Optimal-Transportation Meshfree Approximation Schemes

M. Ortiz

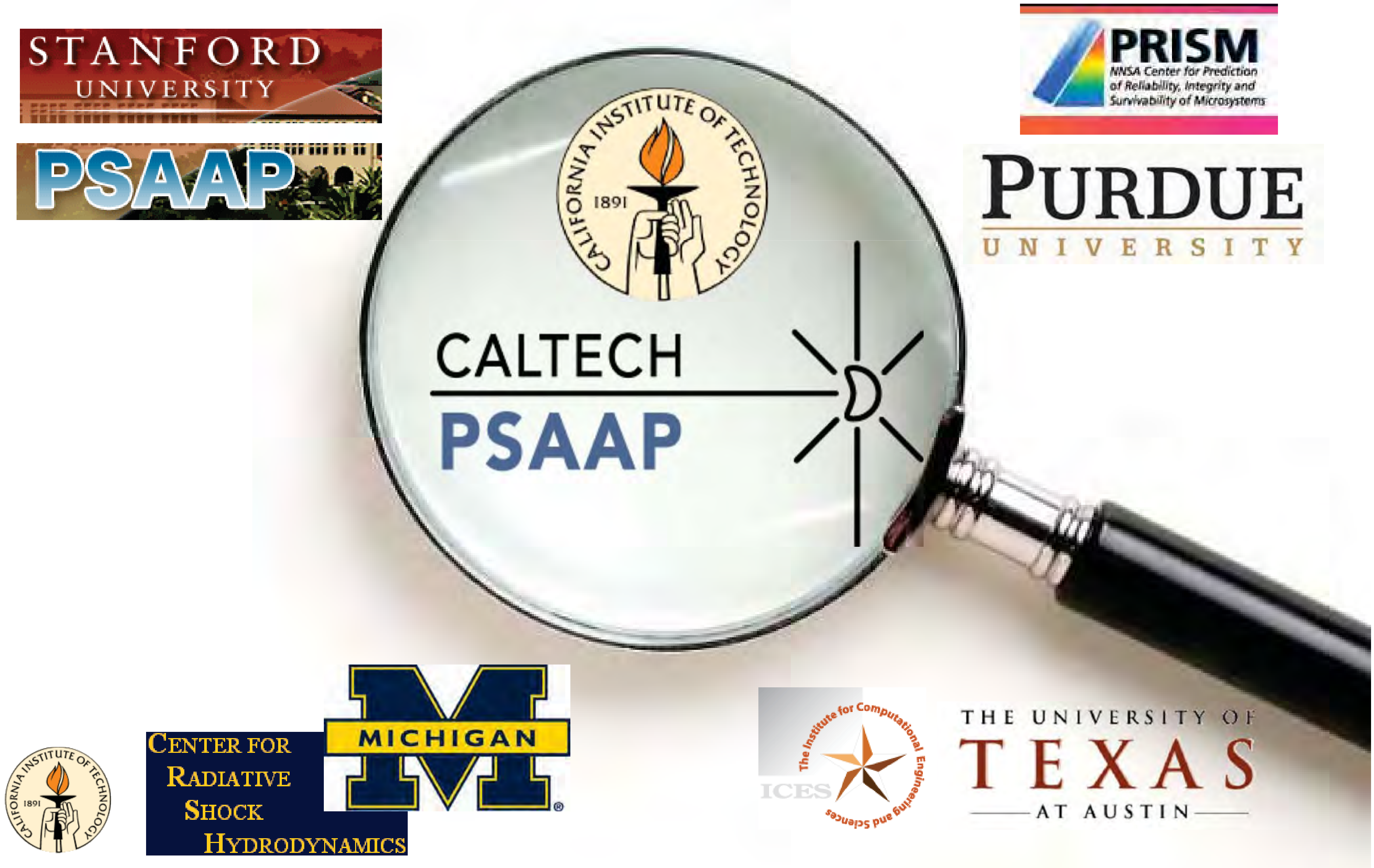
California Institute of Technology

In collaboration with:
Bo Li (Caltech), A. Pandolfi (Milano),
B. Schmidt (Augsburg)

8th European Solid Mechanics Conference
(ESMC2012)

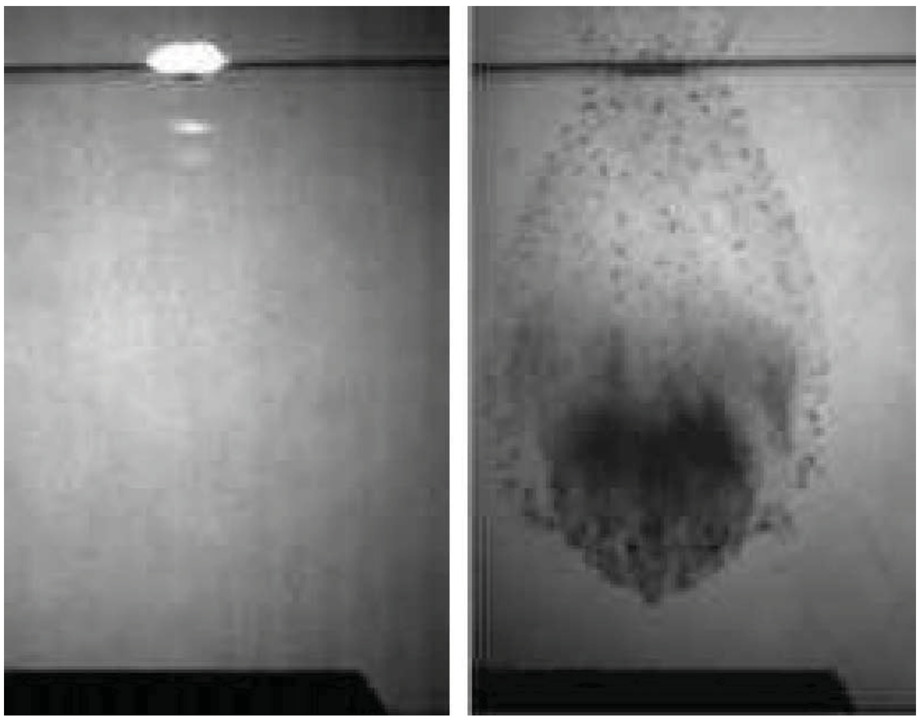
Graz, Austria, July 11, 2012

DoE/ASC/PSAAP Centers

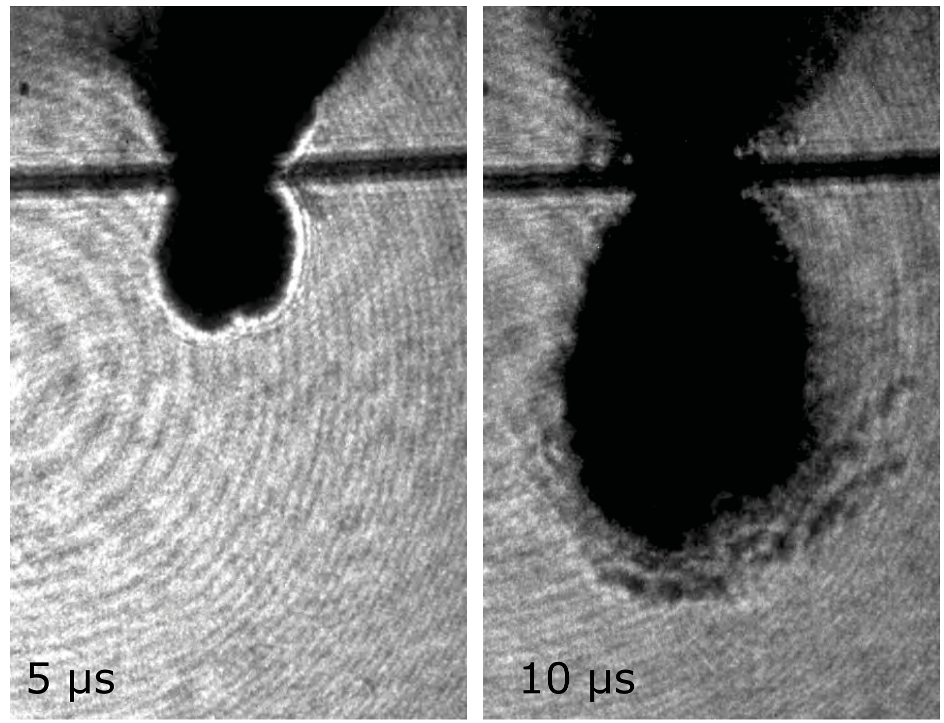


Solids under Extreme Conditions

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



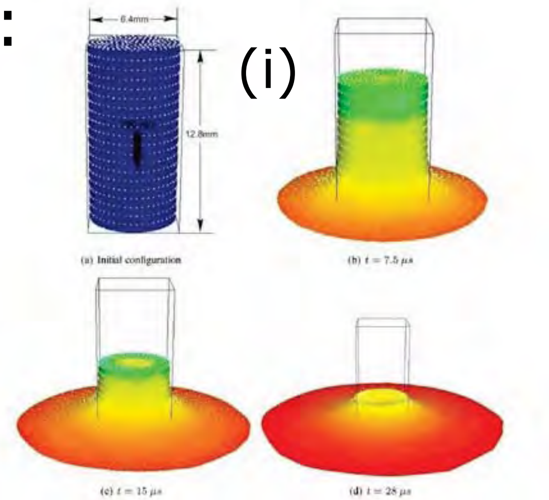
Hypervelocity impact of bumper shield. a) Initial impact flash. b) Debris cloud (Ernst-Mach Inst., Freiburg, Germany).



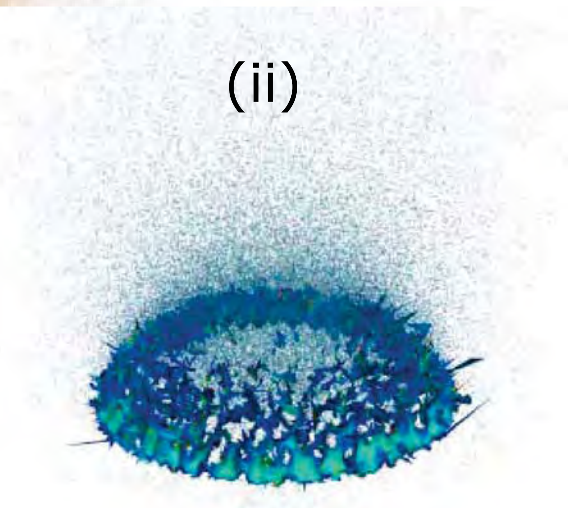
Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

Predictive challenges, tools

- Complex multiphase material behavior: Multiscale modeling…
- Multiphase flows, dynamics, contact: Optimal transportation meshfree (OTM) schemes…
- Fracture, fragmentation: Variational material point erosion (eigenfracture/eigenerosion)…
- Lecture plan:



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



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

Optimal transportation theory

Gaspard Monge
Beaune (1746), Paris (1818)
"*Sur la théorie des déblais et des remblais*" (*Mém. de l'acad. de Paris*, 1781)

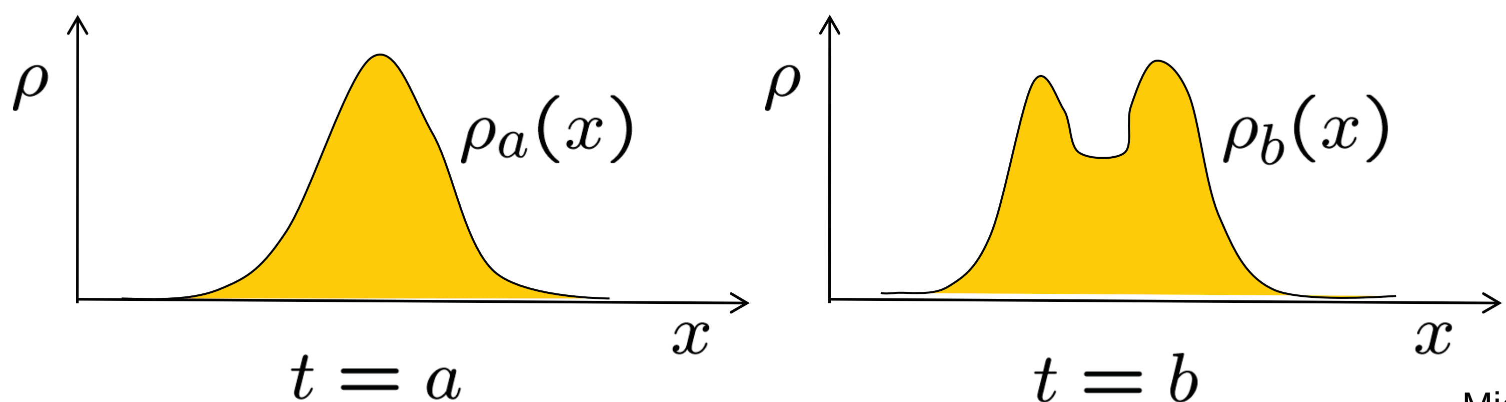
Leonid V. Kantorovich
Saint Petersbourg (1912)
Moscow (1986)
Nobel Prize in Economics (1975)

Mass flows – Optimal transportation

- Flow of non-interacting particles in $\mathbb{R}^n$

$$\left.\begin{aligned}&\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho v)=0\\&\frac{\partial(\rho v)}{\partial t}+\nabla\cdot(\rho v\otimes v)=0\end{aligned}\right\}\quad t\in[a,b]$$

- Initial and final conditions: $\begin{cases}\rho(x,a)=\rho_a(x)\\\rho(x,b)=\rho_b(x)\end{cases}$



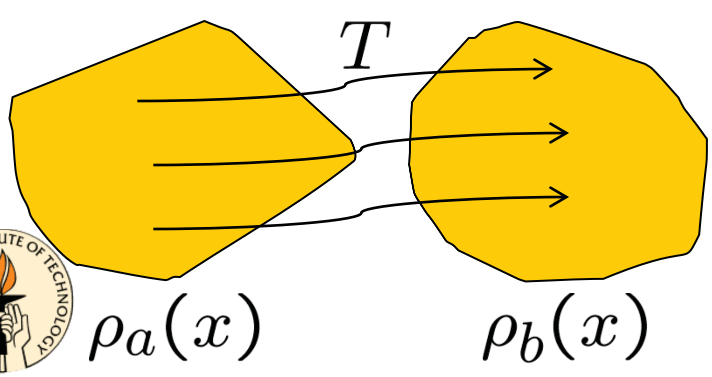
Mass flows – Optimal transportation

- *Benamou & Brenier* minimum principle:

$$\left.\begin{array}{l} \text{minimize: } A(\rho, v) = \int_a^b \int \frac{\rho}{2}|v|^2 \, dx \, dt \\ \text{subject to: } \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \end{array}\right\} \Rightarrow (\rho, v)$$

- Reformulation as optimal transportation problem:

$$\inf A = \inf_T \int |T(x) - x|^2 \rho_a(x) \, dx \equiv d_W^2(\rho_a, \rho_b)$$



- McCann's interpolation:

$$\varphi(x, t) = \frac{b-t}{b-a} x + \frac{t-a}{b-a} T(x)$$

$$\Rightarrow (\rho, v)$$

OT time discretization – Euler fluid

- Semidiscrete action: $A_d(\rho_1, \ldots, \rho_{N-1}) =$

$$\sum_{k=0}^{N-1} \Big\{ \underbrace{\frac{1}{2} \frac{d_W^2(\rho_k, \rho_{k+1})}{(t_{k+1} - t_k)^2}}_{\text{inertia}} - \underbrace{\frac{1}{2}[U(\rho_k) + U(\rho_{k+1})]}_{\text{internal energy}} \Big\} (t_{k+1} - t_k)$$

- Discrete Euler-Lagrange equations: $\delta A_d = 0 \Rightarrow$

$$\frac{2\rho_k}{t_{k+1} - t_{k-1}} \left(\frac{\varphi_{k\to k+1} - \mathrm{id}}{t_{k+1} - t_k} + \frac{\varphi_{k\to k-1} - \mathrm{id}}{t_k - t_{k-1}} \right) = \nabla p_k + \rho_k b_k$$

$$\rho_{k+1} \circ \varphi_{k\to k+1} = \rho_k / \det\left(\nabla \varphi_{k\to k+1}\right)$$

