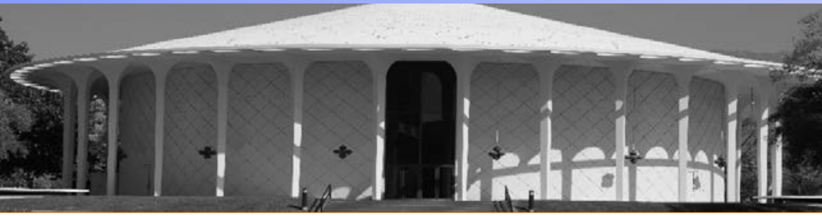

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Optimal Transportation and Particle Methods in Mechanics

Michael Ortiz
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

Workshop on Emergence of Structures in Particle Systems: Mechanics, Analysis and Computation

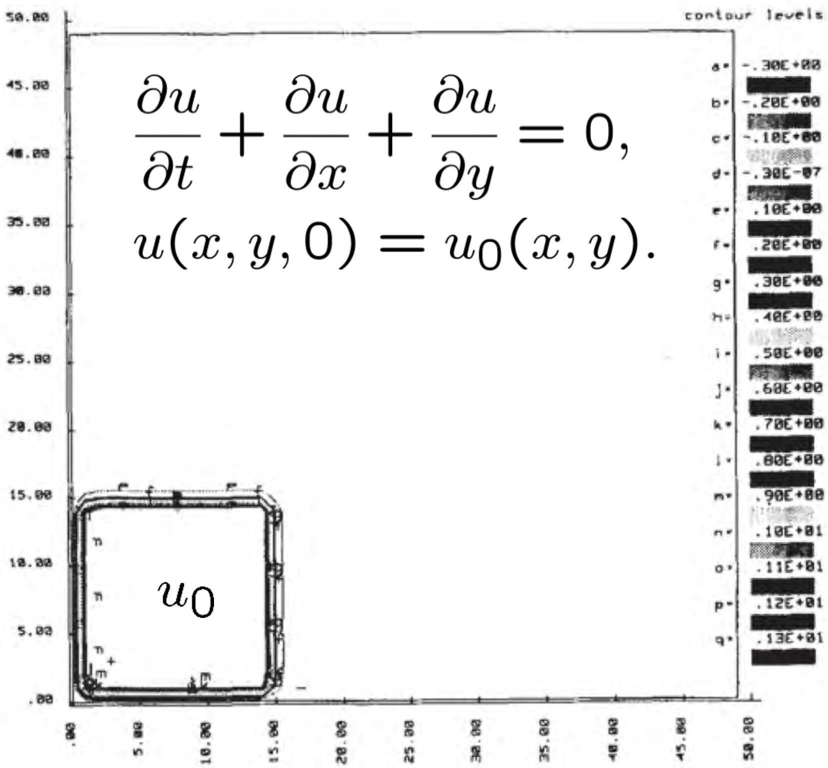
Mathematisches Forschungsinstitut Oberwolfach (MFO)
Oberwolfach, Germany, October 29, 2018

Intro: Particle methods

- *Particle methods* are popular because:
  - *They are meshless and can deal efficiently with unconstrained flows and large geometry changes without mesh entanglement*
  - *They are geometrically exact with respect to advection (push-forward of measures)*
  - *They preserve positivity (no negative densities)*
  - *They have monotonicity properties (no overshoots, no spurious oscillations)*
- Traditional finite-difference/finite-element schemes experience great difficulty in dealing with these issues...

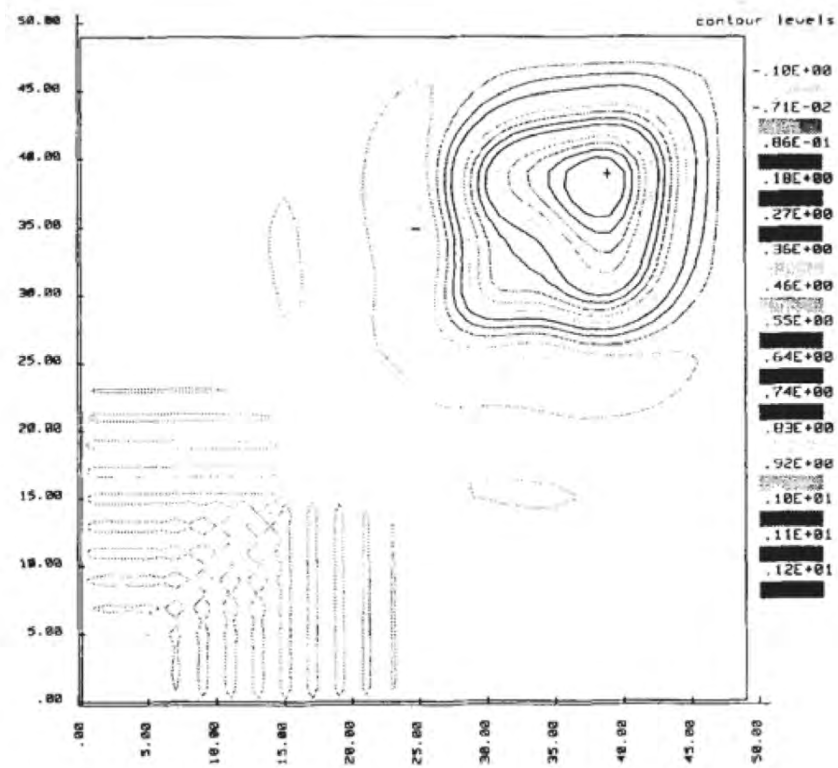
Intro: Particle methods

- Example: Two-dimensional advection



$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = 0,$$
$$u(x, y, 0) = u_0(x, y).$$

Governing equations and initial conditions



Final configuration after application of ALE algorithm[1]

D. J. Benson, *J. Comp. Physics*, **100** (1992) 143.

Intro: Particle methods

Particle methods in engineering = Transport of measures in mathematics

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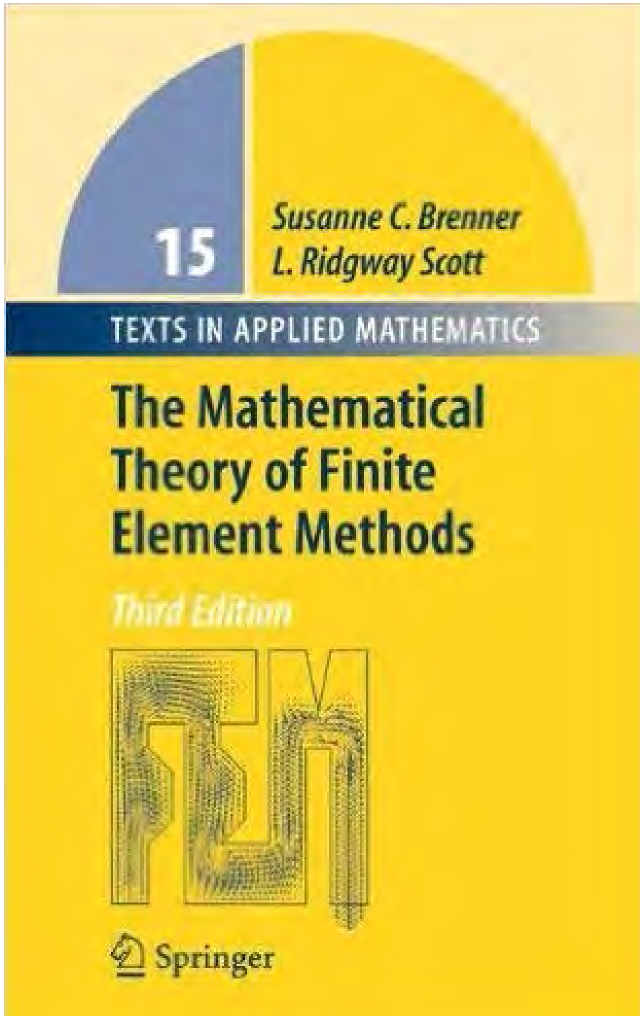
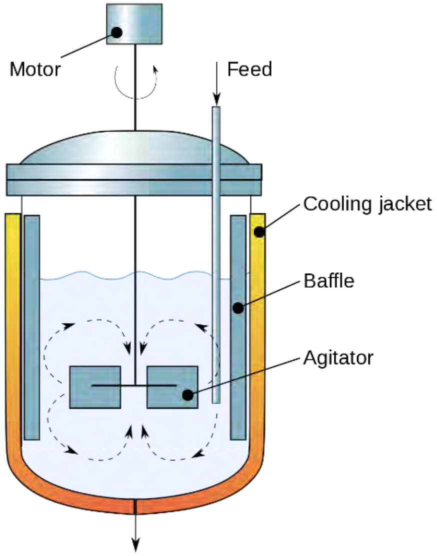
Intro: Particle methods



