Optimal-Transportation Meshfree Approximation Schemes

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In collaboration with:

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Mini-Workshop on Variational Methods for Evolution

Mathematisches Forschungsinstitut Oberwolfach

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Optimal transportation and numerical simulation

- Many applications involve complex fluid and solid (plastic flows)
- Example: Hypervelocity impact:
  - *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)

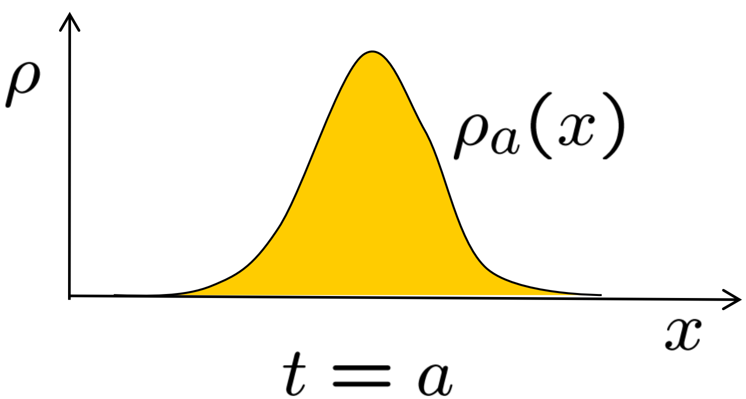
Leonid V. Kantorovich
Saint Petersbourg (1912)
Moscow (1986)
Nobel Prize in Economics (1975)

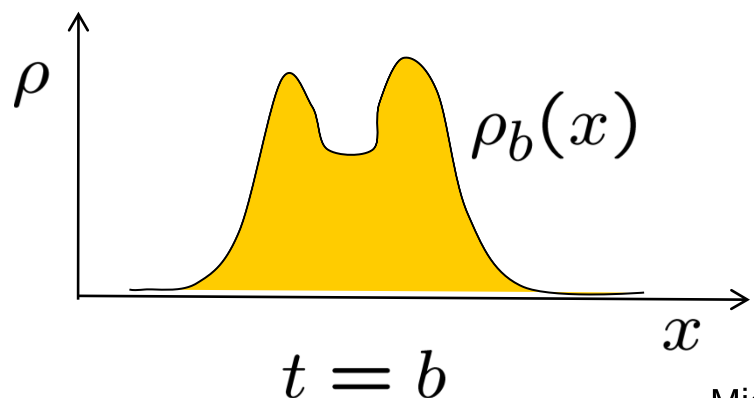
Mass flows – Optimal transportation

- 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: $\left\{\begin{aligned} \rho(x,a) &= \rho_a(x) \\ \rho(x,b) &= \rho_b(x) \end{aligned}\right.$





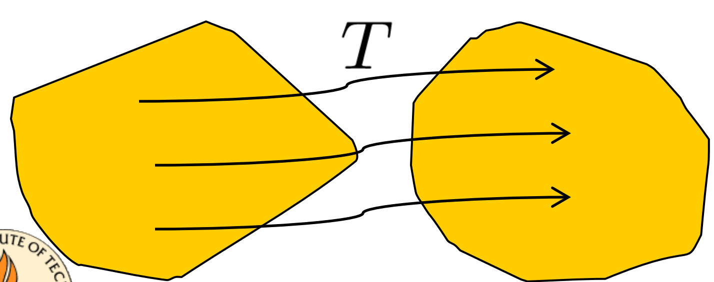
Mass flows – Optimal transportation

- *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:

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



$\rho_a(x)$ $\rho_b(x)$

- McCann's interpolation:

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

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

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: $\delta A_d = 0 \Rightarrow$

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

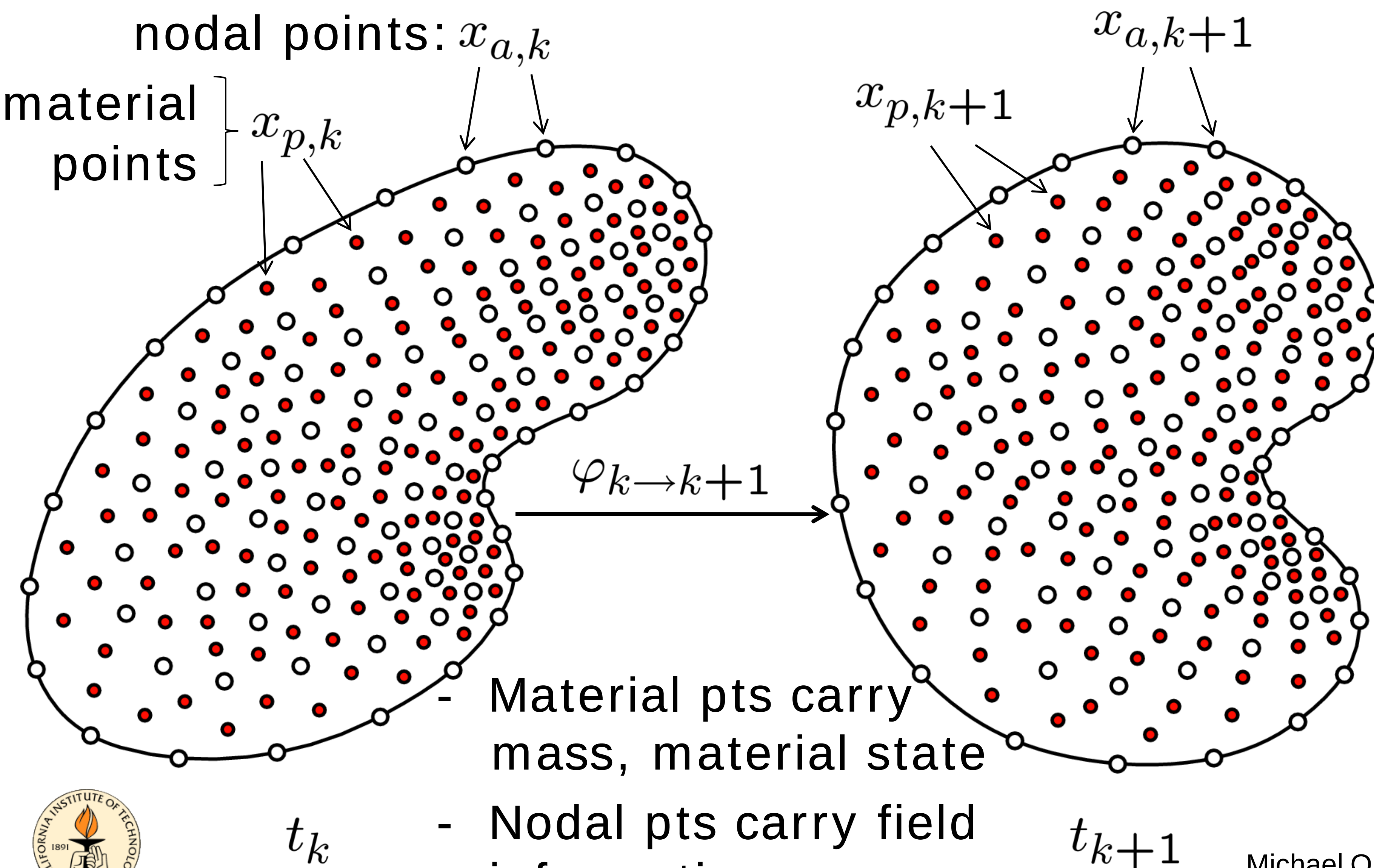
$$\rho_{k+1} \circ \varphi_{k\to k+1} = \rho_k / \det\left(\nabla \varphi_{k\to k+1}\right)$$

geometrically exact mass conservation!

