Predictive Modeling and Simulation of the Dynamic Response of Materials at Caltech

Michael Ortiz
Beijing University of Aeronautics and Astronautics (BUAA)
School of Jet Propulsion
Beijing, March 14, 2011

Caltech & Jet Propulsion Lab (JPL)

CALTECH PSAAP

CALIFORNIA INSTITUTE OF TECHNOLOGY 1891

JPL
Jet Propulsion Laboratory
California Institute of Technology

DoE - ASC/PSAAP Centers

CALTECH PSAAP

STANFORD UNIVERSITY PSAAP

CALIFORNIA INSTITUTE OF TECHNOLOGY 1891

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

PURDUE UNIVERSITY

CALTECH PSAAP

ICES
The Institute for Computational Engineering and Sciences

CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS

MICHIGAN

THE UNIVERSITY OF TEXAS AT AUSTIN

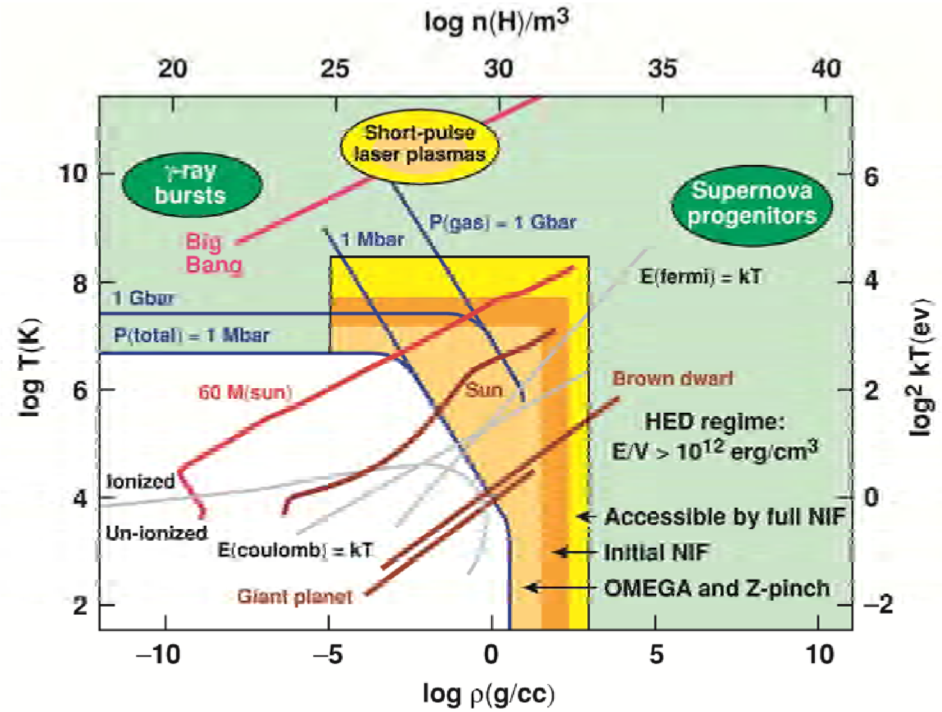
PSAAP: Predictive Science Academic Alliance Program

Overarching objectives – QMU

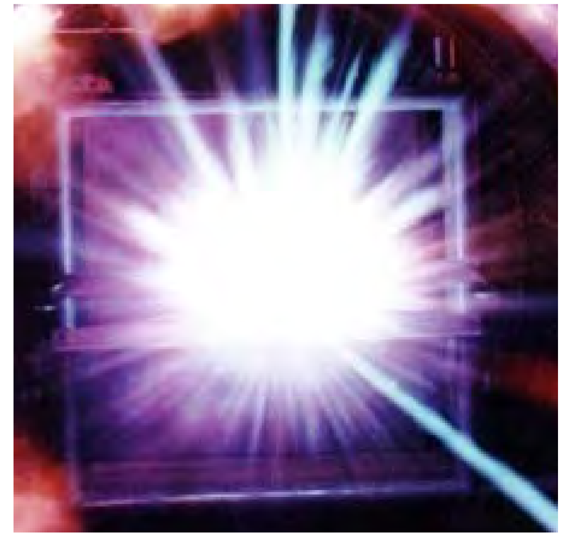
- Aim: *Quantify performance Margin & Uncertainty (QMU) in the behavior of complex physical/engineered systems*
- Example: Short-term weather prediction,
  - Old: Prediction that tomorrow will rain in Beijing…
  - New: *Guarantee* same with 99% confidence…
- *QMU* is important for achieving confidence in high-consequence decisions, designs (e.g., aircraft safety)
- *Paradigm shift* in experimental science, modeling and simulation, scientific computing (*predictive science*):
  - Deterministic → Non-deterministic systems
  - Mean performance → Mean performance + uncertainties
  - Tight integration of experiments, theory and simulation
  - Robust design: Design systems to minimize uncertainty
  - Resource allocation: Eliminate main uncertainty sources

Application: Hypervelocity impact

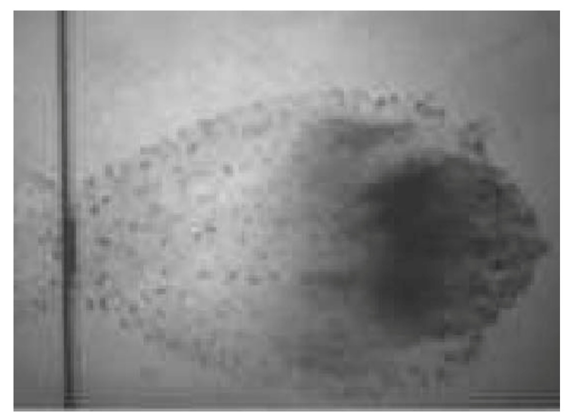
Challenge: Predict *hypervelocity impact* phenomena (10Km/s) with *quantified margins and uncertainties*



Hypervelocity impact test bumper shield (Ernst-Mach Institut, Freiburg Germany)



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



Michael Ortiz

Annual UQ campaigns

CALTECH PSAAP

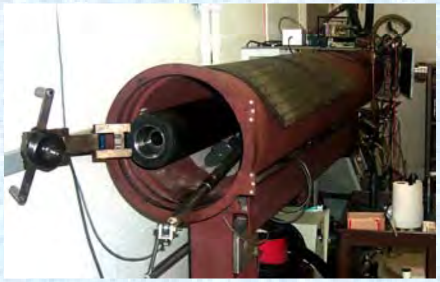
UQ campaign timeline

April 15, 2008

Center starts

Ballistic (SBGG)

- Aluminum plates
- Steel impactor (50g)
- Thickness: 0.125-0.5"
- Velocity: 0.4-1 Km/s



Ballistic (SPHIR)

- Steel/Ta plates
- Steel impactor
- Thick.: 50-105 mils
- Obliquity: 0-30°
- Velocity: 2-3 Km/s

Ballistic (SPHIR)

- Aluminum plates
- Steel impactor
- Thick.: 50-105 mils
- Obliquity: 0-30°
- Velocity: 2-3 Km/s

Hypervelocity (SPHIR)

- Aluminum plates
- Nylon impactor
- Thick.: 10-105 mils
- Obliquity: 0-80°
- Velocity: 3-10 Km/s

Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q

YEAR 1 YEAR 2 YEAR 3 YEA

Hypervelocity impact as system

system inputs:

response function (black box)

performance measures:

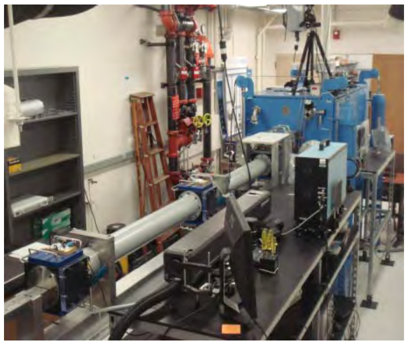
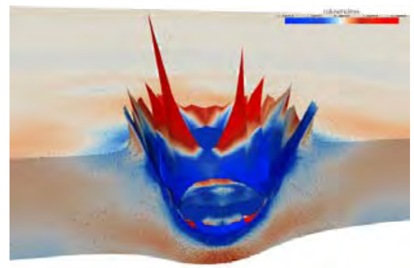
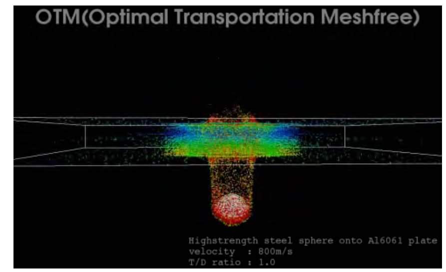
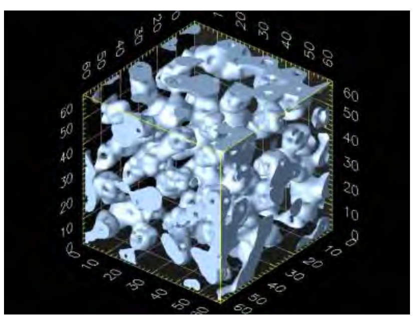
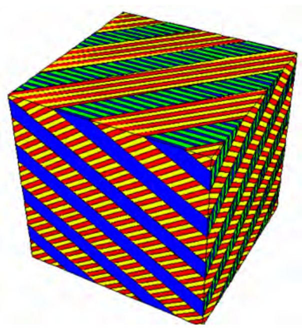
- Random variables
- Known or unknown pdfs
- Controllable
- Uncontrollable
- Unknown-unknowns (Z)

Probability of Failure?

- Observables
- Subject to performance specifications
- Random (due to randomness in inputs, system)
- Noisy (unknown unknowns)

Center's assets

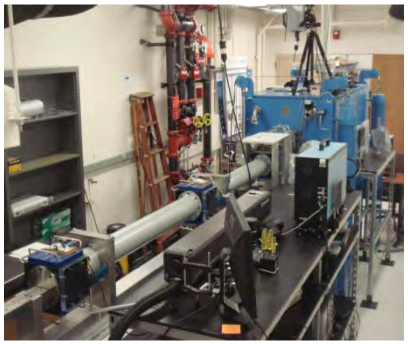
CALTECH PSAAP

Experimental Science		Simulation codes	
			
SPHIR	HSRT	VTF	Eureka
Physics models		**UQ tools**	
			
Plasma/EoS	Strength	Probability/CoM	UQ pipeline

Center's assets

CALTECH PSAAP

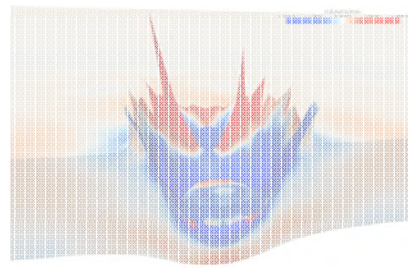
Experimental Science



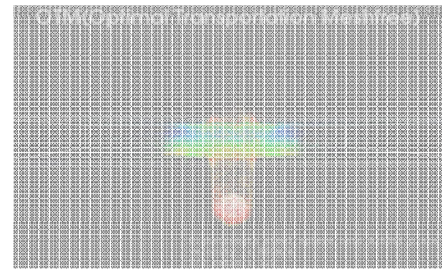
SPHIR

HSRT

Simulation codes

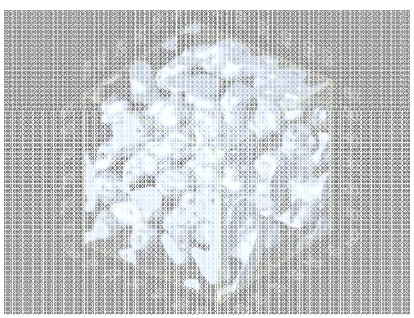


VTF

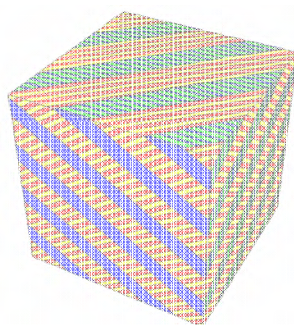


Eureka

Physics models



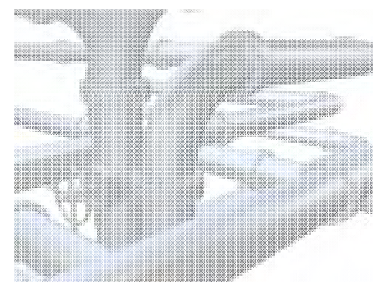
Plasma/EoS



Strength

UQ tools

Probability/CoM



UQ pipeline

Hypervelocity impact at Caltech

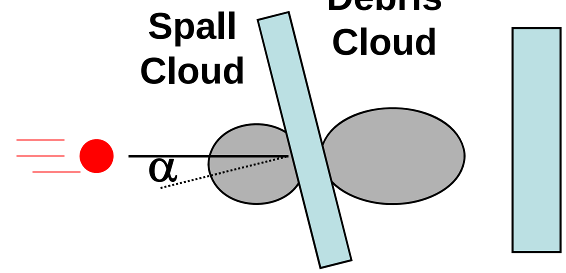
Caltech's Small Particle Hypervelocity Impact Range facility
(Prof. A.J. Rosakis, Director)

Hypervelocity impact at Caltech

CALTECH PSAAP

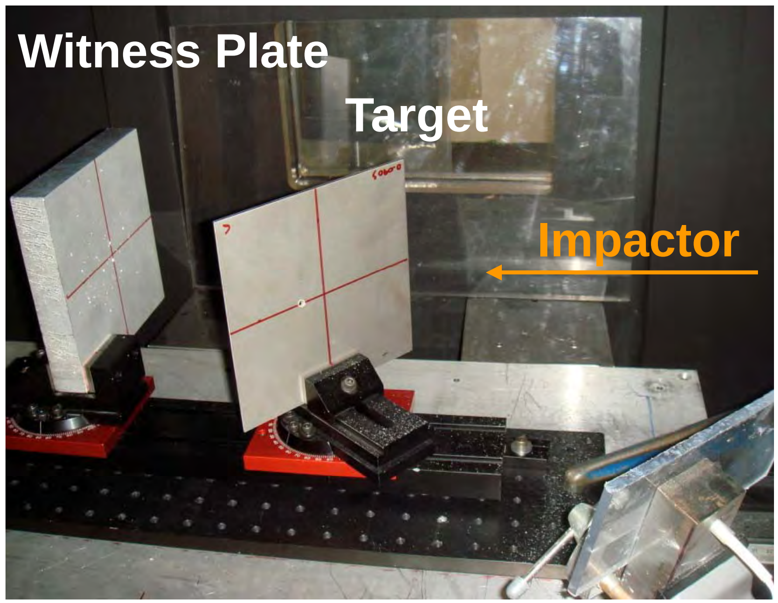
BREECH → PUMP TUBE → LAUNCH TUBE → FLIGHT TUBE → TARGET TANK

STAGE 1 STAGE 2



aluminum witness plates replaced by capture media

<u>Target Materials</u>
- Steel
- Aluminum
- *Tantalum*



- Impact Speeds: 2 to 10 km/s
- Impact Obliquities: 0 to 80 degrees
- Impactor Mass: 1 to 50 mg

