Transport of Currents

$$\frac{\partial T}{\partial t} - \partial(T \wedge v) = 0$$

M. Ortiz
California Institute of Technology

Berlin Mathematics Research Center (MATH+)
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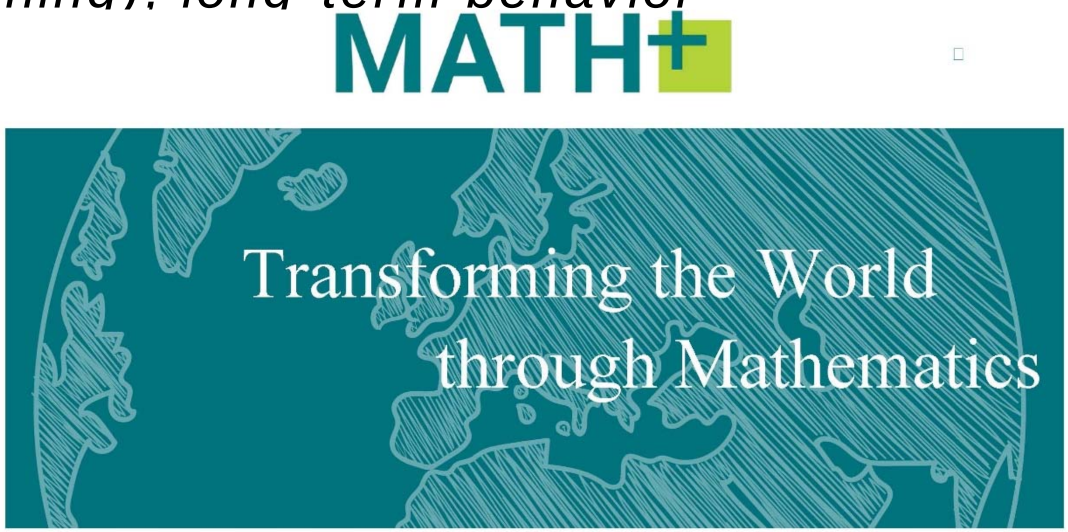
Introduction

- Many *conserved quantities* in physics can be represented mathematically as *currents*
- Currents move and *evolve in time* due to a competition between *energetics, kinetics and inertia*
- Challenge: Bring tools of *geometric measure theory* and *calculus of variations* to bear on the problem:
  - *Analysis: Existence of solutions, relaxation (coase-graining), long-term behavior*
  - *App ... ion*
  - *Phy ... about com*



Current affairs

- Many *conserved quantities* in physics can be represented mathematically as *currents*
- Recall: Vector-valued *smooth p-forms*,

$$\mathcal{D}^p(\Omega;\mathbb{R}^m) = \{\textstyle\sum_{|\alpha|=p} \omega_\alpha dx^\alpha \,:\, \omega_\alpha \in C_c^\infty(\Omega;\mathbb{R}^m)\}$$

- *Exterior derivative:* For every $\omega \in \mathcal{D}^p(\Omega;\mathbb{R}^m)$,

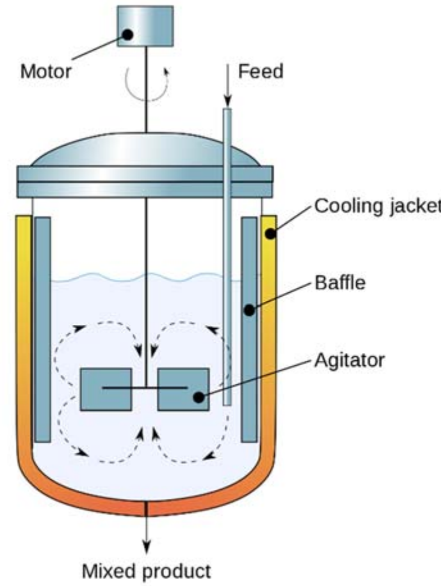
$$d\omega = \textstyle\sum_{|\alpha|=p} d\omega_\alpha \wedge dx^\alpha \in \mathcal{D}^{p+1}(\Omega;\mathbb{R}^m)$$

- A *p-current* is a continuous linear functional on *p-forms*. The space of *p-currents* is $\mathcal{D}_p(\Omega;\mathbb{R}^m)$
- *Boundary operator:* $(\partial T)(\omega) = T(d\omega)$.

Current transport

- *Domain* $\Omega \in \mathbb{R}^d$, open
- *Time-dependent* *p*-current $T : [a, b] \to \mathcal{D}_p(\Omega; \mathbb{R}^m)$
- *Smooth velocity field:* $v : [a, b] \to \mathcal{D}_1(\Omega; \mathbb{R}^n)$
- *Mass* contained in *p*-form ω: $T(\omega)$
- *Inward mass flux* into ω: $T(d(i_v \omega)) := \partial(T \wedge v)(\omega)$
- *Mass conservation:* $\boxed{\dfrac{\partial T}{\partial t} - \partial(T \wedge v) = 0}$
- *NB: The coordinate form of the transport equation depends on the dimension of the current!*

Mass transport



Diffusive transport   Advection-diffusion

- *Mass current* $T := \rho \mathcal{L}^n \in \mathcal{D}_0(\Omega)$, regular measure,

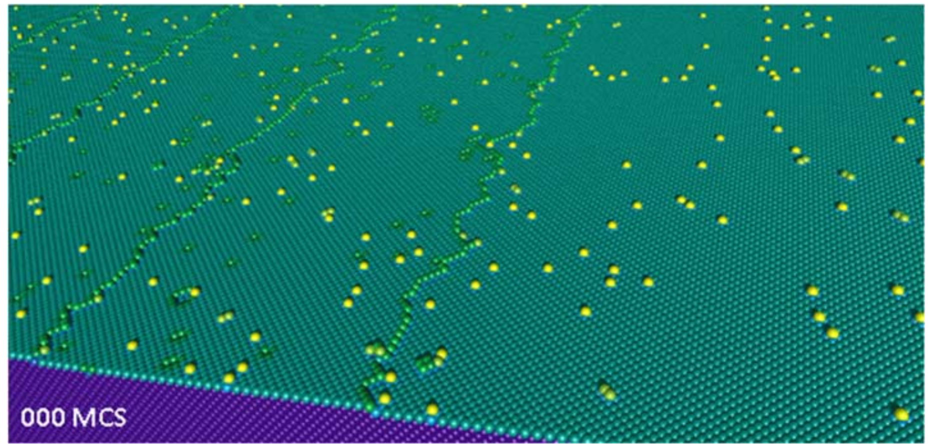
$$T(\omega) = \int_\Omega \rho\omega \, dx, \quad (T \wedge v)(\omega) = \int_\Omega \rho v^i \omega_i \, dx,$$

- *Transport equation:* $\boxed{\dfrac{\partial \rho}{\partial t} + div(\rho v) = 0}$

$\mathcal{D}_0(\Omega)$: Mass transport

Continuous diffusion

Discrete diffusion (© L. Röntzsch)



$$T = \rho \mathcal{L}^d \qquad\qquad T = \textstyle\sum_{i=1}^N m_i \delta_{x_i}$$

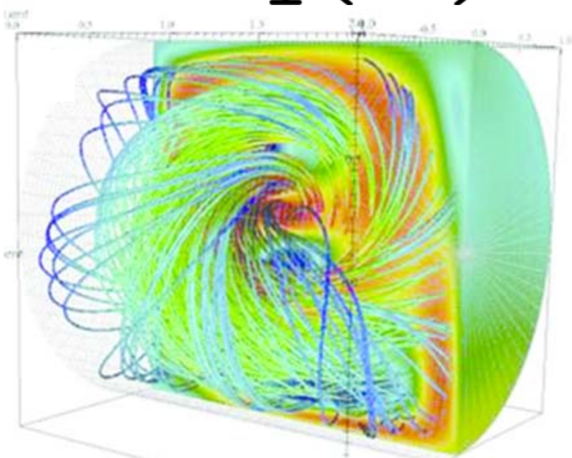
- ***Mass current:*** $T = \rho \mathcal{H}^n \llcorner M$, rectifiable, scalar, flat,

$$T(\omega) = \int_M \rho\omega \, d\mathcal{H}^n, \qquad (T \wedge v)(\omega) = \int_M \rho v^i \omega_i \, d\mathcal{H}^n,$$

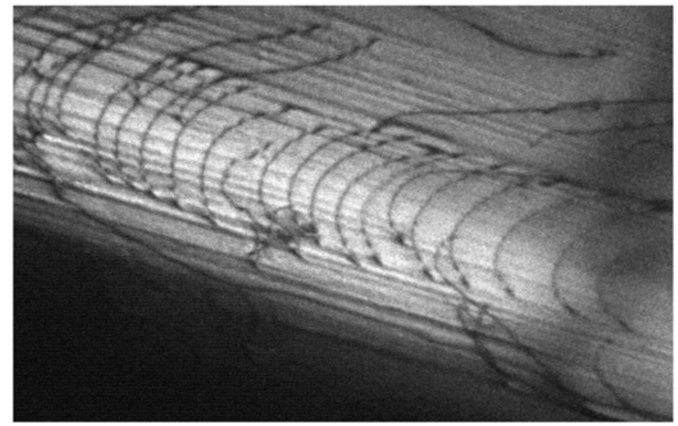
- ***Transport equation:*** (distributionally)

$$\boxed{\frac{\partial \rho}{\partial t} + div(\rho v) = 0}$$

$\mathcal{D}_1(\Omega)$: Line transport



Magnetic field lines in a plasma (Glasser etal 2009)