- Connection between approximation theory and computational science is well-developed in the context of PDEs and functional spaces.
- The connection is comparatively less well-developed in the context of transport of measures (e.g., particle methods)…

Outline

- Introduction (done!)
- *Advection-diffusion problems (scalar)*
- Flow problems (solid/fluid mechanics, vector)
- Dislocation transport (lines, 1-currents)
- Outlook...



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Mass transport

- Advection-diffusion initial-BVP:

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho\, c) = \kappa \Delta \rho, & \text{in } [0,T] \times \Omega\,, \\ \kappa \nabla \rho \cdot \nu = 0, \quad (c \cdot \nu = 0) & \text{on } [0,T] \times \partial\Omega\,, \\ \rho(x,0) = \rho_0(x), & \text{in } \Omega\,. \end{cases}$$

- Transport reformulation (Eulerian):

$$\partial_t \rho + \nabla \cdot (\rho\, v) = 0, \qquad v = c - \kappa \nabla \log \rho$$

- Fokker-Planck equation: $c = \nabla V$
- Existence and uniqueness of smooth solutions, connections with Ito stochastic differential eq...

Mass transport – Time discrete (I)

- Discrete time: $0 = t_0 < t_1 < \cdots < t_N = T$
- Discrete density: $\rho_0, \cdots, \rho_k, \cdots \rho_N$
- Variational principle[1]: $F(\rho_{k+1}) =$

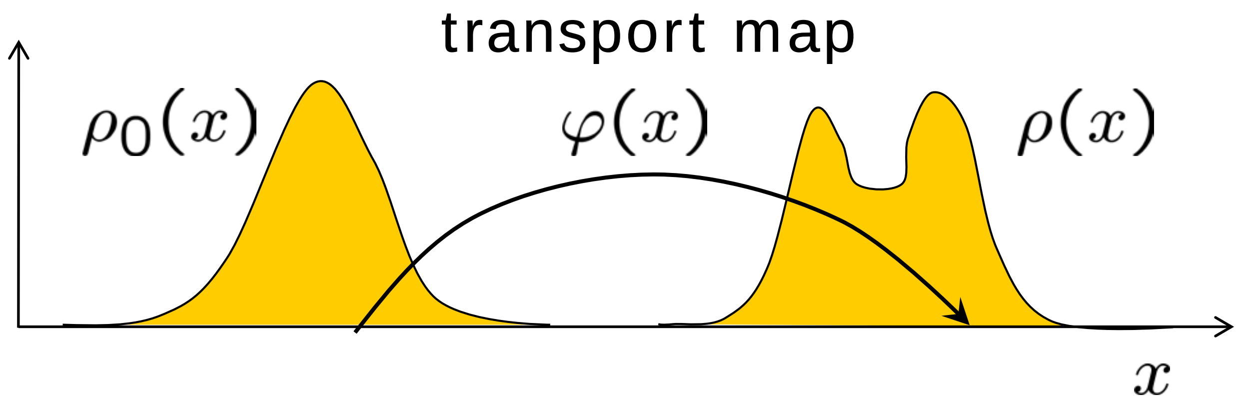
$$\frac{1}{2}\frac{d_W^2(\rho_k, \rho_{k+1})}{t_{k+1} - t_k} + \int_\Omega \kappa \rho_{k+1} \underline{\log \rho_{k+1}} \, dx \to \text{min!}$$

- EL equation: $\dfrac{x - \varphi_{k+1\to k}}{t_{k+1} - t_k} = -\kappa \nabla \log \rho_{k+1}$
- $\underline{\rho_k \in L^1}, \quad \int \rho_k \, dx = 1, \quad \int |x|^2 \rho_k \, dx < +\infty$
- Convergence[1]: $\rho_h \overset{L^1}{\rightharpoonup} \rho \in C^\infty((0, +\infty) \times \mathbb{R}^n)$

[1]Jordan R, Kinderlehrer D, Otto F. *Physica D*, **107** (1997) 265.

Mass transport — Transport maps

Gaspard Monge
Beaune (1746)
Paris (1818)



- Push-forward of $\rho_0\, dx$:

$$\rho \circ \varphi = \rho_0 / \det(\nabla\varphi)$$

- Weak form of push-forward:

$$\int_\Omega \eta(y) \underline{\rho(y)\, dy} = \int_\Omega \eta(\varphi(x)) \underline{\rho_0(x)\, dx}$$

G. Monge, "Sur la théorie des déblais et des Remblais", *Mém. Acad. Paris*, 1781.

Mass transport – Time discrete (II)

- Discrete time: $0 = t_0 < t_1 < \cdots < t_N = T$
- Discrete density: $\rho_0, \cdots, \rho_k, \cdots \rho_N$
- Discrete transport map: $\varphi_{k\to k+1}$
- Weak form of incremental transport equations:

$$\int \eta\, \rho_k\, dx = \int (\eta \circ \varphi^{-1}_{k\to k+1})\, \rho_{k+1}\, dy,$$

$$\int_\Omega \frac{\varphi_{k\to k+1} - x}{t_{k+1} - t_k} \cdot \xi\, \rho_k\, dx = \int_\Omega \kappa\, \mathrm{tr}(\nabla \xi \nabla \varphi^{-1}_{k\to k+1})\, \rho_k\, dx$$

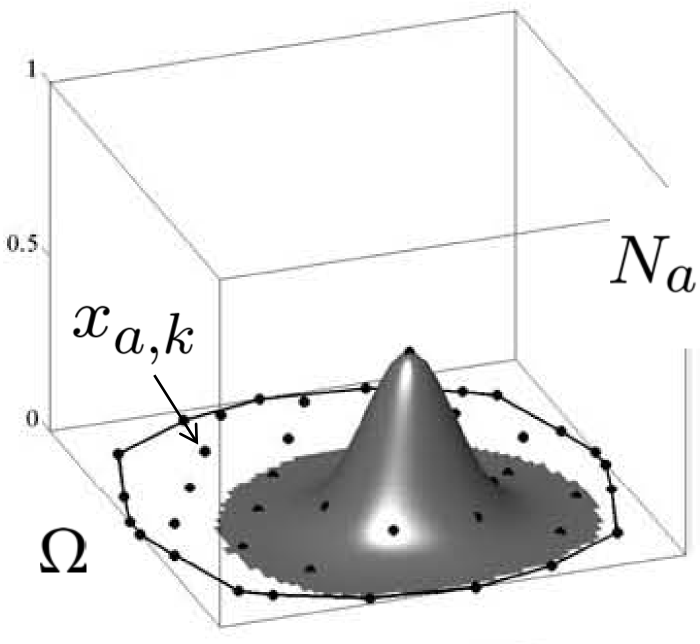
- Particle *ansatz*: $\rho_k(x) = \sum_{p=1}^{M} m_{p,k}\, \delta\big(x - x_{p,k}\big)$

Fedeli L, Pandolfi A, Ortiz M. *IJNME*,**112**(9) (2017) 1175-93.

