Multiscale modeling and simulation of ductile fracture and fragmentation

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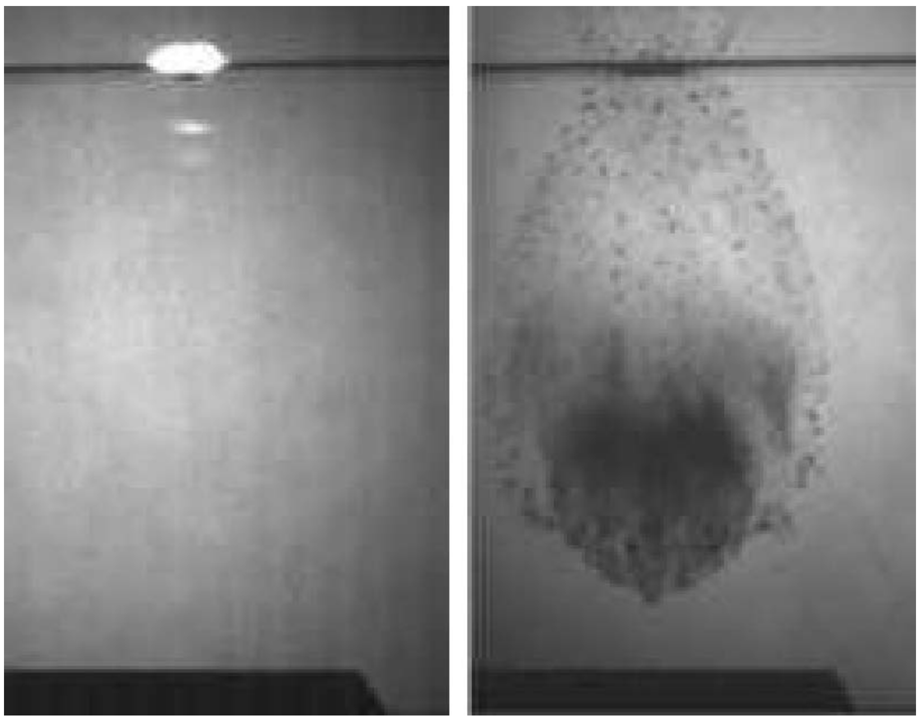
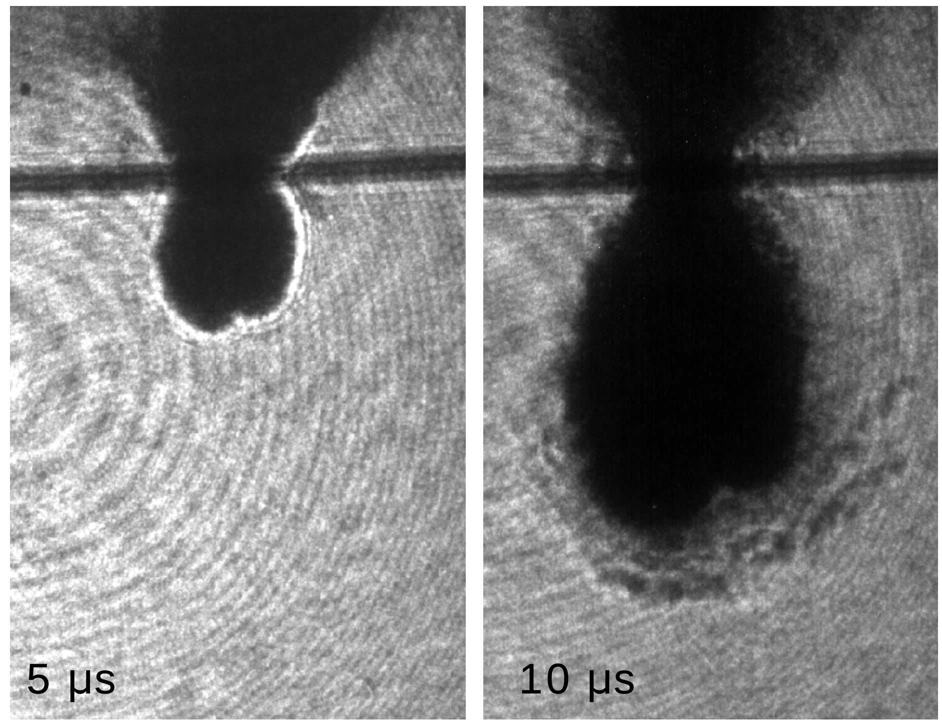
Vienna, Austria, September 10-14, 2012

HVI: Materials at the extreme (XMAT)

How far can we push Computational Mechanics? (and still be predictive)

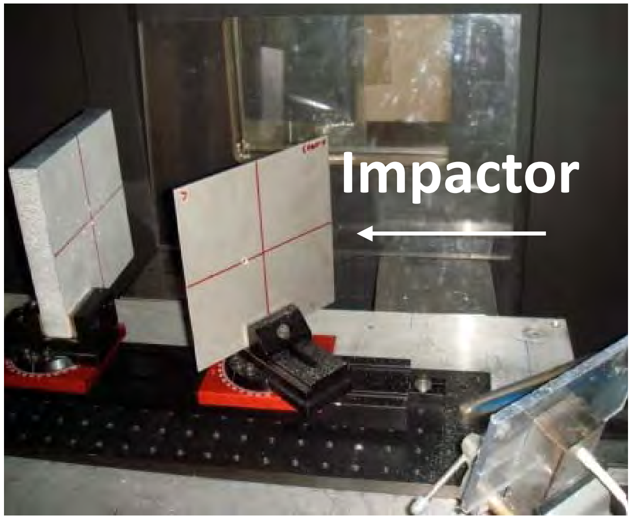


Hypervelocity impact of bumper shield. a) Initial impact flash. b) Debris cloud (Ernst-Mach Inst., Freiburg, Germany).