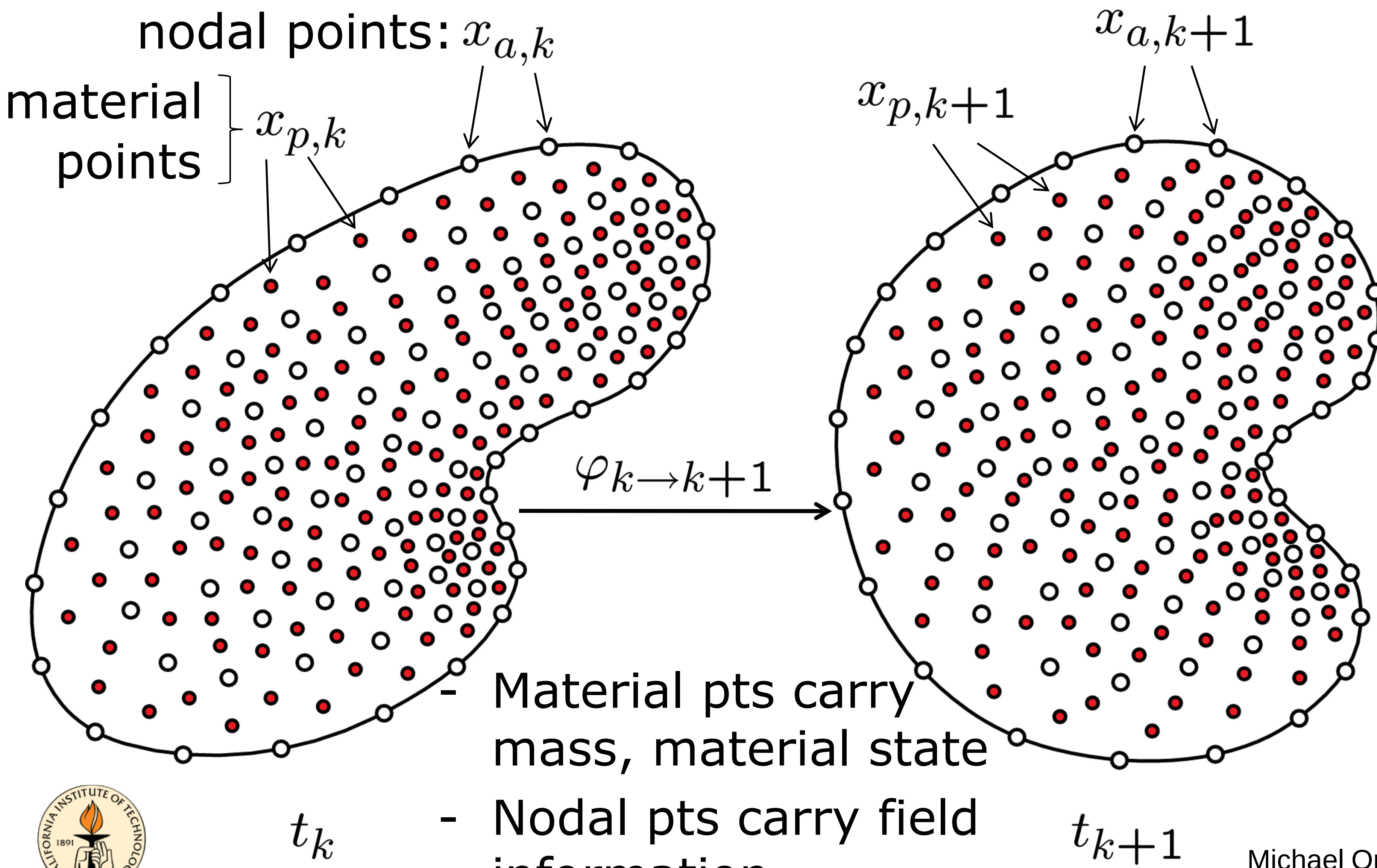
geometrically exact mass conservation!

Li, B., Habbal, F. & MO, *Int. J. Numer. Meth. Eng.*, 83:1541, 2010

OT time discretization

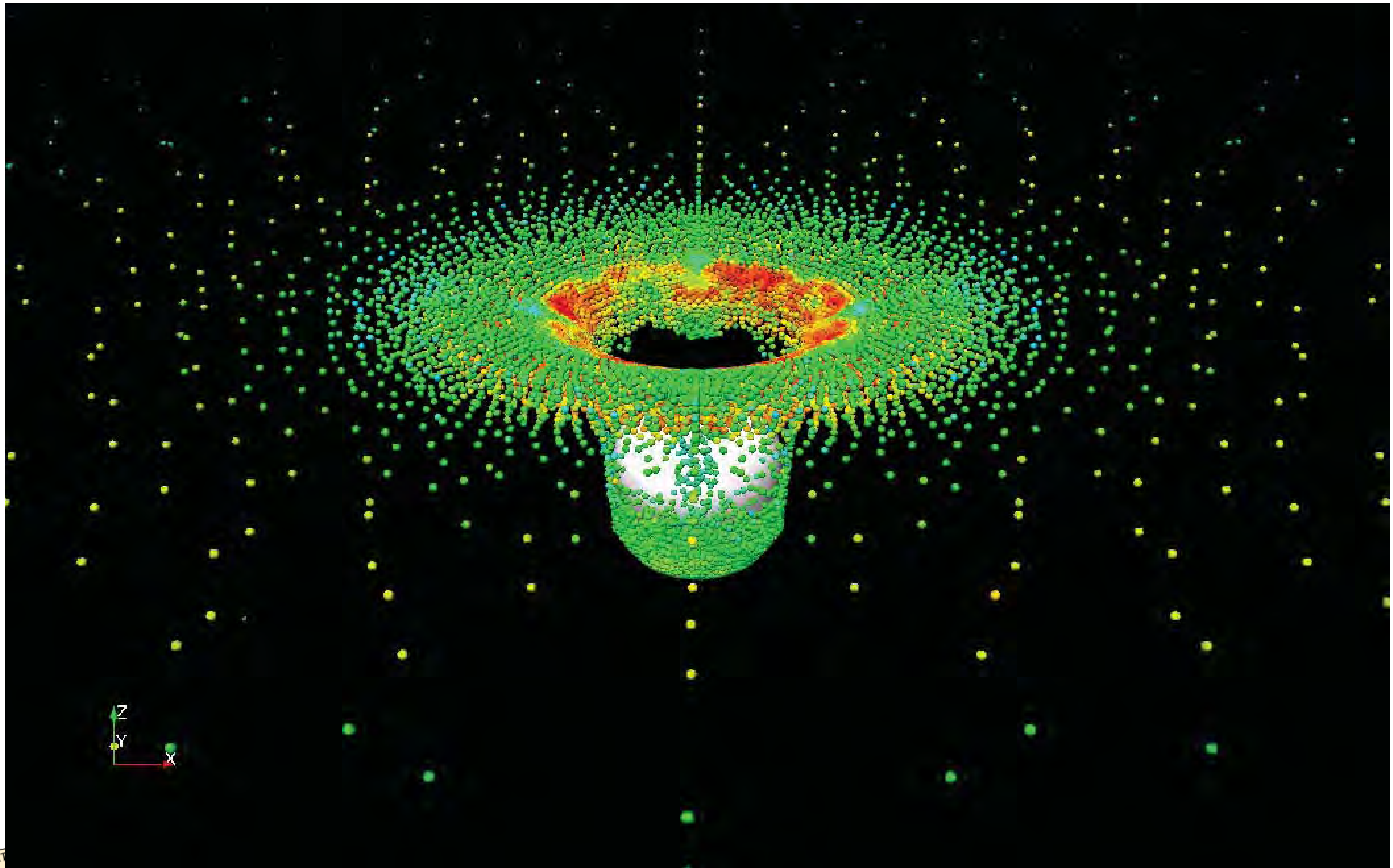
- Optimal transportation theory is a useful tool for generating geometrically-exact discrete Lagrangians for flow problems
- Inertial part of discrete Lagrangian measures distance between consecutive mass densities (in sense of Wasserstein)
- Discrete Hamilton principle of stationary action: Variational time integration scheme:
  - *Symplectic, time reversible*
  - *Exact conservation properties: linear and angular momenta, energy (with time-adaption)*
  - *Strong variational convergence in the sense of Γ-convergence (work in progress…)*