Mass transport — Interpolation

- Incremental transport map interpolation:

$$\varphi_{k\to k+1}(x) = \sum_{a=1}^{N} x_{a,k+1} N_{a,k}(x)$$



- Max-ent shape functions[1,2]:

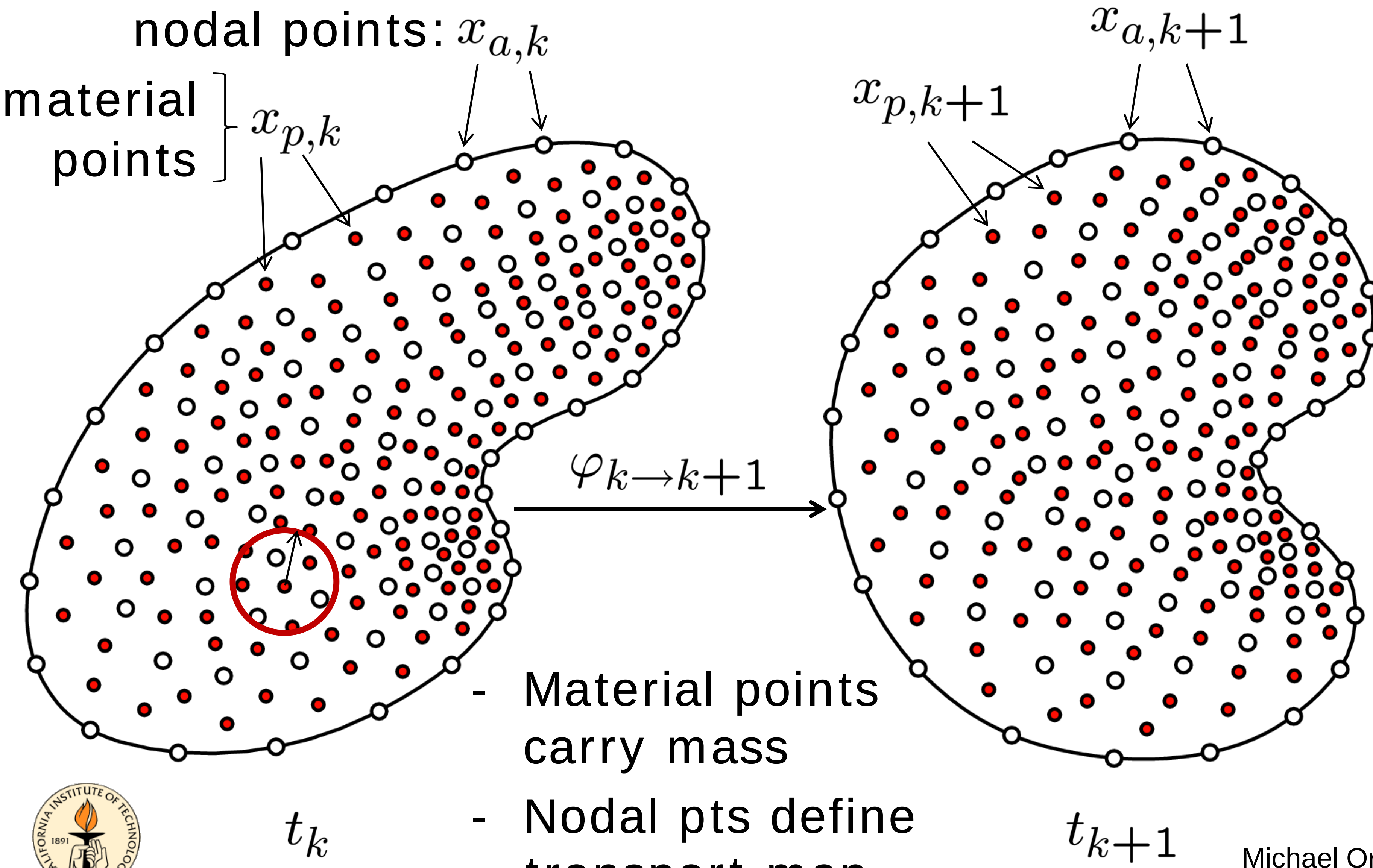
$$N_a(x) = \frac{1}{Z(x)} \mathrm{e}^{-\frac{\beta}{2}|x-x_a|^2 + \lambda(x)\cdot(x-x_a)}$$

- First-order consistency:

$$\sum_{a=1}^{N} x_a N_a(x) = x$$

[1] Arroyo, M. and Ortiz, M., *IJNME*, **65** (2006) 2167.
[2] Bompadre A, Schmidt B and Ortiz M, *SIAM J. Numer. Anal.*, **50** (2012) 1244.

Mass transport – Discretization



- Material points carry mass
- Nodal pts define transport map

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Mass transport — Discretization

- Weak form of incremental transport equations:

$$\int \rho_k \eta \, dx = \int \rho_{k+1} (\eta \circ \varphi_{k \to k+1}^{-1}) \, dy,$$

$$\int_\Omega \rho_k \frac{\varphi_{k \to k+1} - x}{t_{k+1} - t_k} \cdot \xi \, dx = \int_\Omega \kappa \rho_k \text{tr}(\nabla \xi \nabla \varphi_{k \to k+1}^{-1}) \, dx.$$

- Introduce spatial discretization:

$$\begin{cases} m_{p,k+1} = m_{p,k} = \text{constant}, \\ M_k \dfrac{x_{k+1} - x_k}{t_{k+1} - t_k} = f_k = \displaystyle\sum_{p=1}^{M} m_p \, \kappa \, \nabla N_k(x_{p,k}), \end{cases}$$

$$M_{k,ab} = \sum_{p=1}^{M} m_p N_{a,k}(x_{p,k}) N_{b,k}(x_{p,k}).$$

Mass transport – Flow chart

(i) Explicit nodal coordinate update:

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

(ii) Material point update:

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

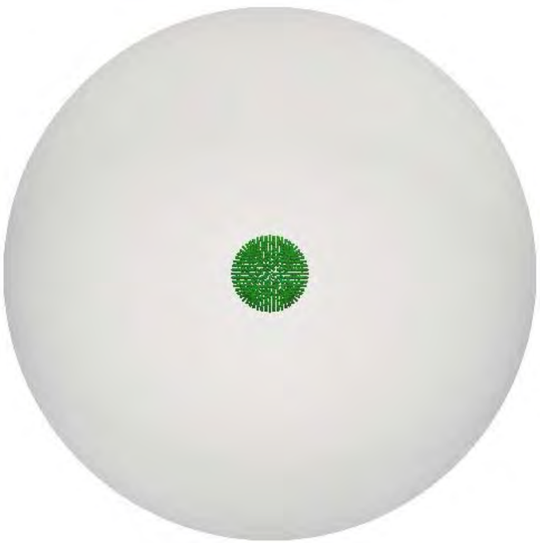
volume: $V_{p,k+1} = \det \nabla\varphi_{k\to k+1}(x_{p,k}) V_{p,k}$

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

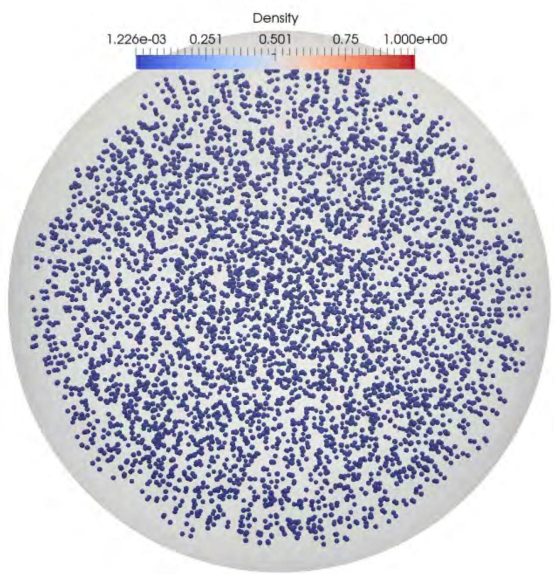
(iii) Reconnect nodal and material points (range searches), recompute max-ext shape functions

Fedeli L, Pandolfi A, Ortiz M. *IJNME*, **112**(9) (2017) 1175-93.