Optimal-Transportation Meshfree (OTM)

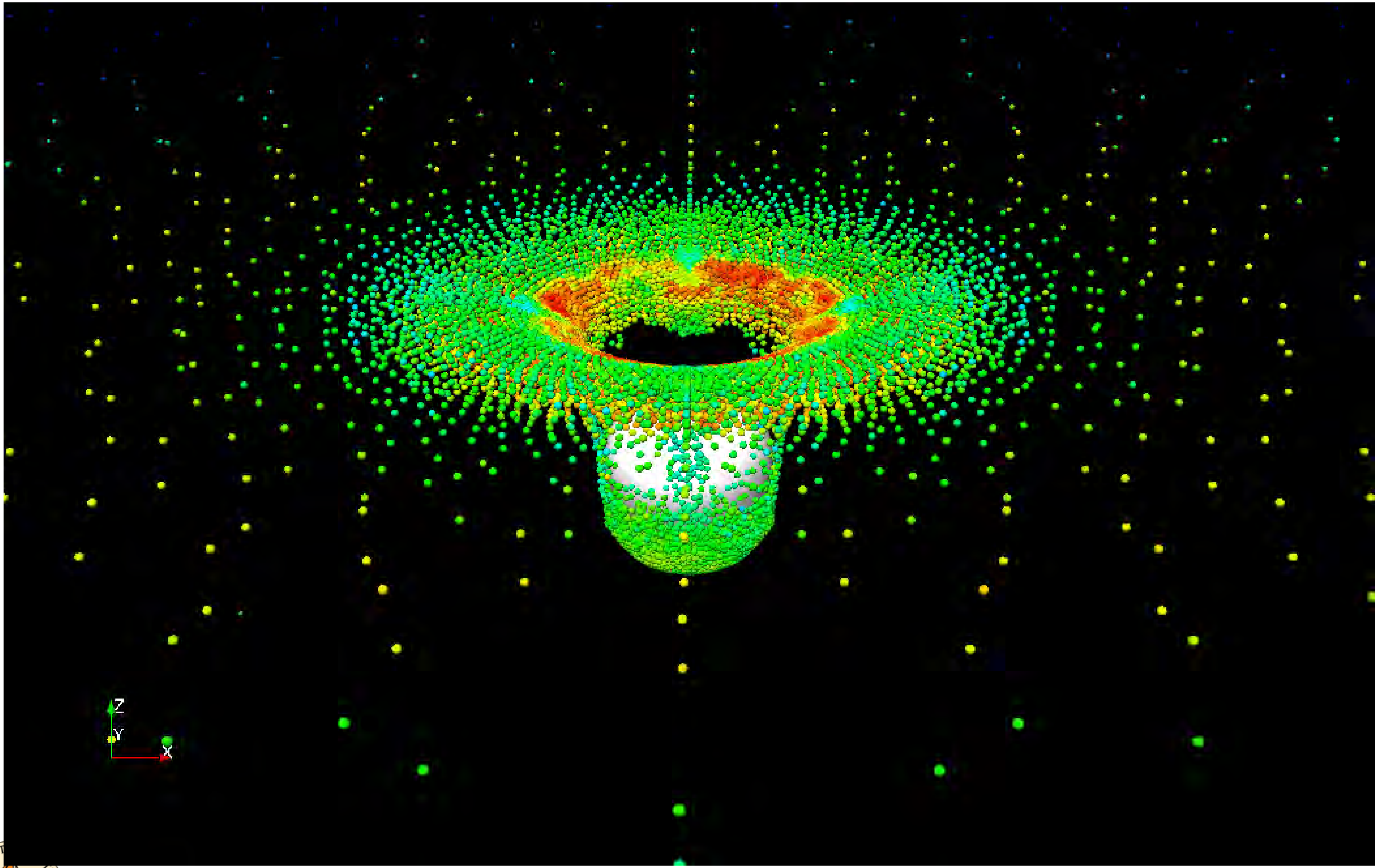
- Optimal transportation theory is a useful tool for generating geometrically-exact discrete Lagrangians for flow problems
- Inertial part of discrete Lagrangian measures distance between consecutive mass densities (in sense of Wasserstein)
- Discrete Hamilton principle of stationary action: Variational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

OTM – Spatial discretization



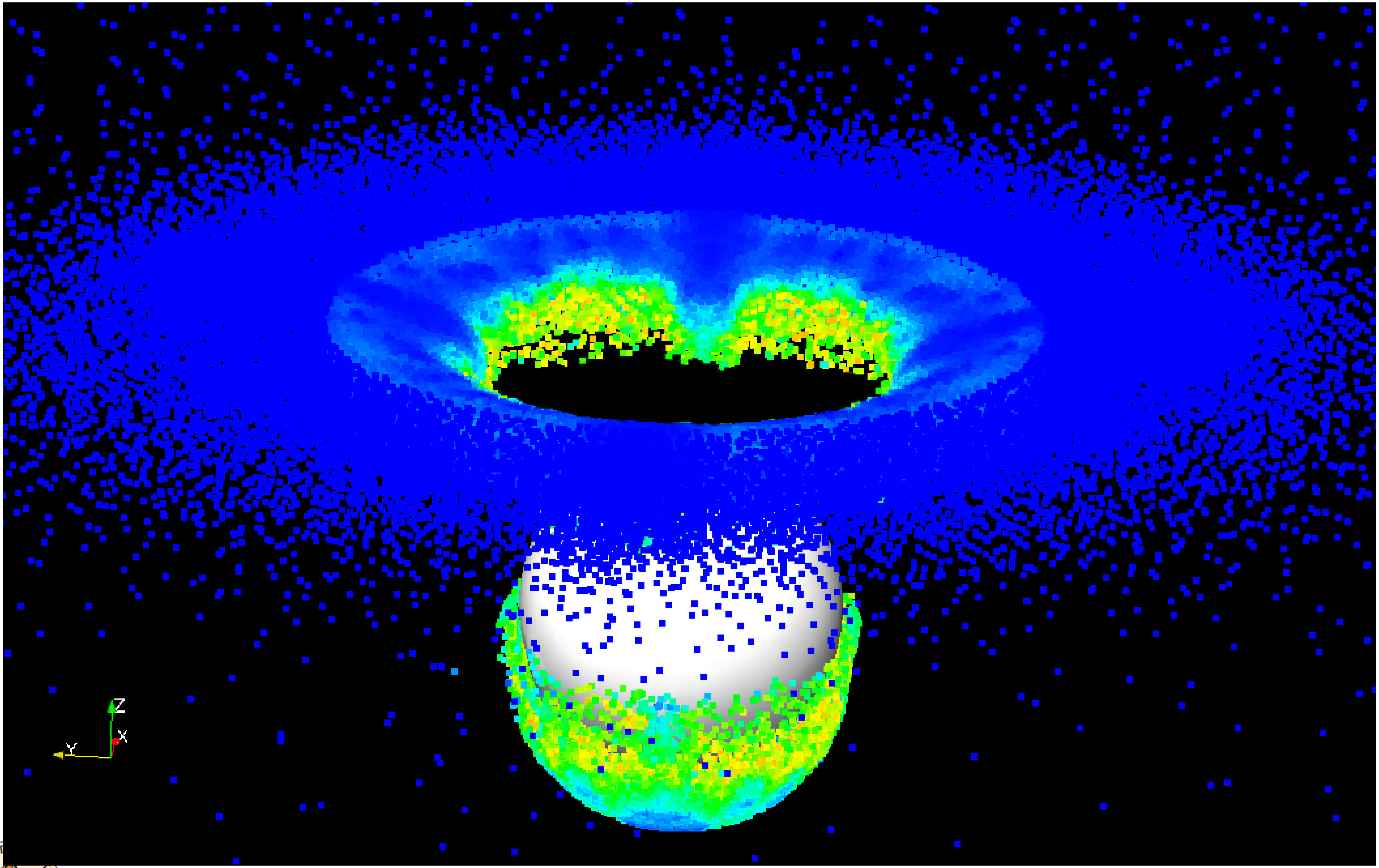
- Material pts carry mass, material state
- Nodal pts carry field information

