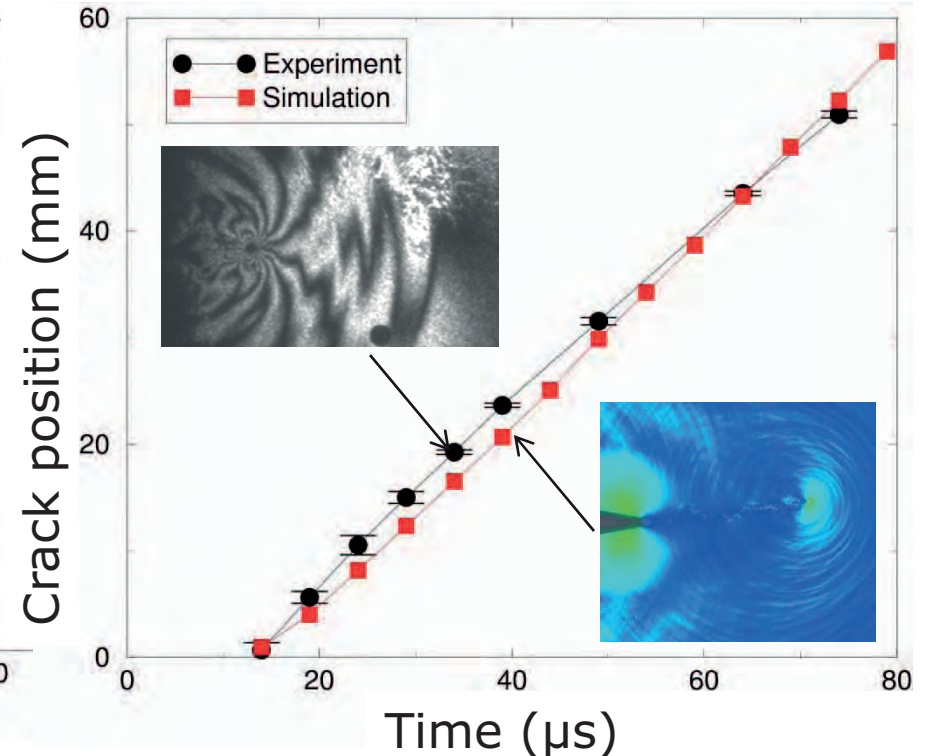
Comparison with experiment

Validation run: ALC, 900 processors, 133 million elements

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Multiscale modeling of ductile fracture and spallation

average opening displacement

local deformation

average traction

$a(t)$

$b(t)$

local stress

QM
MD
KMC

Chao and Shepherd (2004)

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Caltech ASC/ASAP Center (97-07)
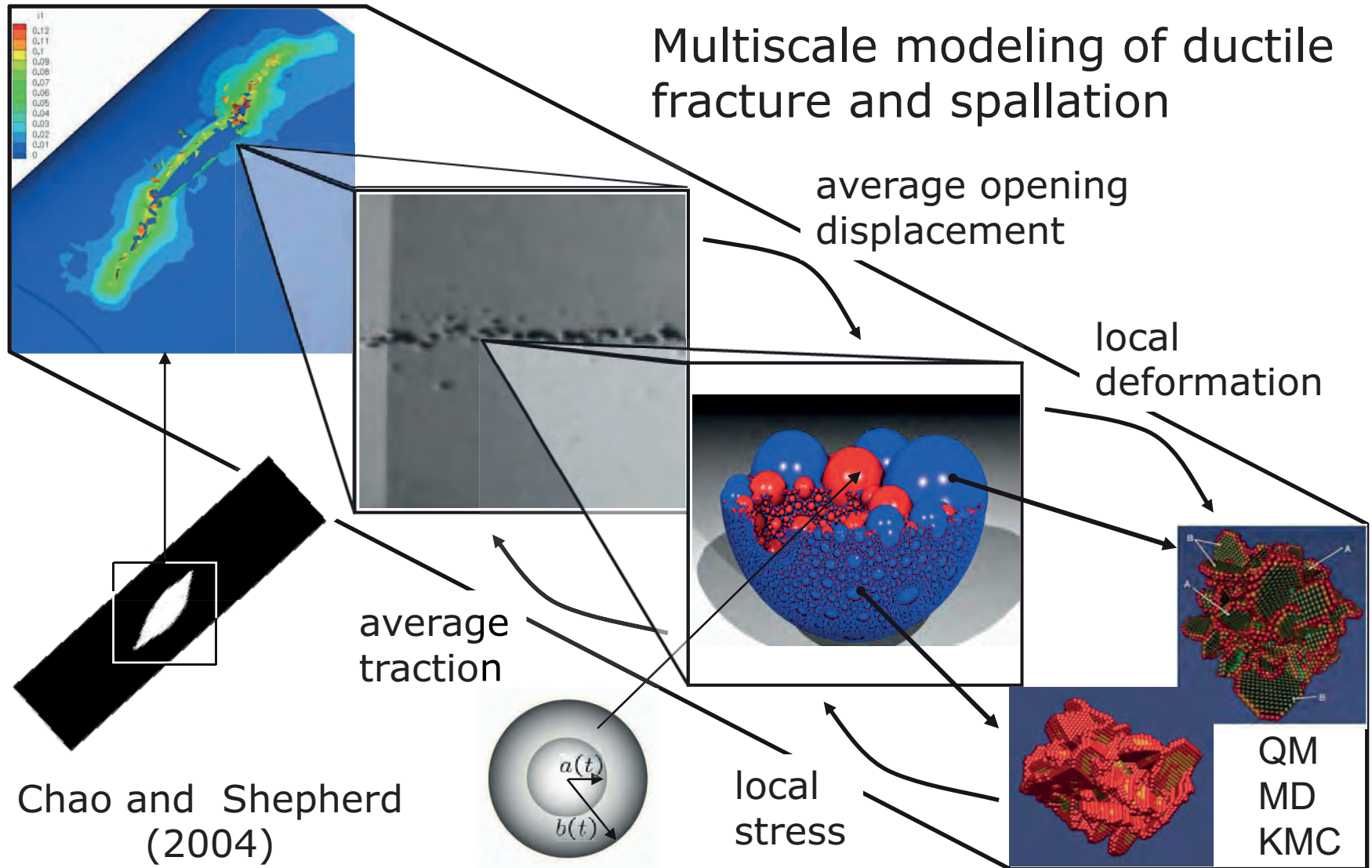
Multiscale modeling of strength of metals

average deformation

local deformation

average stress

Ravichandran *et al.* (2002)

