Transport of Currents

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Overview

- 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:
  - *Physics: Developing a mathematical understanding of behavior of classes of energies and kinetic laws*
  - *Approximation: Spatial and time discretization*
    - *Provably convergent particle methods*
    - *Time-discrete (Wasserstein) gradient flows*
  - *Analysis: Existence of solutions, relaxation (multiscale analysis), long-term behavior…*

Transport

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

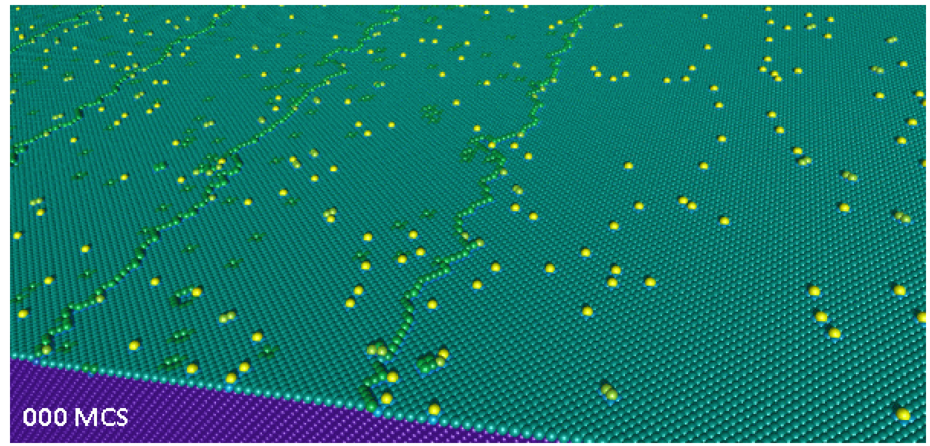
- *Domain* $\Omega \in \mathbb{R}^d$, open
- *Time-dependent* *p*-current $T : [a,b] \to \mathcal{D}_p(\Omega; \mathbb{R}^m)$
- *Smooth velocity field:* $v : [a,b] \to \mathcal{D}_1(\Omega; \mathbb{R}^n)$
- *Mass* contained in *p*-form ω: $T(\omega)$
- *Inward mass flux* into ω: $T(d(i_v \omega)) :=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

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

Continuous diffusion

$$T = \rho \mathcal{L}^d$$

Discrete diffusion (© L. Röntzsch)



$$T = \sum_{i=1}^N m_i \delta_{x_i}$$

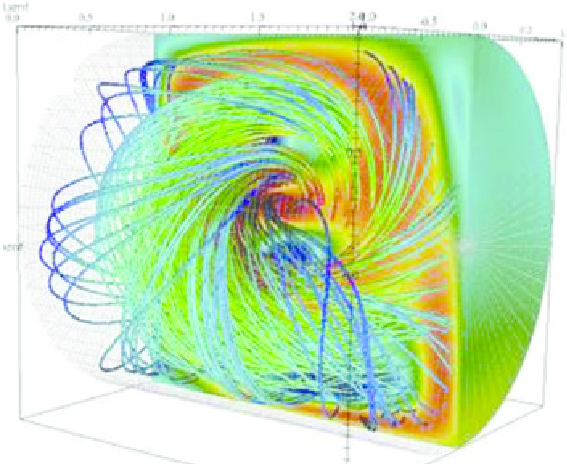
- *Mass current:* $T = \rho \mathcal{H}^n \llcorner M$, rectifiable, scalar, flat,

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

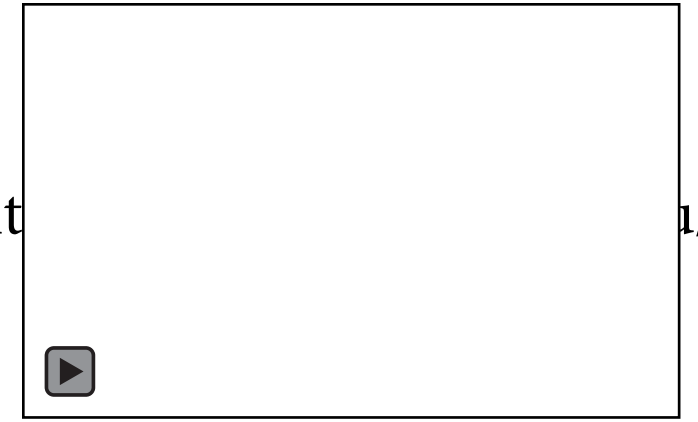
- *Transport equation:* (distributionally)

