Optimal-Transportation Meshfree Approximation Schemes for Fluid and Plastic Flows

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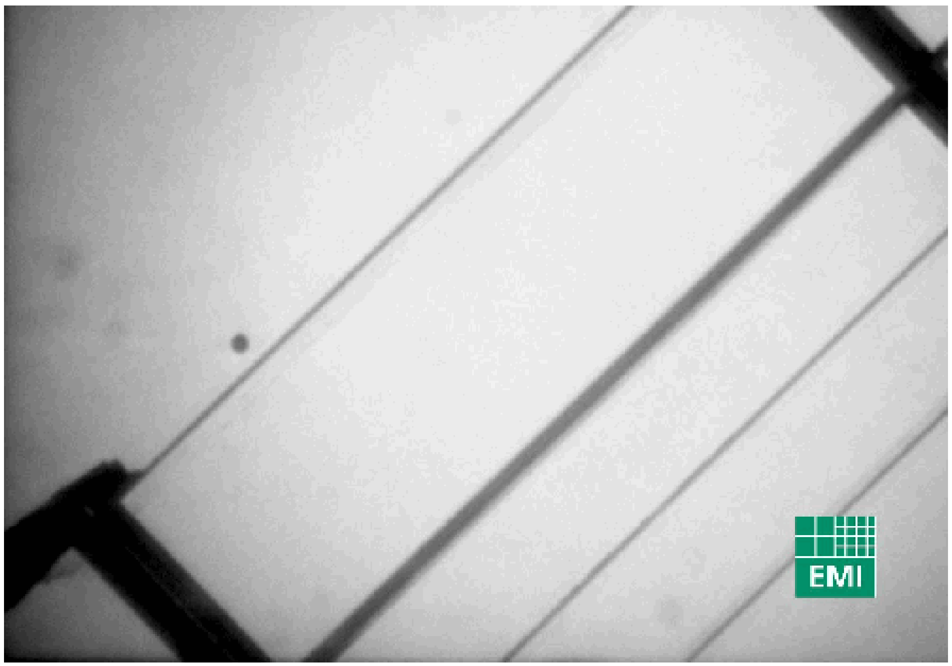
Objective: Hypervelocity impact

- Hypervelocity impact is of interest to a broad scientific community: Micrometeorite shields, geological impact cratering…



Hypervelocity impact test of multi-layer micrometeorite shield (Ernst-Mach Institut, Germany)

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

Simulation requirements

- Hypervelocity impact: Grand challenge in scientific computing
- Main simulation requirements:
  - *Hypersonic dynamics, high-energy density (HED)*
  - *Multiphase flows (solid, fluid, gas, plasma)*
  - *Free boundaries + contact*
  - *Fracture, fragmentation, perforation*
  - *Complex material phenomena:*
    - *HED/extreme conditions*
    - *Ionization, excited states, plasma*
    - *Multiphase equation of state, transport*
    - *Viscoplasticity, thermomechanical coupling*
    - *Brittle/ductile fracture, fragmentation...*

Optimal-Transportation Meshfree (OTM)

- Time integration (OT):
  - *Optimal transportation methods:*
    - *Geometrically exact, discrete Lagrangians*
  - *Discrete mechanics, variational time integrators:*
    - *Symplecticity, exact conservation properties*
  - *Variational material updates, inelasticity:*
    - *Incremental variational structure*
- Spatial discretization (M):
  - *Max-ent meshfree nodal interpolation:*
    - *Kronecker-delta property at boundary*
  - *Material-point sampling:*
    - *Numerical quadrature, material history*
  - *Dynamic reconnection, 'on-the-fly' adaptivity*

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)

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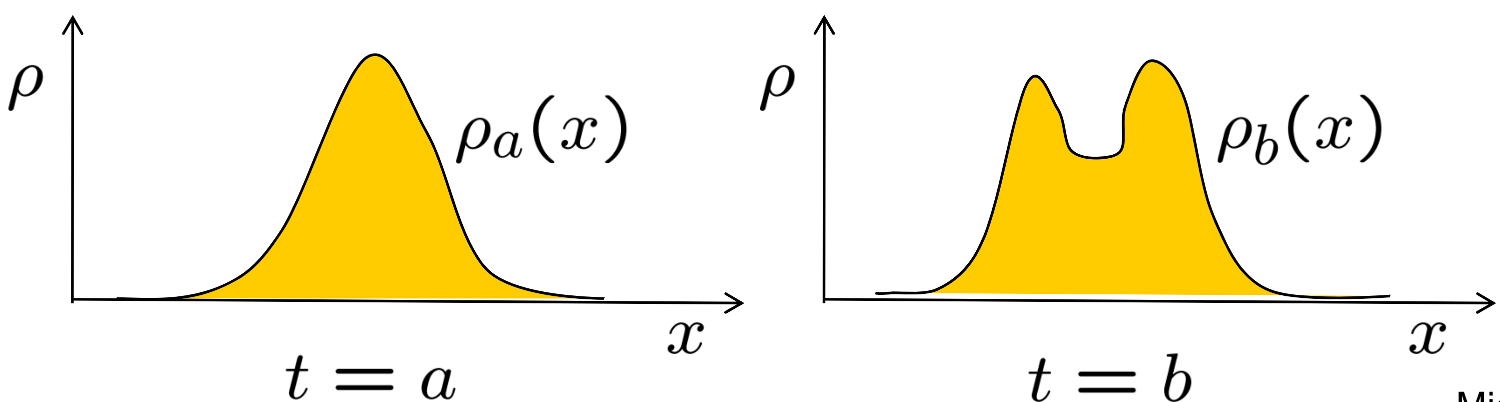
Mass flows – Optimal transportation

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



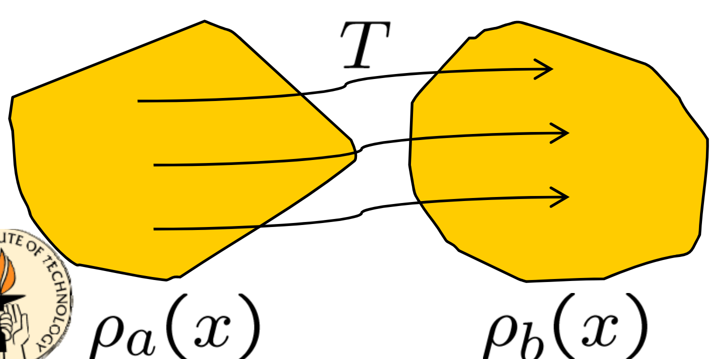
Mass flows – Optimal transportation

- *Benamou & Brenier* minimum principle:

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

- 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:

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

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

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Euler flows – Optimal transportation

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

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

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

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

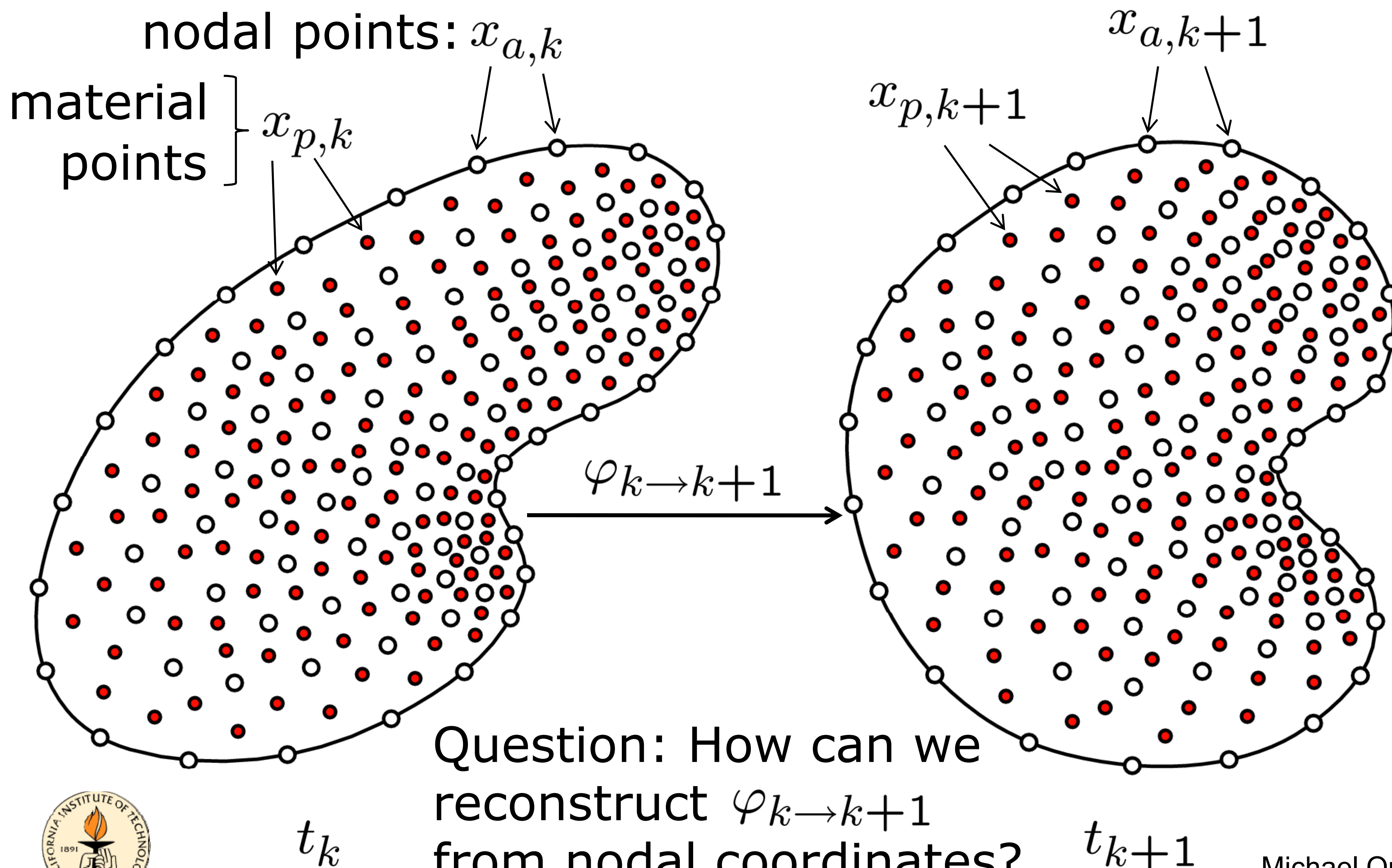
$$\rho_{k+1} \circ \varphi_{k\to k+1} = \rho_k / \det\left(\nabla \varphi_{k\to k+1}\right)$$

geometrically exact mass conservation!

Optimal-Transportation Meshfree (OTM)

- 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)*
  - *Strong variational convergence (in sense of Γ-convergence, non-linear phase error analysis)*

OTM – Spatial discretization



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

OTM – Max-ent interpolation

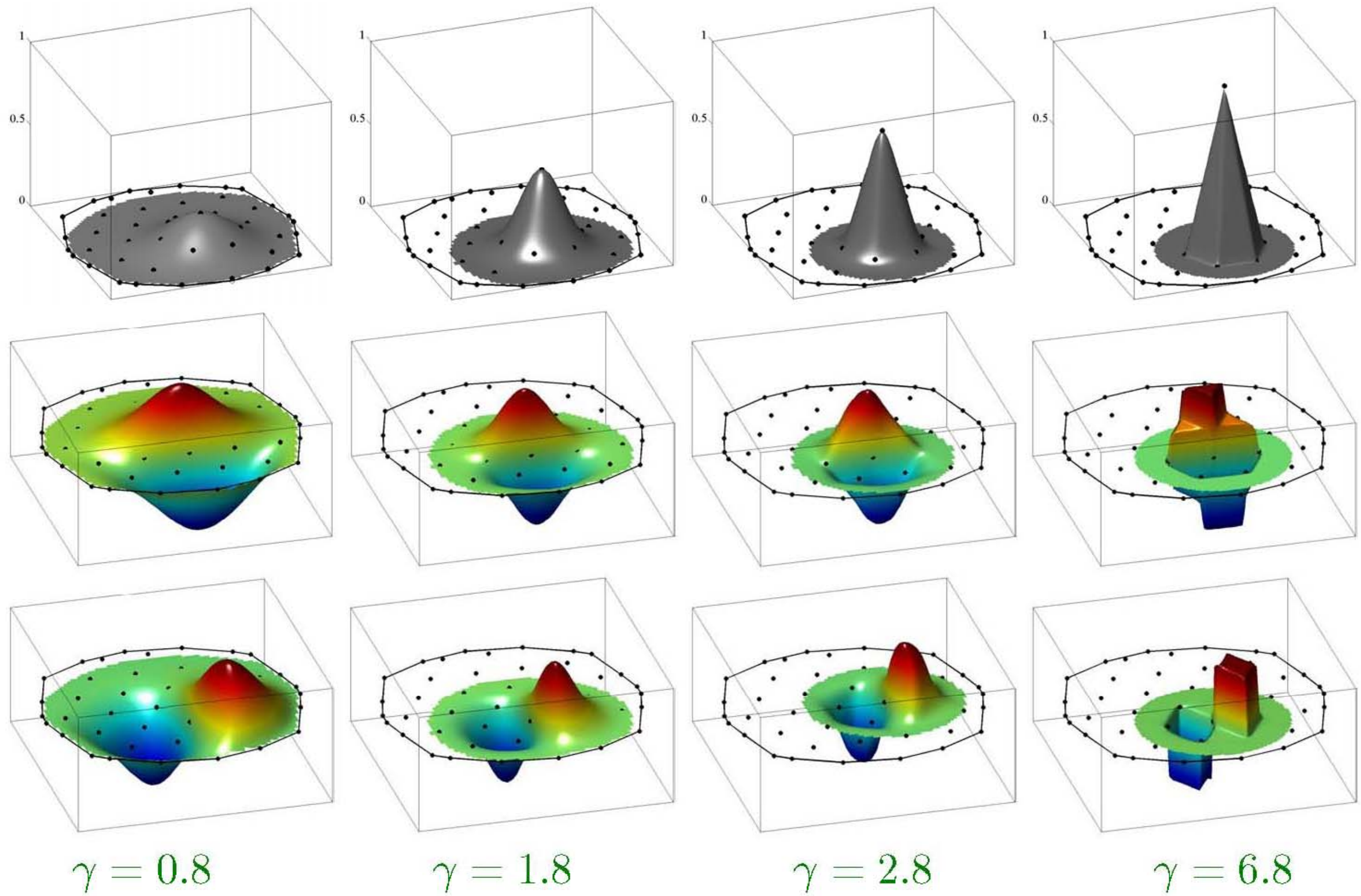
- Problem: Reconstruct function $u(x)$ from nodal sample $\{u(x_a),\ a = 1, \dots, N\}$ so that:
  - Reconstruction is *least biased*
  - Reconstruction is *most local*