local stress

QM
MD
KMC

STAINLESS STEEL
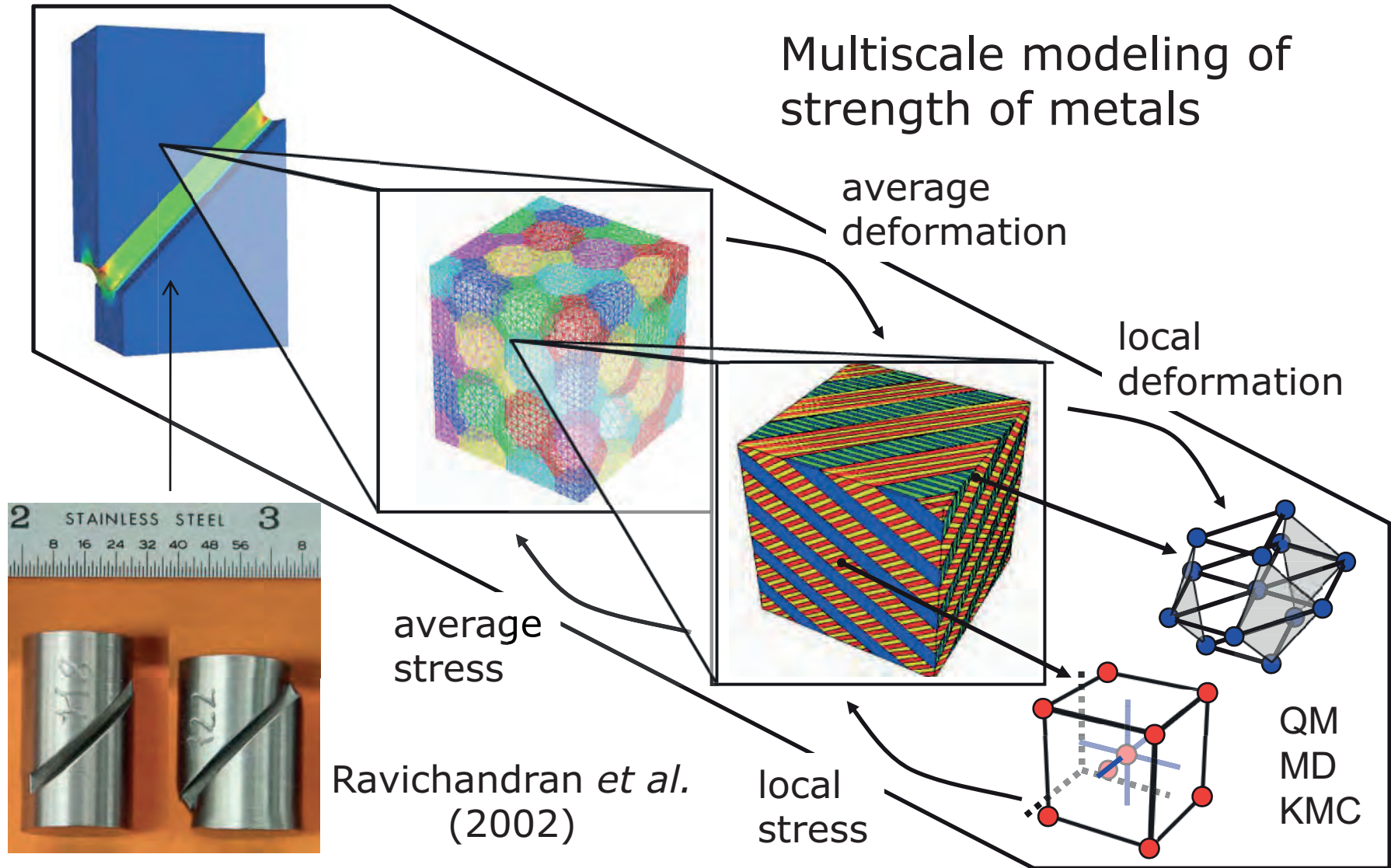
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The ASAP→PSAAP phase transition

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?

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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

Caltech's ASC/PSAAP Center

- Hypervelocity normal and oblique impact of projectiles/targets at impact velocities of up to 10 km/s
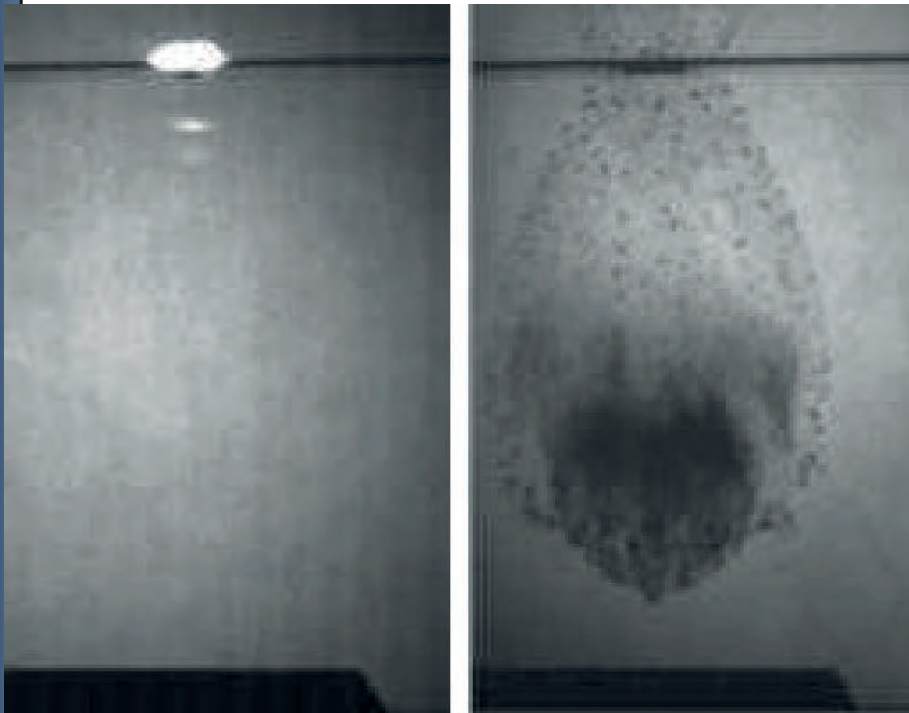
Hypervelocity impact of bumper shield.
a) Initial impact flash. b) Debris cloud
(Ernst-Mach Institut, Freiburg Germany).
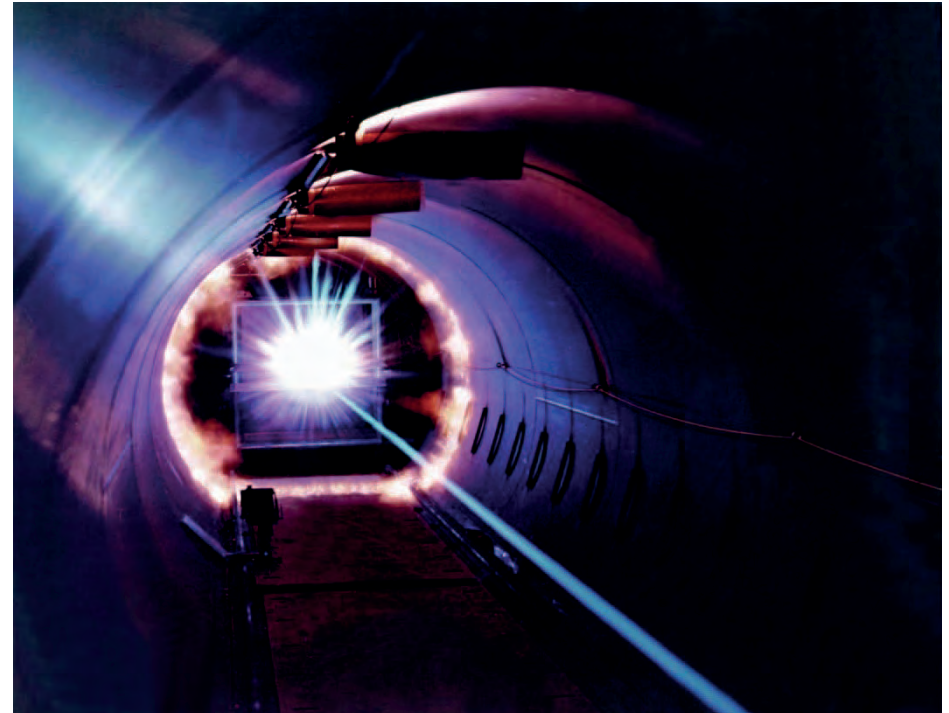
NASA Ames Research Center
Energy flash from hypervelocity test
at 7.9 Km/s