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

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



Magnetic field lines in a plasma (Glasser *etal* 2009)



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

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

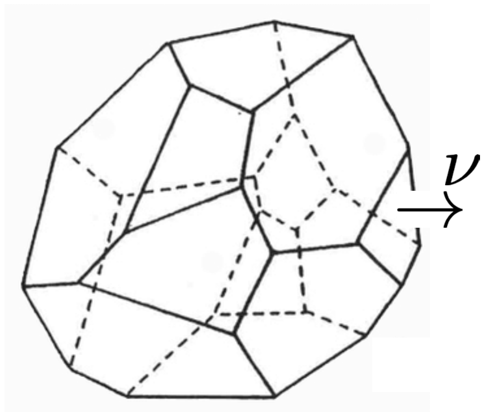
- *Line current:* $T = B\mathcal{H}^n \llcorner M$, rectifiable, vector, flat,

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

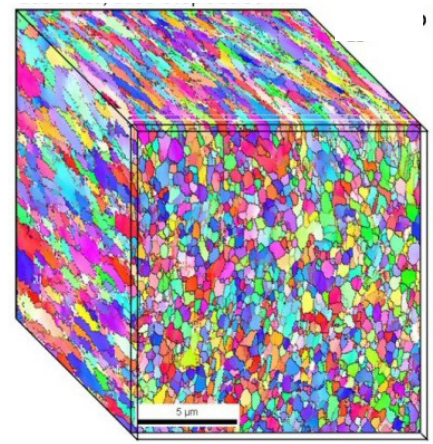
- *Transport equation:* (distributionally)

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

$\mathcal{D}_2(\Omega)$: 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,

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

- *Transport equation:* (distributionally)

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

Kinetics and energetics

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

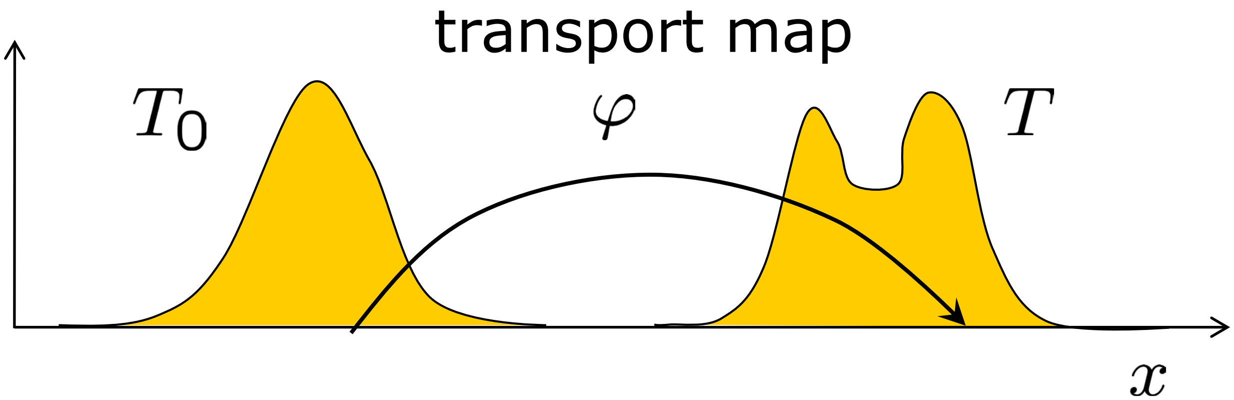
$$T = \theta\, \mathcal{H}^n \llcorner M \wedge \vec{T}, \qquad \|T\| = \theta\, \mathcal{H}^n \llcorner M$$

- 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:* $T = \varphi_{\#} T_0$. Then, there is v such that

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

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

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

- Non-cooperative *game* with players $v(t)$!

