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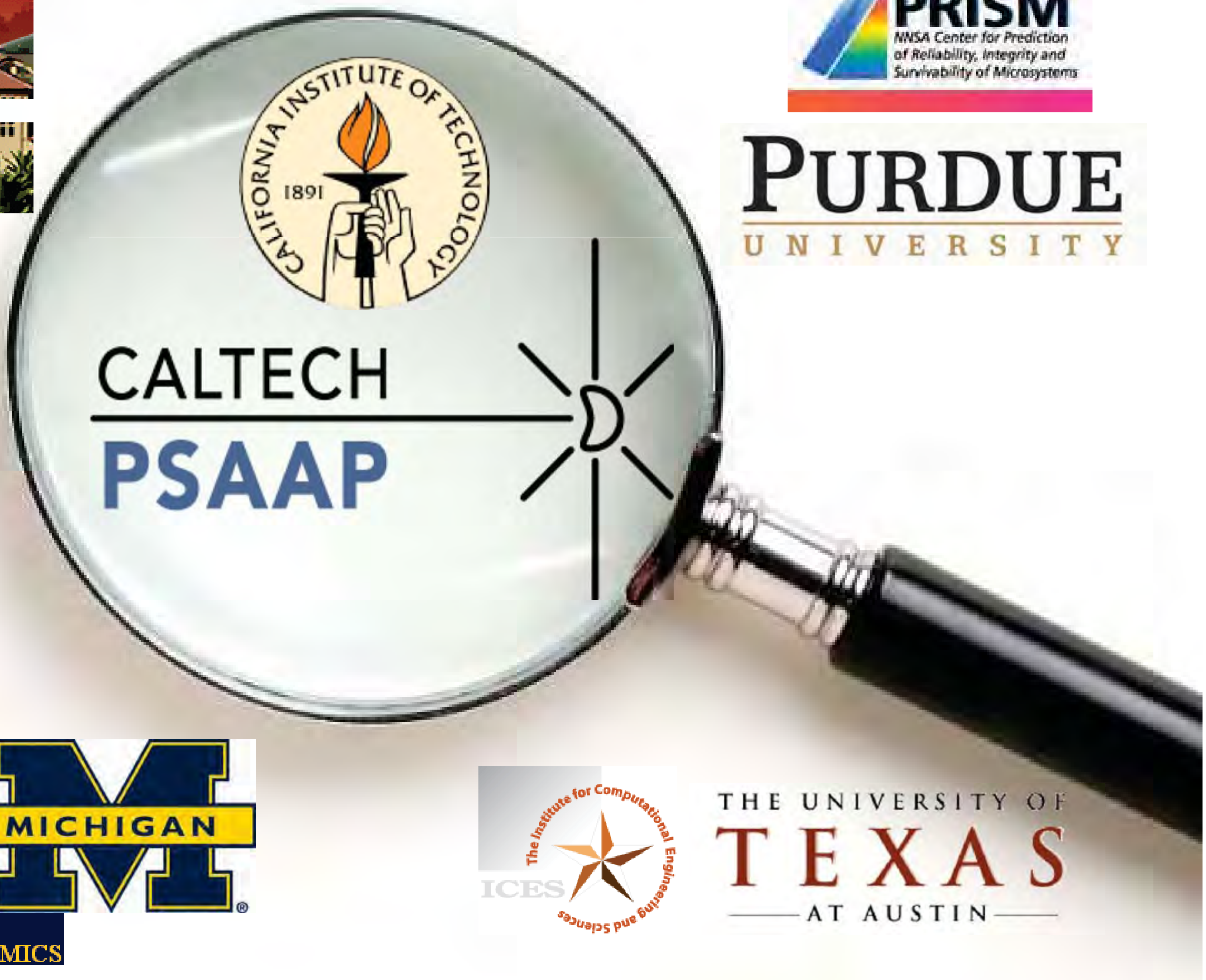
Multiscale Modeling of Materials: Linking Microstructure and Macroscopic Behavior

Michael Ortiz

DOE CSGF Conference
Krell Institute, July 27, 2012

DoE/ASC/PSAAP Centers



STANFORD UNIVERSITY

PSAAP

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

PURDUE UNIVERSITY

CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS

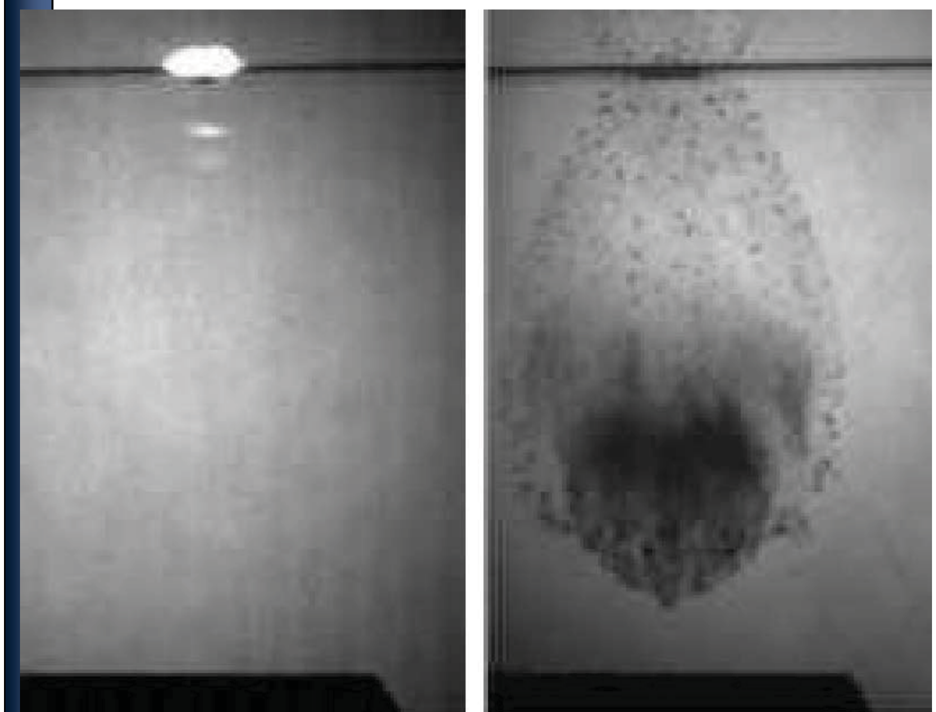
MICHIGAN

The Institute for Computational Engineering and Sciences
ICES

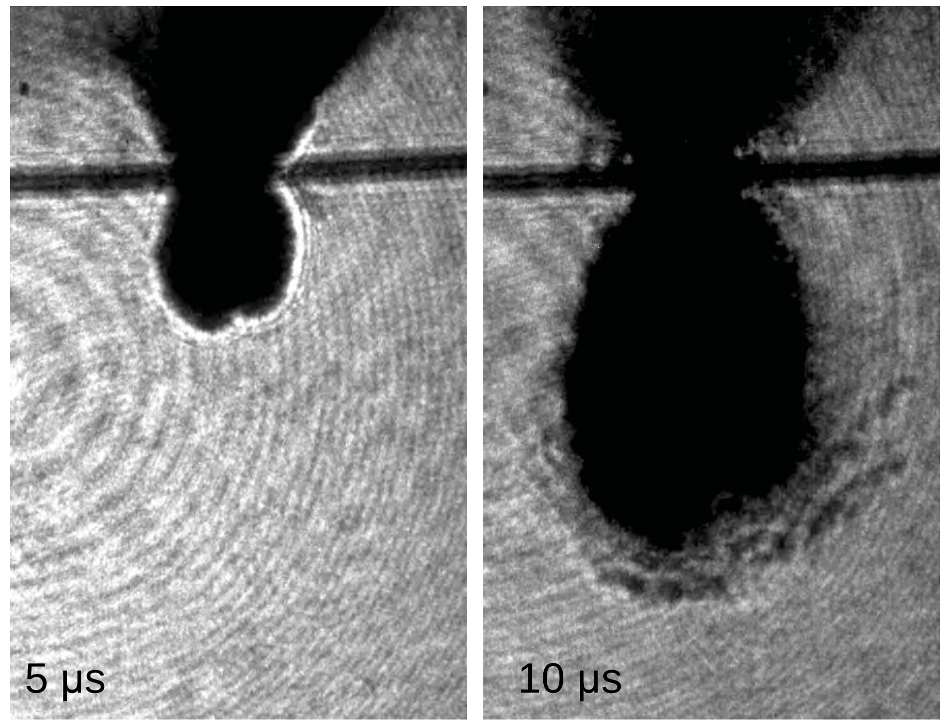
THE UNIVERSITY OF TEXAS AT AUSTIN

Solids under Extreme Conditions

How far can we push Modeling and Simulation?
(and still be predictive)



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



Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

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Hypervelocity impact - Simulation

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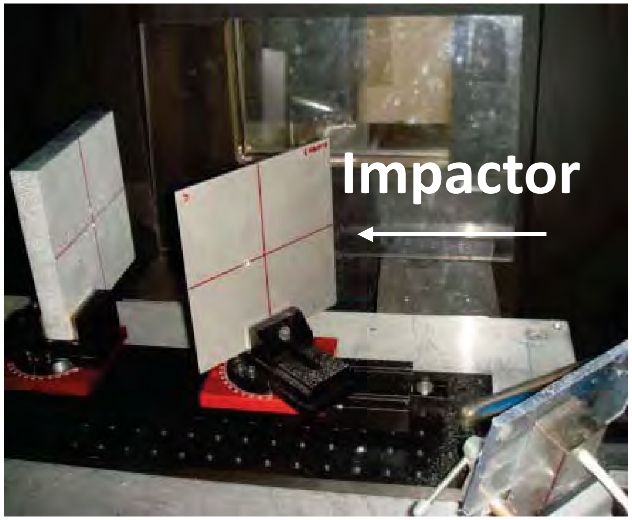
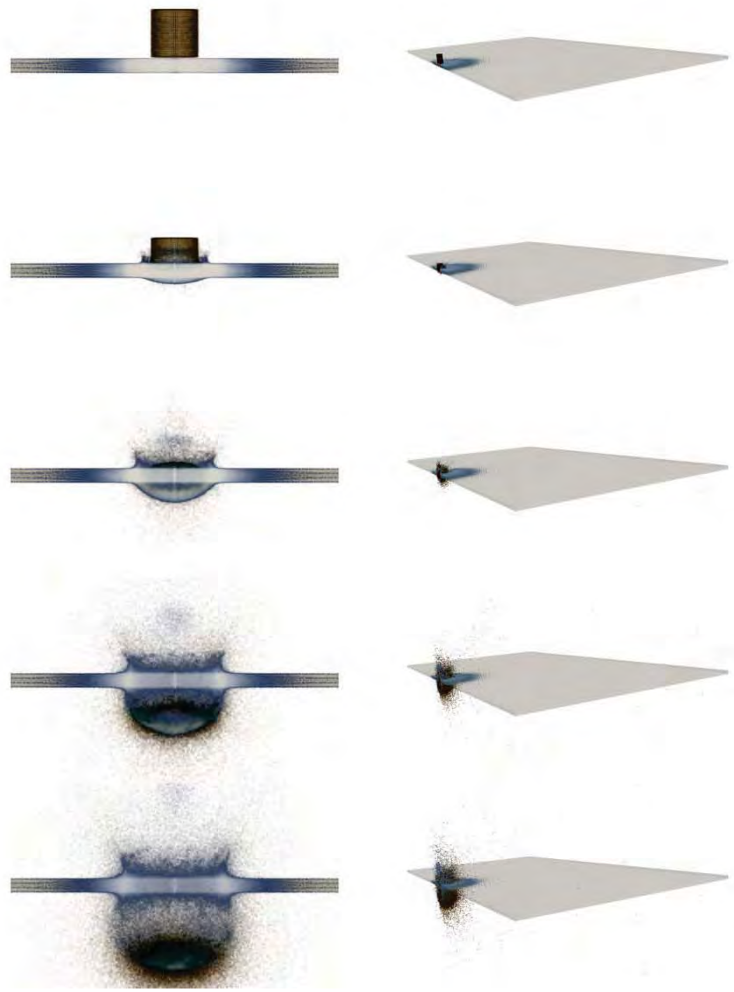
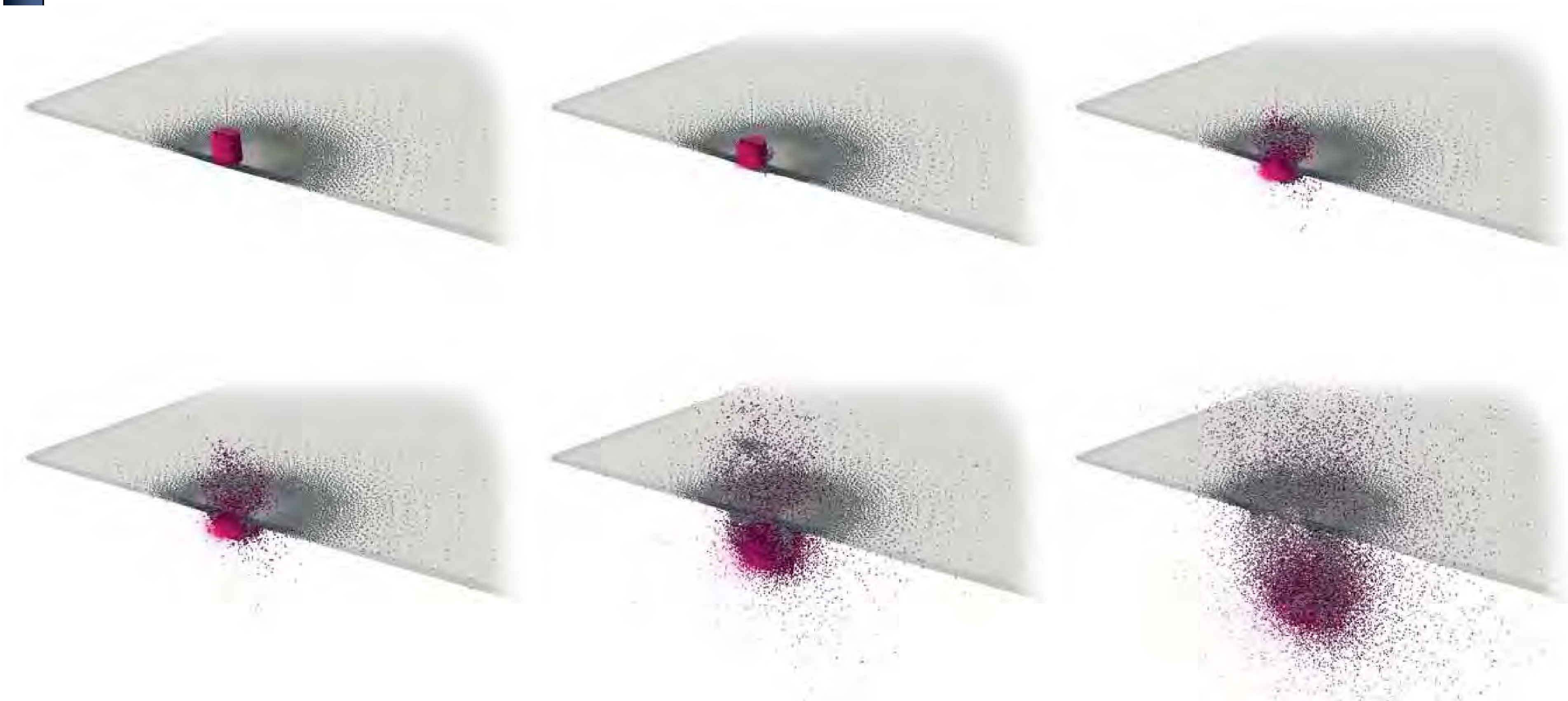