TEM imaging of dislocations in α-Ti (Kacher etal 2019)

$$T = B\mathcal{L}^d \qquad\qquad T = b \otimes t\,\mathcal{H}^1 \llcorner \gamma$$

- ***Line current:*** $T = B\mathcal{H}^n \llcorner M$, rectifiable, vector, flat,

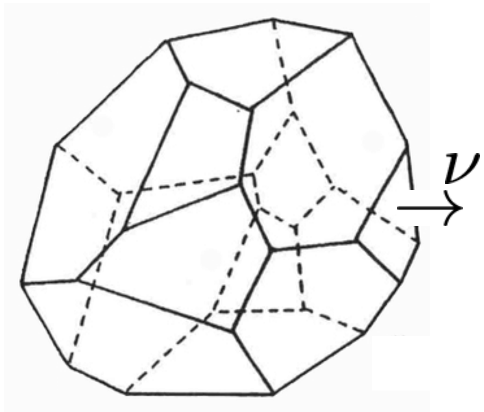
$$T(\omega) = \int_M B(\omega)\, d\mathcal{H}^n, \qquad (T \wedge v)(\omega) = \int_M (B \wedge v)(\omega)\, d\mathcal{H}^n,$$

- ***Transport equation:*** (distributionally)

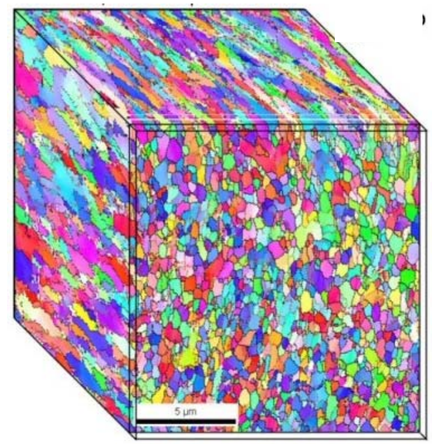
$$\boxed{\frac{\partial B}{\partial t} + curl(B \times v) = 0}$$

Michael Ortiz

$\mathcal{D}_2(\Omega)$: Surface transport



Sharp-interface model
of grain (Smith etal 2015)



3D EBSD reconstruction of
ECAP CuZr (Raabe etal 2011)

$$T = b \otimes *\nu \, \mathcal{H}^2 \llcorner \sigma$$

- *Surface current:* $T = B\mathcal{H}^n \llcorner M$, rectifiable, vector,

$$T(\omega) = \int_M B(\omega)\, d\mathcal{H}^n, \qquad (T \wedge v)(\omega) = \int_M (B \wedge v)(\omega)\, d\mathcal{H}^n,$$

- *Transport equation:* (distributionally)

$$\boxed{\frac{\partial(*B)}{\partial t} + curl((*B) \times v) = 0}$$

Kinetics and energetics

- Currents move and *evolve in time* due to a competition between *energetics, kinetics and inertia*
- Assume current is *integral* and *rectifiable*,

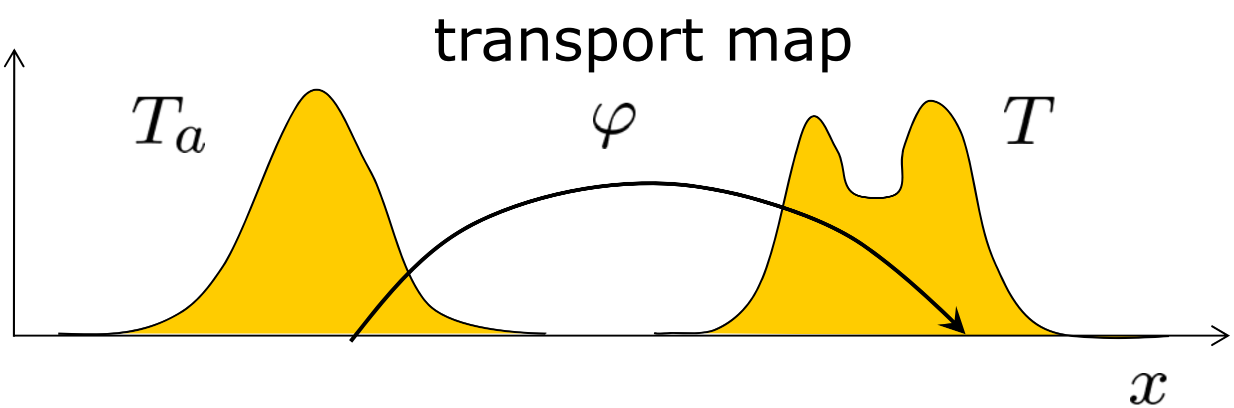
$$T = \theta\, \mathcal{H}^n \llcorner M \wedge \vec{T}, \qquad \|T\| = \theta\, \mathcal{H}^n \llcorner M$$

- The *kinetics* of current motion (mobility law) is encoded into the *dissipation potential*

$$\Psi(v, T) = \int_M \psi(v(x); \theta(x), \vec{T}(x))\, d\mathcal{H}^n$$

- *Energy function:* $E(T)$, not necessarily local:
  - *Entropy of mixing*
  - *Line/surface tension (local)*
  - *Elastic interaction (long range)*

The rate problem



- *Transport map:* $\varphi : \Omega \to \Omega$, sufficiently regular
- *Suppose:* $T = \varphi_{\#} T_a$. Then, there is v such that

$$\frac{\partial T}{\partial t} - \partial(T \wedge v) = 0, \qquad \frac{d}{dt} E(T) = DE(T) v$$

- *Rate problem: At all times, for given* T,

$$F(v) = \Psi(v, T) + DE(T) v \to \min!$$

Weighted Energy-Dissipation functionals

- *WED functionals:* For $\epsilon > 0$, $\varphi(a) = \text{id}$,

$$F_\epsilon(\varphi) = \int_a^b \Big(\Psi(v,T) + DE(T)v\Big)\, w_\epsilon(t)\, dt \to \text{min!}$$

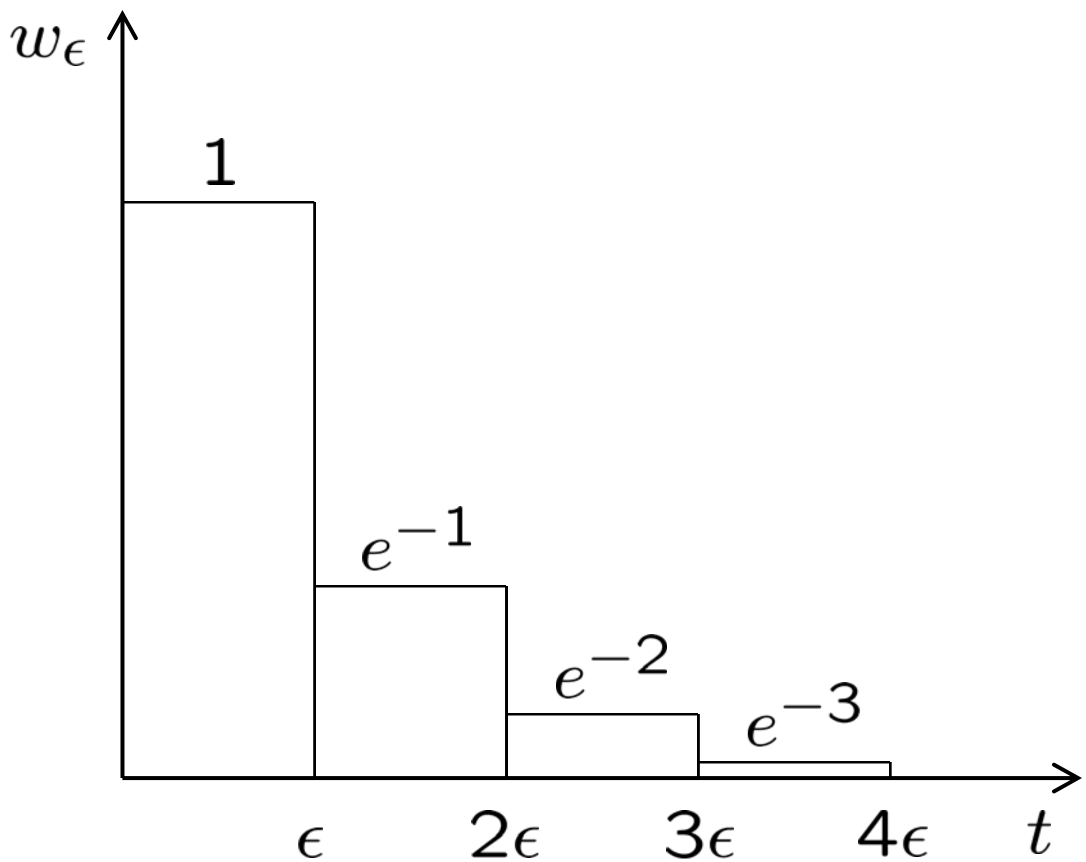
- *Weighting function* w_ϵ positive, decreasing and

$$\lim_{\epsilon\to 0} \frac{w_\epsilon(t)}{w_\epsilon(s)} = 0, \quad \forall s,t \in [a,b], \quad s < t$$