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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 $10^{11}s^{-1}$ } states of matter 'of interest'
  - High temperatures (4,000-36,0000 K)

- 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

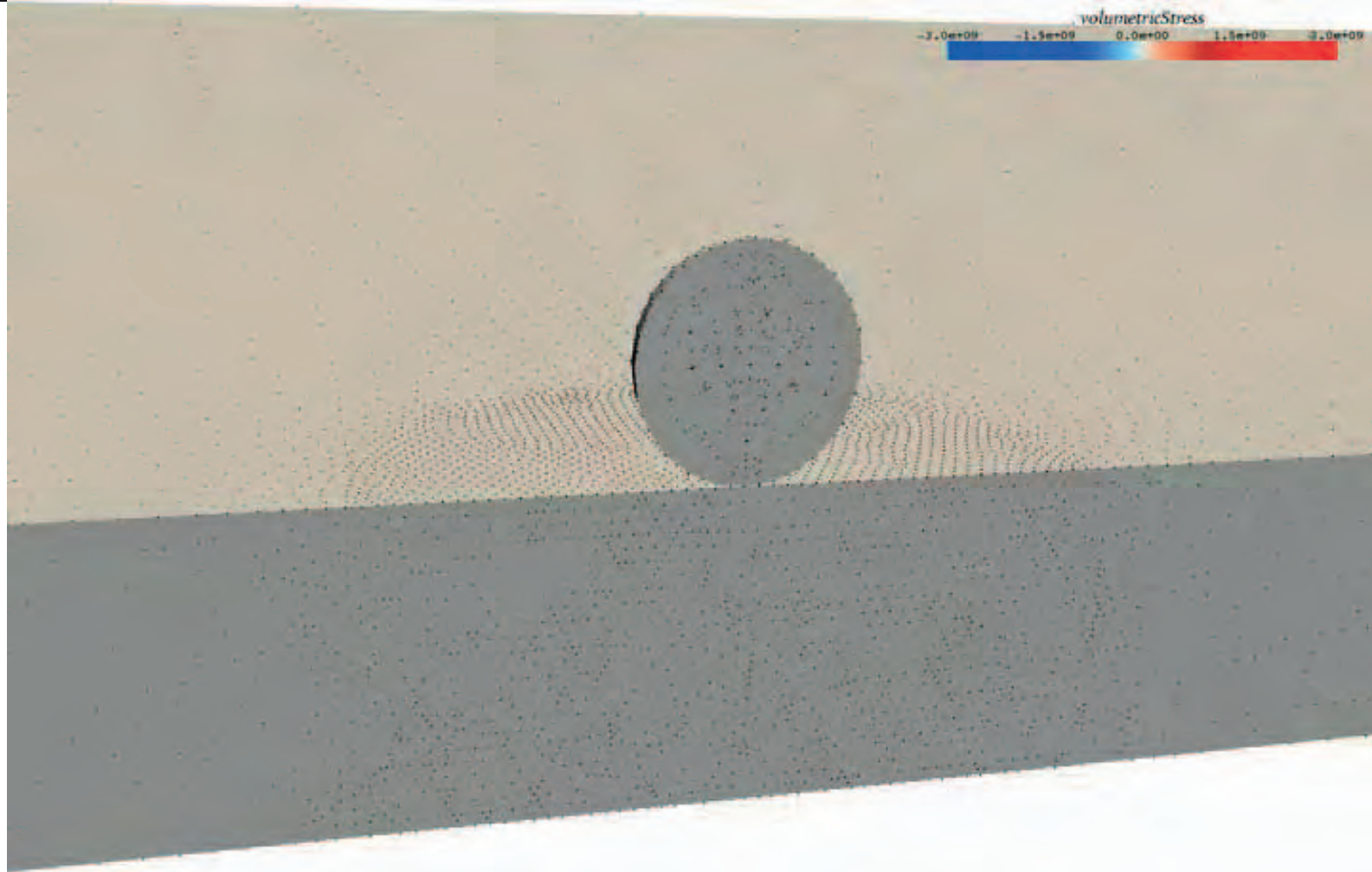The International Space Station uses 200 different types of shield to protect it from impacts