Caltech's hypervelocity Impact facility



OTM simulation, 5.2 Km/s, Nylon/Al6061-T6, 20 million points

Hypervelocity impact - Simulation



OTM simulation, 5.2 Km/s, Nylon/Al6061-T6,
20 million points

Modeling and Simulation Paradigm

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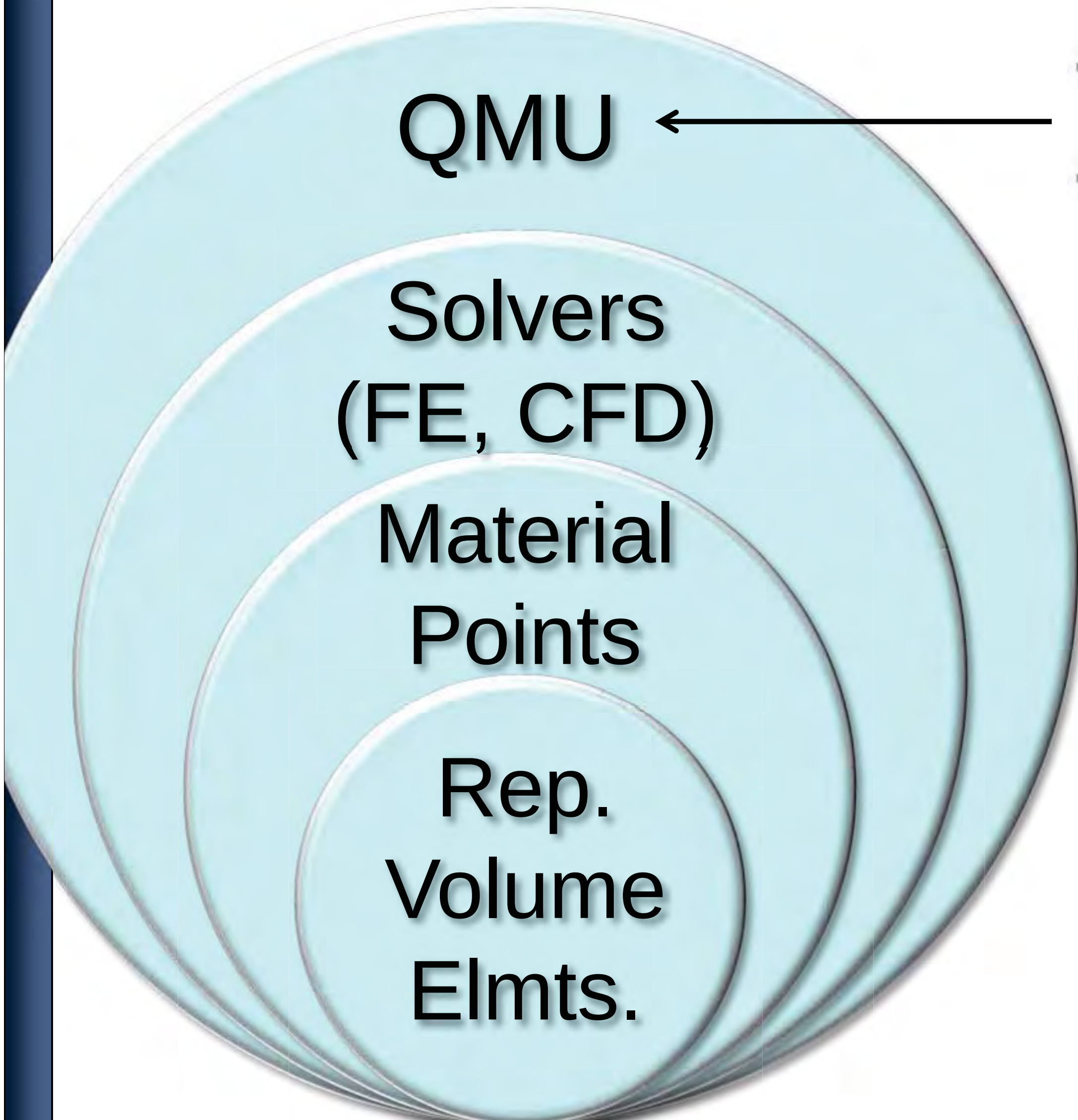

Ensembles of calculations:
- Statistics (sampling)
- Design Margins
- Uncertainties (UQ)…

Modeling and Simulation Paradigm

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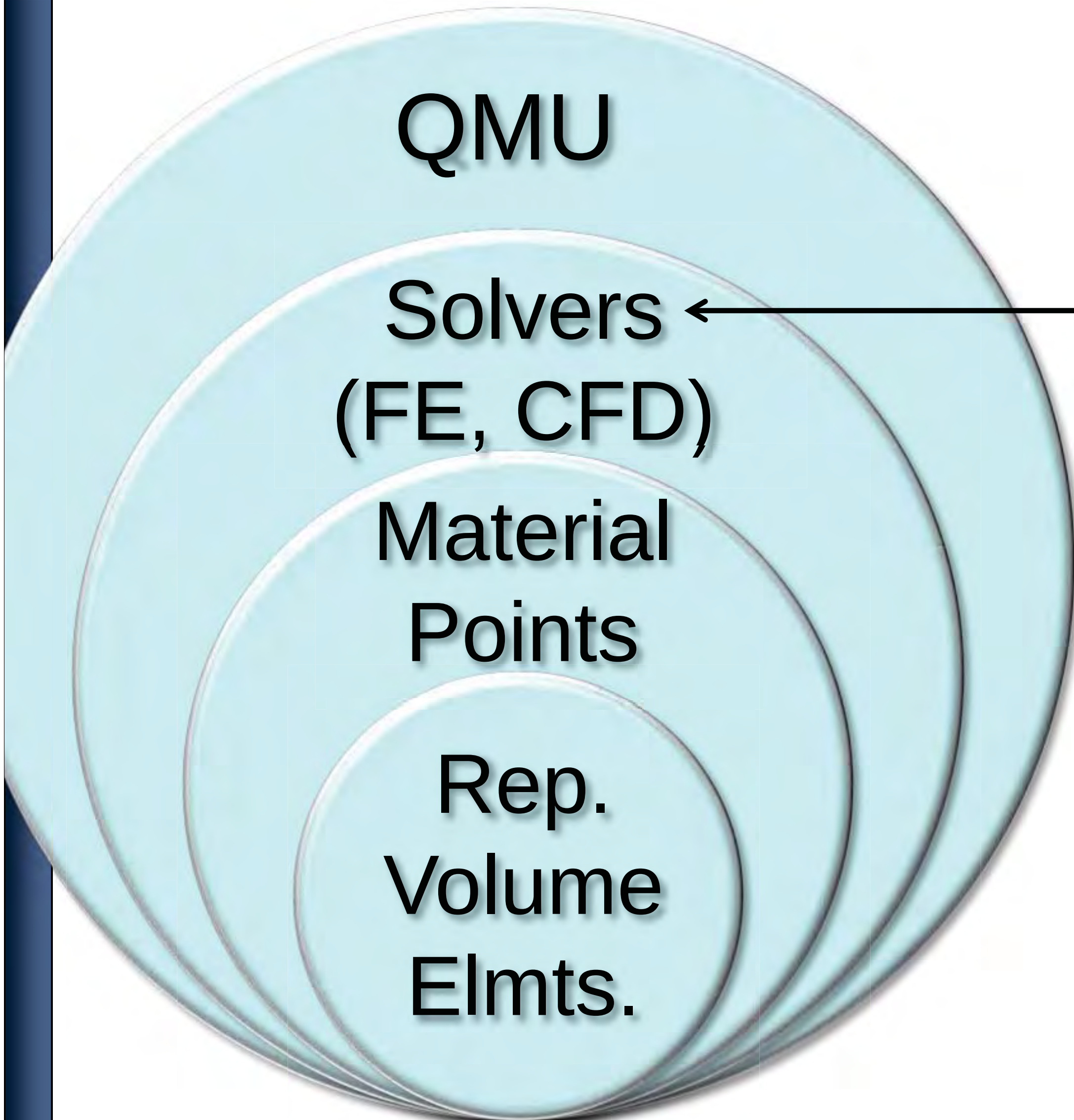
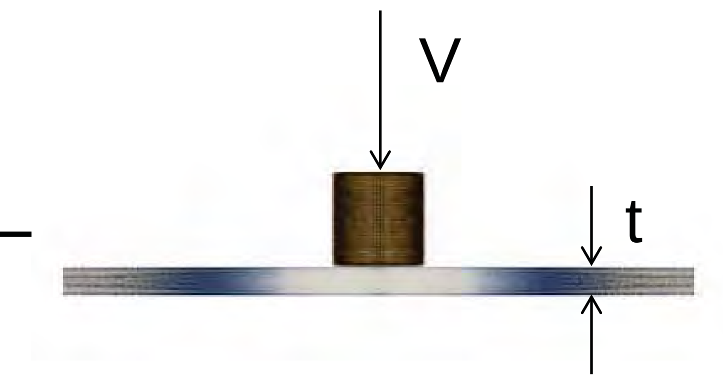
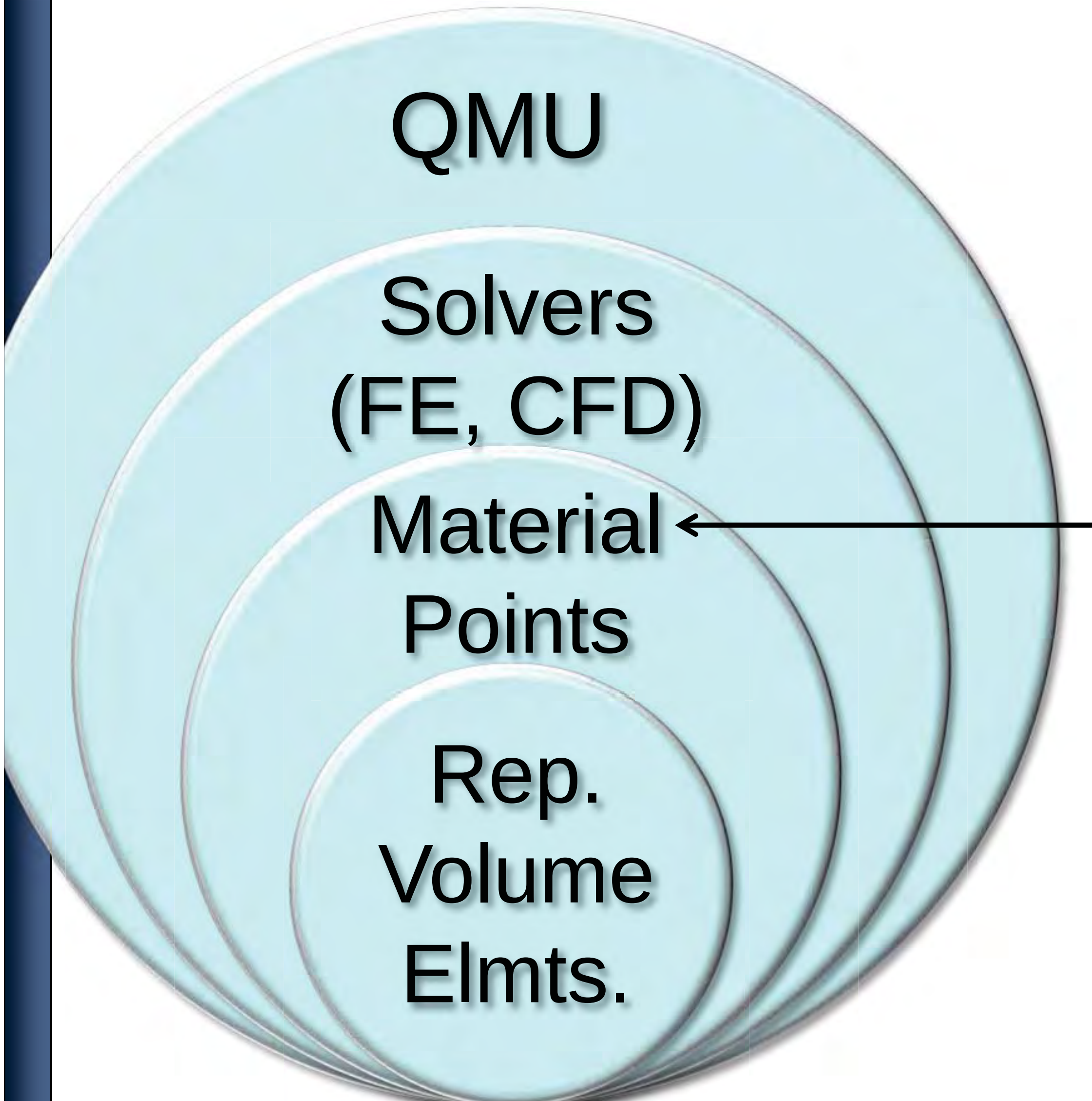


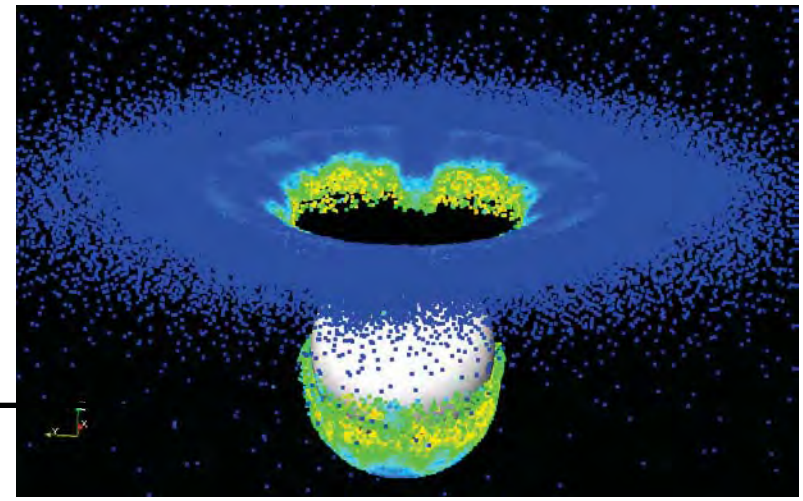


Individual calculation:

- Geometry (CAD)
- Boundary conditions
- Initial conditions
- Loads, actions…
- Global solvers…

Modeling and Simulation Paradigm





Material points:

- Local material elements
- Insulated from global data
- ‘See’ local conditions only
- Material laws…

Modeling and Simulation Paradigm

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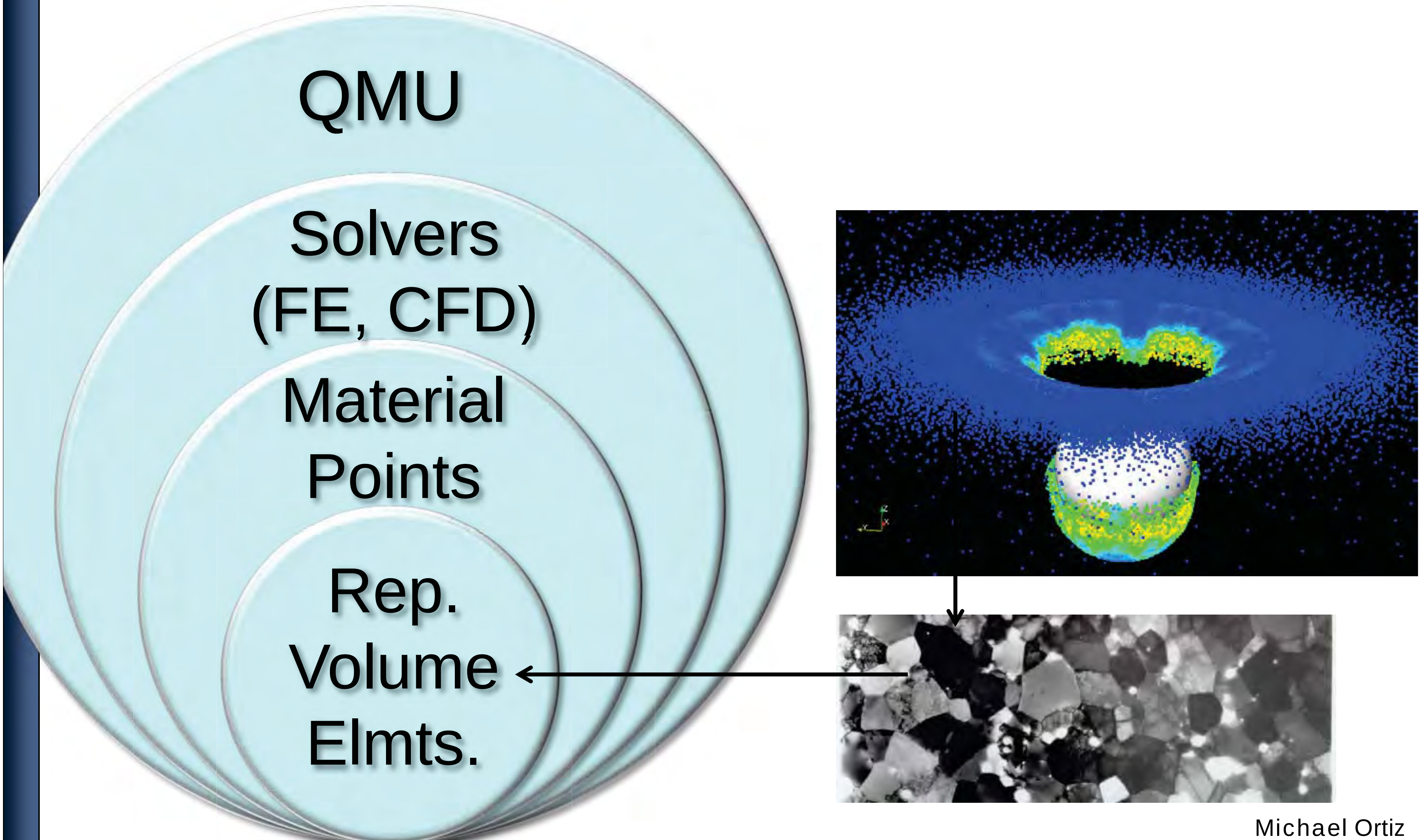