- Optimal shape functions (Arroyo & MO, *IJNME*, 2006):

Minimize: $$\underbrace{\sum_{a=1}^{N} |x - x_a|^2 N_a(x)}_{\text{shape function width}} + \beta \underbrace{\sum_{a=1}^{N} N_a(x) \log N_a(x)}_{\text{information entropy}}$$

Subject to: $$\sum_{a=1}^{N} N_a(x) = 1, \qquad \sum_{a=1}^{N} x_a N_a(x) = x.$$

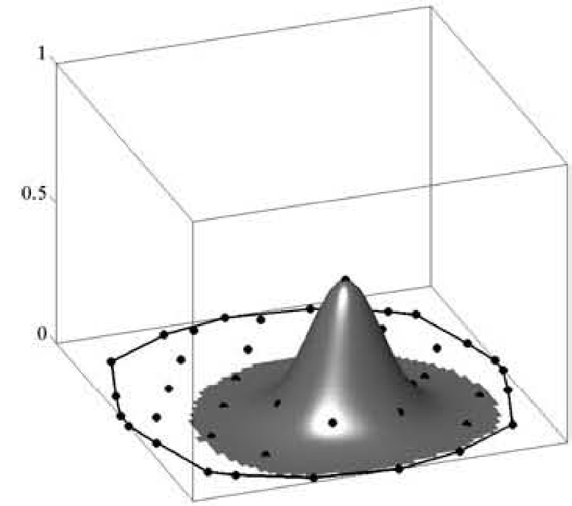
OTM – Max-ent interpolation

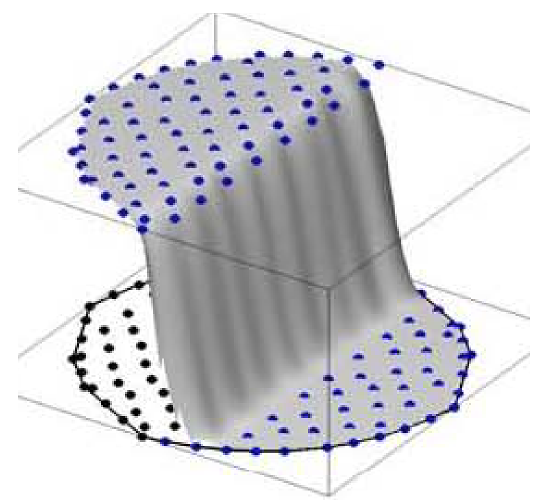


Max-ent shape functions, $\gamma = \beta h^2$

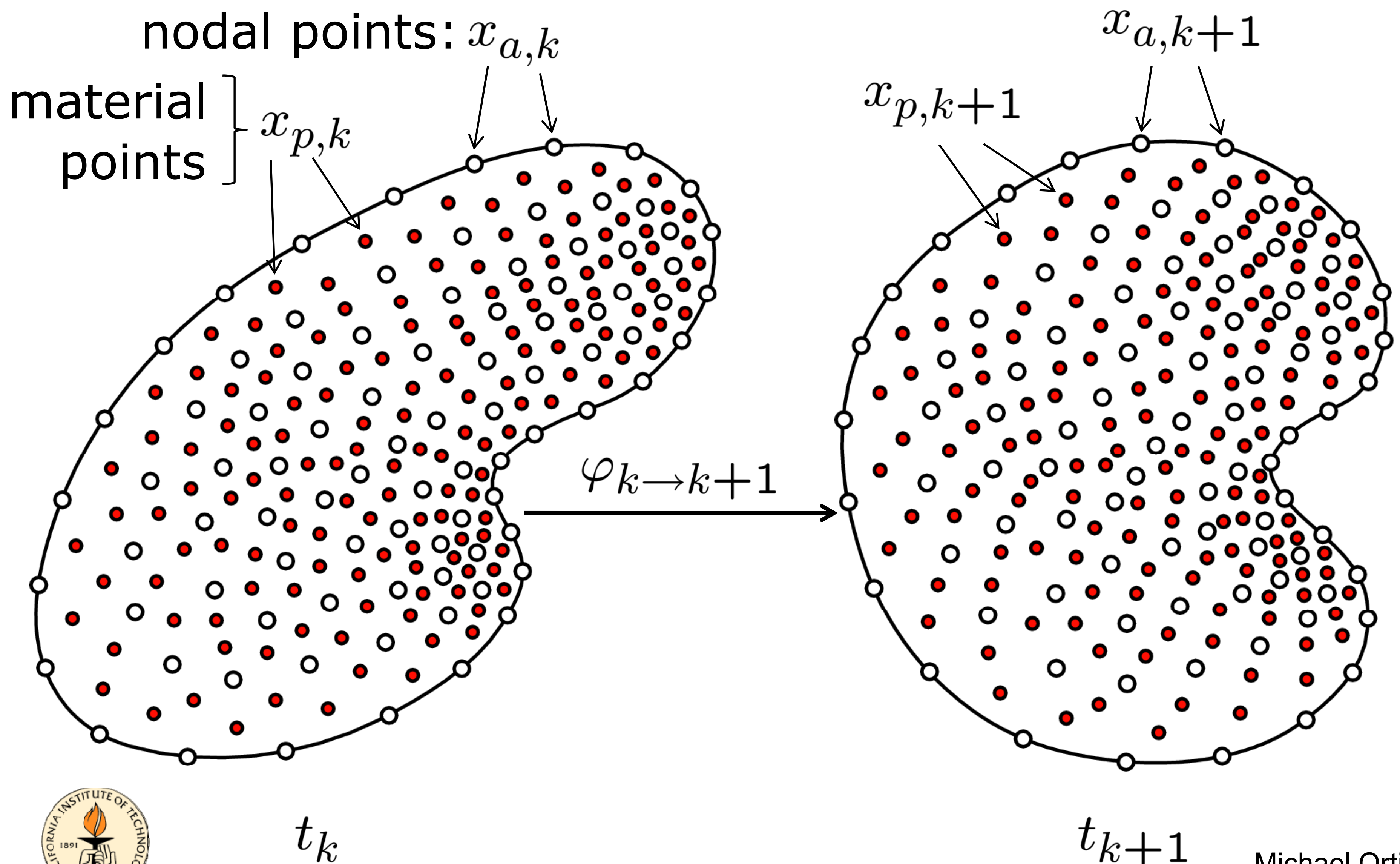
OTM — Max-ent interpolation

- Max-ent interpolation is smooth, meshfree
- Finite-element interpolation is recovered in the limit of $\beta \to \infty$
- Rapid decay, short range
- Monotonicity, maximum principle
- Good mass lumping properties
- Kronecker-delta property at the boundary:
  - *Displacement boundary conditions*
  - *Compatibility with finite elements*





OTM – Spatial discretization



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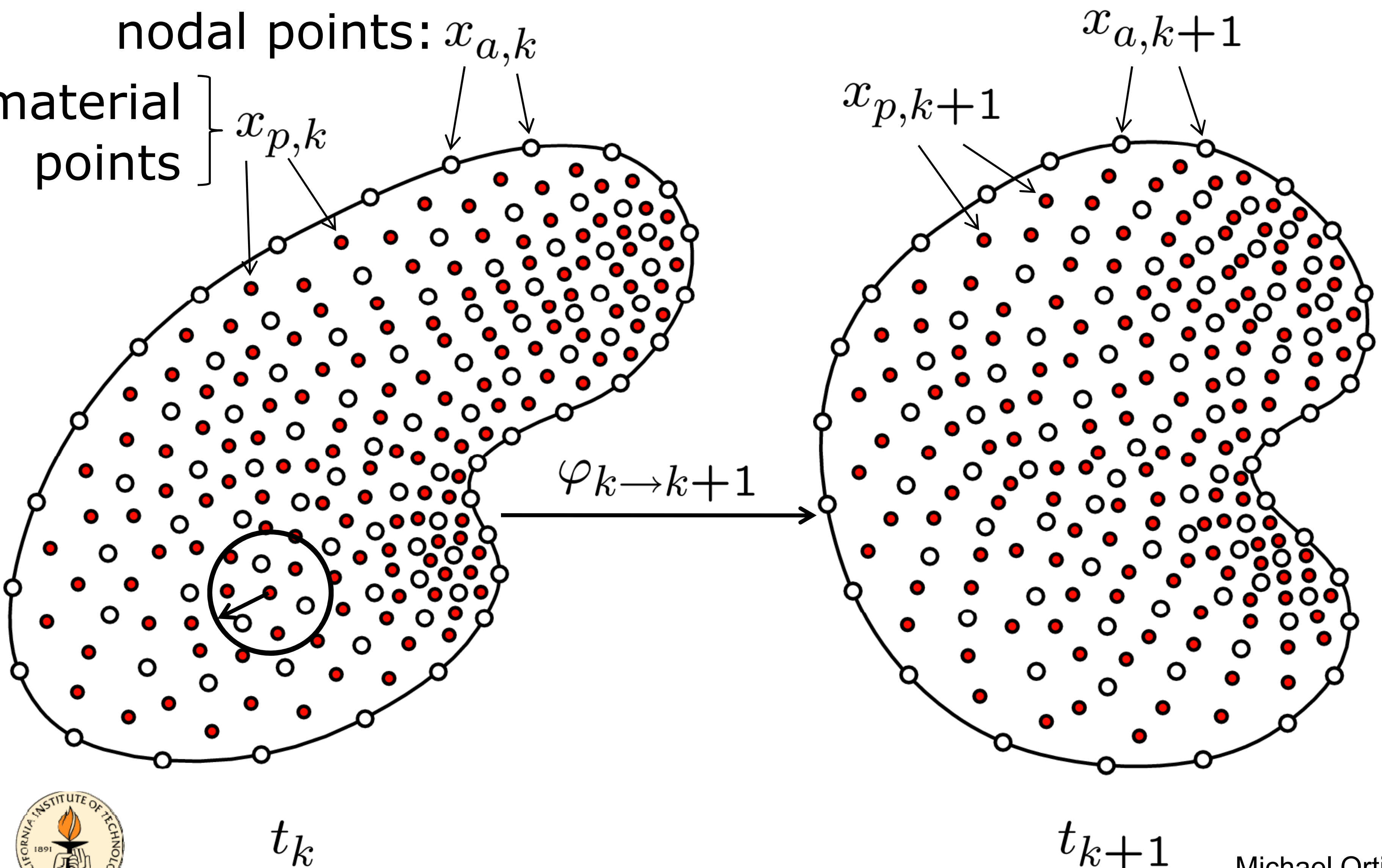
OTM – Spatial discretization