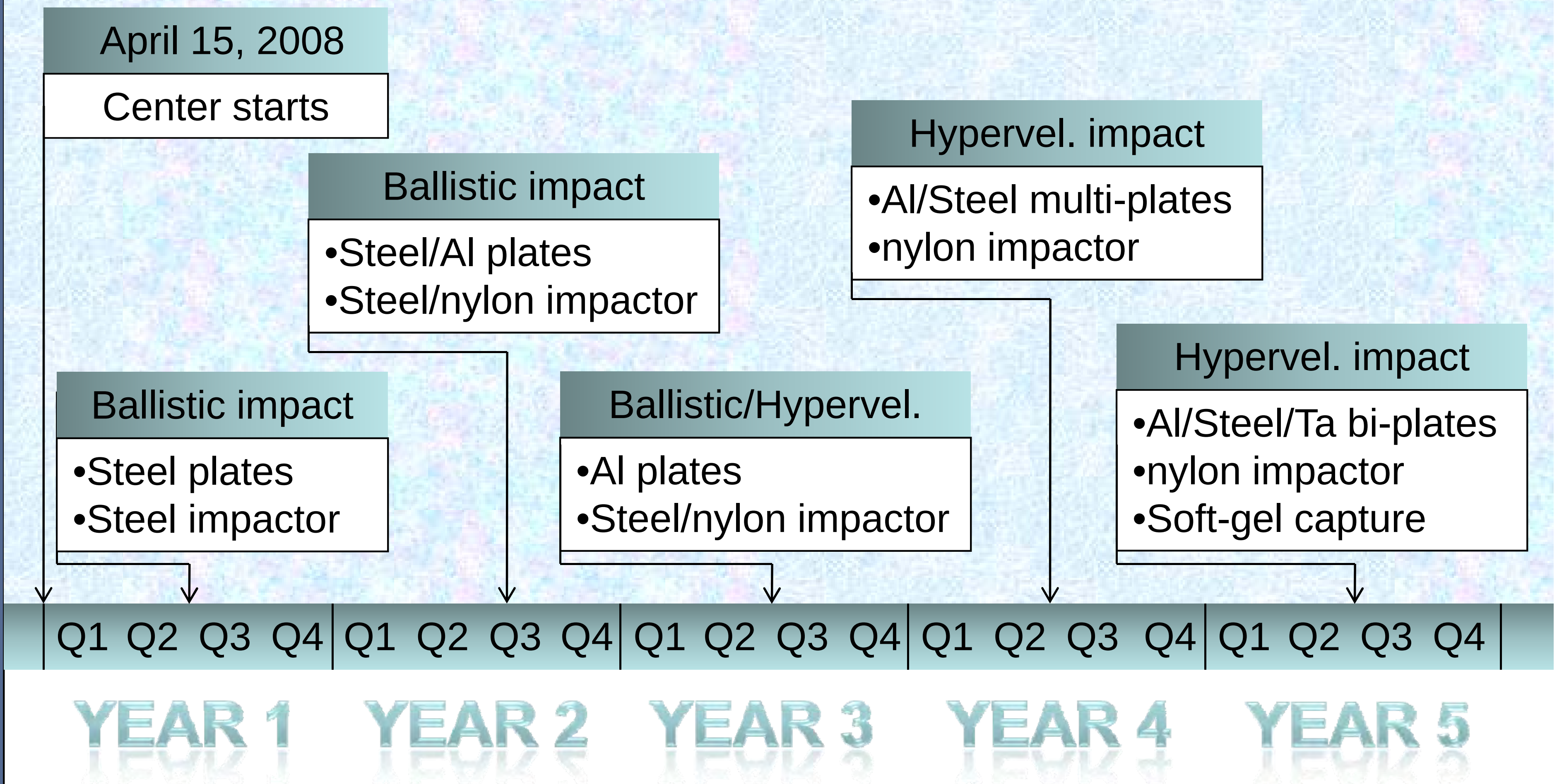
Ø 71 mil ($1\text{x}10^{-3}$ in) launch tube bore

<u>Impactor Materials</u>
- Steel
- Nylon

SPHIR – A reconfigurable facility

CALTECH PSAAP

SPHIR configuration timeline



Hypervelocity impact at Caltech

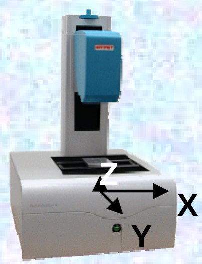
CALTECH PSAAP

Diagnostic deployment timeline

April 15, 2008
Center starts

Perforation area
Olympus SZ61 Microscope

Profilometry
Optimet MiniConoscan 3000

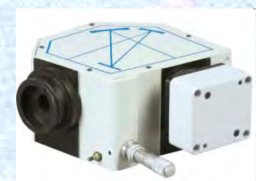


Velocimetry
Valyn Multi-Beam VISAR

Real-time CGS
Full-field surface slopes

Backlighting
Real-time shadowgraph imaging

Spectrometry
Real-time spectra



Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q

YEAR 1 YEAR 2 YEAR 3 YEA

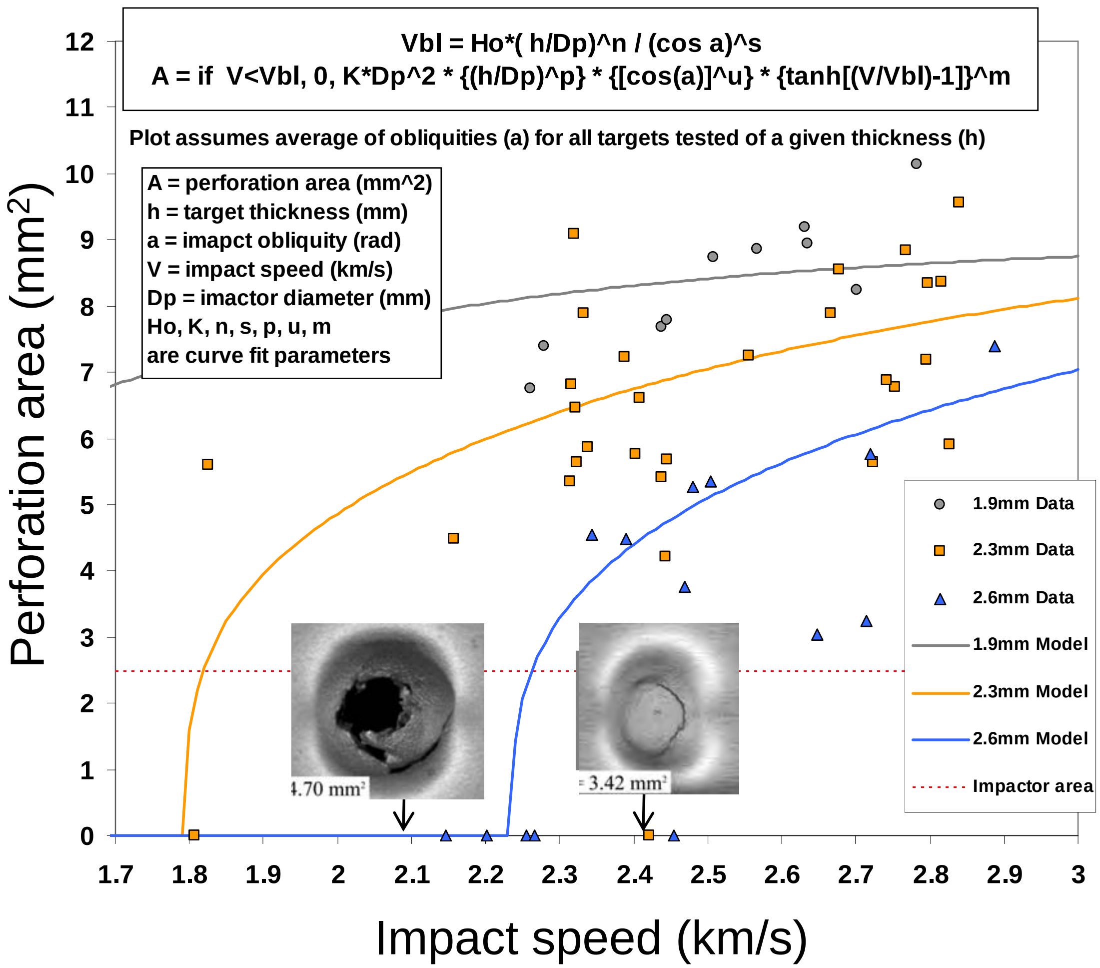
Michael Ortiz

SPHIR – Inputs and Metrics

CALTECH PSAAP

System inputs (X)	System Outputs (Y)	
	Diagnostics	**Metrics**
Projectile velocity		
Projectile mass	Conoscope	Profilometry Perforation area, Slope Contour Area
Number of target plates	Backlighting shadowgraph	Real-time back-surface bulge and ejecta/debris cloud formation
Plate thicknesses	VISAR	Real-time, back-surface velocimetry
Plate obliquities	CGS	Real-time, full-field back-surface deformation
Projectile/plate materials	Spectro-photometer	Impact flash, debris and spall clouds, spectra over IR to UV range

SPHIR - Sample data



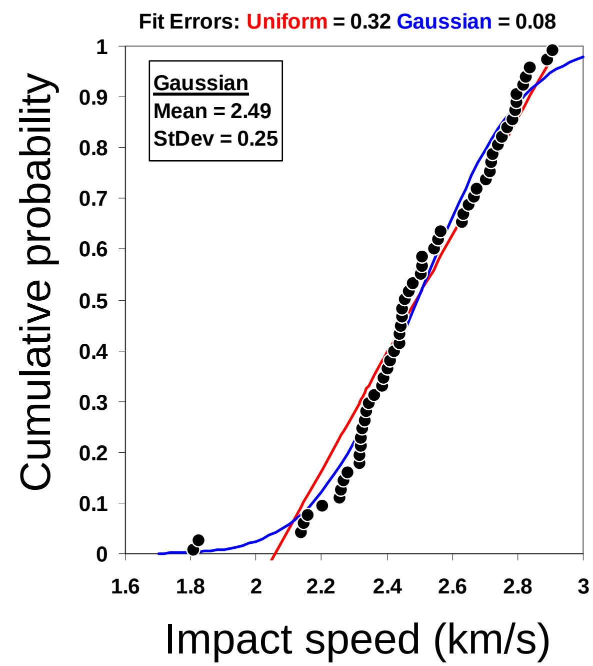
Experimental ballistic curves (SPHIR)

440 C Steel spherical projectiles

304 Stainless Steel plate targets

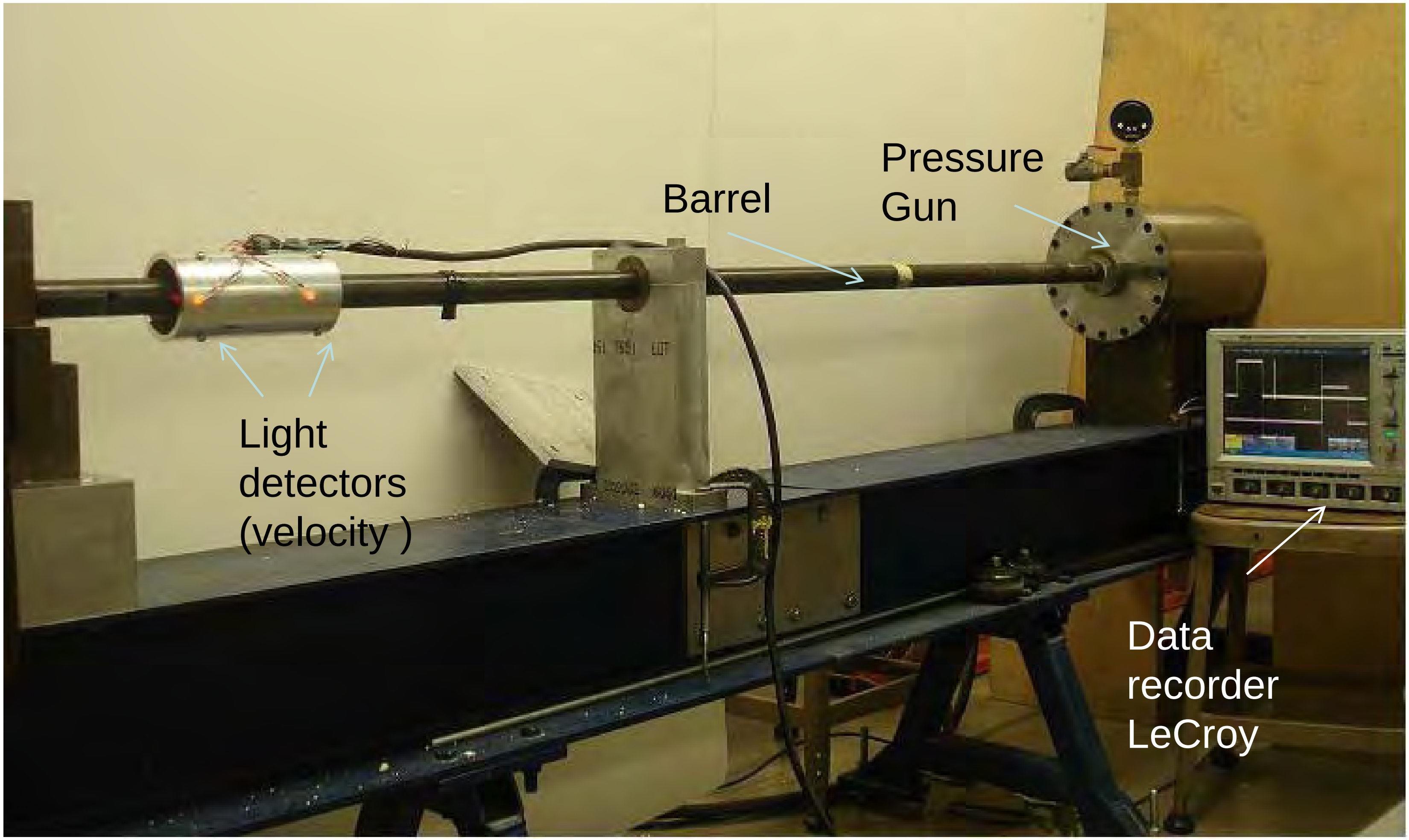
- Added challenges:
  - Experimental scatter!
  - Impact velocity uncontrollable!

Measured speed distribution



Michael Ortiz

Ballistic impact – GALCIT Small Bore Gas Gun (SBGG) facility



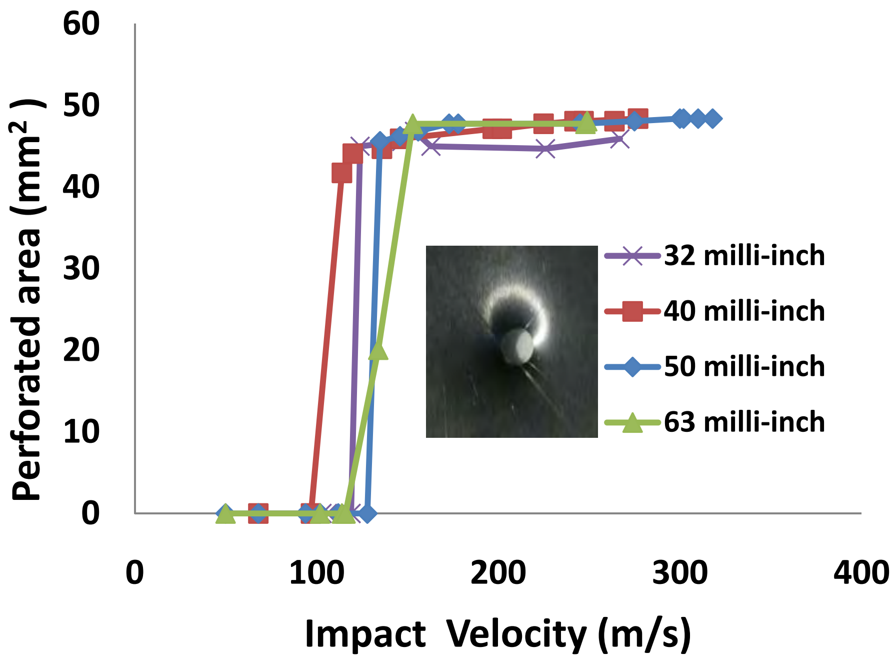
Caltech's Small Bore Gas Gun (SBGG) facility
(Prof. G. Ravichandran, Director)

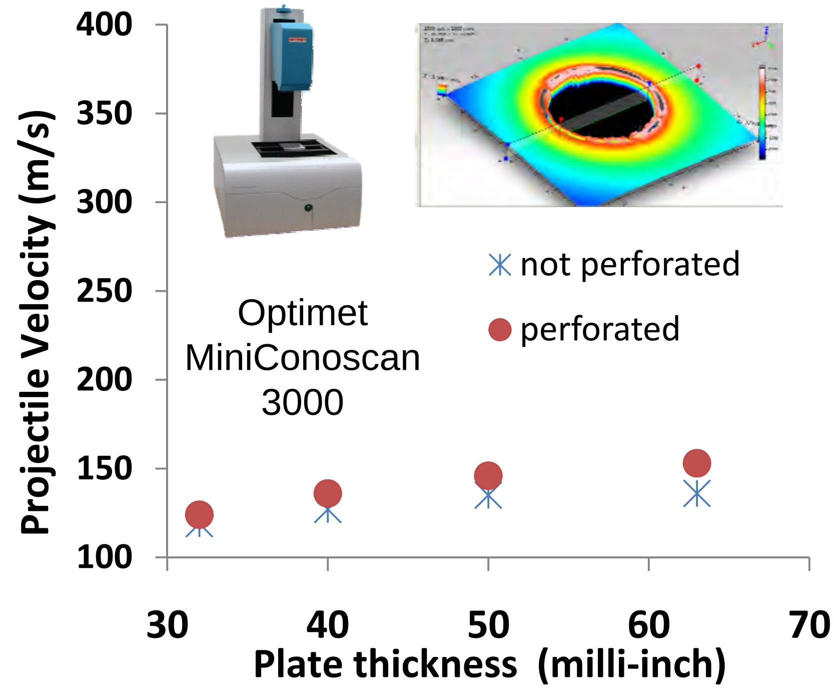
Ballistic impact – SBGG

System inputs (X)	System Outputs (Y)	
	Diagnostics	Metrics
Projectile velocity		
Plate thickness	Conoscope	Profilometry Perforation area
Projectile/plate materials		

Ballistic impact - Sample data

CALTECH PSAAP





Perforation area *vs*. impact velocity
(note small data scatter!)