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The case for multiscale modeling

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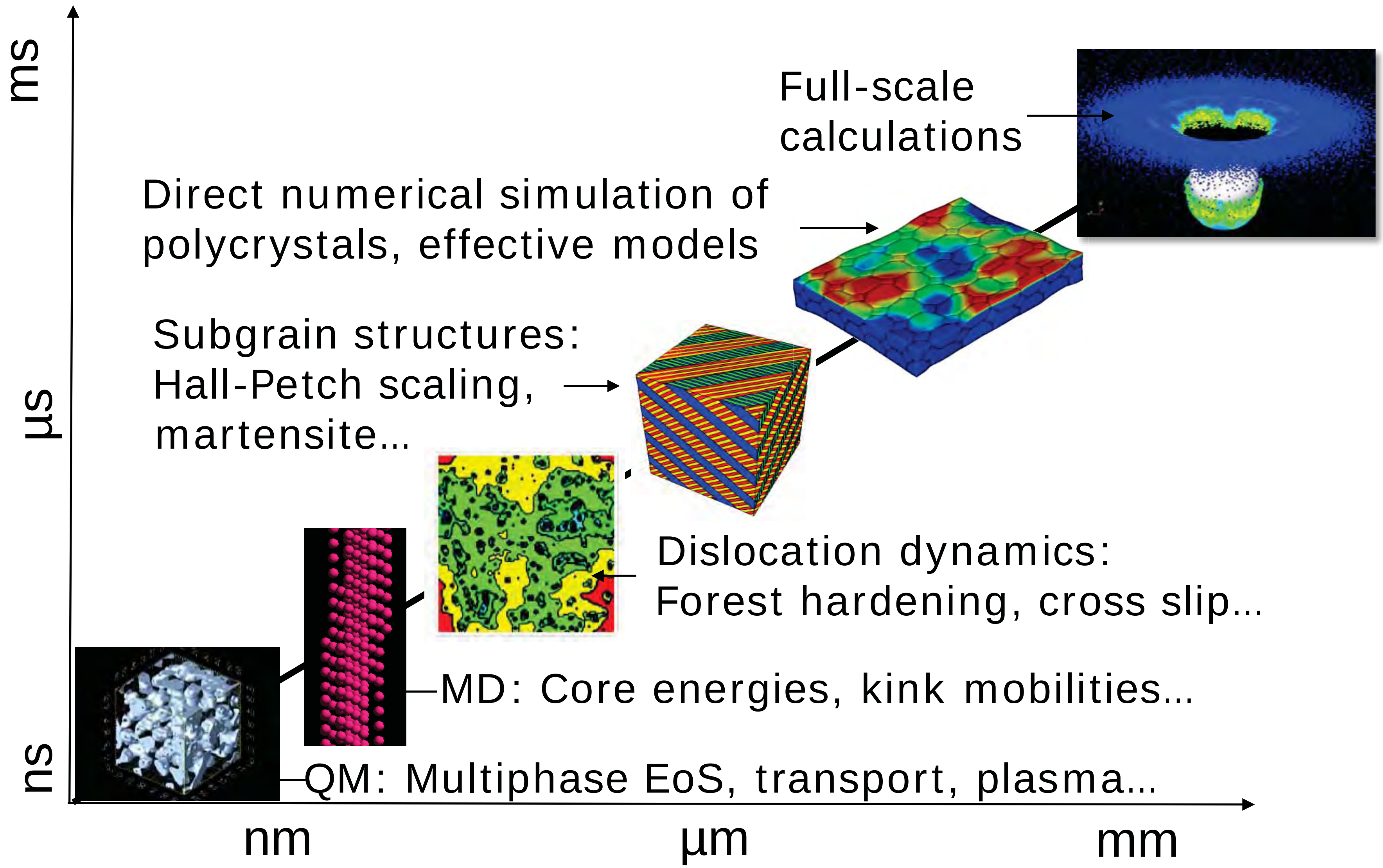
- Material models 'sit' at the core of full system simulations, describe the behavior of local material elements (independently of global geometry, boundary conditions…)
- Simulations are only as good as the material models used, never better! (material models are a critical 'predictive' bottleneck)
- Need high-fidelity material models, up to and including extreme conditions of deformation, pressure, temperature…
- Only game in town: **Multiscale modeling!**

Multiscale modeling - Strength



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Multiscale modeling - Challenges

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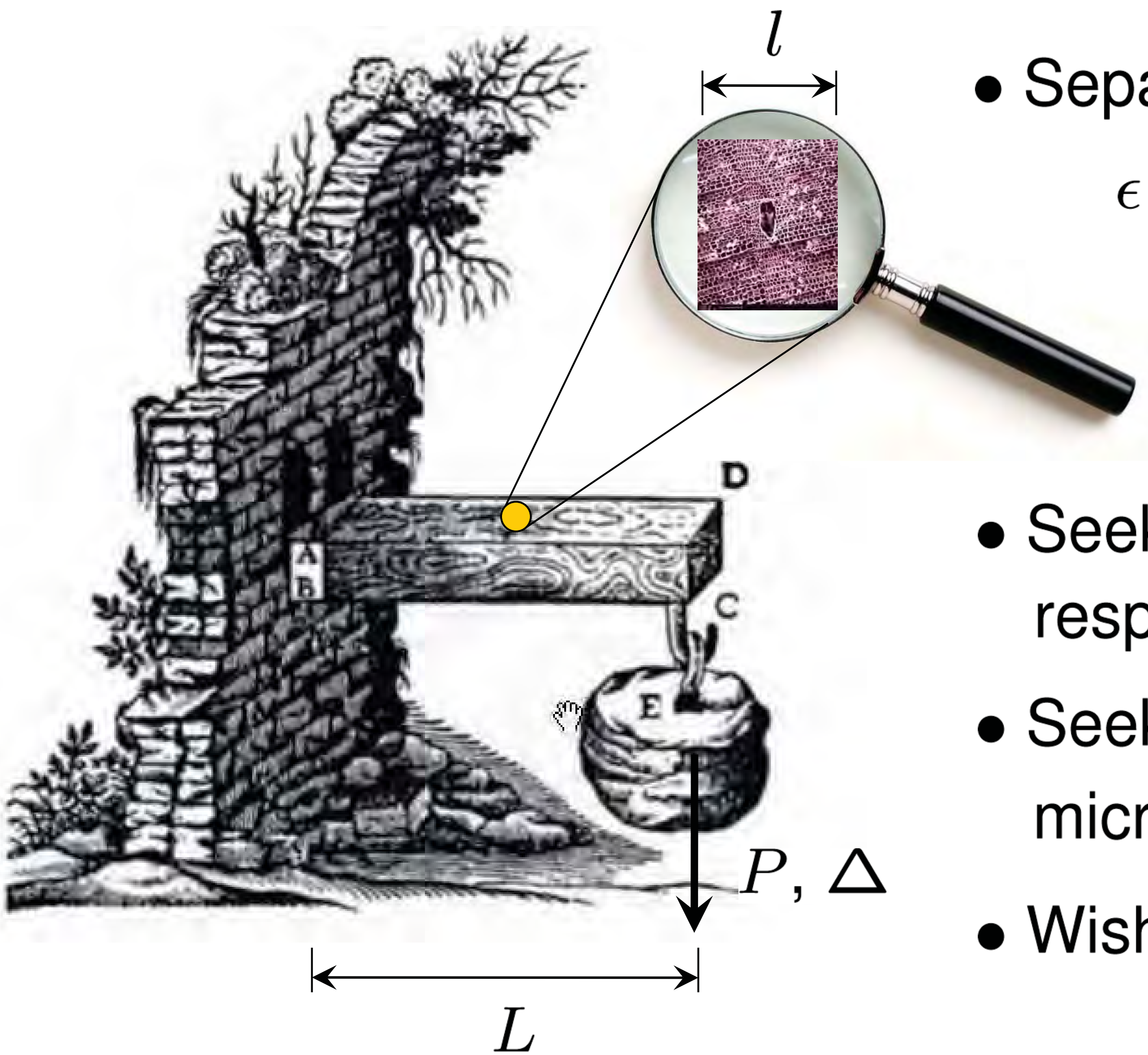
- The essential difficulty: Vastly disparate scales,
  - Atomic level rate-limiting processes: Thermal vibrations, lattice defects, transport …
  - Macroscopic processes of interest: Ductile fracture, GB embrittlement, irradiation damage, aging…
- Time-scale gap: From molecular dynamics (MD) (femptosecond) to macroscopic (seconds-years)
- Spatial-scale gap: From lattice defects (Angstroms) to macroscopic (mm-m)
- No computational asset/scheme, present or future, capable of resolving all length/time scales explicitly and concurrently by brute force alone
- Need: **Multiscale Modeling & Simulation!**

Multiscale - Separation of scales



- Separation of scales:

$$\epsilon = l/L \to 0$$

- Seek macroscopic response P-Δ
- Seek to eliminate microscopic scale
- Wish return option...

Multiscale - Separation of scales

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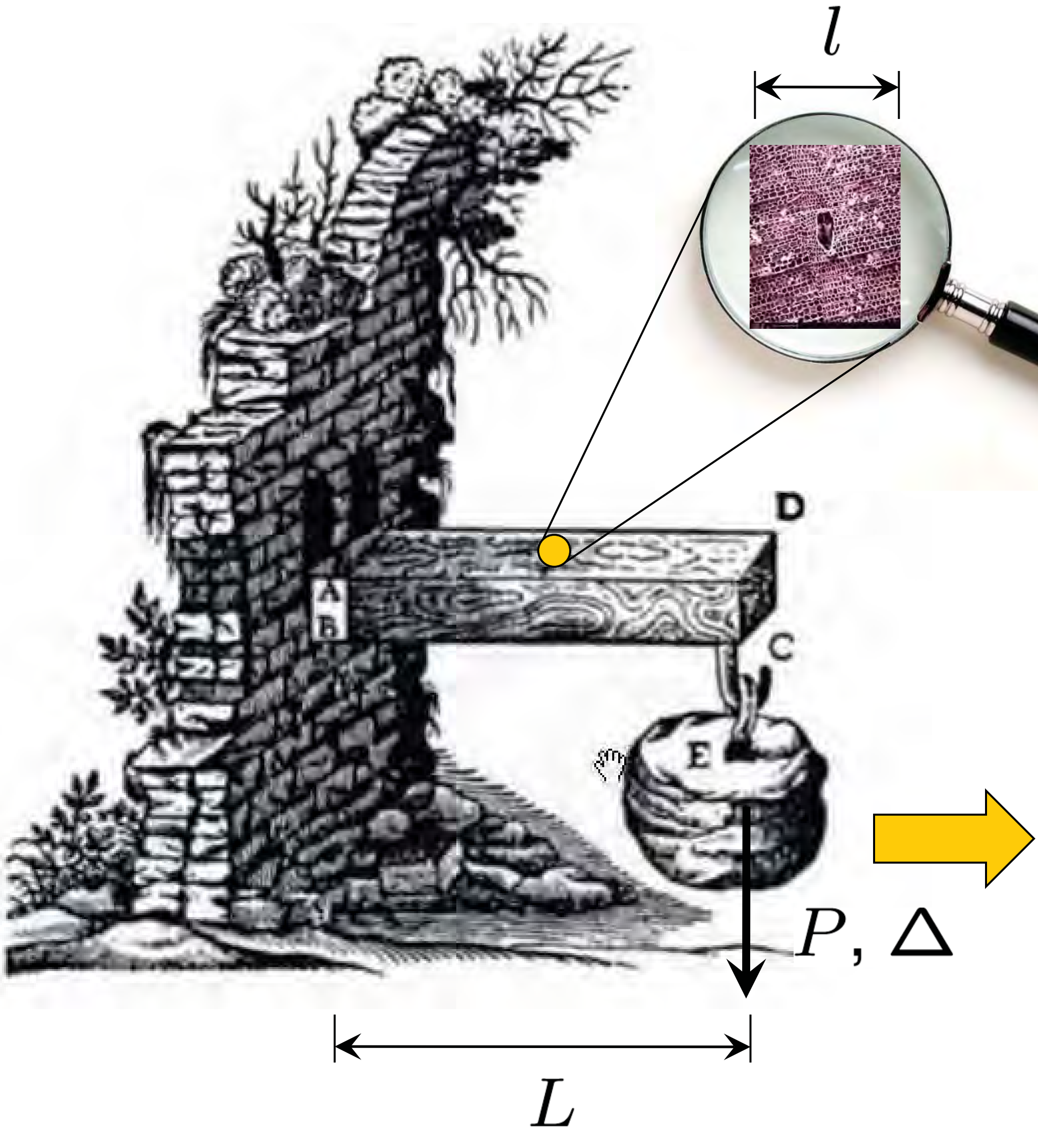
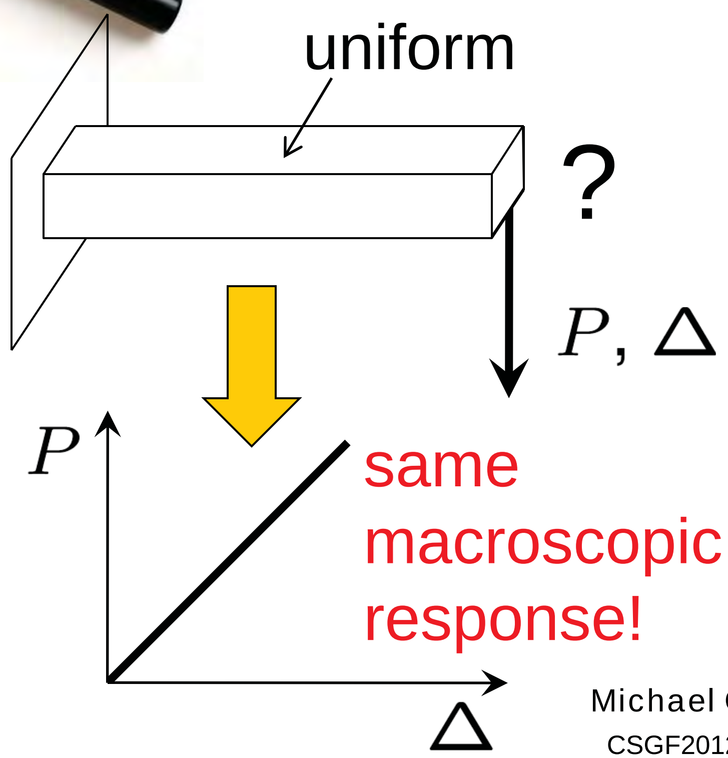
- Separation of scales:

$$\epsilon = l/L \to 0$$



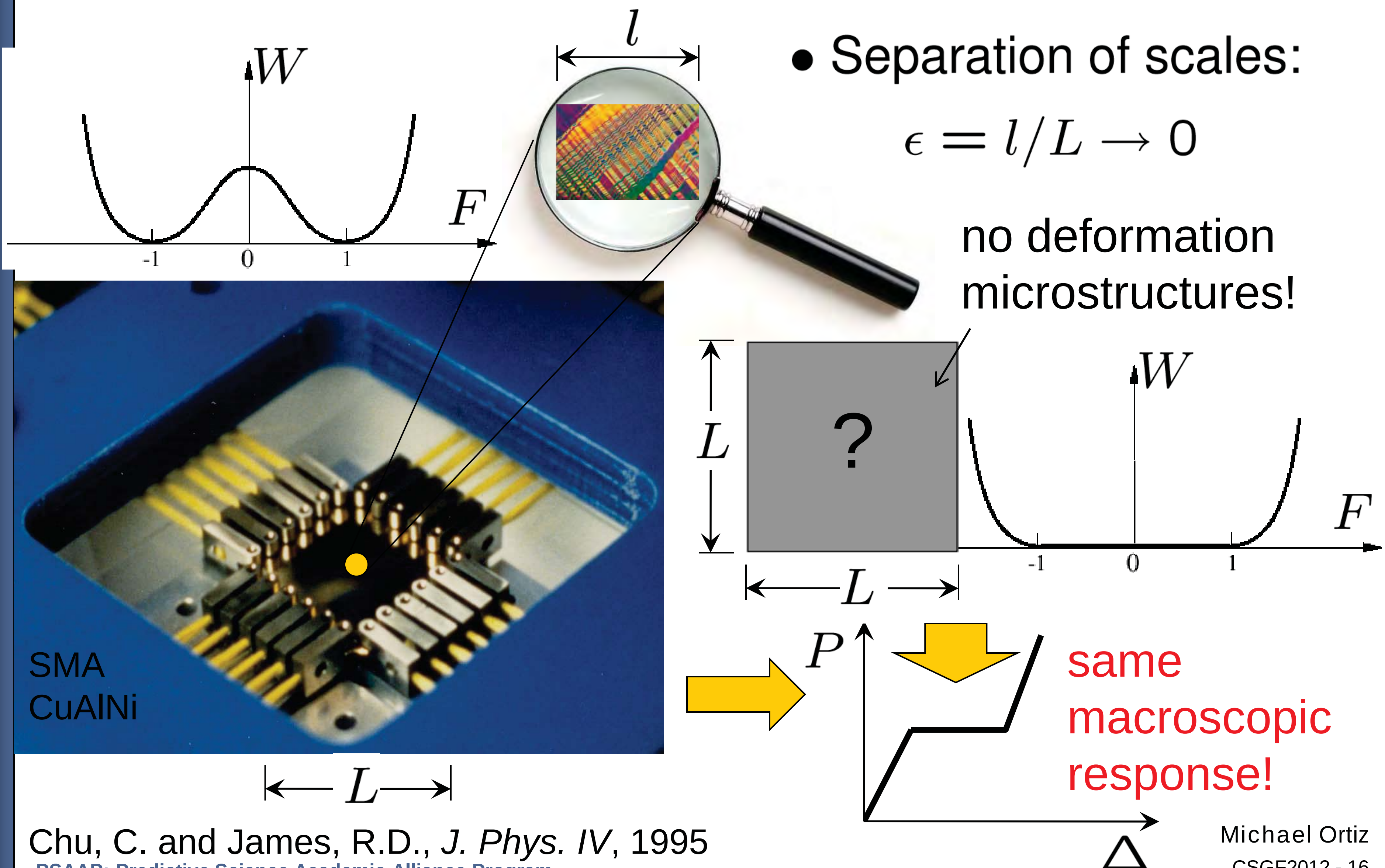


Multiscale - Separation of scales

- Separation of scales:

$$\epsilon = l/L \to 0$$

no deformation microstructures!



same macroscopic response!