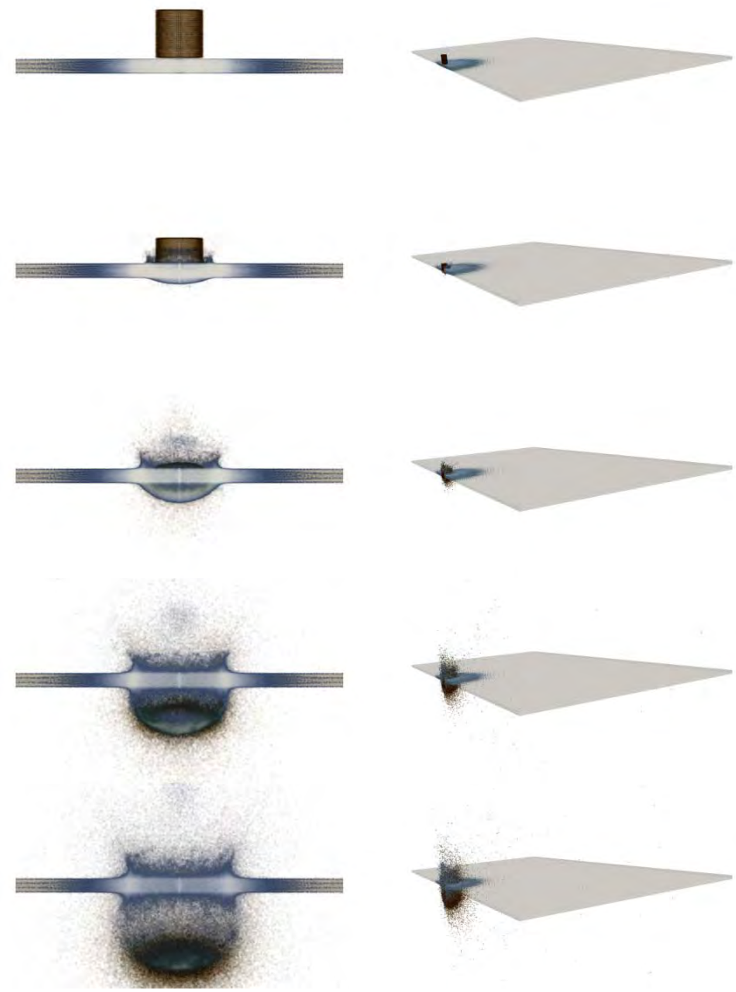


Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

Hypervelocity impact - Simulation

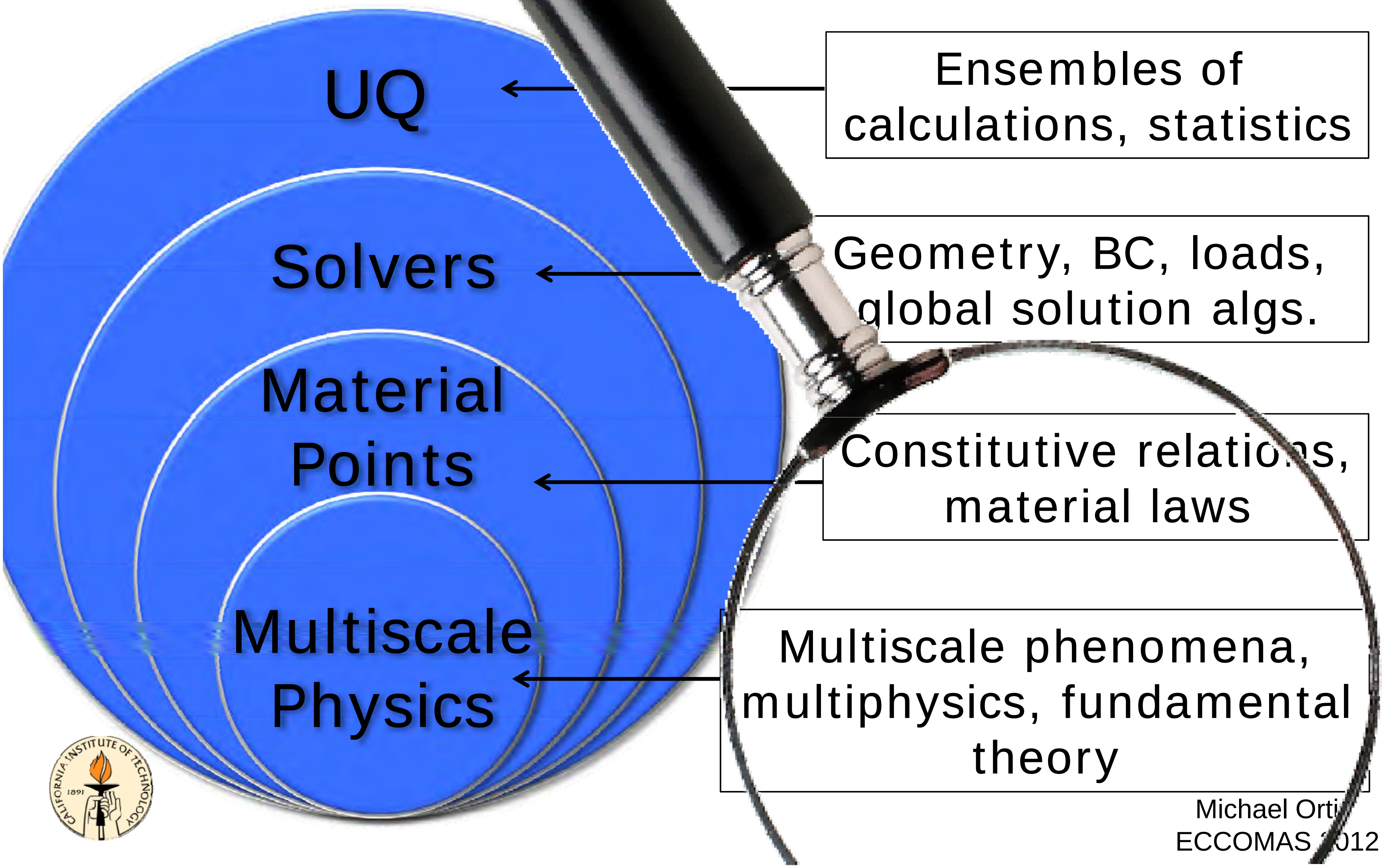


Caltech's hypervelocity Impact facility



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

Anatomy o mputational campaign



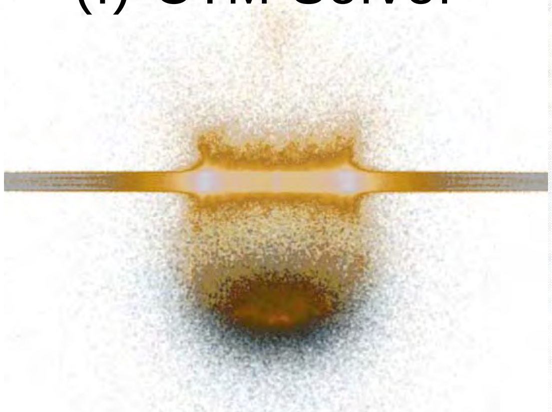
The case for multiscale modeling

- Material models sit at the core of computational campaigns: ***Predictive bottleneck!***
- Often, the *experimental data* is scarce, noisy, provide partial coverage of conditions of interest
- Often, *empirical models* are unavailable, especially for complex phenomena, or unreliable
- What else? Physics-based ***multiscale modeling!***
- ***Essential difficulty****:* The standard *relaxation* (homogeneization) scheme *does not apply to fracture* (localization, internal length scales...)
- What else? ***Optimal scaling!***

Lecture plan

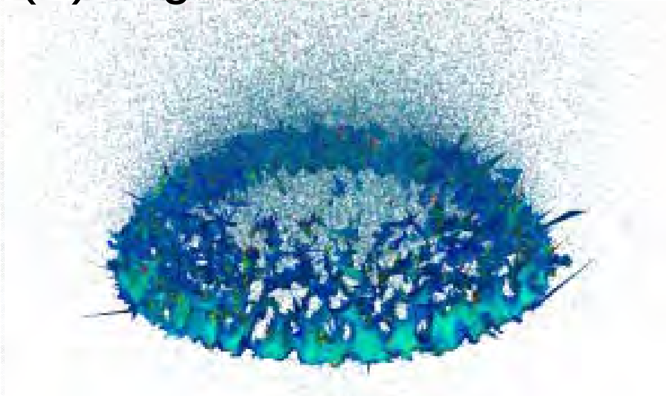
- The application framework: Hypervelocity Impact (HVI) of metallic targets @ 5-10 Km/s
- The computational framework: Optimal transportation meshfree + eigenerosion
- Focus: Multiscale modeling of ductile fracture

(i) OTM Solver



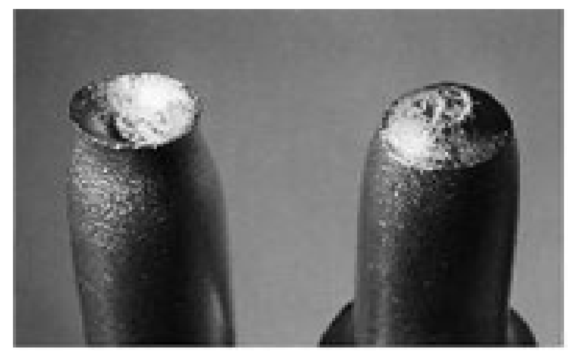
Li, B., Habbal, F. & MO, *IJNME*, **83**:1541, 2010

(ii) Eigenerosion Solver



Schmidt, B., Fraternali, F. & MO, SIAM Multiscale, **7**:1237, 2009

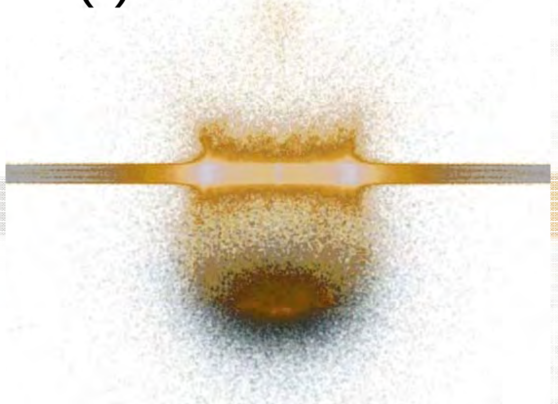
(iii) Ductile fracture



Fokoua, L., Conti, S. & MO, (in progress)

Lecture plan

(i) OTM Solver



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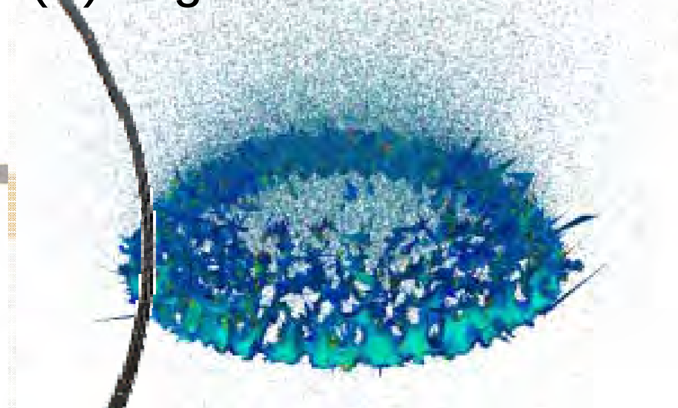
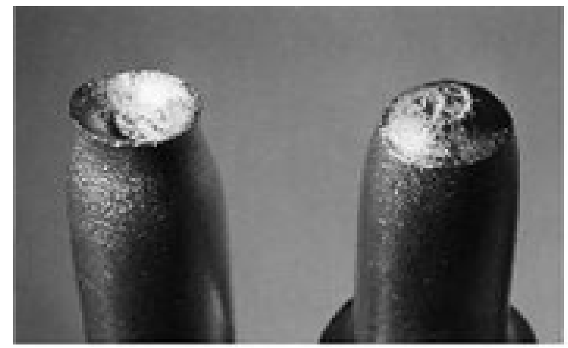


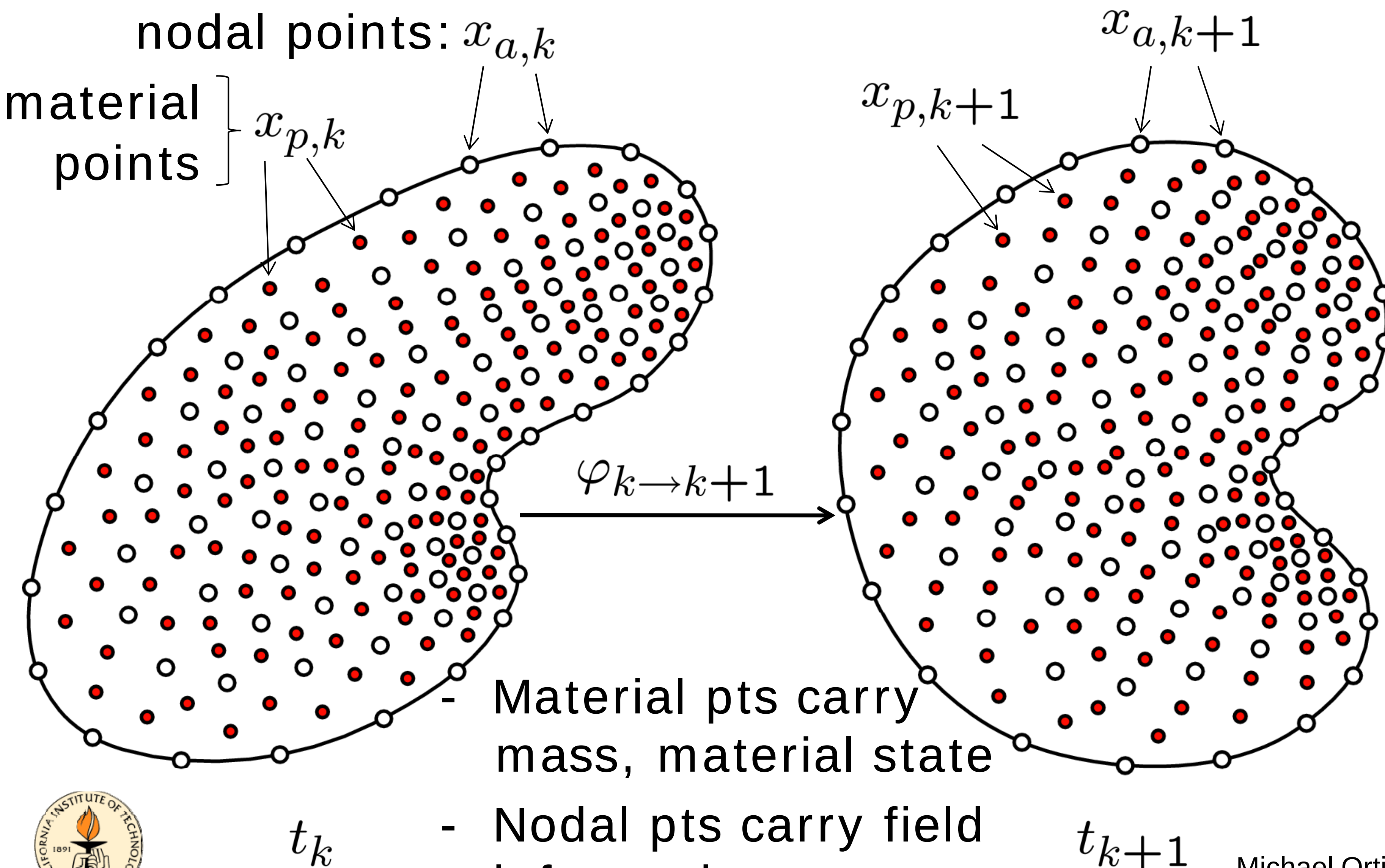
Schmidt, B., Fraternali, F. & MO, SIAM Multiscale, **7**:1237, 2009