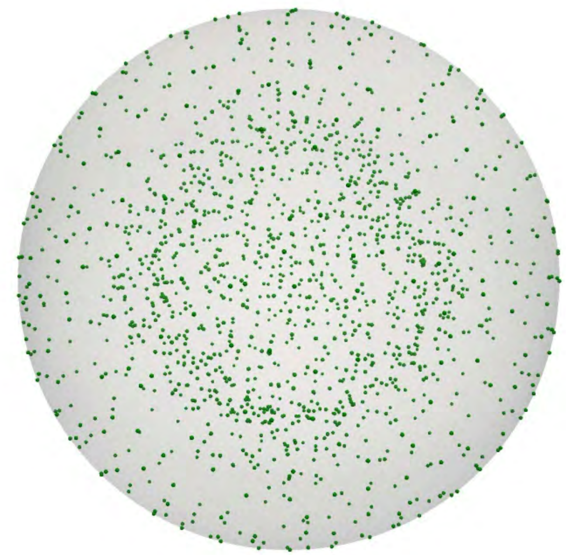
Pure diffusion in spherical domain



Initial distribution of nodes



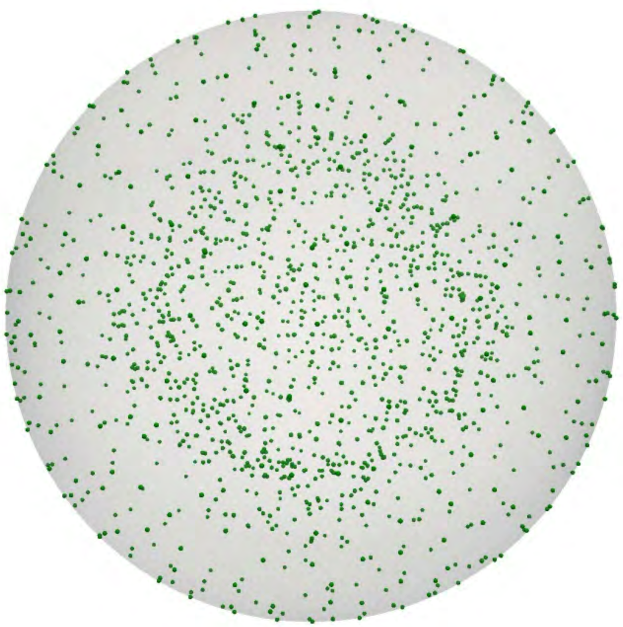
Final distribution of material points

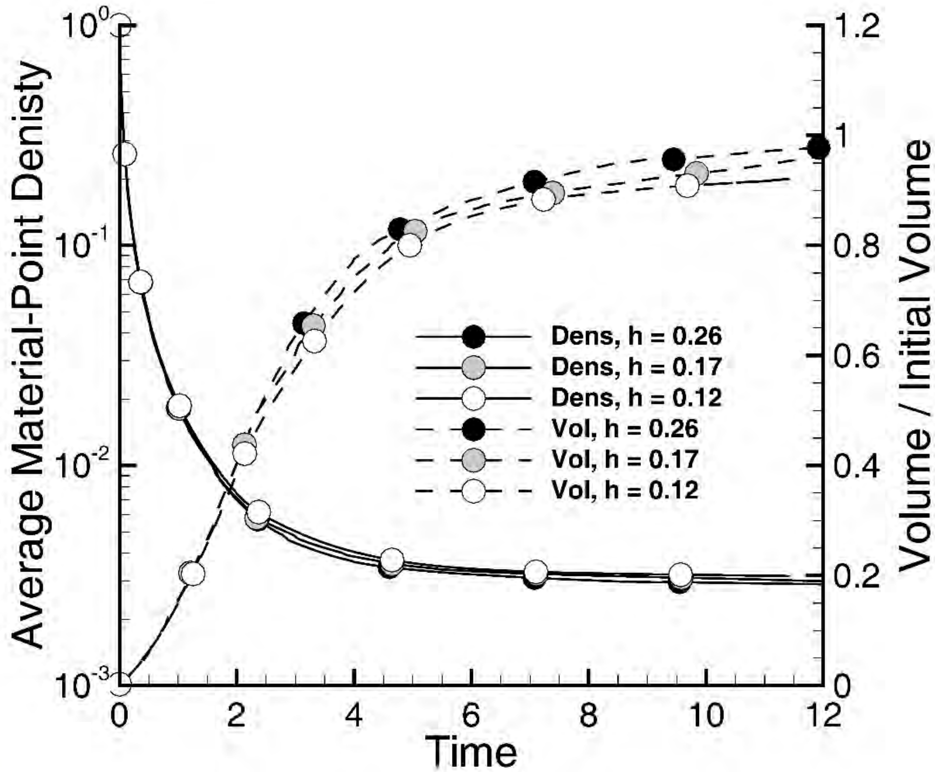


Final distribution of nodes

Fedeli L, Pandolfi A, Ortiz M. *IJNME*,**112**(9) (2017) 1175-93.

Mass transport – Convergence





Final distribution of nodes

Time evolution for three discretizations

Fedeli L, Pandolfi A, Ortiz M. *IJNME*,**112**(9) (2017) 1175-93.

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Outline

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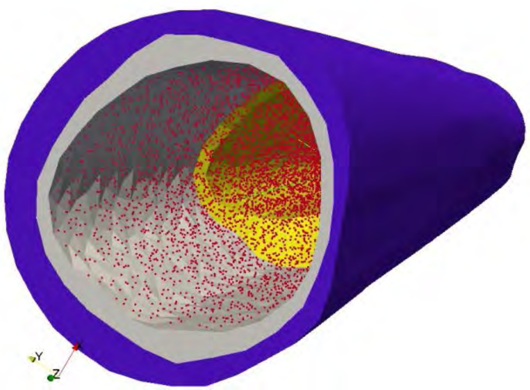
- Advection-diffusion problems (scalar)
- *Flow problems (solid/fluid mechanics, vector)*
- Dislocation transport (lines , 1-currents)
- Outlook...



Particle simulations of arterial blood flow
accounting for wall elasticity, plaque
(with Stefanie Heyden, Bo Li, Anna Pandolfi)

Flow problems

- Mass + linear-momentum transport (Eulerian):

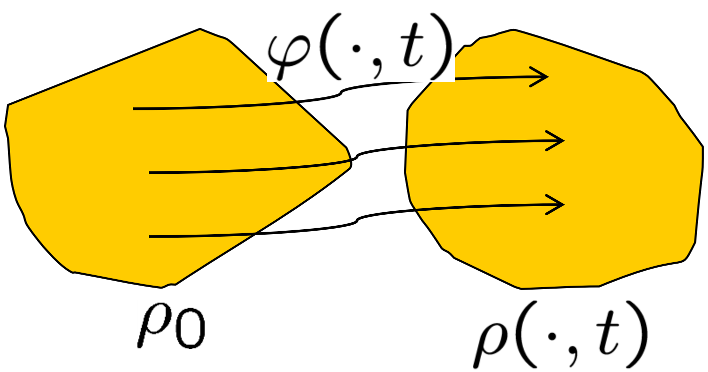
$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho\, v) = 0, & \text{in } [0,T] \times \Omega_t\ , \\ \partial_t(\rho v) + \nabla \cdot (\rho\, v \otimes v) = \nabla \cdot \sigma, & \text{in } [0,T] \times \Omega_t\ , \\ (\rho v \otimes v - \sigma)\nu = 0, & \text{on } [0,T] \times \partial\Omega_t \end{cases}$$

- Lagrangian reformulation: $\partial_t\, \varphi = v \circ \varphi,$

$$\rho \circ \varphi = \rho_0 / \det(\nabla\varphi),$$

$$\sigma = \sigma(D\varphi, Dv, \text{history})$$

- Transport map = $\varphi(\cdot, t)$



Flow problems — Time-discrete

- Semidiscrete action: $A_d(\varphi_1, \ldots, \varphi_{N-1}) =$

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

with: $\rho_{k+1} \circ \varphi_{k\to k+1} = \rho_k / \det\big(\nabla \varphi_{k\to k+1}\big)$

(geometrically exact mass conservation!)