Chu, C. and James, R.D., *J. Phys. IV*, 1995

Multiscale - The relaxation scheme

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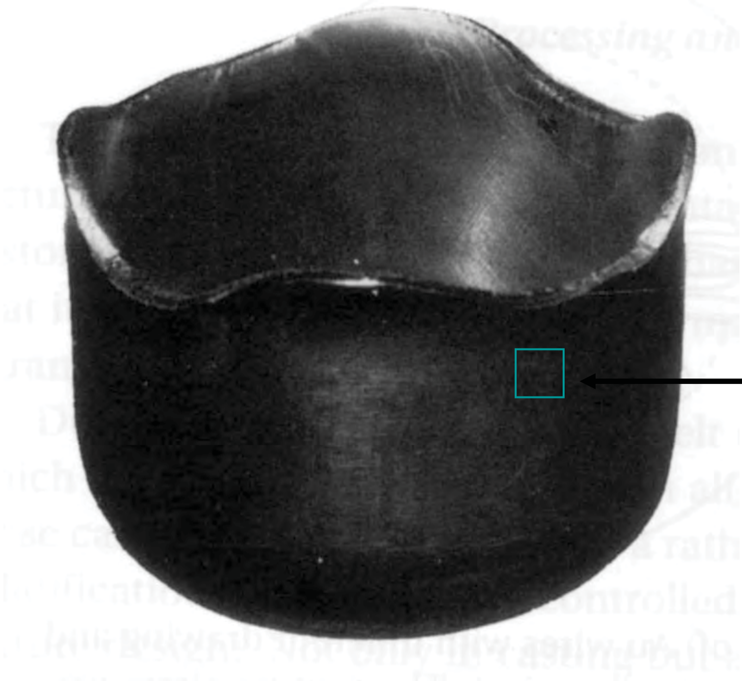
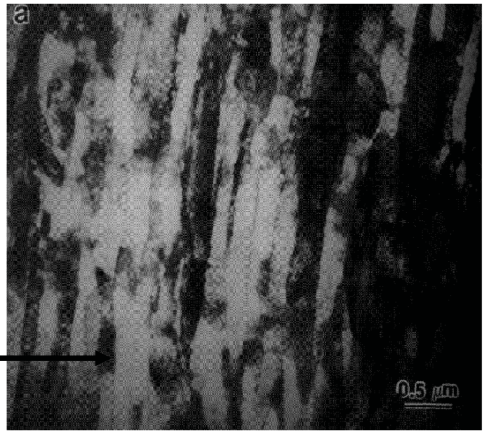
The effective macroscopic model (in some cases) follows from a 'representative volume' calculation



Macroscopic problem (e.g., deep drawing)



- Representative volume:
  - Pre-evaluate all possible microstructures
  - Determine 'most efficient' microstructure
  - Compute average properties…

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Multiscale - The relaxation scheme

- The relaxed and unrelaxed problems deliver the same macroscopic response (they are indistinguishable under macroscopic testing)
- All microstructures are pre-accounted for by the relaxed problem (no physics lost)
- Microstructures can be reconstructed from the solution of the relaxed problem (no loss of information: *return* option!)
- Return option is important when the extreme values of the solution, and not just averages, are of concern: failure, nucleation, initiation…

Example - High Explosives (HE)

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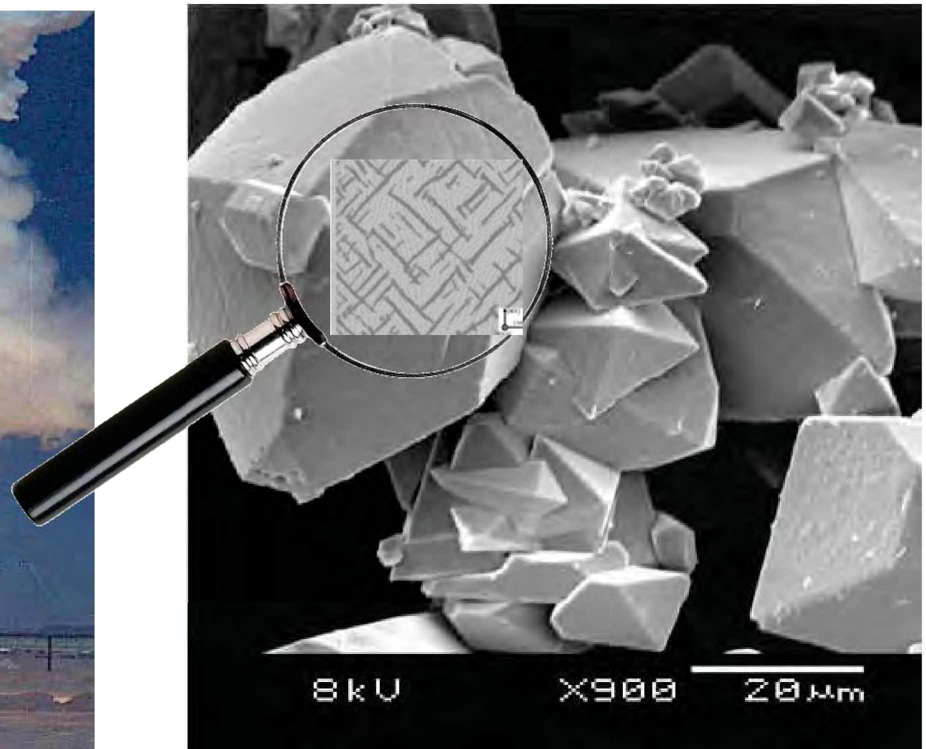
Detonation of high-explosive (RDX, PETN, HMX)



SEM image of RDX (Kline *et al*., 2003)

M. J. Cawkwell et al.
Phys. Rev. B **78, 8**014107 2008

- Can subgrain microstructure development (partially) explain hot spots, detonation sensitivity?

HE – The relaxation 'boomerang'

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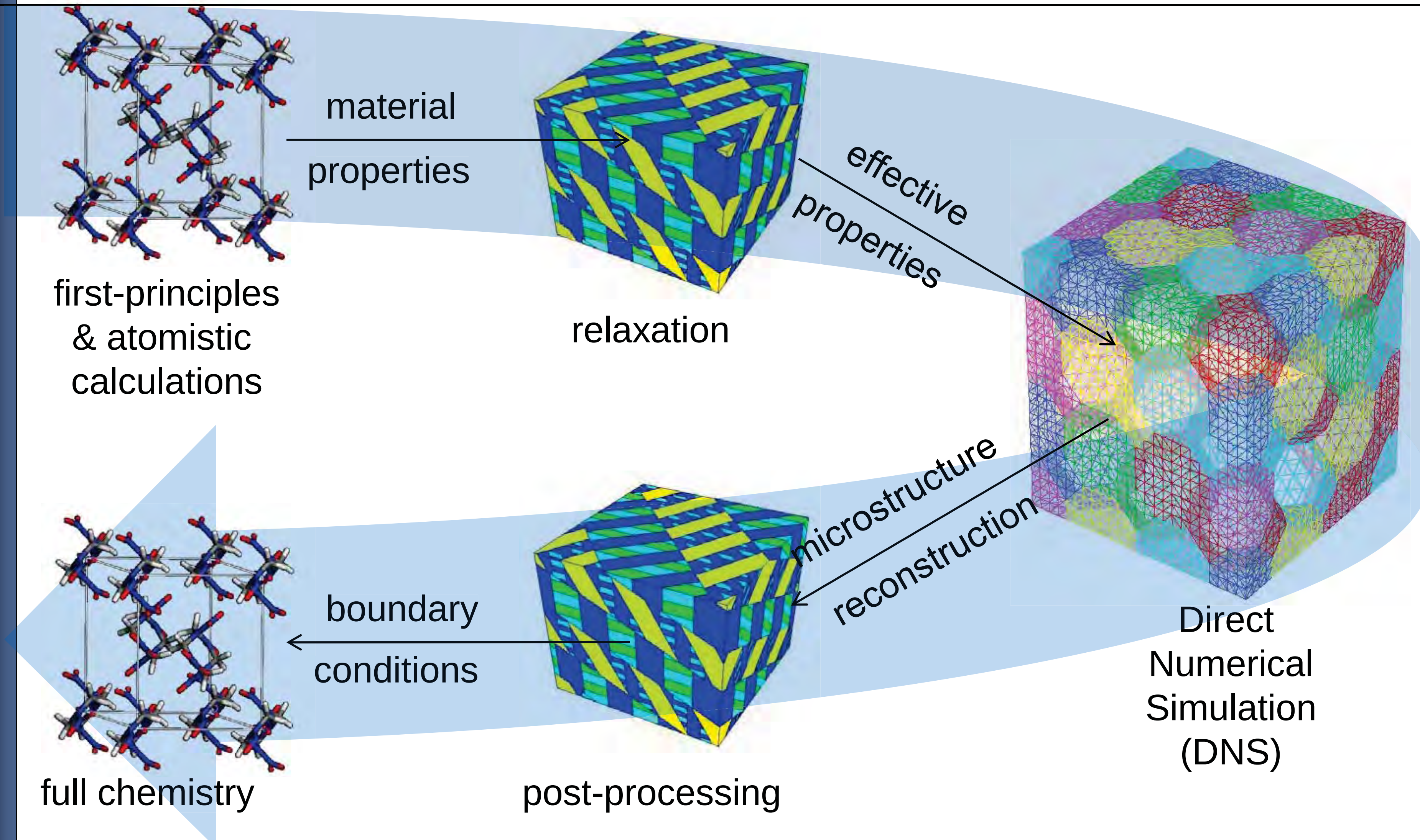
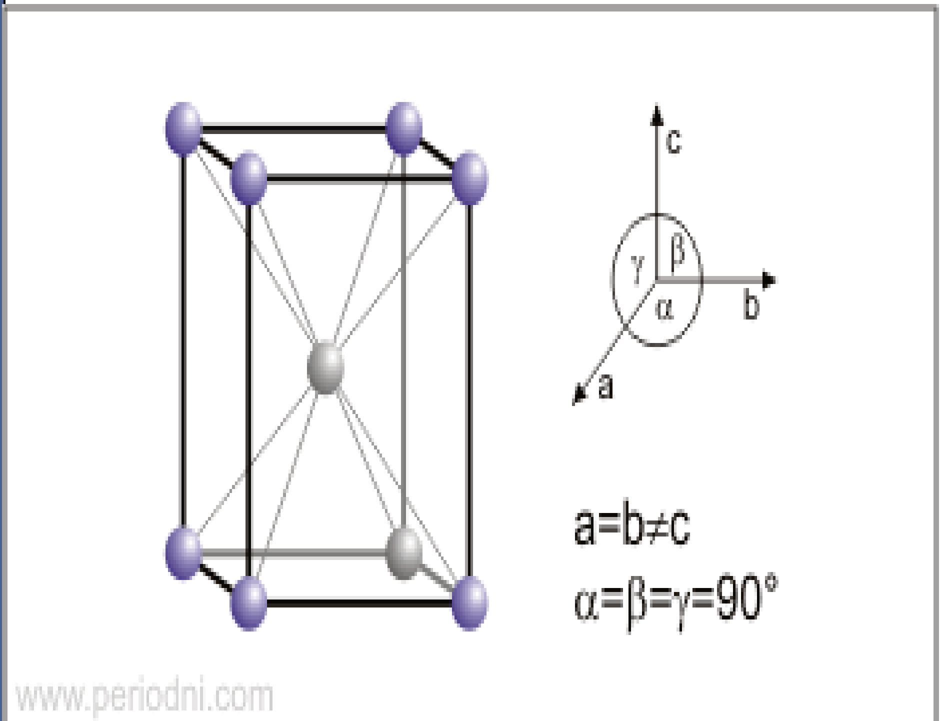


Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

PETN – Elastic constants

Body Centered Tetragonal Lattice



a=b=9.380A and c=6.710A

- Elastic Constants(GPA): (Winey and Gupta, 2001)

C_{11}=17.22 C_{33}=12.17
C_{44}=5.04 C_{66}=3.95
C_{12}=5.44 C_{13}=7.99

- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

$$C_{ij}(\theta, p) = \frac{\theta - \theta_{\text{melt}}(p)}{\theta_0 - \theta_{\text{melt}}(p)}$$

- Menikoff and Sewell (2002):

$$\theta_{\text{melt}}(p) = \theta_{\text{melt}}(p_0)\left(1 + a\frac{\Delta V}{V_0}\right)$$

where a = 2(Γ-1/3), Γ ~ 1.2 = Grüneisen constant

PETN – Slip systems

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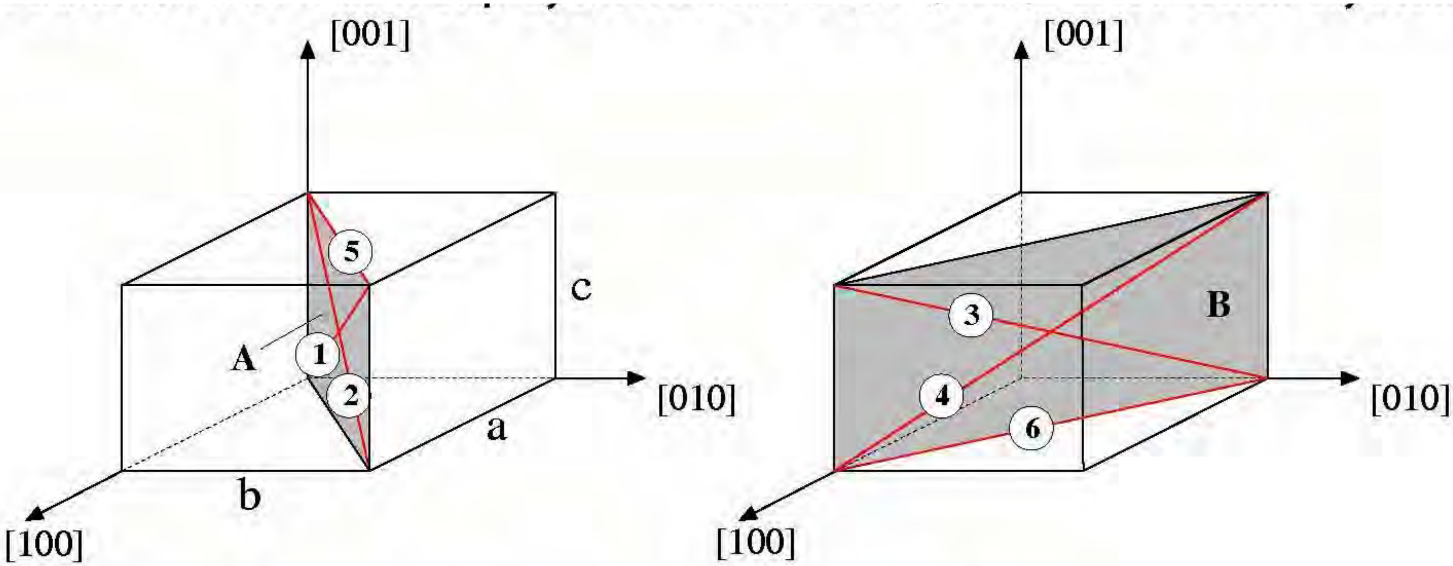