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

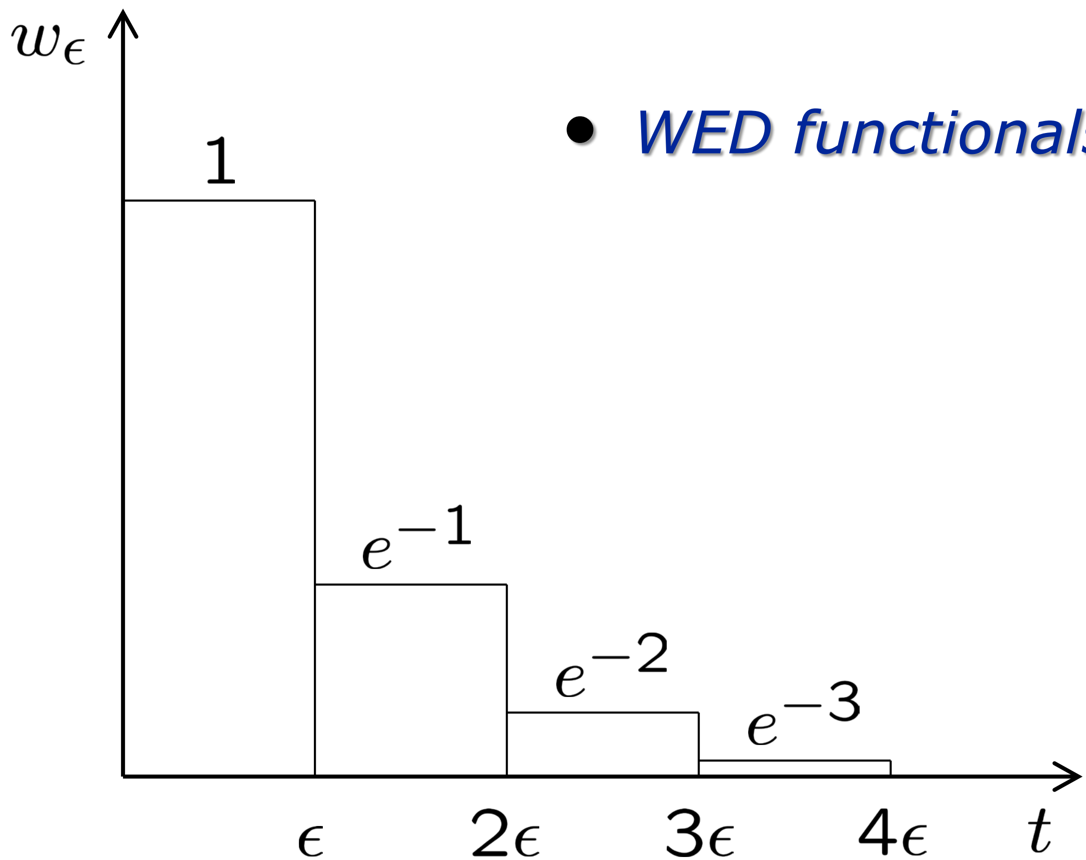
$$\lim_{\epsilon\to 0} \frac{w_\epsilon(t)}{w_\epsilon(s)} = 0, \quad \forall s,t \in [a,b], \quad s < t$$

- Expected properties of WED functionals:
  - *Causal limit:* (Approximate) minimizers φ_ϵ of F_ϵ converge to solutions of the (relaxed) problem[1]
  - *Approximation:* Convergence stable with respect to Gamma convergence[1] $\Psi_h \to \Psi$, $E_h \to E$

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

Numerics

Variational time discretization



- *WED functionals:*

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

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

Variational space–time discretization

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

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

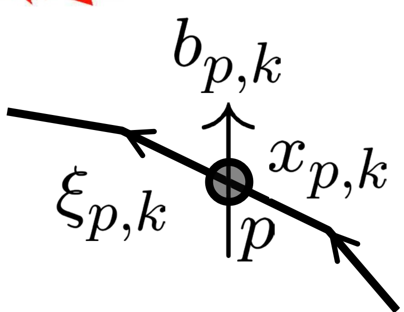
- *Dissipation cost* (a la Wasserstein):