Meshfree spatial discretization



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

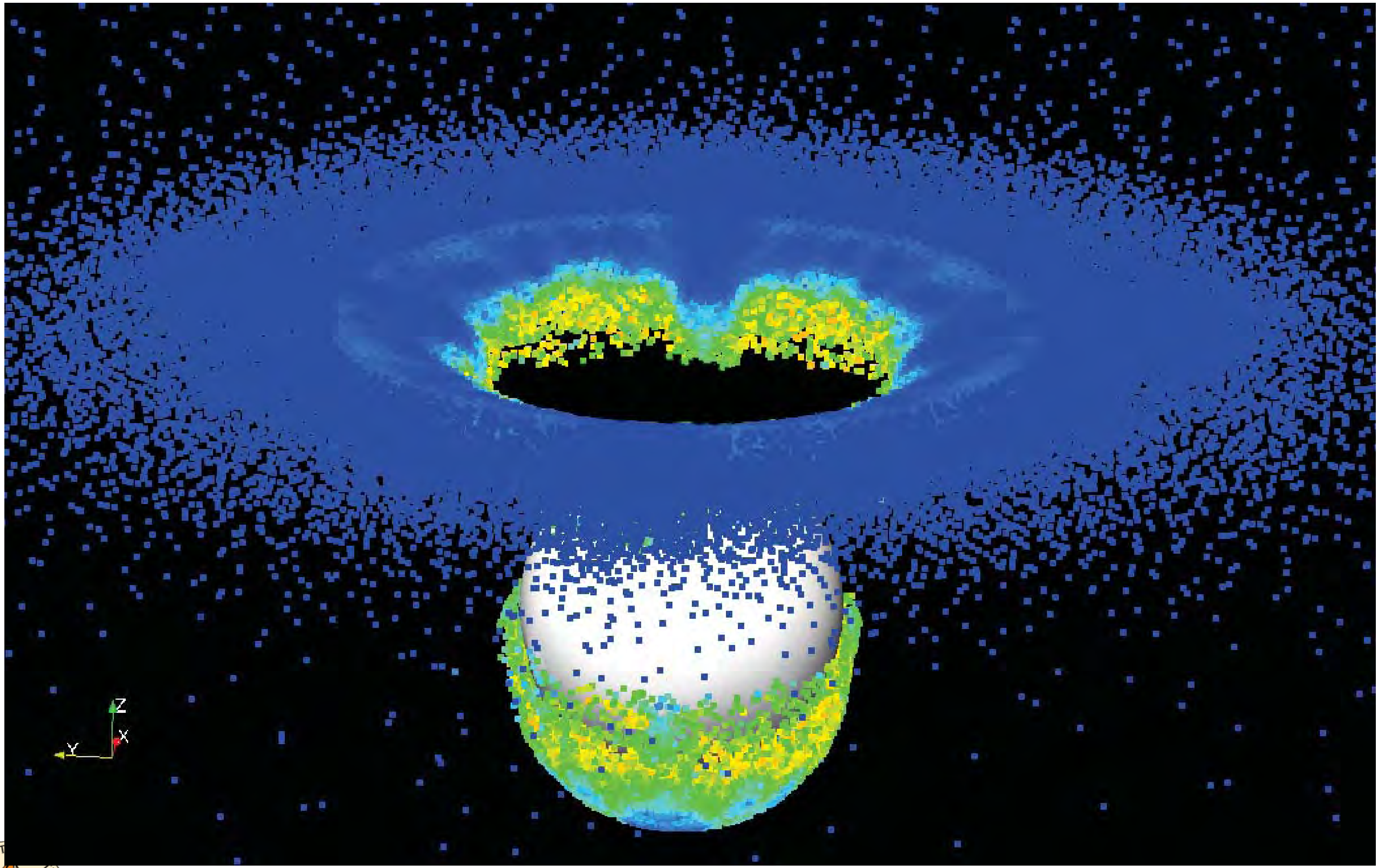
Meshfree spatial discretization



Steel projectile/aluminum plate: Nodal set

Michael Ortiz
ESMC2012

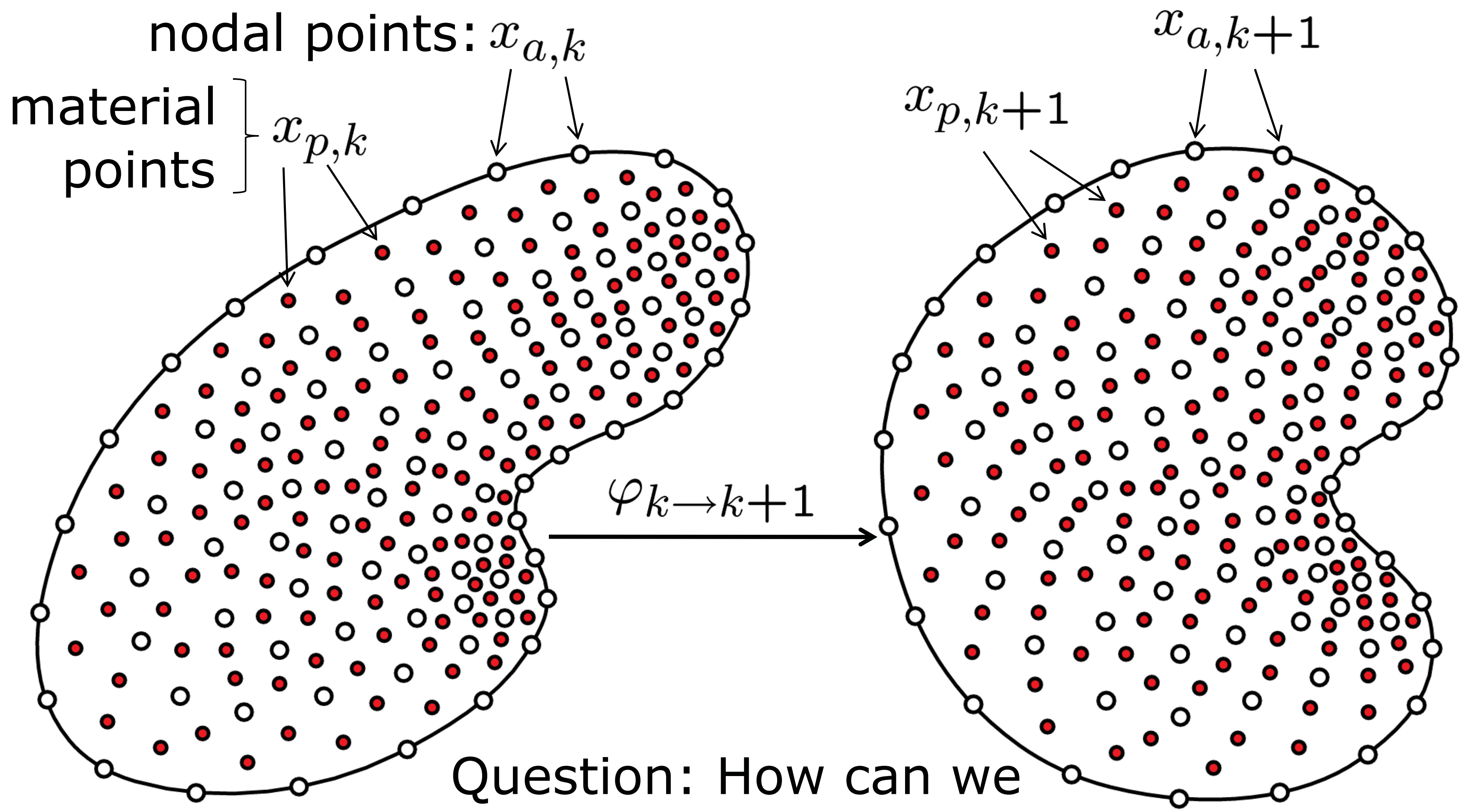
Meshfree spatial discretization



Steel projectile/aluminum plate: Material point set

Michael Ortiz
ESMC2012

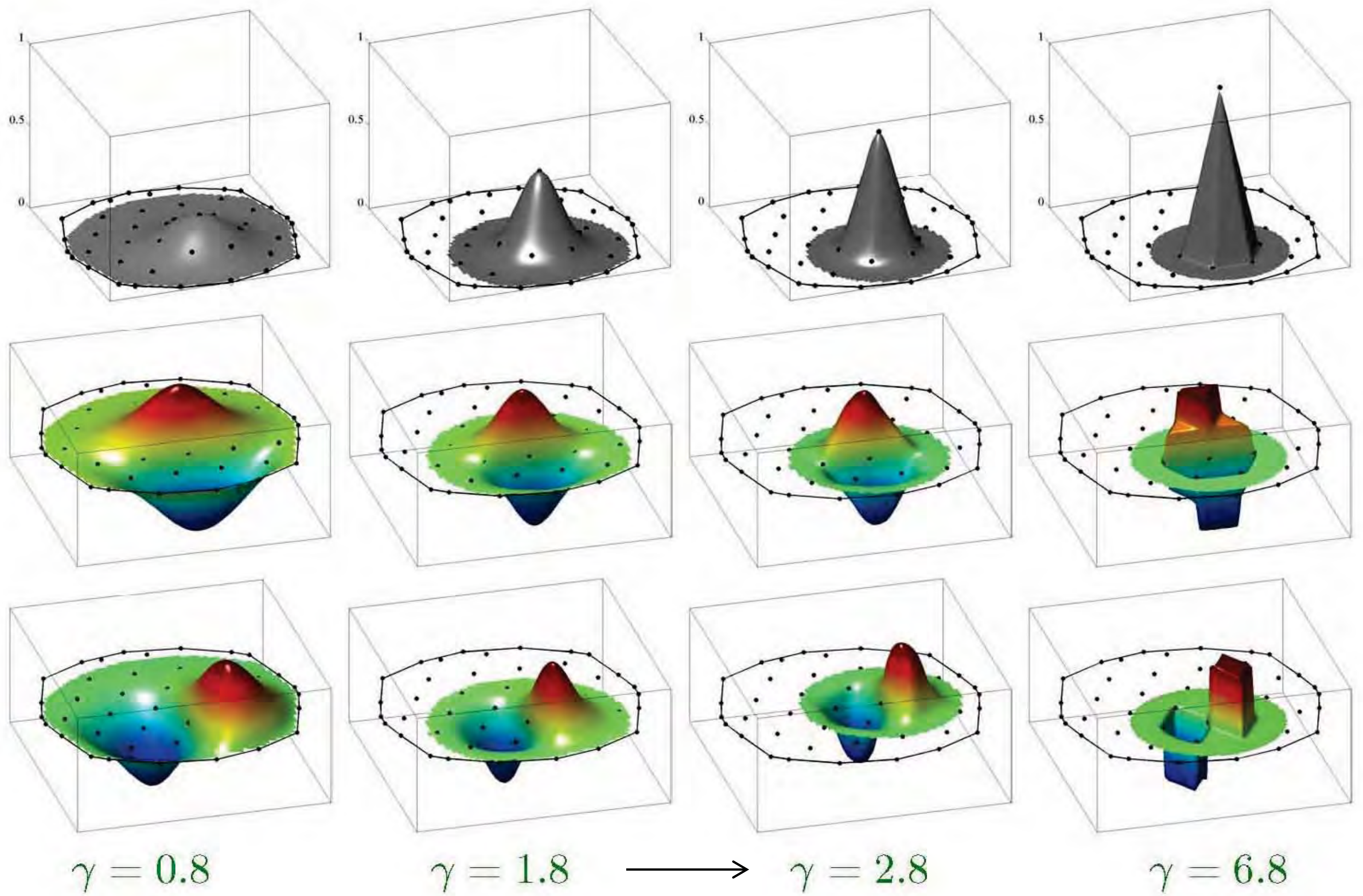
Meshfree spatial discretization



Question: How can we reconstruct $\varphi_{k \to k+1}$ from nodal coordinates?

t_k t_{k+1}

Max-ent spatial interpolation

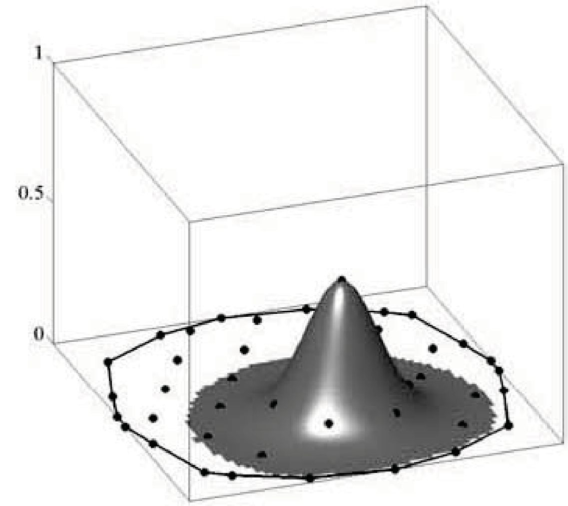


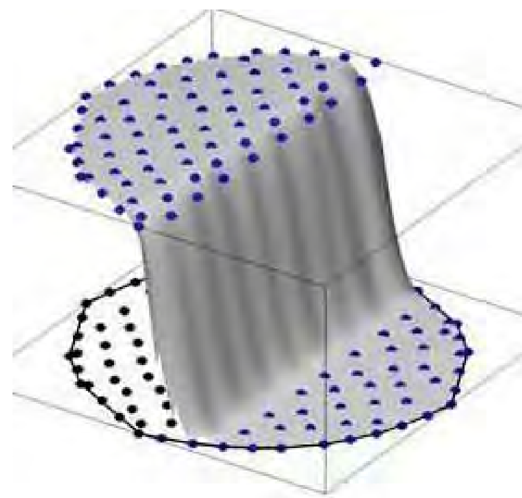
Max-ent shape functions of decreasing entropy

Arroyo, M. & MO, *Int. J. Numer. Meth. Engr.*, 65:2167-2202, 2006

Max-ent spatial interpolation

- Shape functions determined by node set directly (meshfree)
- Max-ent interpolation is smooth, local (rapid decay), monotonic
- Simplicial Delaunay interpolation is recovered in the limit of $\beta \to \infty$
- Kronecker-delta property at the boundary (enables essential BC)
- Density in $W^{k,p}$, $k \geq 1$, $1 < p < \infty$: Convergence for problems (with p-growth) of any order

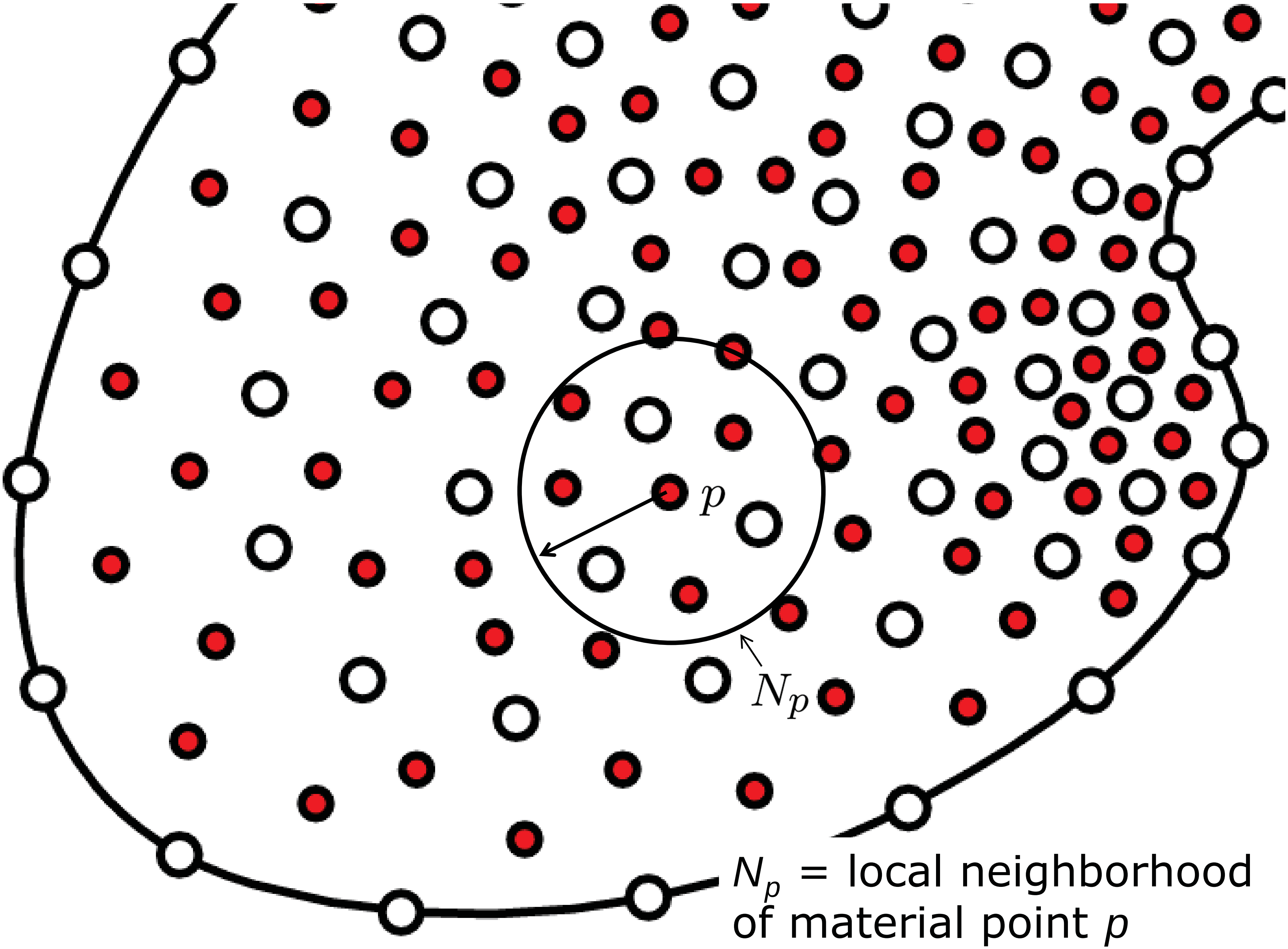




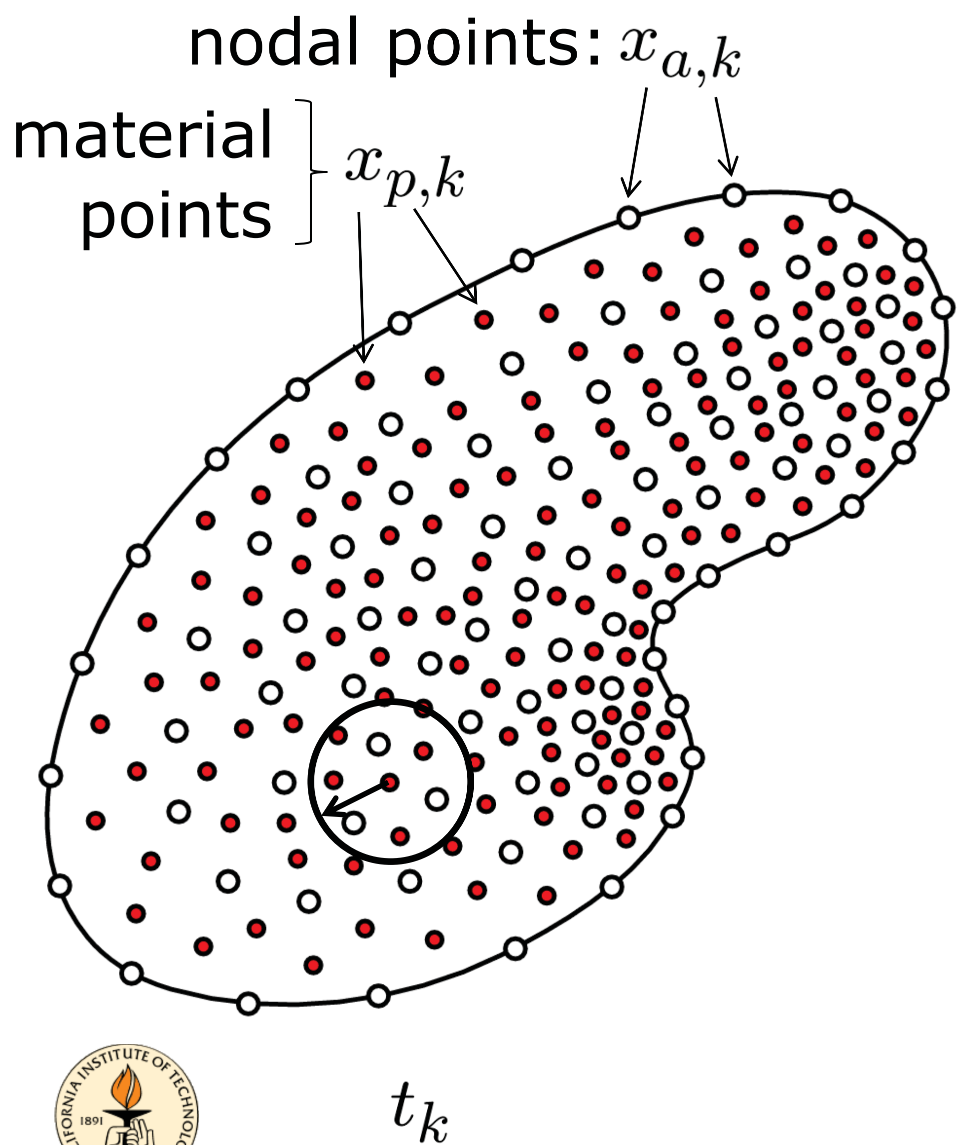
Max-ent interpolation

Bompadre, A., Schmidt, B. & MO, *SIAM J. Numer. Anal.*, 50:1344-1366, 2012.

Bompadre A., Perotti, L.E., Cyron, C.J. & MO CMAME, 221-222:80-103, 2012.


p
N_p
N_p = local neighborhood
of material point p

Max-ent spatial discretization



- Max-ent interpolation at material point *p* determined by nodes in its local environment N_p *only*
- Local environments determined 'on-the-fly' by range searches
- Local environments evolve continuously during flow (dynamic reconnection)
- Dynamic reconnection requires no remapping of history variables!

OTM – Flow chart

(i) Explicit nodal coordinate update:

$$x_{k+1} = x_k + (t_{k+1} - t_k)(v_k + \frac{t_{k+1} - t_{k-1}}{2} M_k^{-1} f_k)$$

(ii) Material point update:

position: $x_{p,k+1} = \varphi_{k \to k+1}(x_{p,k})$

deformation: $F_{p,k+1} = \nabla \varphi_{k \to k+1}(x_{p,k}) F_{p,k}$

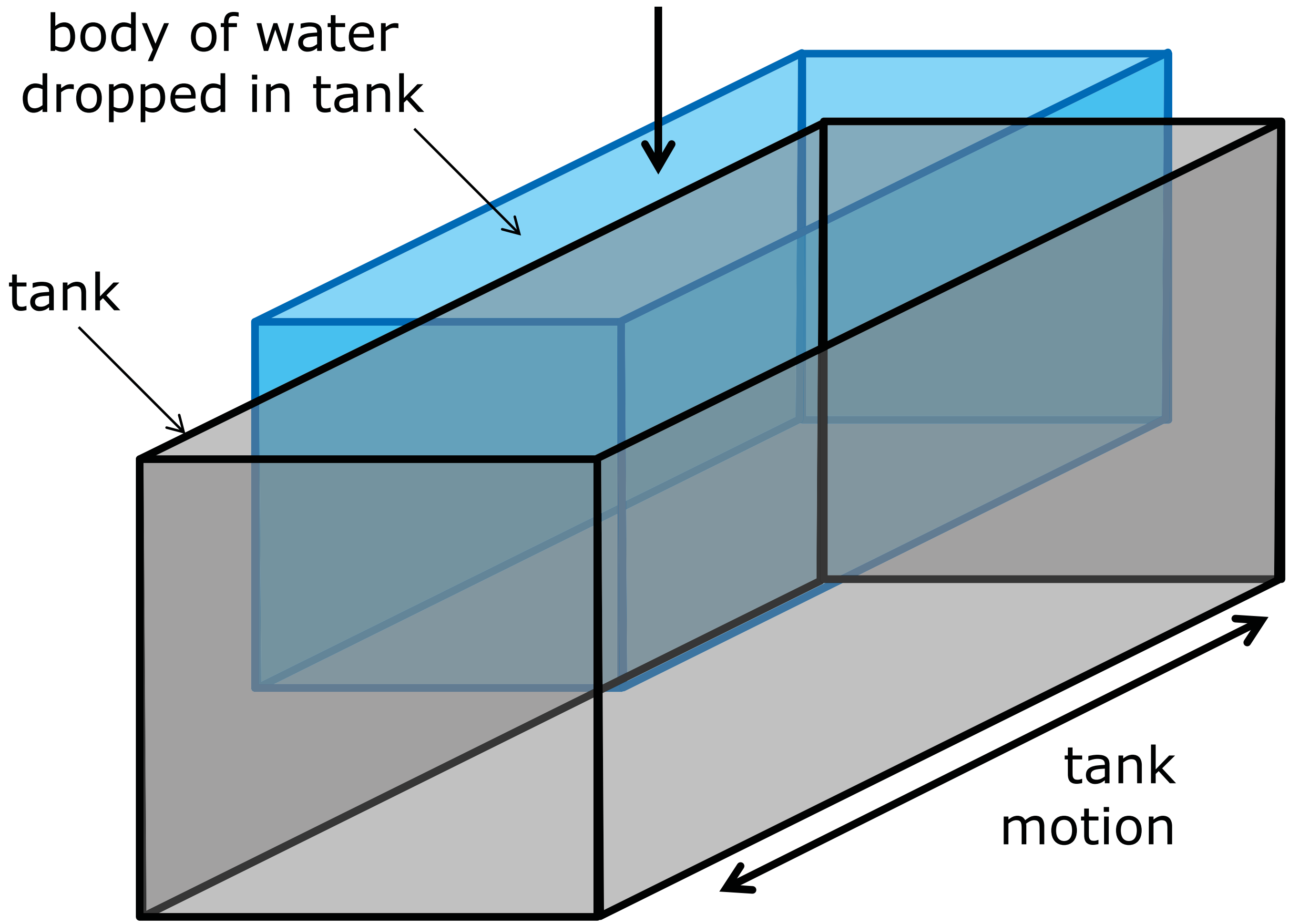
volume: $V_{p,k+1} = \det \nabla \varphi_{k \to k+1}(x_{p,k}) V_{p,k}$