OTM – Spatial discretization



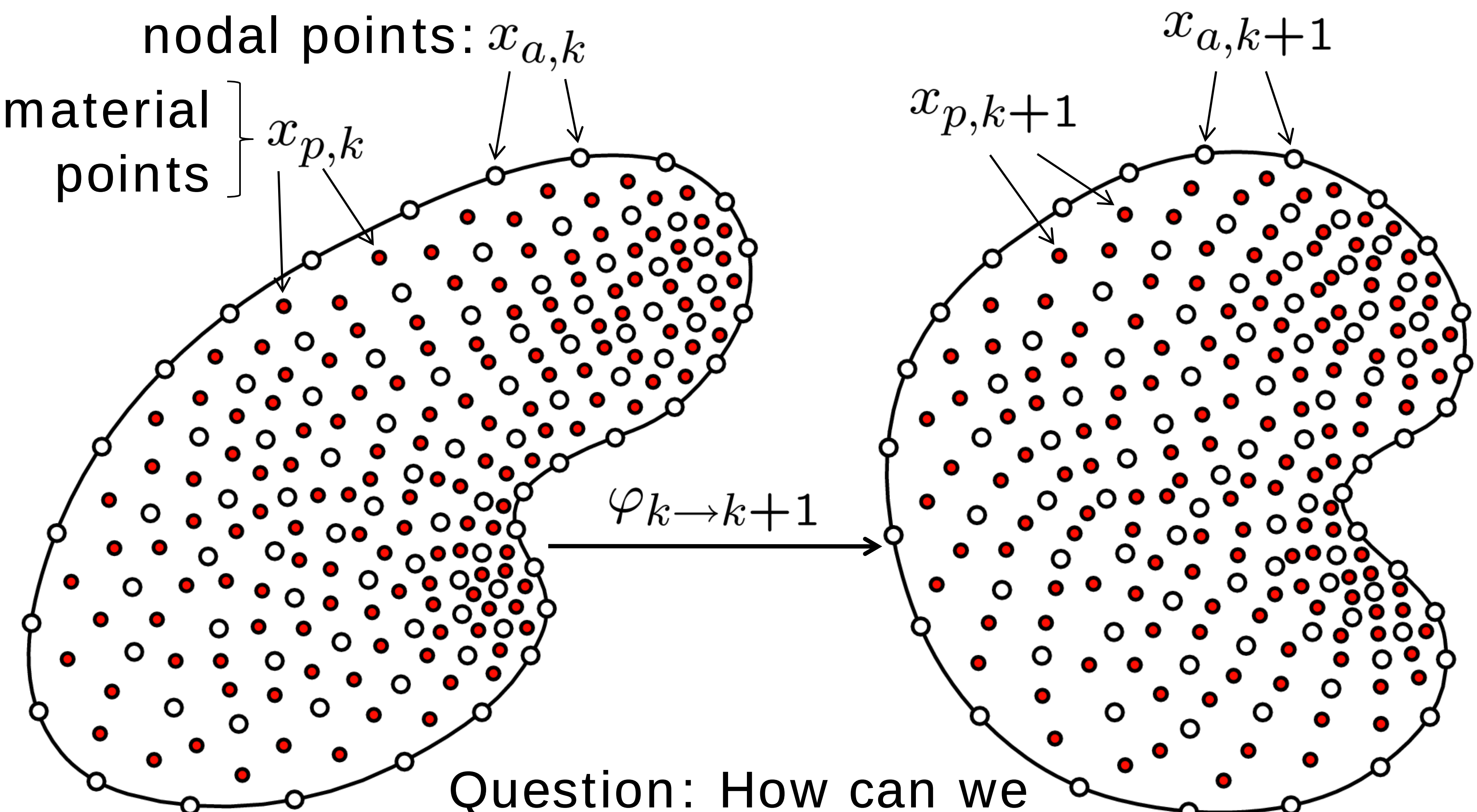
Steel projectile/aluminum plate: Nodal set

OTM – Spatial discretization



Steel projectile/aluminum plate: Material point set

OTM – Spatial discretization



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

OTM — Max-ent interpolation

- Problem: Reconstruct incremental deformation mapping $\varphi_{k\to k+1}(x)$ from nodal coordinates:

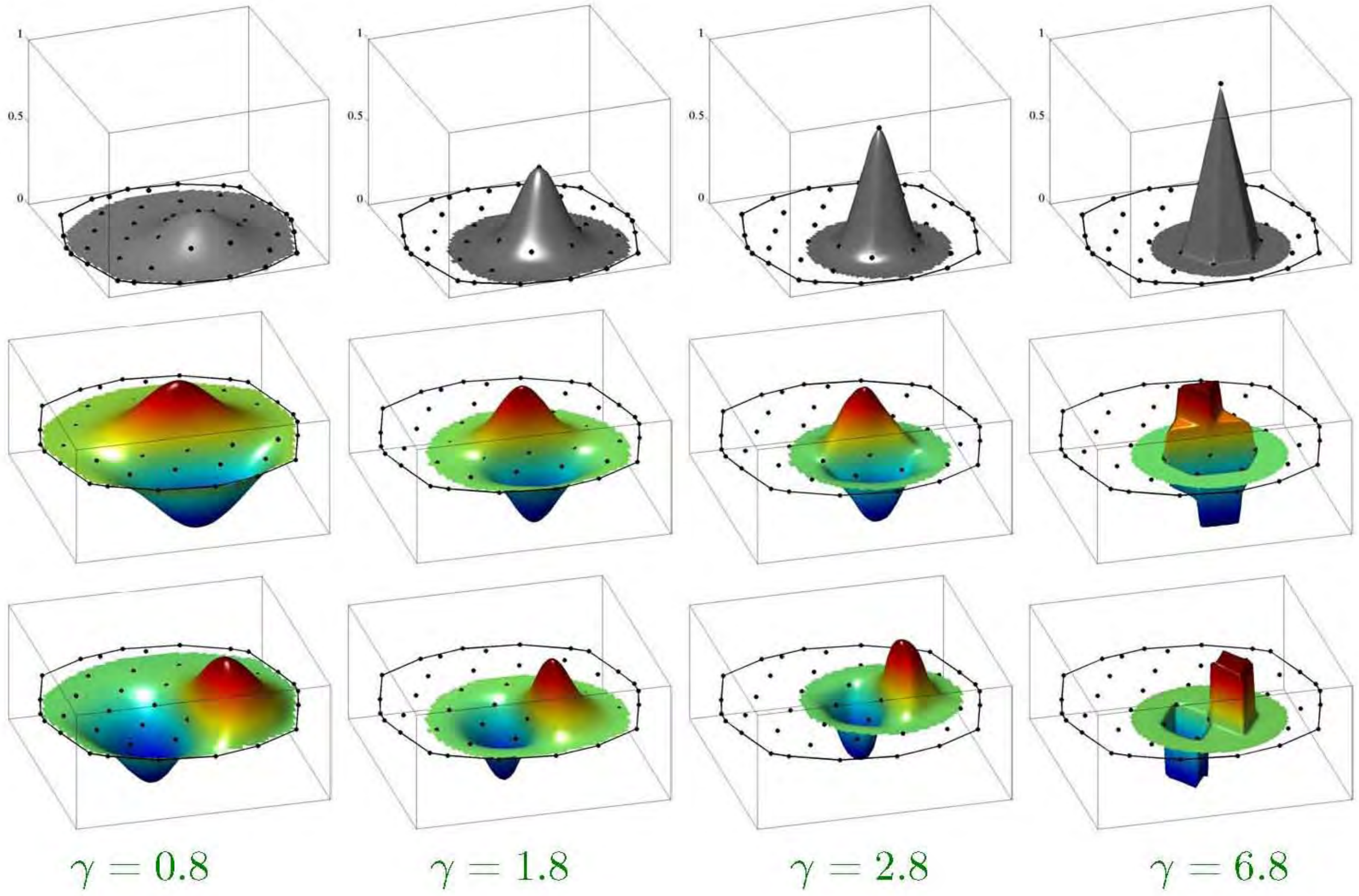
$$\varphi_{k\to k+1}(x) = \sum_{a=1}^{N} x_a(t_{k+1}) w_a(x, t_{k+1})$$

- Optimal interpolation (Arroyo & MO, 2006):

$$\text{Minimize:} \quad \underbrace{\sum_{a=1}^{N} |x - x_a|^2 w_a(x)}_{\text{nodal weight } \textbf{costs}} + \beta \underbrace{\sum_{a=1}^{N} w_a(x) \log w_a(x)}_{\text{information } \textbf{entropy}}$$