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

- *Geometrically exact update:*

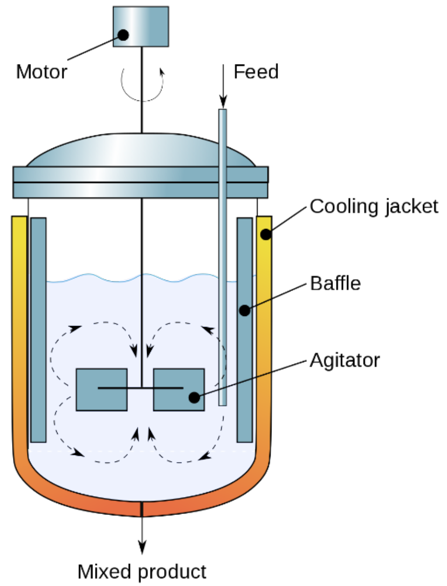
$$T_{k+1} = (\varphi_{k\to k+1})_\# T_k$$

- *Particle discretization* (Dirac masses):



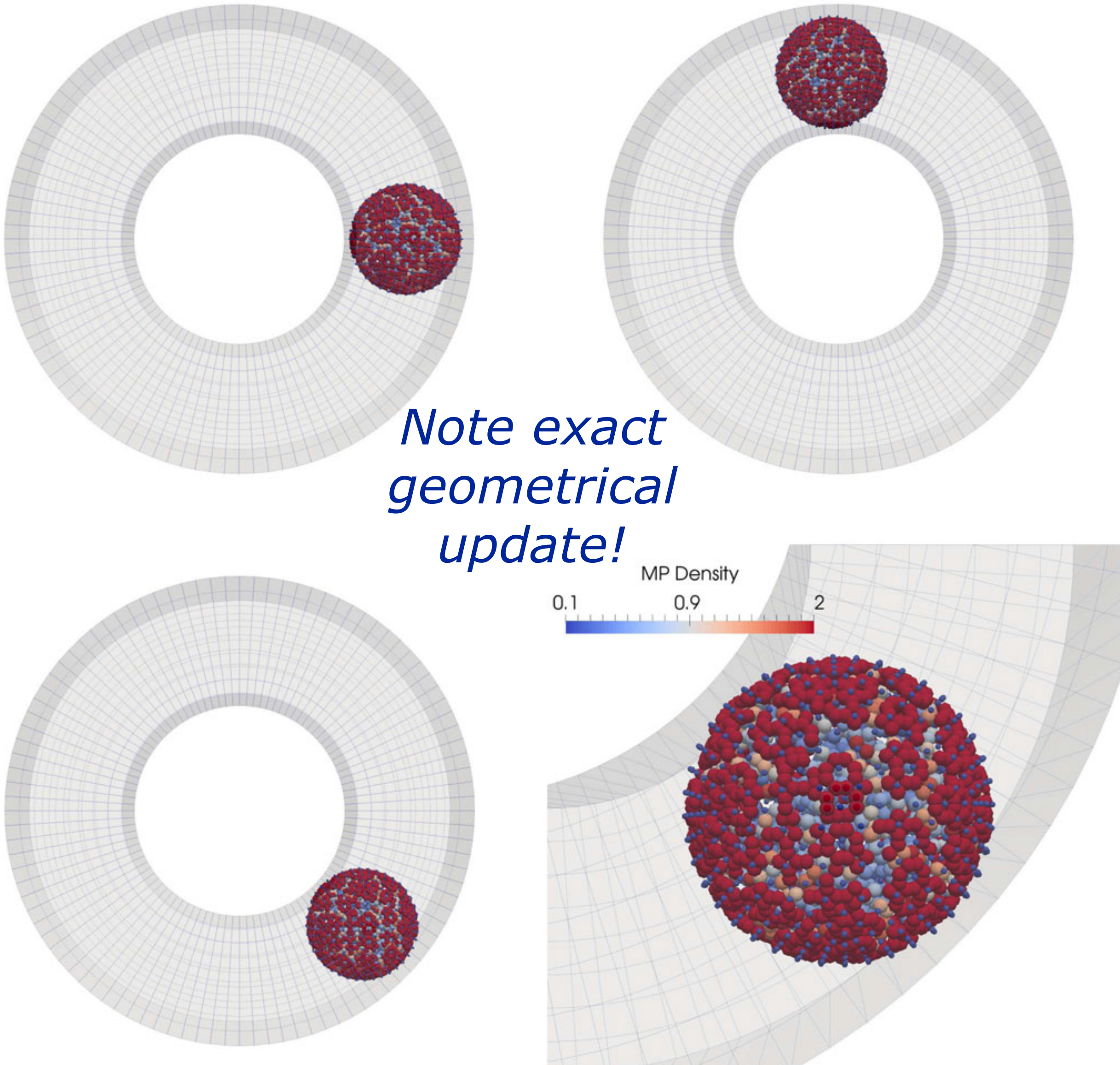
$$T_k = \textstyle\sum_{p=1}^N b_{p,k} \otimes \xi_{p,k}\, \delta_{x_{p,k}}$$