density: $\rho_{p,k+1} = m_p / V_{p,k+1}$

(iii) Constitutive update at material points

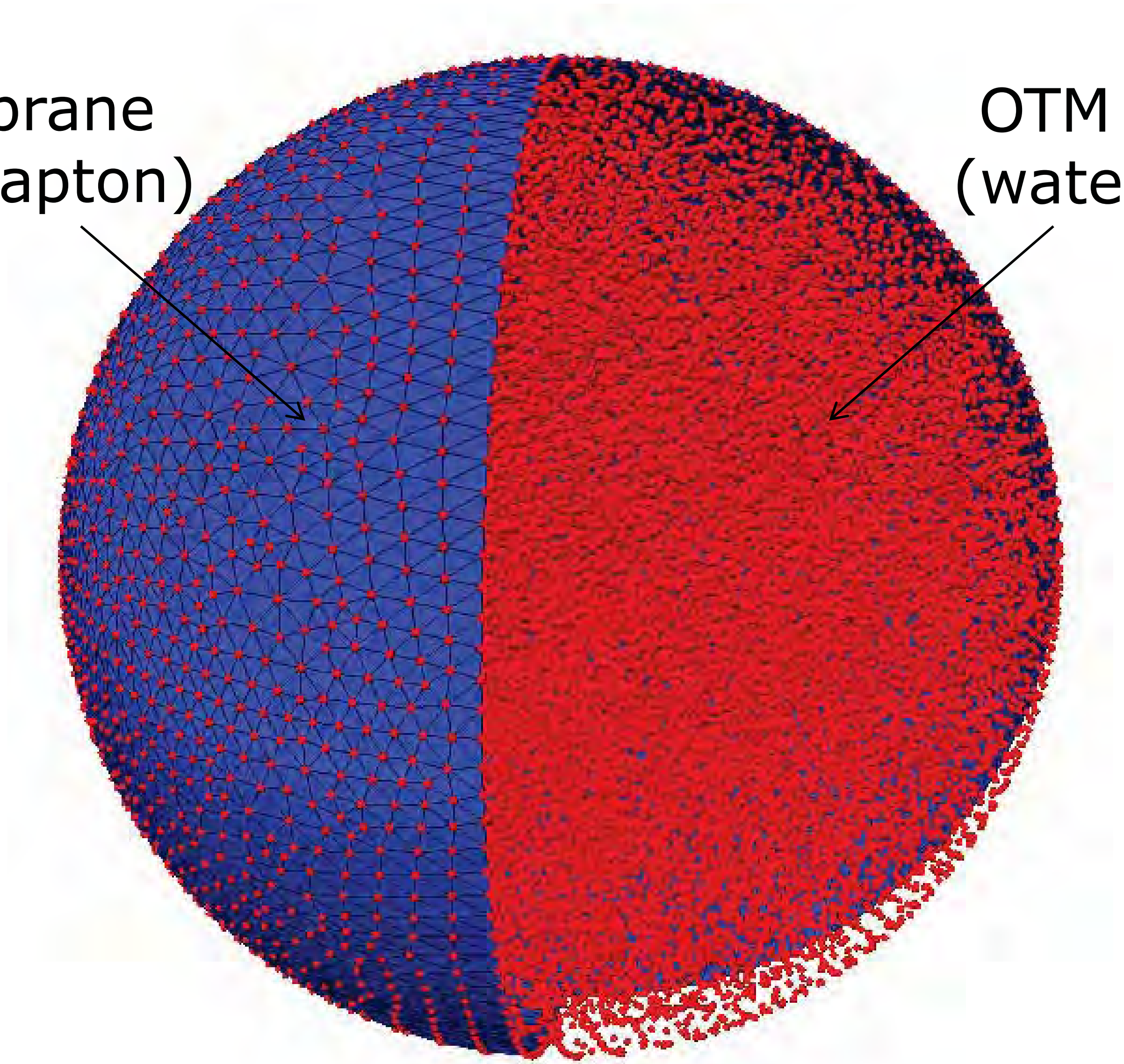
(iv) Reconnect nodal and material points (range searches), recompute max-ext shape functions

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



Dirk Hartmann, Siemens AG, Munich
Corporate Research and Technologies

Example – Bouncing balloons



Li, B., Habbal, F. & MO, *Int. J. Numer. Meth. Eng.*, 83:1541, 2010

Convergence – Non-interacting particles

- Action (Benamou & Brenier): $A = \int_a^b \int \frac{\rho}{2} |v|^2 \, dx \, dt$
- Discrete mass: $\rho_{h,k}(x) = \sum_{p=1}^{M} m_p \delta(x - x_{p,k})$
- Fully-discrete action:

$$A_{M,N} = \sum_{k=0}^{N-1} \sum_{p=1}^{M} \frac{m_p}{2} \frac{|x_{p,k+1} - x_{p,k}|^2}{t_{k+1} - t_k}$$

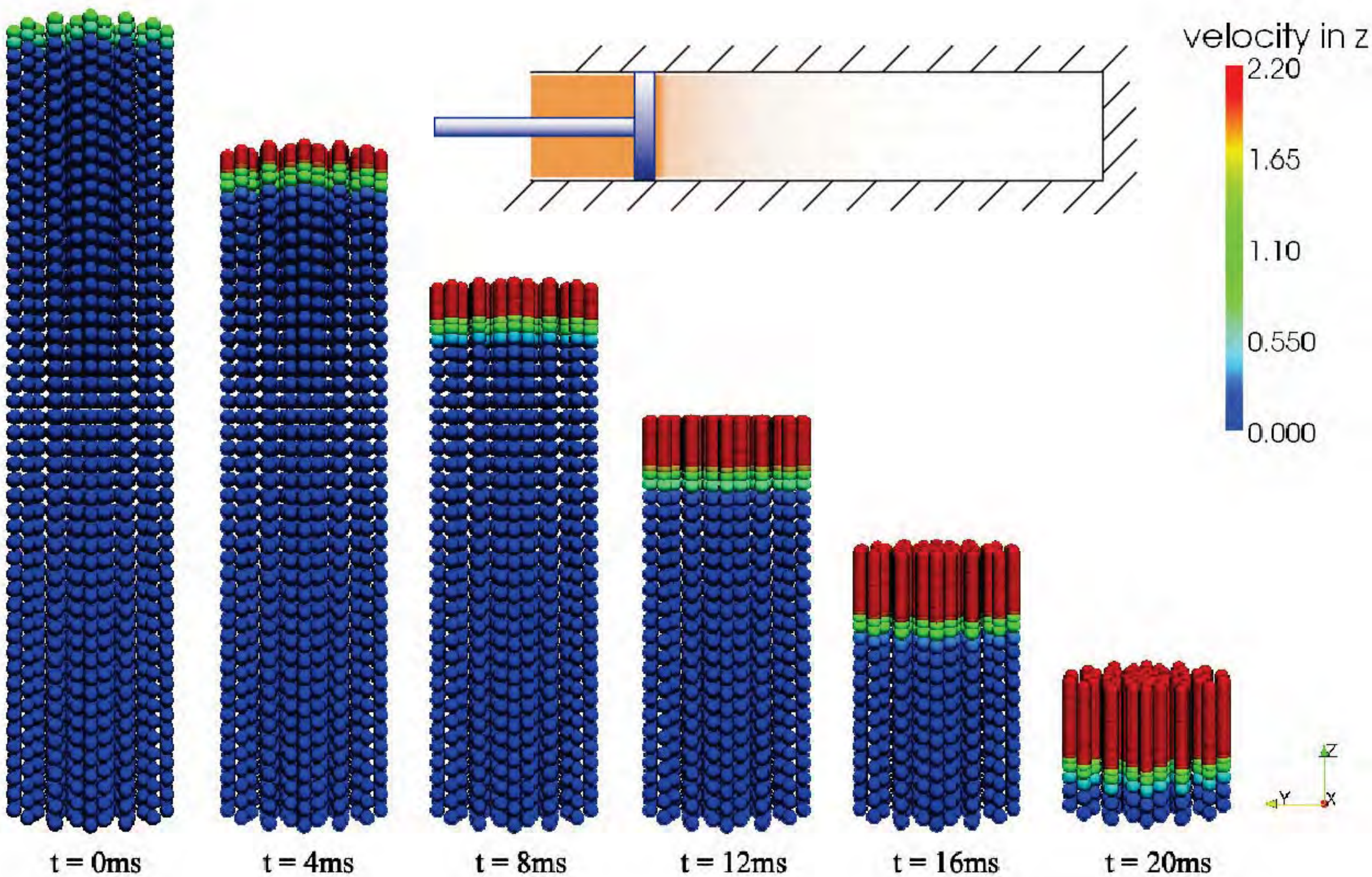
- **Theorem** (B. Schmidt) $A_{M,N} \xrightarrow{\Gamma} A$ as $M, N \to \infty$.
- Remarks:

  i) Theorem applies to particles in a field of force

  ii) Theorem implies convergence of minimizers

  iii) Case of interacting particles remains open!

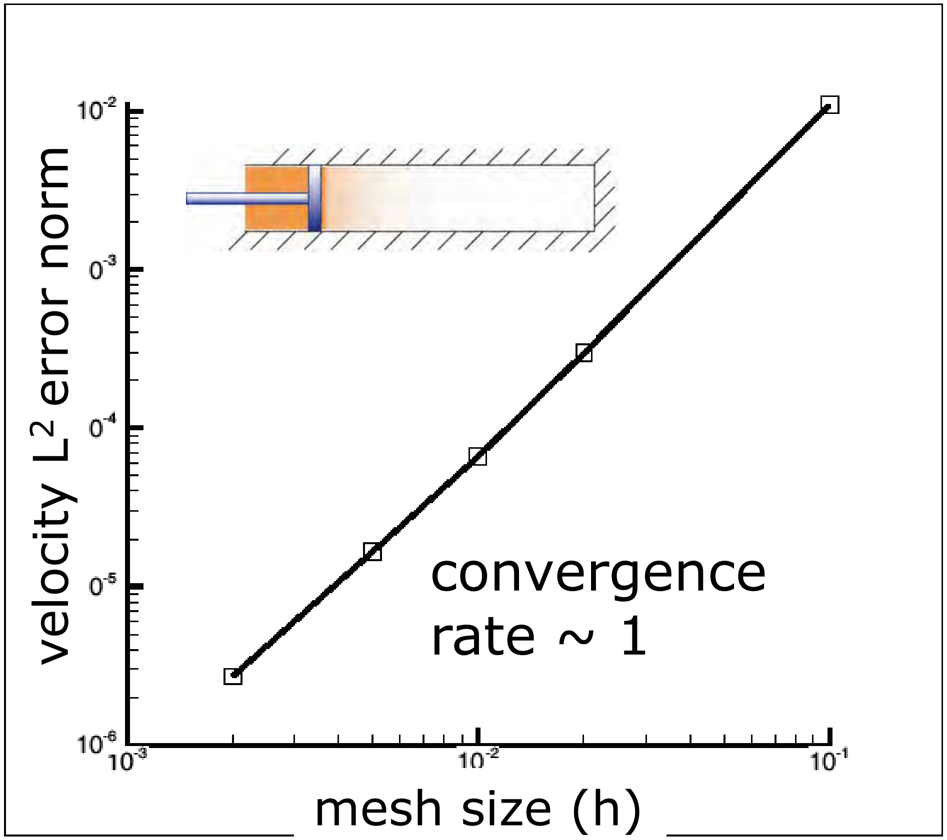
OTM verification – Shock tube problem

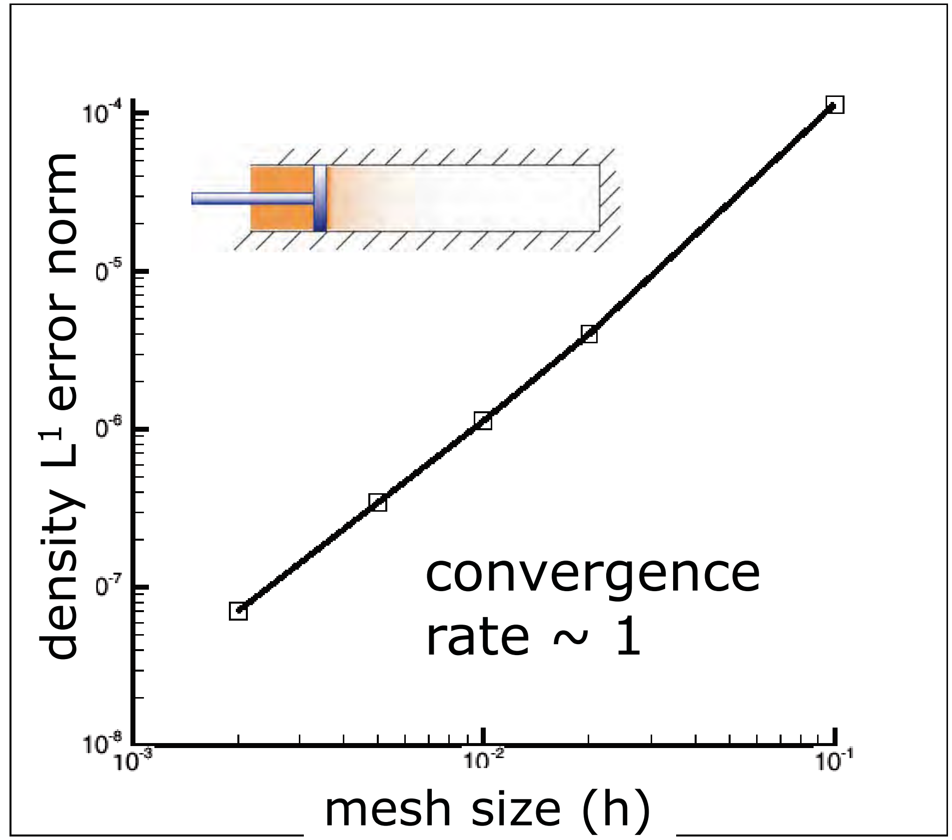


Shock tube problem – velocity snapshots

Li, B., Habbal, F. & MO, *Int. J. Numer. Meth. Eng.*, 83:1541, 2010

OTM verification – Shock tube problem





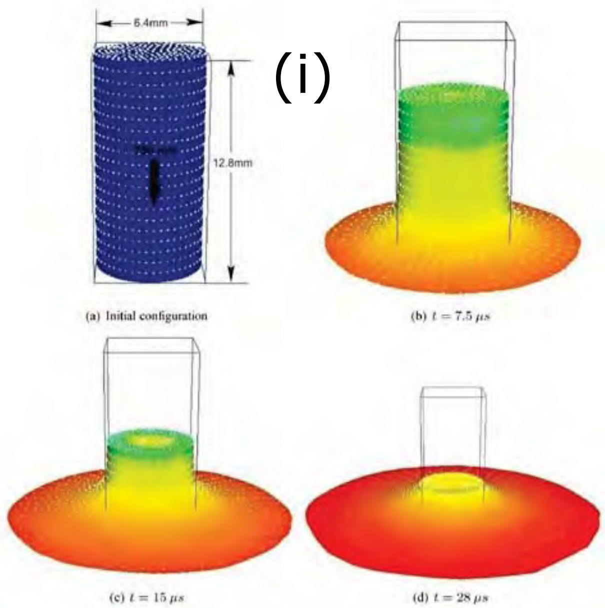
velocity convergence (L^2 norm)

density convergence (L^1 norm)