- Expected properties of WED functionals:
  - *Causal limit:* (Approximate) minimizers φ_ϵ of F_ϵ converge to solutions of the (relaxed) problem
  - *Approximation:* Convergence stable with respect to Gamma convergence $\Psi_h \to \Psi$, $E_h \to E$

A. Mielke and M. Ortiz, ESAIM: COCV 14 (2008) 494–516.

Variational time discretization



- *Stepwise weighting function*: For $k = 0, 1, \dots,$

$$w_\epsilon = \mathrm{e}^{-k}, \qquad k\epsilon \leq t - a < (k+1)\epsilon$$

Variational time discretization

- *Stepwise WED functionals:* For $\epsilon > 0$, $\varphi_0 = \mathrm{id}$,

$$F_\epsilon(\varphi) = \sum_{k\in\mathbb{N}} \Big(D_\epsilon(\varphi_k, \varphi_{k+1}) + E(\varphi_{k+1}) - E(\varphi_k) \Big) \, \mathrm{e}^{-k}$$

- *Dissipation cost* (a la Wasserstein):

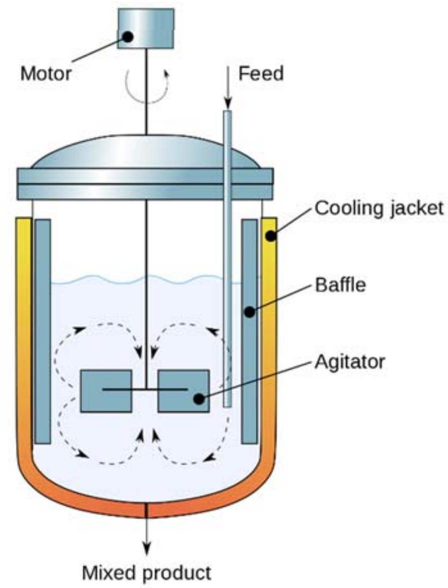
$$D_\epsilon(\varphi_k, \varphi_{k+1}) = \inf_{\text{paths } \varphi_k \to \varphi_{k+1}} \int_0^\epsilon \Psi(v(s), T(s)) \, ds$$

- *Geometrically exact update:*

$$T_{k+1} = (\varphi_{k\to k+1})_\# T_k$$

- *NB: Fundamental departure from traditional time discretization methods based on divided differences!*

Mass transport – Advection/diffusion



- Transport equation: $\partial_t \rho + \nabla \cdot (\rho v) = 0$
- Dissipation functional: $\Psi(v, \rho) = \int_\Omega \frac{1}{2} \rho |v|^2 \, dx$
- Energy functional: $E(\rho) = \int_\Omega \kappa \rho \log \rho \, dx$

Mass transport — Time discrete (I)

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

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

- EL equation: $\dfrac{x - \varphi_{k+1\to k}}{t_{k+1} - t_k} = -\kappa\nabla \log \rho_{k+1}$
- Push-forward: $\rho_{k+1} = \rho_k / \det(\nabla\varphi_{k\to k+1})$

geometrically exact! 

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

Mass transport – Time discrete

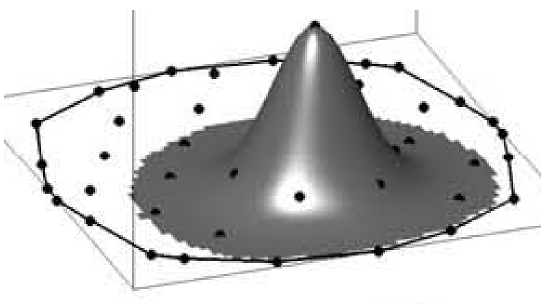
- Weak form of incremental transport equations:

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

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

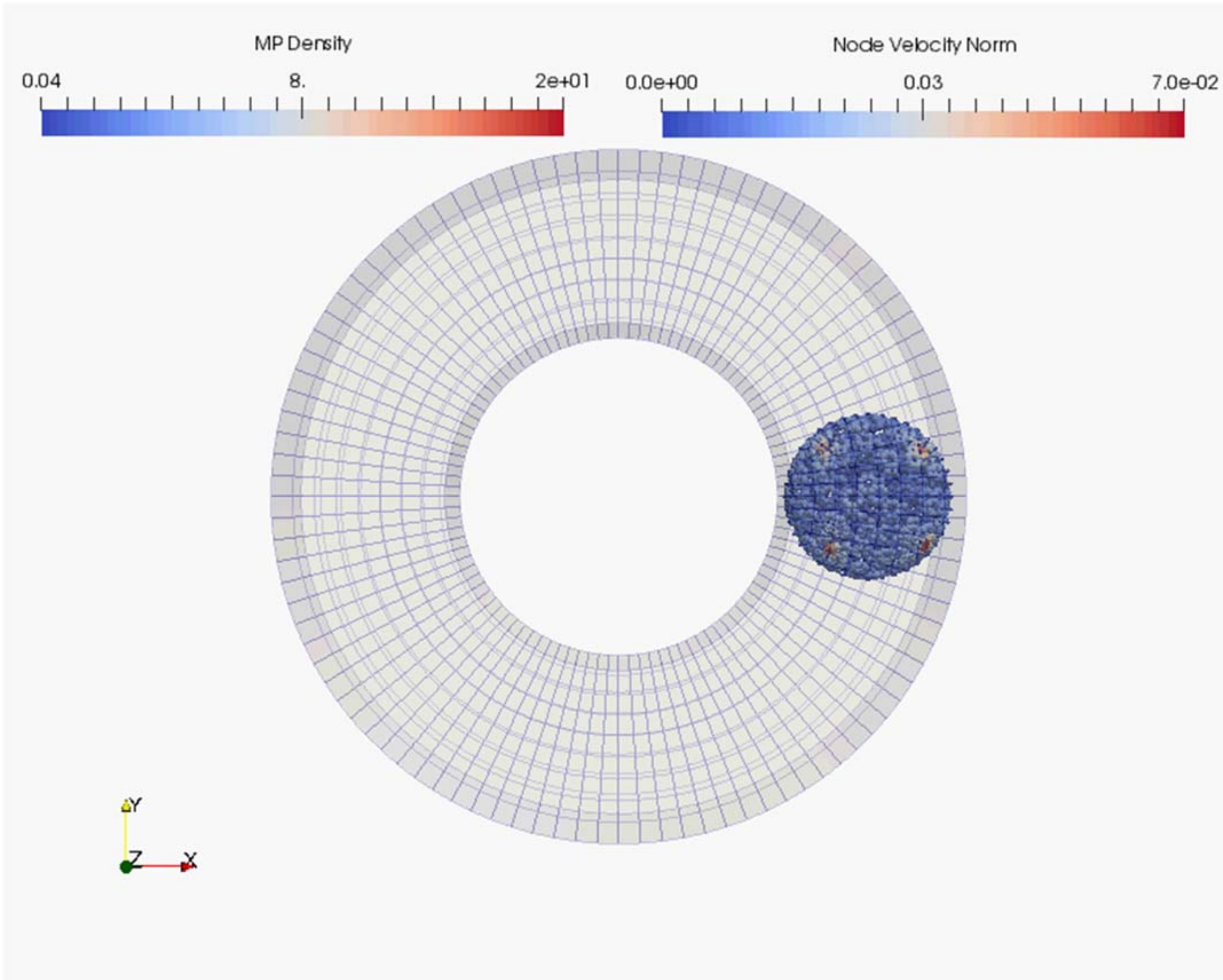
- Particle *ansatz*: $\rho_k(x) = \sum_{p=1}^{h} m_{p,k}\, \delta\big(x - x_{p,k}\big)$

- Incremental transport map interpolation:



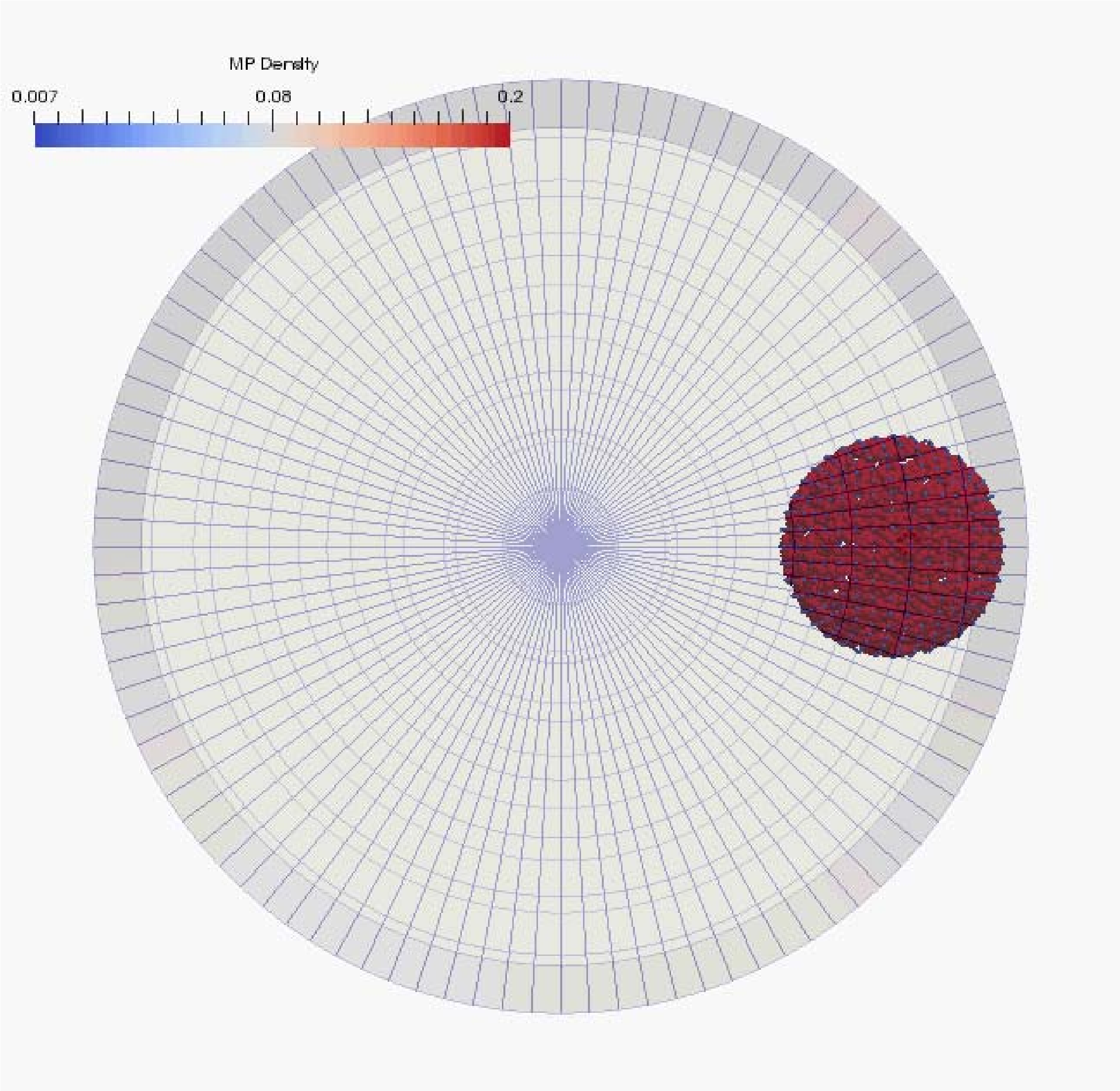
$$\varphi_{k\to k+1}(x) = \sum_{a=1}^{h} x_{a,k+1} N_{a,k}(x)$$

Pure advection in cylindrical channel



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

Advection-diffusion in rotating flow cell



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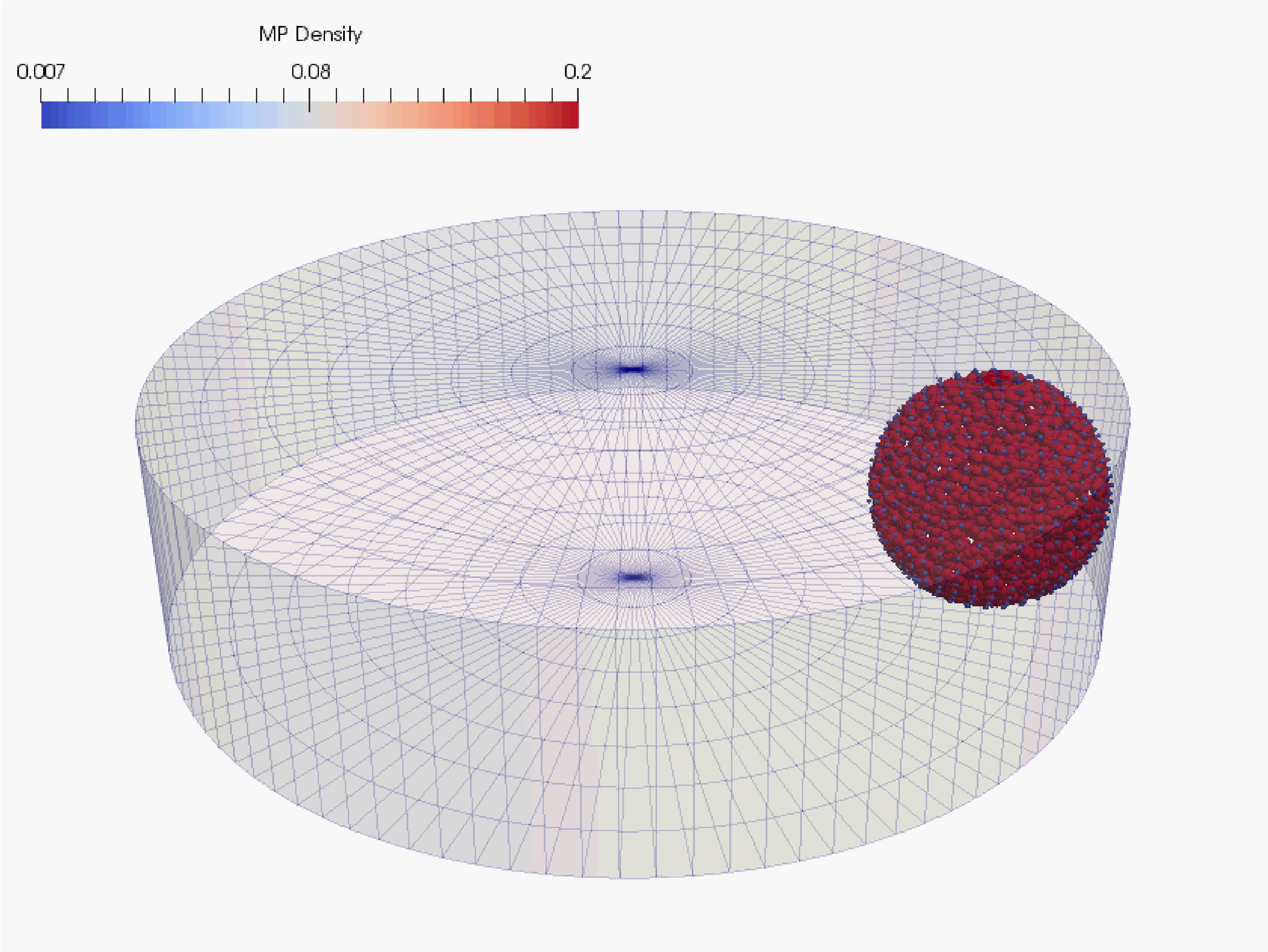
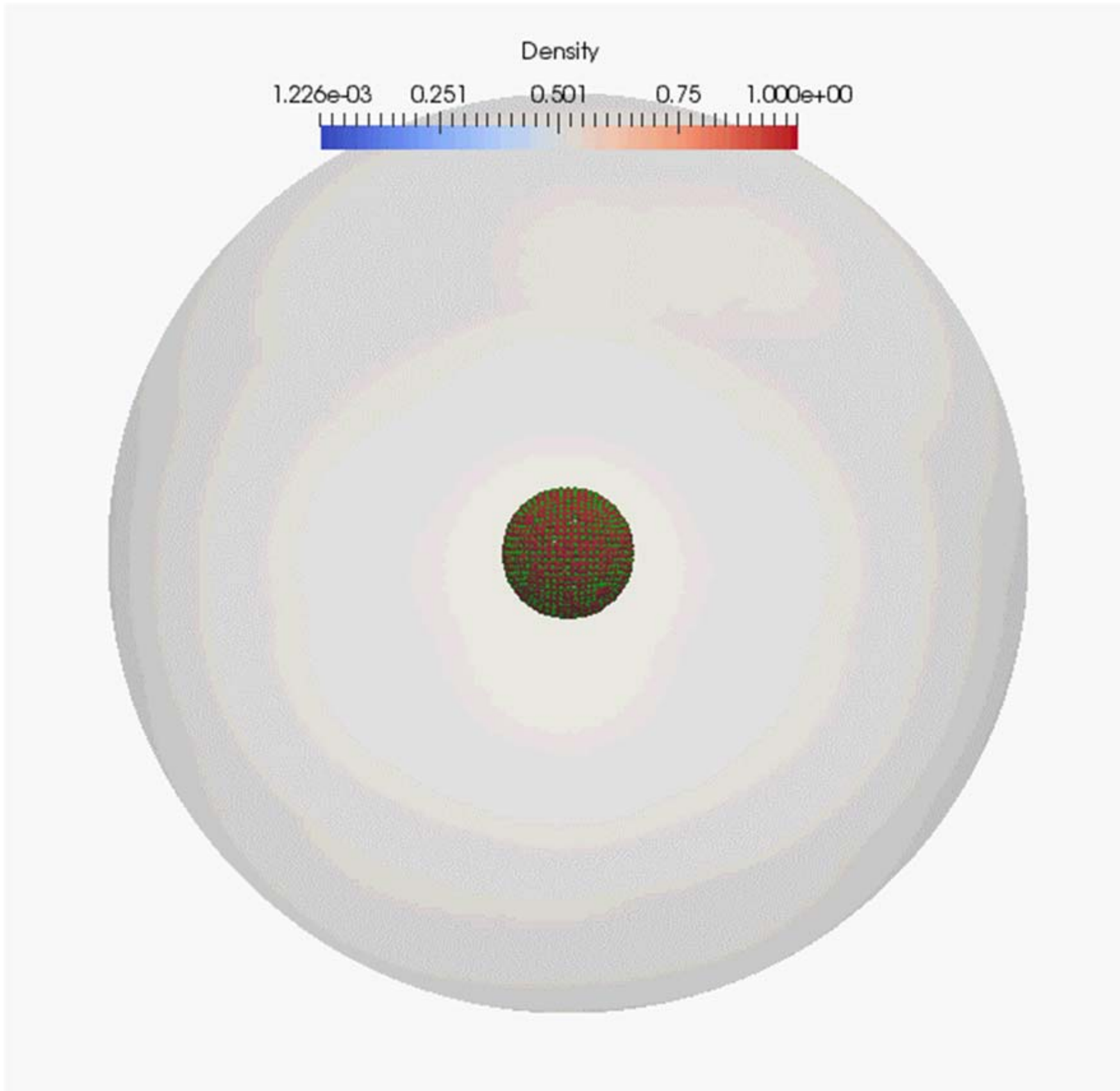
Advection-diffusion in rotating flow cell