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: $E(\rho) = \int_\Omega \kappa \rho \log \rho \, dx$

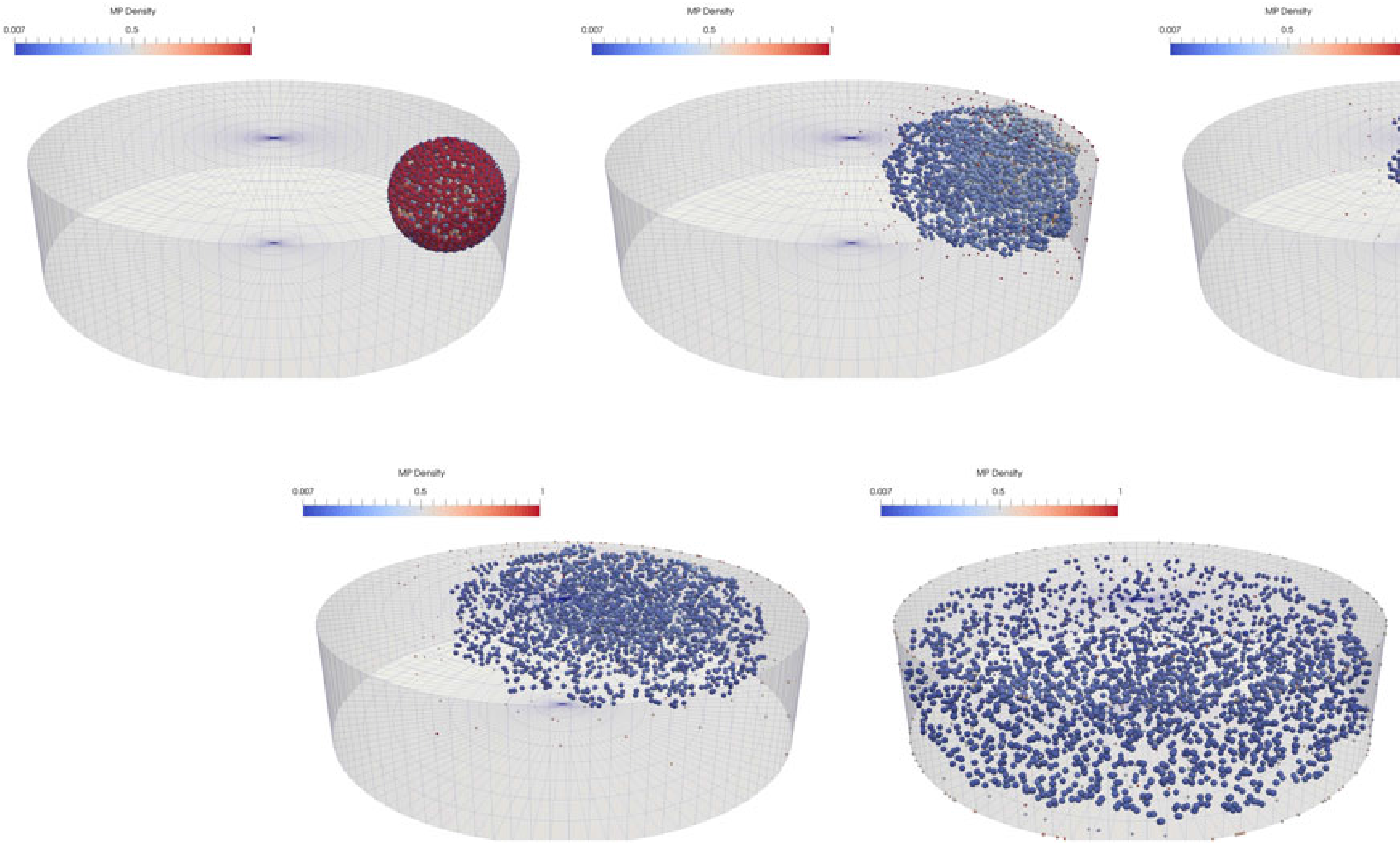
Pure advection in cylindrical channel



Note exact geometrical update!