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

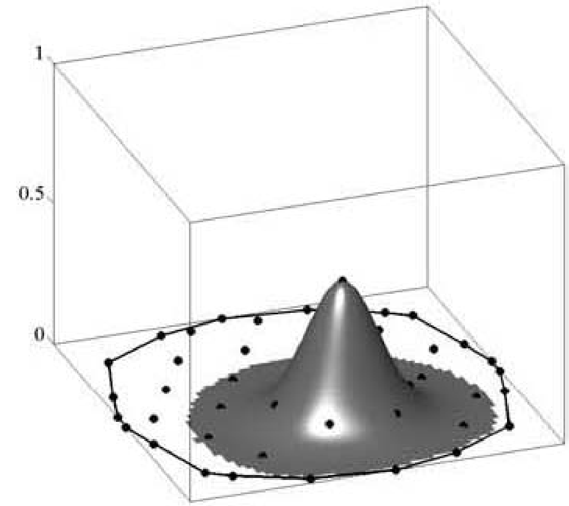
OTM – Max-ent interpolation

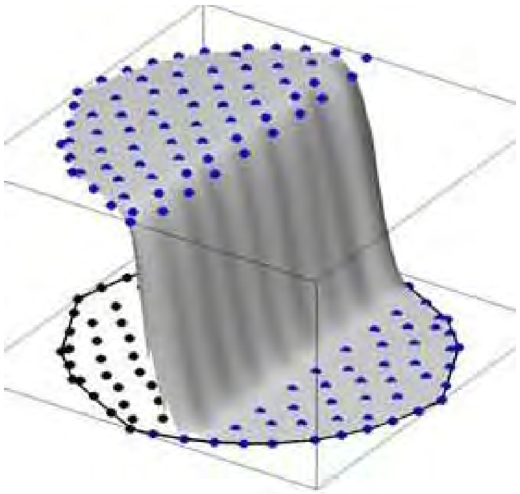


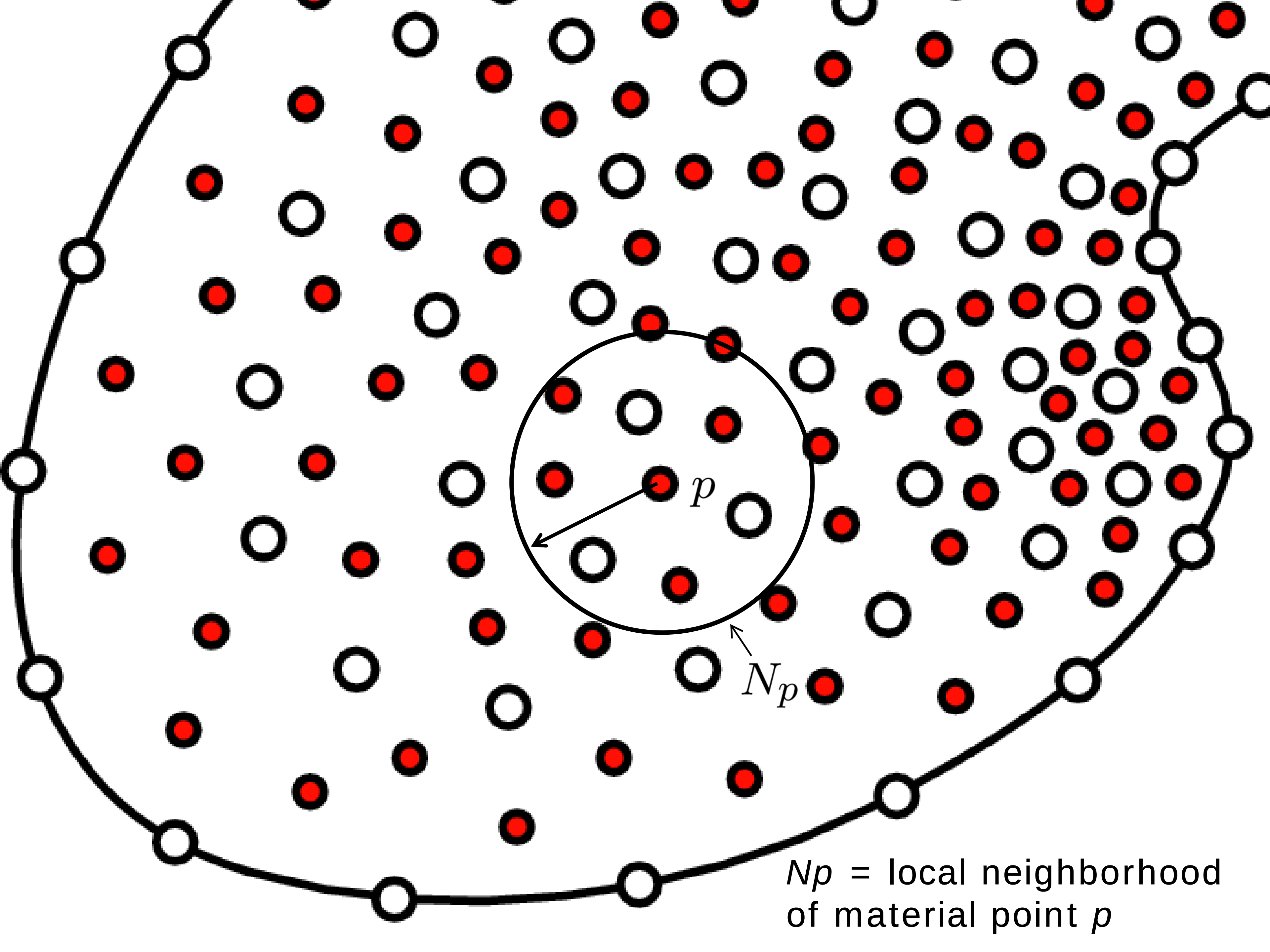
Max-ent shape functions, $\gamma = \beta h^2$

OTM — Max-ent interpolation

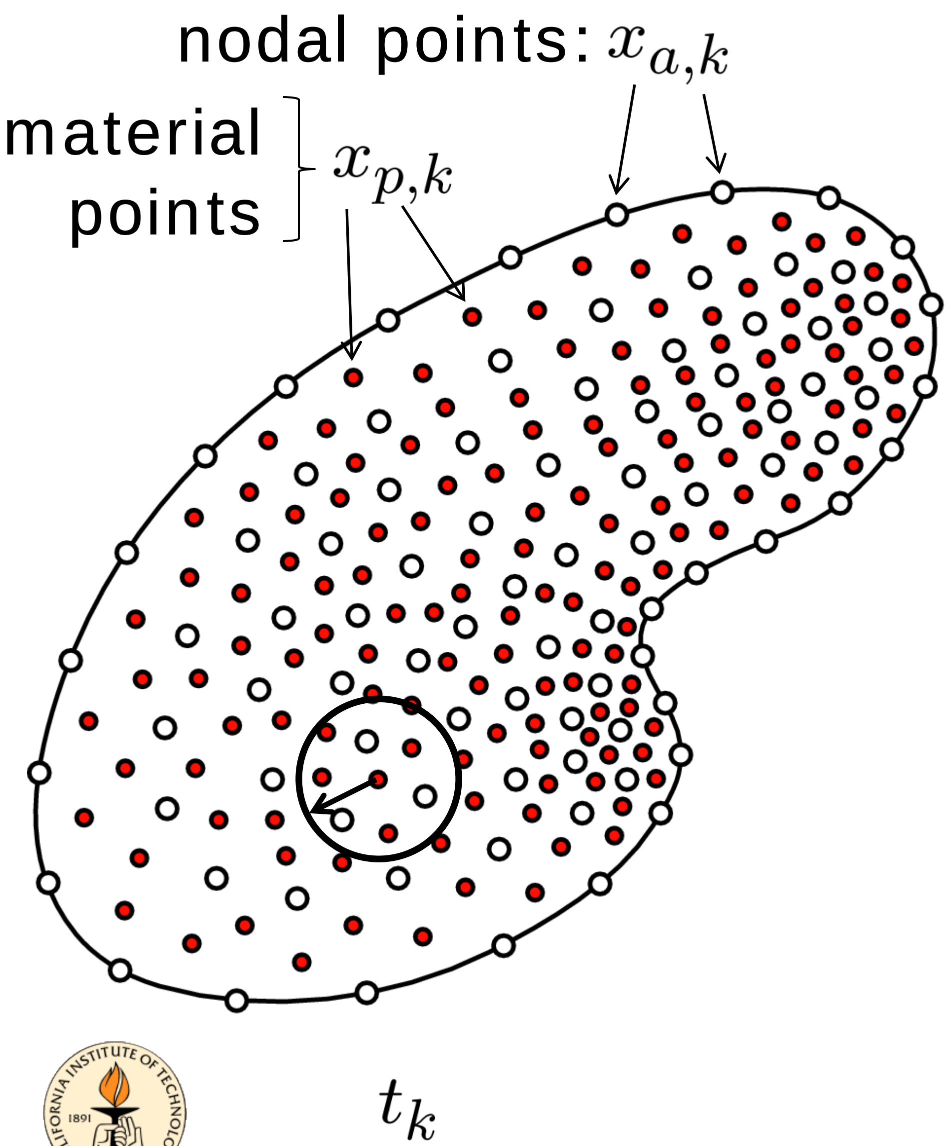
- Optimal weight functions can be computed exactly in close form
- Max-ent interpolation is smooth, meshfree, monotonic, rapid decay, short range
- Simplicial Delaunay interpolation is recovered in the limit of $\beta \to \infty$
- Kronecker-delta property at the boundary (interpolation on the boundary depends on boundary data only)
- Density in $W^{1,p}$ (A. Bompadre, MO, B. Schmidt)






p
N_p
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 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!