(iii) Ductile fracture

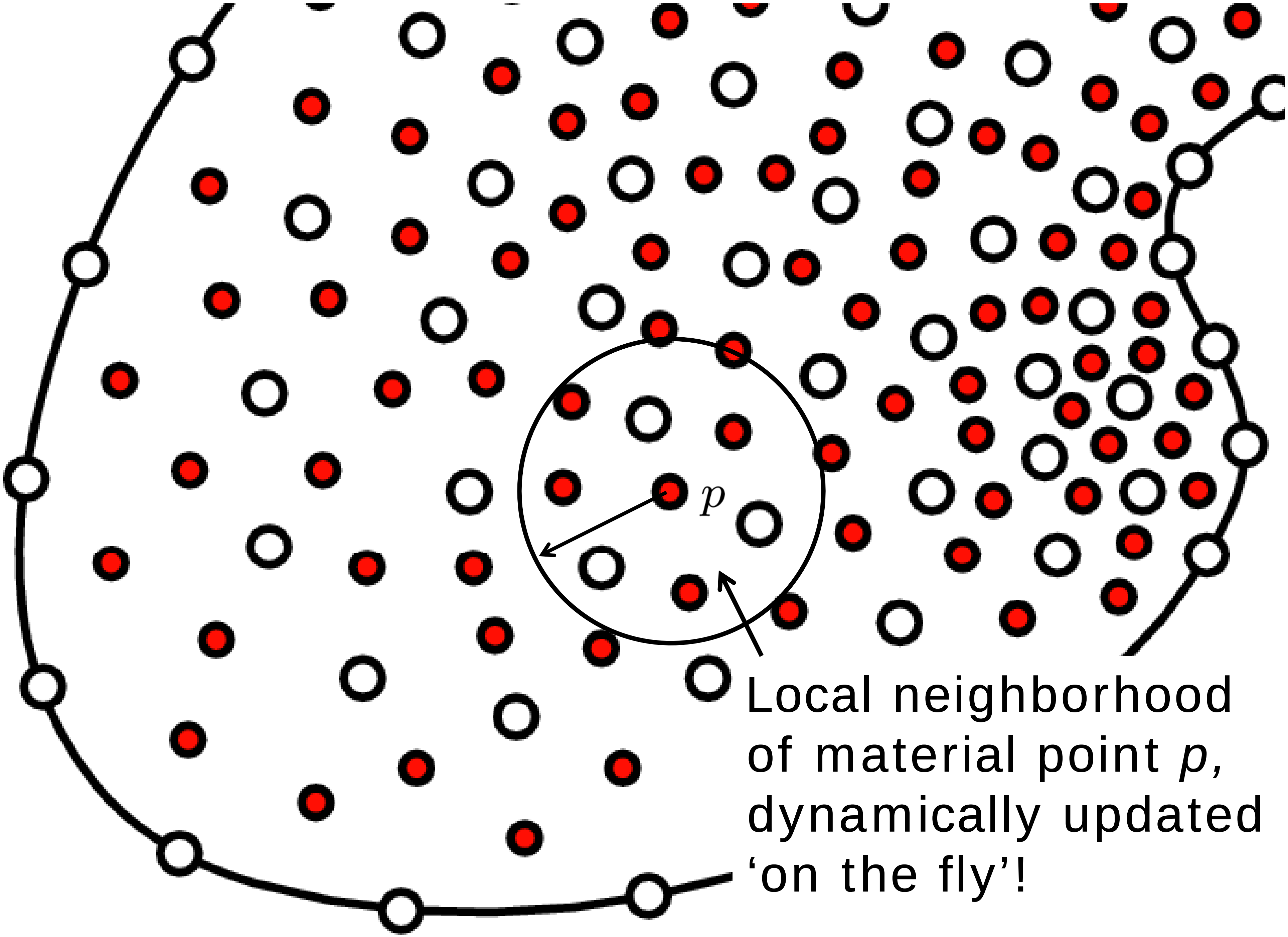


Fokoua, L., Conti, S. & MO, (in progress)

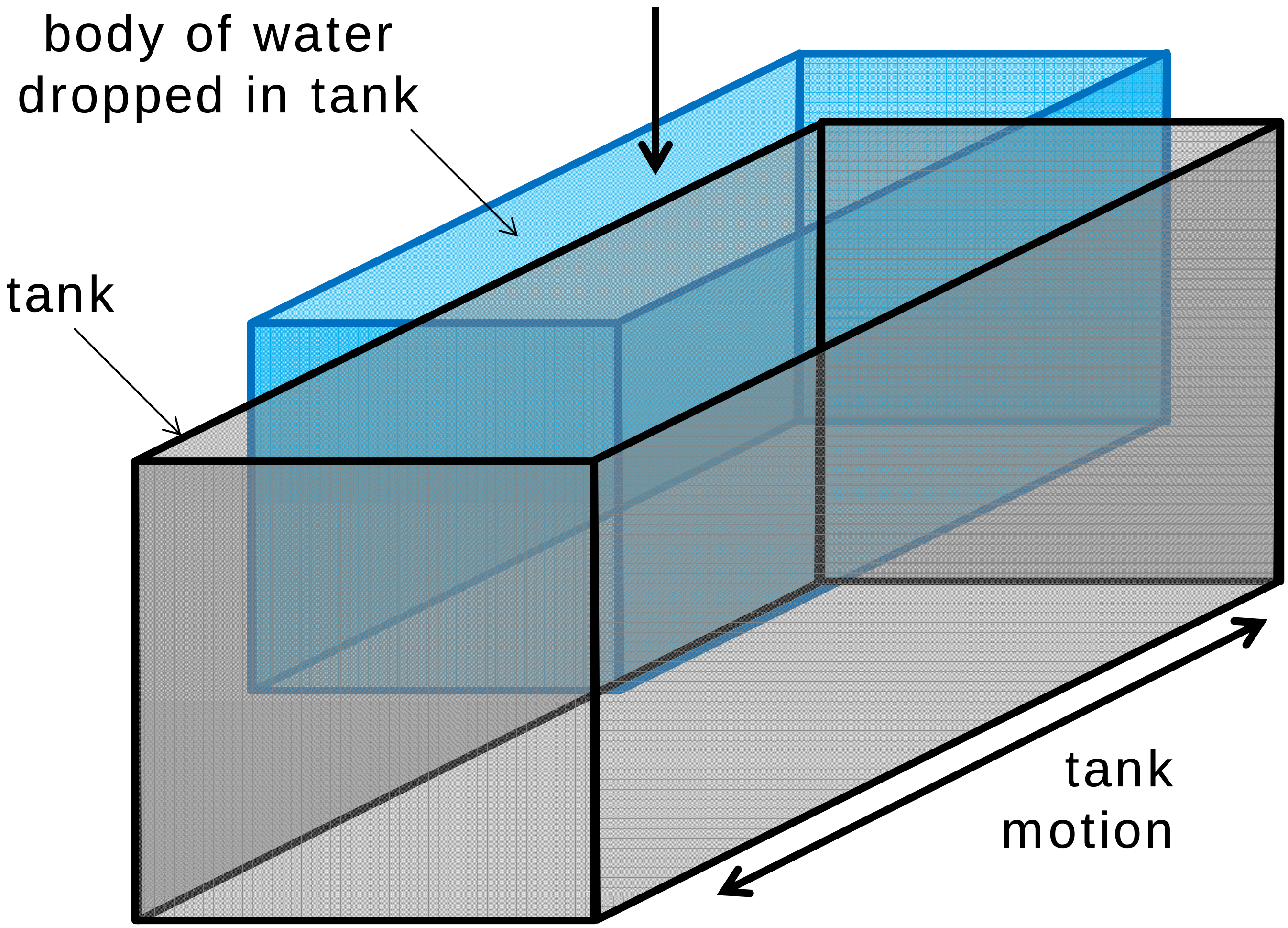
OTM Solver – Spatial discretization



- Material pts carry mass, material state
- Nodal pts carry field information


p
Local neighborhood
of material point *p*,
dynamically updated
‘on the fly’!

Example: Water sloshing in tank (free-surface, compressible NS)



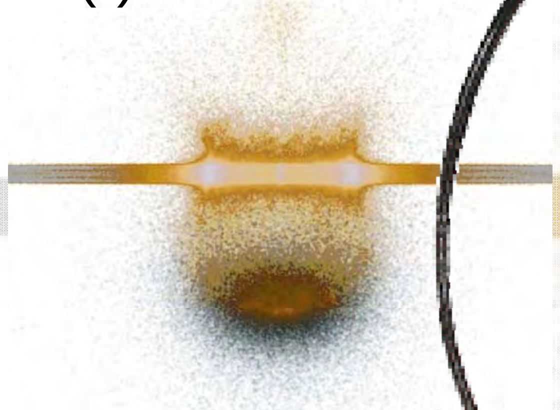
Dirk Hartmann, Siemens AG, Munich
Corporate Research and Technologies

Solver: Optimal Transportation Meshfree

- *Optimal transportation theory* generates *geometrically-exact* discrete Lagrangians for flow problems (solid, fluid, solid+fluid...)
- Inertial part of discrete Lagrangian measures *distance* between consecutive mass densities (in sense of *Wasserstein*)
- Discrete Hamilton principle of stationary action, *variational time integration scheme*:
  - *Symplectic, time reversible*
  - *Exact momenta conservation properties*
  - *Geometrically-exact mass transport*
  - *Variational convergence, in the sense of Γ-convergence (B. Schmidt, work in progress...)*

Lecture plan

(i) OTM Solver



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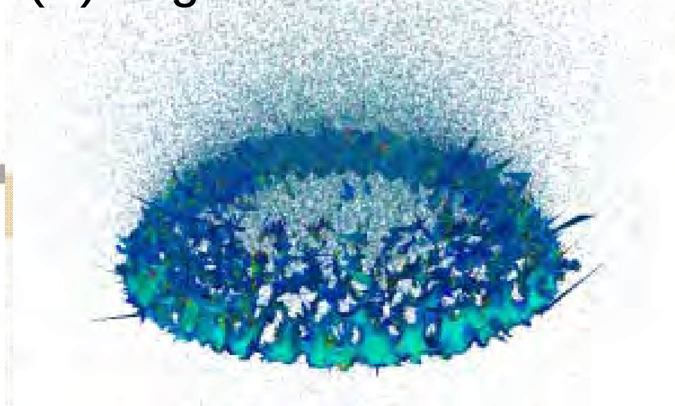
(ii) Eigenerosion Solver