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SPHIR

Small Particle Hypervelocity Impact Range

Caltech's ASC/PSAAP Center

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

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Caltech's ASC/PSAAP Center
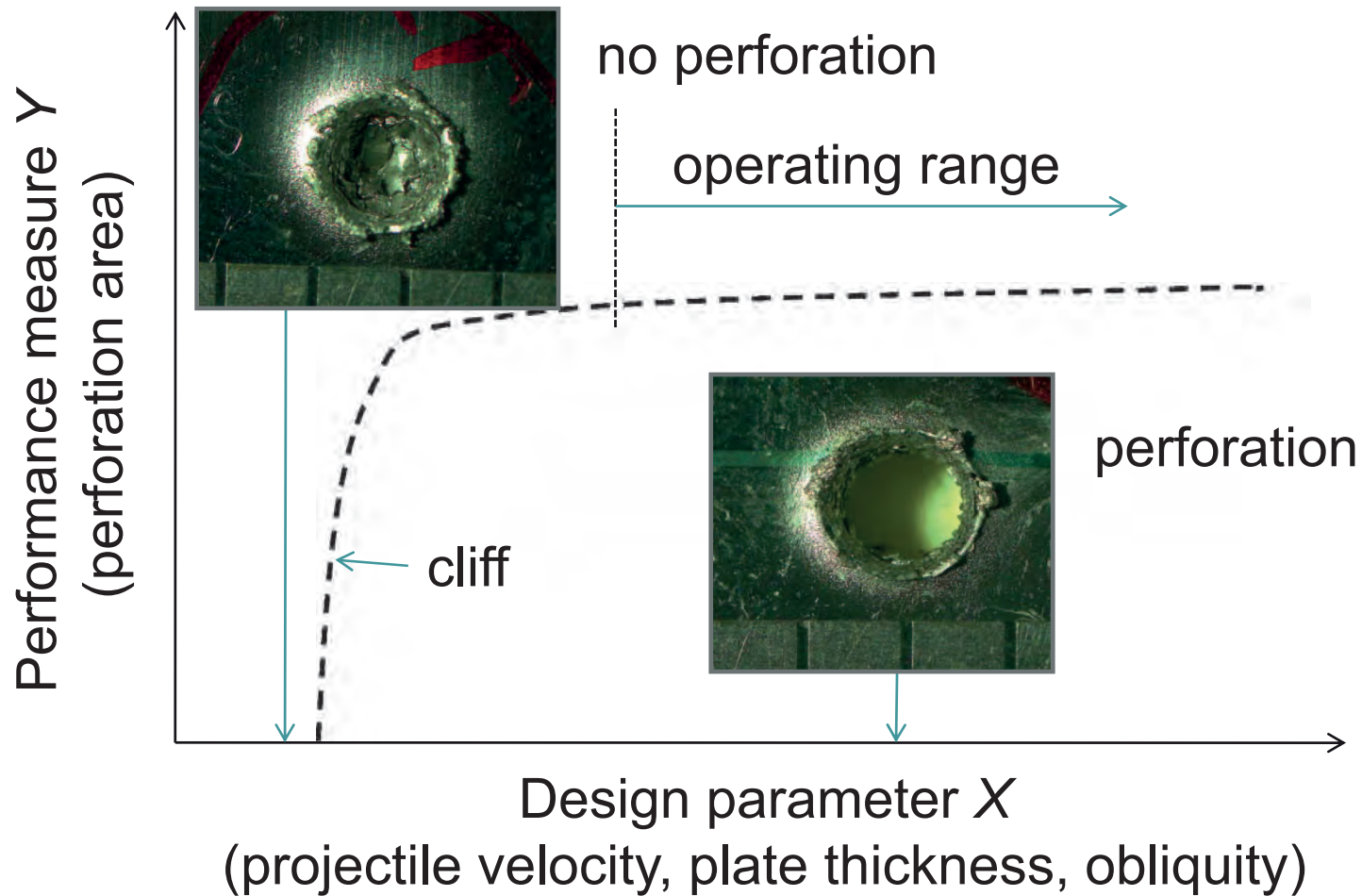
- ***Fundamental question***: How can we use physics models AND experiments to certify the performance of a complex system?

- ***Our strategy***: Formulate, evaluate, rigorous ***upper bounds on the probability of failure*** of the system → 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.
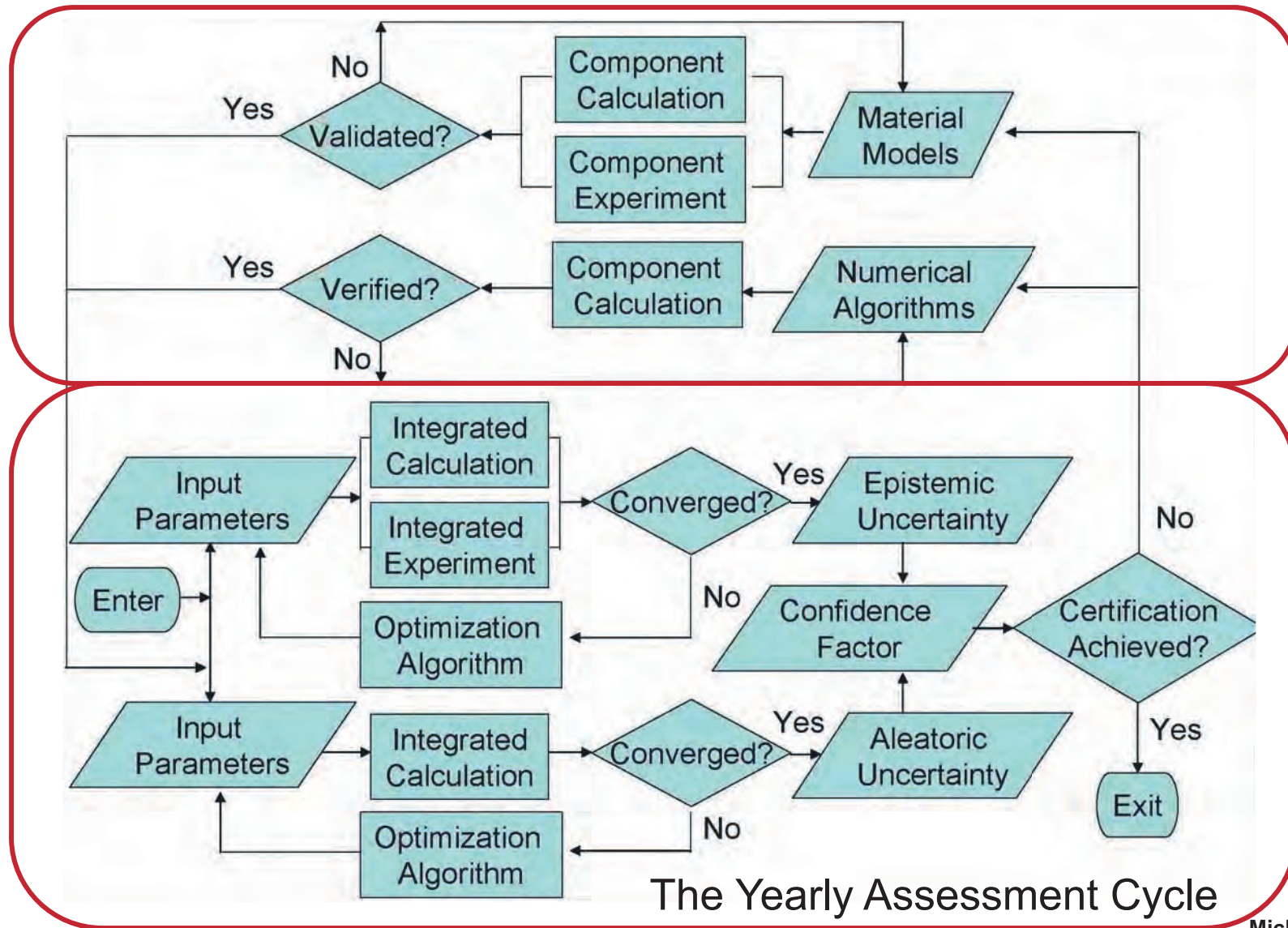
The Yearly Assessment Cycle