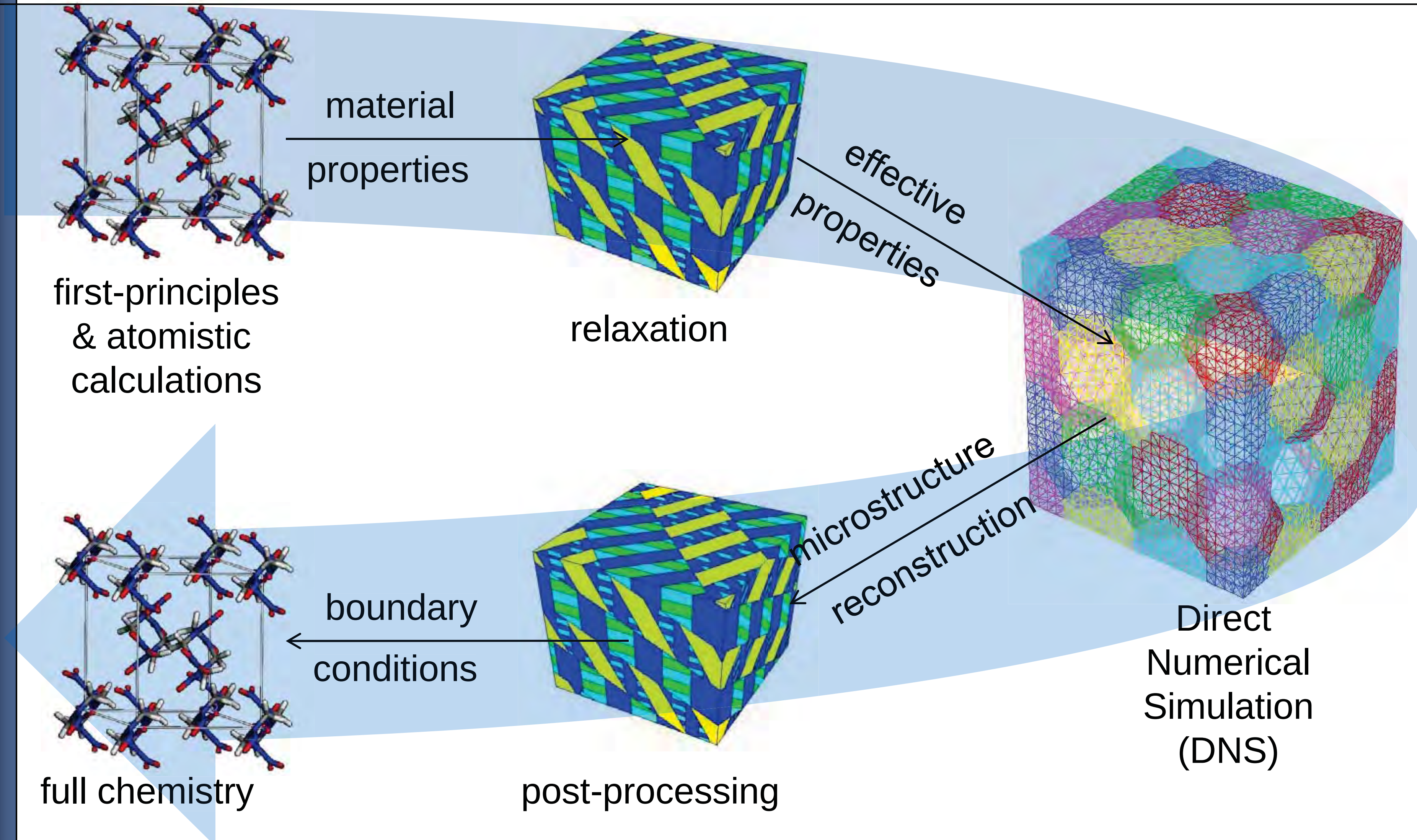
$a = b = 9.380\text{Å} \qquad c = 6.710\text{Å}$

- $\tau_c(\theta)$ fitted to data of Amuzu *et al*. (1976) and:

Slip System	B3	B4	A1	A2	B6	A5
s^α	$\pm[1\bar{1}1]$	$\pm[1\bar{1}\bar{1}]$	$\pm[111]$	$\pm[11\bar{1}]$	$\pm[1\bar{1}0]$	$\pm[\bar{1}\bar{1}0]$
m^α	(110)	(110)	$(1\bar{1}0)$	$(1\bar{1}0)$	(110)	$(1\bar{1}0)$
τ_c [GPa]	1.0	1.0	1.0	1.0	2.0	2.0

P. Xu, S. Zybin, S. Dasgupta, and W. A. Goddard III, private communication

HE – The relaxation 'boomerang'



Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

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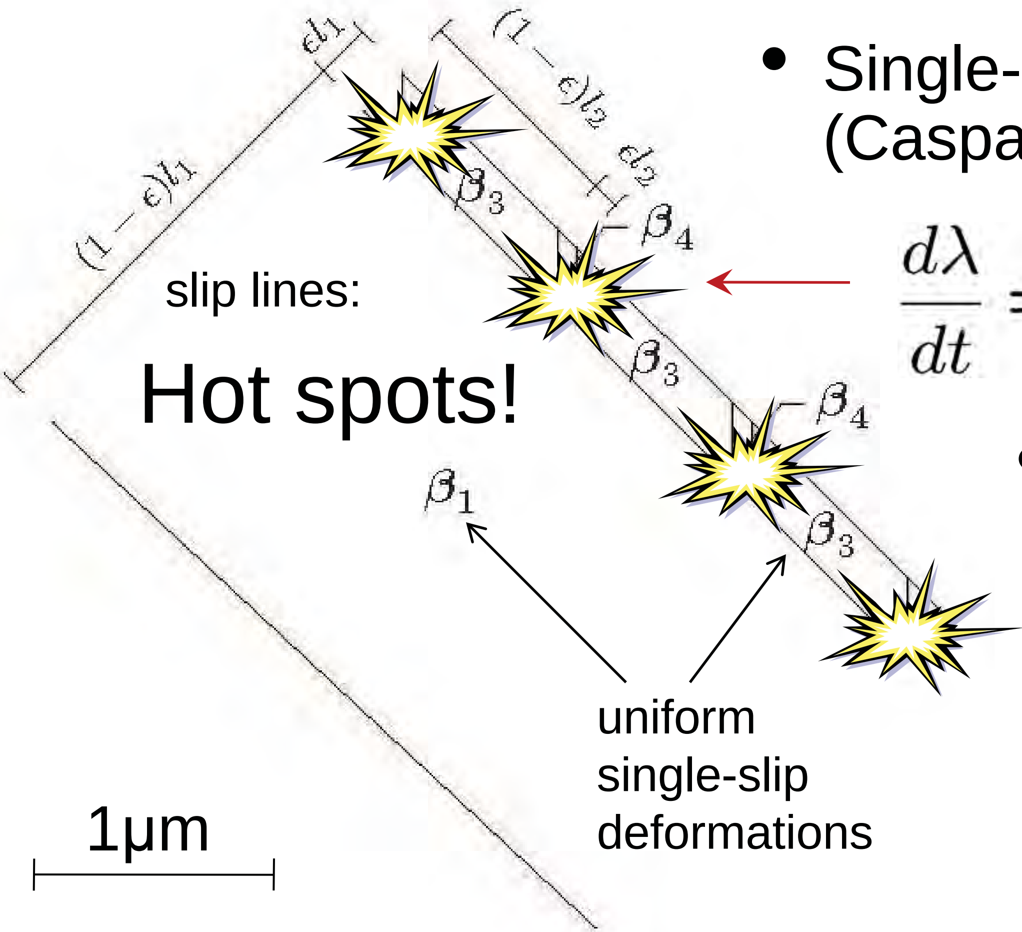
PETN – Chemistry



- Single-step reaction kinetics (Caspar *et al*., 1998):

$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{ER}{\theta}\right)$$

- Activation energy E and rate constant Z from Rogers (1975):

R	8.314 J/mol/K
E	196.742×10^3 J/mol
Z	6.3×10^{19} s^{-1}

- Temperature computed assuming adiabatic heating, full conversion of plastic work to heat, heat capacity

PETN – Plate impact test

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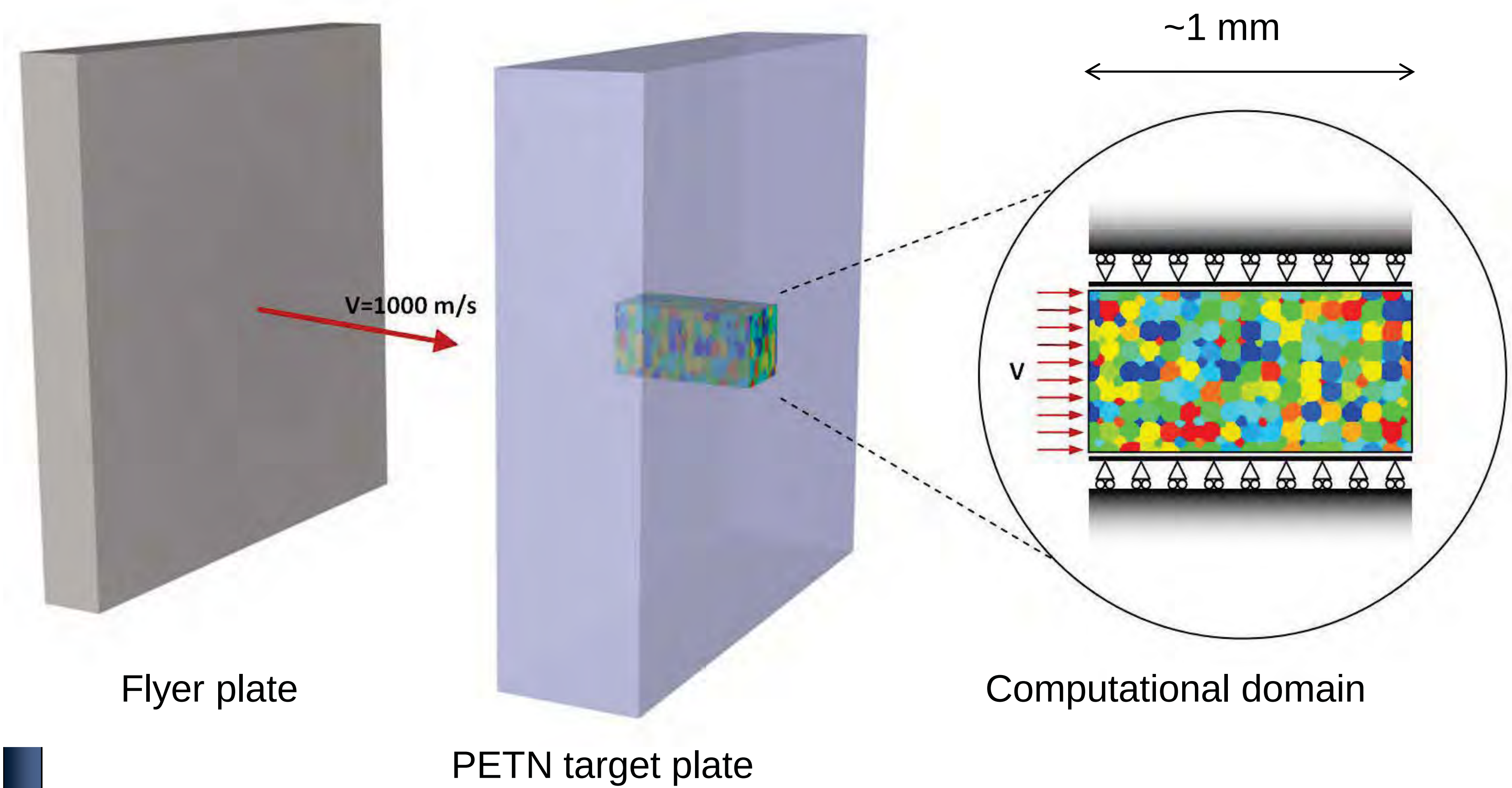
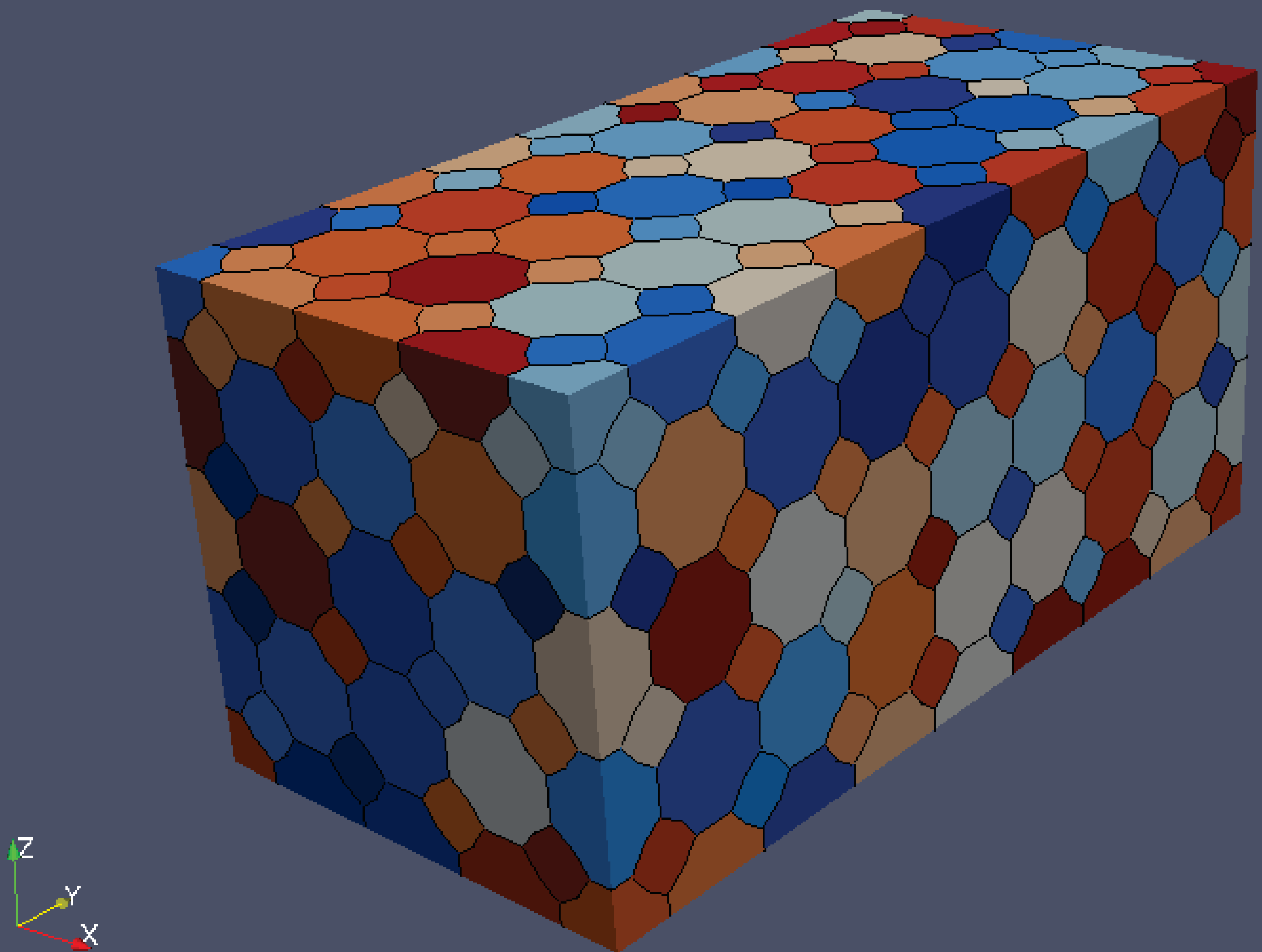


