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

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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 Petersburg (1912), Moscow (1986)
Nobel Prize in Economics (1975)
Mass flows — Optimal transportation

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

$$\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \otimes v) = 0$$

- Initial and final conditions:

$$t \in [a, b]$$

$$\rho(x, a) = \rho_a(x)$$

$$\rho(x, b) = \rho_b(x)$$

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Mass flows — Optimal transportation

- **Benamou & Brenier minimum principle:**

\[
\begin{align*}
\text{minimize: } & A(\rho, v) = \int_a^b \int \frac{\rho}{2} |v|^2 \, dx \, dt \\
\text{subject to: } & \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0
\end{align*}
\]

\[\Rightarrow (\rho, v)\]

- 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:

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

\[\Rightarrow (\rho, v)\]
Euler flows — Optimal transportation

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

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

inertia \hspace{1cm} \text{internal energy}

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

\[
\frac{2\rho_k}{t_{k+1} - t_{k-1}} \left( \frac{\varphi_{k\rightarrow k+1} - \text{id}}{t_{k+1} - t_k} + \frac{\varphi_{k\rightarrow k-1} - \text{id}}{t_k - t_{k-1}} \right) = \nabla p_k + \rho_k b_k
\]

\[
\rho_{k+1} \circ \varphi_{k\rightarrow k+1} = \rho_k / \det(\nabla \varphi_{k\rightarrow k+1})
\]

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 $\varphi_{k \rightarrow k+1}$ from nodal coordinates?
OTM — Max-ent interpolation

• Problem: Reconstruct function \( u(x) \) from nodal sample \( \{u(x_a), \ a = 1, \ldots, N\} \) so that:
  
  – Reconstruction is \textit{least biased}
  
  – Reconstruction is \textit{most local}

• Optimal shape functions (Arroyo & MO, \textit{IJNME}, 2006):

\[
\begin{align*}
\text{Minimize:} & \quad \sum_{a=1}^{N} |x-x_a|^2 N_a(x) + \beta \sum_{a=1}^{N} N_a(x) \log N_a(x) \\
\text{Subject to:} & \quad \sum_{a=1}^{N} N_a(x) = 1, \quad \sum_{a=1}^{N} x_a N_a(x) = x.
\end{align*}
\]
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

nodal points: $x_{a,k}$

material points $x_{p,k}$

$\varphi_{k \rightarrow k+1}$

$t_k$, $t_{k+1}$
OTM — Spatial discretization

nodal points: \( x_{a,k} \)

material points \( x_{p,k} \)

\( \varphi_{k \rightarrow k+1} \)

\( t_k \)

\( t_{k+1} \)
$N_p = \text{local neighborhood of material point } p$
OTM — Spatial discretization

- Max-ent interpolation at node $p$ determined by nodes in its local environment $N_p$
- 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:
\[ x_{k+1} = x_k + (t_{k+1} - t_k) \left( v_k + \frac{t_{k+1} - t_{k-1}}{2} M_{k-1} f_k \right) \]

(ii) Material point update:
- position: \[ x_{p,k+1} = \varphi_{k\rightarrow k+1}(x_{p,k}) \]
- deformation: \[ F_{p,k+1} = \nabla \varphi_{k\rightarrow k+1}(x_{p,k}) F_{p,k} \]
- volume: \[ V_{p,k+1} = \det \nabla \varphi_{k\rightarrow k+1}(x_{p,k}) V_{p,k} \]
- density: \[ \rho_{p,k+1} = \frac{m_p}{V_{p,k+1}} \]

(iii) Constitutive update at material points

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

computed vs. exact wave structure
OTM — Shock tube problem

Shock tube problem – velocity snapshots
OTM — Shock tube problem

Shock tube problem – convergence plots

velocity convergence (L² norm)

density convergence (L¹ norm)

convergence rate ~ 1

mesh size (h)

velocity L² error norm
density L¹ error norm
OTM — Taylor anvil test

Copper rod @ 750 m/s

t=0

t=7.5 µs

t=15 µs

t=28 µs
OTM — Taylor anvil test

copper rod @ 750 m/s
OTM — Bouncing balloons

FE membrane (rubber, Kapton)

OTM fluid (water, air)
OTM — Bouncing balloons

FE membrane (rubber, Kapton)

OTM fluid (water, air)
OTM — Bouncing balloons

FE membrane (rubber, Kapton)

OTM fluid (water, air)
OTM — Bouncing balloons

FE membrane (rubber, Kapton)

OTM fluid (water, air)
OTM — Terminal ballistics

1500 m/s

steel projectile

aluminum plate
OTM — Terminal ballistics

1500 m/s

steel projectile

aluminum plate

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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...