Caltech's ASC/PSAAP Center

no perforation

operating range

Performance measure Y (perforation area)

cliff

perforation

Design parameter X
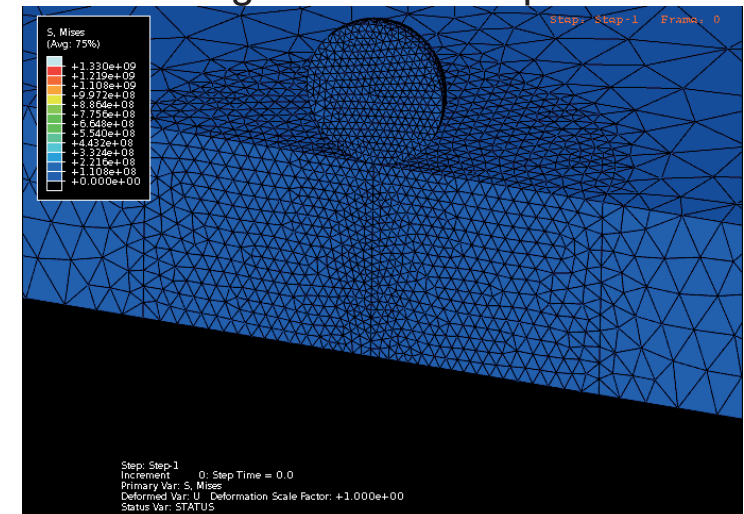(projectile velocity, plate thickness, obliquity)

Y1 UQ analysis scope

Caltech's ASC/PSAAP Center

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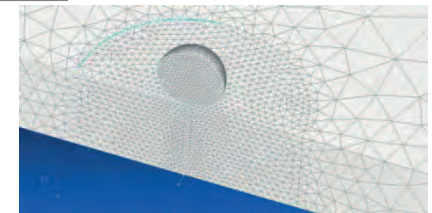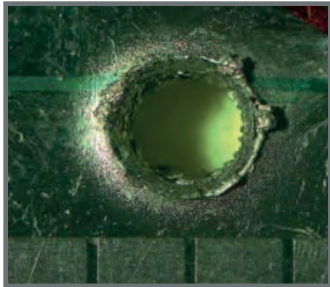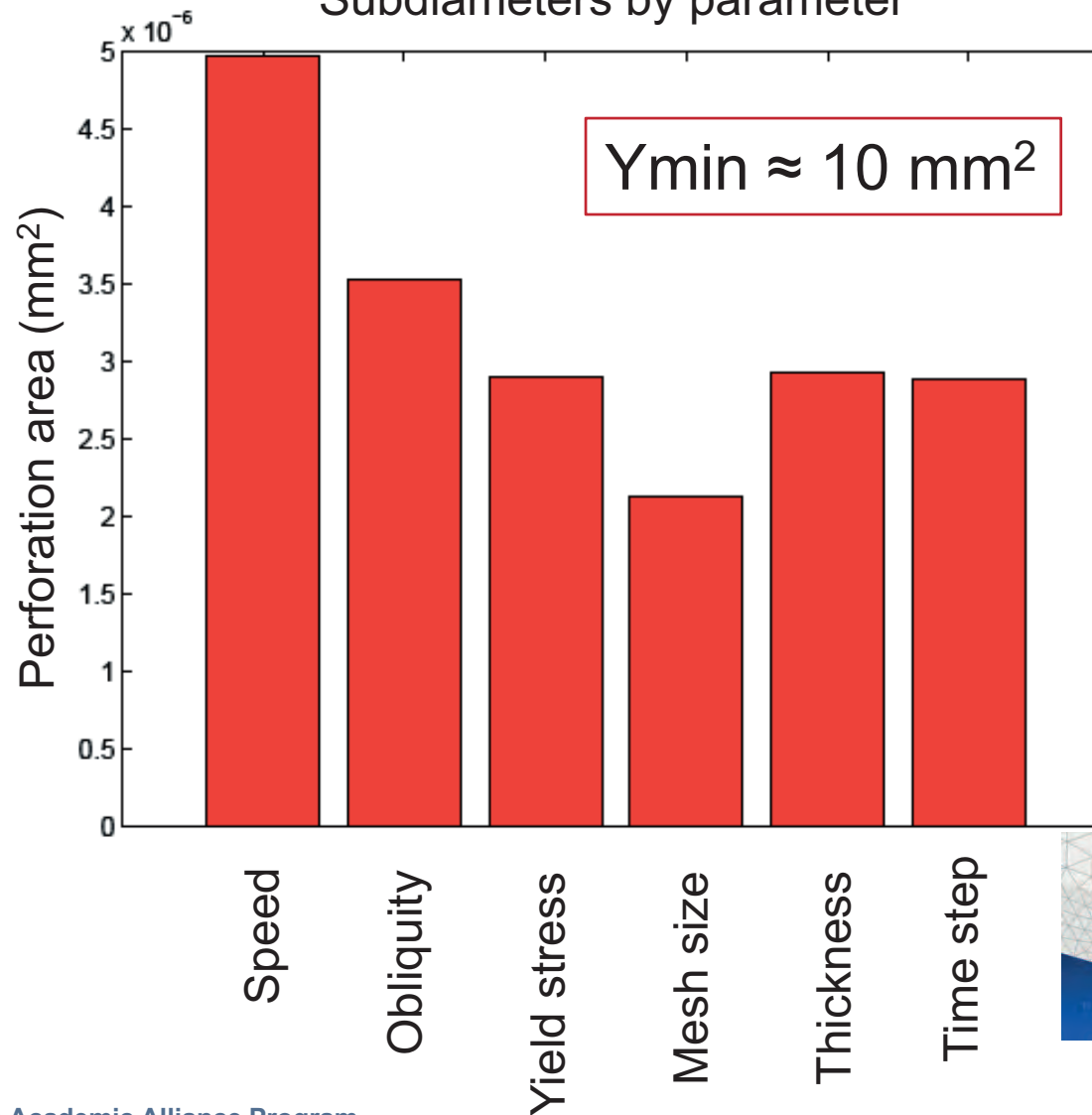- ABAQUS model
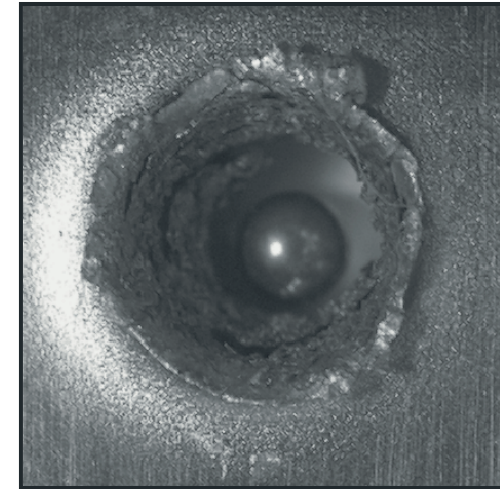
Steel-on-steel, 2.6 km/s damage zone and impactor