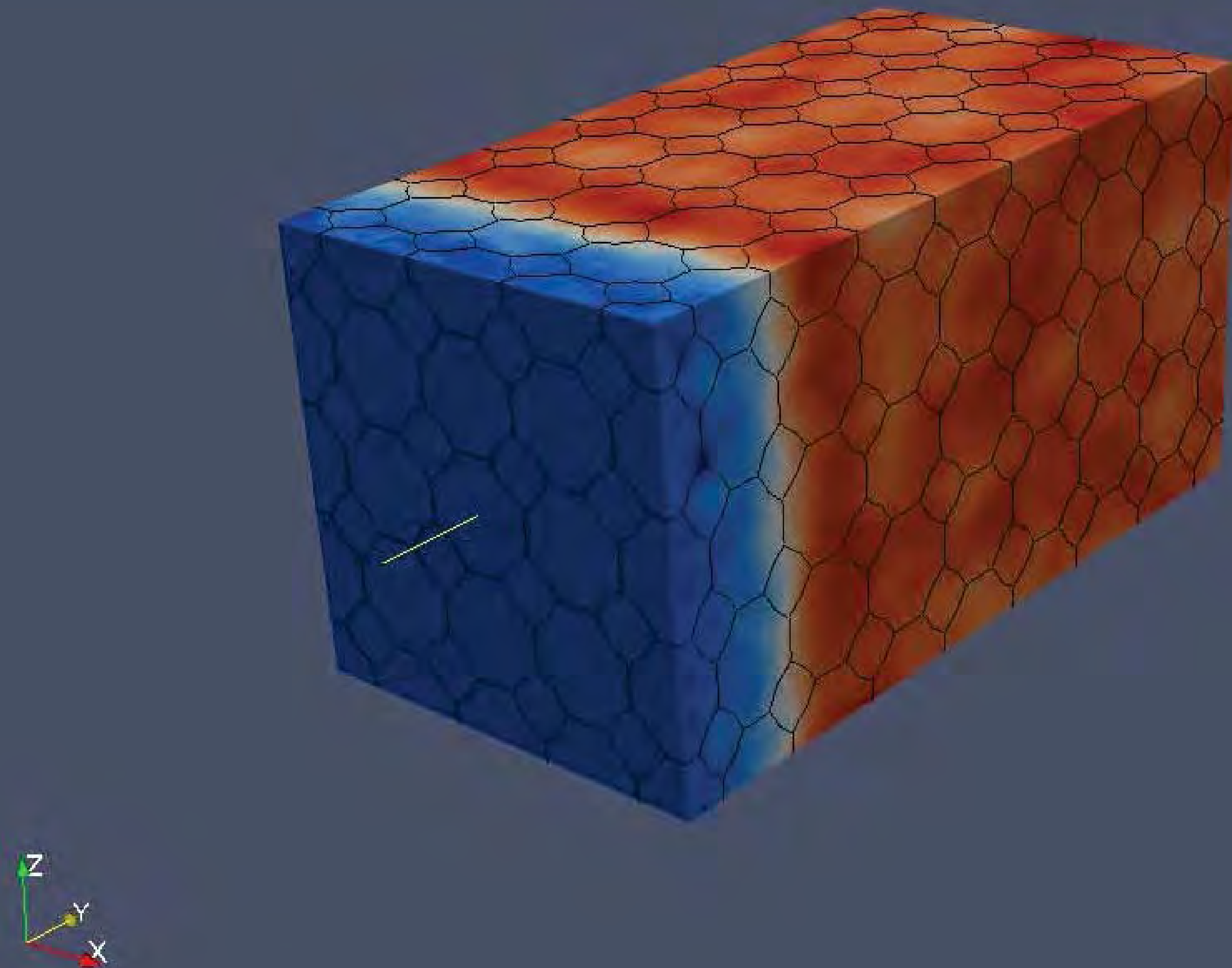
Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

High-Explosives Detonation Initiation

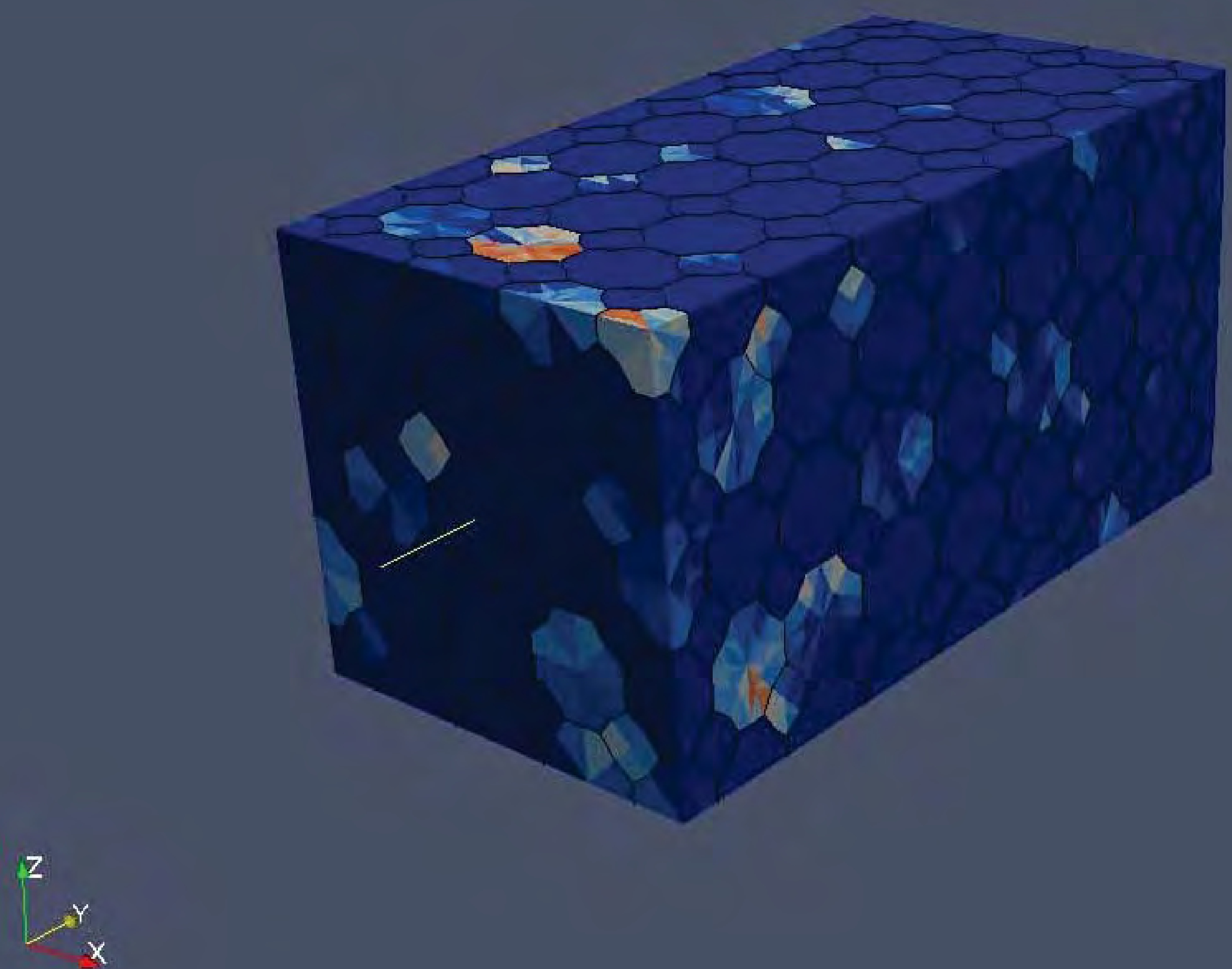


Polycrystal model and grain boundaries

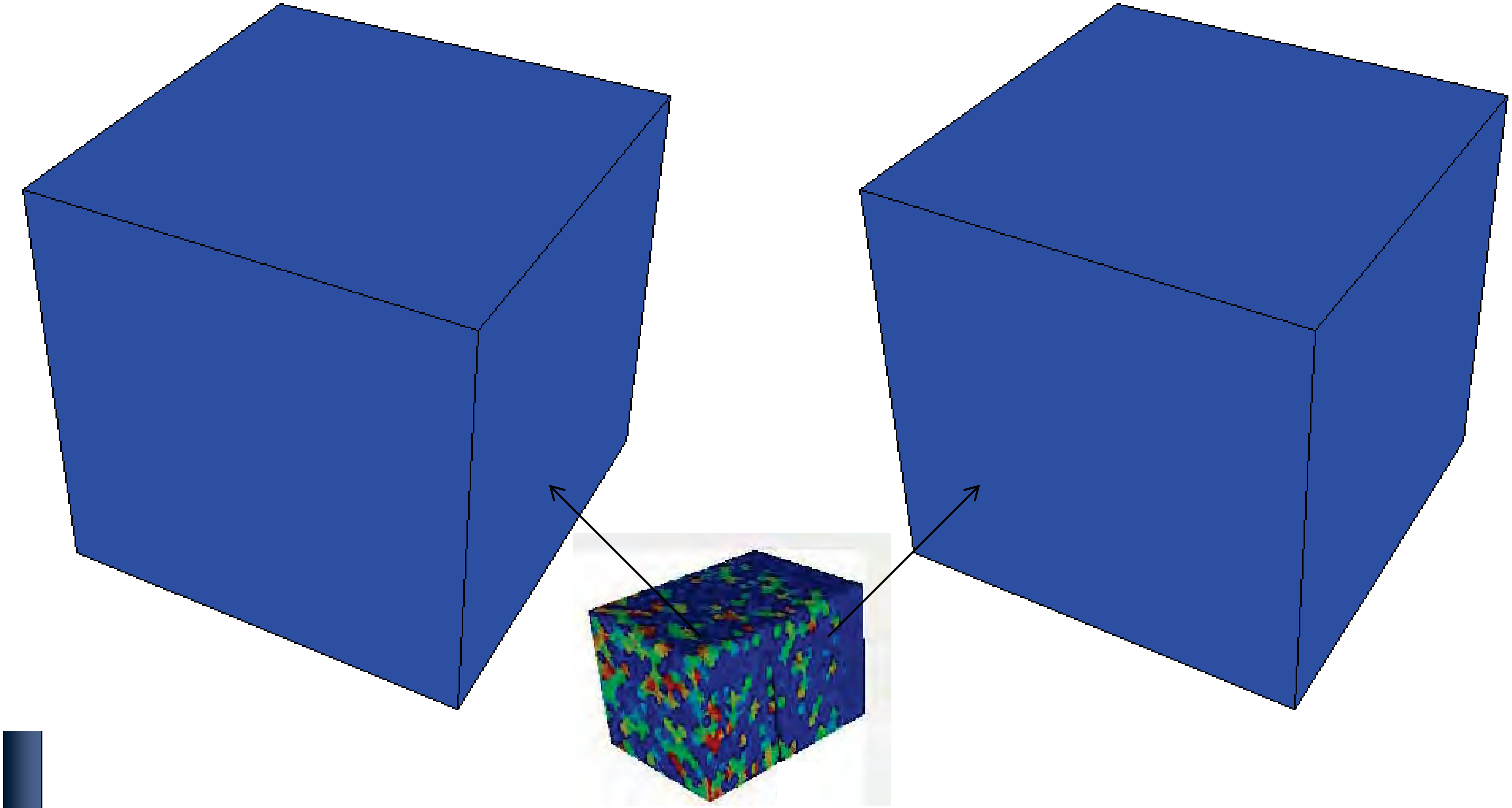
PETN plate impact - Velocity



PETN plate impact - temperature

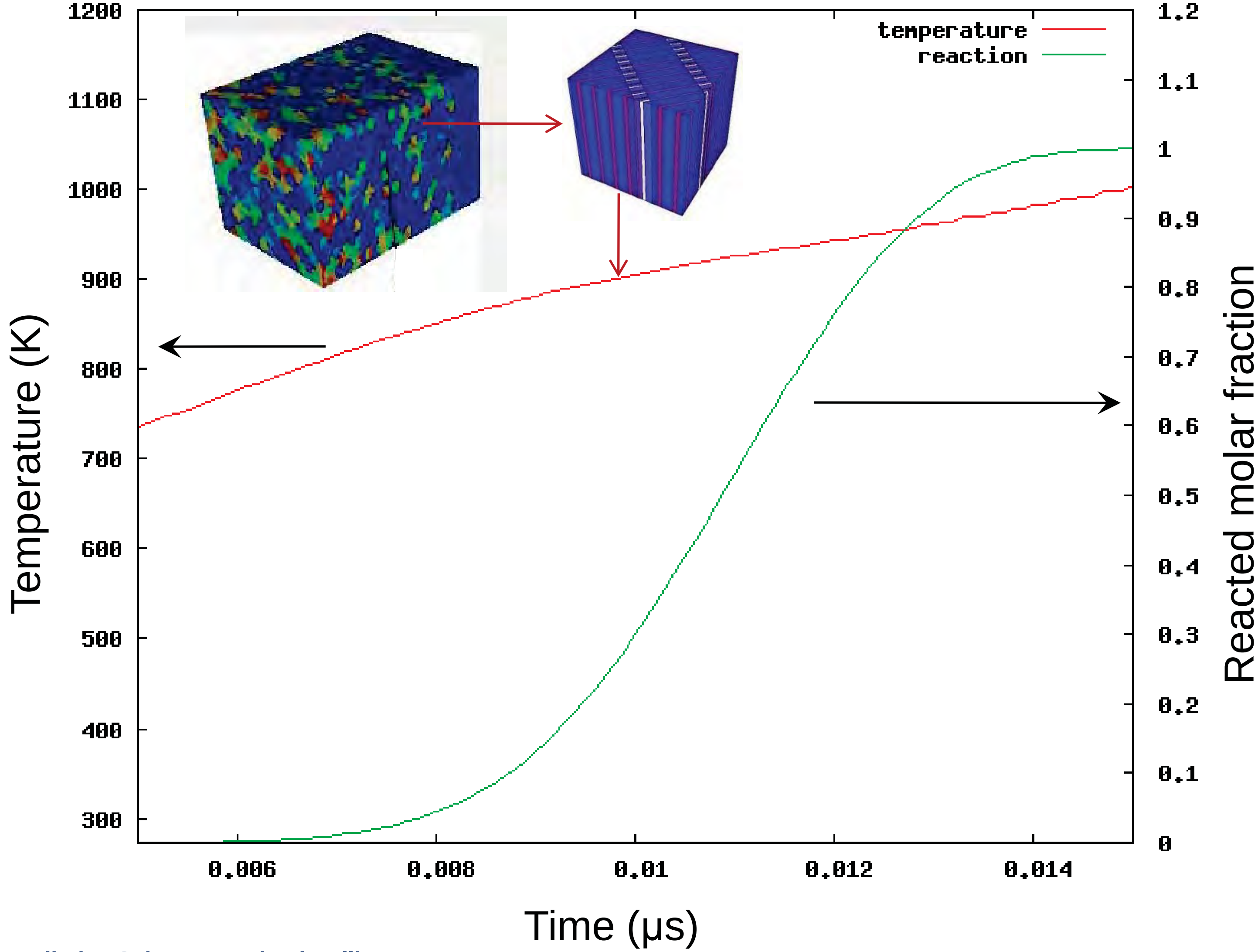


PETN plate impact – Subgrain microstructures



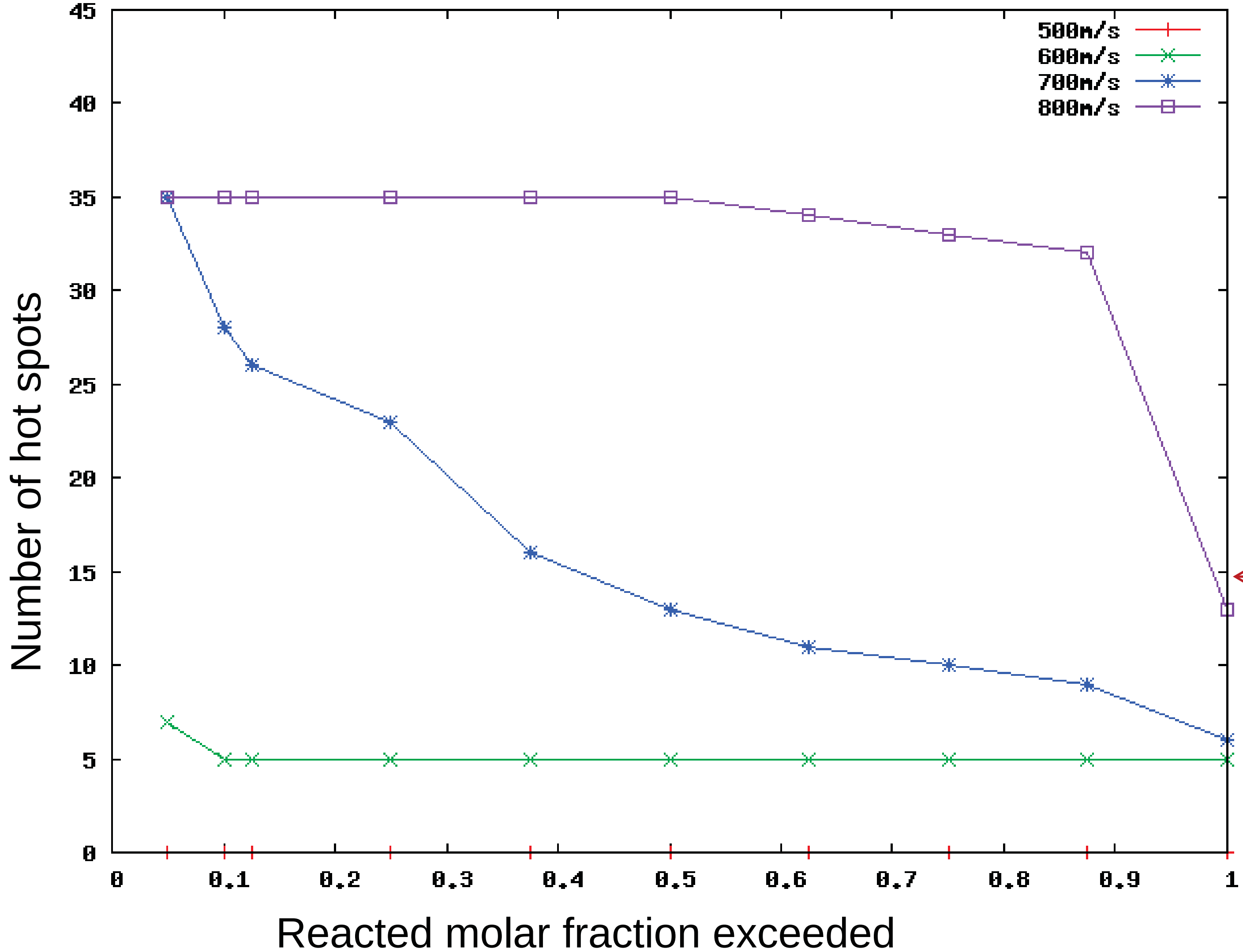
Microstructure evolution at selected material points