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

Pure diffusion in spherical domain



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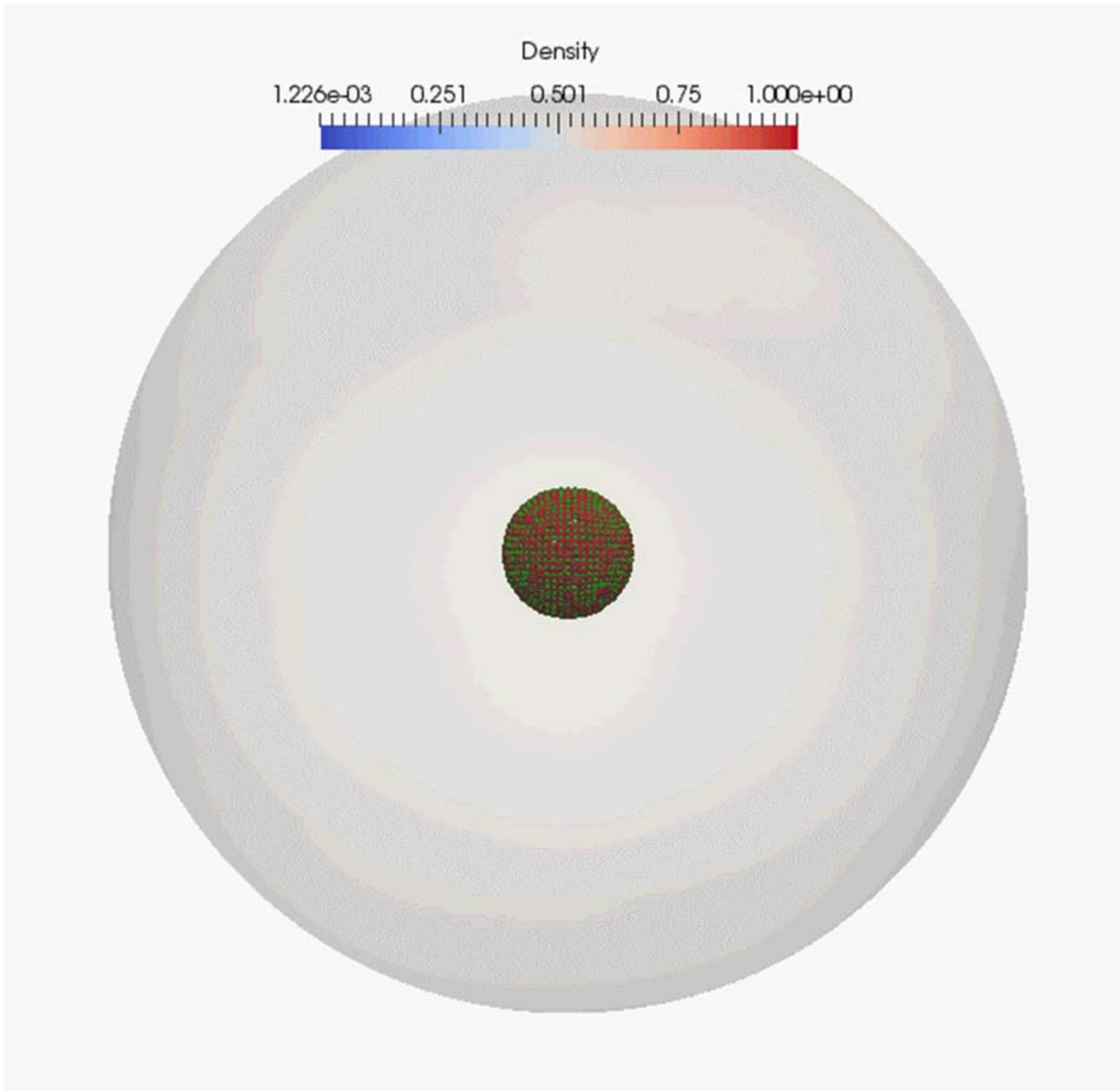
Pure diffusion in spherical domain



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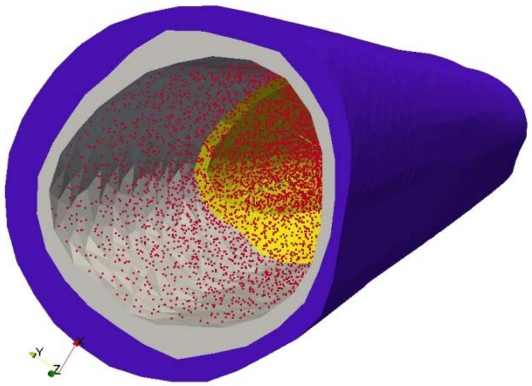
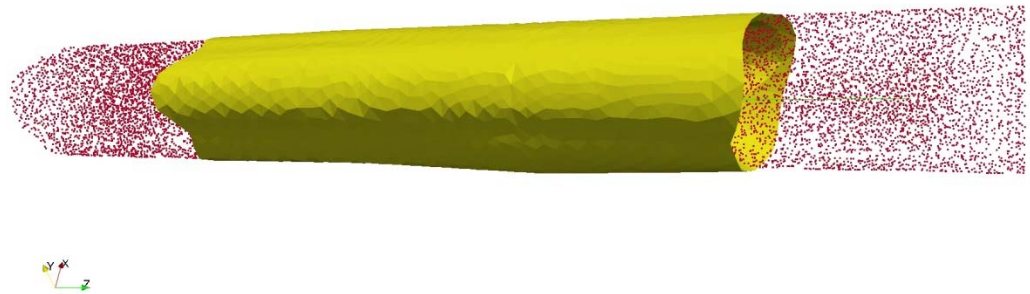
Flow problems





- Mass + linear-momentum transport:

$$\partial_t \rho + \nabla \cdot (\rho\, v) = 0,$$

$$\partial_t (\rho v) + \nabla \cdot (\rho\, v \otimes v) = \nabla \cdot \sigma,$$

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

Flow problems – Time-discrete

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

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

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

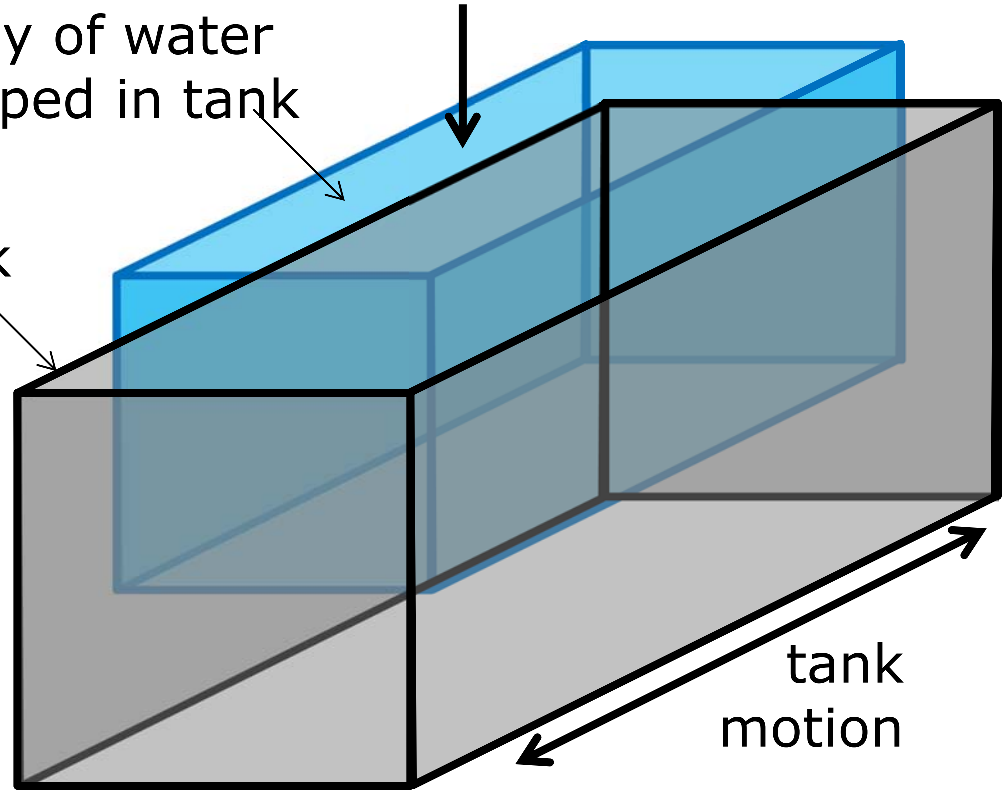
(geometrically exact mass conservation!)