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

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

Li, B., Habbal, F. and Ortiz, M. , *IJNME*, **83** (2010) 1541.

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

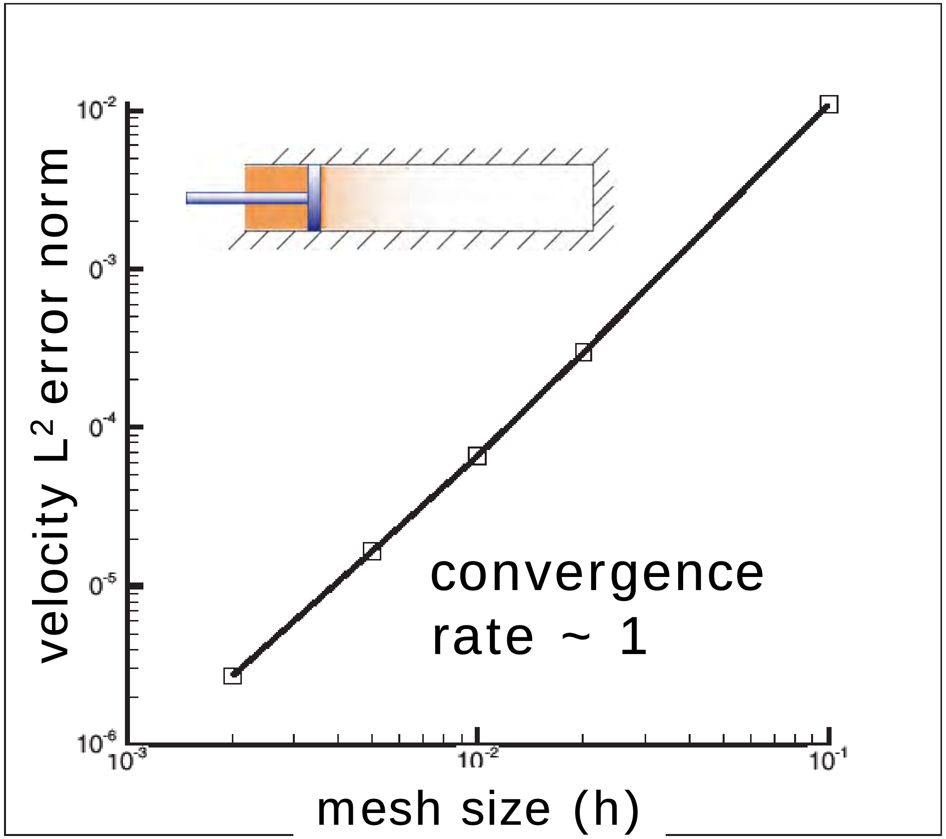
volume: $V_{p,k+1} = \det \nabla\varphi_{k\to k+1}(x_{p,k}) V_{p,k}$

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

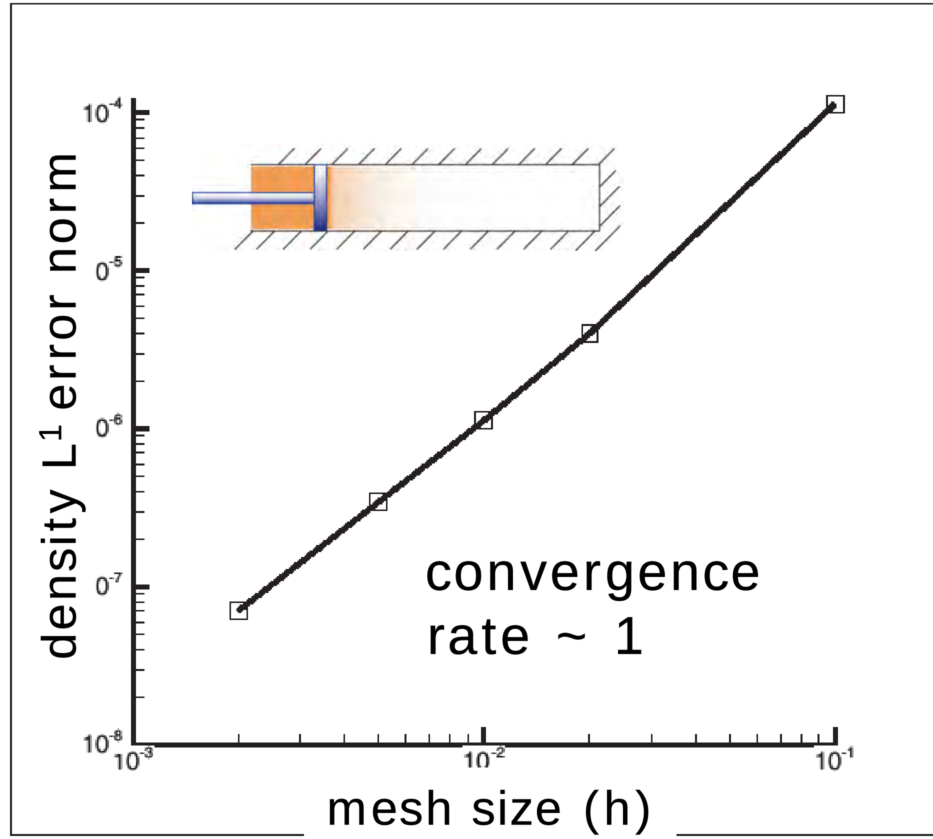
(iii) Constitutive update at material points

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

Flow problems — Riemann problem



velocity convergence
(L^2 norm)



density convergence
(L^1 norm)

Li, B., Habbal, F. and Ortiz, M. , *IJNME*, **83** (2010) 1541.

Flow problems – 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 $M, N \to \infty$.

i) Theorem applies to particles in a field of force

ii) Theorem implies convergence of minimizers

iii) Case of interacting particles remains open!

Schmidt, B. *Multiscale Modeling & Simulation*, **12** (2014) 265.

Outline

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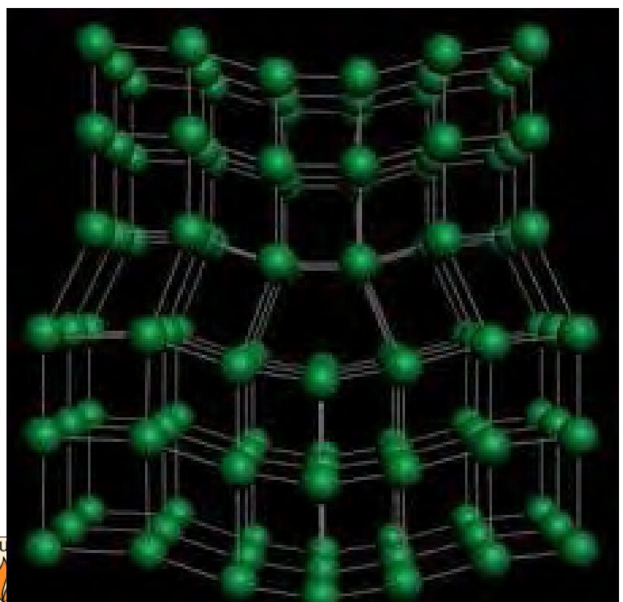
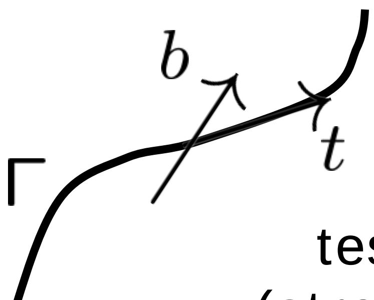
- *Dislocation transport (lines, 1-currents)*
- Outlook…