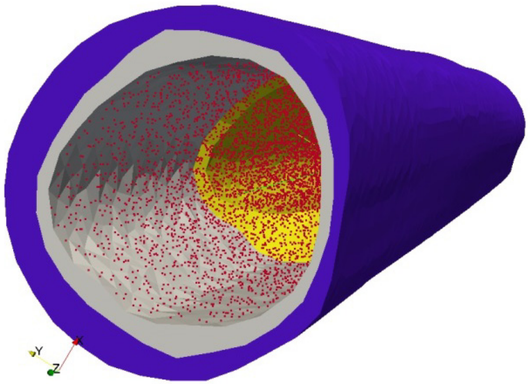
Fedeli L, Pandolfi A, Ortiz M. *IJNME,* **112**(9) (2017) 1175-93.

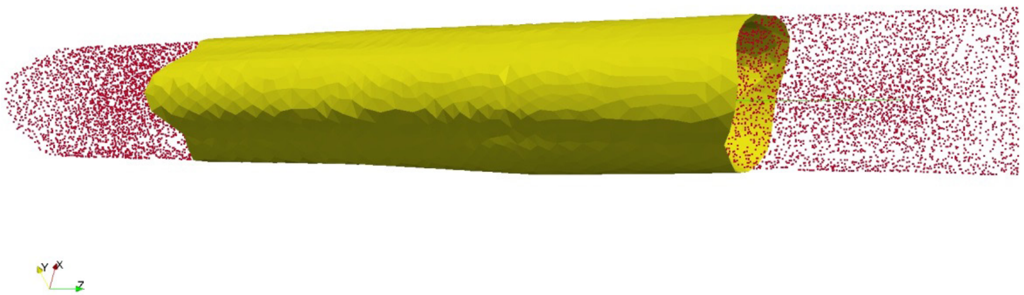
Advection-diffusion in rotating flow cell