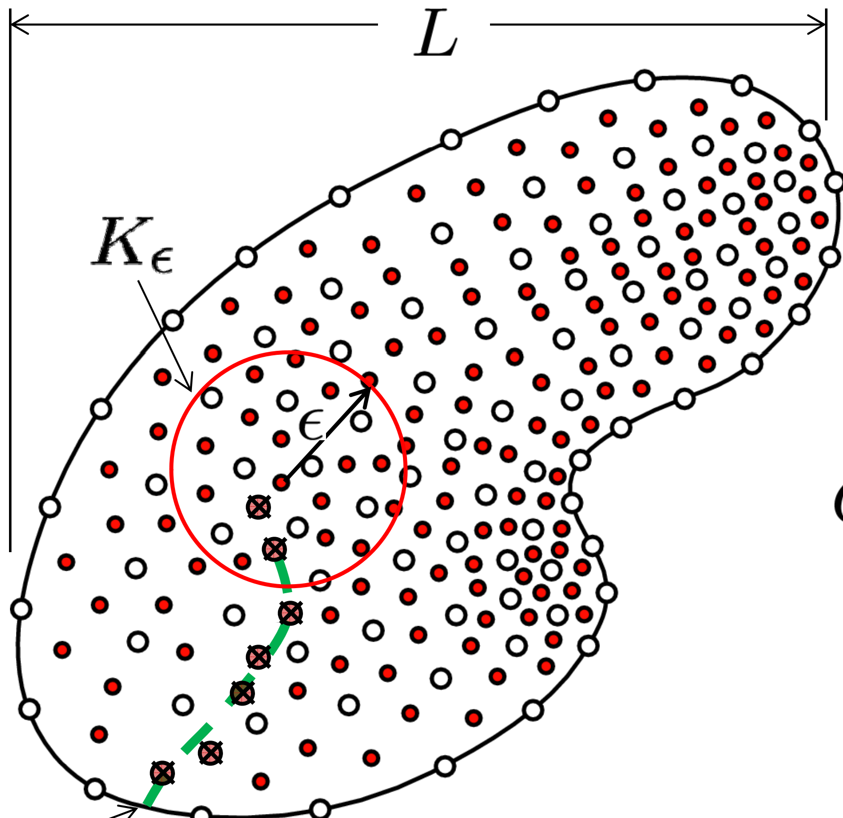


Schmidt, B., Fraternali, F. & MO, SIAM Multiscale, **7**:1237, 2009

(iii) Ductile fracture

Fokoua, L., Conti, S. & MO, (in progress)

Fracture – Material-point erosion



crack ⊗ Failed material pts

Schematic of ε-neighborhood construction

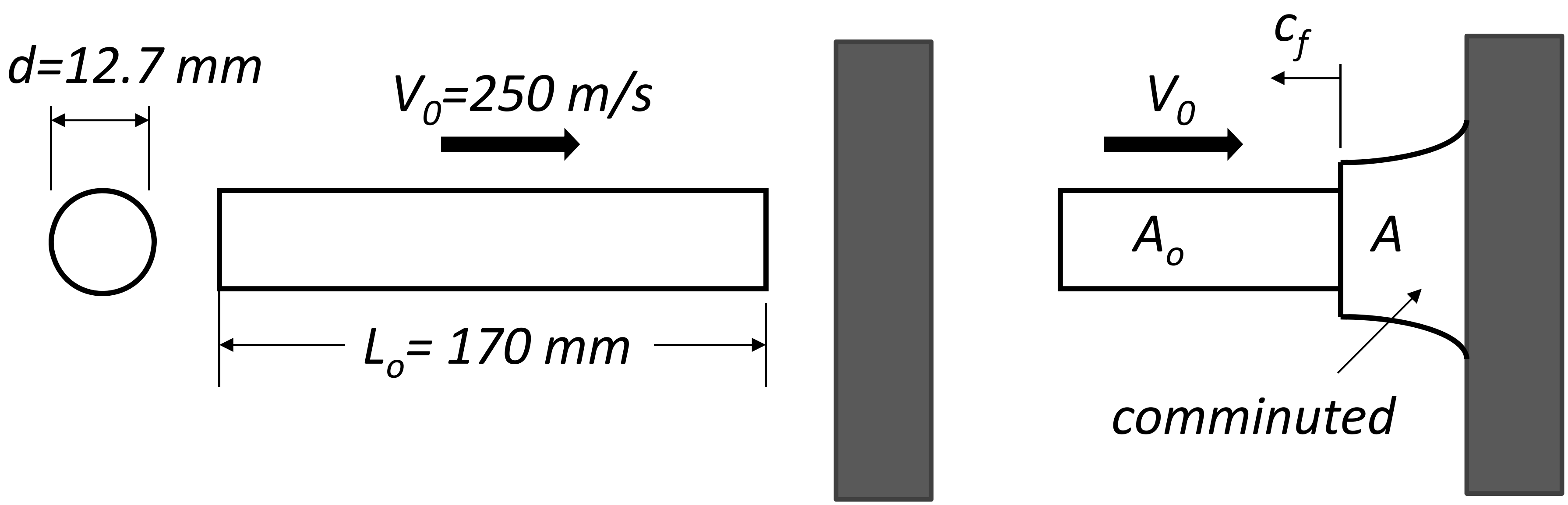
- ε-neighborhood construction: Choose h << ε << L
- Erode material point if

$$G_\epsilon \sim \frac{h^2}{|K_\epsilon|} \int_{K_\epsilon} W(\nabla u)\, dx \geq G_c$$

- Proof of convergence to Griffith fracture:
  - *Schmidt, B., Fraternali, F. & MO, SIAM J. Multiscale Model. Simul.*, **7**(3):1237-1366, 2009.

Validation – Failure waves in glass rods

- Brittle fracture: G_c = constant!

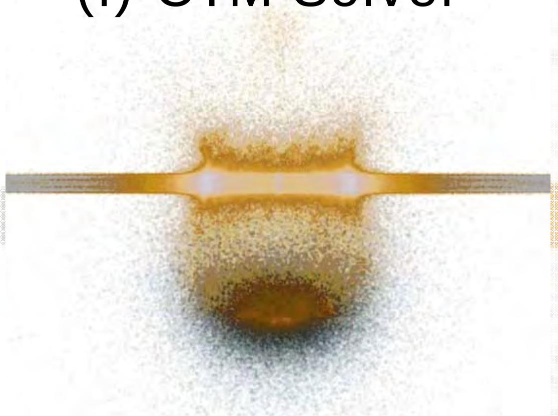


- V_0=225 m/s, c_f = 3.6 Km/s (Brar & Bless, 1991)
- V_0=250 m/s, c_f = 3.0 Km/s (Repetto et al., 2000)
- V_0=250 m/s, c_f = 3.63 Km/s (present)

Brar, N.S. and Bless, S.J., *Appl. Phys. Let*., **59:**3396, 1991
Repetto, E.A. *et al*., *CMAME*, **183**:3, 2000

Lecture plan

(i) OTM Solver



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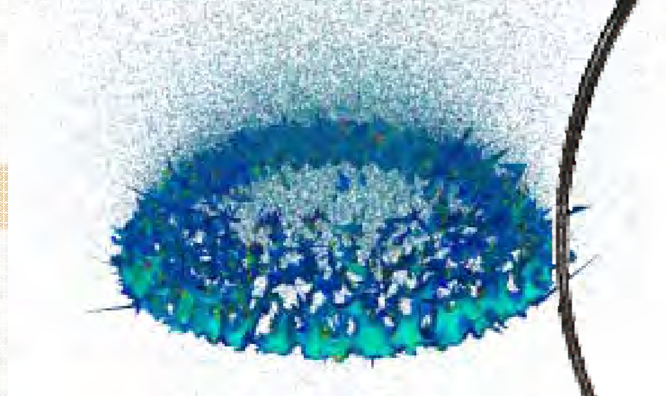

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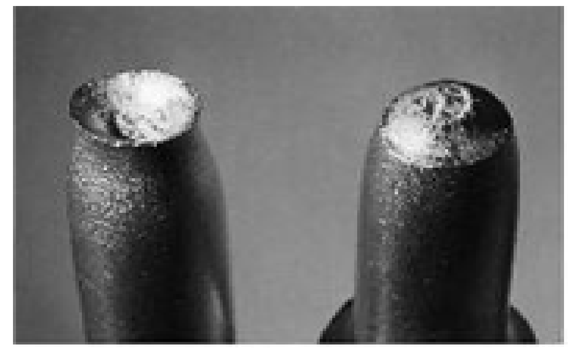
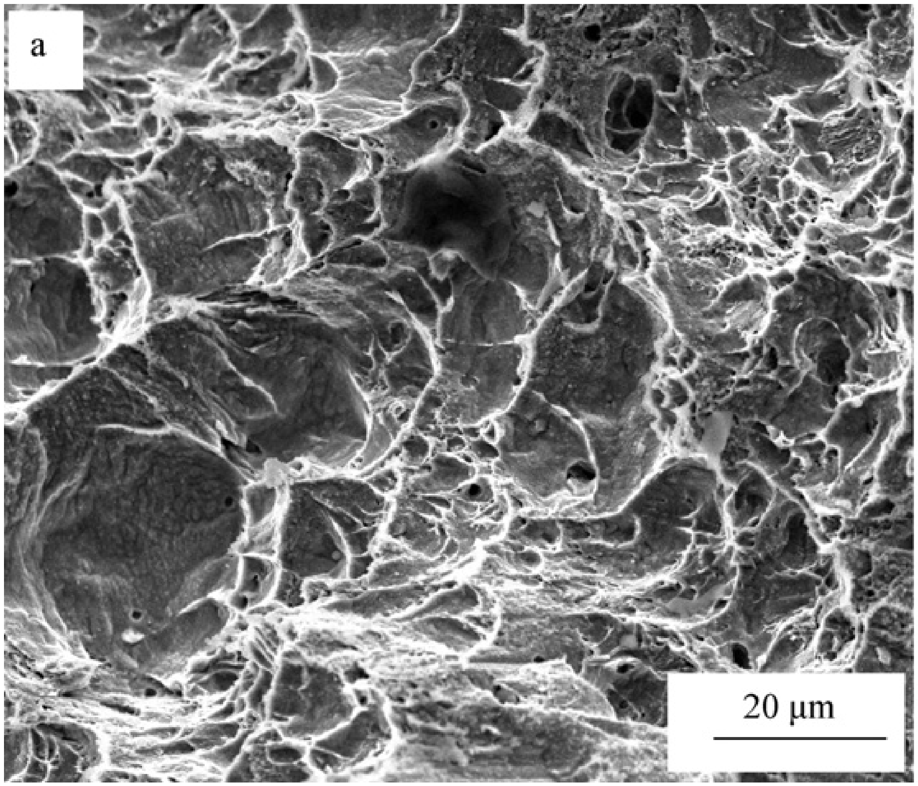
(iii) Ductile fracture