J. Kacher, Materials Science and Engineering, Georgia Tech.

Dislocation transport

- Dislocations: *line-defects* in crystals consisting of lines carrying *Burgers vector* ‘charge’
- Representation as vector-valued *1-currents*:



$$\int_\Omega \chi \cdot d\alpha = \oint_\Gamma \chi\, b \cdot t \, ds$$

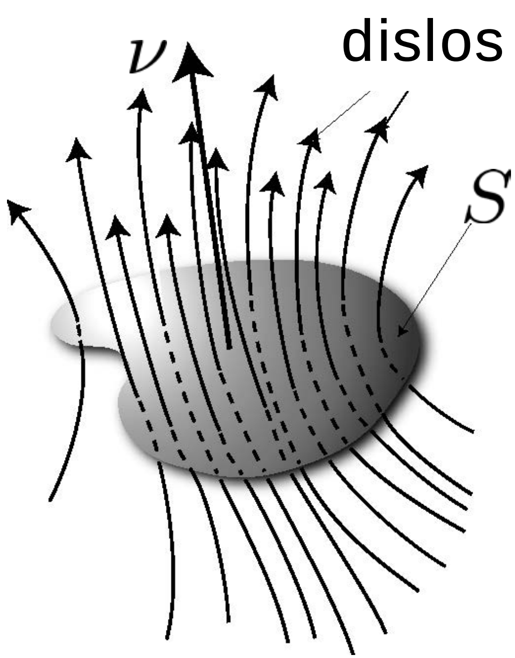
← arc-length differential

test function (stress potential) · dislocation measure · Burgers vector · tangent vector

- Closedness: $\operatorname{div} \alpha = 0$, or $\int_\Omega \nabla \eta \cdot d\alpha = 0$
- Aim: *Transport of dislocations as 1-currents*
- Particle approximation? (*monopoles*)

S. Conti, A. Garroni, and A. Massaccesi, *CoV & PDEs*, **54**(2):1847, 2115.

Dislocation transport equation



- Total Burgers vector through S:

$$b(S,t) = \int_S d\alpha\, \nu$$

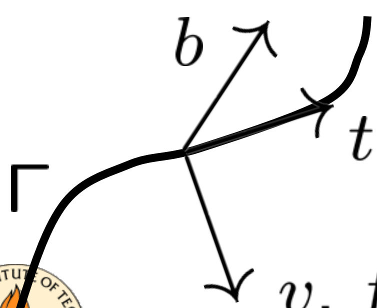
- Flux of Burgers vector into S:

$$\dot{b}(S,t) = \int_{\partial S} d\alpha \cdot (t \times v)$$

- Stokes theorem, transport eq.:

$$\dot{\alpha} + \text{curl}\,(\alpha \times v) = 0$$

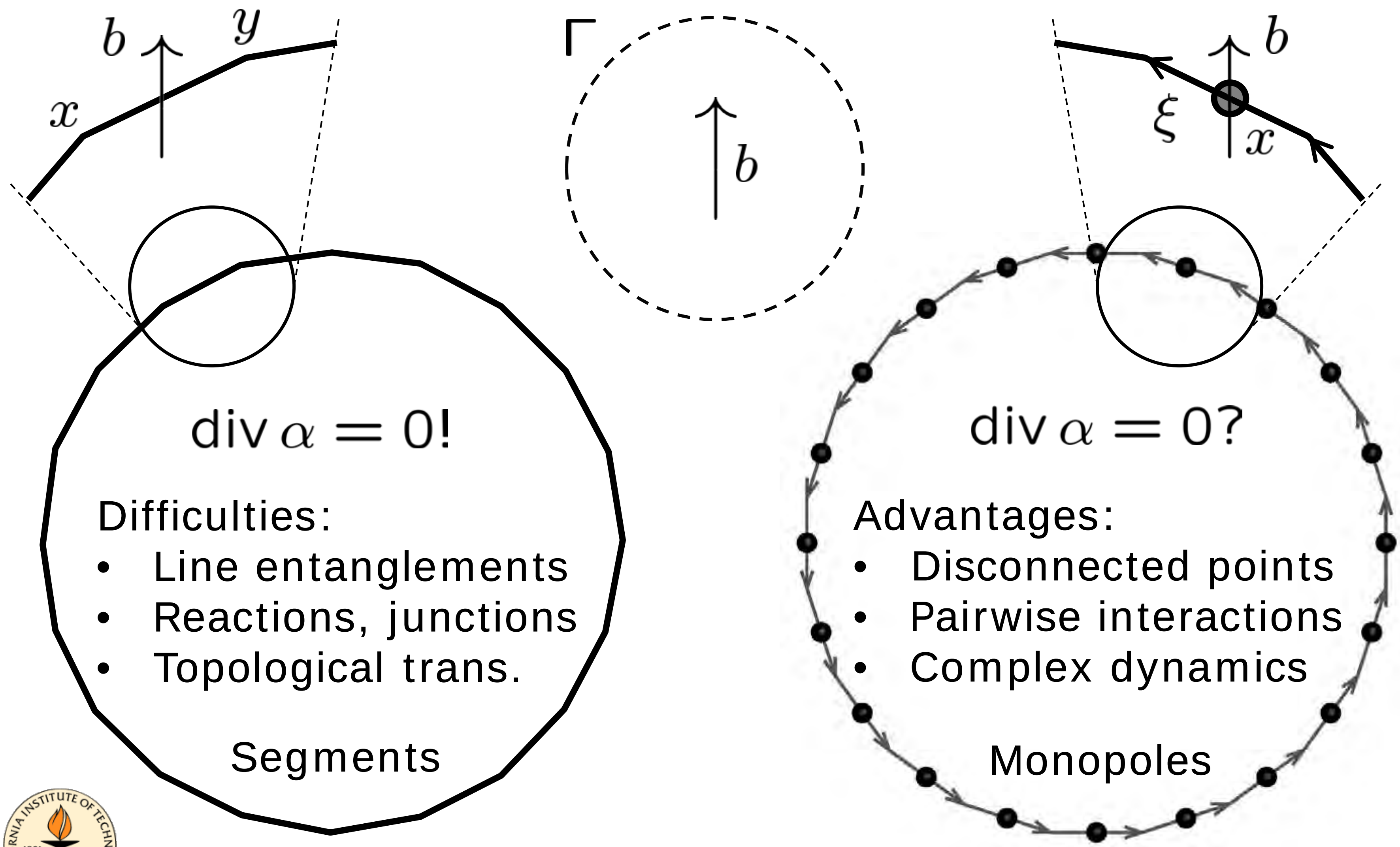
- Dislocation mobility: $f = D\psi(v)$



v, $f = \sigma b \times t$ (Peach-Koehler force)