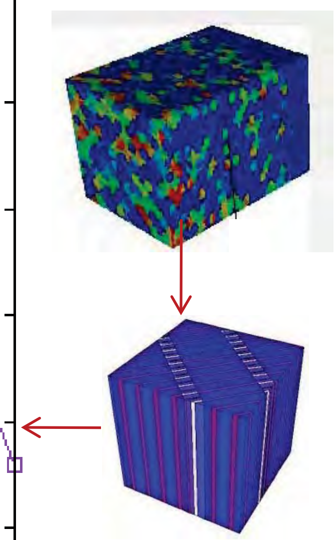
PETN plate impact - temperature and reaction evolution at selected hot spot



PSAAP: Predictive Science Academic Alliance Progran.

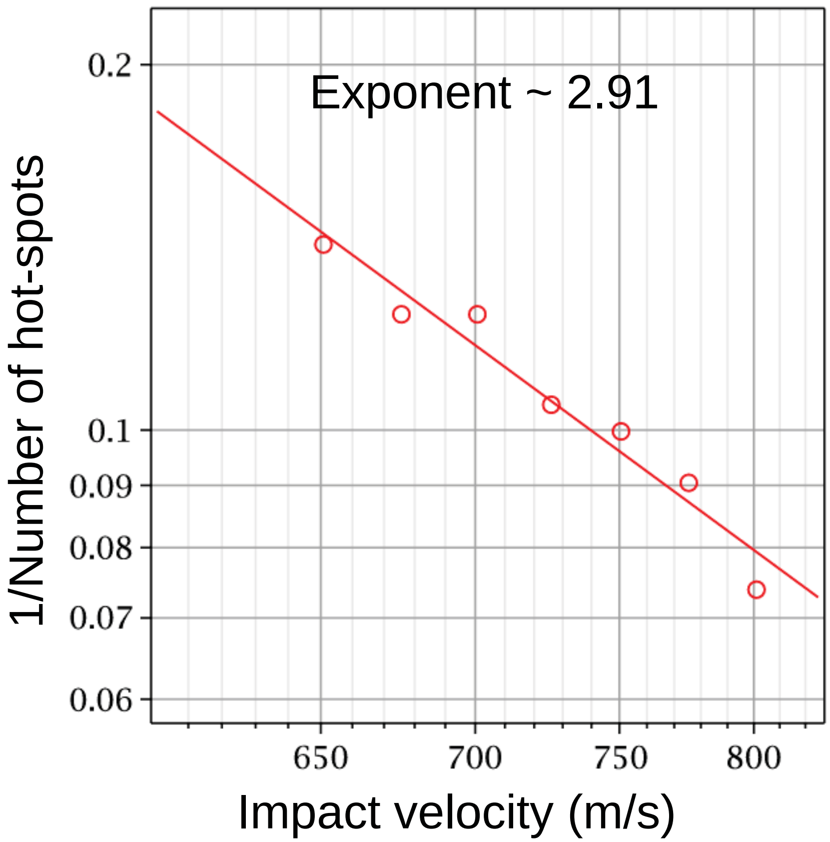
PETN plate impact - Number of hot spots



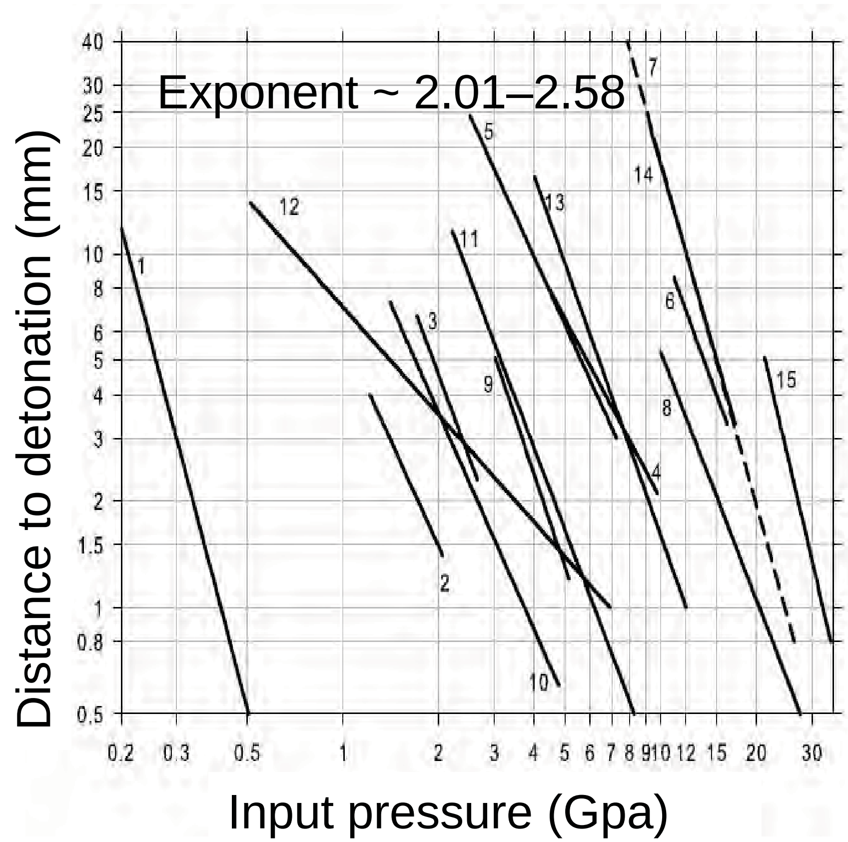


PETN plate impact – Pop plots

Impact velocity (m/s)



Multiscale model



S.A. Sheffield and R. Engelke (2009)

Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

Multiscale – The relaxation scheme

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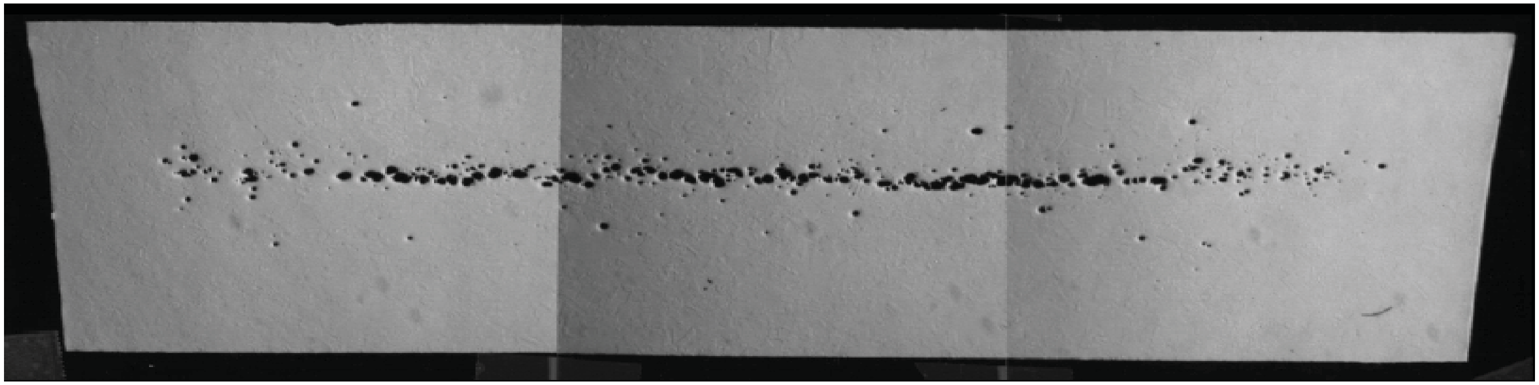
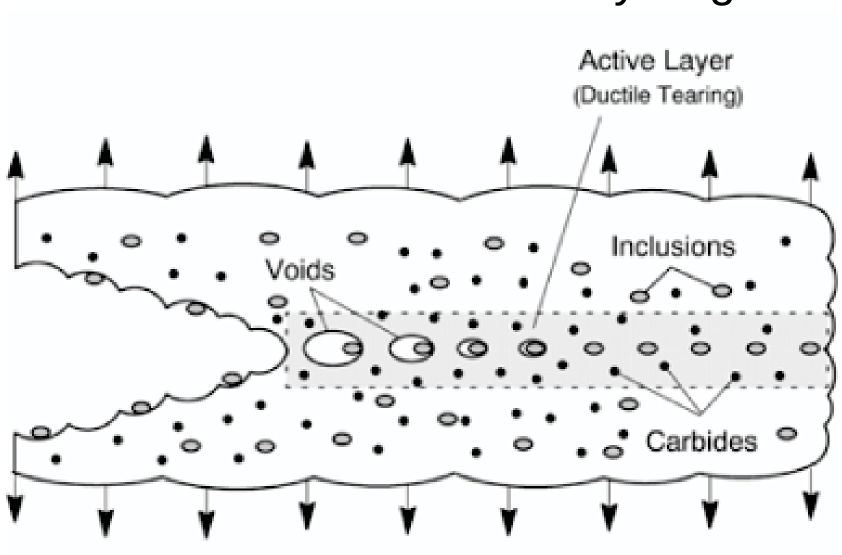
- Relaxation: Pre-evaluate the effect of all possible microstructure, determine effective behavior.
- Relaxation eliminates fine-scale microstructural features from consideration in macroscopic calculations, but provides a 'return option': The microstructures can be reconstructed at *post-processing* stage (from macroscopic solution)
- Return option is important when the extreme values of the solution, and not just averages, are of concern: failure, nucleation, initiation…
- Application to HE initiation, contact with engineering test data, would not have been possible without multiscale modeling and simulation!

Multiscale modeling – Fracture

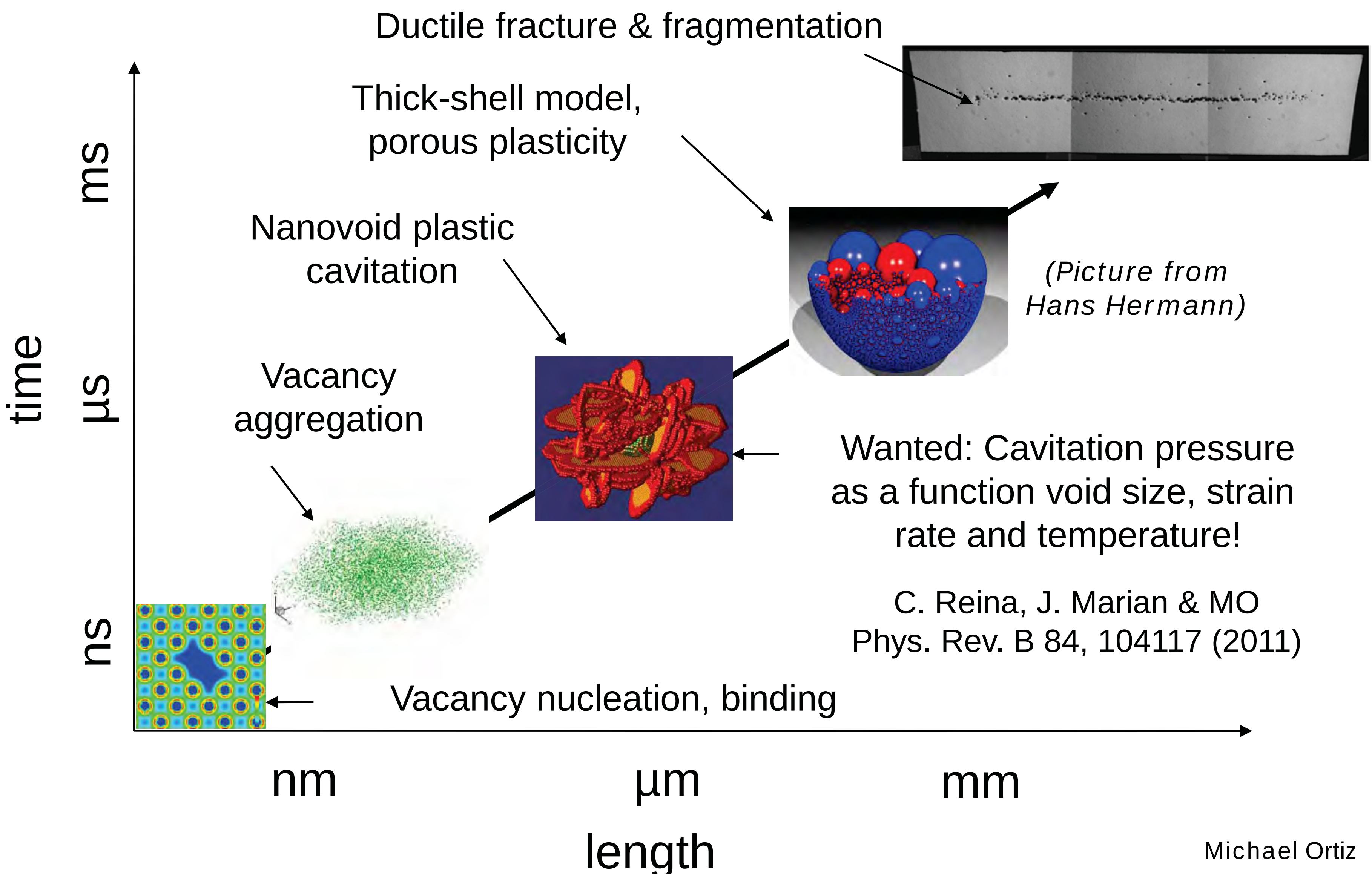


R. Becker "How Metals Fail", *Science and Technology Review*, LLNL, July/August 2002



C. Ruggieri, J. of the Braz. Soc. of Mech. Sci. & Eng., Vol. XXVI, No. 2 (2004) 190-198.

Multiscale modeling – Fracture



Multiscale modeling - Fracture

- Ductile fracture is the end result of:
  - Void nucleation (nanoscale, e.g., second-phase particles)
  - Void growth (mesoscale, distributed damage, porosity)
  - Void coalescence (macroscale, void sheets, fracture)
- Fracture provides an example of a multiscale process where the relaxation scheme fails due to localization of damage to failure planes (void sheets)
- Instead of relaxation: Optimal scaling (bounds)
- Optimal scaling gives the fracture energy as a function of strength (strain hardening, temperature, strain rate) and surface energy (non-local plasticity, size effect)
- Macroscopic fracture and fragmentation modeled by material point failure and erosion