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

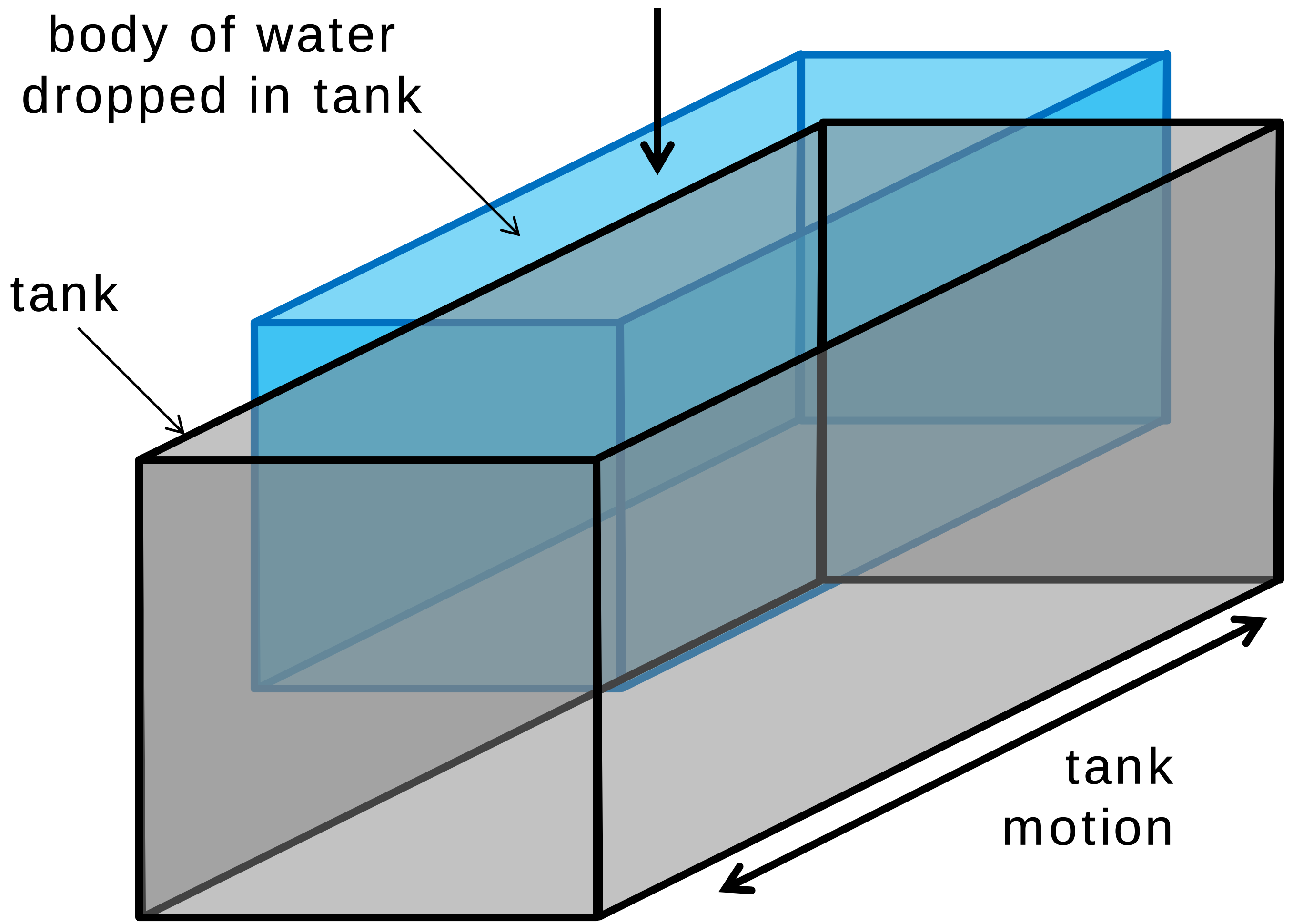
volume: $V_{p,k+1} = \det \nabla\varphi_{k\to k+1}(x_{p,k}) V_{p,k}$

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

(iii) Constitutive update at material points

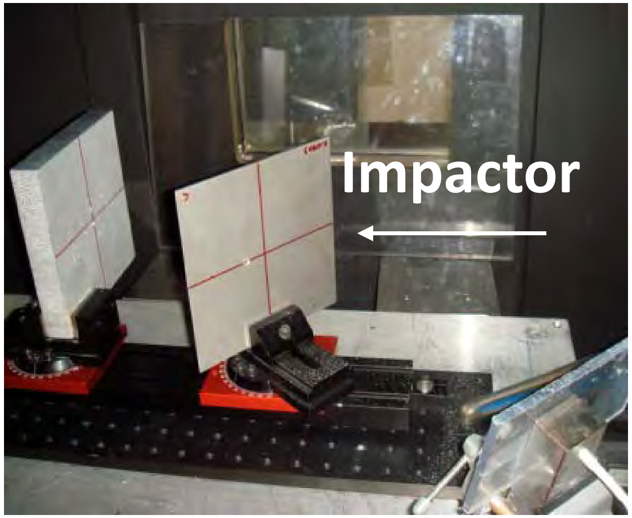
(iv) Reconnect nodal and material points (range searches), recompute max-ext shape functions

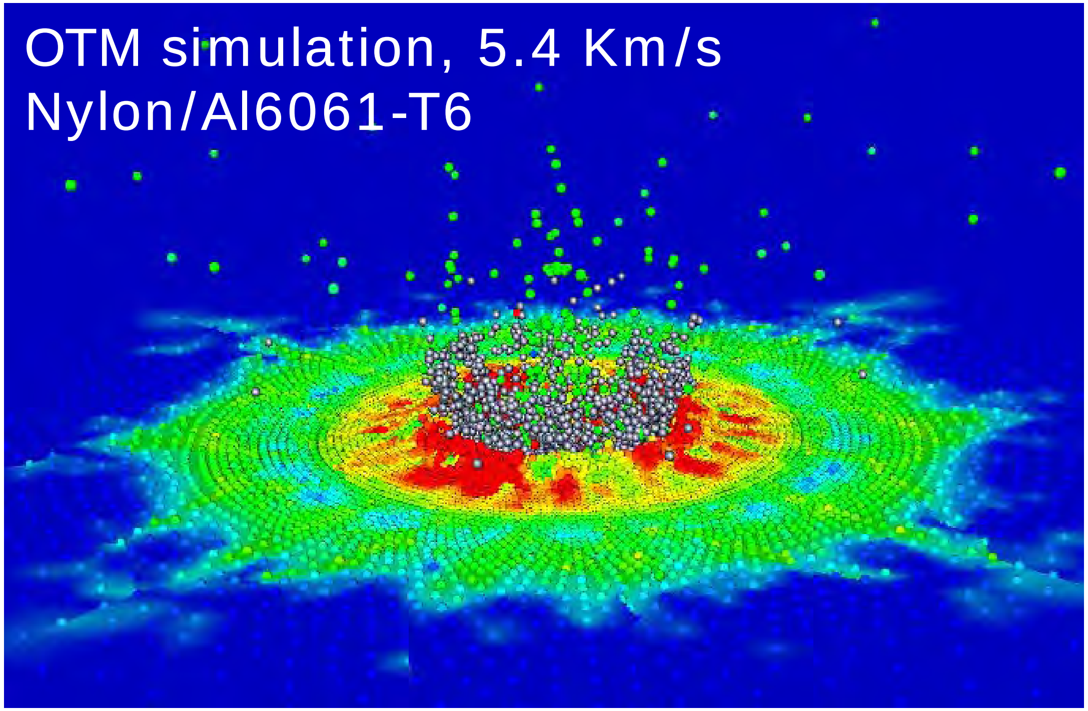
Example: Water sloshing in tank (free-surface, compressible NS)