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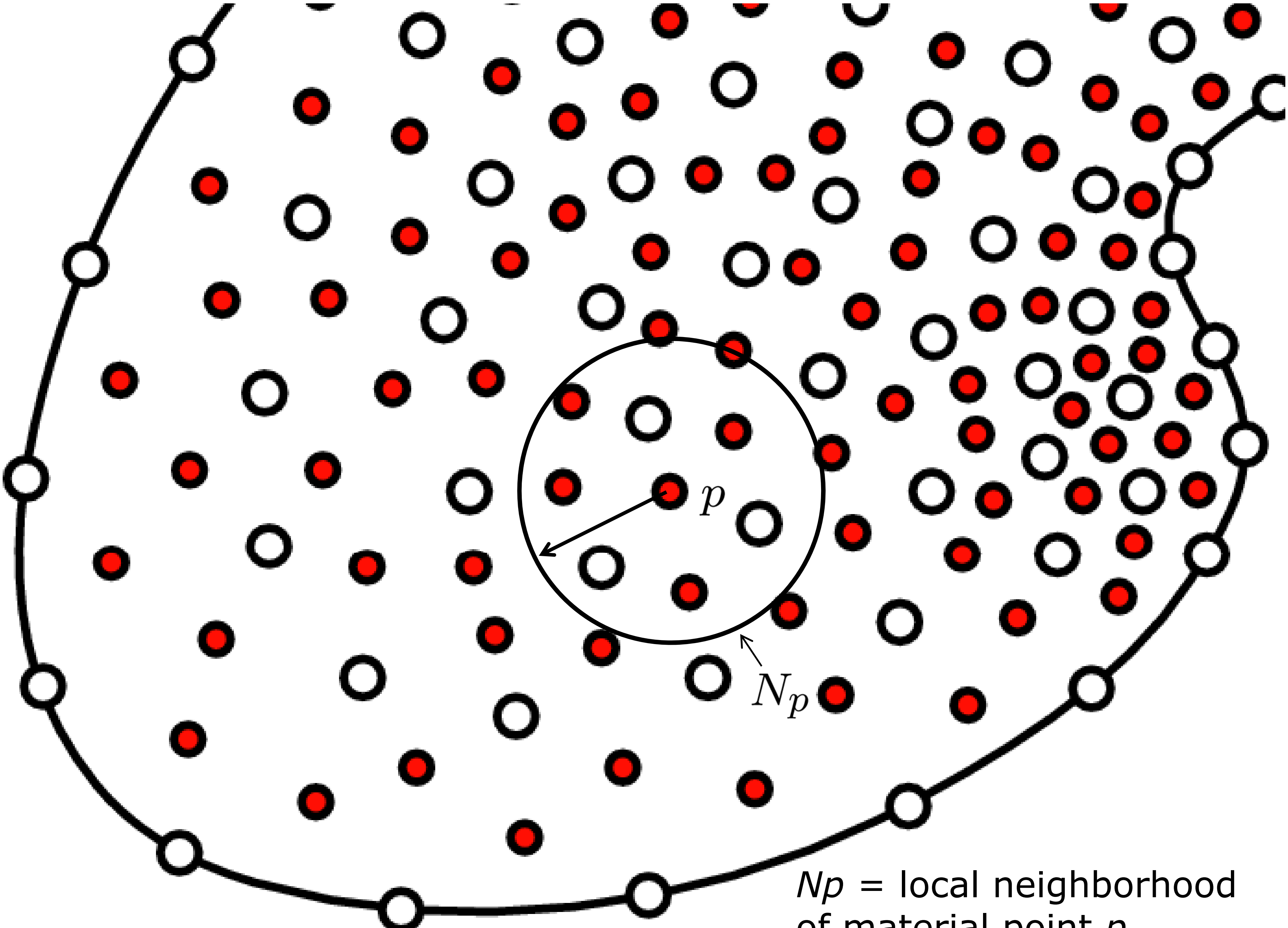
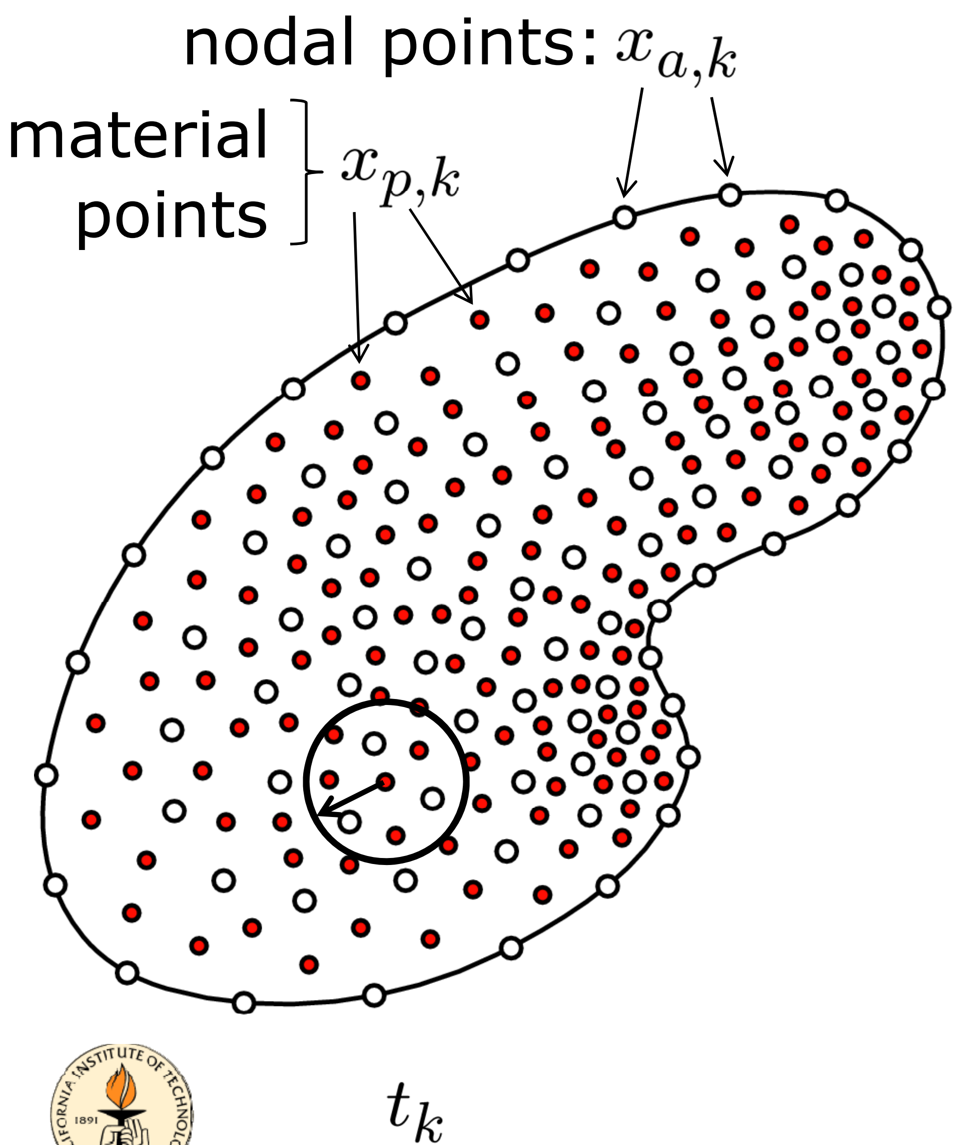


Np = local neighborhood of material point *p*

OTM – Spatial discretization



- Max-ent interpolation at material point *p* determined by nodes in its local environment *Np*
- 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: $F_{p,k+1} = \nabla \varphi_{k \to k+1}(x_{p,k}) F_{p,k}$

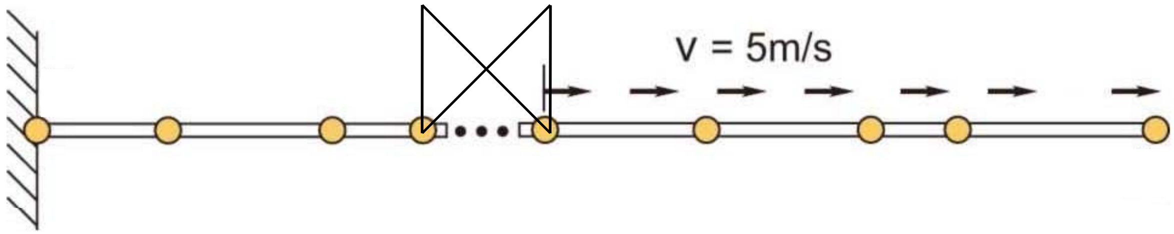
volume: $V_{p,k+1} = \det \nabla \varphi_{k \to k+1}(x_{p,k}) V_{p,k}$

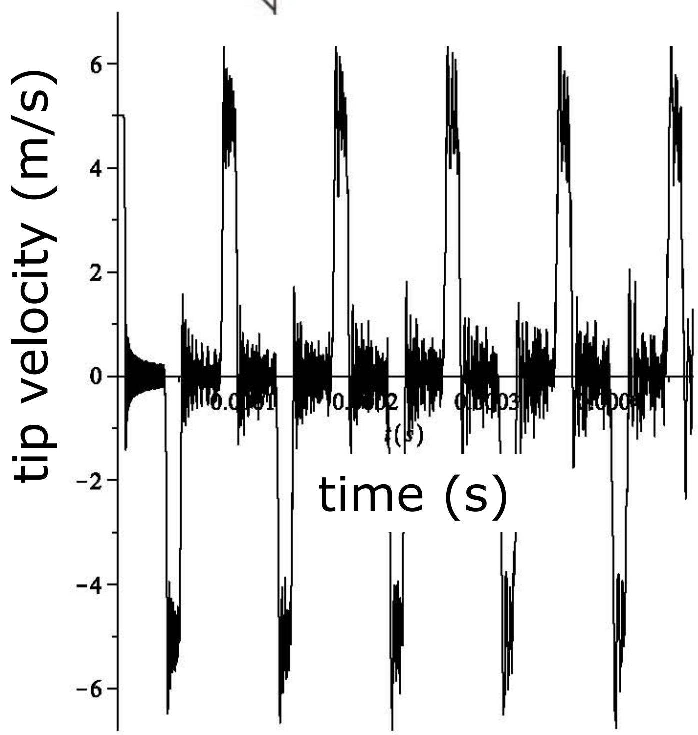
density: $\rho_{p,k+1} = m_p / V_{p,k+1}$

(iii) Constitutive update at material points

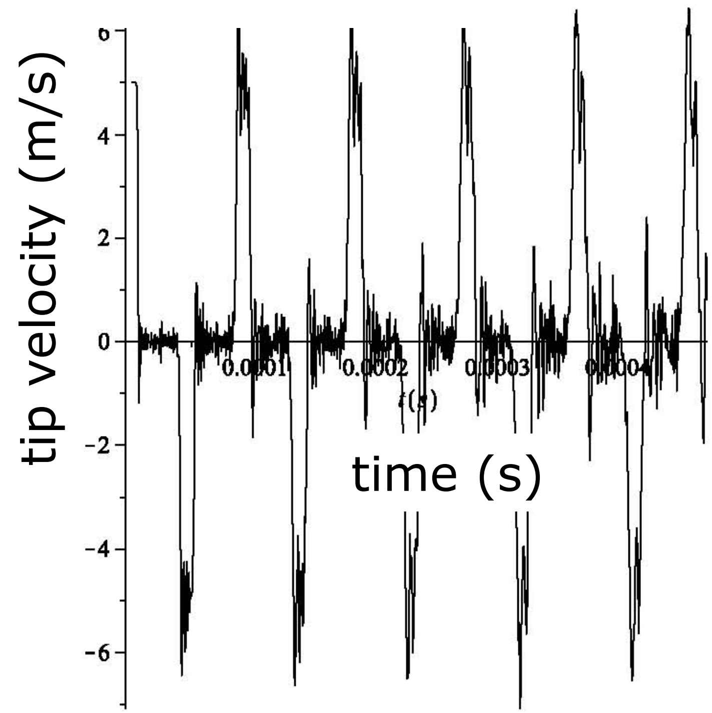
(iv) Reconnect nodal and material points (range searches), recompute max-ext shape functions

OTM – Tensile stability





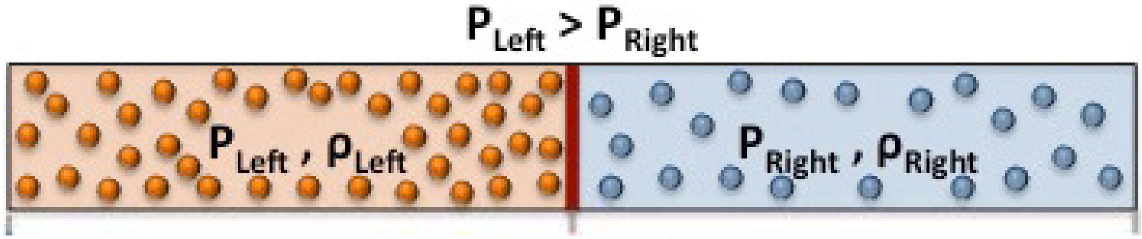
Finite elements

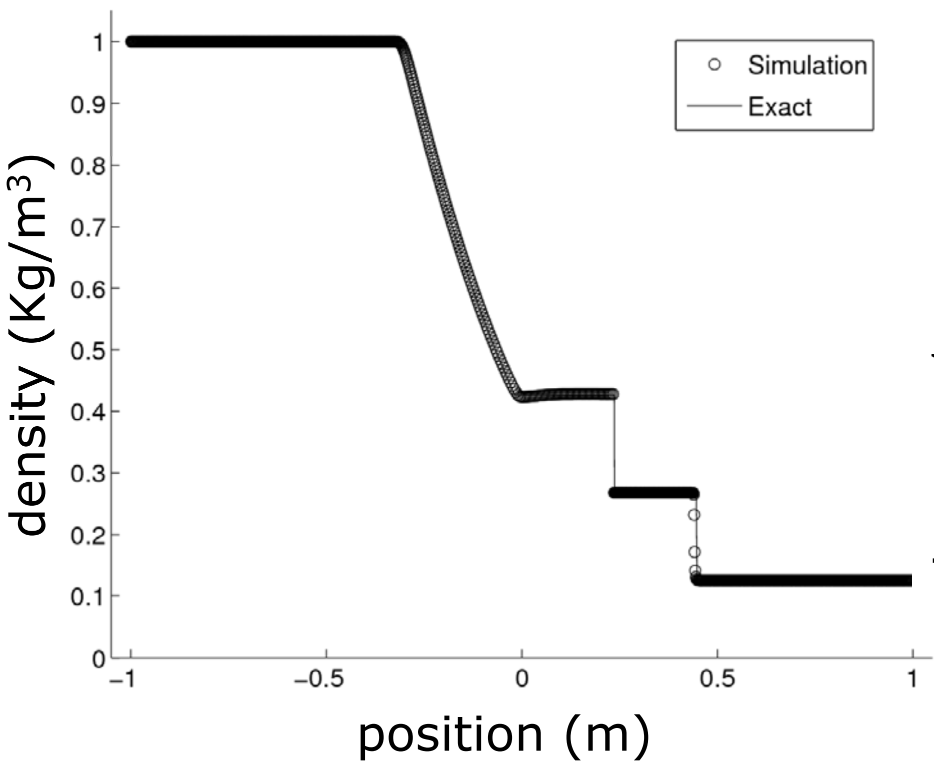


OTM

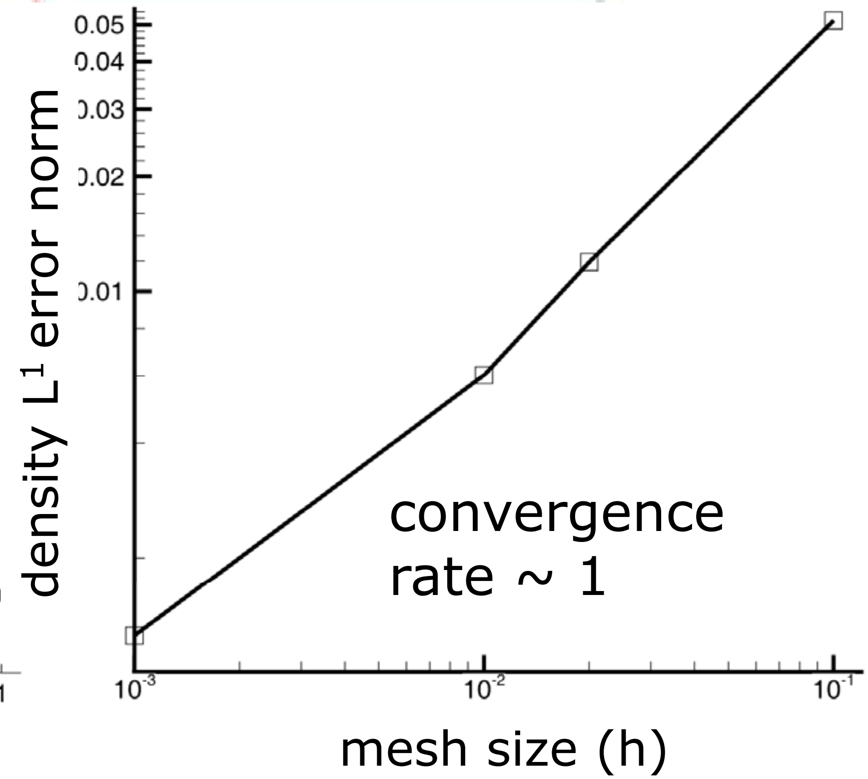
OTM is free from tensile instabilities!