Validation – Explosively driven cap

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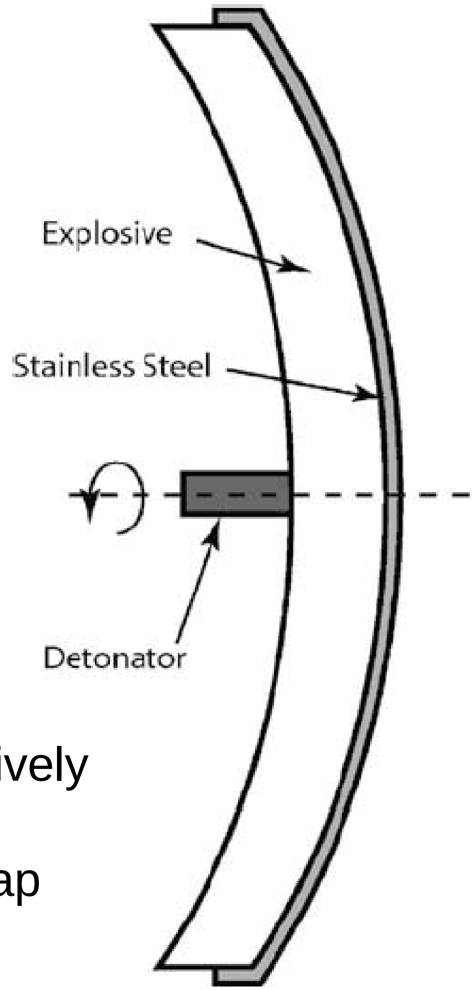
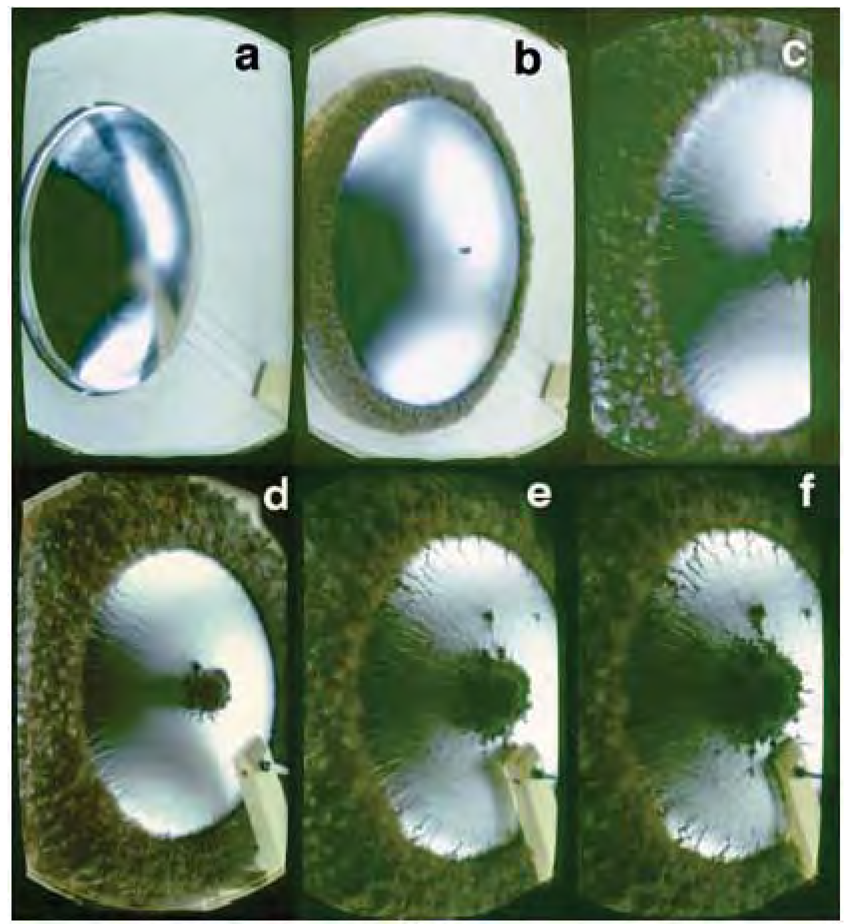


Explosively driven steel cap

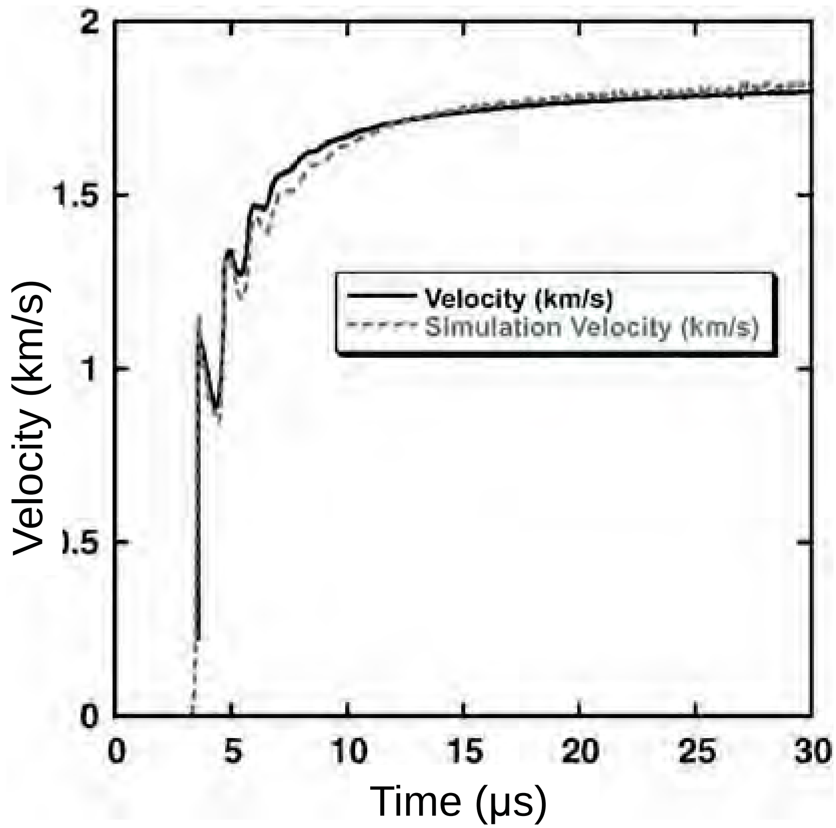


Optical framing camera records

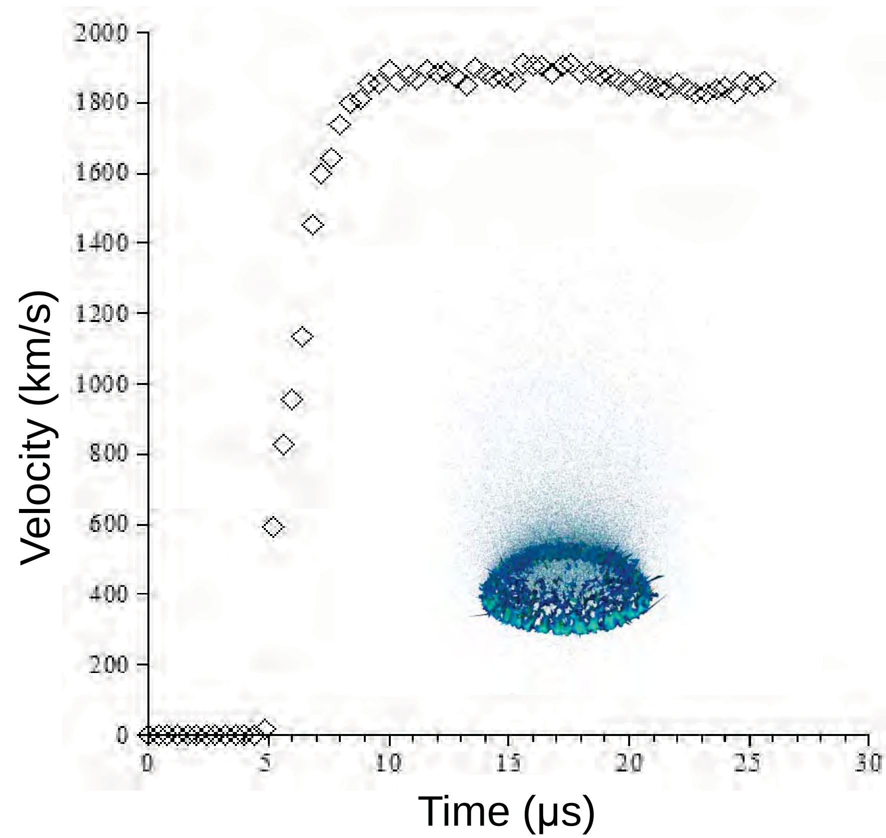
G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Validation – Explosively driven cap

Experiment



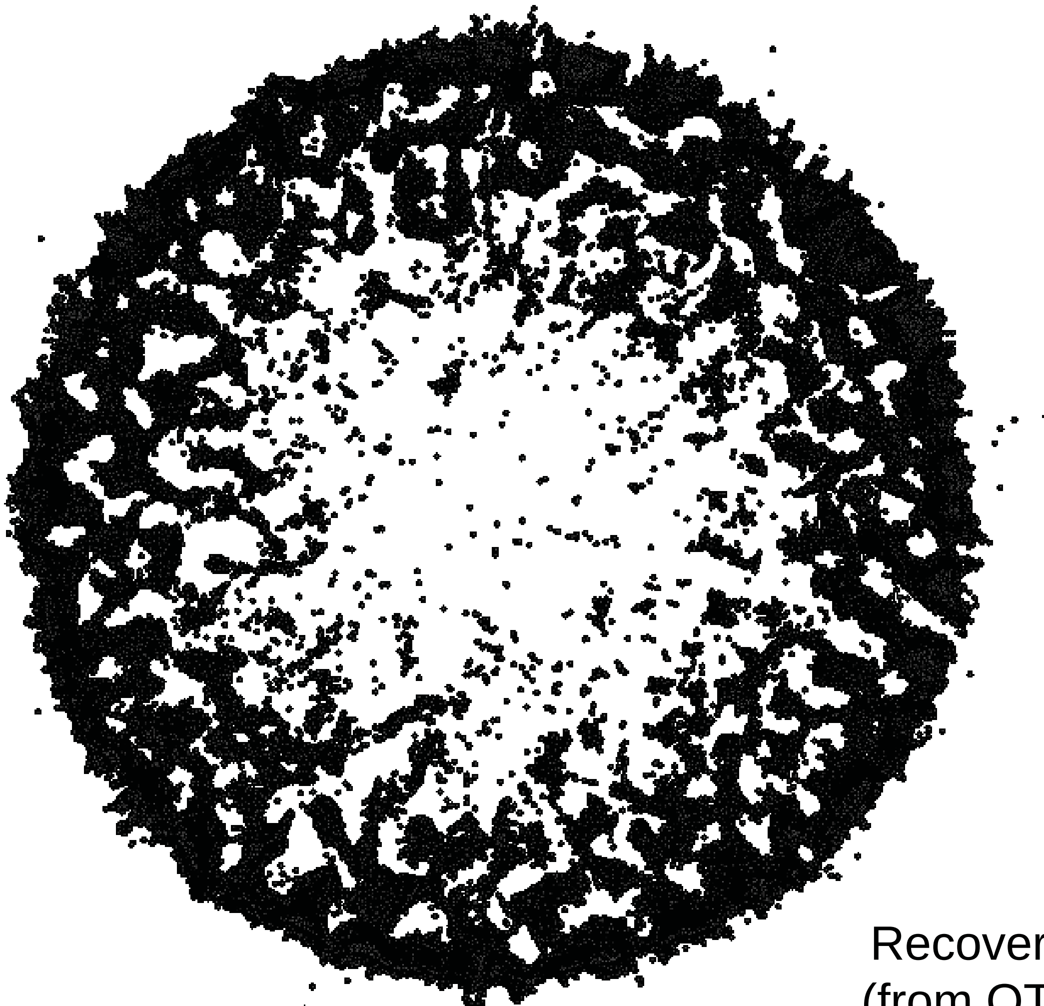
OTM simulation



Surface velocity for spot midway between pole and edge

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Validation – Explosively driven cap



Recovered fragments
(from OTM simulation)

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Validation – Explosively driven cap

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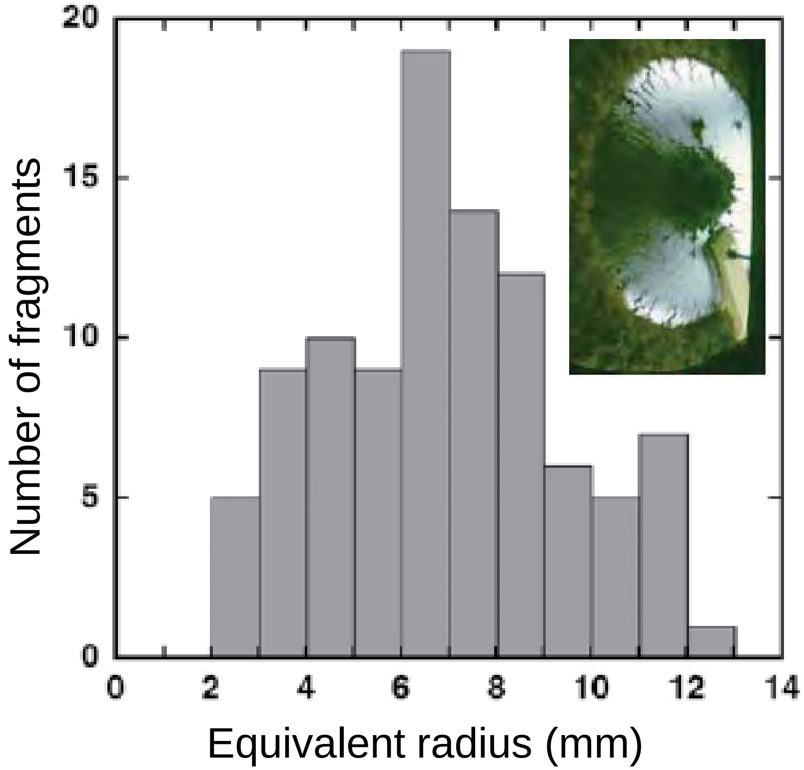
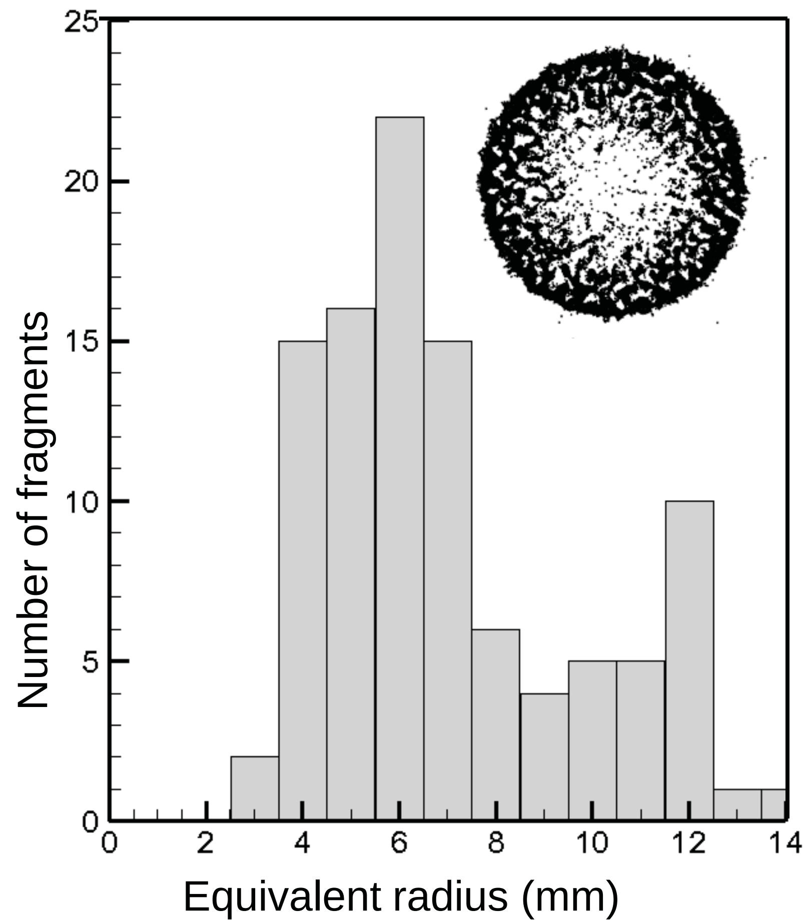
Experiment



OTM simulation



Histograms of equivalent fragment radii

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

The case for multiscale modeling

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- No computational asset/scheme, present or future, capable of resolving all length/time scales explicitly and concurrently by brute force alone (exascale beware!)
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Thank you!