Perforation/non-perforation
boundary

Experimental ballistic curves (SBGG)
S2 Steel spherical projectiles
Al 6061 plate targets

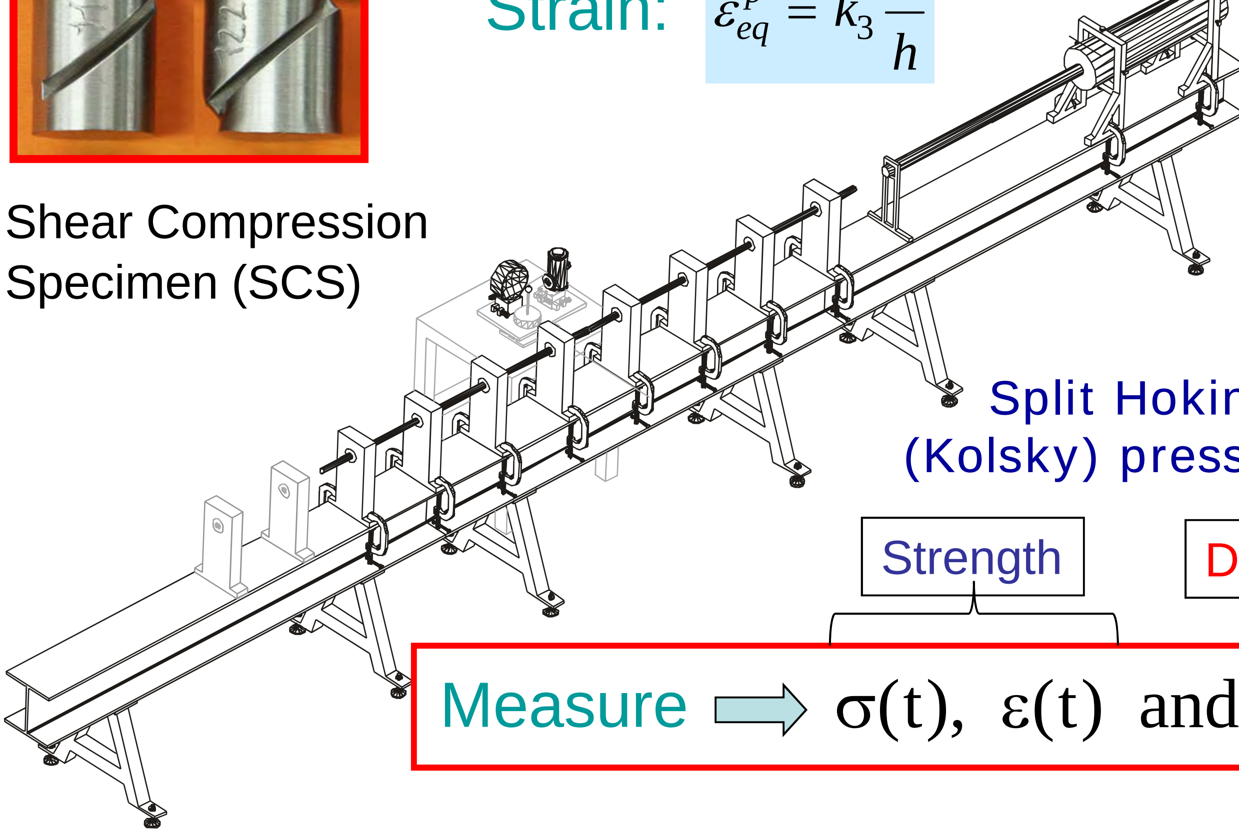
High Strain-Rate Testing (HSRT)

CALTECH PSAAP

Shear Compression Specimen (SCS)

Stress: $\sigma_{eq} = k_1 (1 - k_2 \varepsilon_{eq}^p) \frac{P}{Dt}$

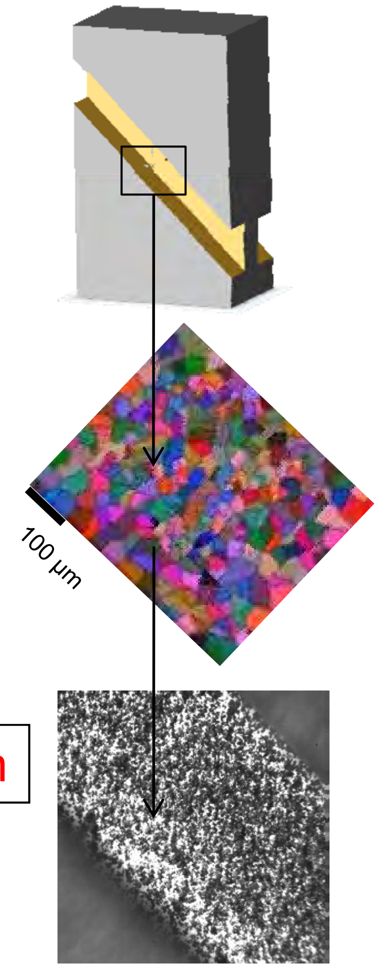
Strain: $\varepsilon_{eq}^p = k_3 \frac{d}{h}$



Split Hokinson (Kolsky) pressure bar

Strength | Dissipation

Measure ⟹ $\sigma(t)$, $\varepsilon(t)$ and $\theta(t)$



Full-field imaging, Sub-grain resolution

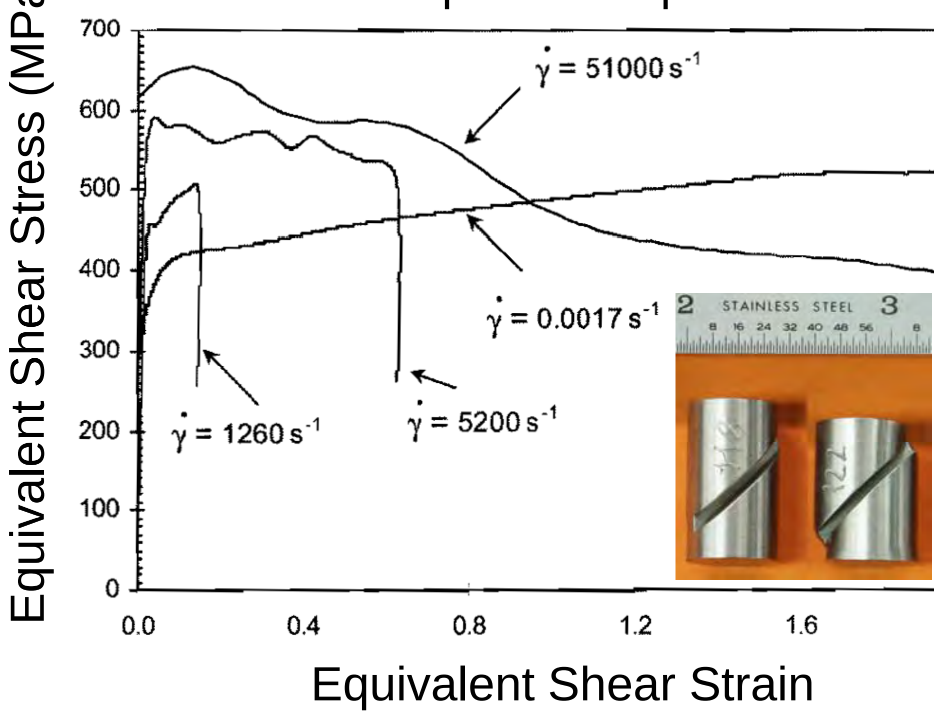
Caltech's High Strain-Rate Testing (HSRT) facility
(Prof. G. Ravichandran, Director)

Conventional validation - Examples

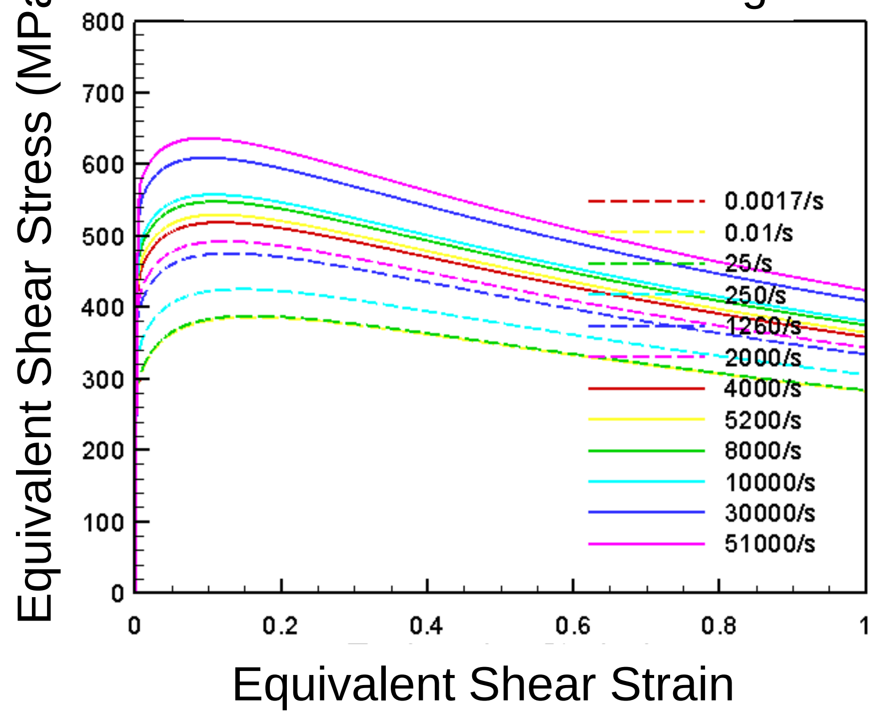
CALTECH PSAAP

Power-law strain-rate sensitivity

Shear compression specimen



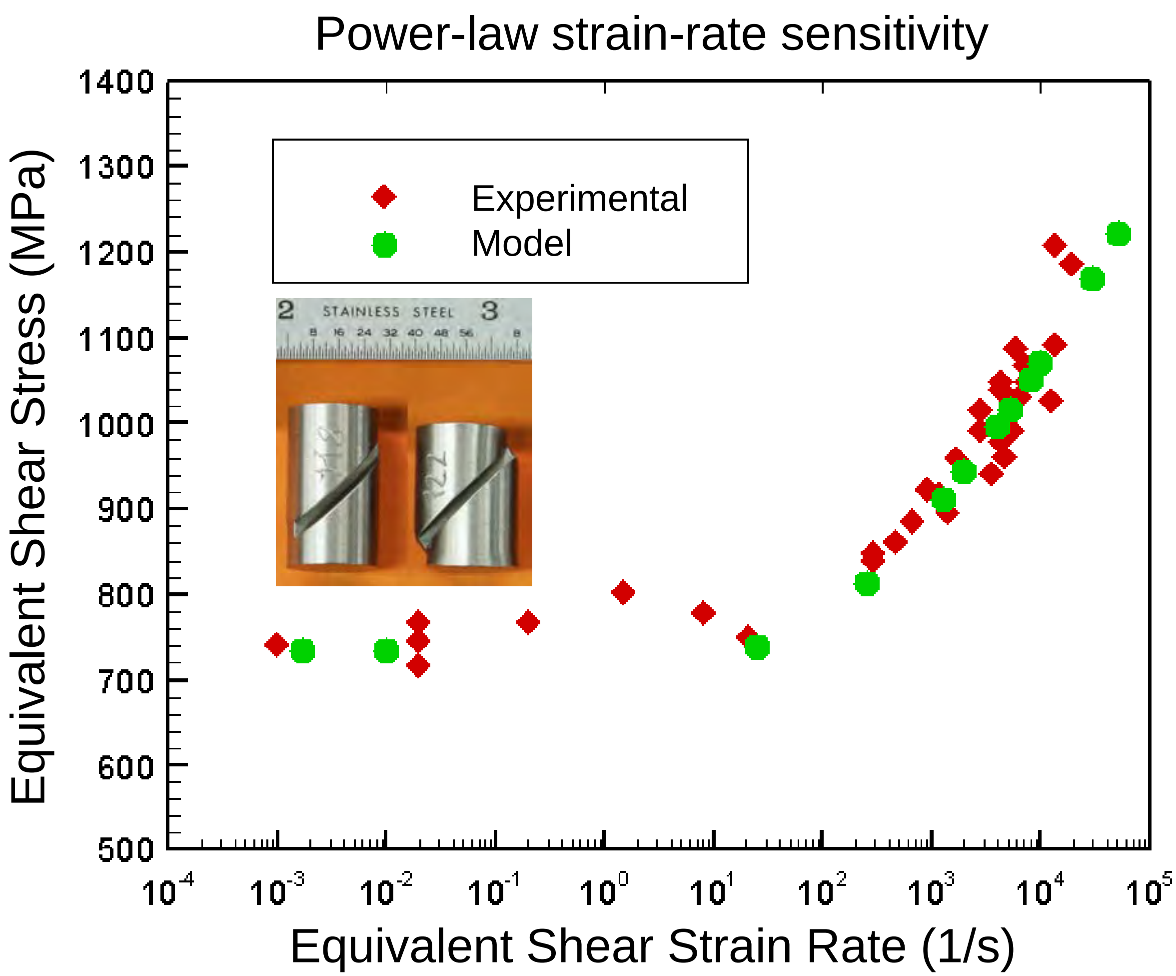
Power-law work hardening



M. Vural, D. Rittel and G. Ravichandran, “Large strain mechanical behavior of 1018 cold-rolled steel over a wide range of strain rates,” *Metallurgical and Materials Transactions A*, Vol. 34A (2003) p. 2873.