OTM – Riemann problem





computed *vs*. exact wave structure



density convergence (L^1 norm)

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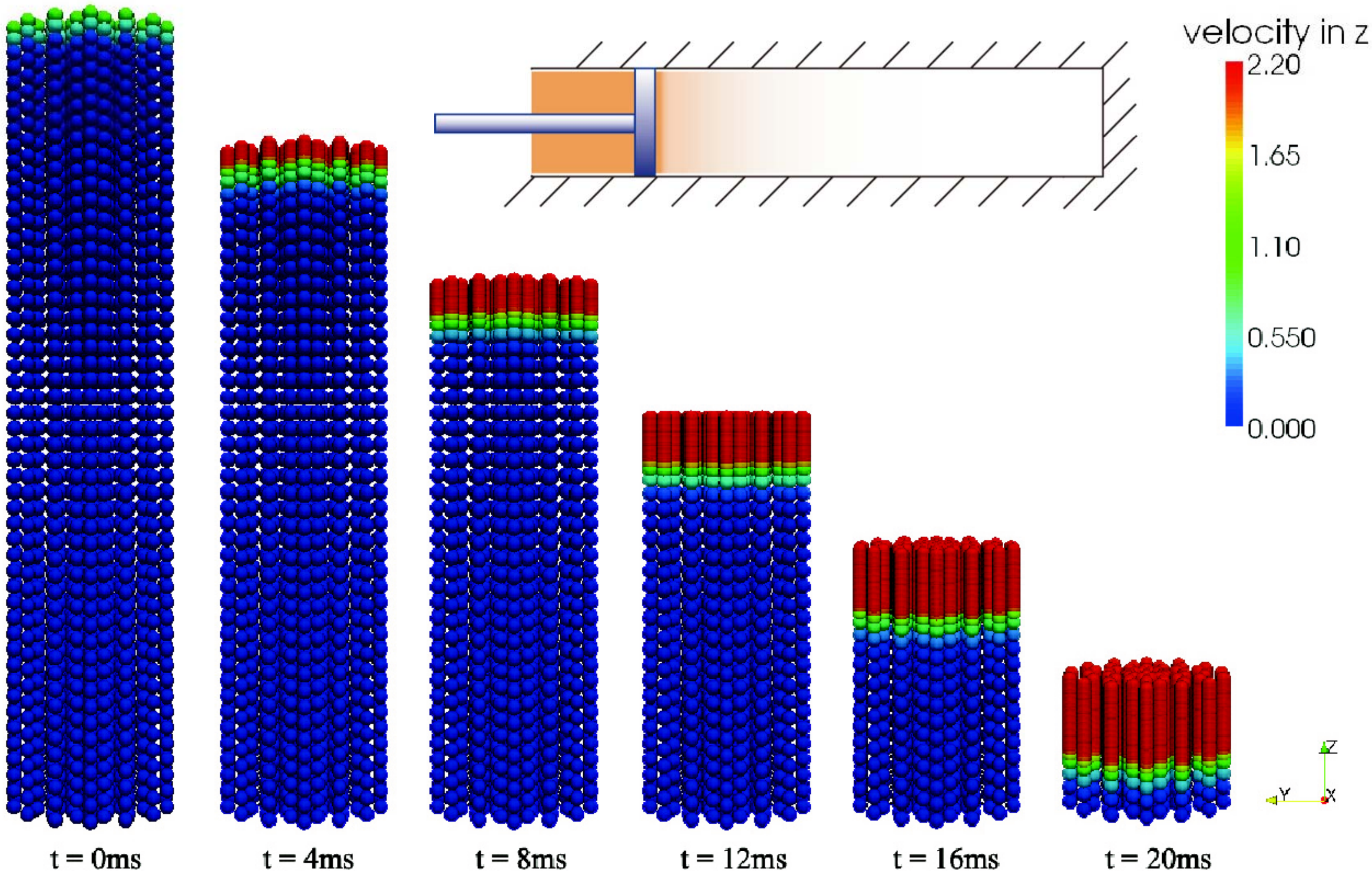
OTM – Shock tube problem



Shock tube problem – velocity snapshots

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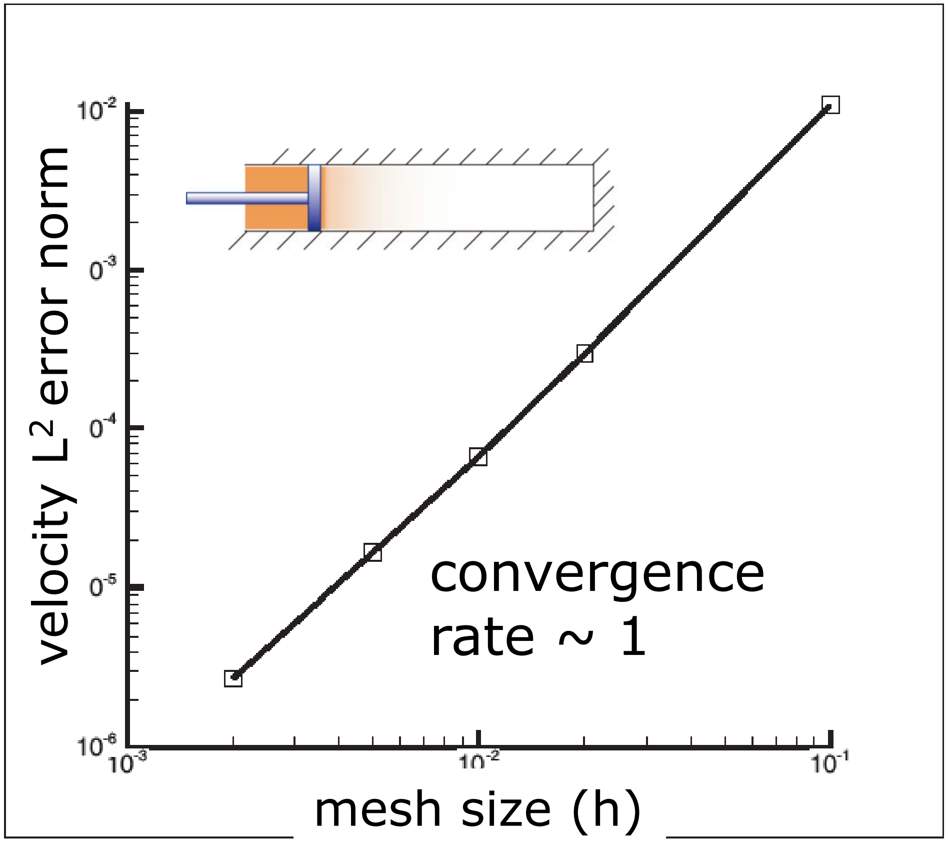
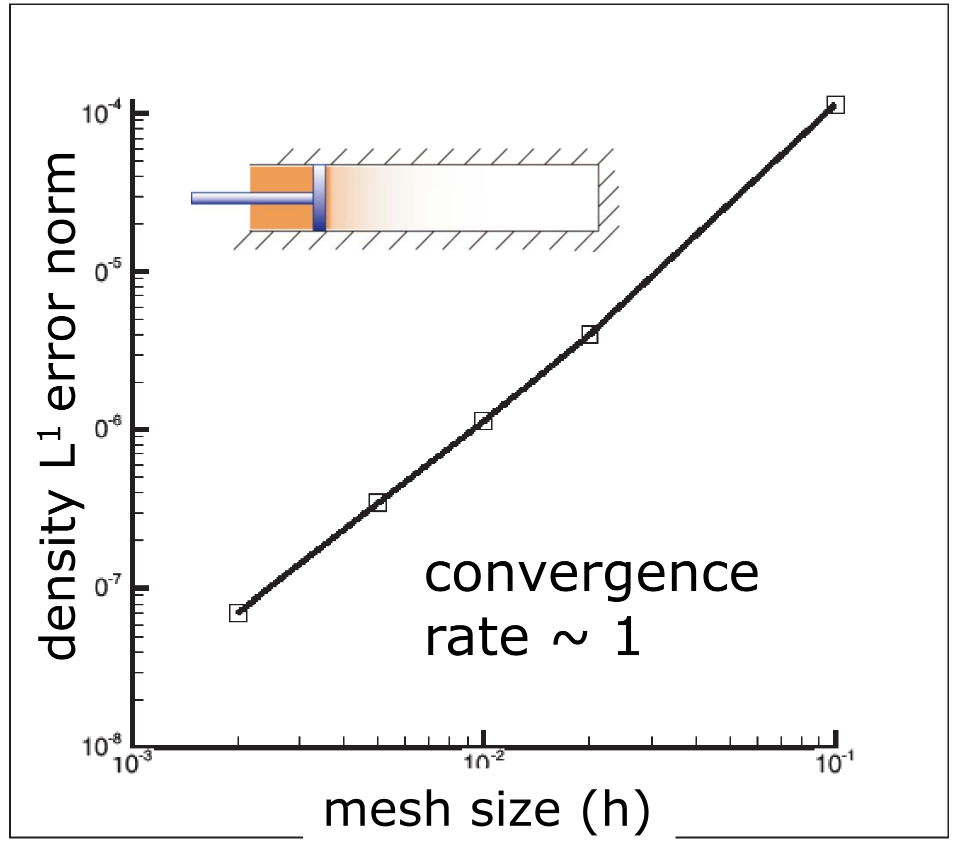
OTM – Shock tube problem



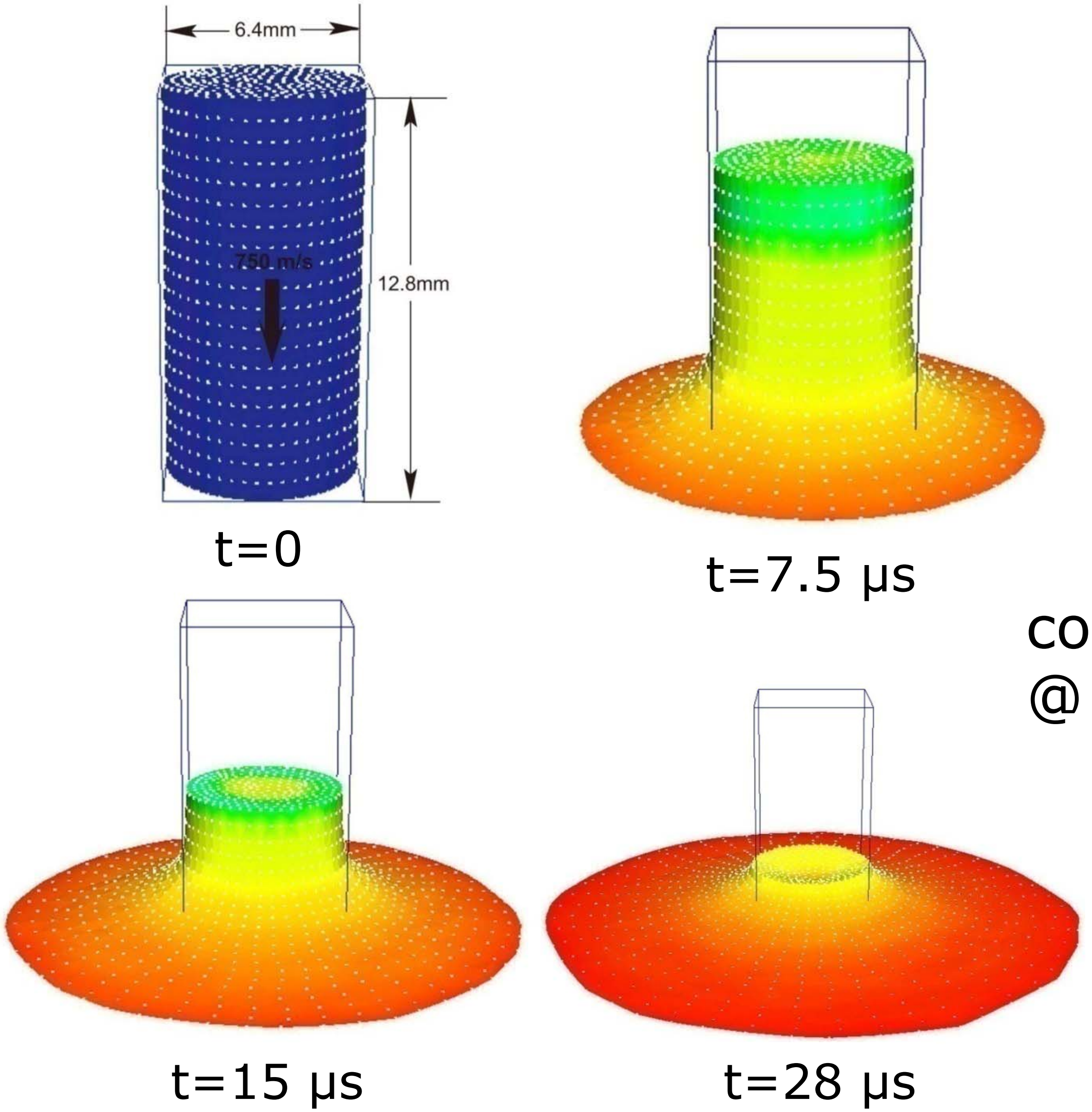
velocity convergence
(L^2 norm)



density convergence
(L^1 norm)