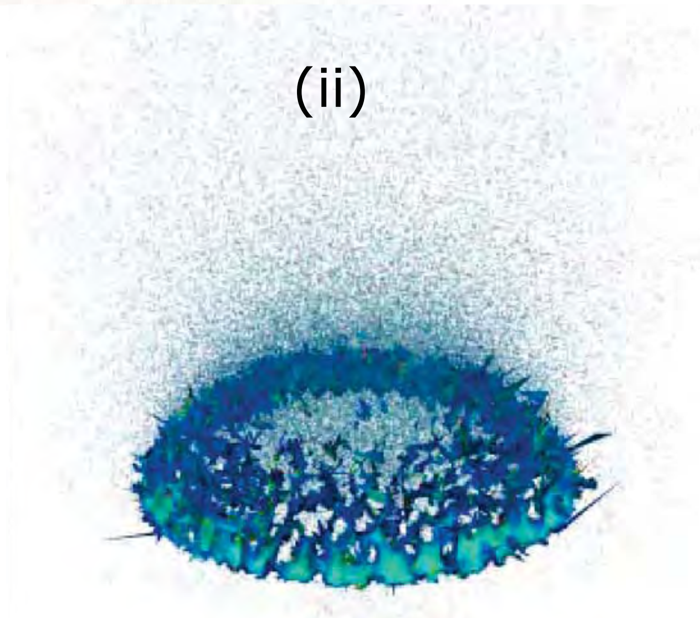
Shock tube problem – convergence plots

Li, B., Habbal, F. & MO, *Int. J. Numer. Meth. Eng.*, 83:1541, 2010

Lecture plan

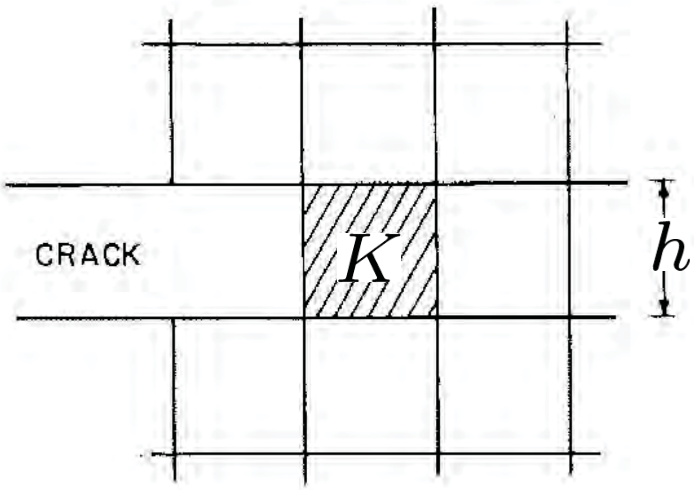


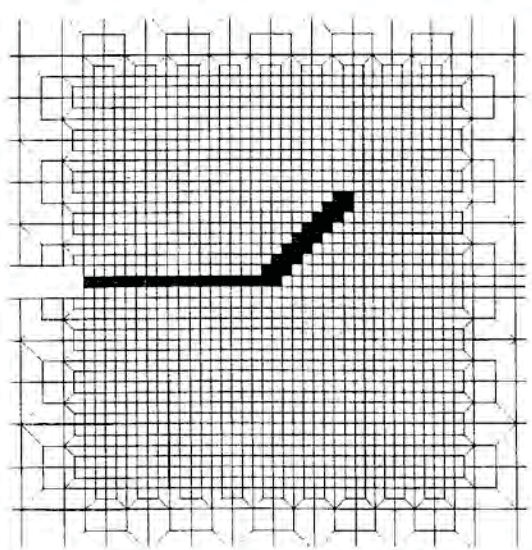
Li, B., Habbal, F. & MO,
IJNME, 83:1541, 2010



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

Fracture – Element erosion





Mixed-mode crack growth

- Energy-release rate:

$$G \sim \frac{1}{h} \int_K W(\nabla u)\, dx$$

- Erosion criterion:

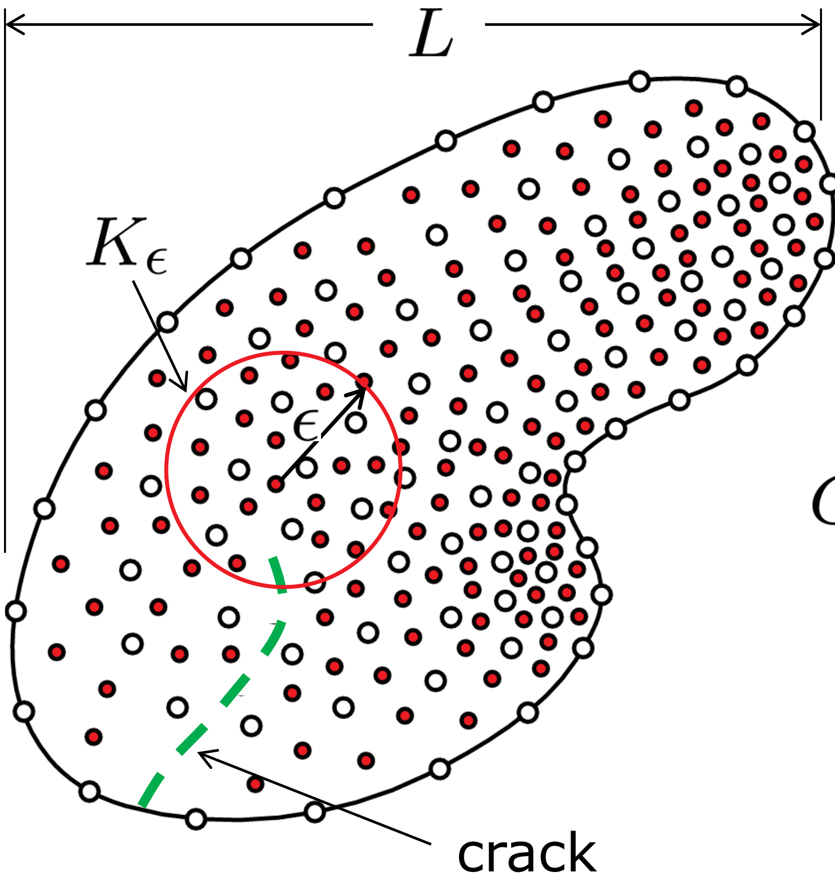
$$G \geq G_c$$

- Fracture energy over-estimated as $h \to 0$!
- Non-convergence for general paths, meshes!

J.R. Rice, *Fracture*, 2:191, 1968

MO & A.E. Giannakopoulos, *Int. J. Fracture*, 44:233-258, 1990

OTM – Material-point erosion



Schematic of ε-neighborhood construction

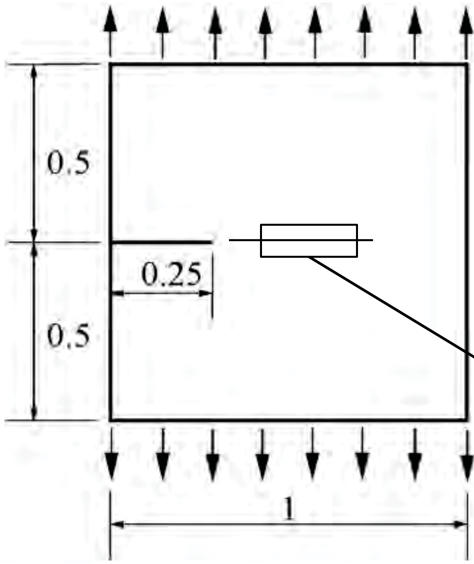
- ε-neighborhood construction: Choose h << ε << L
- Erode material point if

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

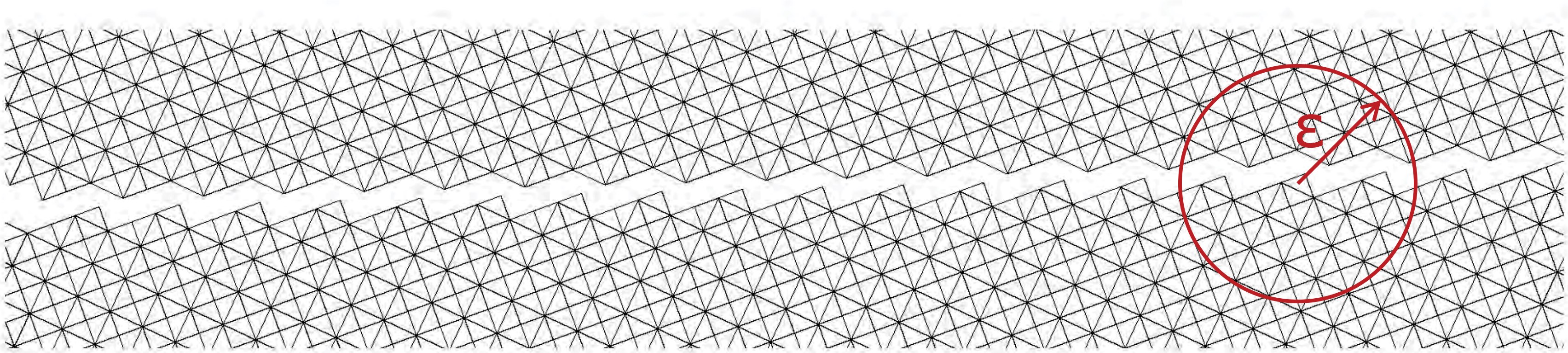
- Proof of convergence to Griffith fracture:
  – *Schmidt, B., Fraternali, F. & MO, SIAM J. Multiscale Model. Simul.*, **7**(3):1237-1366, 2009.

Michael Ortiz
ESMC2012

Verification – Mode-I edge-crack panel

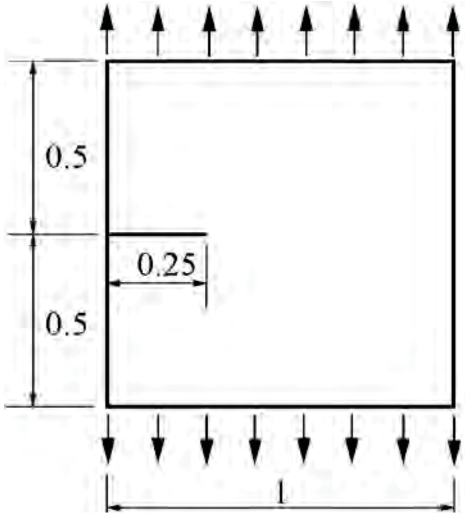


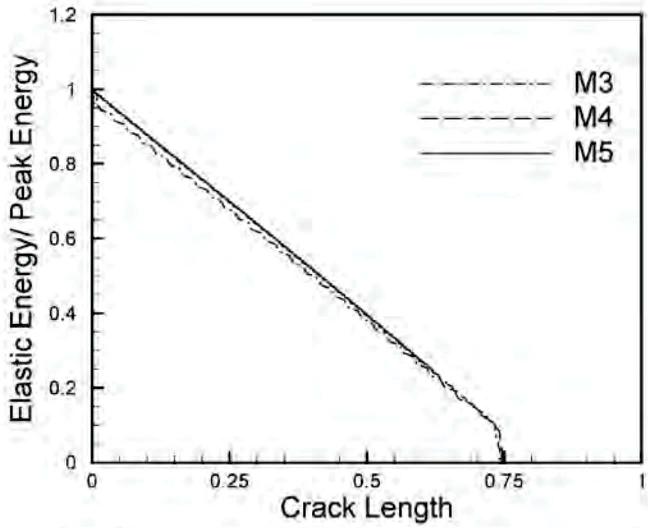
- Mesh slanted at 20° to crack plane
- ε-construction compensates for slant and tracks the exact crack path *on average*



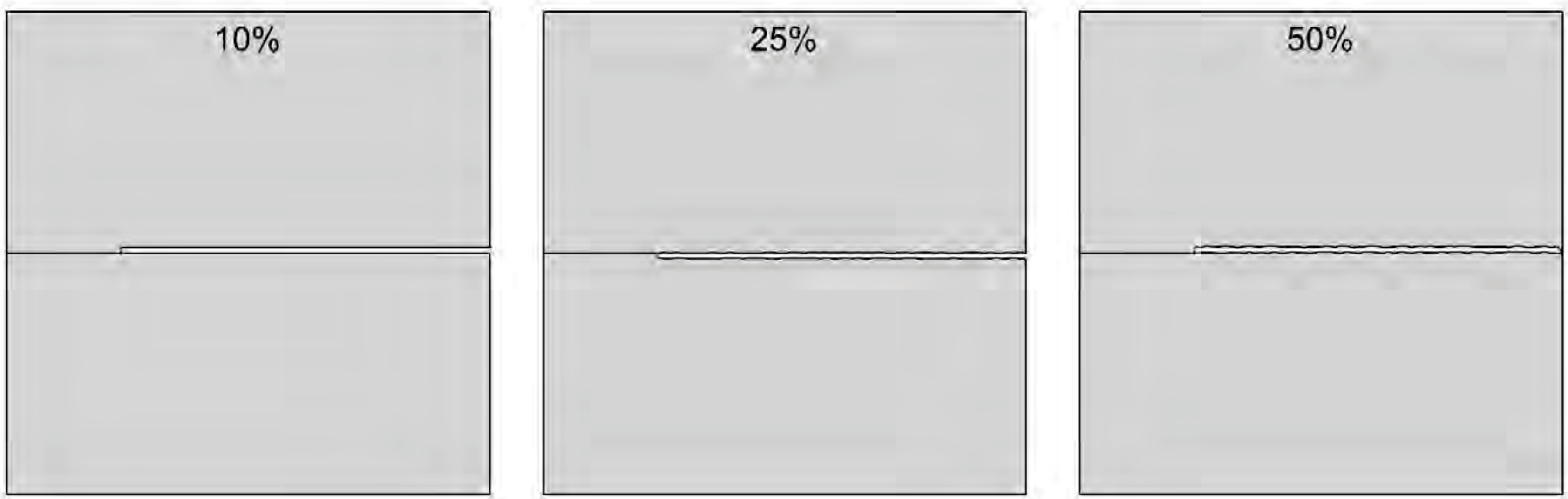
Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