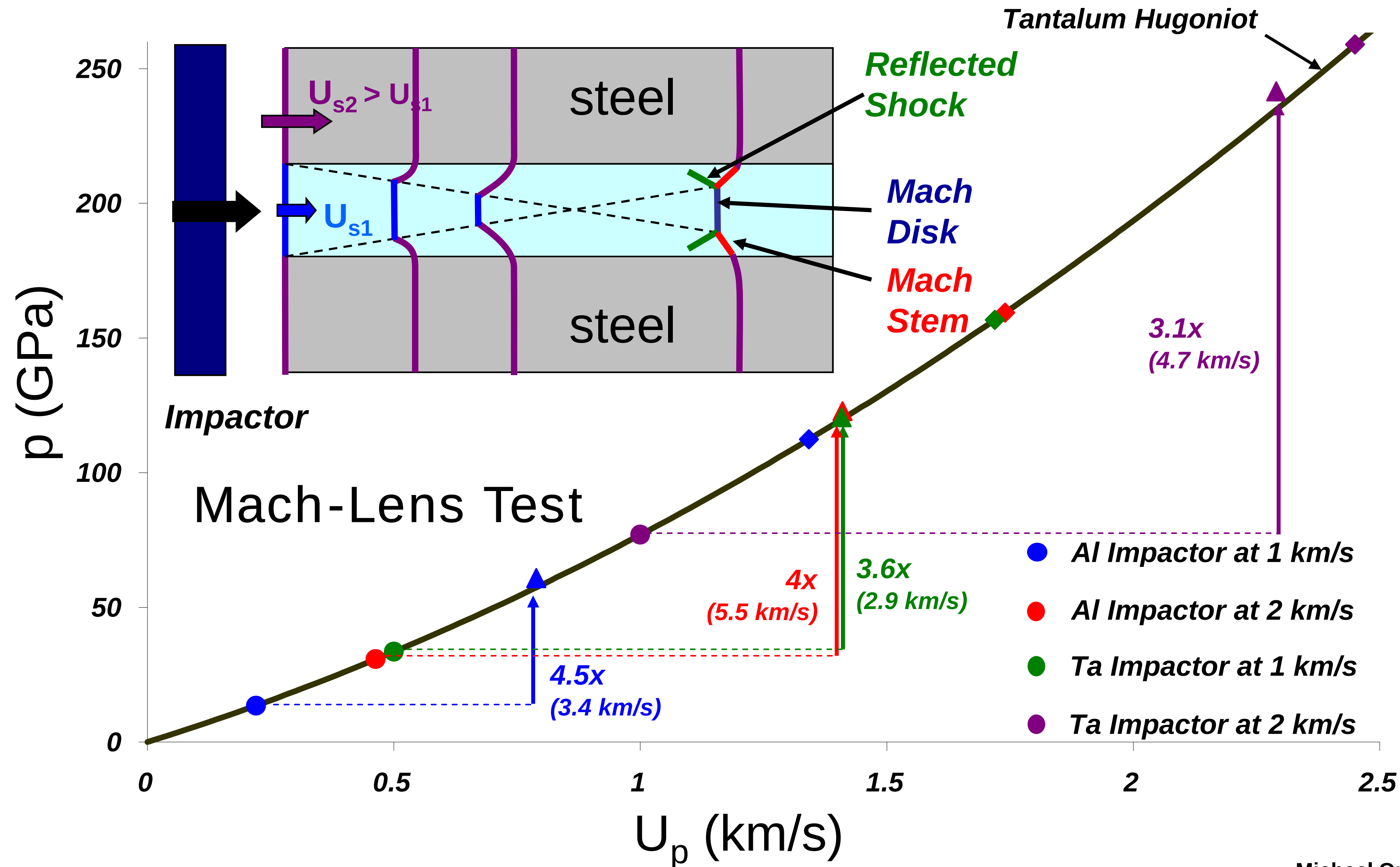
Conventional validation - Examples

CALTECH PSAAP



M. Vural, D. Rittel and G. Ravichandran, "Large strain mechanical behavior of 1018 cold-rolled steel over a wide range of strain rates," *Metallurgical and Materials Transactions A*, Vol. 34A (2003) p. 2873.

High Strain-Rate Testing (HSRT)



Michael Ortiz

Experimental data at Caltech

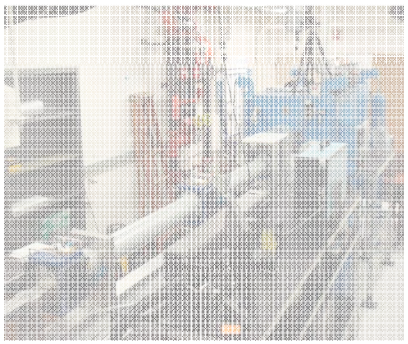
CALTECH PSAAP

- The Caltech center has its own in-house experimental facilities:
  - Small Particle Hypervelocity Impact Range
  - Small Bore Gas Gun Facility (ballistics)
  - High-Strain Rate Facility (constitutive characterization)
- Experimental facilities are reconfigurable and may be regarded as black boxes mapping inputs to outputs
- Experimental facilities supply specific instances of systems to be modeled, tested and certified
- Experimental facilities supply data in for purposes of Uncertainty Quantification
  - Integral 'data on demand' at fixed inputs
  - Integral legacy data (by accumulation)
  - Component data (e.g., constitutive data)

Center’s assets

CALTECH PSAAP

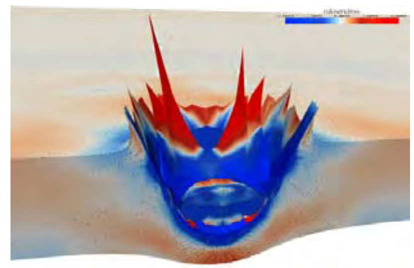
Experimental Science



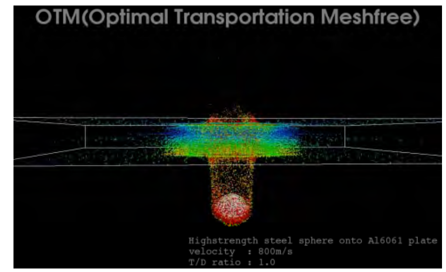
SPHIR

HSRT

Simulation codes

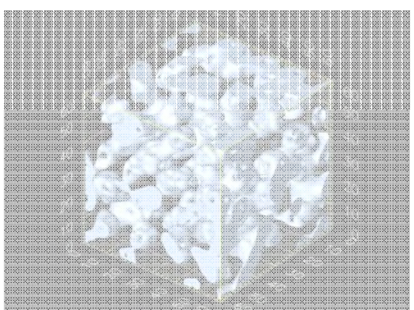


VTF

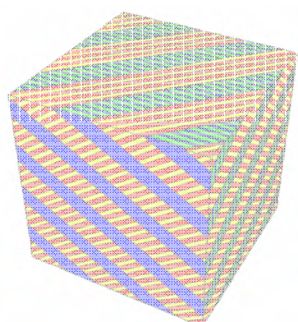


Eureka

Physics models

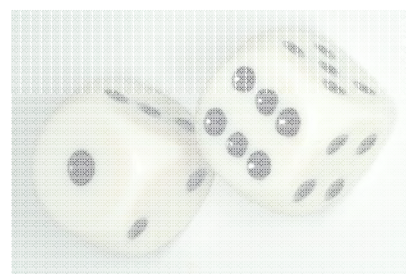


Plasma/EoS

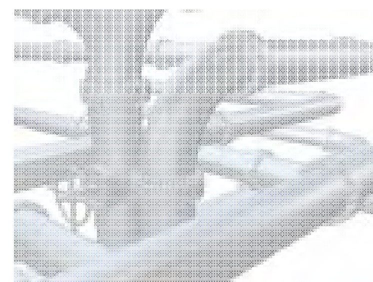


Strength

UQ tools



Probability/CoM



UQ pipeline

Focus simulation - Roadmap

CALTECH PSAAP

Simulation roadmap

April 15, 2008

Center starts

ABAQUS Explicit

- Lagrangian FEM
- Explicit dynamics
- Explicit contact
- Element erosion
- Engr. Models
- Serial

Lagrangian VTF

- Lagrangian FEM
- Explicit dynamics
- Proxy-ball contact
- Element erosion
- Engr. Models/EoS
- Massively parallel

Eureka OTM

- Update-Lagrange
- Optimal transport
- Meshfree/MPM
- Variational dyns
- Seizing contact
- Erosion/fracture
- Multiscale models

Eulerian VTF

- Eulerian AMR
- FD/WENO
- EoS/strength
- Multiphase/BC
- Ghost fluid
- Massive parallel

Serial | Parallel

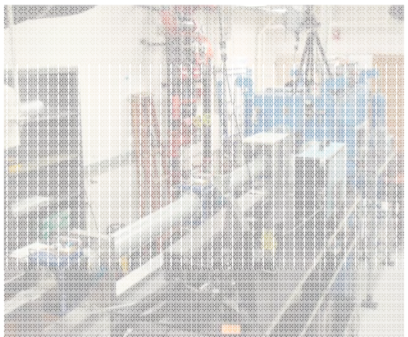
Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q