Dirk Hartmann, Siemens AG, Munich
Corporate Research and Technologies

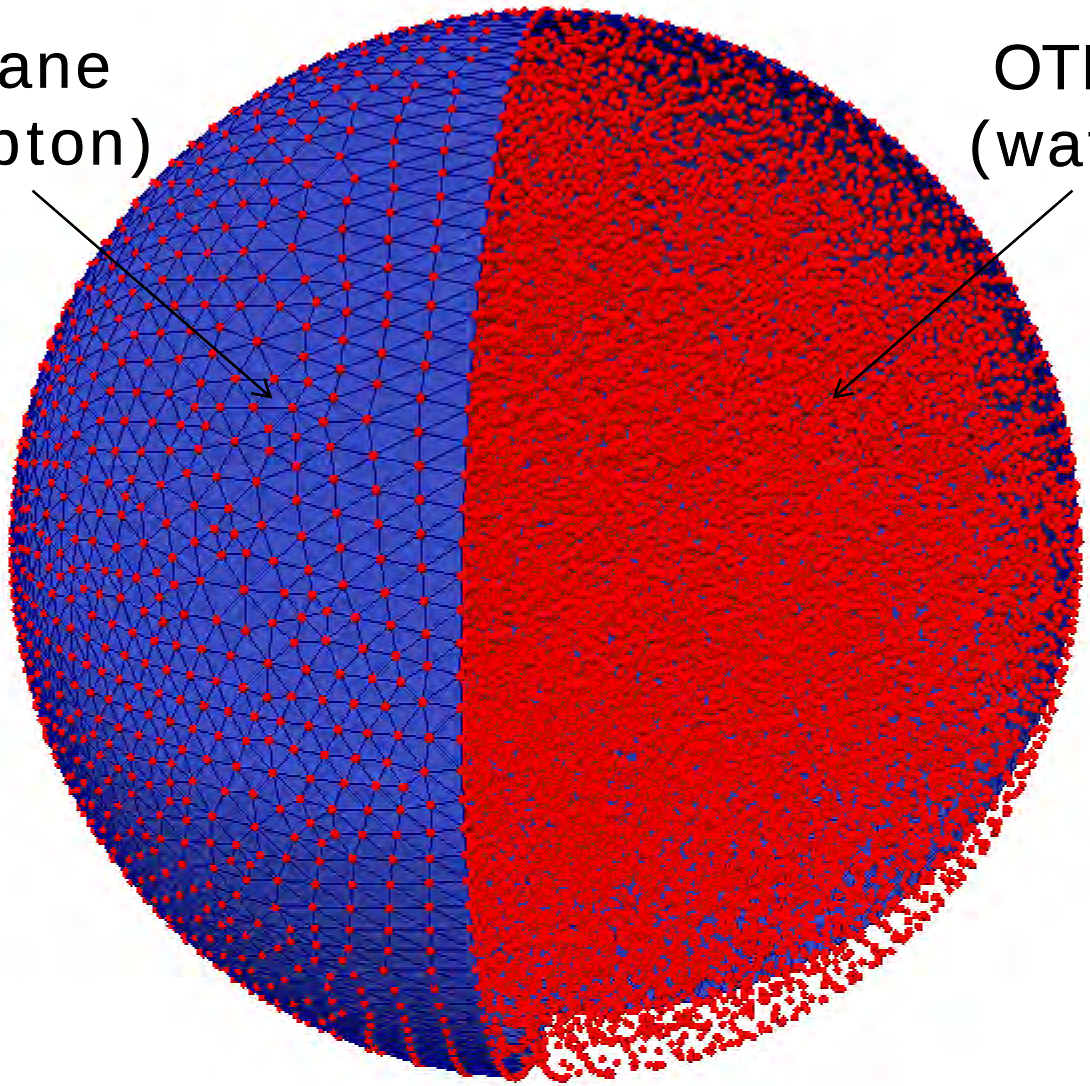
Example: Hypervelocity impact





Caltech's SPHIR facility

Example – Bouncing balloons



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OTM – Convergence analysis

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

$$\sum_{k=0}^{N-1} \left\{ \frac{1}{2} \frac{d_W^2(\rho_k, \rho_{k+1})}{(t_{k+1} - t_k)^2} - \frac{1}{2}[U(\rho_k) + U(\rho_{k+1})] \right\} (t_{k+1} - t_k)$$

- Non-interacting particles: $U = 0$
- Discrete mass: $\rho_{h,k}(x) = \sum_{p=1}^{M} m_{p,k} \delta(x - x_{p,k})$
- Conservation of mass: $m_{p,k} =$ constant
- Fully-discrete action:

$$A_h(\rho_{h,1}, \ldots, \rho_{h,N-1}) = \sum_{k=0}^{N-1} \sum_{p=1}^{M} \frac{m_p}{2} \frac{|x_{p,k+1} - x_{p,k}|^2}{t_{k+1} - t_k}$$

OTM – Convergence analysis

- Over stationary discrete trajectories:

$$A_h(\rho_{h,0}, T) = \frac{1}{2(b-a)} \int_{\mathbb{R}^n} |Tx - x|^2 \, d\rho_{h,0}$$

where $\rho_{h,N} = T\#\rho_{h,0}$.

- Coarse-graining procedure: $\rho_{h,0} = S_h\#\rho_a(x)dx$,

$S_h : \Omega \to \mathbb{R}^n$ piecewise constant, $S_h \to$ id uniformly

- Then: $\rho_{h,N} = TS_h\#\rho_a dx$,

$$A_h(\rho_{h,0}, T) = \frac{1}{2(b-a)} \int_{\mathbb{R}^n} |TS_h x - S_h x|^2 \, \rho_a(x) \, dx$$

OTM – Convergence analysis

Theorem (Γ-convergence and compactness)

Let $\rho_a,\, \rho_b \in L^1(\mathbb{R}^n)$, *compactly supported.*

i) $T_h S_h \# \rho_a dx \overset{*}{\rightharpoonup} \rho_b dx$ *in* $\mathcal{M},\ A_h(S_h \# \rho_a, T_h) < C < +\infty \Rightarrow \exists T \in L^\infty(\Omega)$, *subsequence s. t.*

i.a) $T_h S_h \rightharpoonup T$ *in* $L^2(\Omega, \rho_a dx)$

i.b) $\liminf_{h\to 0} A_h(S_h \# \rho_a, T_h) \geq A(T)$

ii) $\forall T \in L^\infty(\Omega), \exists T_h$ *s. t.* $S_h T_h \overset{*}{\rightharpoonup} T$ *and*

$$\lim_{h\to 0} A_h(S_h \# \rho_a, T_h) = A(T)$$

OTM – Convergence analysis

Theorem (Strong conv. of recovery sequences)

Let $T_h S_h \rightharpoonup T$ *in* $L^2(\Omega, \rho_a dx)$, $\lim_{h\to 0} A_h(S_h \# \rho_a, T_h) = A(T)$. *Then,* $T_h S_h \to T$ *strongly in* $L^2(\Omega, \rho_a dx)$ *and* $T \# \rho_a = \rho_b$.