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Subdiameters by parameter

Ymin ≈ 10 mm^2

Perforation area (mm^2)

Speed, Obliquity, Yield stress, Mesh size, Thickness, Time step

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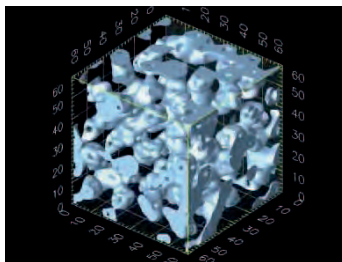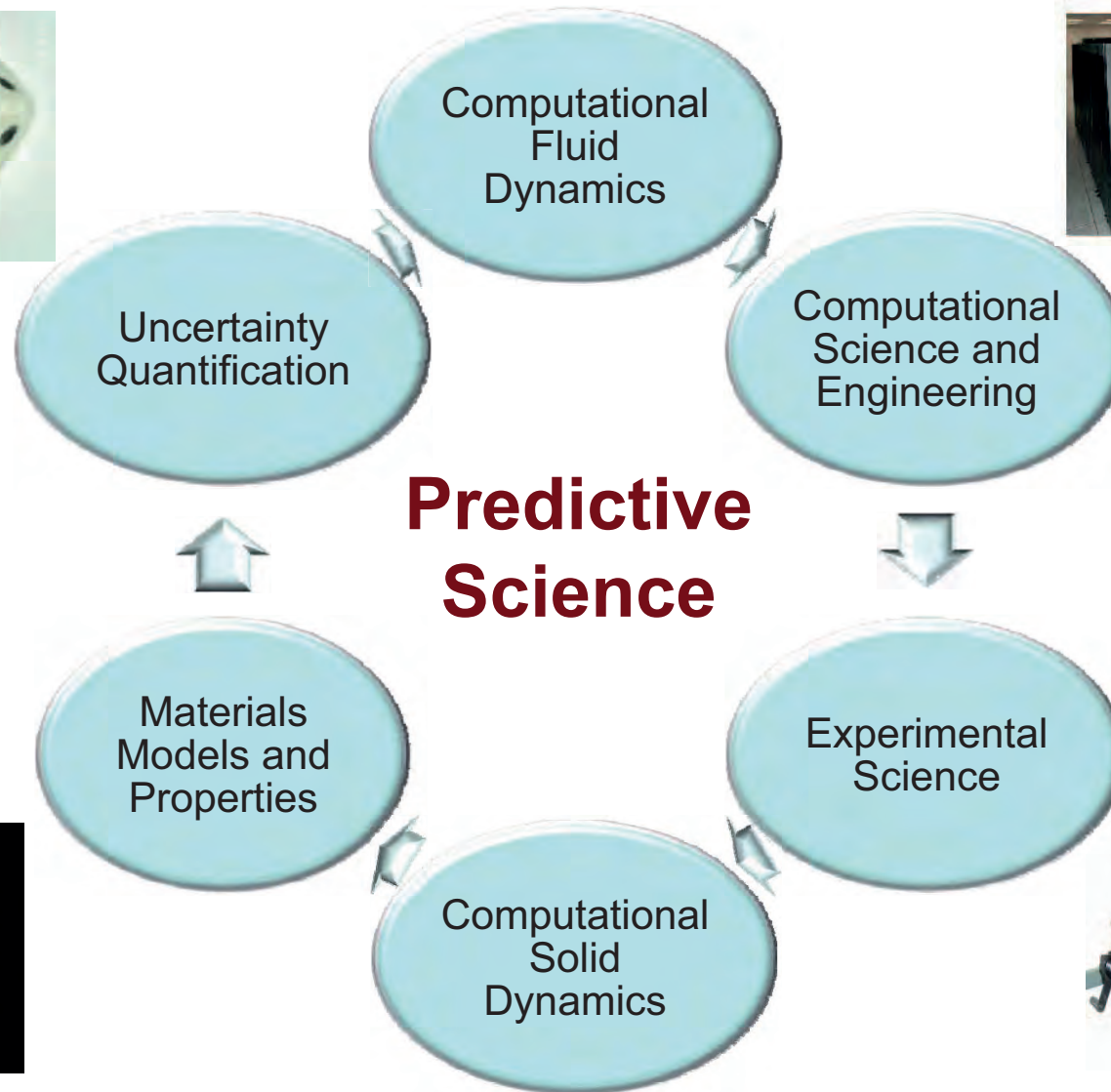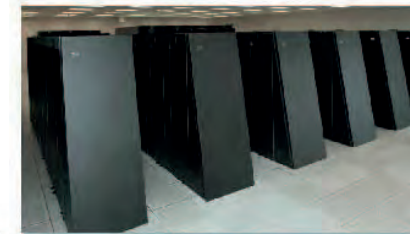
- Quantified uncertainties are too high near the cliff!