YEAR 1 YEAR 2 YEAR 3 YEA

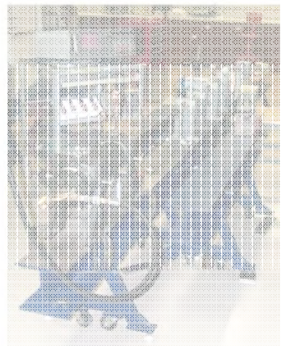
Center's assets

CALTECH
PSAAP

Experimental Science

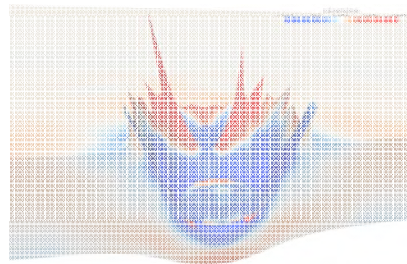


SPHIR

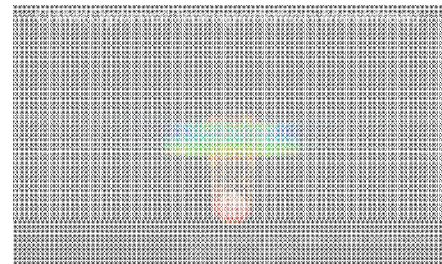


HSRT

Simulation codes

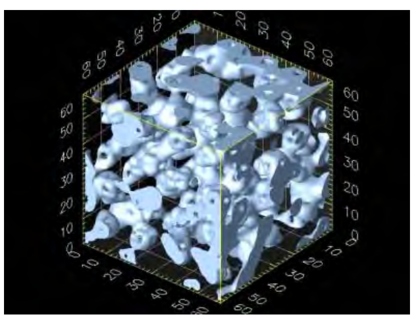


VTF

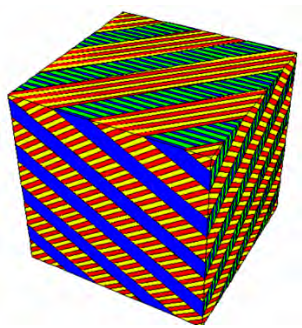


Eureka

Physics models

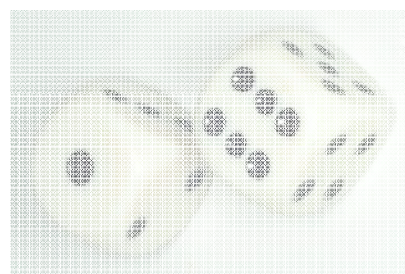


Plasma/EoS

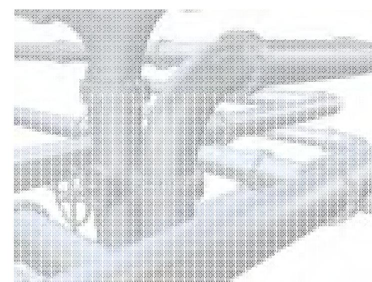


Strength

UQ tools

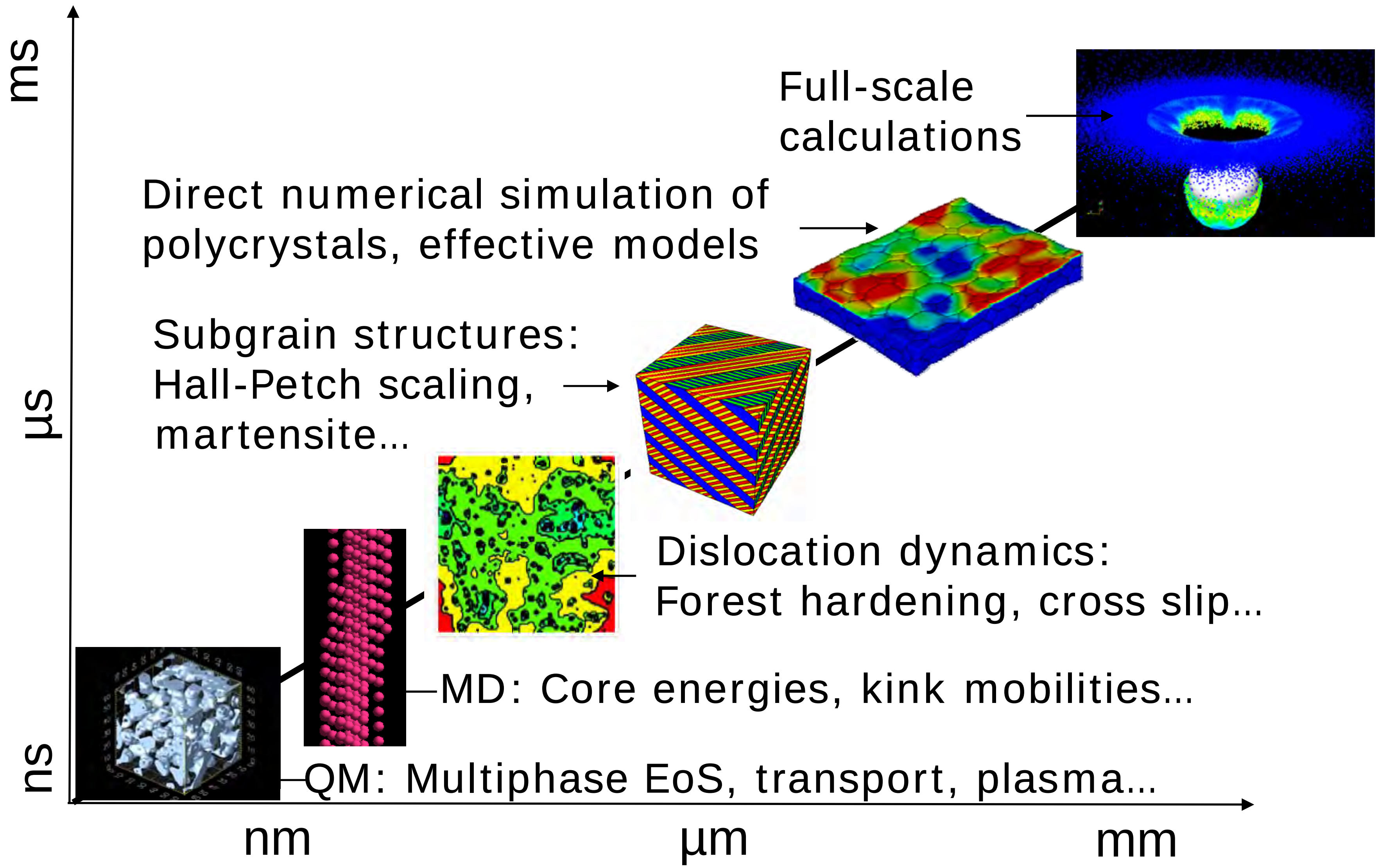


Probability/CoM

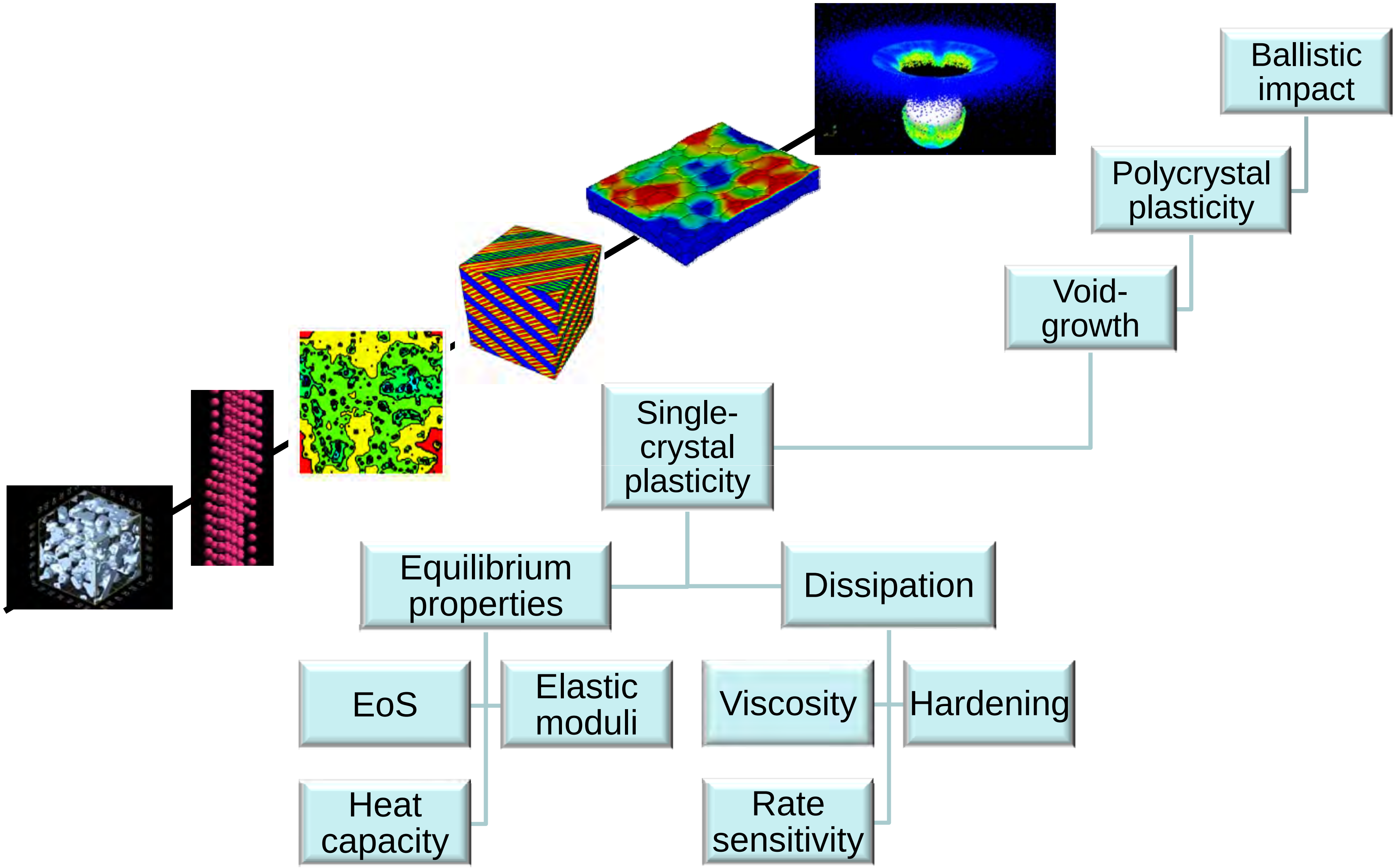


UQ pipeline

Multiscale models - Strength

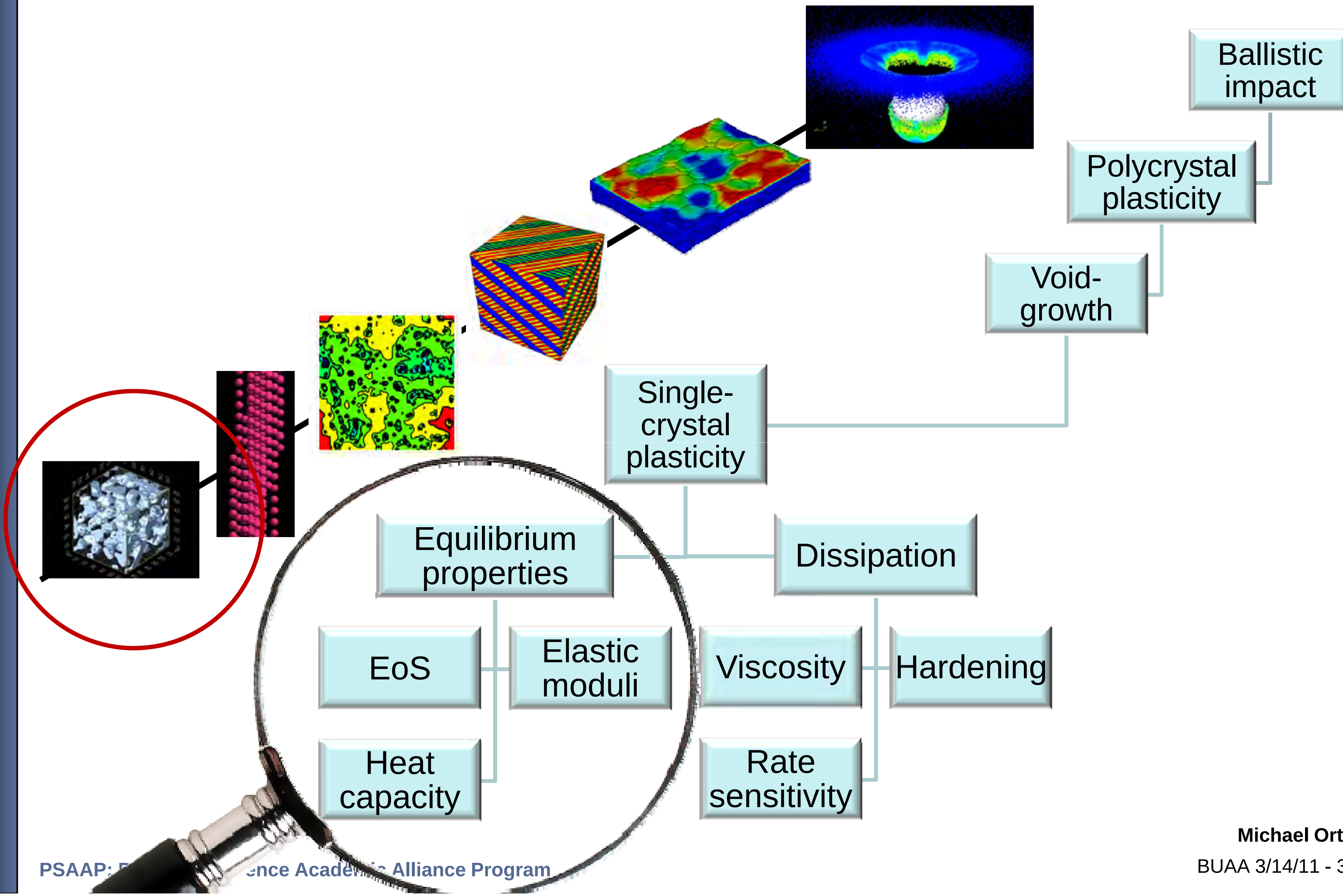


Multiscale Modeling - Strength

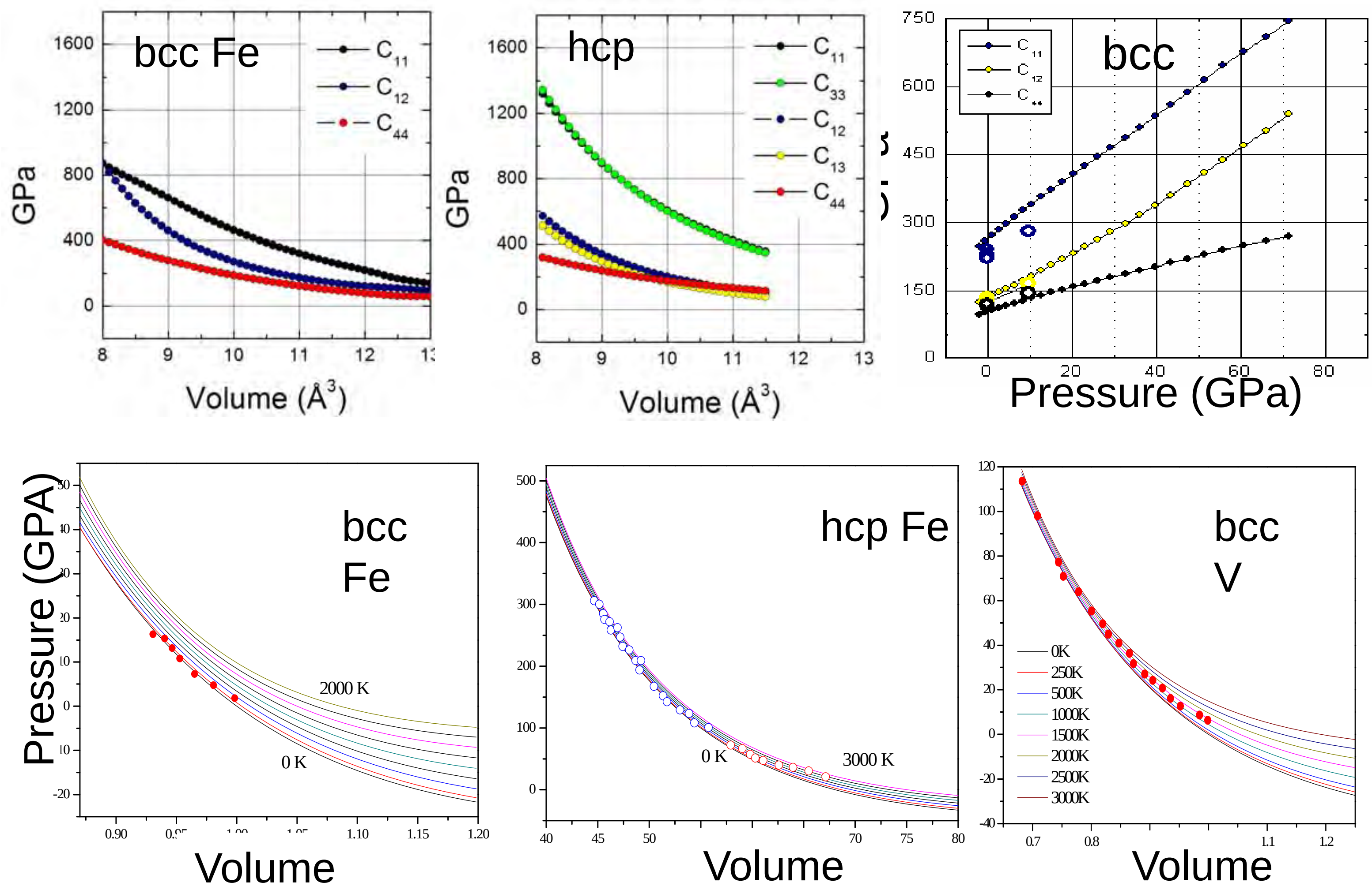


Multiscale Modeling - EoS

CALTECH PSAAP



Multiscale Modeling – Computed EoS

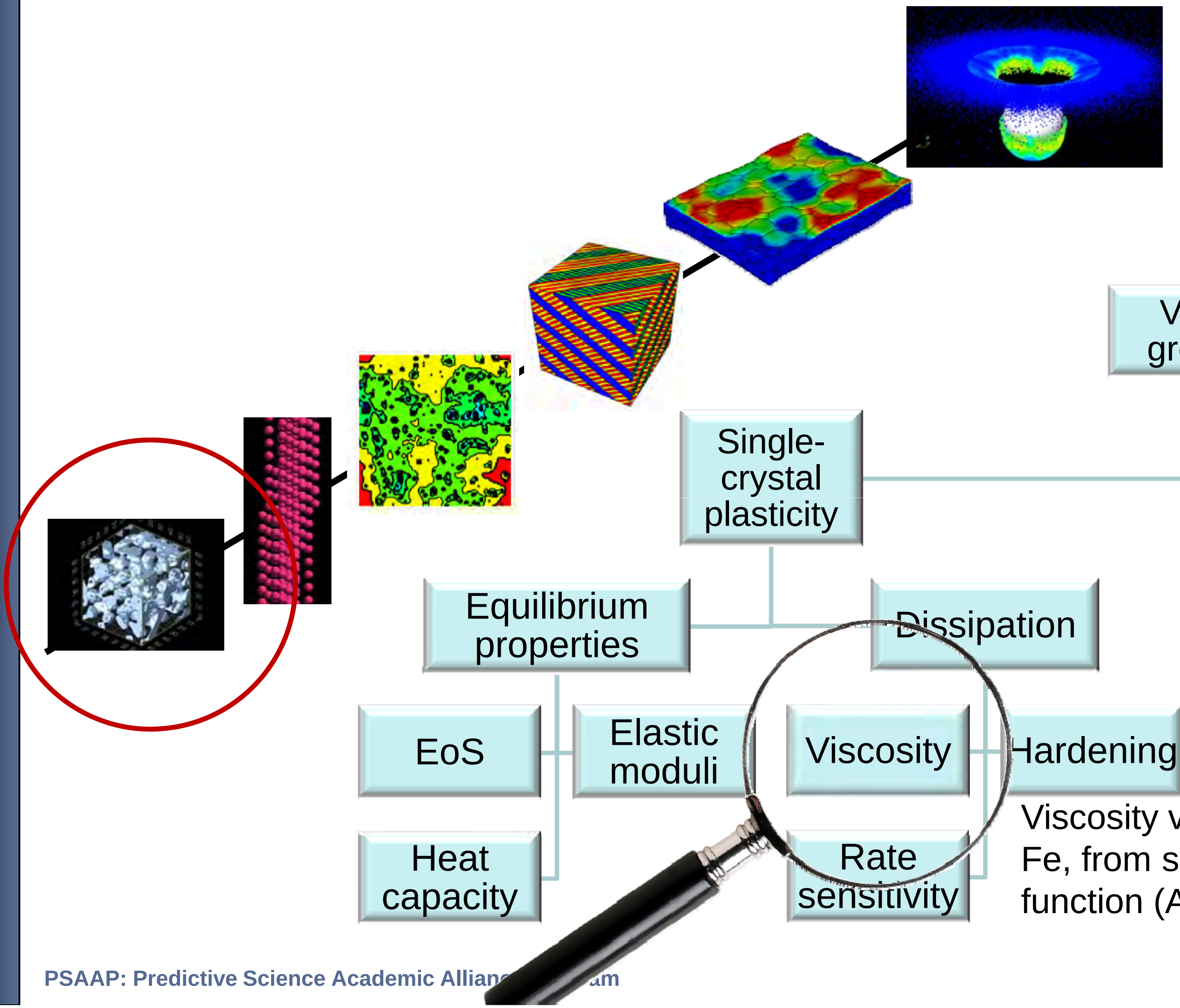


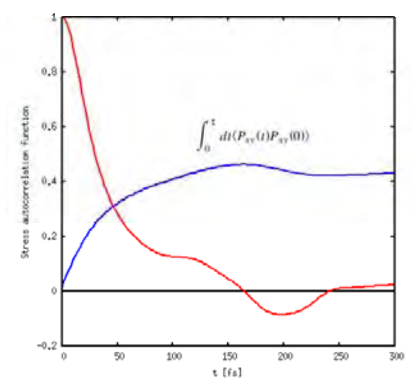
First-principles EoS, heat capacity, elastic moduli

(Wasserman, Stixrude and Cohen, PRB 53, 8296, 1996)