Shock tube problem – convergence plots

OTM – Taylor anvil test



copper rod
@ 750 m/s

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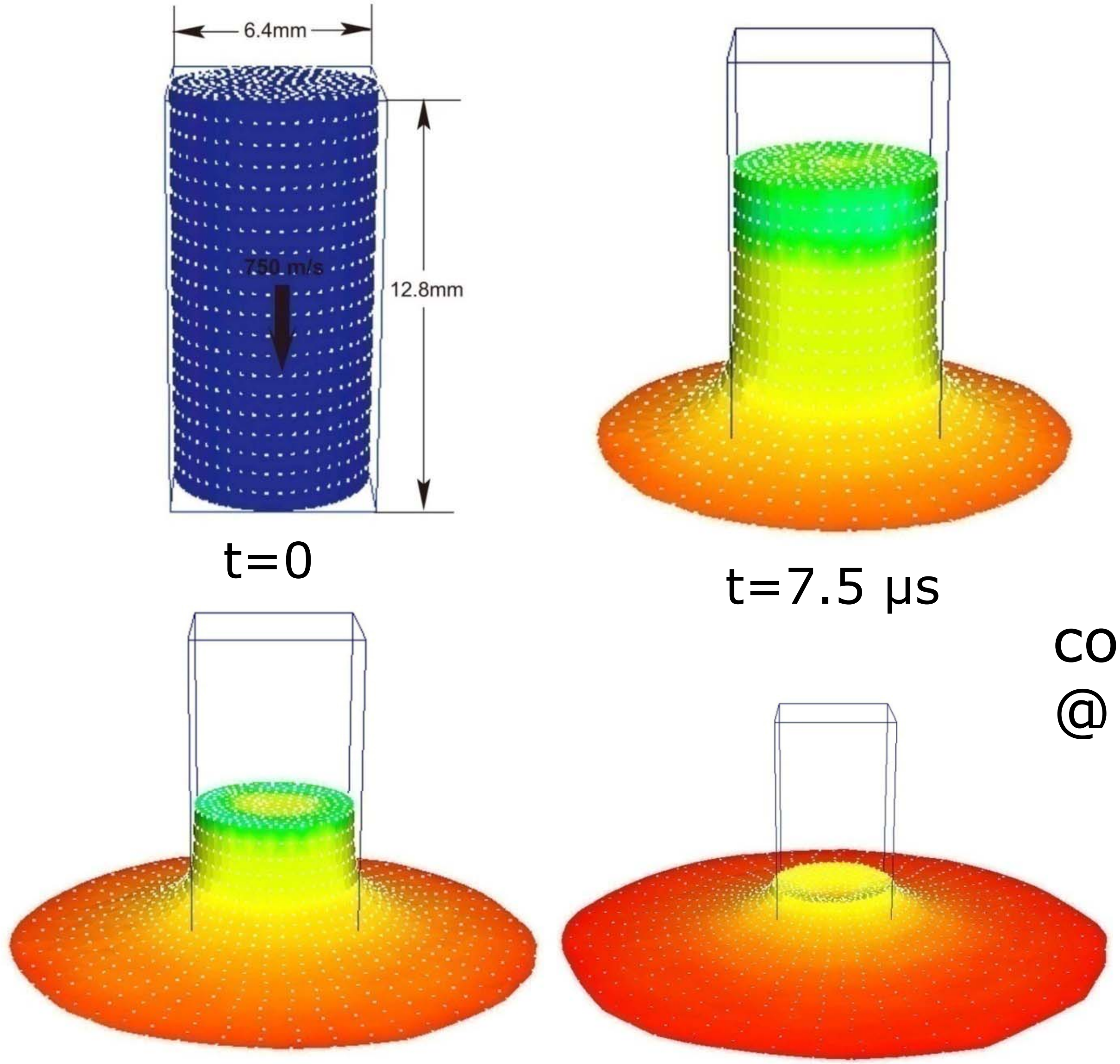
OTM – Taylor anvil test



t=0

t=7.5 μs

t=15 μs

t=28 μs

copper rod
@ 750 m/s

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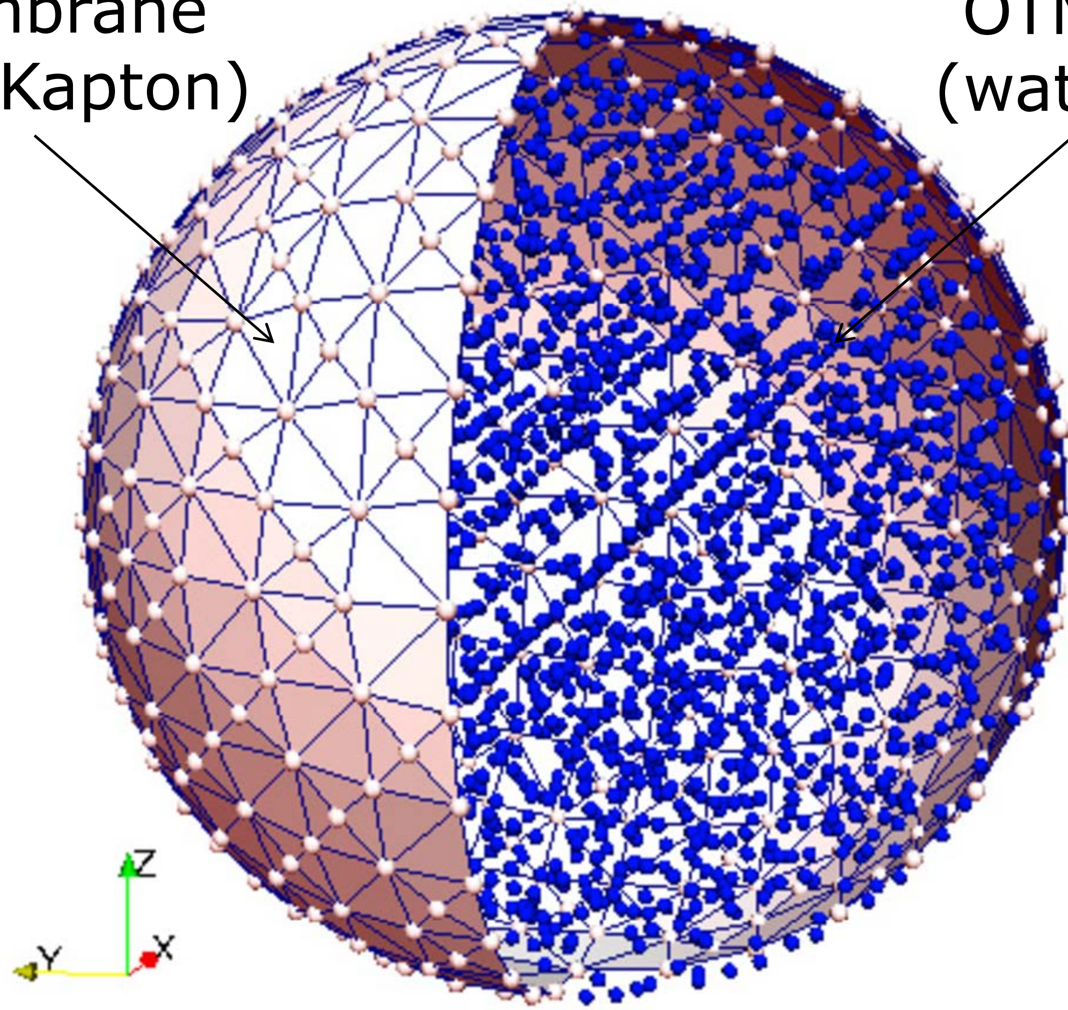
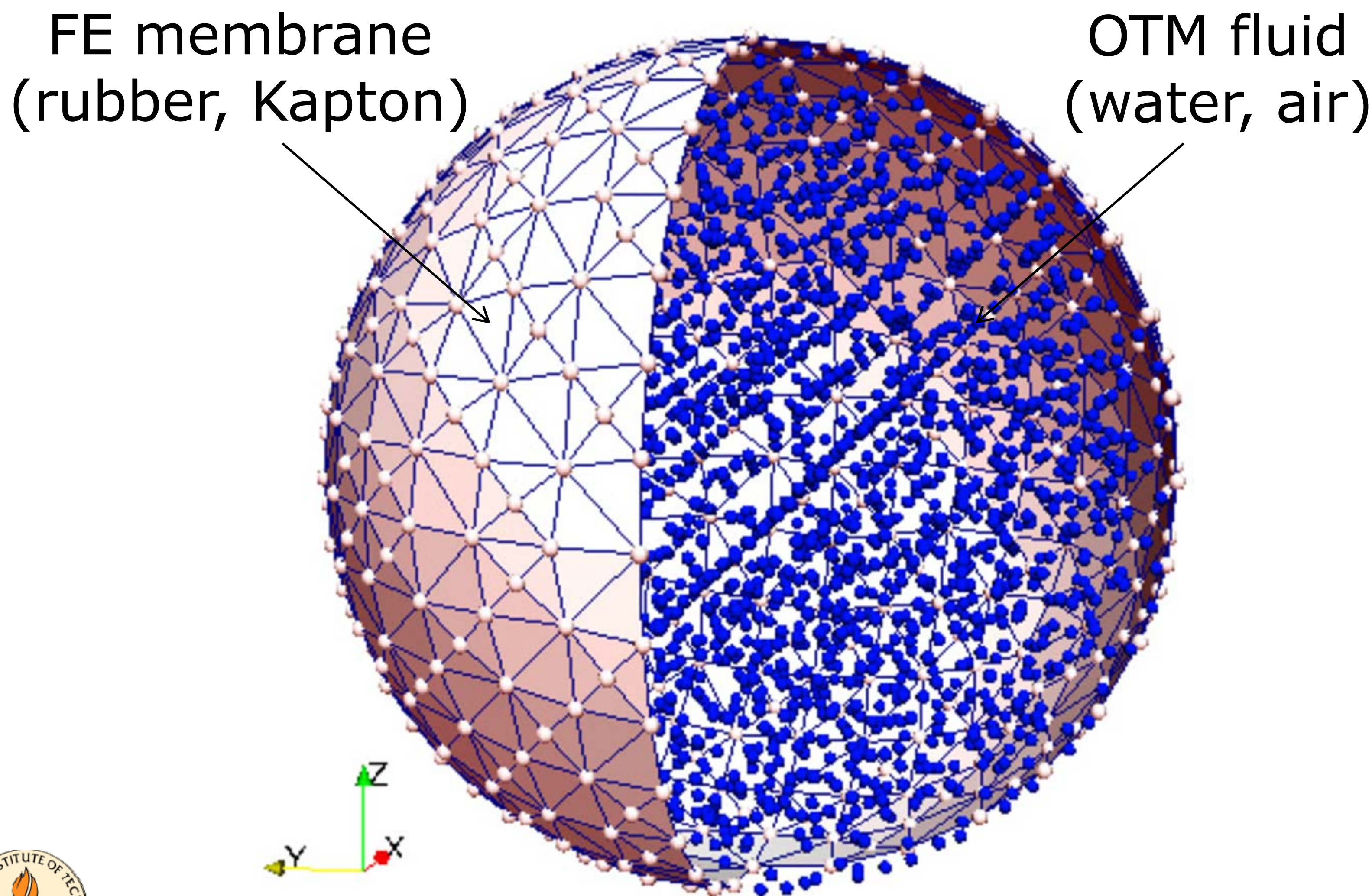
OTM – Bouncing balloons

FE membrane
(rubber, Kapton)

OTM fluid
(water, air)



OTM – Bouncing balloons



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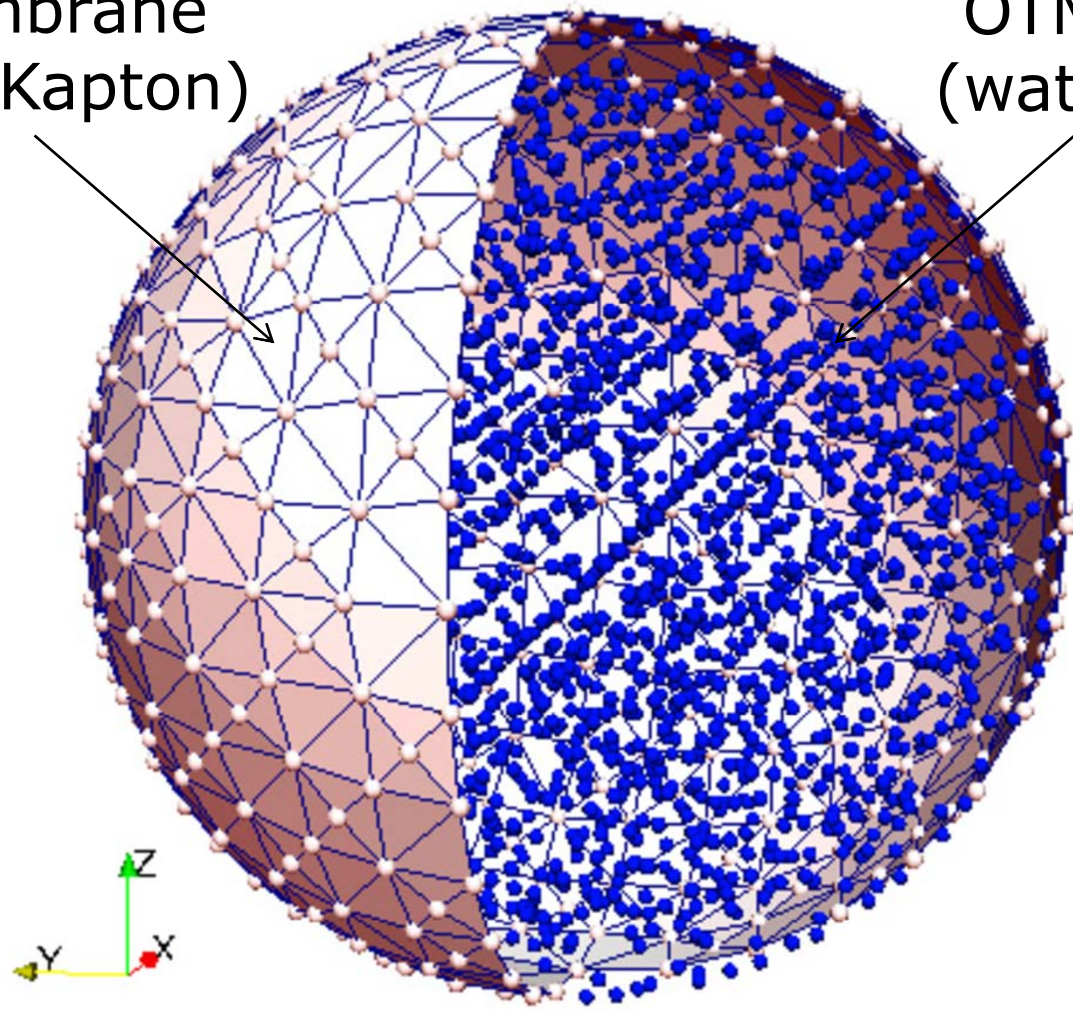