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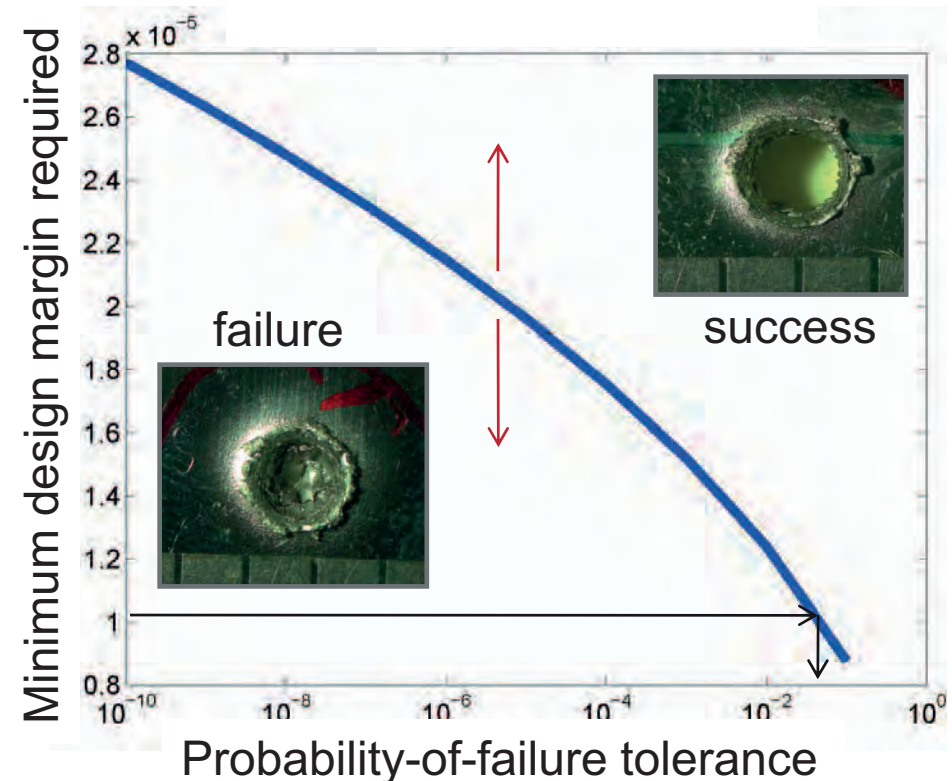
Design margin requirements resulting from Y1 UQ analysis for impact velocities near ballistic limit of target plate

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Predictive Science

- Computational Fluid Dynamics
- Computational Science and Engineering
- Experimental Science
- Computational Solid Dynamics
- Materials Models and Properties
- Uncertainty Quantification

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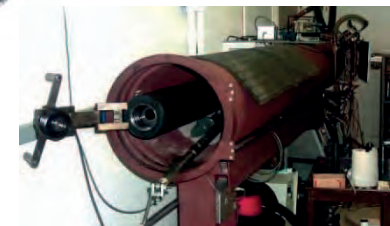
Student co-mentoring program
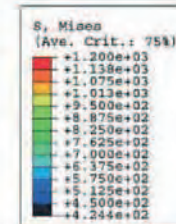

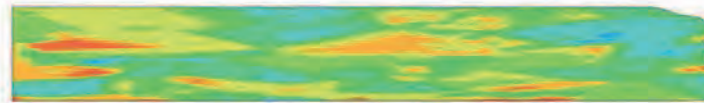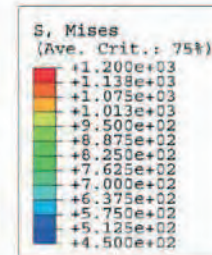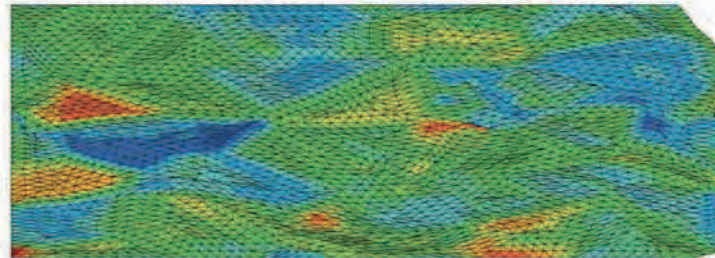MS 200 Sec: 13 - Advanced Work in Materials Science   FA 2006-07
Ortiz, Michael

Hansen
Benjamin Lee
G4 (MS)
bhansen@caltech.edu

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
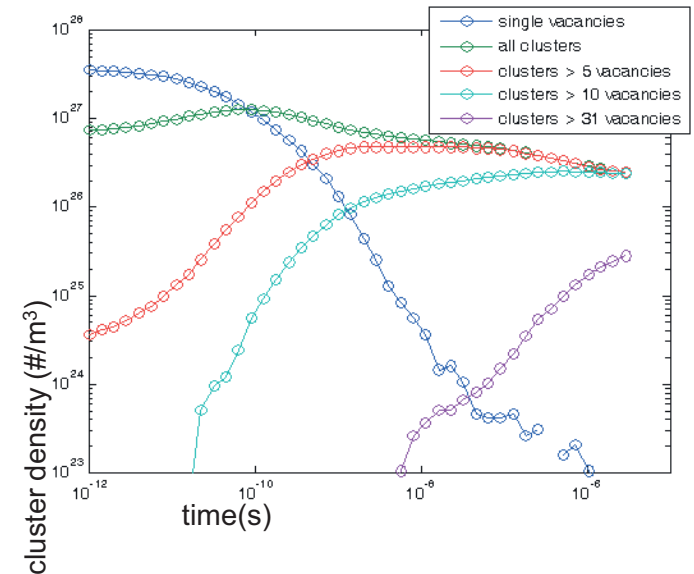
Caltech's ASC/PSAAP Center