Michael Ortiz

Multiscale Modeling - Viscosity

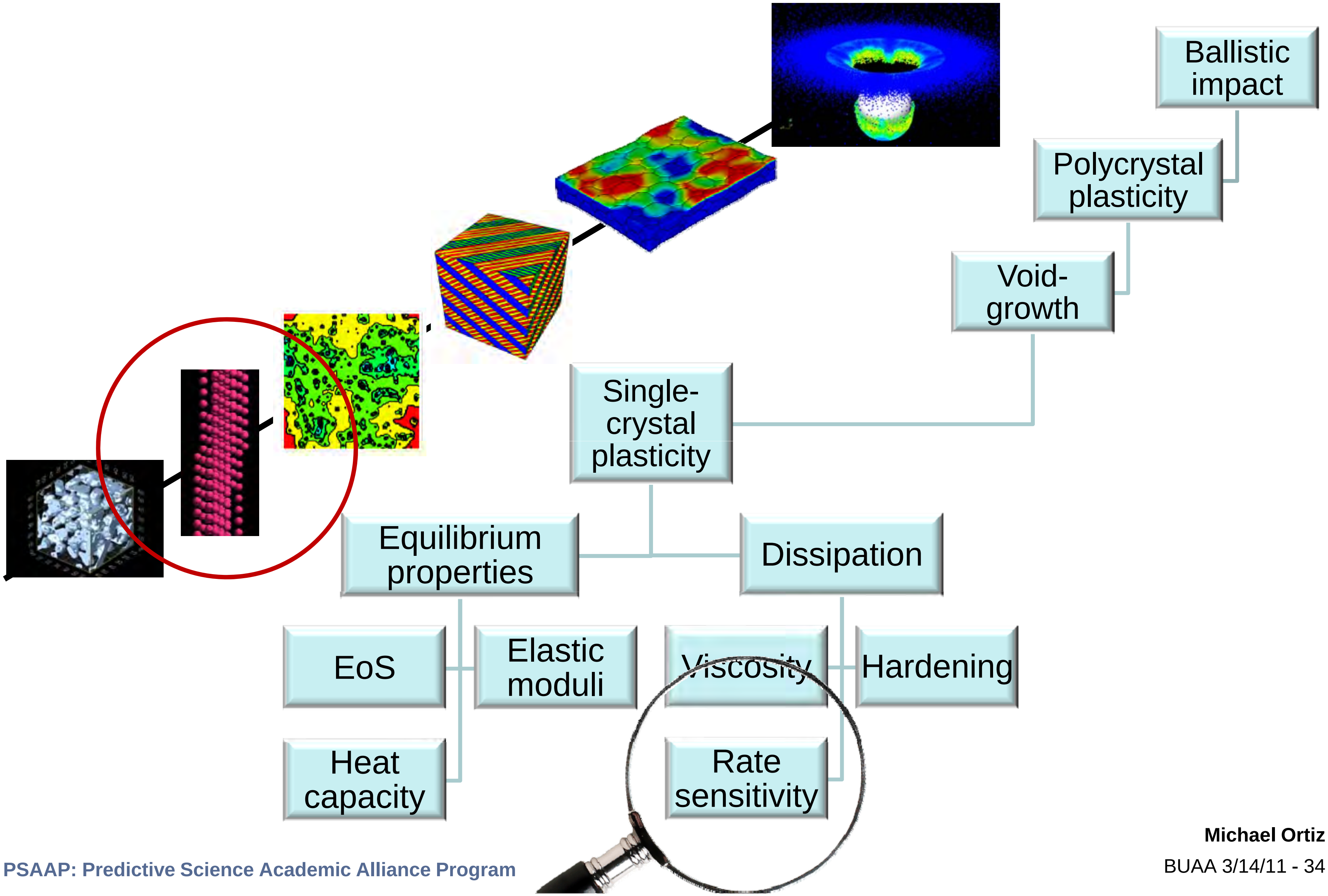




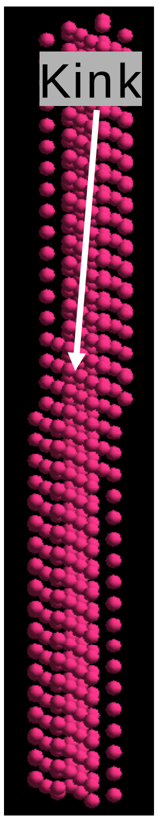
Viscosity vs (p,T) for liquid Ta, Fe, from shear stress autocorr. function (Axel van de Walle)

Michael Ortiz

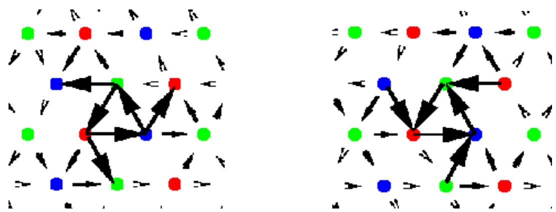
Multiscale Modeling - Transport



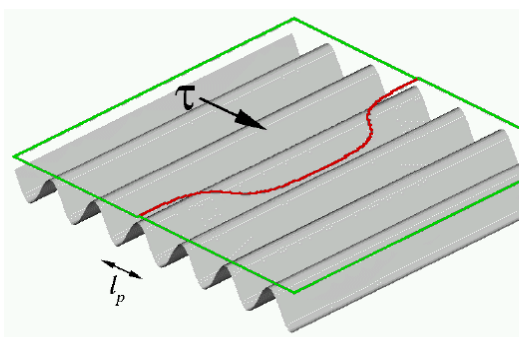
Multiscale Modeling – Rate sensitivity

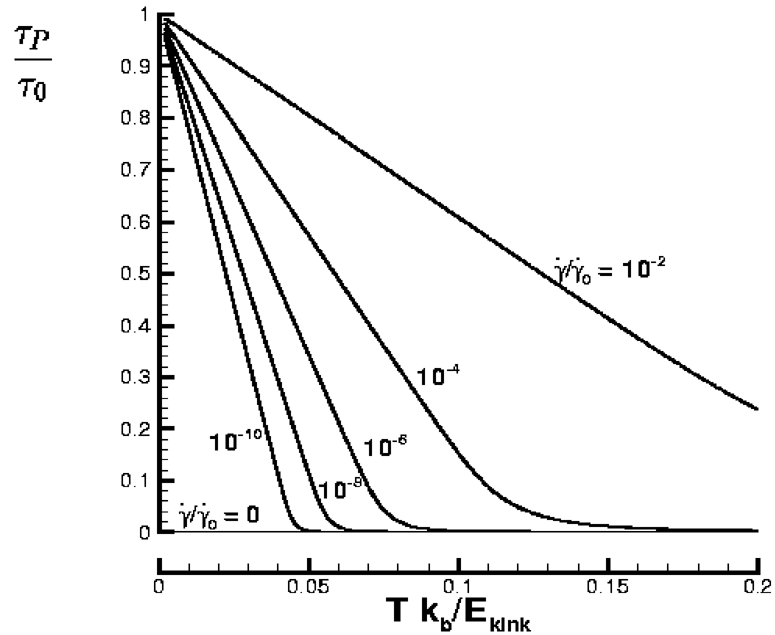


1/2<111> screw dislocation
Single Kinks (<112> kink)



Negative core (n)
Positive core (p)



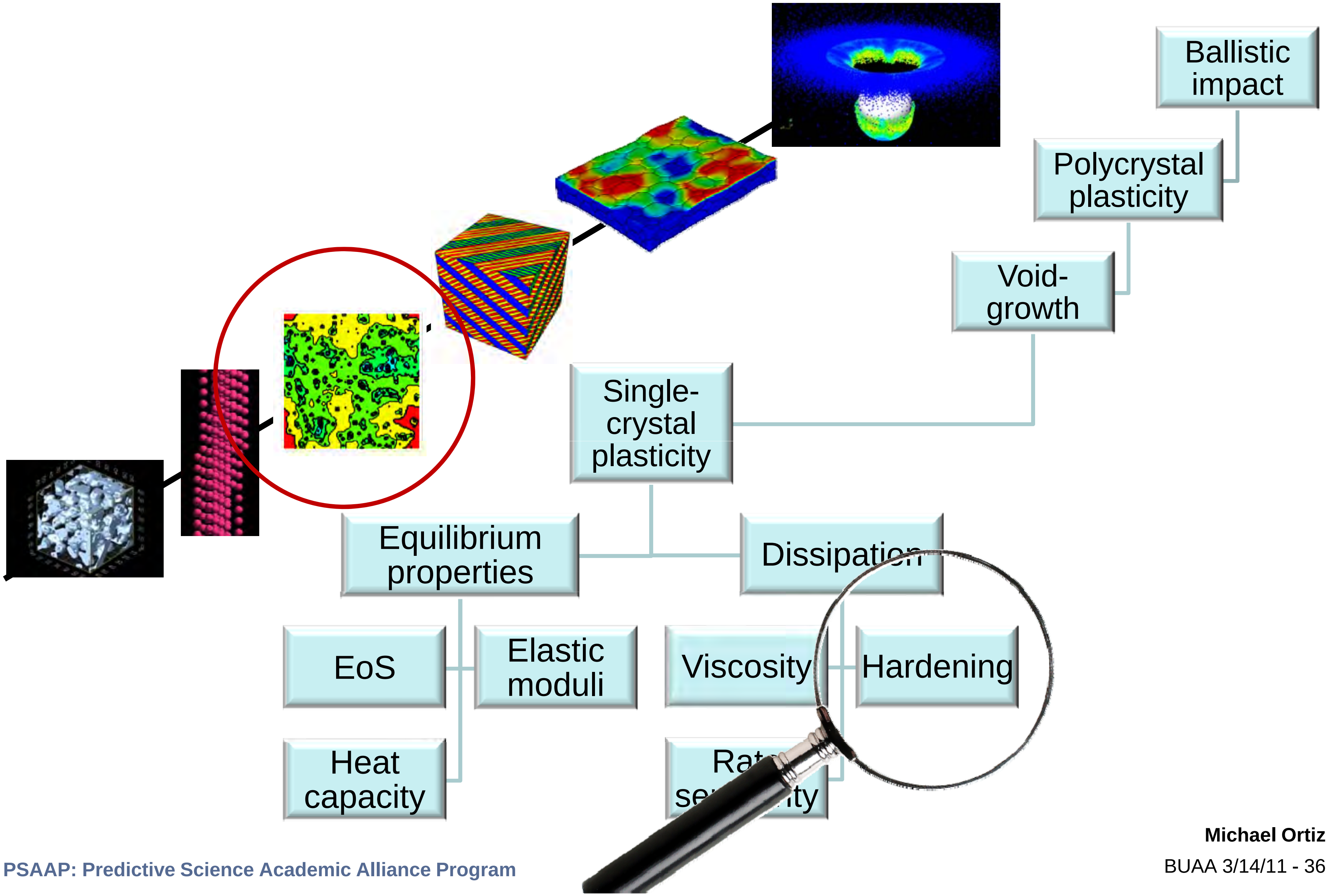


- From kink dynamics (MD):
  - Formation energies
  - Migration energy barriers
- From thermal activation theory:
  - Dislocation mobility
  - Rate sensitivity

Michael Ortiz

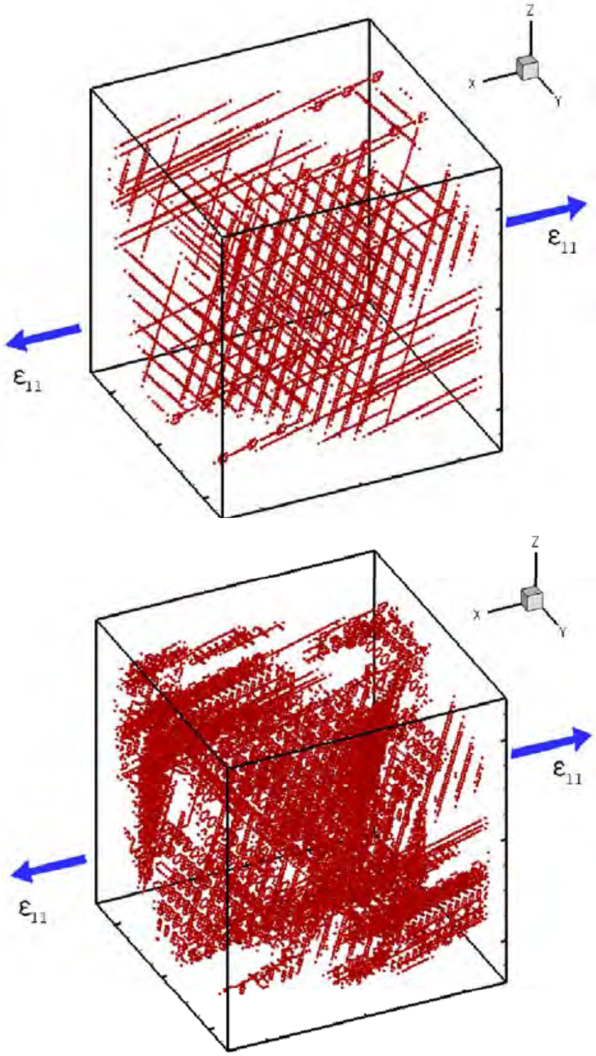
Multiscale Modeling - Hardening

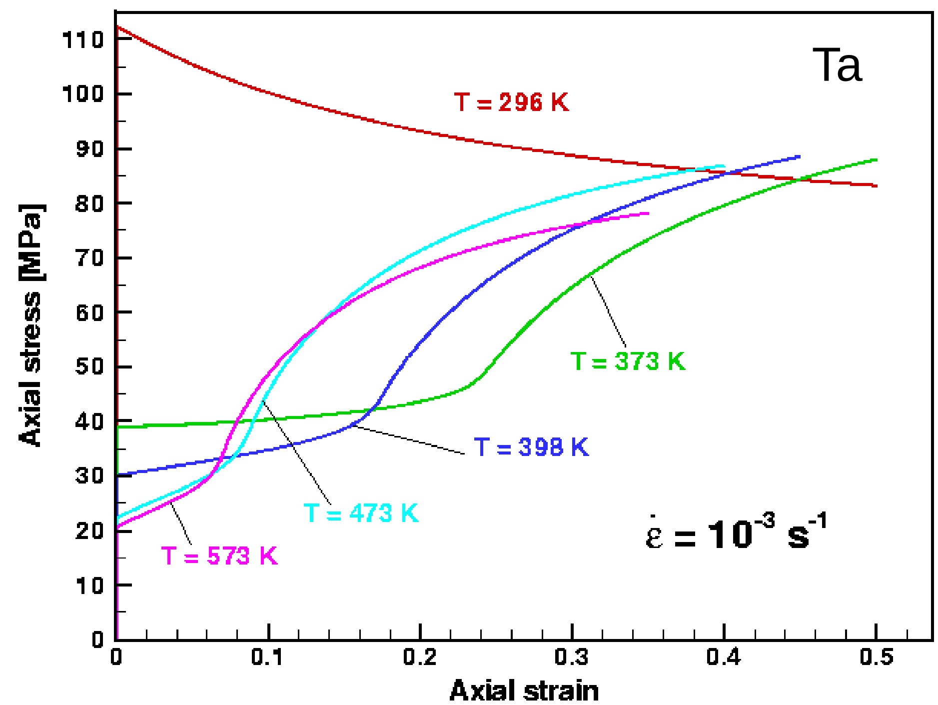
CALTECH PSAAP



Multiscale Modeling – Hardening

CALTECH PSAAP



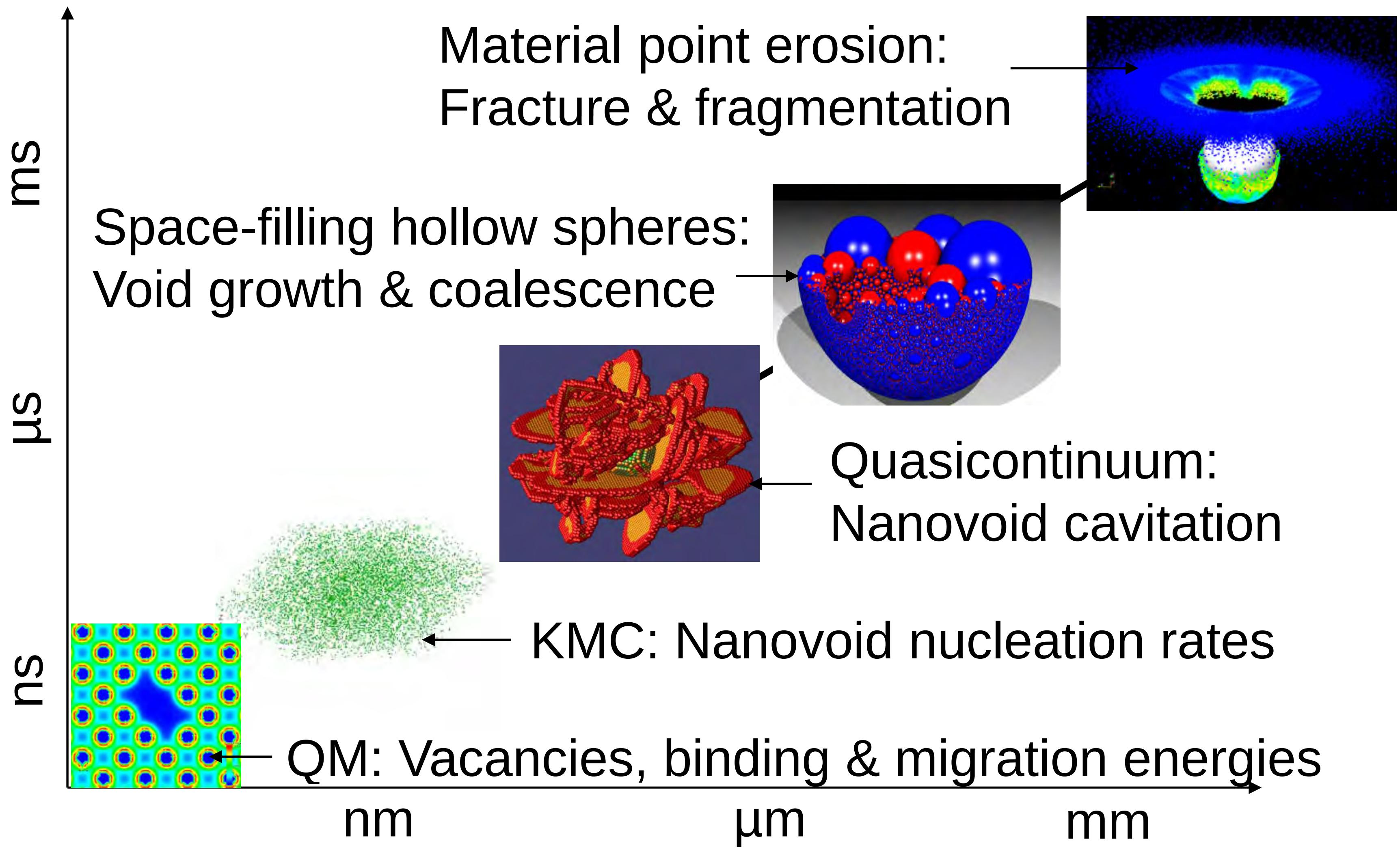


- From dislocation dynamics:
  - Anisotropic line tension
  - Secondary dislocations
  - Dislocation multiplication
- Percolation analysis (Kocks):
  - Hardening relations (analytical)