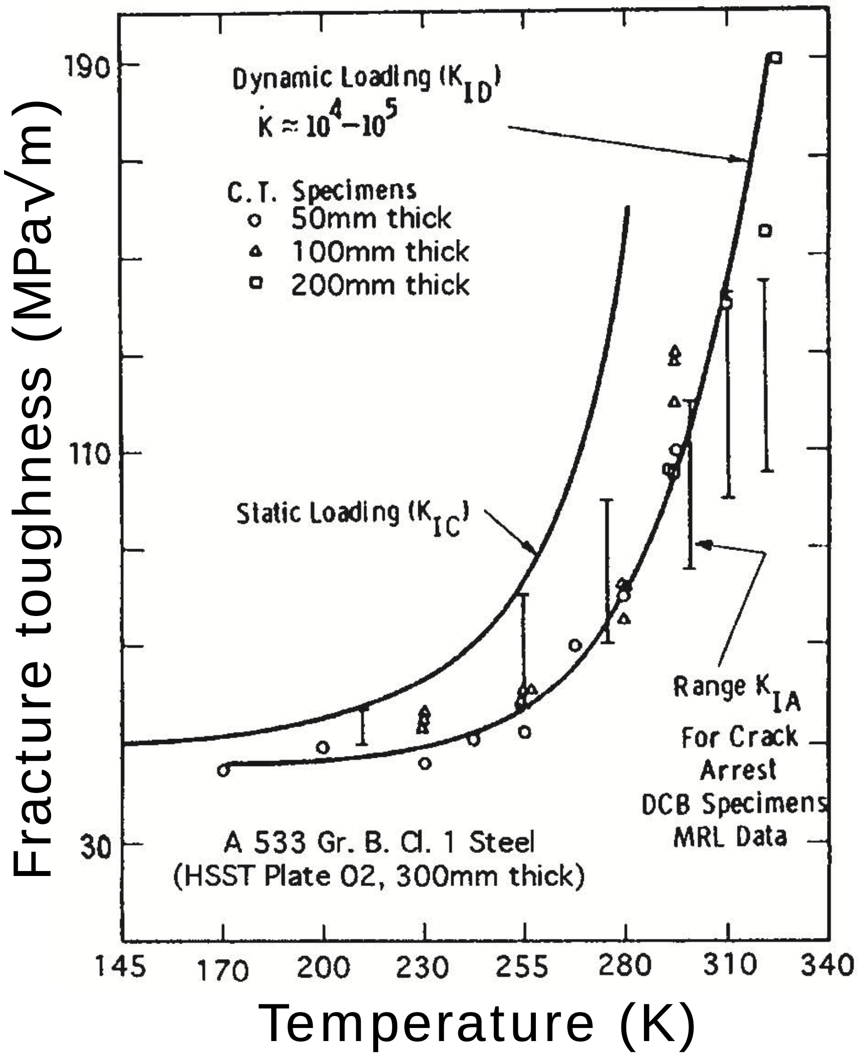
Fokoua, L., Conti, S.
& MO, (in progress)

Ductile fracture – Experimental data



Fracture surface in SA333 steel (room temp., $d\varepsilon/dt = 3\times10^{-3}s^{-1}$)

S.V. Kamata, M. Srinivasa and P. R. Rao, Mater. Sci. Engr. A, ***528*** *(2011) 4141–4146*

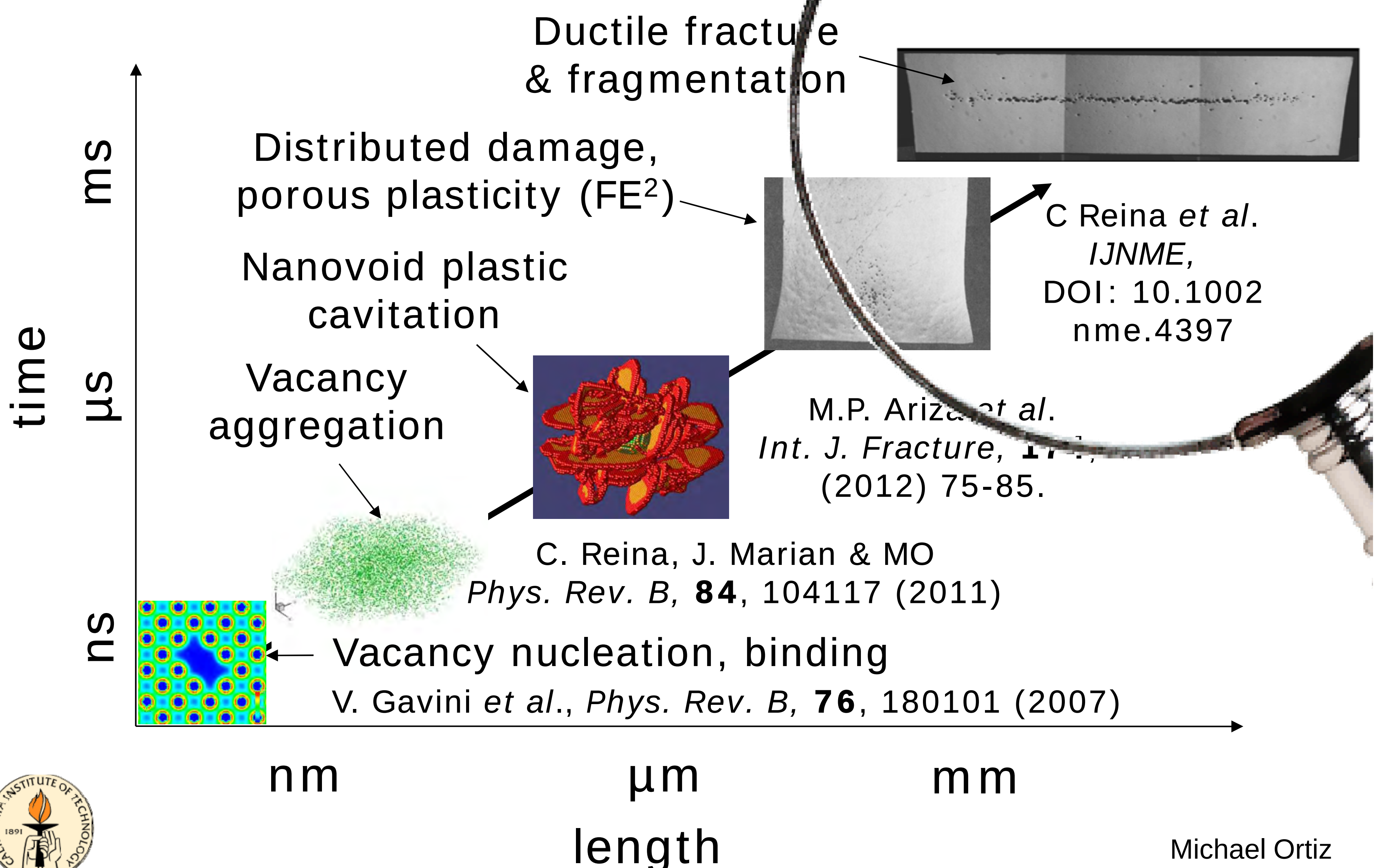


J. D. Landes, *Metall. Trans. A*, **21A** (1990) 1097–1104.

Ductile fracture – Empirical models?

- *Complex dependence* of specific fracture energy (G_c) on temperature, pressure, rate of deformation, history, processing...
- *Complex coupling* to plasticity, dislocation dynamics, surface energy/phenomena...
- *Paucity of experimental data* in general, especially under extreme conditions...
- *Lack of*—poor prospects for—predictive *empirical models* (behavior too complex!)...
- What instead? ***Multiscale modeling!***

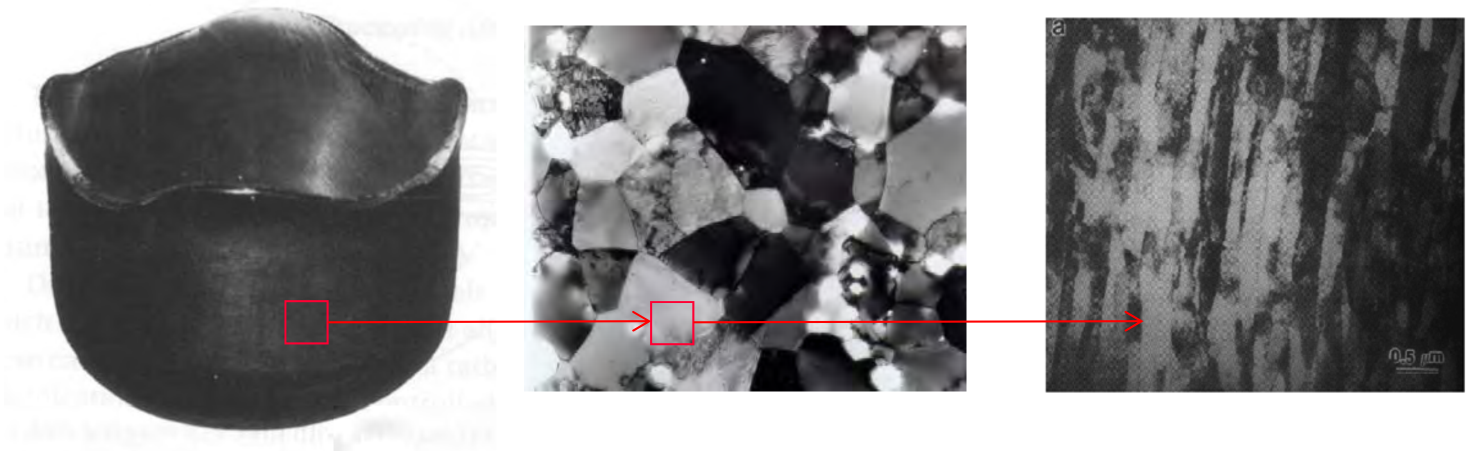
Ductile fracture – Multiscale hierarchy



Michael Ortiz
ECCOMAS 2012

Multiscale - Homogeneization

- Effective macroscopic model follows (in some cases) from a ‘representative volume’ calculation