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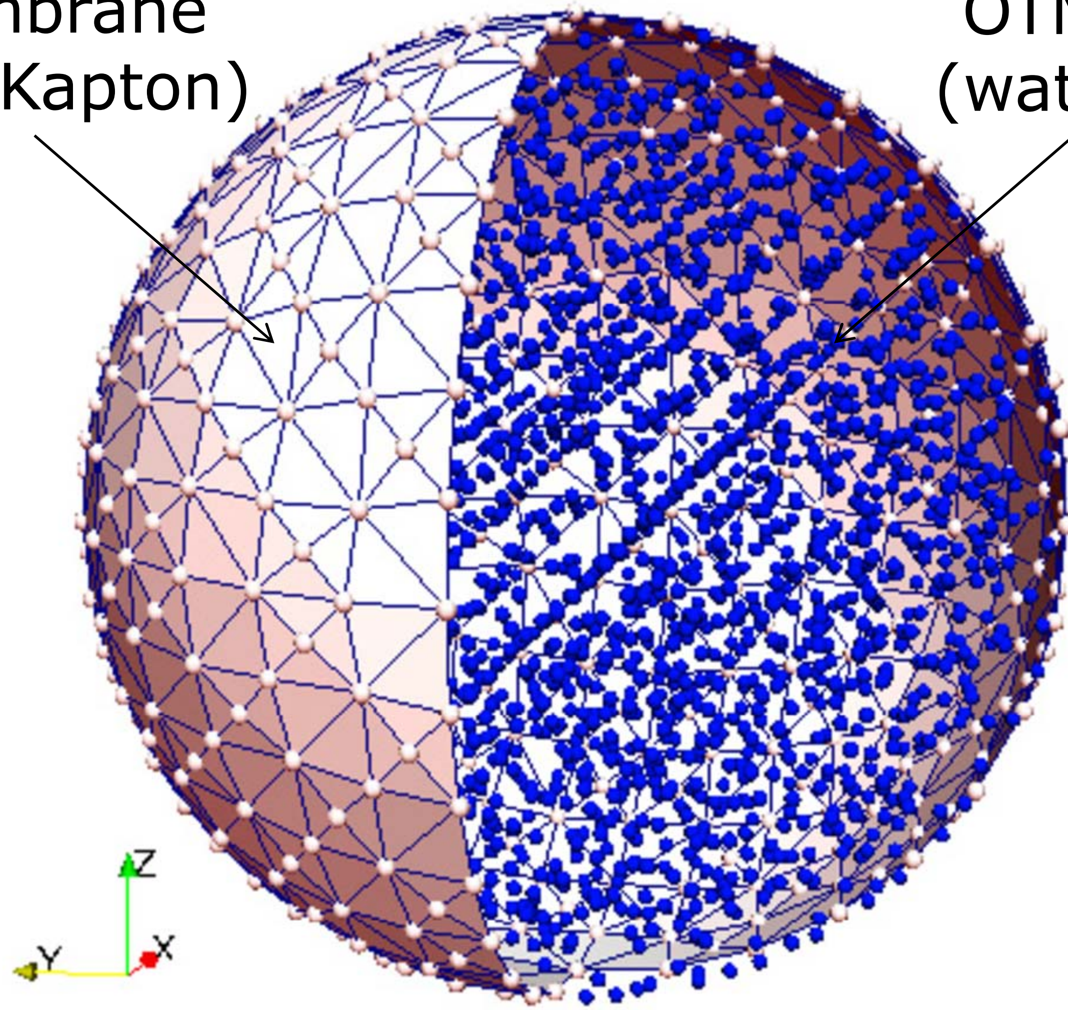
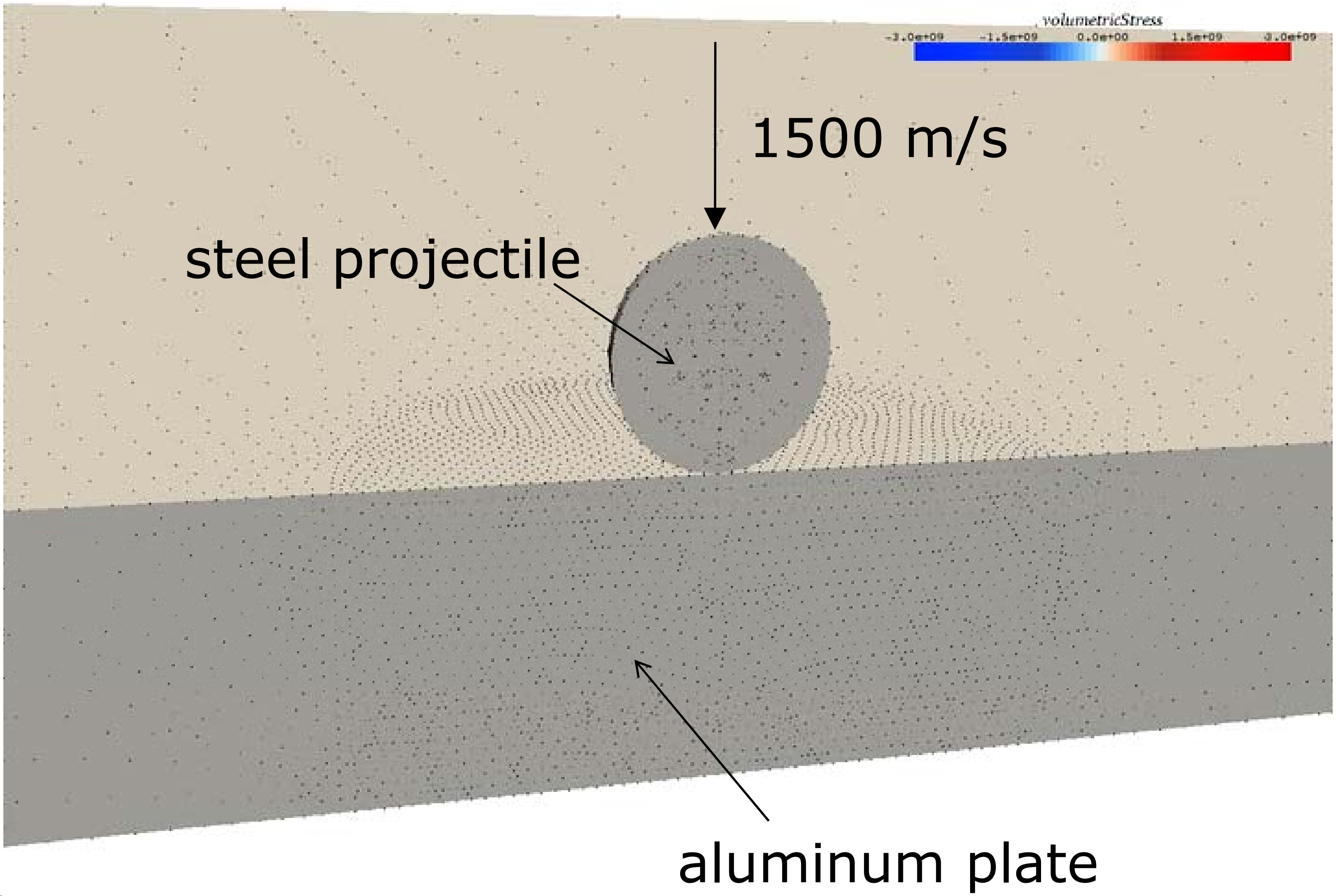
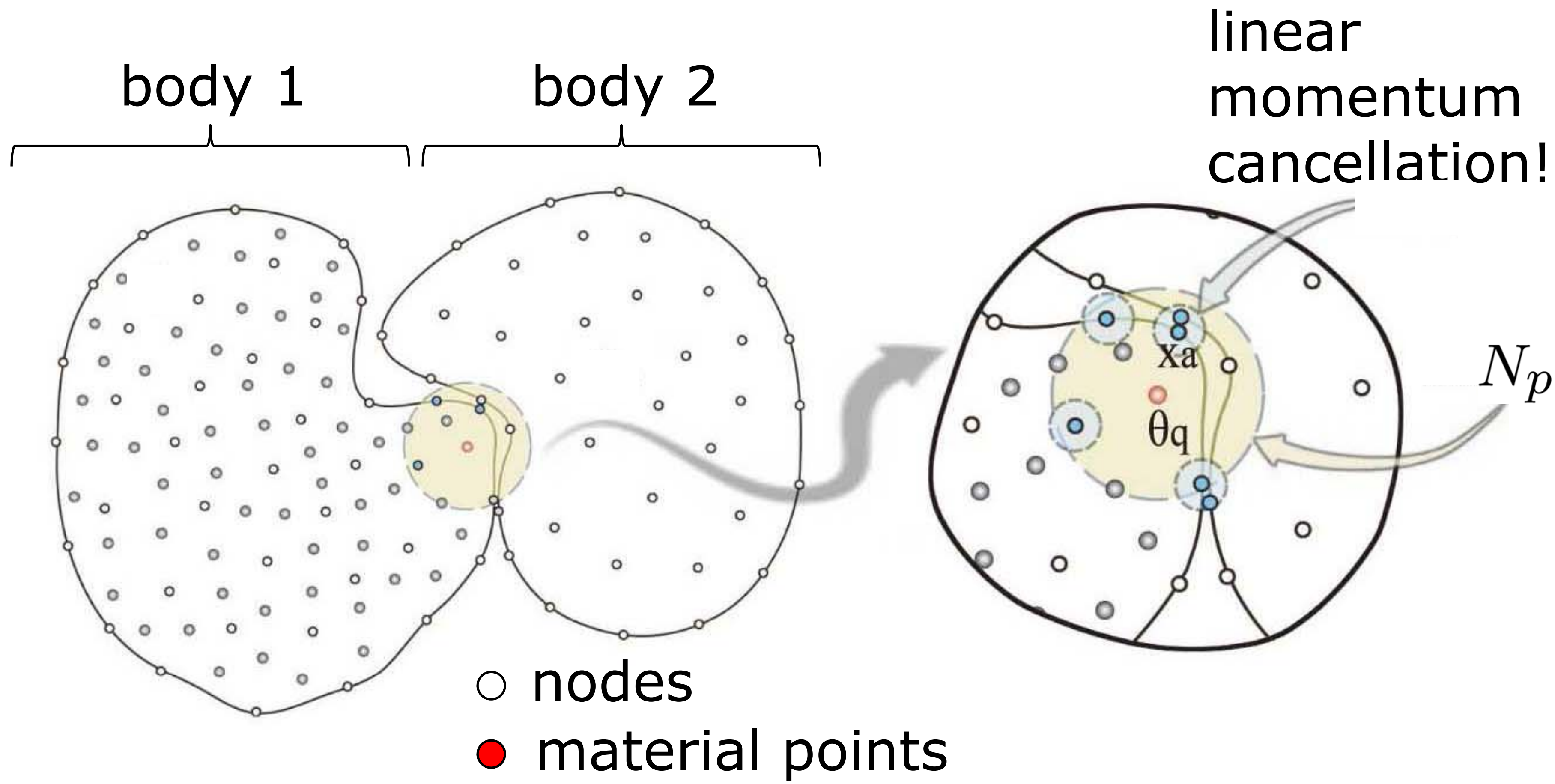


OTM – Terminal ballistics

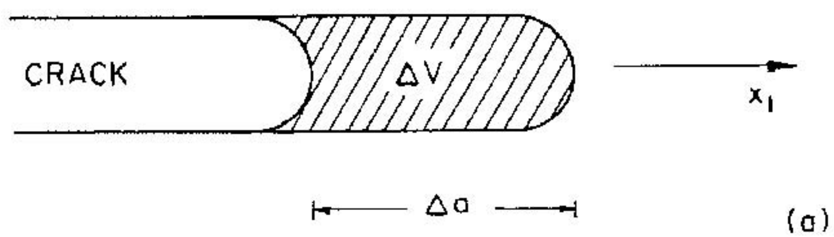


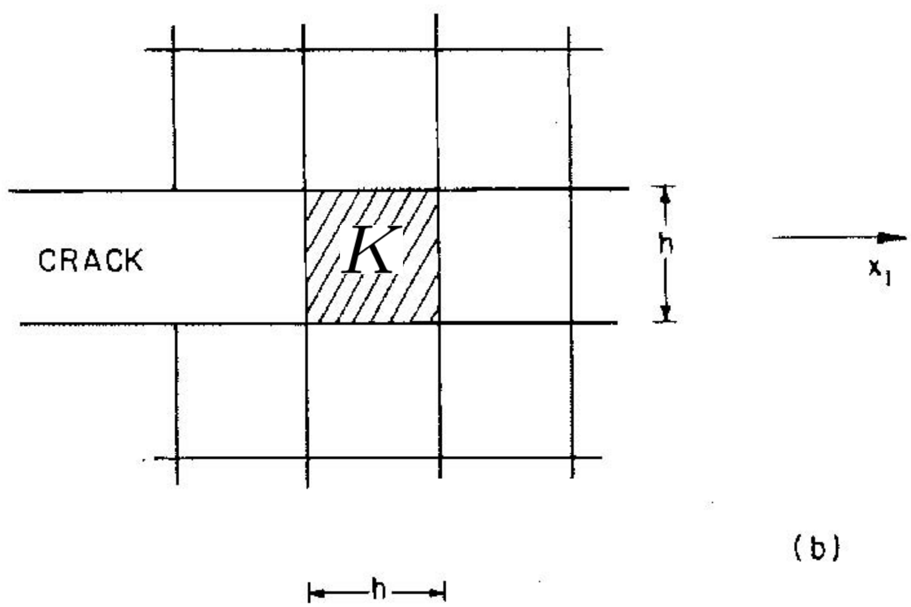
OTM – Seizing contact



Seizing contact (infinite friction)
is obtained for free in OTM!
(as in other material point methods)

Variational Fracture & fragmentation





- Energy-release rate:

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

- Erosion criterion:

$$G \geq G_c$$

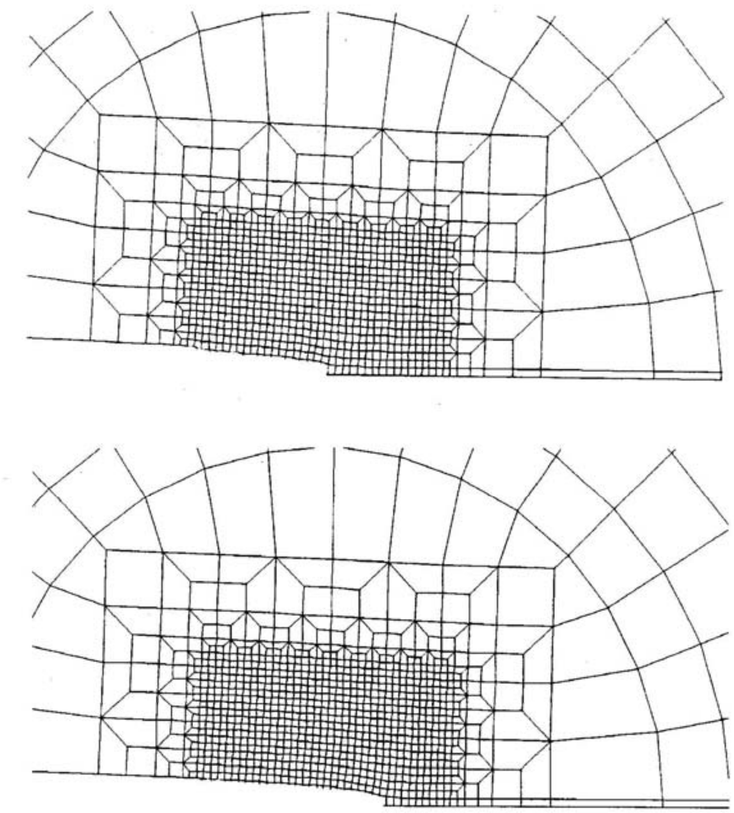
- Implementation:

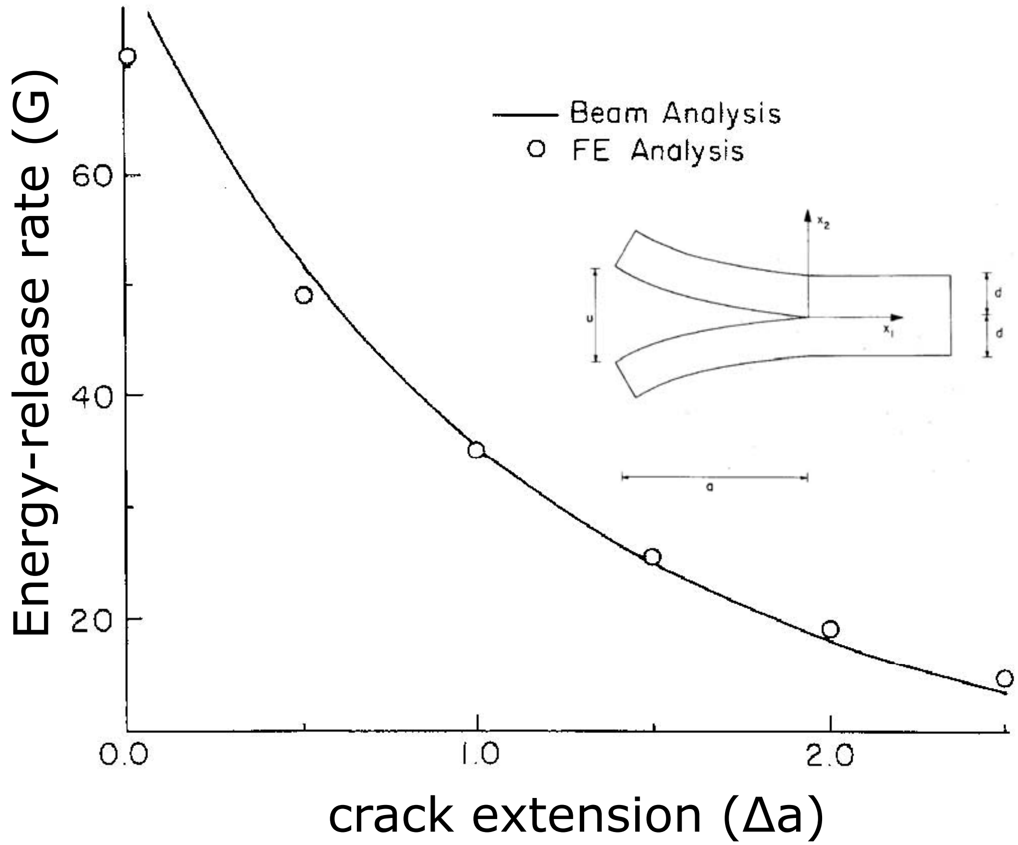
  i) Order elements by G

  ii) Pop top element

M. Ortiz and A.E. Giannakopoulos,
Int. J. Fracture, **44** (1990) 233-258.

Variational Fracture & fragmentation





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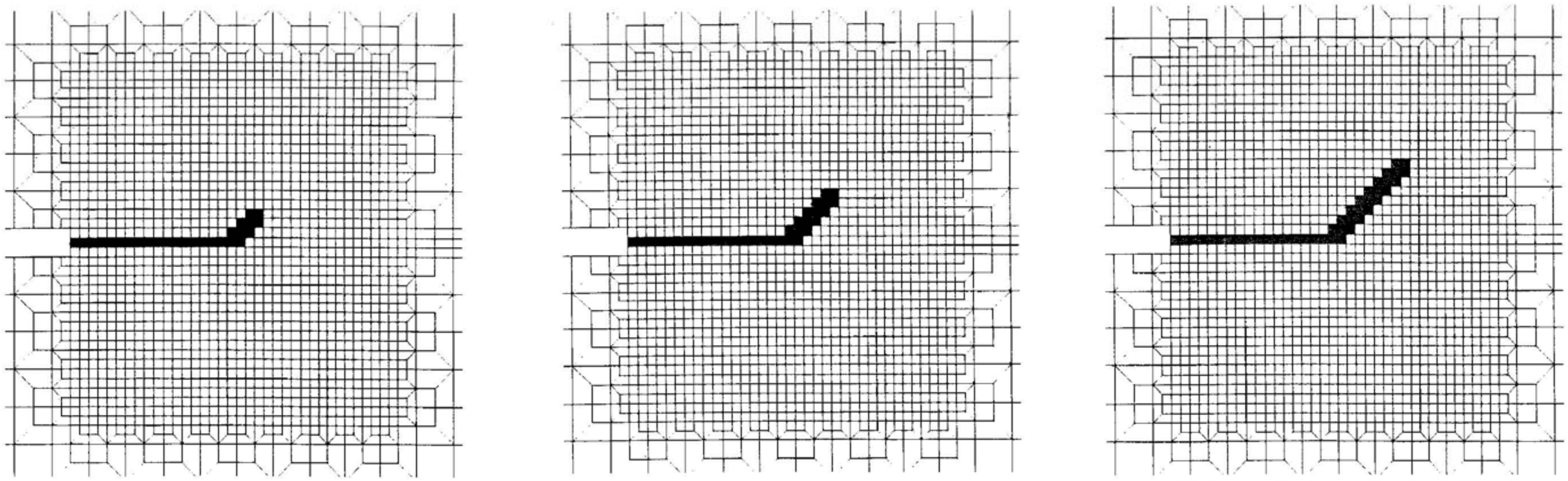
OTM – Fracture & fragmentation

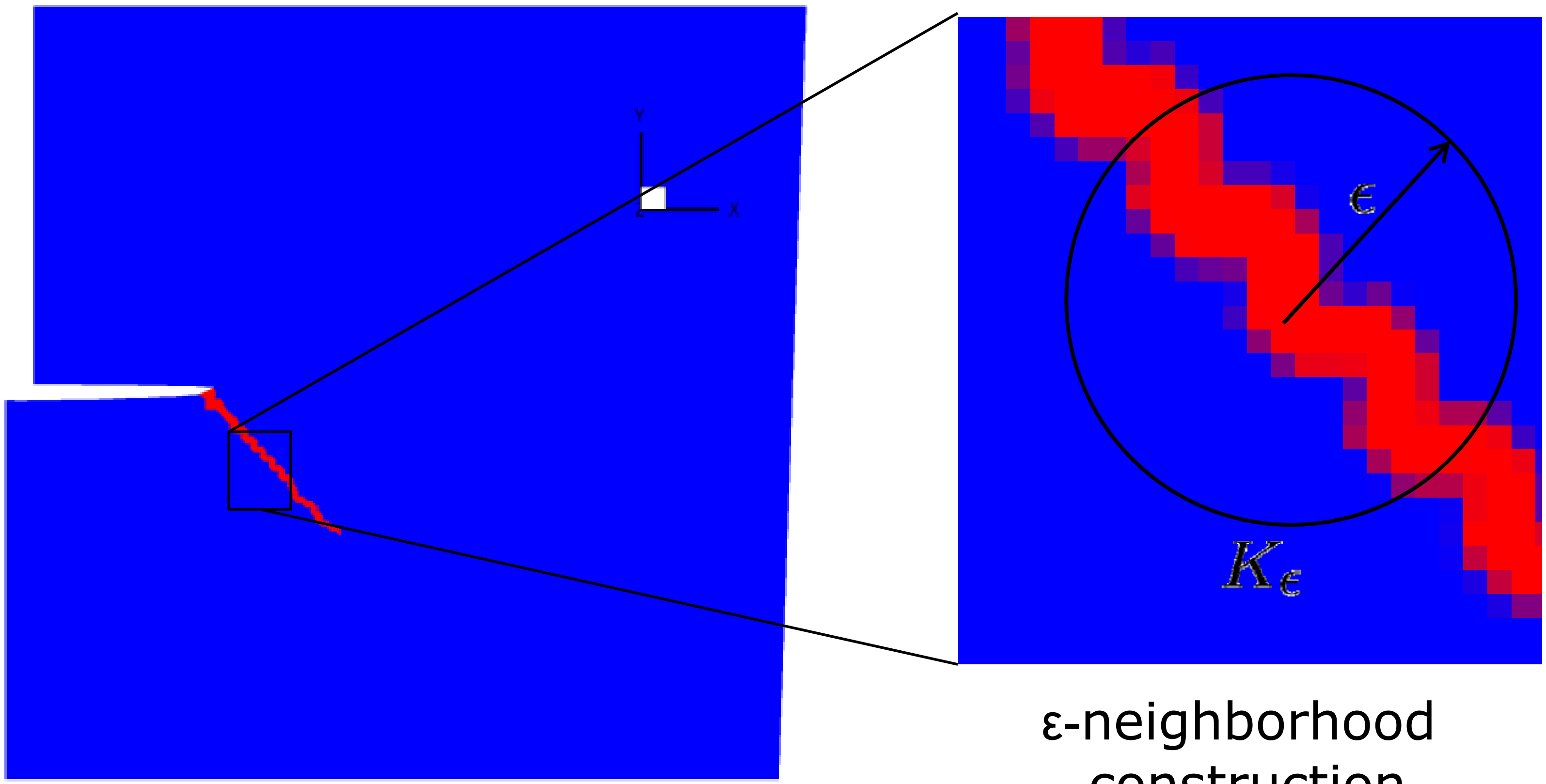


Crack growth in mixed mode

M. Ortiz and A.E. Giannakopoulos,
Int. J. Fracture, **44** (1990) 233-258.

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

OTM – Fracture & fragmentation



ε-neighborhood construction

- Energy-release rate due to element erosion:

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

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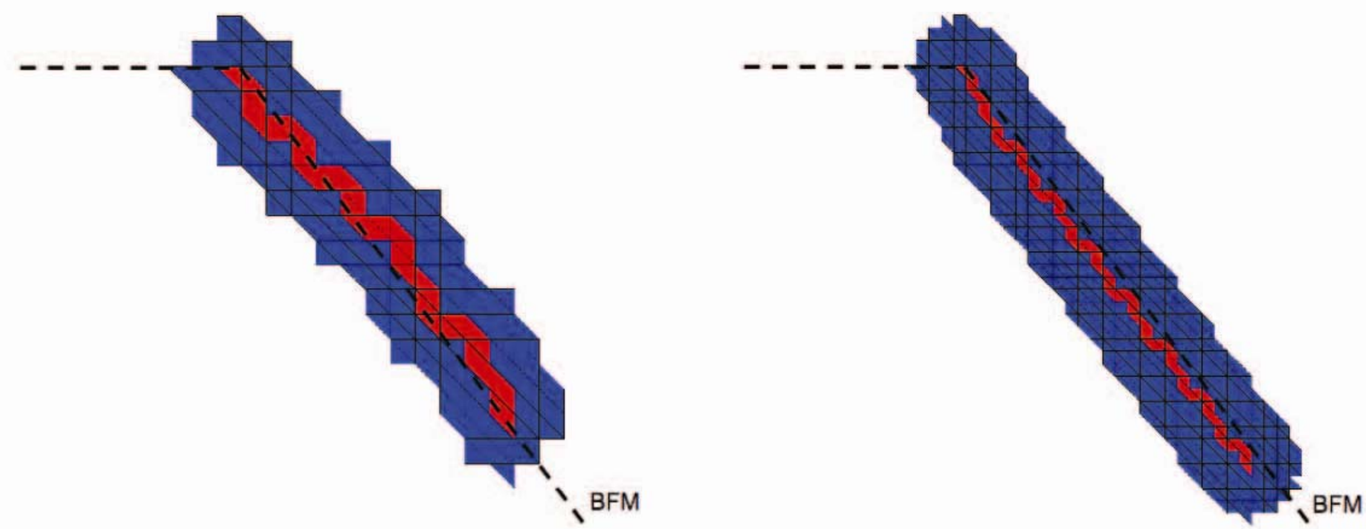
Variational Fracture & fragmentation