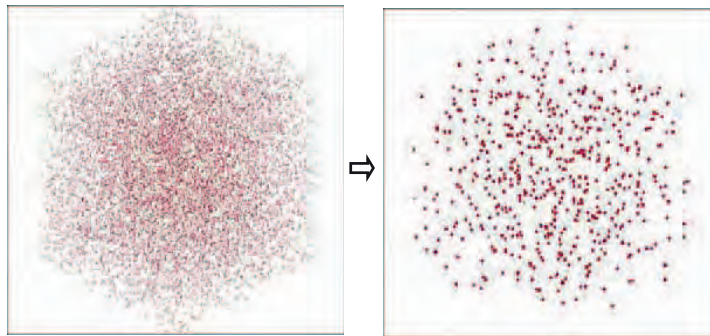## Summer practica at NNSA labs

**Reina Romo
Celia**
G3(Ae)
celia@caltech.edu

Evolution of cluster density in Al

Jaime Marian – Chemistry, Materials and Life Sciences Directorate

Lawrence Livermore National Laboratory

Michael Ortiz

Caltech's ASC/PSAAP Center

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
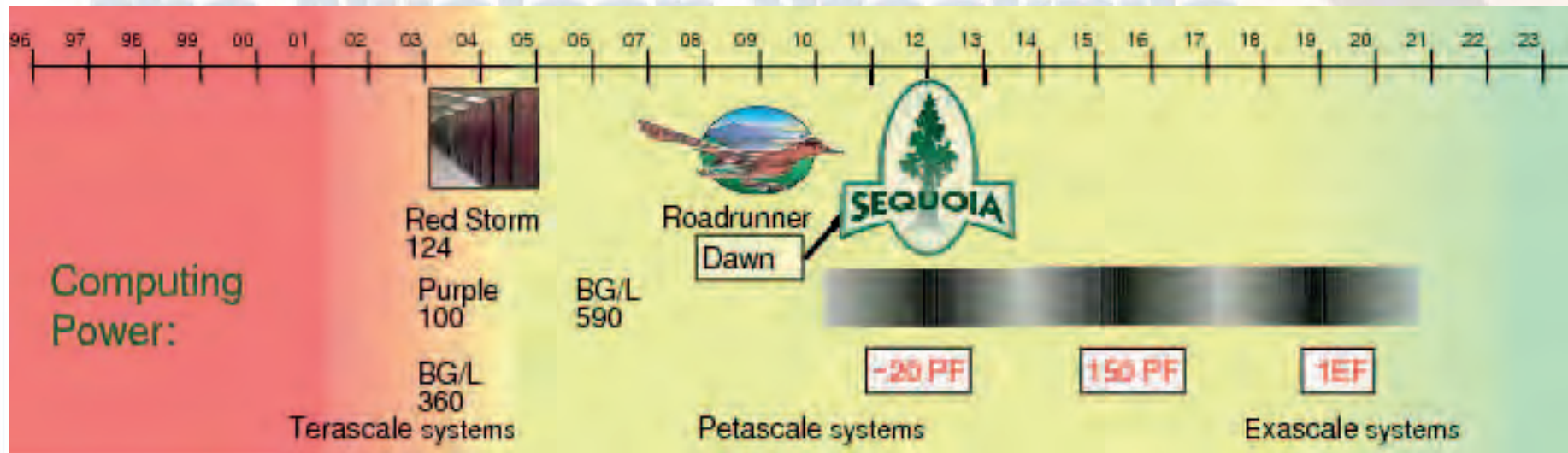Stanford

- Our alumni are our most enduring legacy…
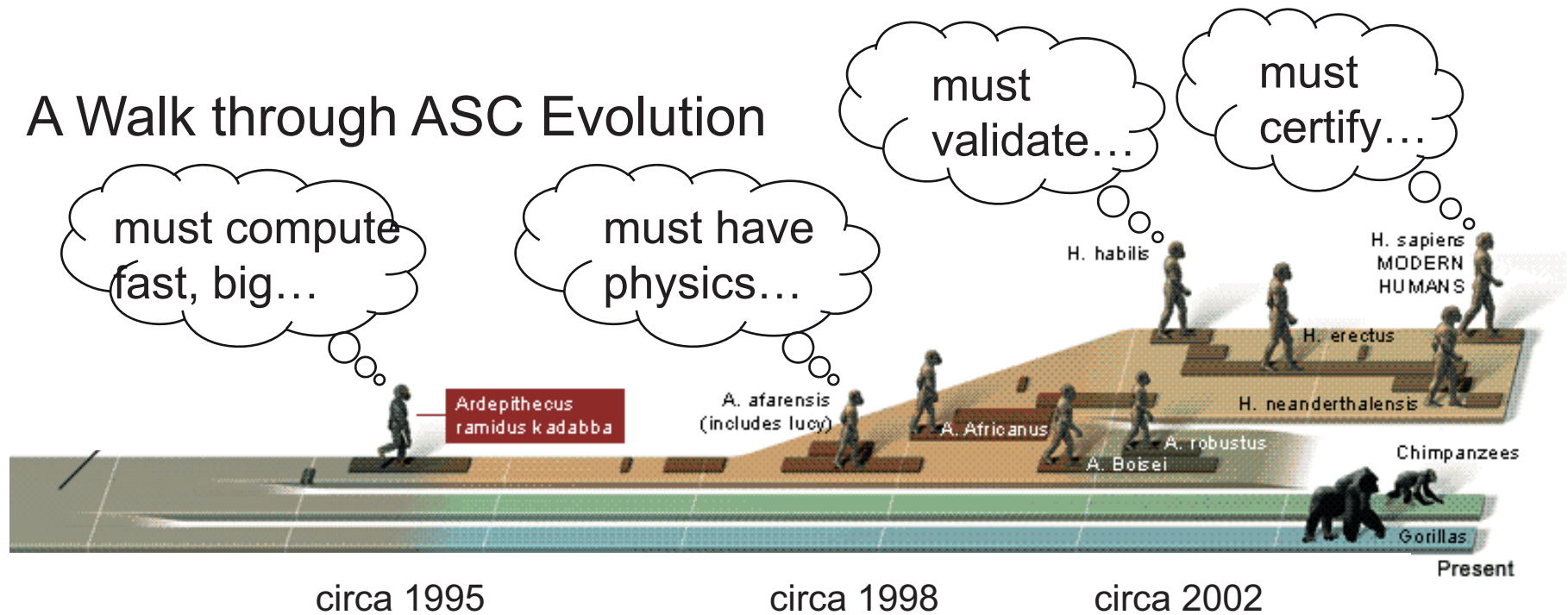
ASC – Towards exascale computing

Purple – 0.1PF/s

BlueGene/L – 0.4

Computing Power:

Red Storm 124

Purple 100

BG/L 360

BG/L 590

Roadrunner

Dawn

SEQUOIA

~20 PF

150 PF

1EF

Terascale systems

Petascale systems

Exascale systems

Our vision for predictive science…

A Walk through ASC Evolution

must compute fast, big…

must have physics…

must validate…

must certify…

circa 1995   circa 1998   circa 2002

- 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!

Thank you!

Michael Ortiz