Theorem (Convergence of minimizers)

Let ρ_a, $\rho_b \in L^1(\mathbb{R}^n)$, *compactly supported.*

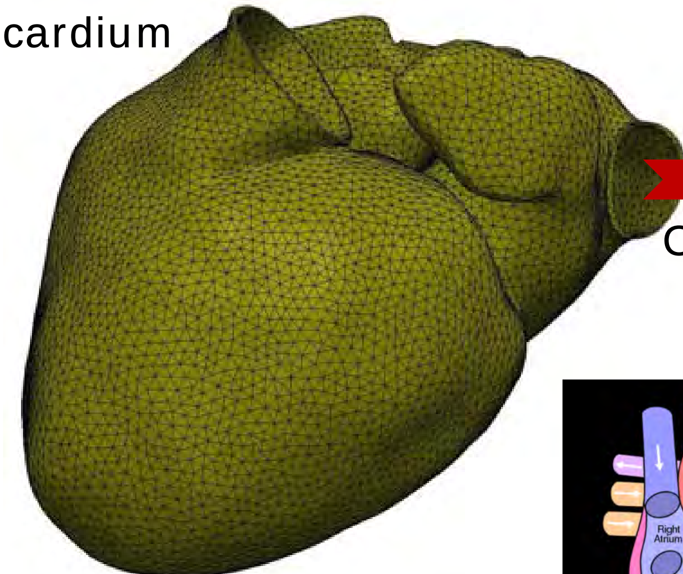
Let T_h *be a sequence of minimizers of* $A_h(S_h \# \rho_a, T)$, *subject to* $T S_h \rho_{h,0} = \rho_{h,N}$, *where* $\rho_{h,N} \overset{*}{\rightharpoonup} \rho_b dx$ *in* $\mathcal{M}$. *Then,* $T_h S_h \rightharpoonup T$ *in* $L^2(\Omega, \rho_a dx)$, *where* T *is a minimizer of* A *(with respect to* ρ_a *and* ρ_b*).*

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*
- Outlook:
  - *Extend convergence analysis to compressive-Euler flows, solid flows*
  - *Applications, applications, applications...*

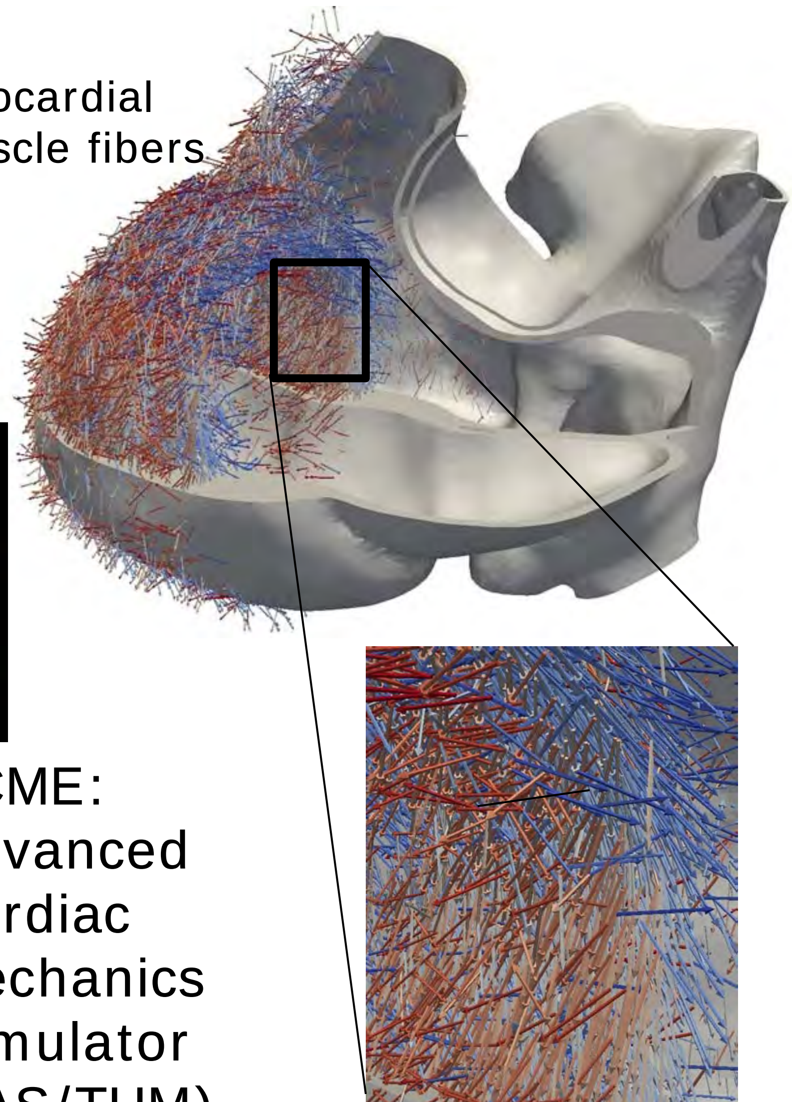
OTM – Summary and outlook

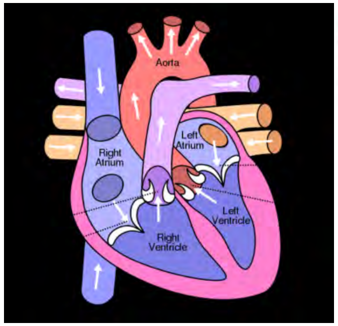
myocardium
(FE)



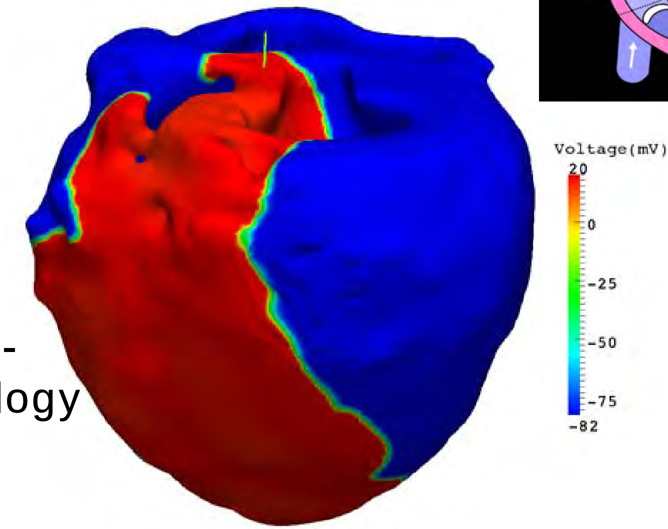
OTM blood

myocardial
muscle fibers





electro-
physiology



ACME:
Advanced
Cardiac
Mechanics
Simulator
(IAS/TUM)

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OTM – Summary and outlook

Thank you!

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