- 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.

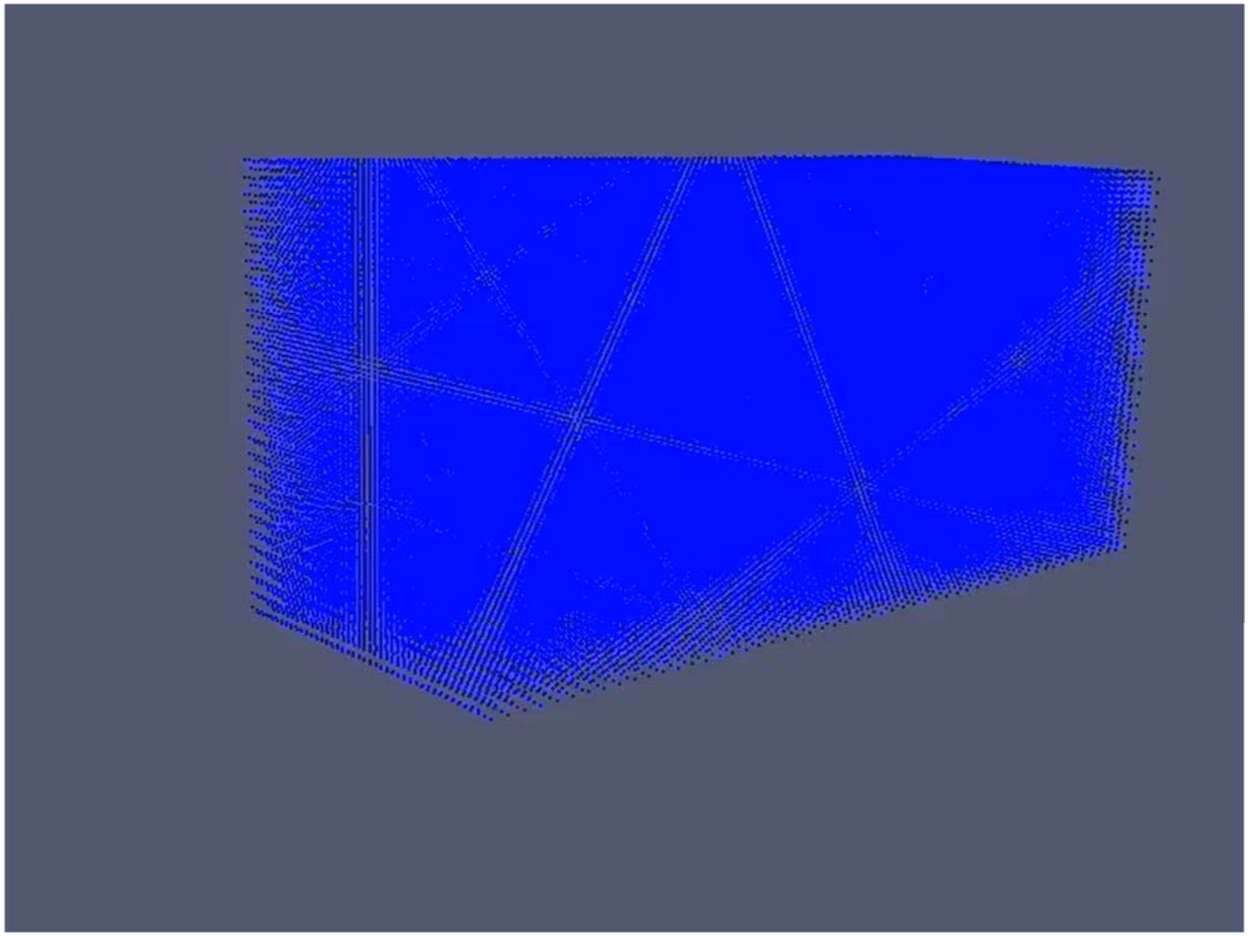
Flow problems – Sloshing



Dirk Hartmann, Siemens AG, Munich (2011).

Dreier, N.A., Engwer, C. and Hartmann, D., *IJNMF*, **88** (2018) 100.

Flow problems – Tank sloshing

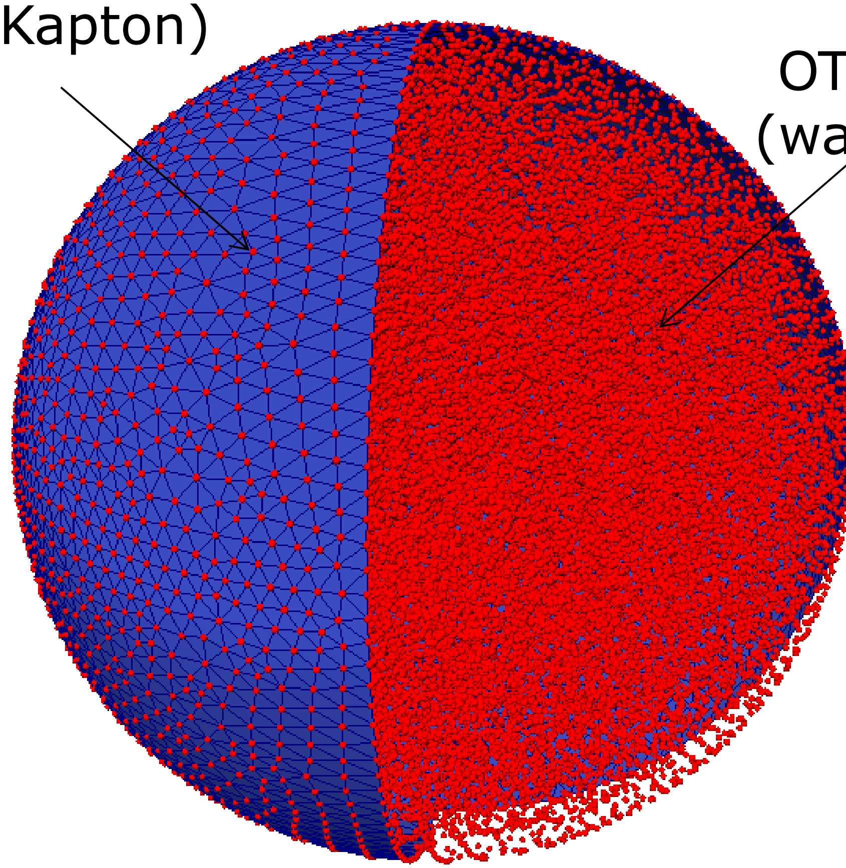


Dirk Hartmann, Siemens AG, Munich (2011).
Dreier, N.A., Engwer, C. and Hartmann, D., *IJNMF*, **88** (2018) 100.

Flow problems – Balloons

Balloon system for Spirit rover Mars landing (JPL, 2004)

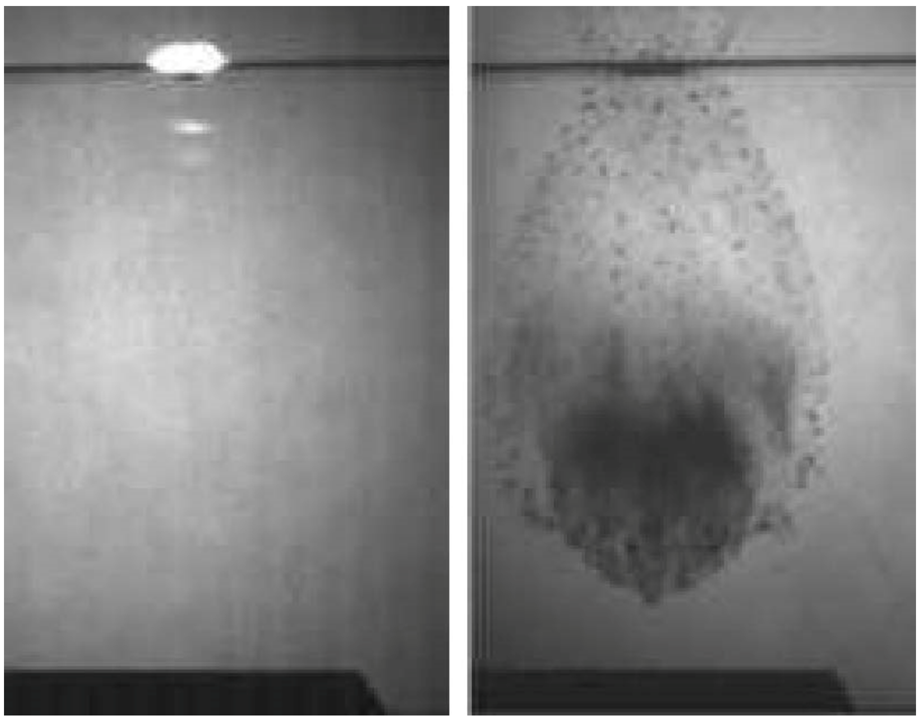
FE membrane (rubber, Kapton)