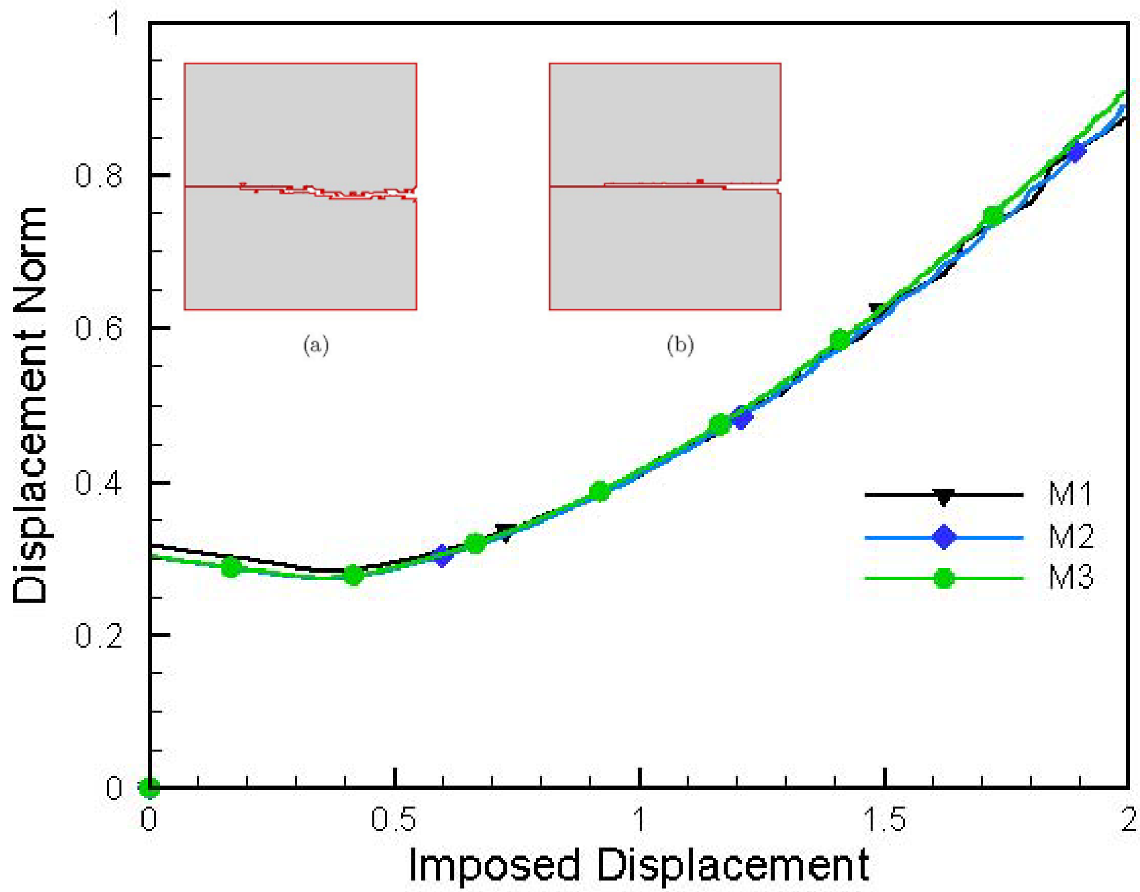
- Proof of convergence of variational element erosion to Griffith fracture:
  - *Schmidt, B., Fraternali, F. and Ortiz, M. "Eigenfracture: An eigendeformation approach to variational fracture," SIAM J. Multiscale Model. Simul.,* **7**(3) (2009) 1237-1366*.*



$\alpha = 15$ deg, $h = \varepsilon/2 = 0.0125$

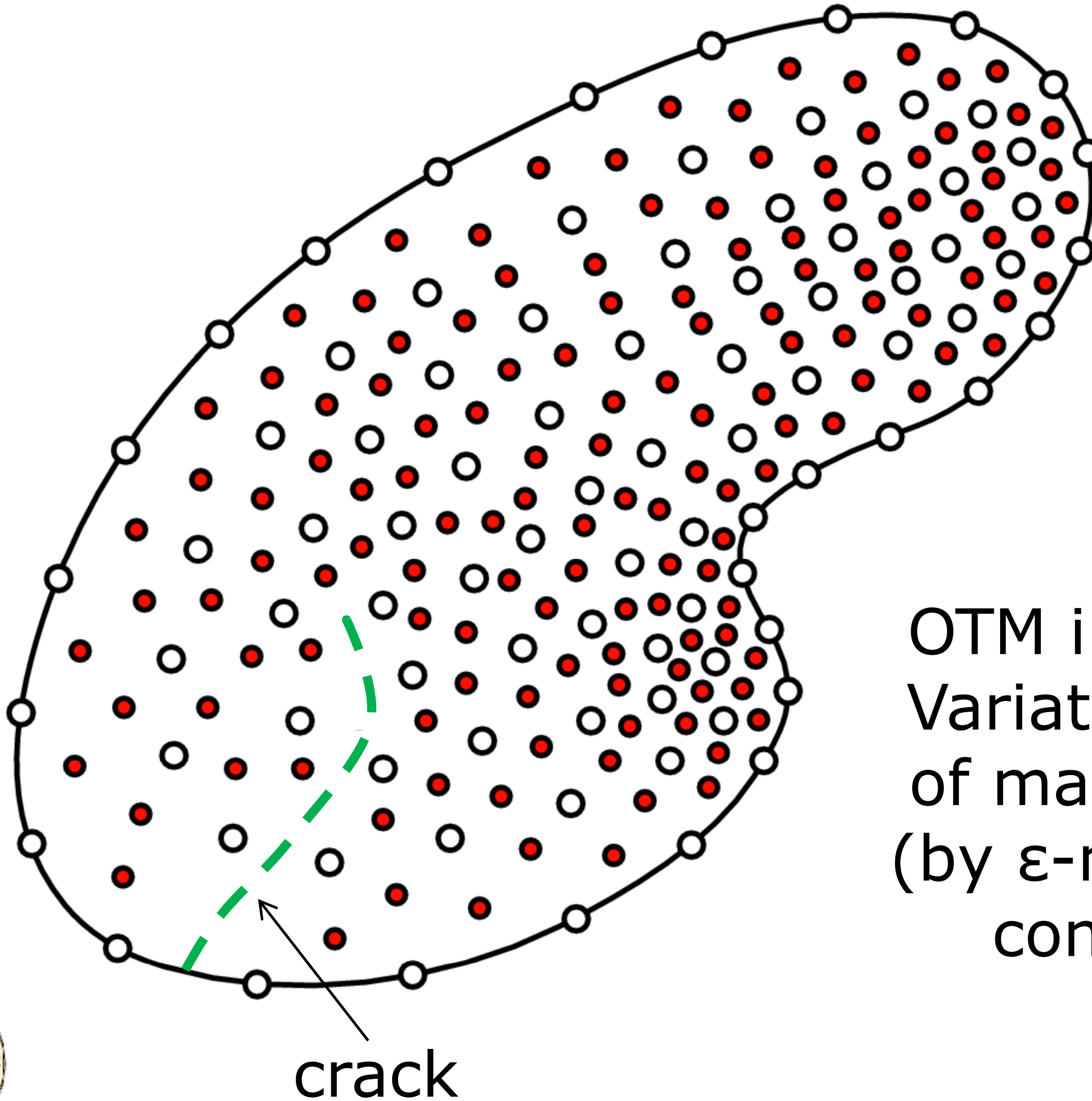
$\alpha = 15$ deg, $h = \varepsilon/4 = 0.00625$

Variational Fracture & fragmentation



Displacement convergence in L1-norm
Mode I propagation through random mesh
(courtesy Anna Pandolfi)

OTM – Fracture & fragmentation



OTM implentation:
Variational erosion
of material points!
(by ε-neighborhood
construction)

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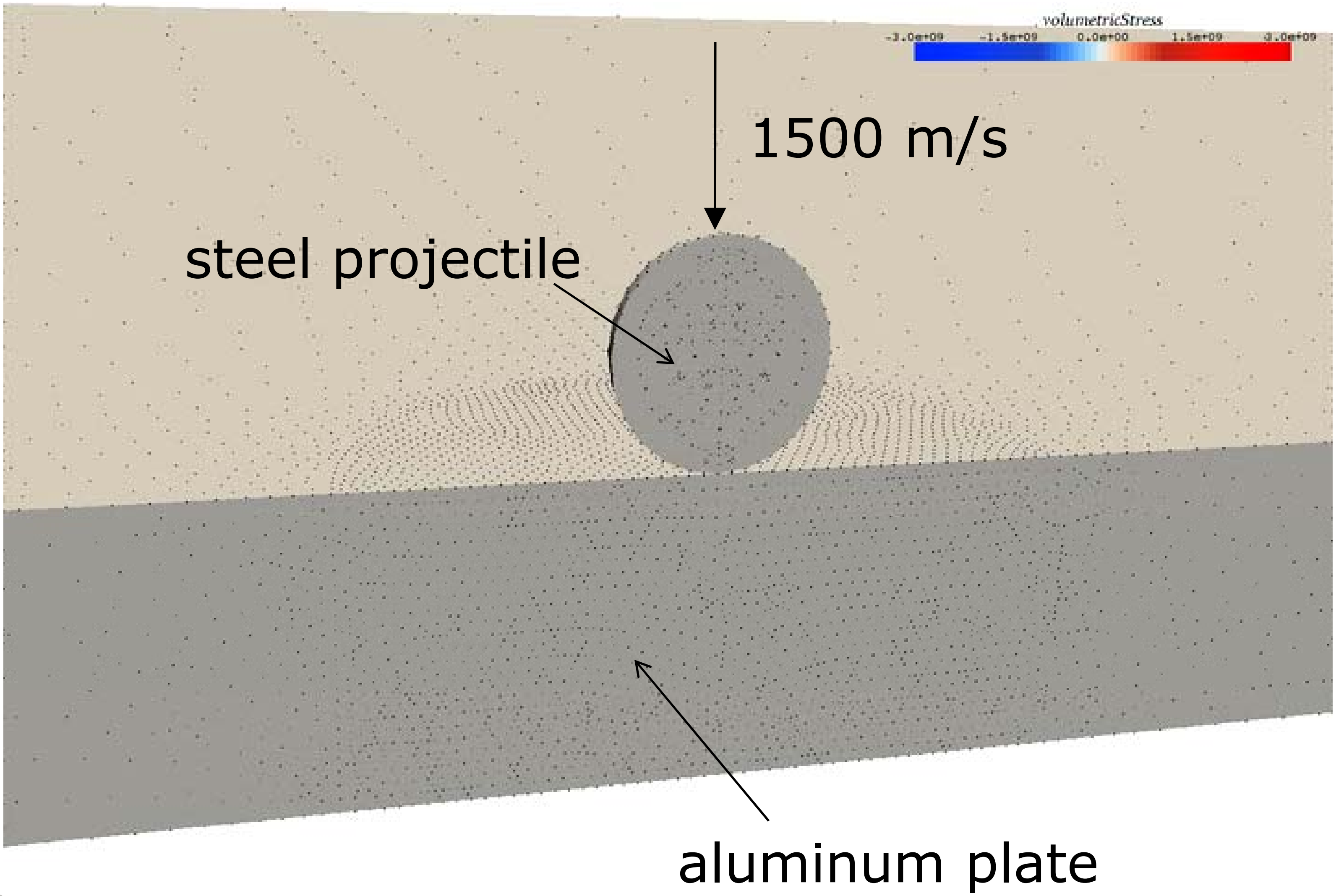
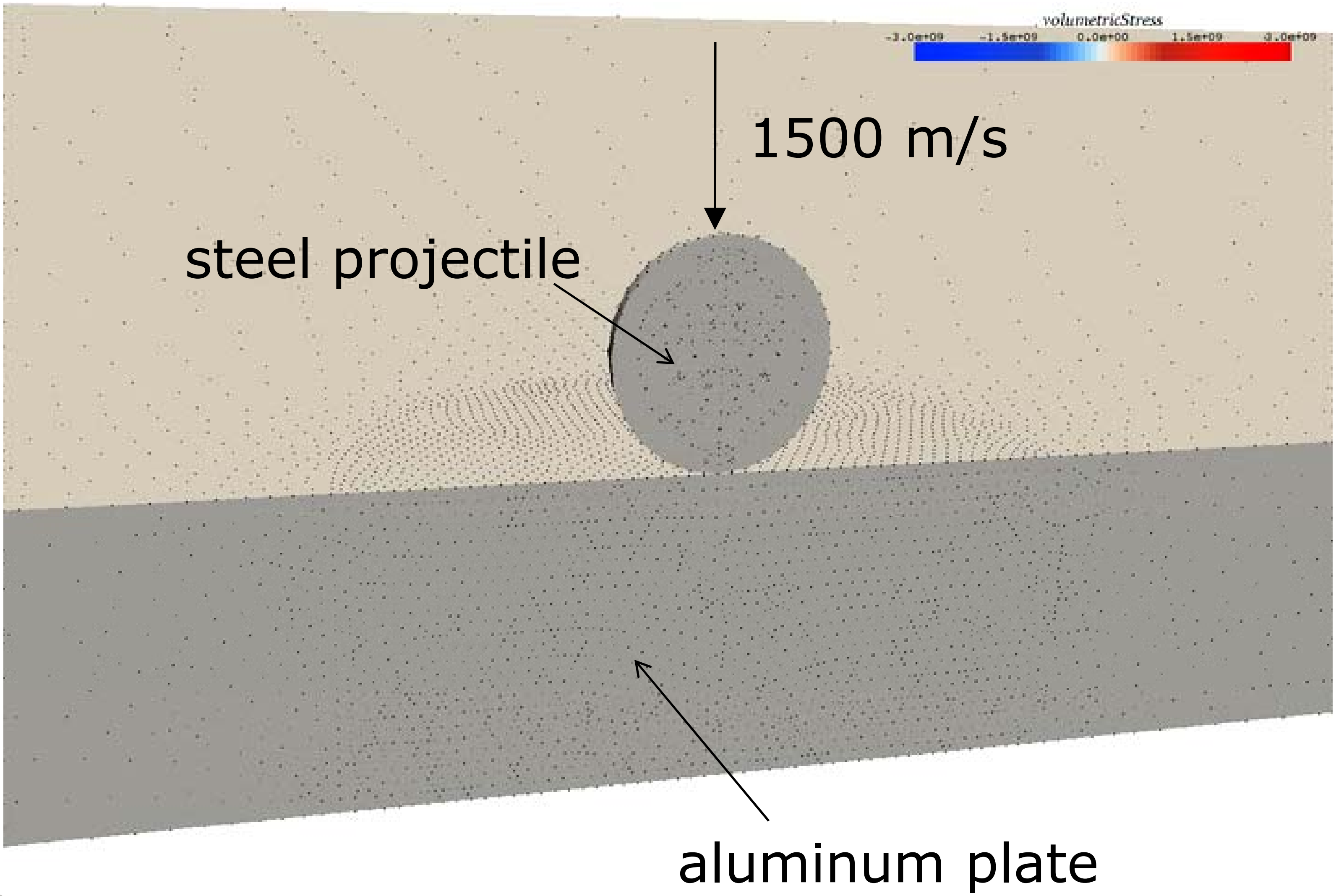
OTM – Back to terminal ballistics



OTM – Back to terminal ballistics



OTM – Summary and outlook

- Optimum-Transportation-Meshfree method:
  - *OT is a useful tool for generating geometrically-exact discrete Lagrangians for flow problems*
  - *Max-ent approach supplies an efficient meshfree, continuously adaptive, remapping-free, FE-compatible, interpolation scheme*
  - *Material-point sampling effectively addresses the issues of numerical quadrature, history variables*
- Extensions include:
  - *Contact (seizing contact for free!)*
  - *Fracture and fragmentation (provably convergent)*
- Outlook: Parallel implementation, UQ…

OTM – Summary and outlook

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