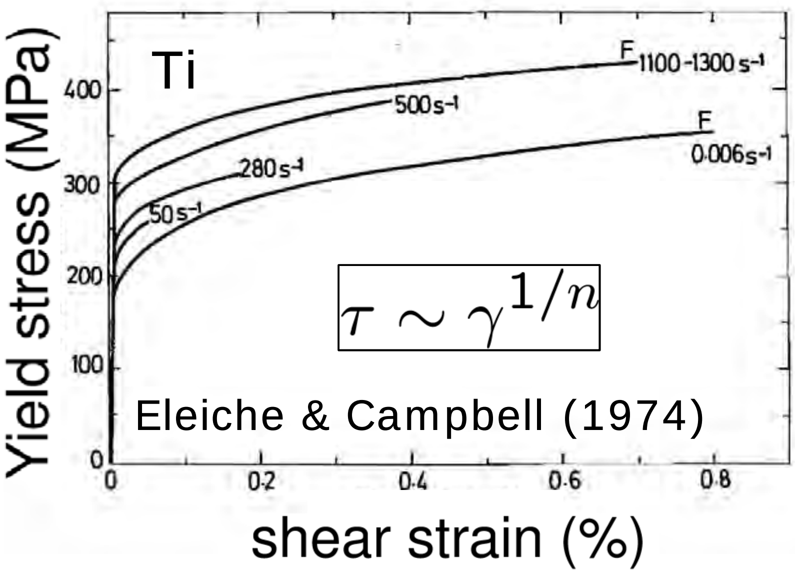
Macroscopic problem

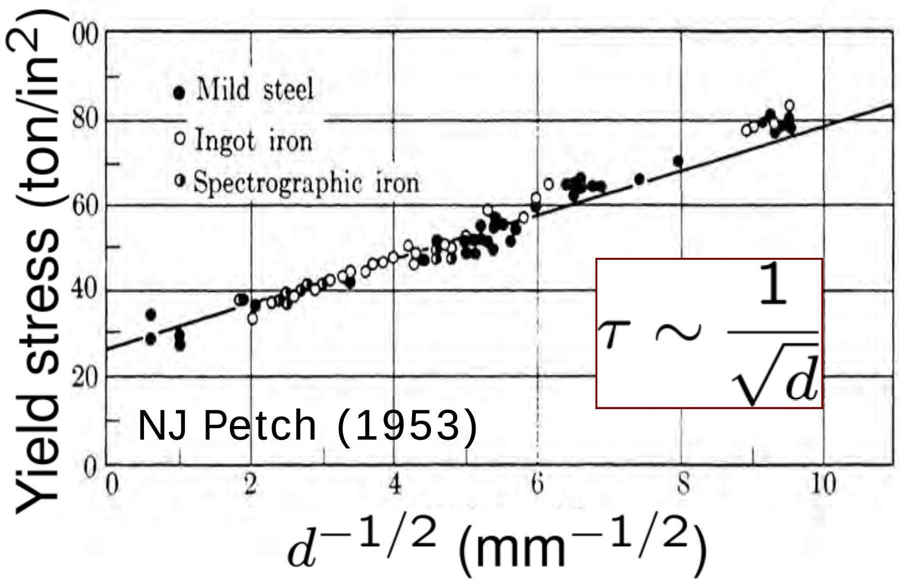
Representative volume: Pre-evaluate all microstructures

- **But**: Relaxation requires superlinear energy growth, ‘bulk’ energy scaling’: In R^d,

$$(\text{length}) \to \lambda(\text{length}) \Rightarrow (\text{energy}) \to \lambda^d(\text{energy})$$

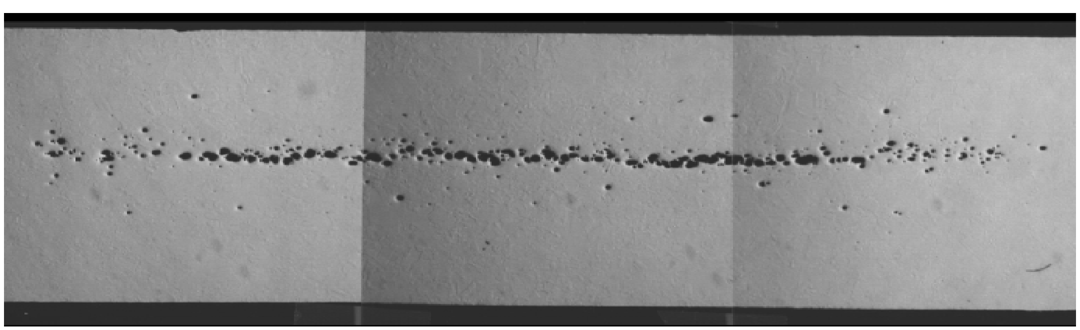
Homogeneization fails for ductile fracture!





Sublinear-energy growth
(necking @ Considère condition)

Internal length scales
(scaling and size effect)



R. Becker
"How Metals Fail",
Sci. &Tech. Rev., LLNL,
July/August 2002

Localization, no 'bulk' energy scaling!

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Ductile fracture – Multiscale modeling?

- Homogeneization fails for ductile fracture due to sub-linear growth of energy and the attendant damage localization (voids sheets)
- What instead? ***Optimal scaling!***
- Suppose: Energy $= E(u, \epsilon_1, \ldots, \epsilon_N)$
- Optimal (matching) upper and lower bounds:

$$C_L \epsilon_1^{n_1} \ldots \epsilon_N^{n_N} \leq \inf E(\cdot, \epsilon_1, \ldots, \epsilon_N) \leq C_U \epsilon_1^{n_1} \ldots \epsilon_N^{n_N}$$

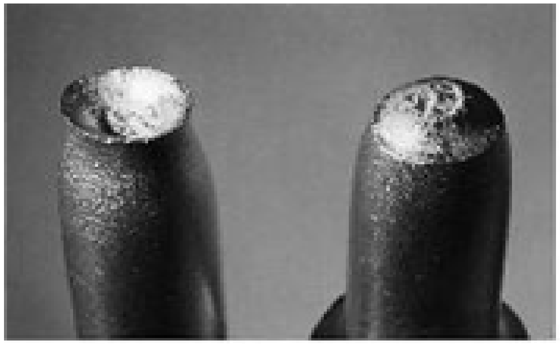
- Originally applied to branched microstructures in martensite (Kohn-Müller 92, 94; Conti 00)
- Applications to micromagnetics (Choksi-Kohn-Otto 99), thin films (Belgacem *et al* 00)…

Optimal scaling laws in ductile fracture

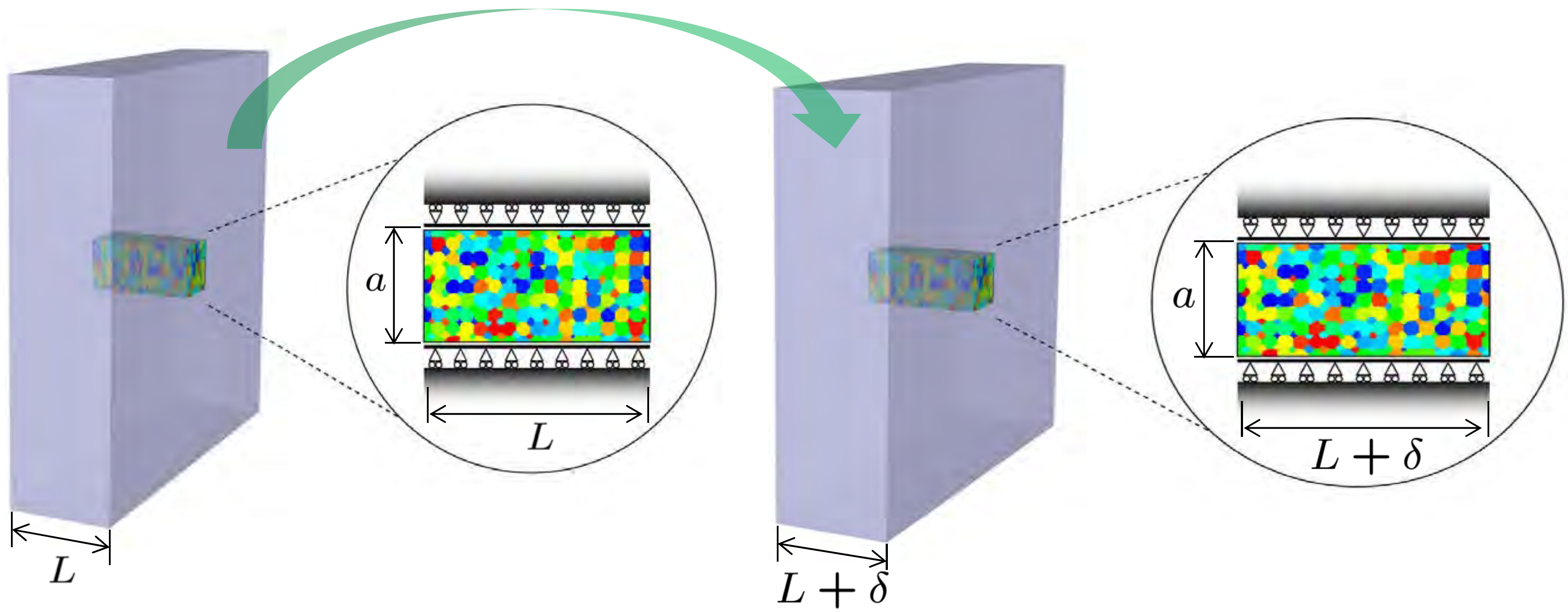
- Assumptions of optimal-scaling analysis:
  - Deformation theory of plasticity (finite kinematics)
  - Strain-gradient theory of plasticity
  - Rigid-plastic behavior (negligible elastic strains)
  - Isotropic hardening, no plastic spin
- Assume energy growth of the form:

$$c_L \int_\Omega (|F|^p + \epsilon |DF|)\, dx \leq E \leq c_U \int_\Omega (|F|^p + \epsilon |DF|)\, dx$$

- Assume hardening exponent $n > 1$
- Growth exponent $p = 1/n < 1$
- Necking, localization, fracture...



Optimal scaling laws in ductile fracture



- Geometry, BC: $\Omega = [0,a]^2 \times [0,L]$, $L \to L + \delta$.