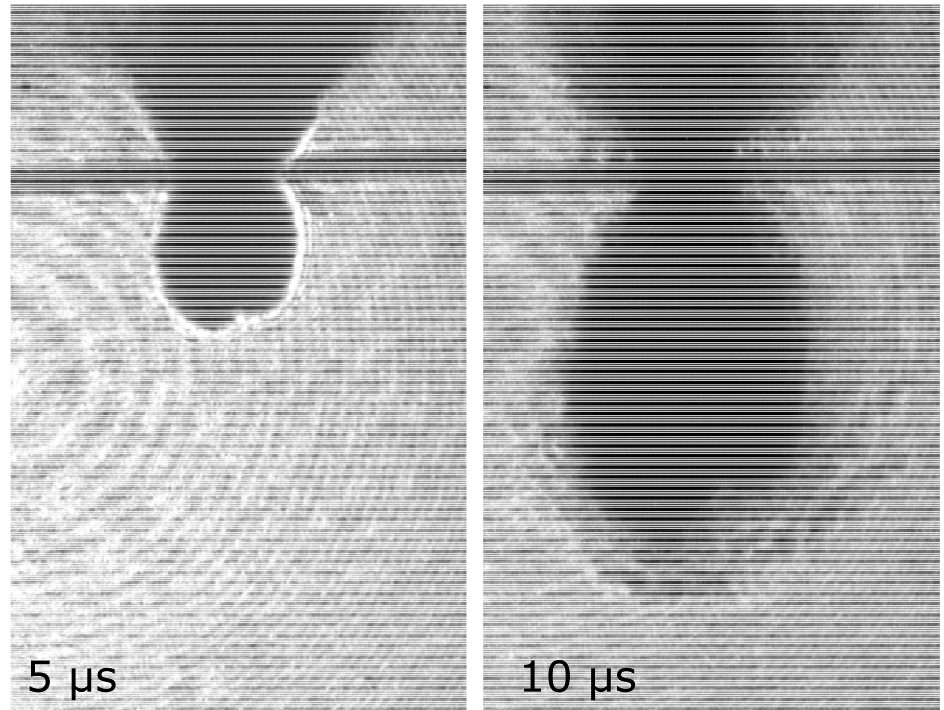
OTM fluid (water, air)

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

Flow problems – HV impact



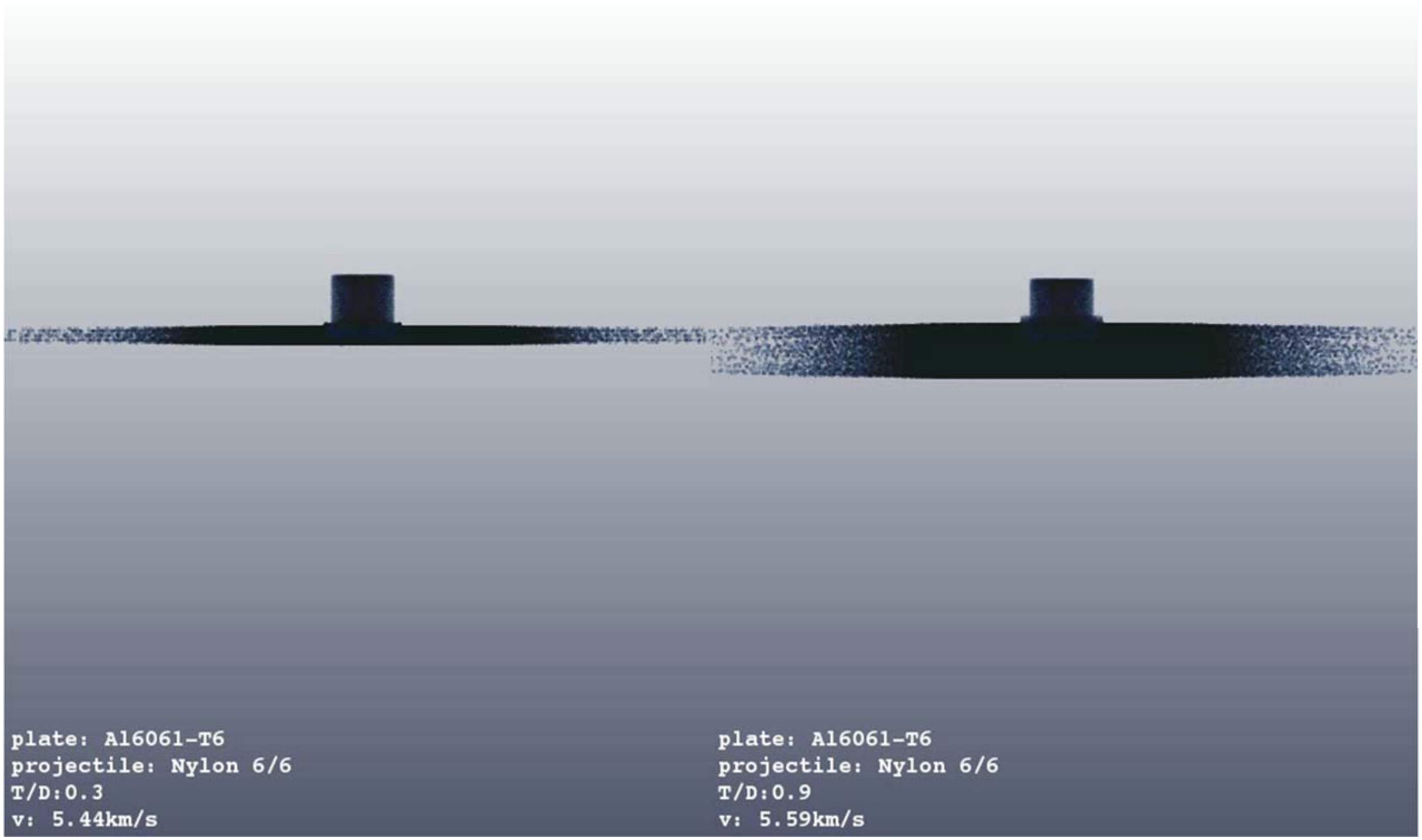
Hypervelocity impact of bumper shield. a) Initial impact flash. b) Debris cloud (Ernst-Mach Inst., Freiburg, Germany).



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

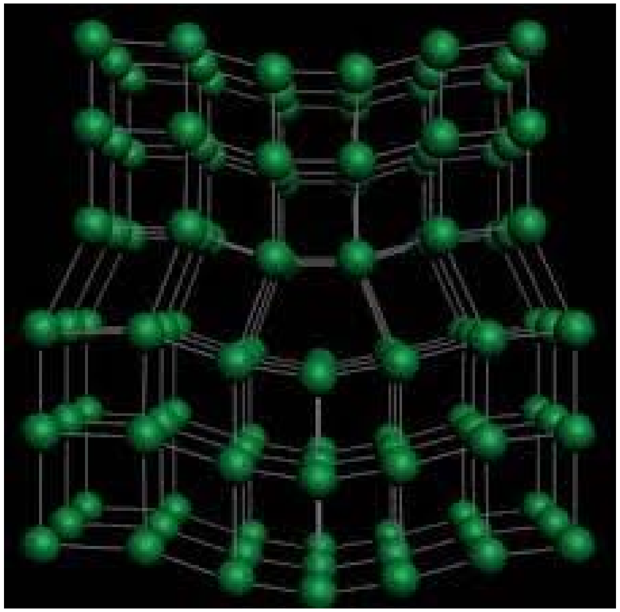
Li, B., Habbal, F. and Ortiz, M. , *IJNME*, **83** (2010) 1541.
Li, B. et al., *Procedia Engineering*, **58** (2013) 320.
Li, B., Stalzer, M. and Ortiz, M., *IJNME*, **100** (2014) 40.