T. Mura, *Micromechanics of Defects in Solids*, Martinus Nijhoff, 1987.

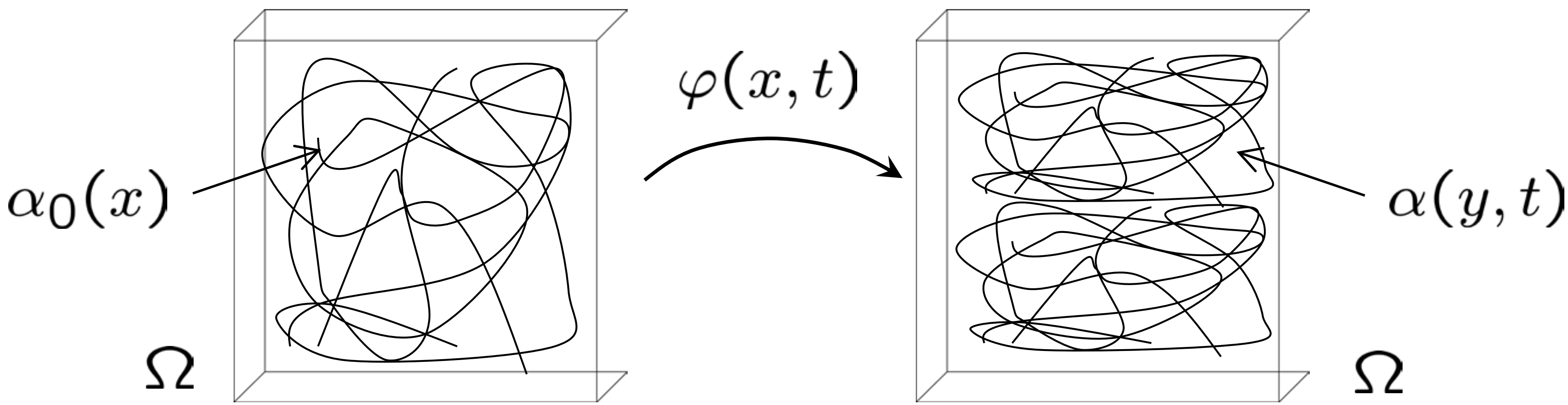
Dislocation transport – Line-free



Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Dislocation transport – Transport maps

- Representation of general dislocation measure dynamics by means of a transport maps:



- Push-forward for line-currents: $\alpha = \varphi_{\#}\alpha_0$ if

$$\int_\Omega \eta(y)\cdot \underline{d\alpha(y,t)} = \int_\Omega \Big(\eta(\varphi(x,t))\nabla\varphi(x,t)\Big)\cdot \underline{d\alpha_0(x)}$$

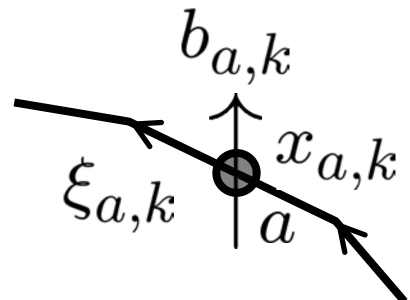
- Divergence: $\text{div}\,\alpha_0(x) = 0 \Rightarrow \text{div}\,\alpha(y,t) = 0$!

Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Dislocation transport – Discrete

- Discrete time: $0 = t_0 < t_1 < \cdots < t_N = T$.
- Discrete measure: $\alpha_0, \cdots, \alpha_k, \cdots \alpha_N$.
- Geometric update: $\alpha_{k+1} = (\varphi_{k \to k+1})_\# \alpha_k$.
- Monopole discretization:

$$\alpha_k = \sum_{a=1}^{M} b_{a,k} \otimes \xi_{a,k} \, \delta_{x_{a,k}}$$



- Incremental transport map discretization:

$$\varphi_{k \to k+1}(x) = x + \sum_{a=1}^{M} (x_{a,k+1} - x_{a,k}) N_{a,k}(x)$$

- Max-ent: $N_{a,k}(x) = \frac{1}{Z_k} \exp\left(-\frac{\beta_a}{2} |x - x_{a,k}|^2 \right)$

Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Dislocation transport – Discrete

- Incremental dissipation function:

$$D(\alpha_k, \alpha_{k+1}) = \inf_{\substack{\alpha_k = \varphi(t_k)_\# \alpha_0, \\ \alpha_{k+1} = \varphi(t_{k+1})_\# \alpha_0}} \int_{t_k}^{t_{k+1}} \Psi(\varphi(t), \dot{\varphi}(t))\, dt$$

- Incremental energy-dissipation function:

$$F(\varphi_k, \varphi_{k+1}) = D(\alpha_k, \alpha_{k+1}) + E(\alpha_{k+1}) - E(\alpha_k)$$

with $\alpha_{k+1} = (\varphi_{k \to k+1})_\# \alpha_k$

- Incremental minimum principle:

$$\varphi_{k+1} \in \operatorname{argmin} F(\varphi_k, \cdot\,)$$

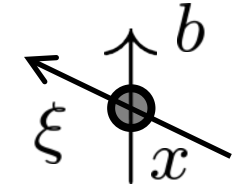
Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Dislocation transport – Discrete

- Insert *ansätze* into weak for of push-forward:

  i) $b_{a,k+1} = b_{a,k}$

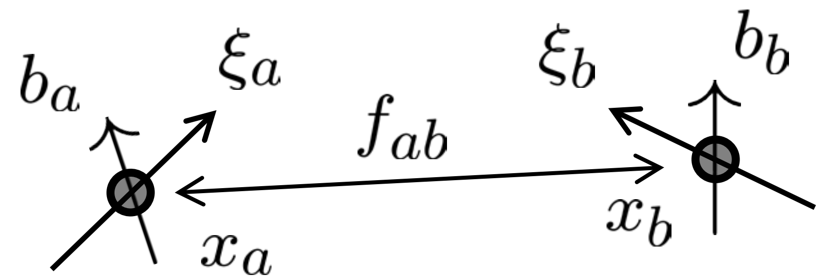
  ii) $\xi_{a,k+1} = \nabla\varphi_{k\to k+1}(x_{a,k})\xi_{a,k}$



monopole

- Exact Burgers vector conservation!
- Dislocation line rotation and stretching!
- Incremental minimum principle:

$$f_{a,k+1} = \frac{\partial F}{\partial x_{a,k+1}} = 0$$



- Linear elasticity: pairwise interactions!

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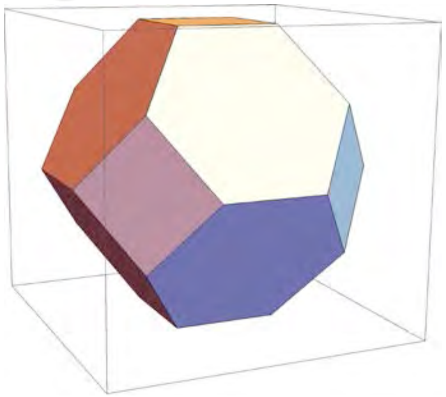
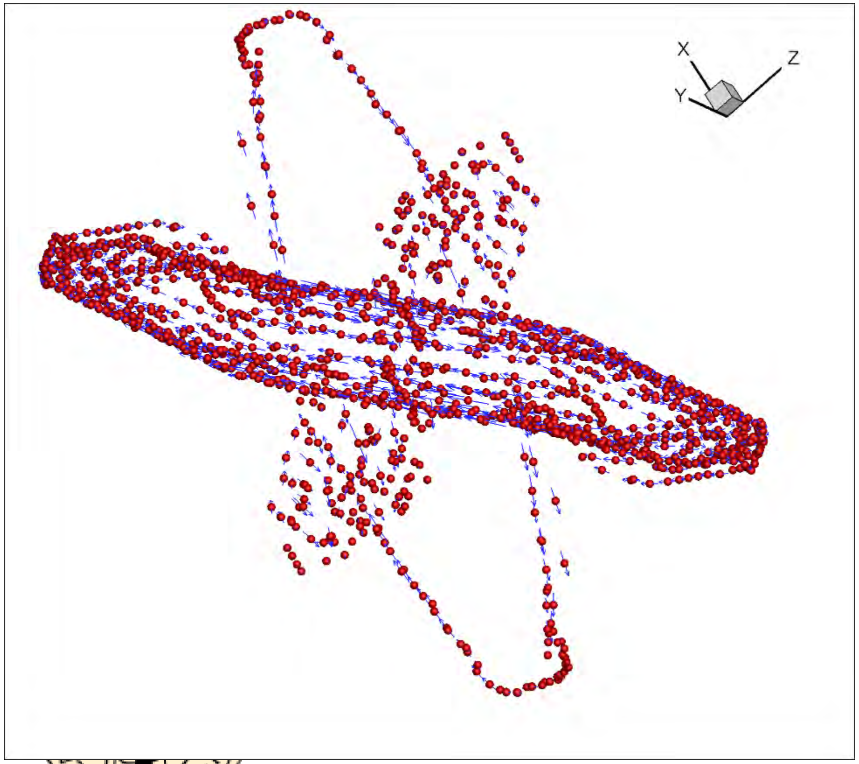
Dislocation transport – BCC grain