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

Flow problems





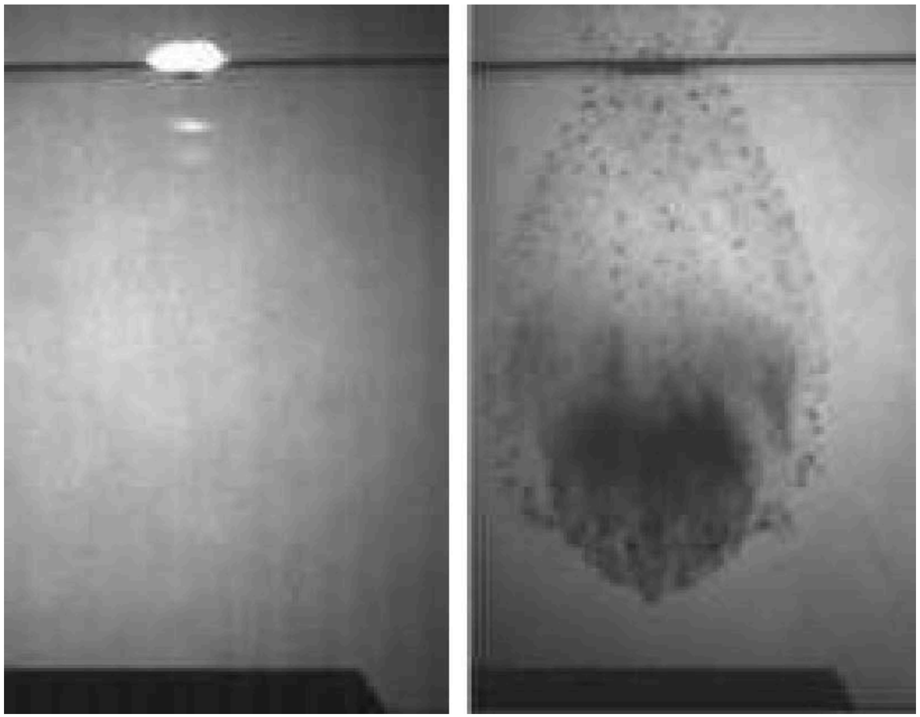
- Mass + linear-momentum transport:

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

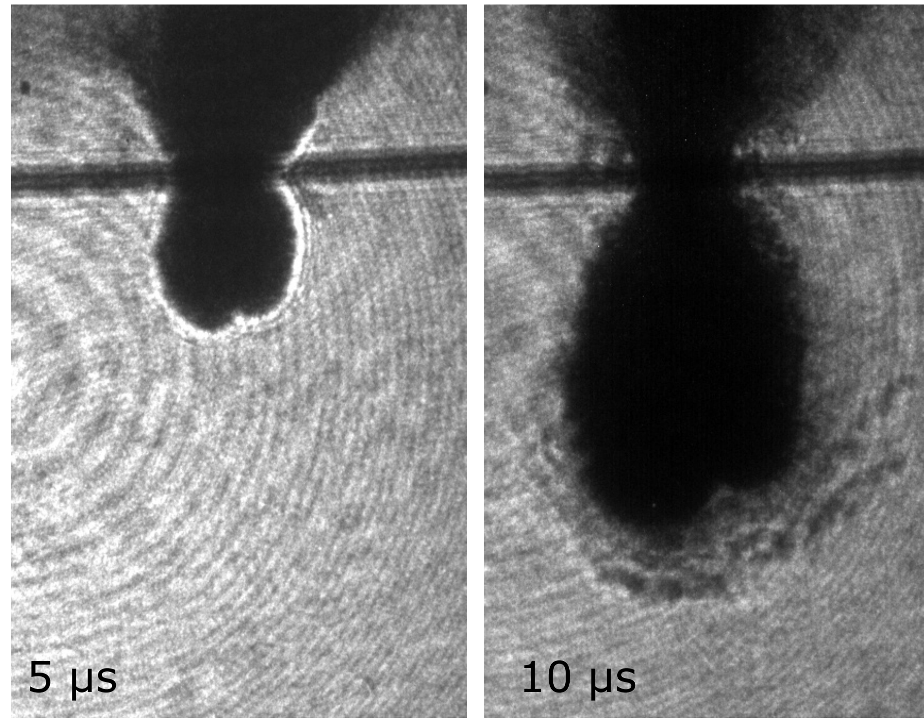
$$\partial_t (\rho v) + \nabla \cdot (\rho\, v \otimes v) = \nabla \cdot \sigma,$$