Theorem [L. Fokoua, S. Conti & MO]

$$C_L a^2 \delta^{\frac{1}{2-p}} \epsilon^{\frac{1-p}{2-p}} \leq \inf E \leq C_U a^2 \delta^{\frac{1}{2-p}} \epsilon^{\frac{1-p}{2-p}}$$

Optimal scaling laws in ductile fracture

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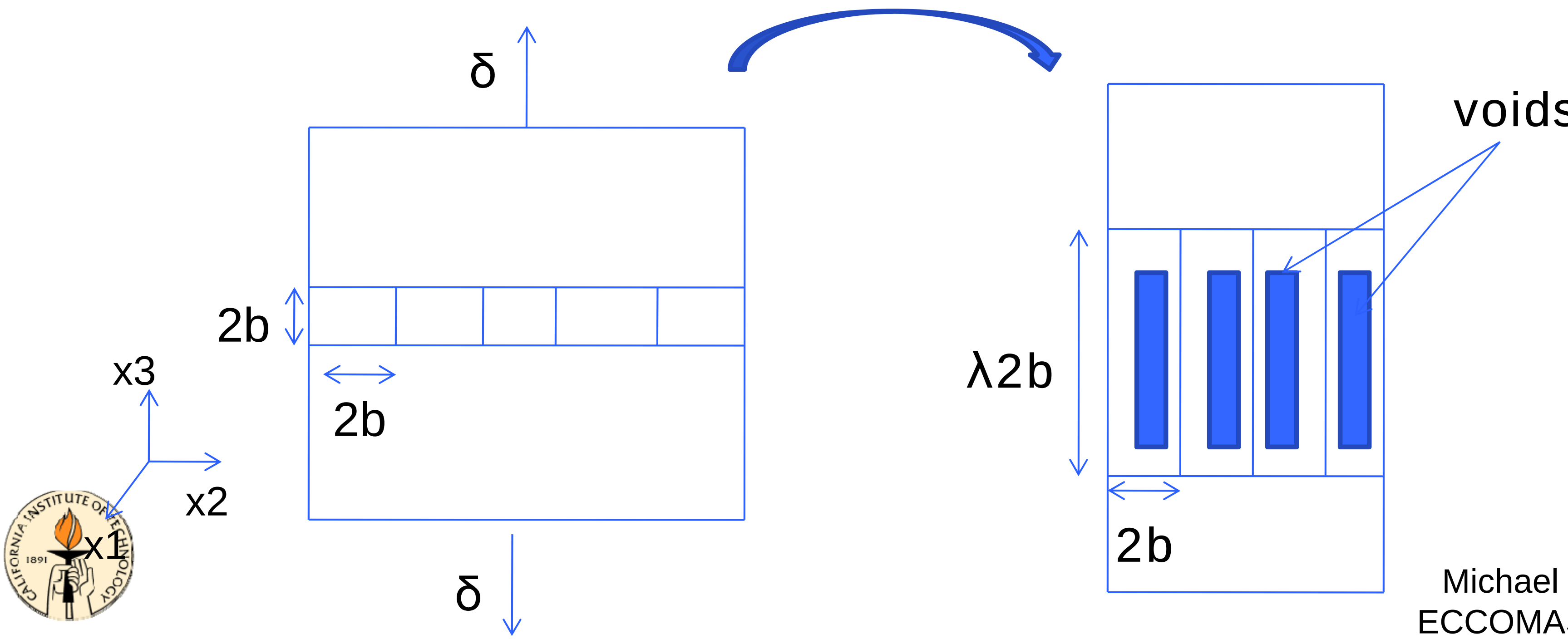
- Upper bound: *Void-sheet construction!*



Optimal scaling laws in ductile fracture

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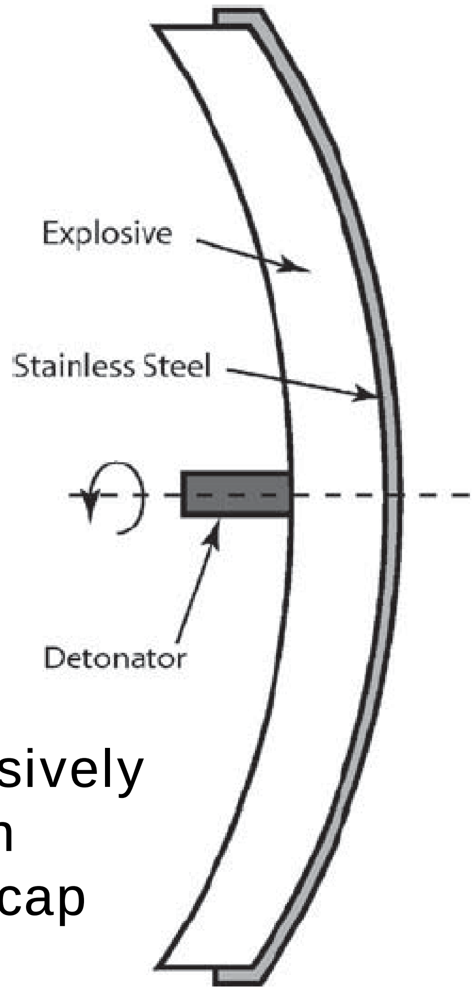
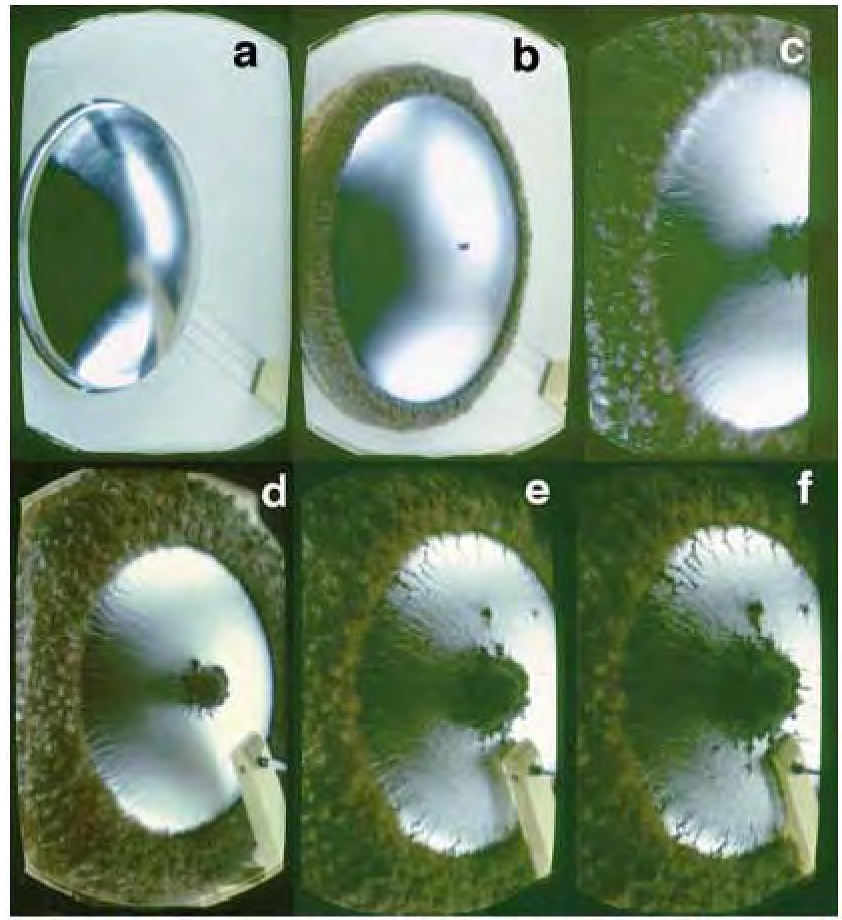
$$C_L a^2 \delta^{\frac{1}{2-p}} \epsilon^{\frac{1-p}{2-p}} \leq \inf E \leq C_U a^2 \delta^{\frac{1}{2-p}} \epsilon^{\frac{1-p}{2-p}}$$

- Deformation localizes to void sheet (fracture)
- Minimum energy scales with area (fracture)
- Fracture energy obeys power law in opening displacement, with exponent 1/(2-p)
- Cohesive law: $\sigma \sim \delta^{-(1-p)/(2-p)}$ (non-Griffith!)
- Power dependence on intrinsic length scale ε
- *Dependence of G_c on temperature, strain rate, upscaled directly from microscopic plasticity!*