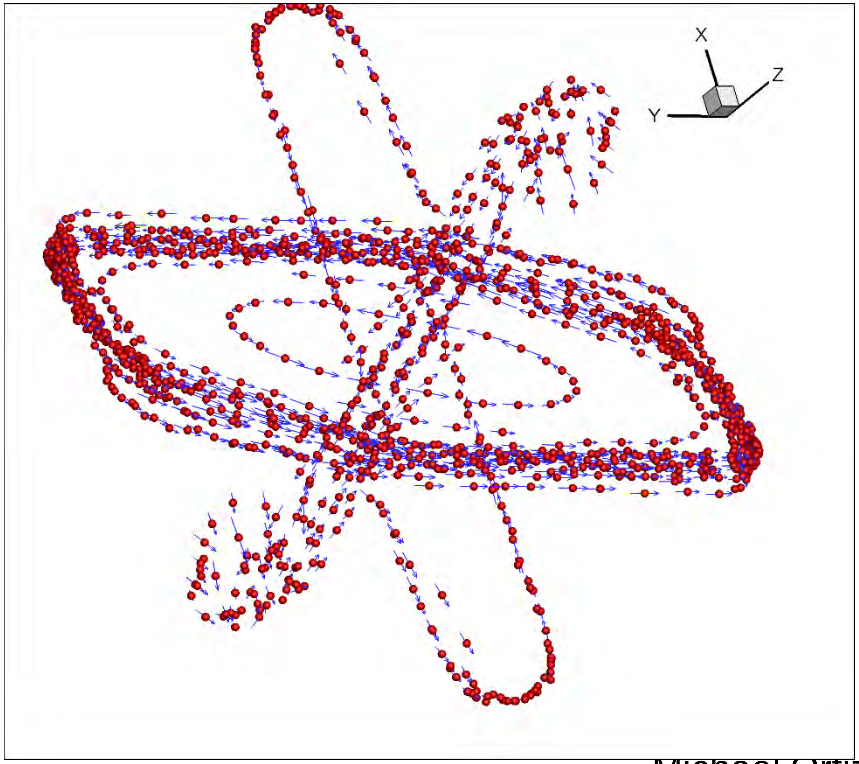


- Slip systems:

$m_{A2} = (0\ -1\ 1)$ $m_{A3} = (1\ 0\ 1)$ $m_{A6} = (1\ 1\ 0)$

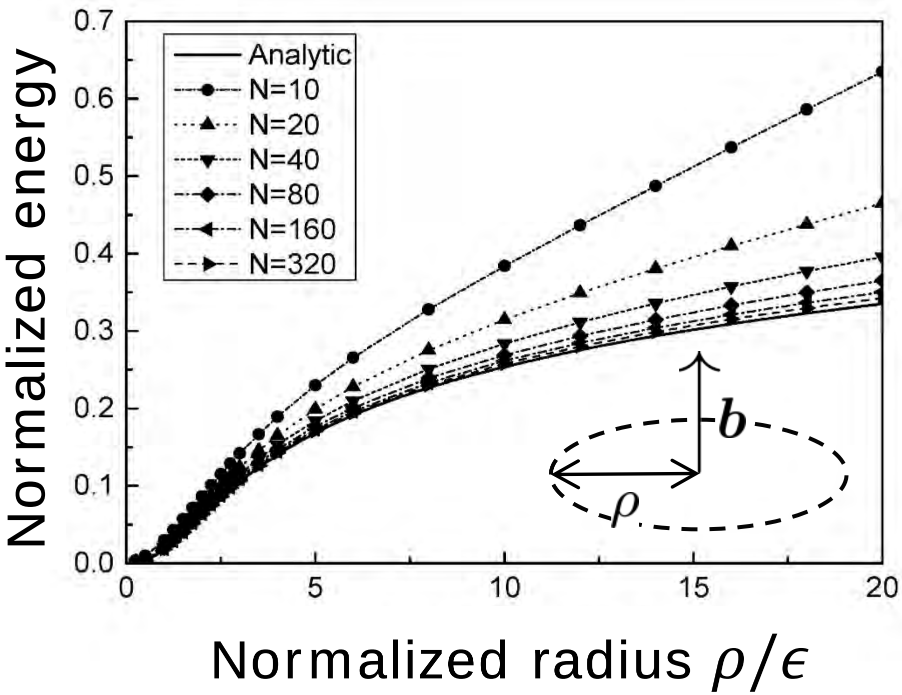
$b_{A2} = [-1\ 1\ 1]$ $b_{A3} = [-1\ 1\ 1]$ $b_{A6} = [-1\ 1\ 1]$

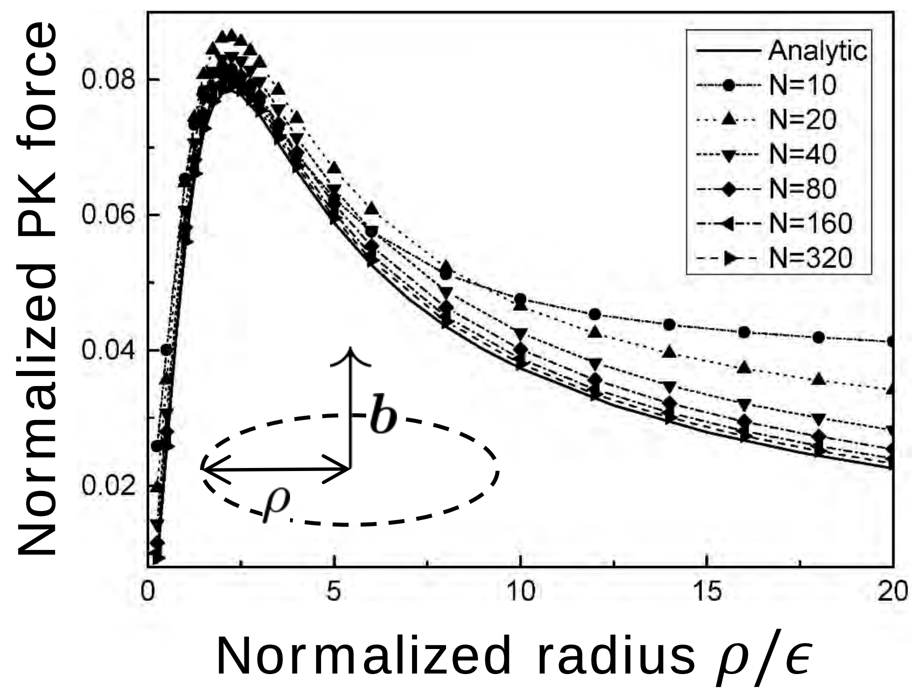




Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Dislocation transport – Convergence





- Convergence to exact elastic force and energy with increasing number of monopoles!

Deffo, A., Ariza, M.P., Ortiz, M., *JMPS*, **122** (2019) 566-589.

Michael Ortiz
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Concluding Remarks

- *Transport problems* belong in *spaces of measures* (NB: pretending otherwise results in loss of opportunity and severe penalties)
- *Particle methods = transport of measures* (but formulation of transport problem must make sense for general measures, including Diracs)
- Powerful *optimal transport* tools:
  - *Wasserstein-type metrics (action, dissipation…)*
  - *Push-forward operations (exact geometrical updates)*
  - *Transport maps (updated Lagrangian formulation)*
- Particle schemes deal simply and effectively with phenomena of staggering *complexity*
- So far *math-free* ☹ Need convergence *analysis!*

Adopt a measure

Michael Ortiz
OW 10/29/18