Michael Ortiz

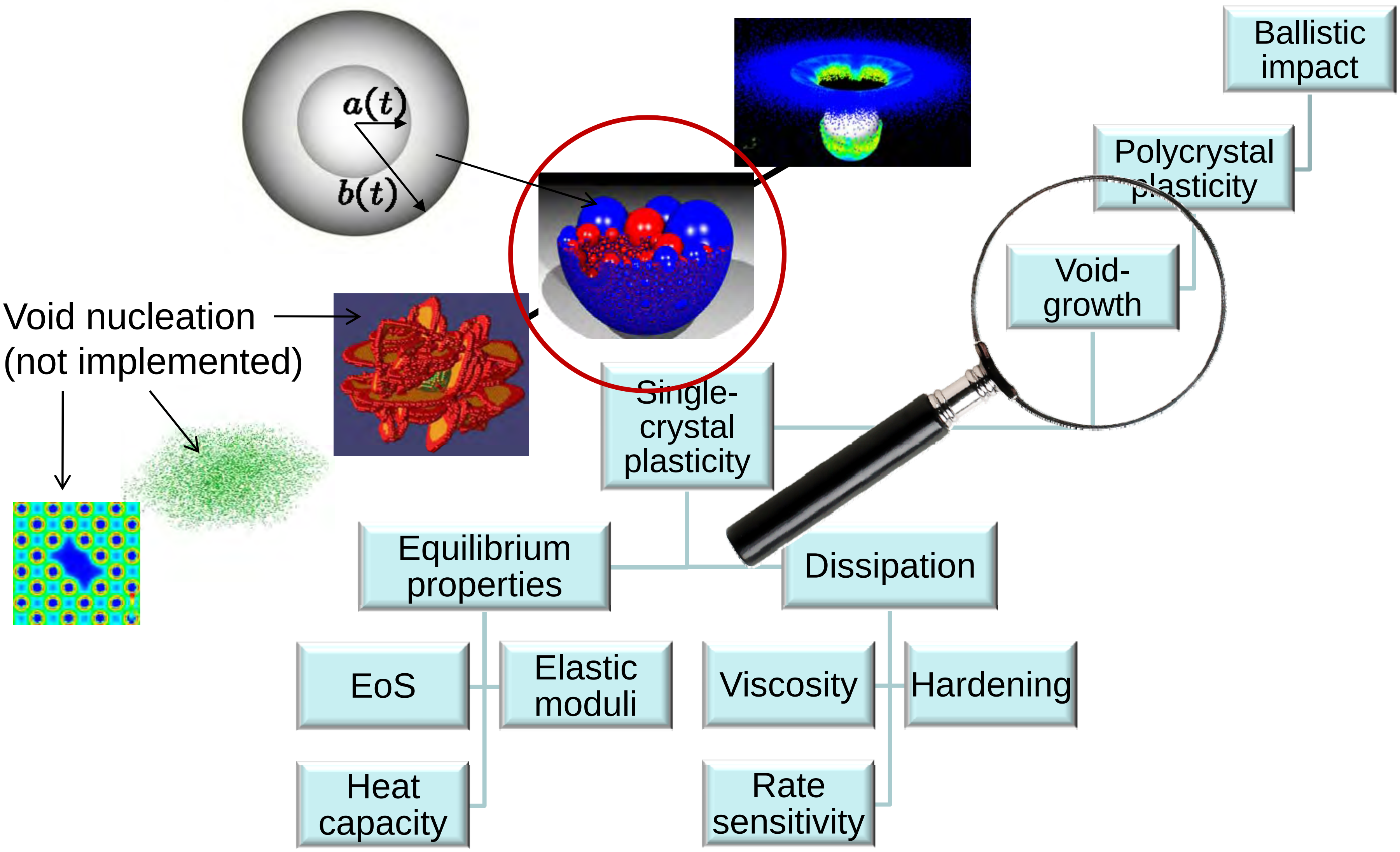
Multiscale models – Ductile fracture

CALTECH PSAAP



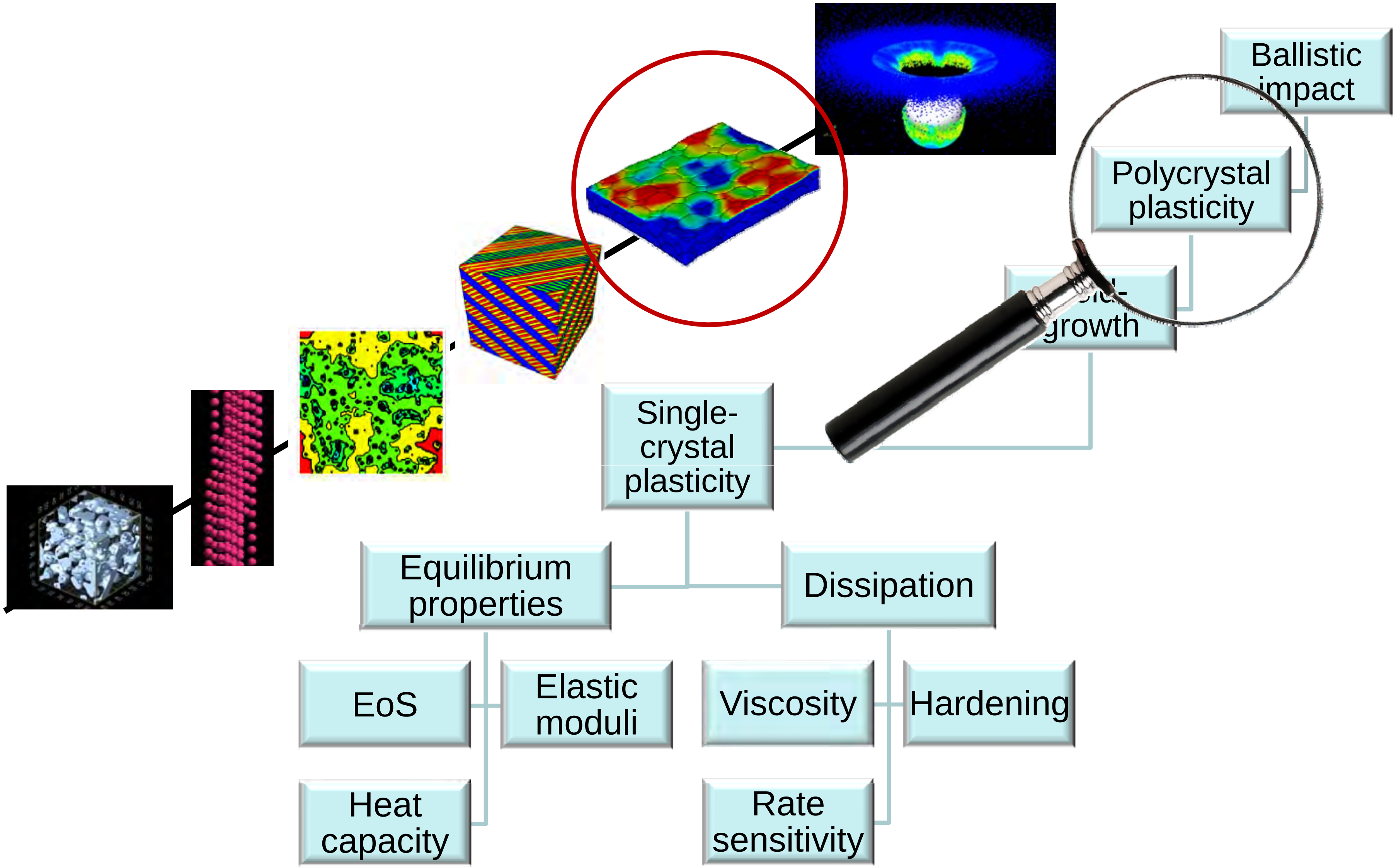
Multiscale Modeling – Fracture (FE^2)

CALTECH PSAAP



Michael Ortiz

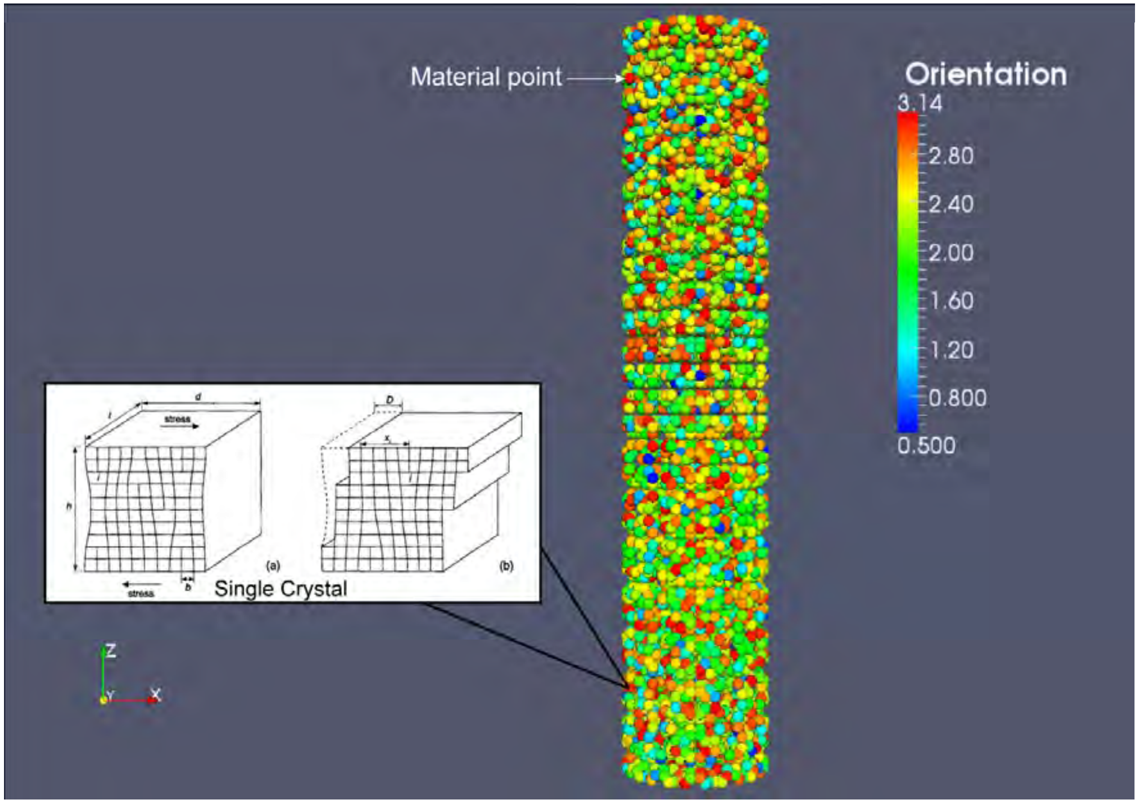
Multiscale Modeling - Polycrystal

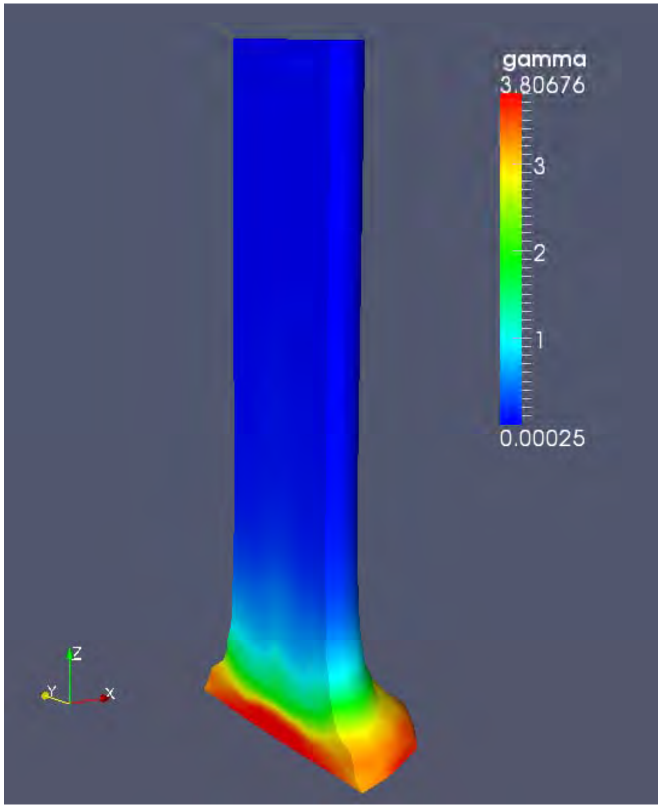


Multiscale Modeling - Polycrystal

CALTECH PSAAP

- Multiscale models integrated into full-scale simulations!





OTM simulation where each material point represents a randomly oriented crystal

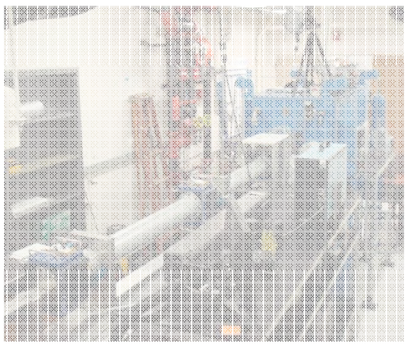
Copper cylinder striking frictionless rigid wall at 227m/s