Validation – Explosively driven cap



Explosively driven steel cap

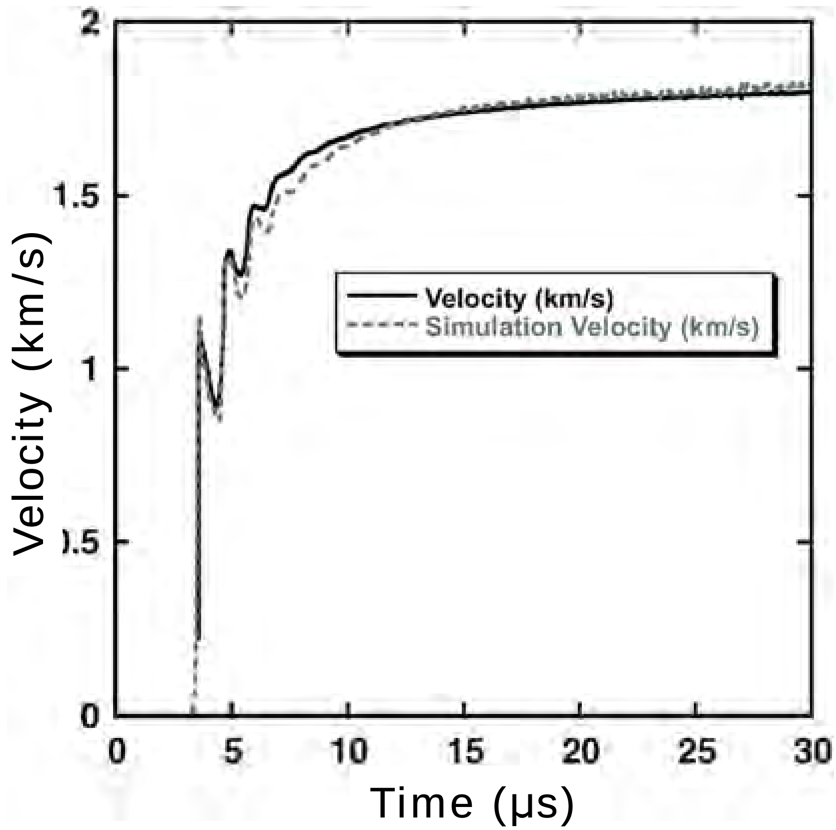


Optical framing camera records

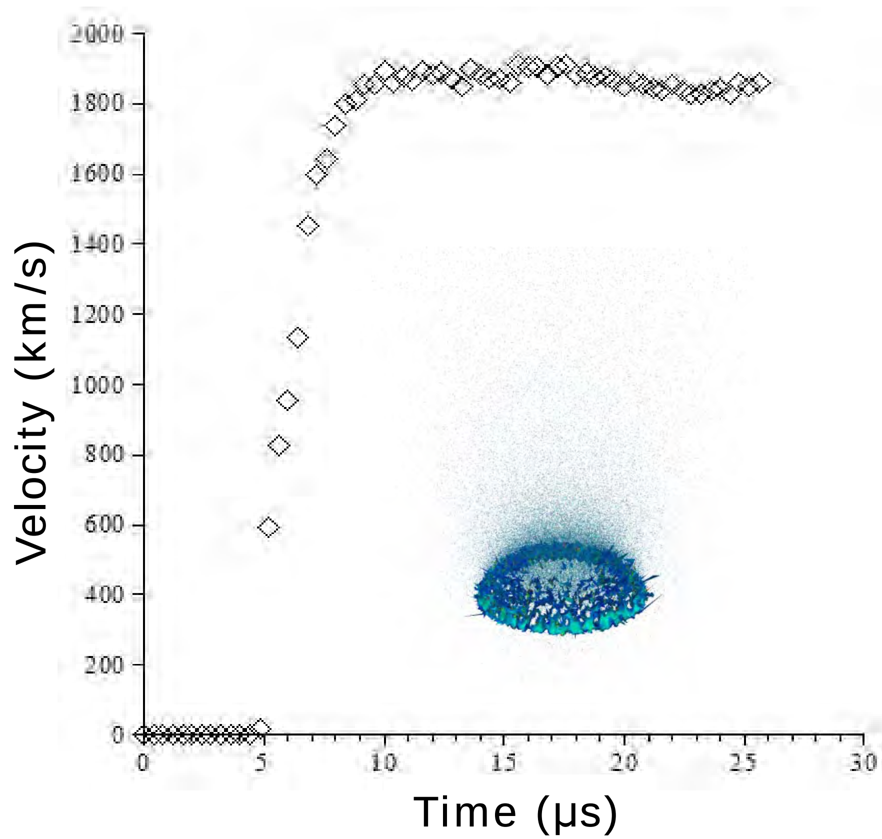
G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Validation – Explosively driven cap

Experiment



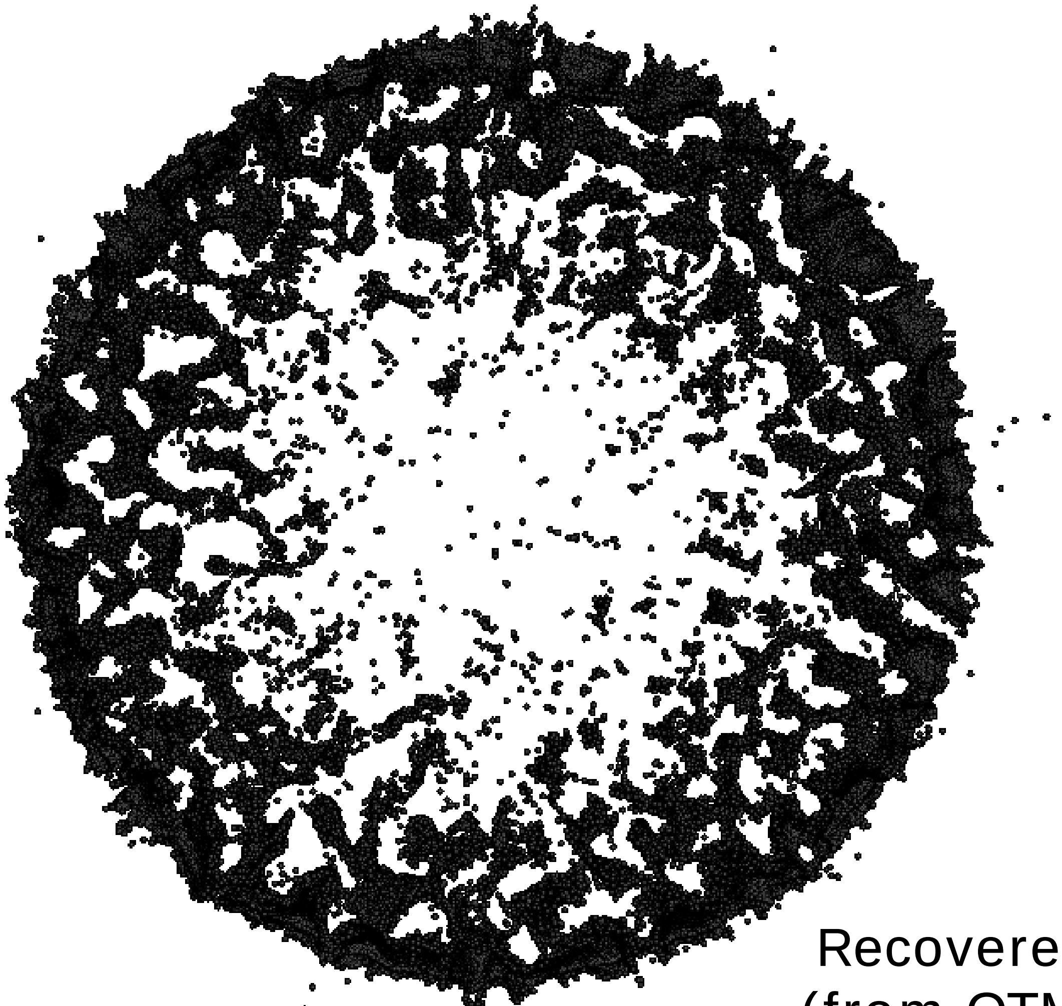
OTM simulation



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

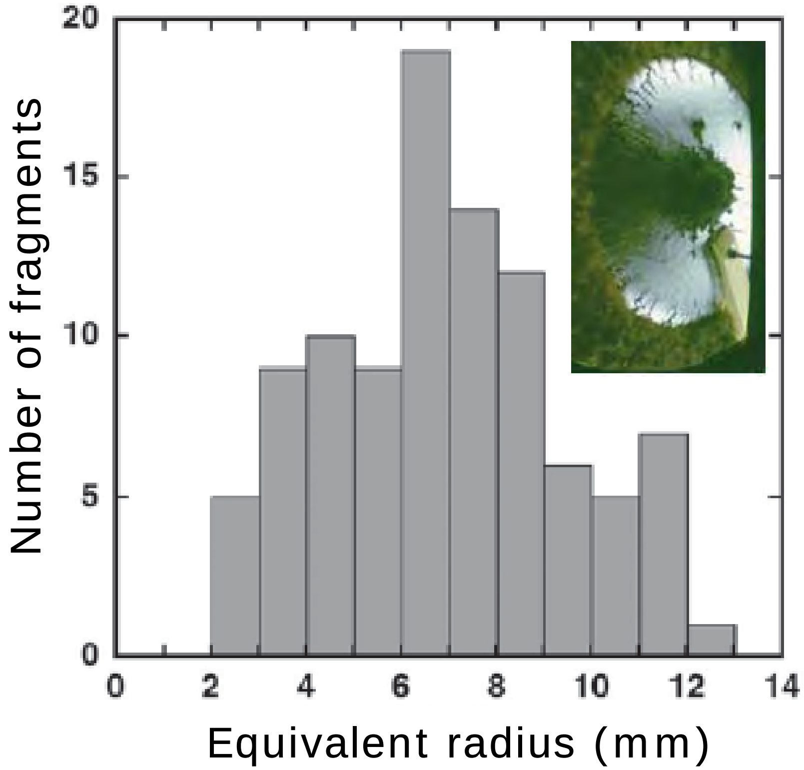


Recovered fragments
(from OTM simulation)

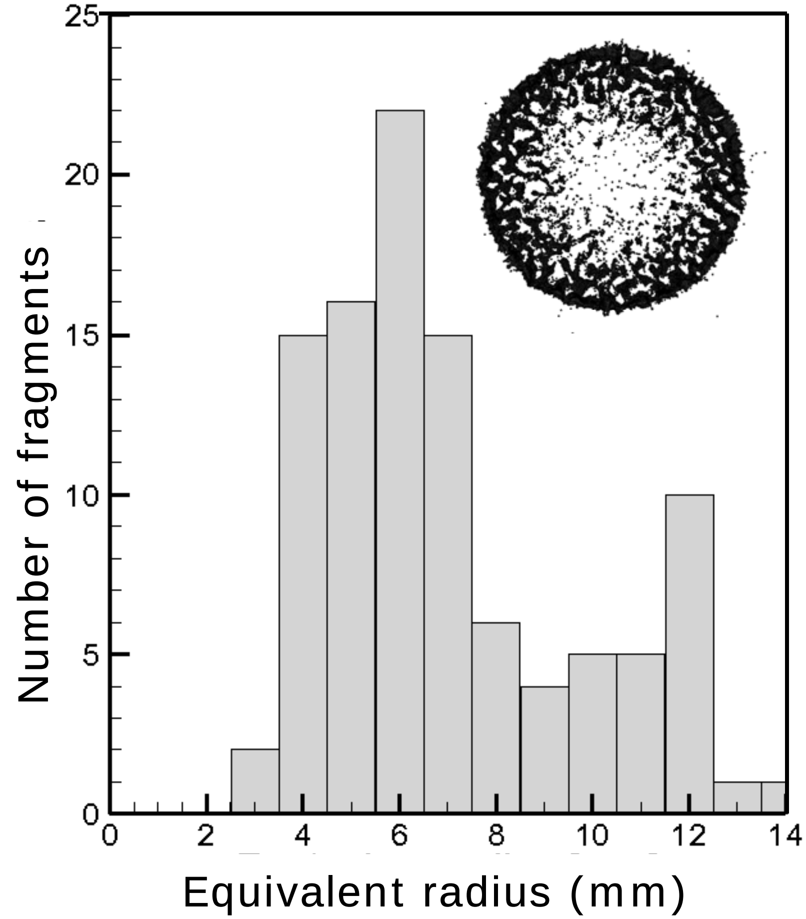
G.H. Campbell, G. C. Archbold, O. A. Hurricane and
P. L. Miller, *JAP*, **101**:033540, 2007

Validation – Explosively driven cap

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

Summary

- Modeling of *fracture* under *extreme conditions* requires characterization of fracture energy as function of temperature, pressure, strain rate
- *Deficit* of experimental data, empirical models
- Conventional *homogeneization* (relaxation) scheme *fails* due to sublinear energy growth
- Instead: Effective fracture energy delivered by *optimal scaling* (void-sheet construction)
- Scaling laws indicative of *cohesive behavior* at the macroscale, sensitivity to intrinsic length
- *Temperature and rate-dependence of fracture energy upscaled from microscopic plasticity!*

Thank you!