Verification – Mode-I edge-crack panel

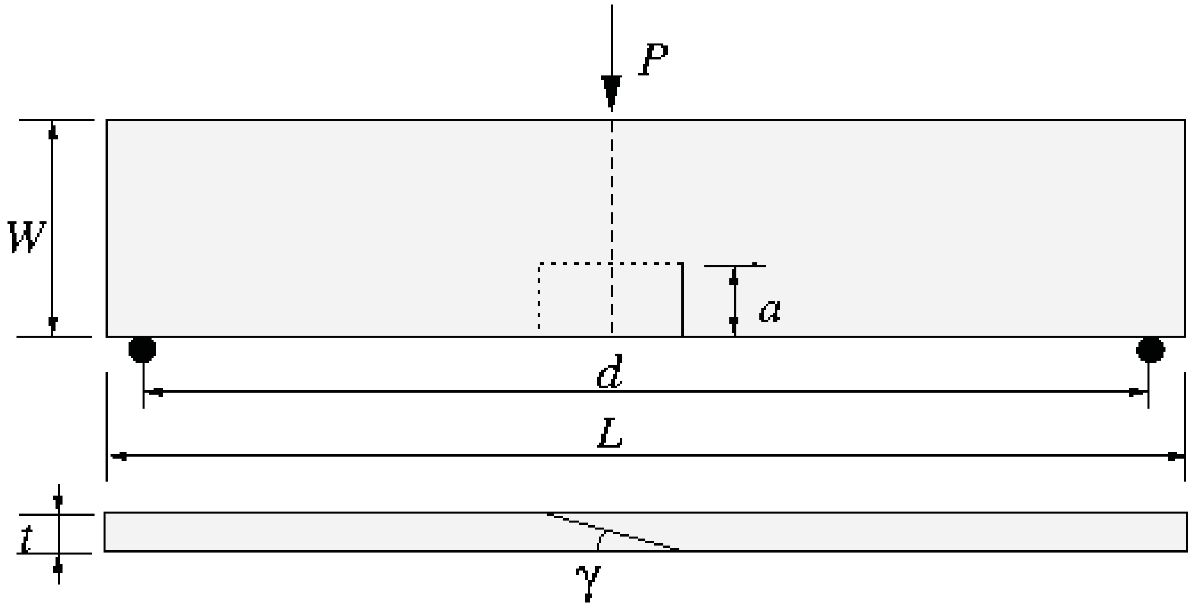




- Random mesh:
  - Convergence
  - Mesh insensitive
  - Good accuracy



Verification: Mode I-III 3-point bending

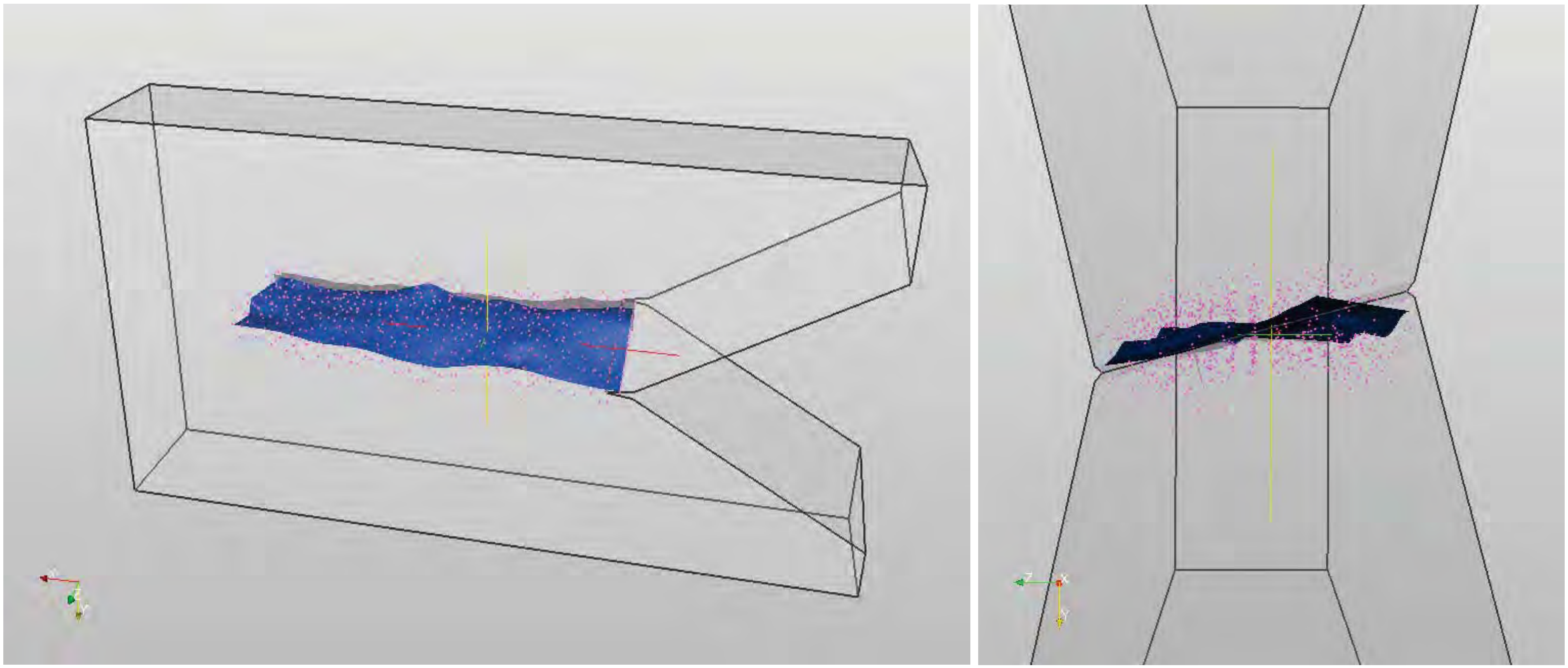


- Mixed-mode 3-point bending tests, PMMA plates (260x60x10 mm, a = 20 mm)
- Inclination of notch: 75°, 60°, 45°
- E = 2800 MPa, n = 0.38, G_c = 0.54 N/mm

Lazarus, V. *et al.*, *IJF*, 153:141, 2008

Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

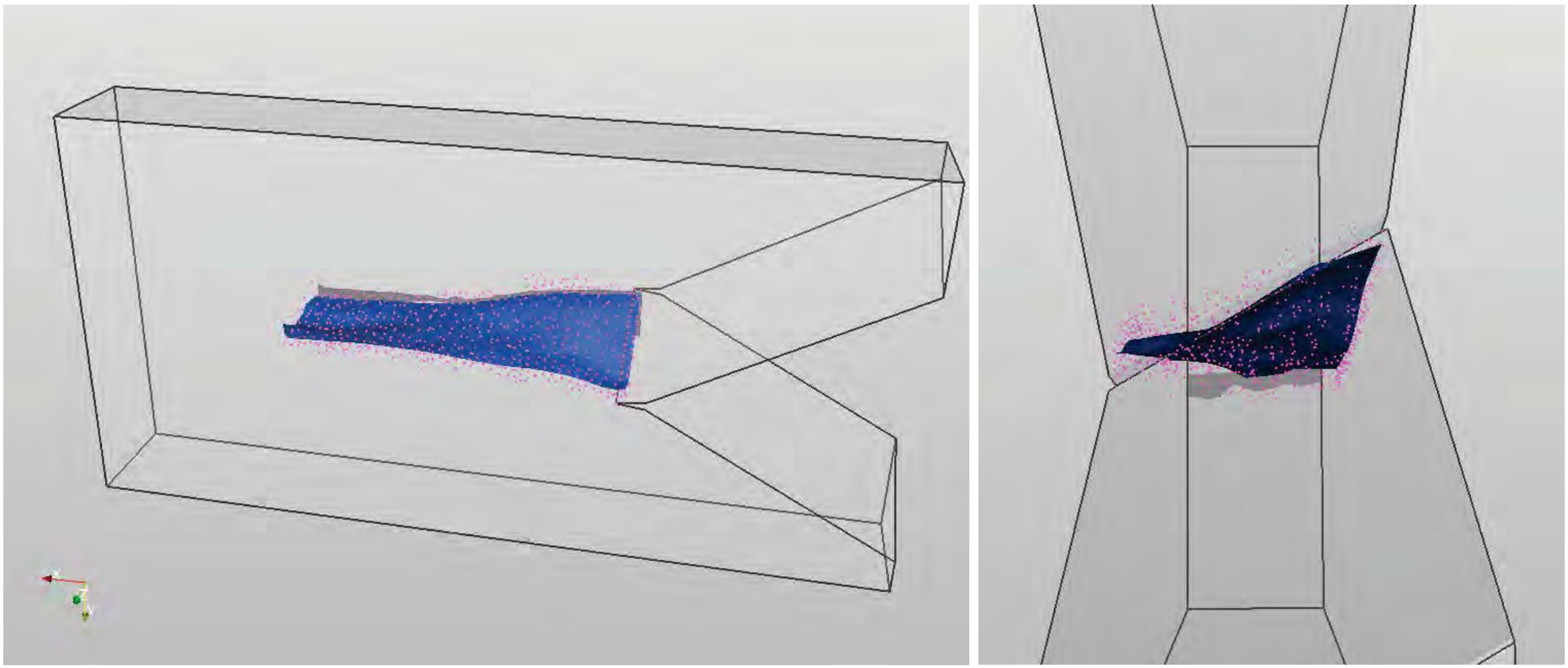
Predominant Mode I (γ = 75°)



Mixed mode I-III crack growth in three-point bending

Lazarus, V. *et al.*, *IJF*, 153:141, 2008
Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

Mixed Mode I-III ($\gamma = 60°$)

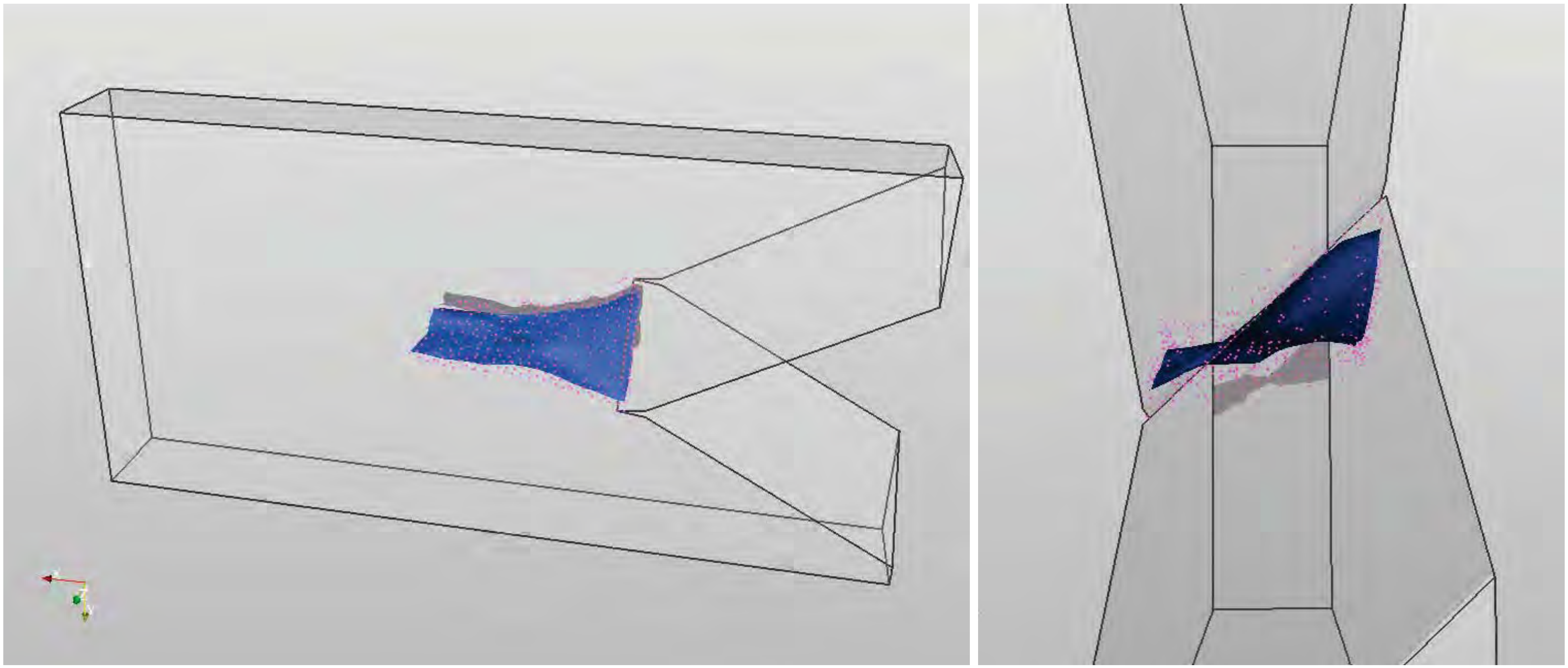


Mixed mode I-III crack growth in three-point bending

Lazarus, V. *et al.*, *IJF*, 153:141, 2008

Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

Predominant Mode III (γ = 45°)

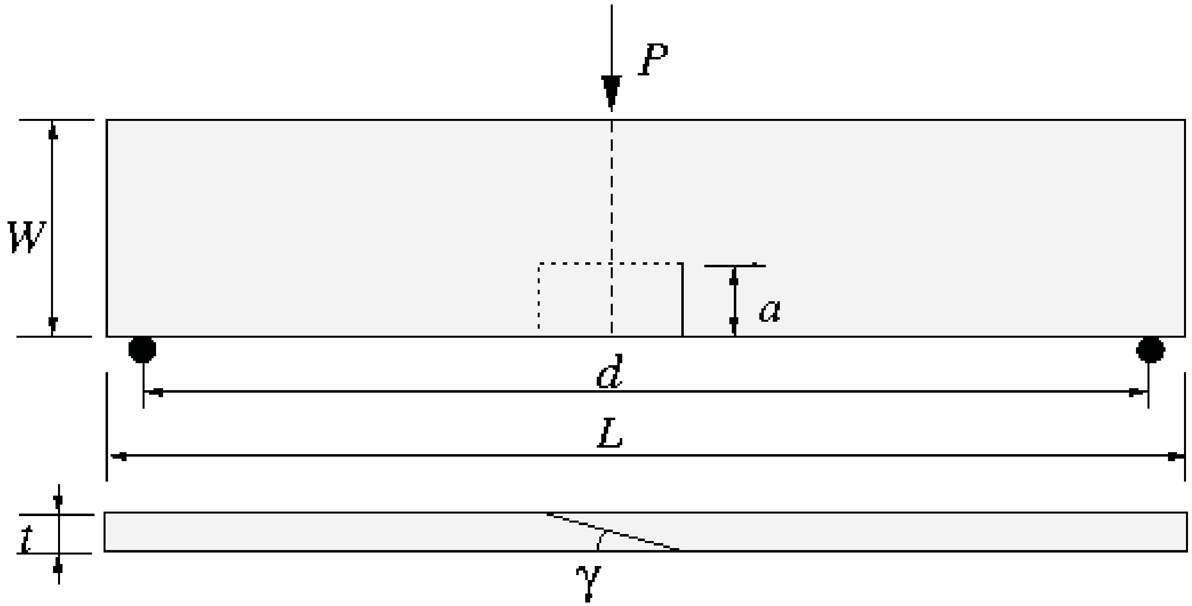


Mixed mode I-III crack growth in three-point bending

Lazarus, V. *et al.*, *IJF*, 153:141, 2008

Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

Verification: Mode I-III 3-point bending

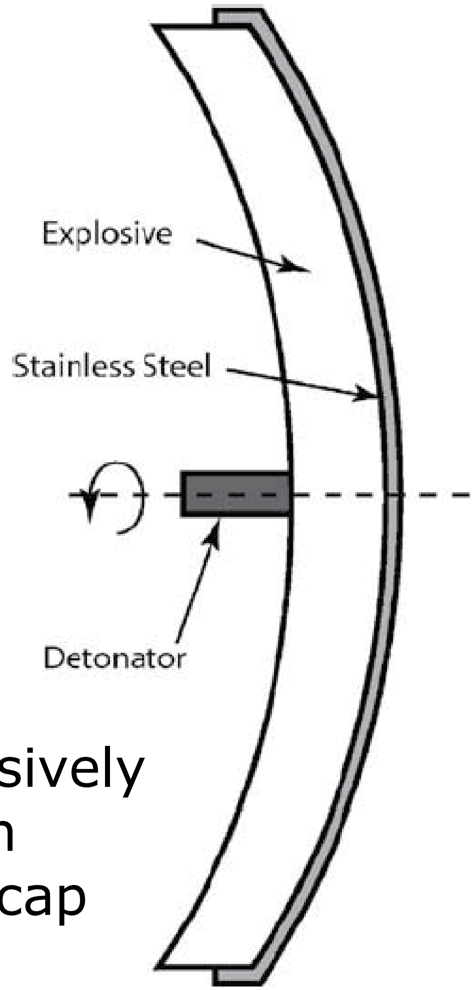


γ	α Lazarus et al. [2008]	α_R	α_L	α	error %
75	21.1	22	18	20.0	5.1
60	38.4	36	35	35.5	7.6
45	61.9	57	58	57.5	7.1