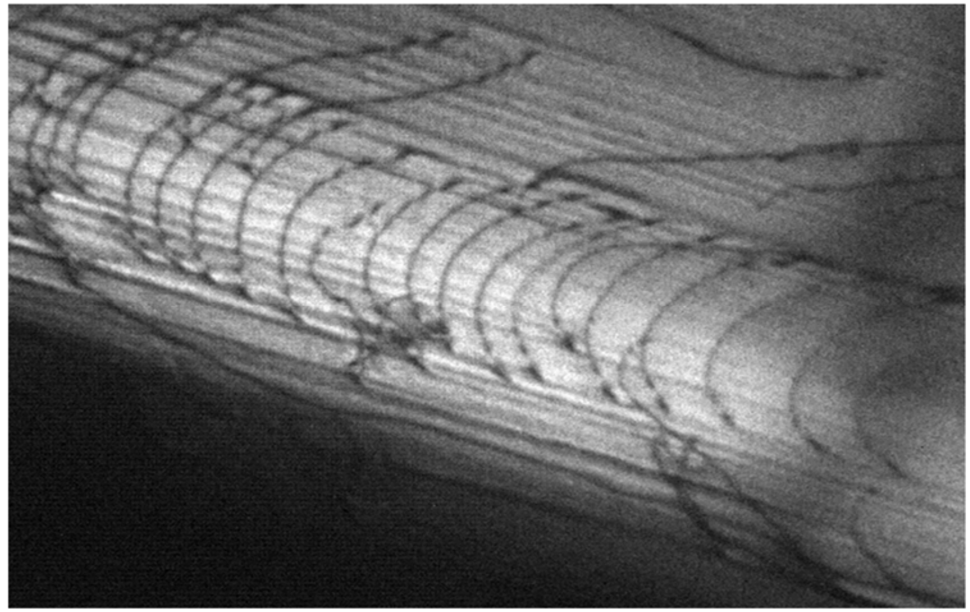
Flow problems – HV impact



Li, B., Habbal, F. and Ortiz, M. , *IJNME*, **83** (2010) 1541.
Li, B. et al., *Procedia Engineering*, **58** (2013) 320.
Li, B., Stalzer, M. and Ortiz, M., *IJNME*, **100** (2014) 40.

Dislocation transport



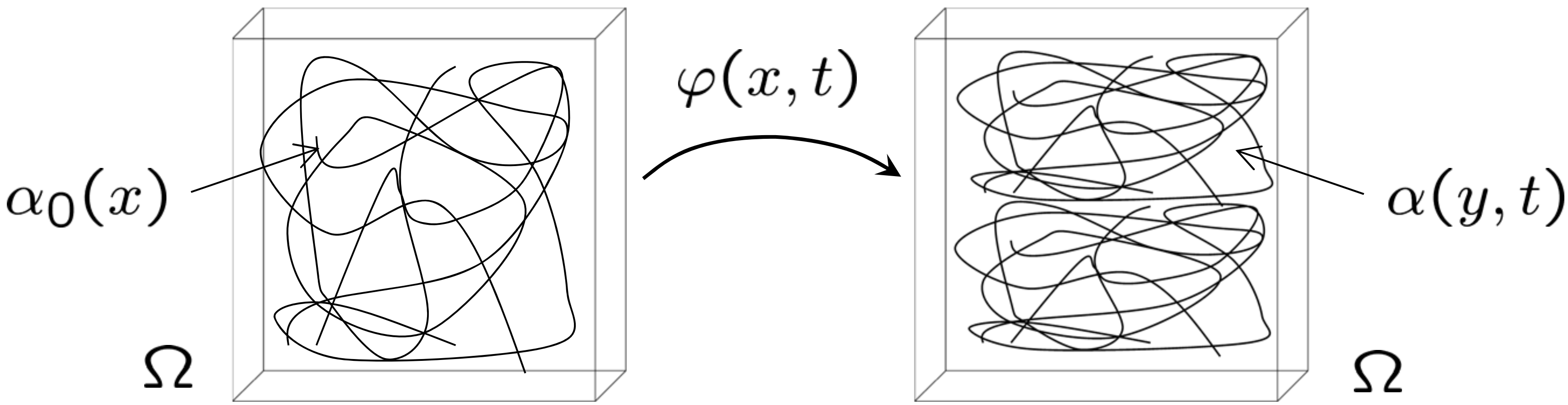


- Dislocation current: $\alpha = b \otimes t \, \mathcal{H}^1 \llcorner \gamma$
- Transport equation: $\dot{\alpha} + \mathrm{curl}\,(\alpha \times v) = 0$
- Dislocation mobility + elastic interaction

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

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

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

- Incremental minimum principle:

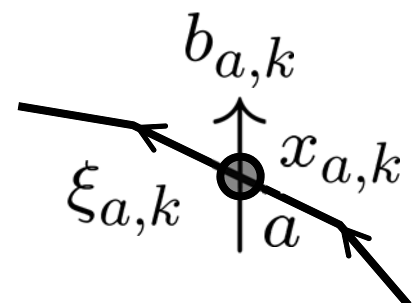
$$\varphi_{k+1} \in \operatorname{argmin} F(\varphi_k, \cdot\,)$$

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

Dislocation transport – Discrete

- 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:

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



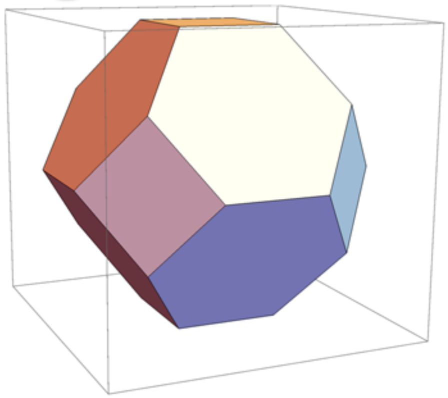
- Incremental transport map discretization:

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

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

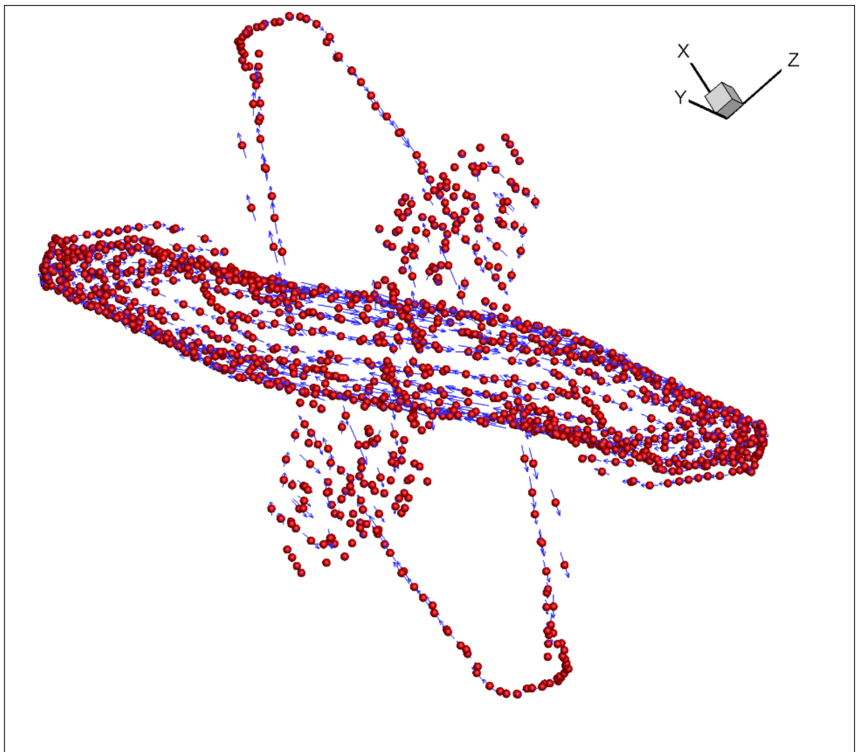
Deffo, A., Ariza, M.P., Ortiz, M., *JMPS,* **122** (2019) 566-589.

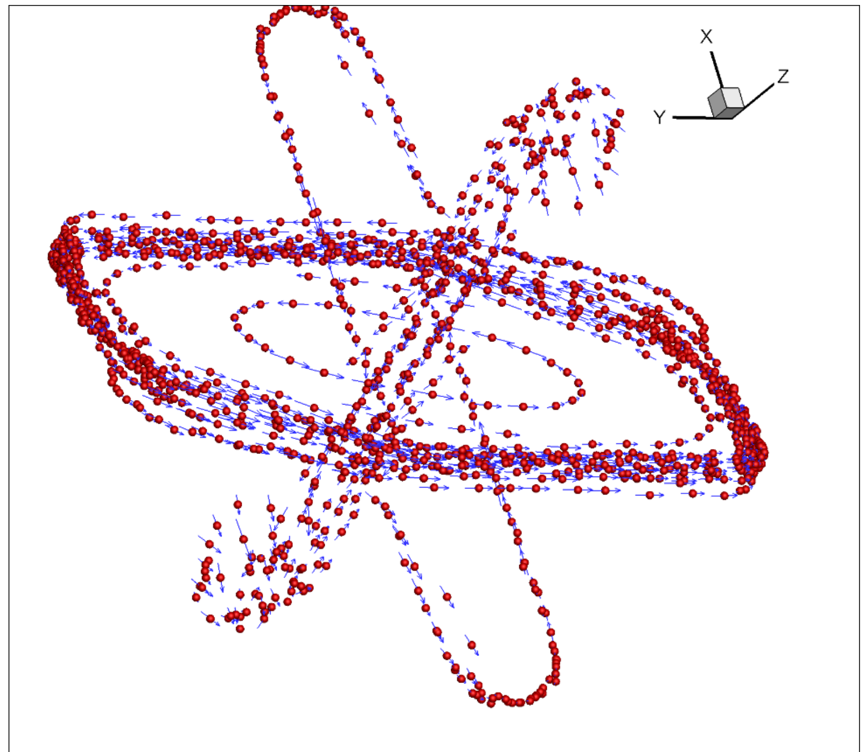
Dislocation transport – BCC grain



- 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.

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*

Adopt a measure

Michael Ortiz
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