Michael Ortiz

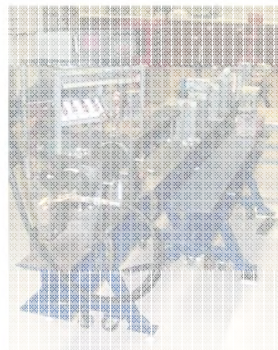
Center's assets

CALTECH PSAAP

Experimental Science

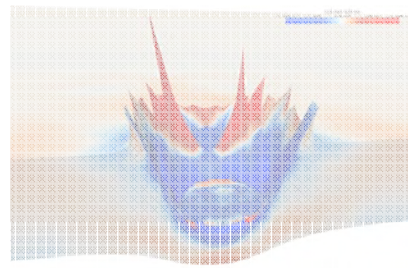


SPHIR

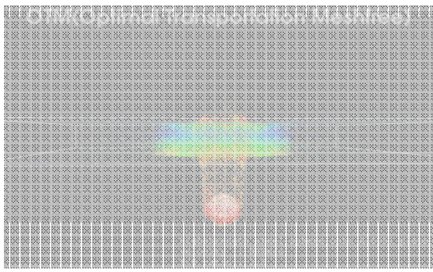


HSRT

Simulation codes

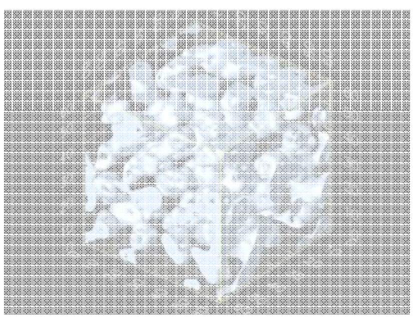


VTF

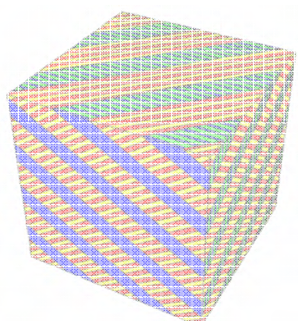


Eureka

Physics models



Plasma/EoS



Strength

UQ tools

Probability/CoM

UQ pipeline

Development of UQ methodology

UQ methodology timeline

April 15, 2008
Center starts

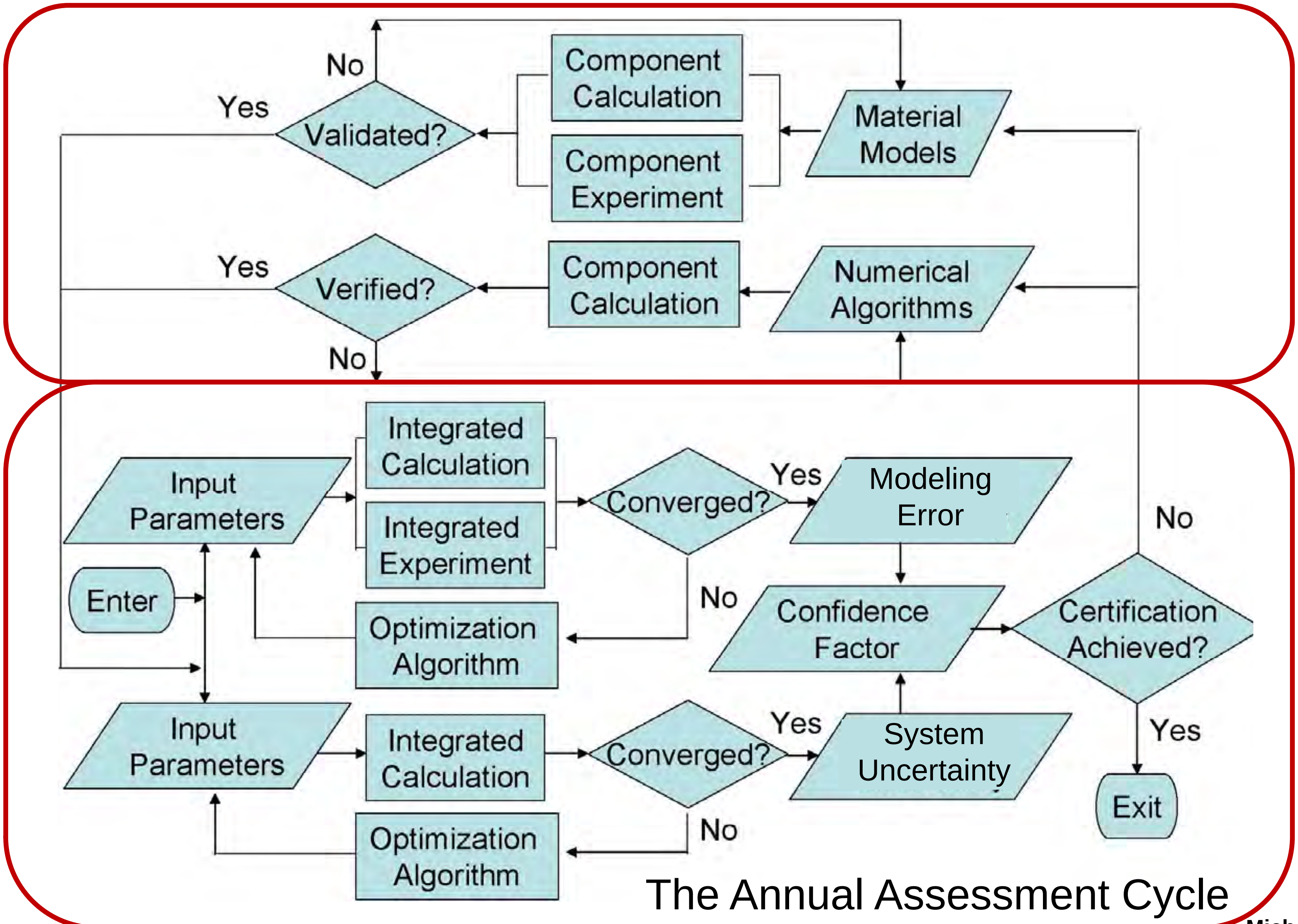
Data-on-Demand Protocol (I)	Data-on-Demand Protocol (II)	Legacy-Data Protocol
McDiarmid Inequality Noiseless data Controllable inputs	McDiarmid inequality Noisy data Uncontrollable inputs	McDiarmid inequality Lipschitz constants Noisy data

Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q3 Q4 | Q1 Q2 Q

YEAR 1 YEAR 2 YEAR 3 YEA

The data-on-Demand UQ protocol

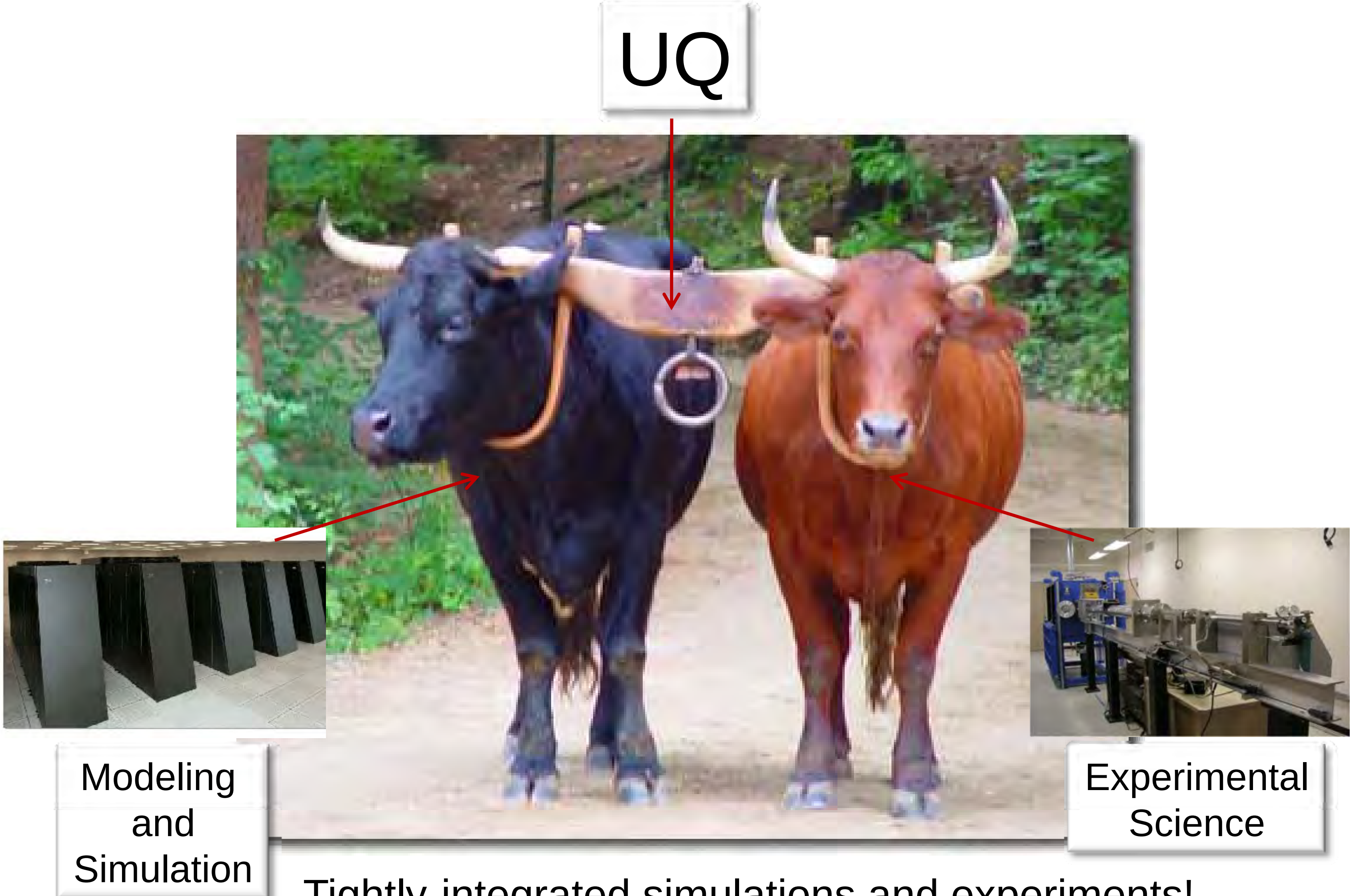
CALTECH PSAAP



Michael Ortiz

The data-on-Demand UQ Protocol

CALTECH PSAAP

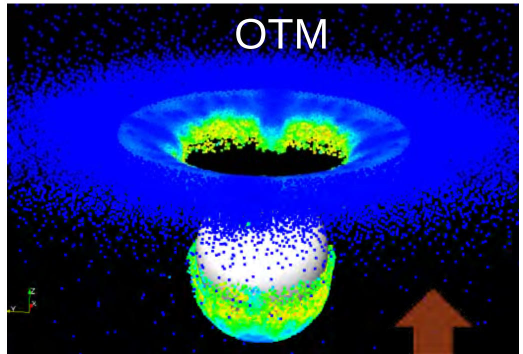


Tightly-integrated simulations and experiments!

Caltech's UQ pipeline - CSE

Effort led by Caltech's Center for Advanced Computing Research

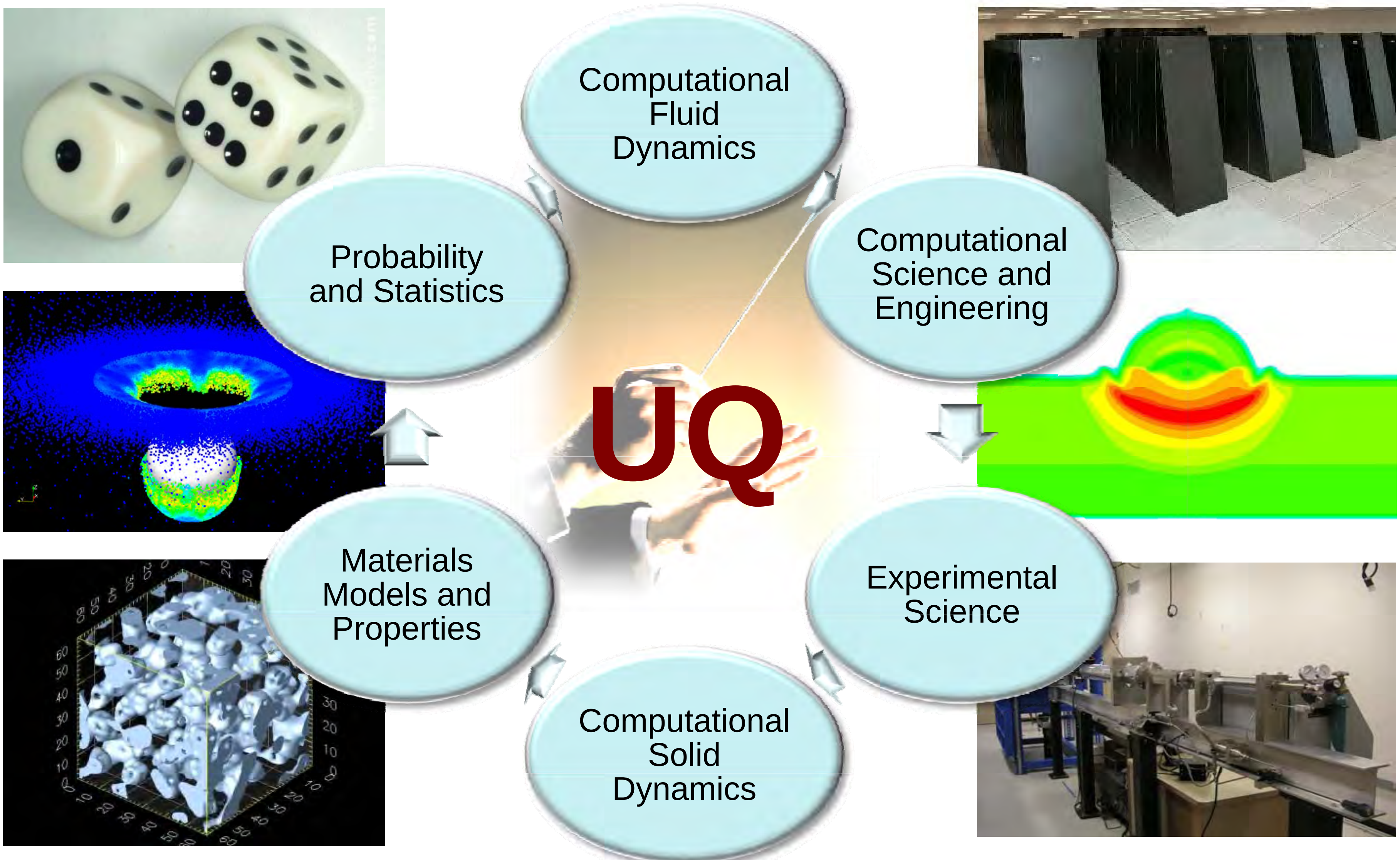
Challenge: Develop Computational Science and Engineering (CSE) infrastructure for uncertainty quantification (UQ) analysis.



Michael Ortiz

UQ orchestrates all activities

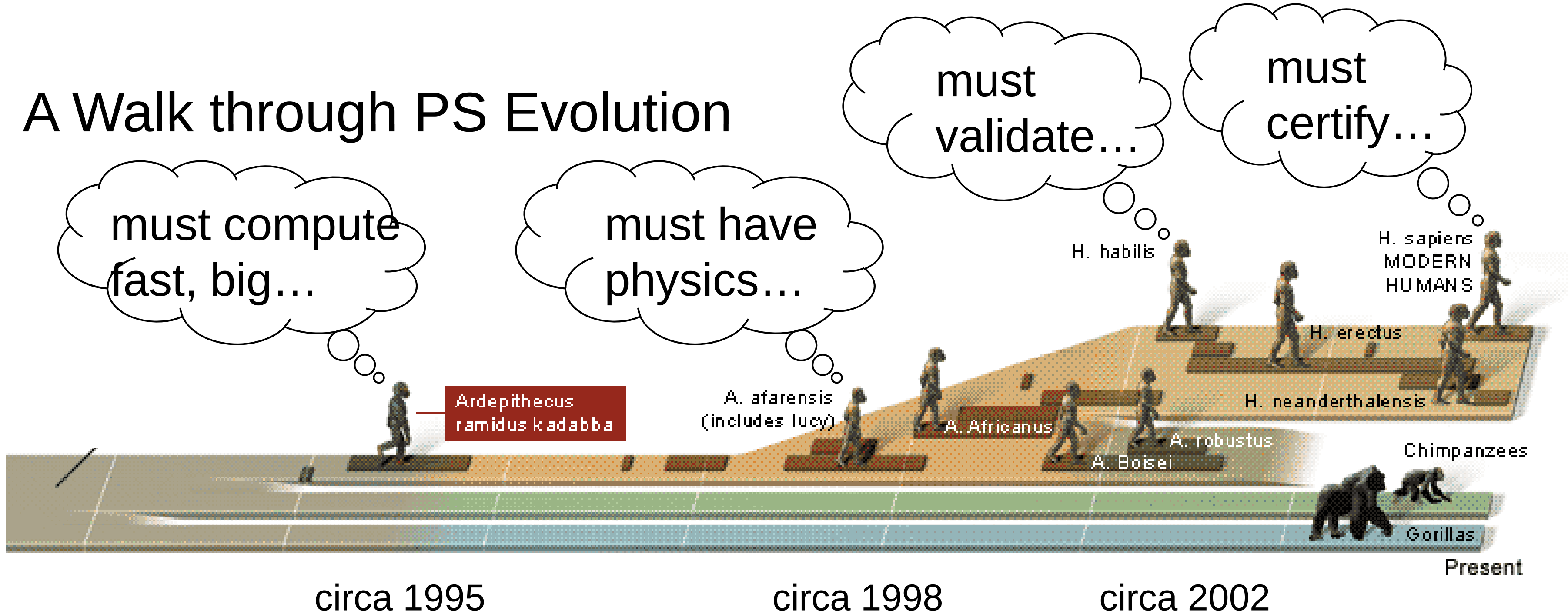
CALTECH PSAAP



Our vision for Predictive Science…

CALTECH PSAAP

A Walk through PS Evolution



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

Overview