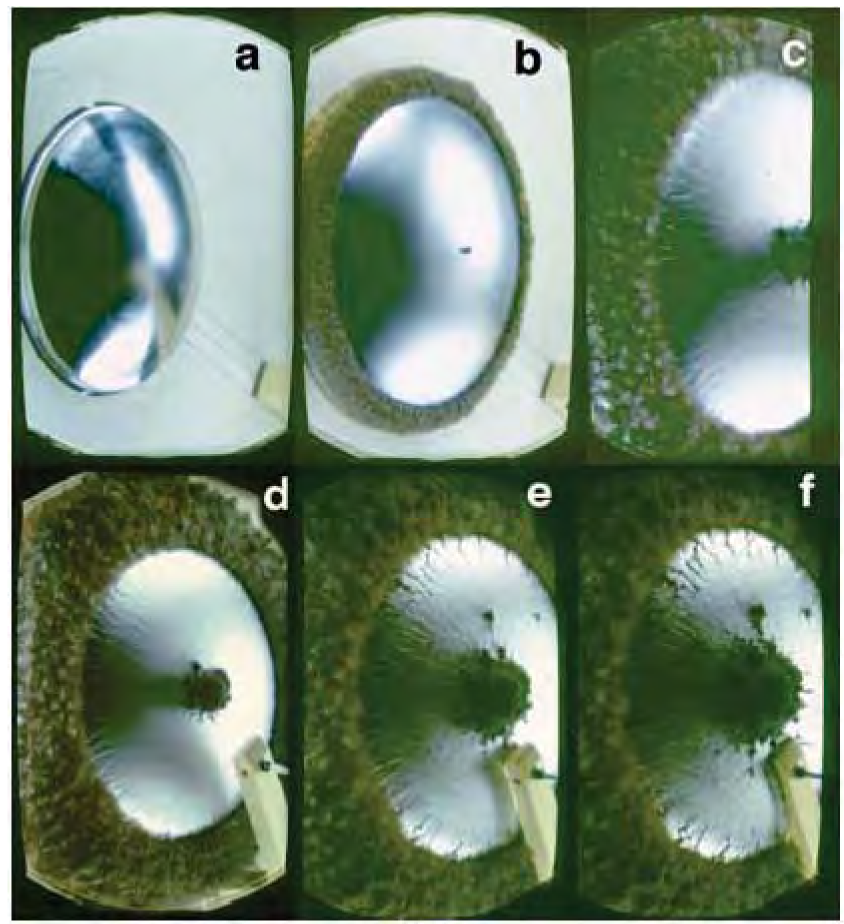
Lazarus, V. *et al.*, *IJF*, 153:141, 2008

Pandolfi, A. and Ortiz, M., *IJNME* (in press) 2012

Validation – Explosively driven cap



Explosively driven steel cap

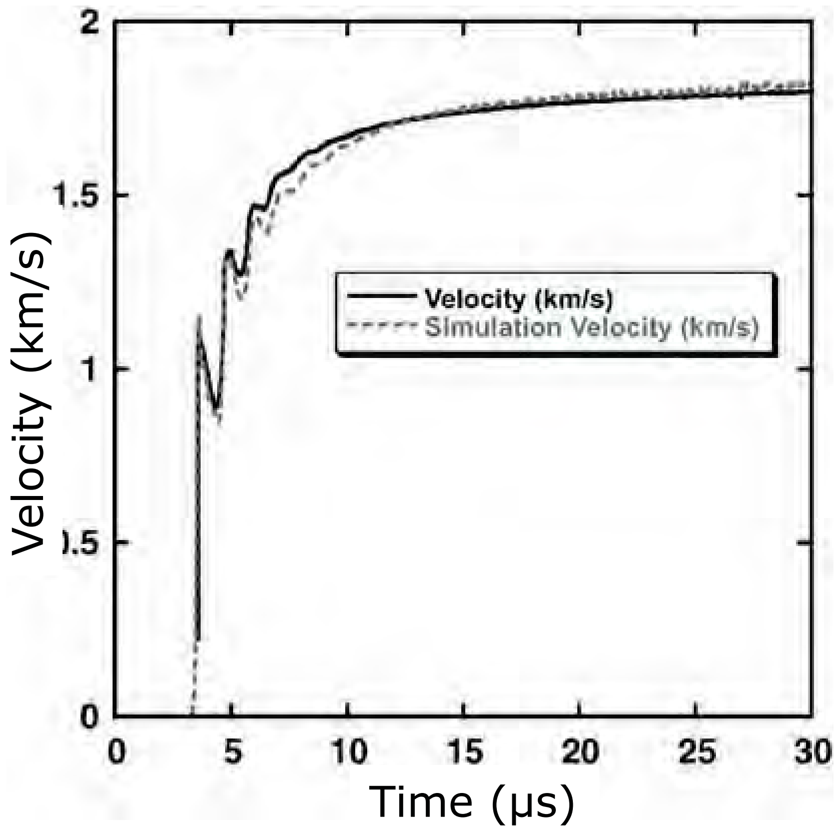


Optical framing camera records

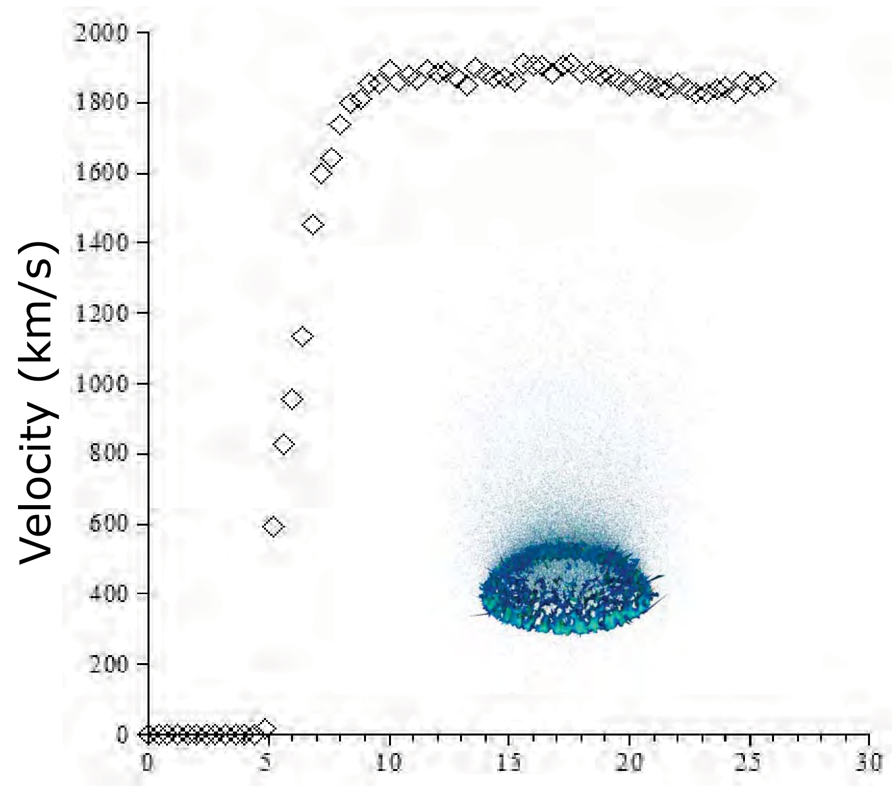
G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, 101:033540, 2007

Validation – Explosively driven cap

Experiment



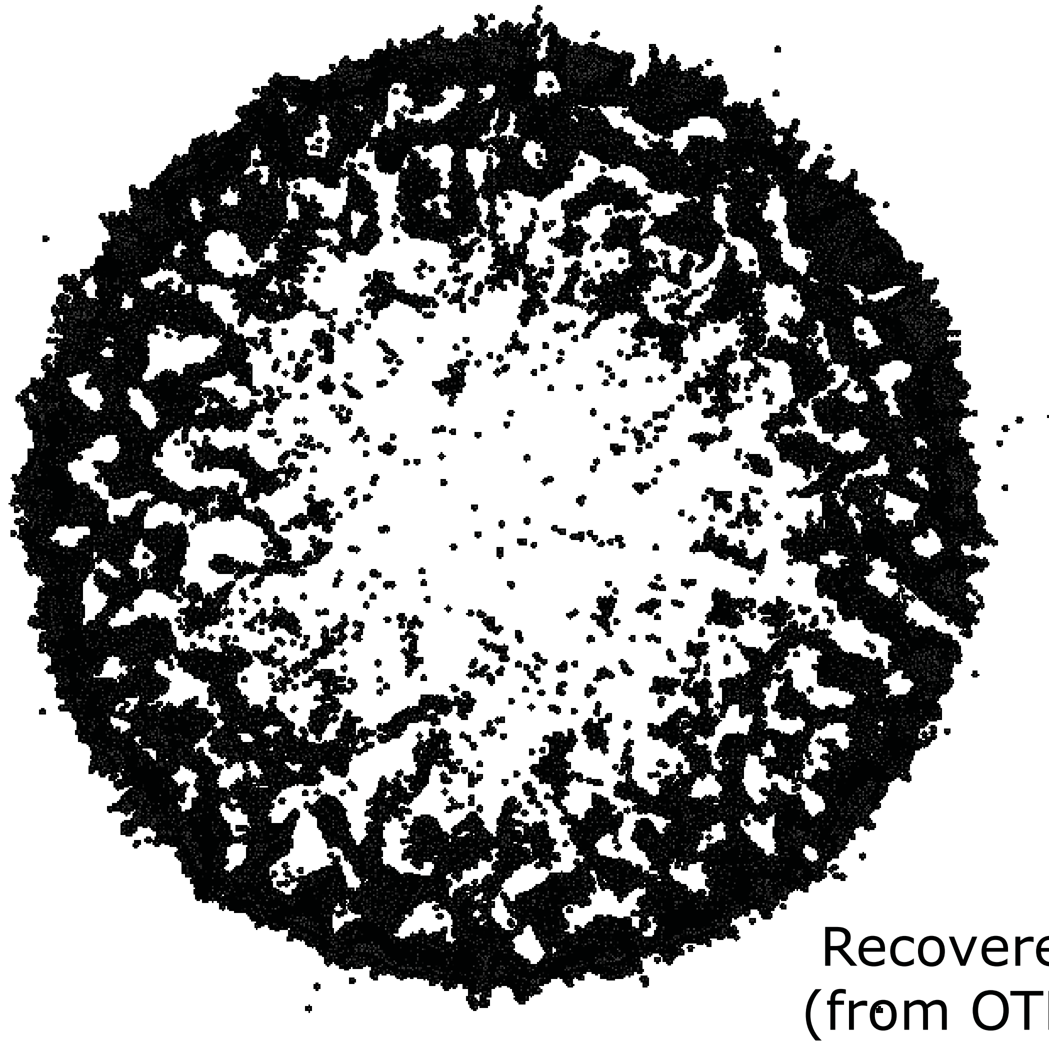
OTM simulation



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

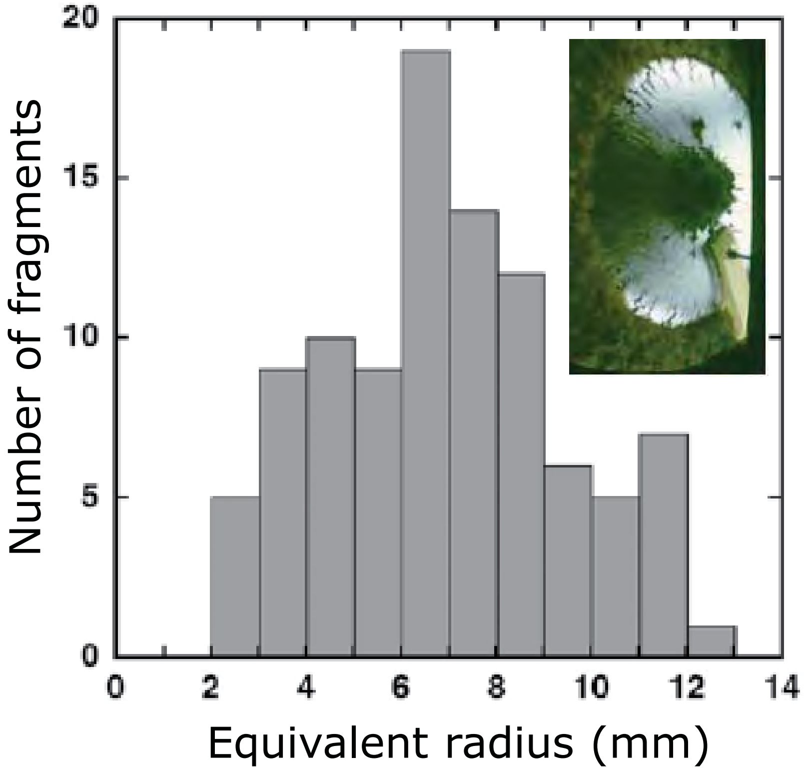


Recovered fragments
(from OTM simulation)

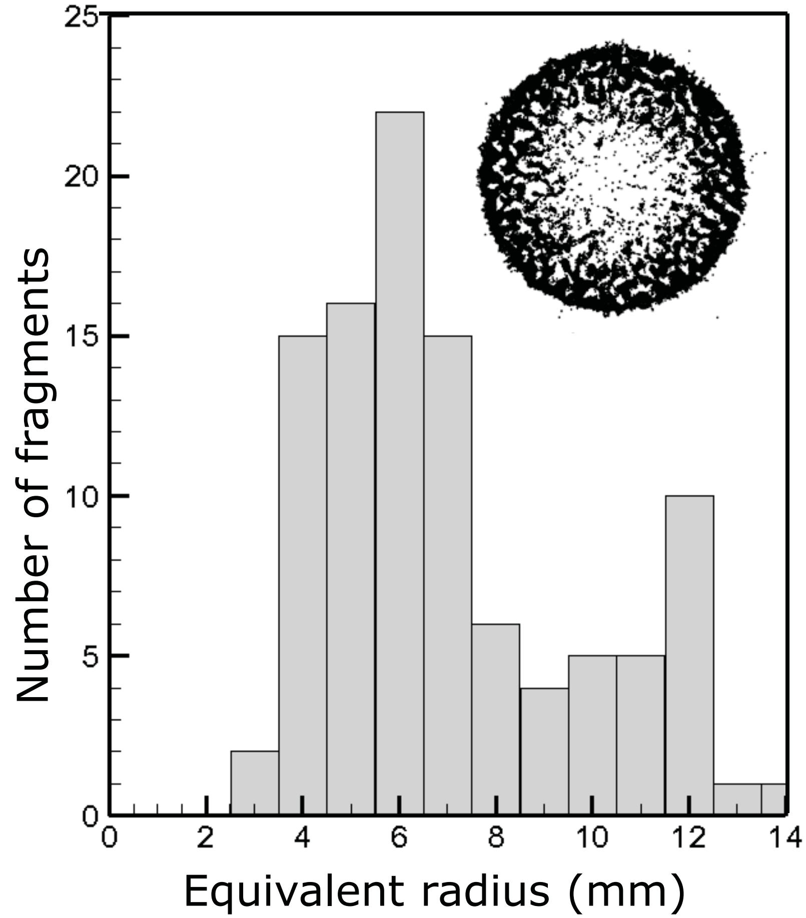
G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, 101:033540, 2007

Validation – Explosively driven cap

Experiment



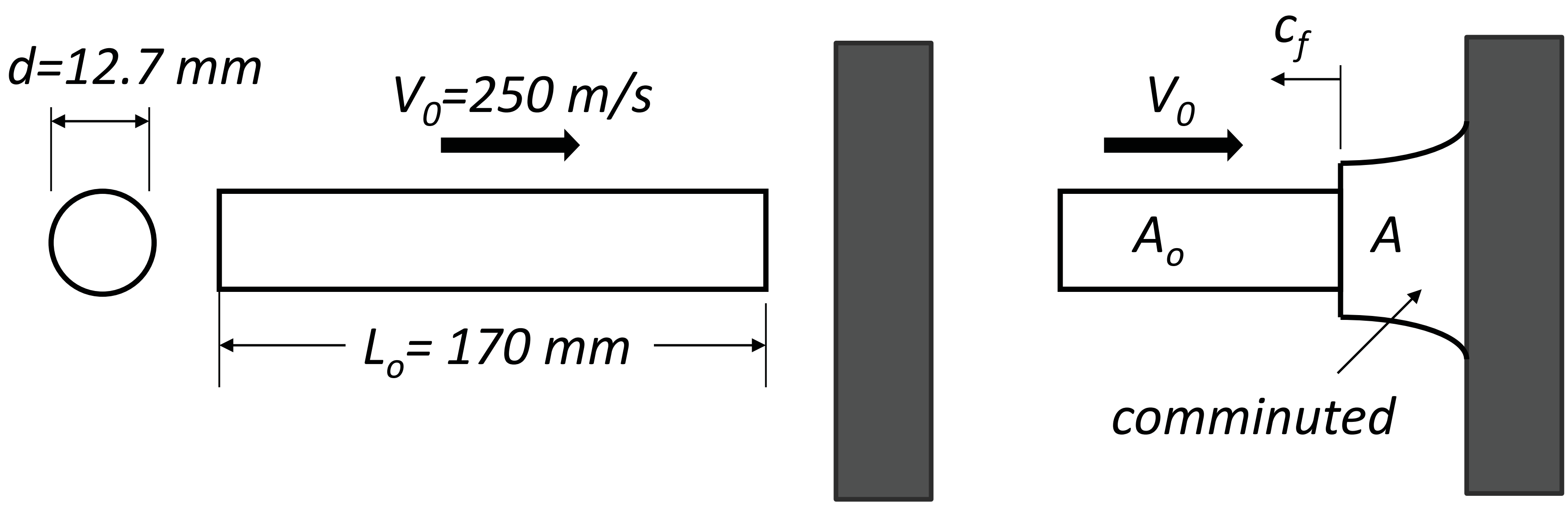
OTM simulation



Histograms of equivalent fragment radii

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

Validation – Failure waves in glass rods

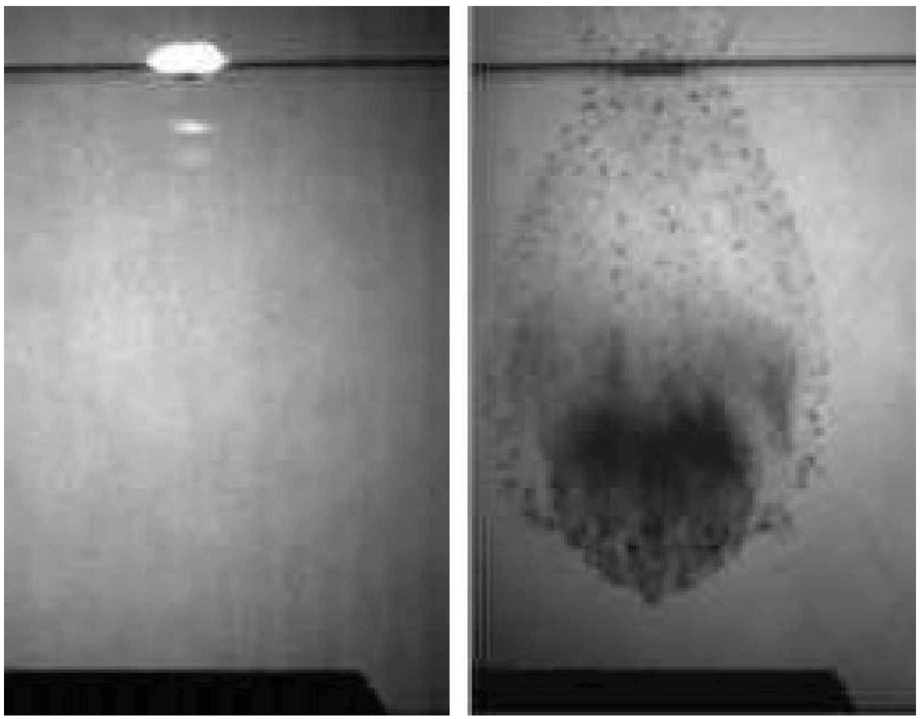


- V_0=225 m/s, c_f = 3.6 Km/s (Brar & Bless, 1991)
- V_0=250 m/s, c_f = 3.0 Km/s (Repetto et al., 2000)
- V_0=250 m/s, c_f = 3.63 Km/s (present)

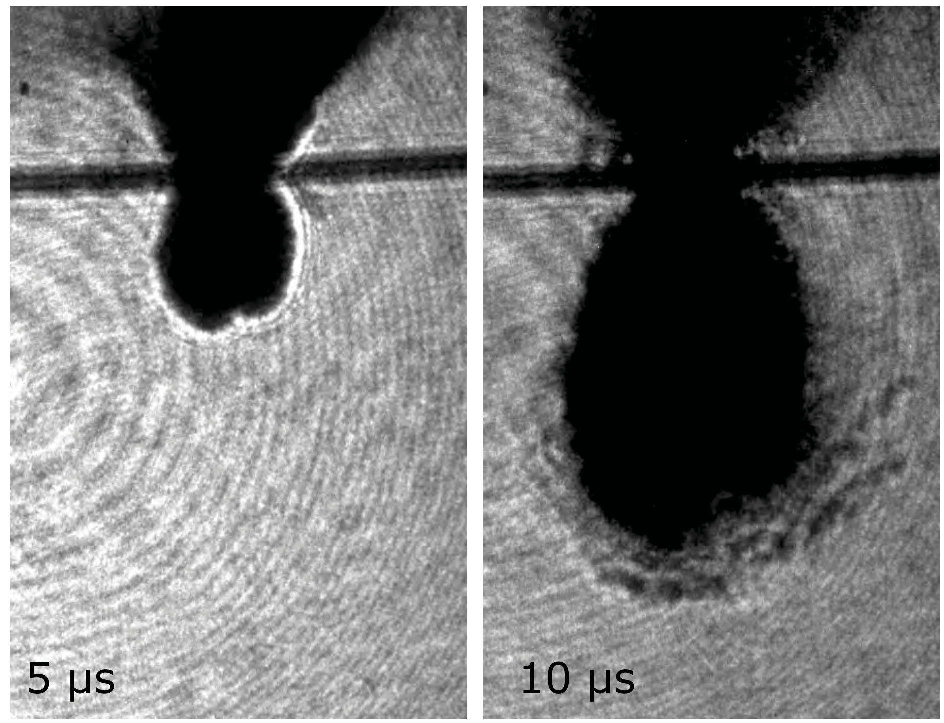
Brar, N.S. and Bless, S.J., *Appl. Phys. Let*., 59:3396, 1991
Repetto, E.A. *et al*., *CMAME*, 183:3, 2000

Solids under Extreme Conditions

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



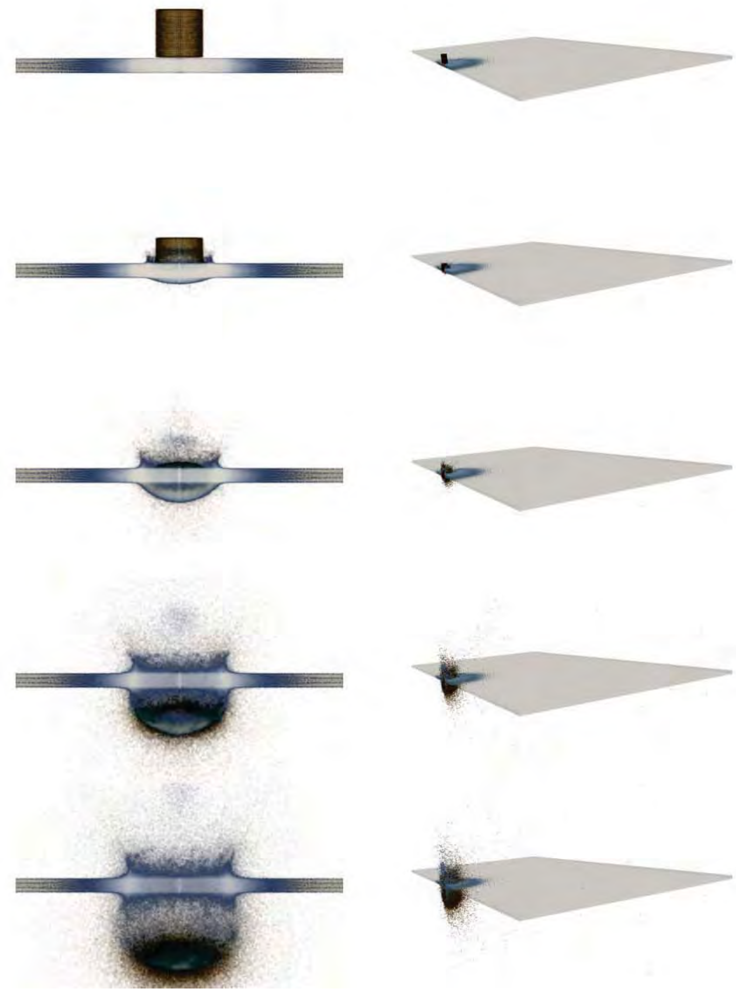
Hypervelocity impact of bumper shield. a) Initial impact flash. b) Debris cloud (Ernst-Mach Inst., Freiburg, Germany).



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

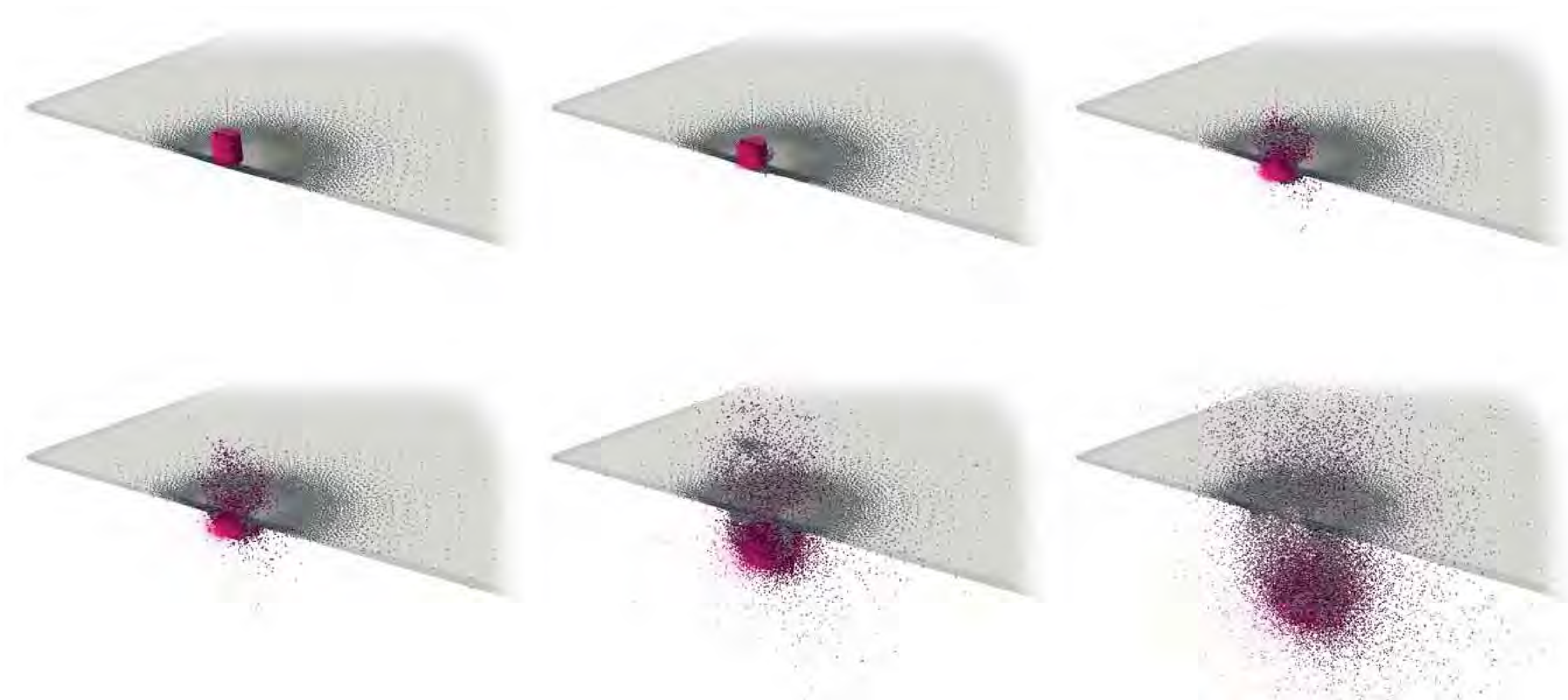
Application to hypervelocity impact

Caltech's hypervelocity Impact facility



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

Application to hypervelocity impact

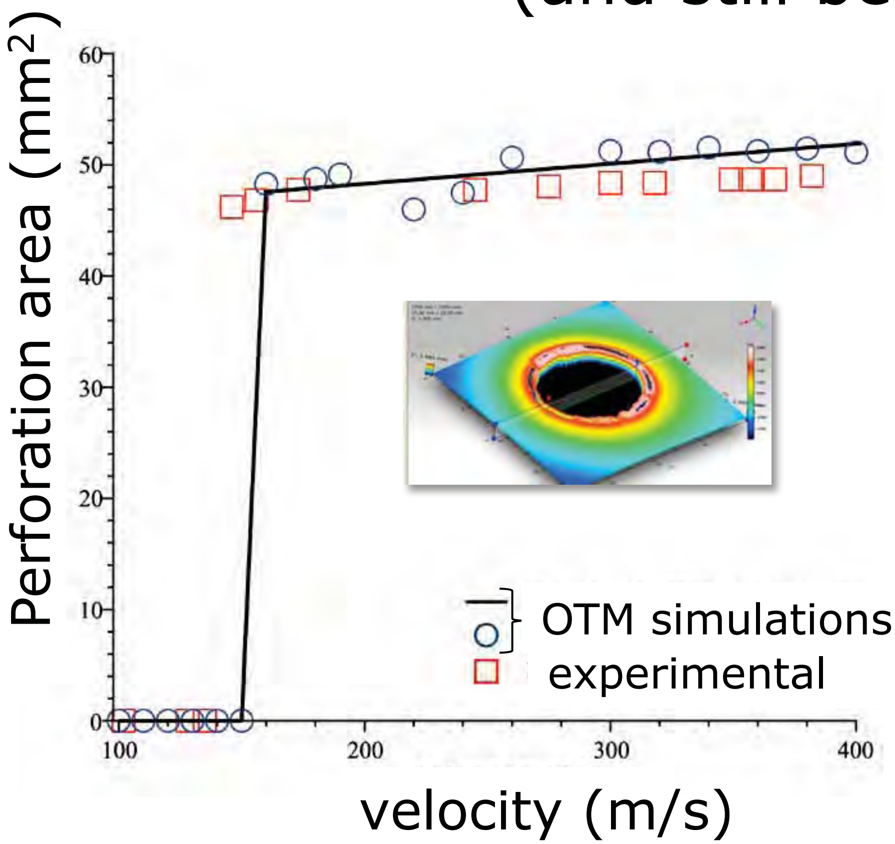


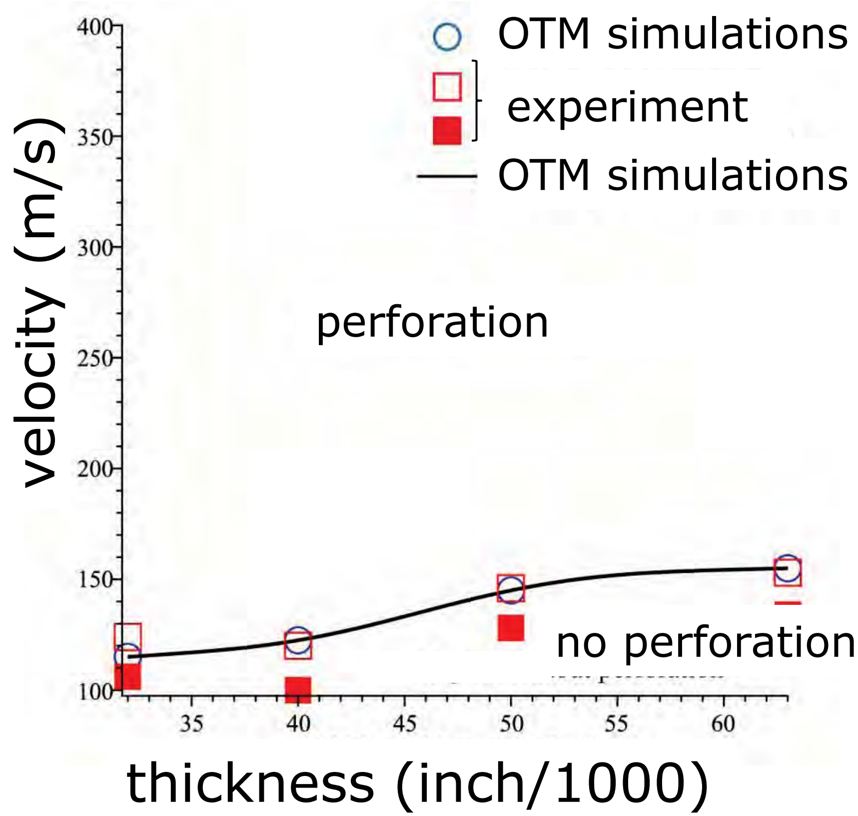
OTM simulation, 5.2 Km/s, Nylon/Al6061-T6,
20 million points

Michael Ortiz
ESMC2012

Validation – Hypervelocity impact

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





Measured *vs*. computed perforation area:
Small modeling error, uncertainty…

OTM – Summary

- *Optimal transportation* is a useful tool for generating geometrically-exact discrete Lagrangians for flow problems
- *Max-ent interpolation* supplies an efficient meshfree, continuously adaptive, remapping-free, FE-compatible, interpolation scheme
- *Material point sampling* effectively addresses the issues of numerical quadrature, history variables
- *Eigen-erosion*: Convergent material-point erosion scheme for approximating fracture and fragmentation

Thank you!