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

Flow problems — HV impact



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



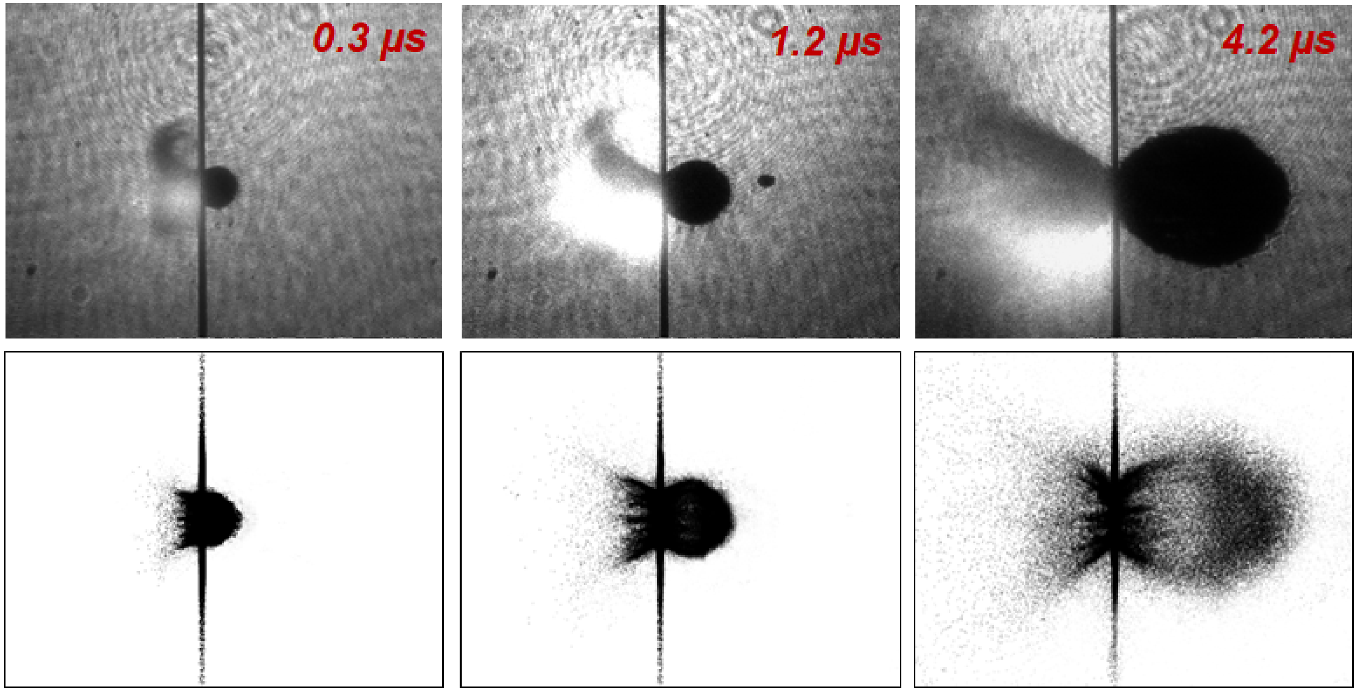
Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

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

Nylon 6/6, L/D=1 Cylinder
6061-T6 Al. Target

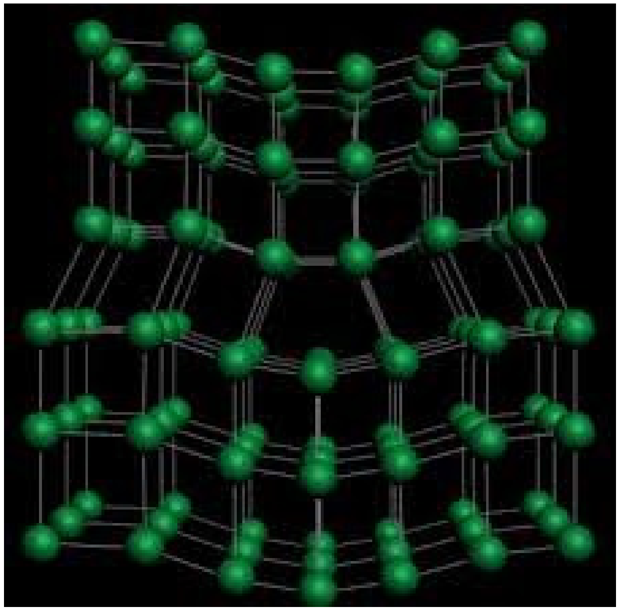
v_{impact} = 5.84 km/s
h = 0.5 mm (20 mil) at 0°

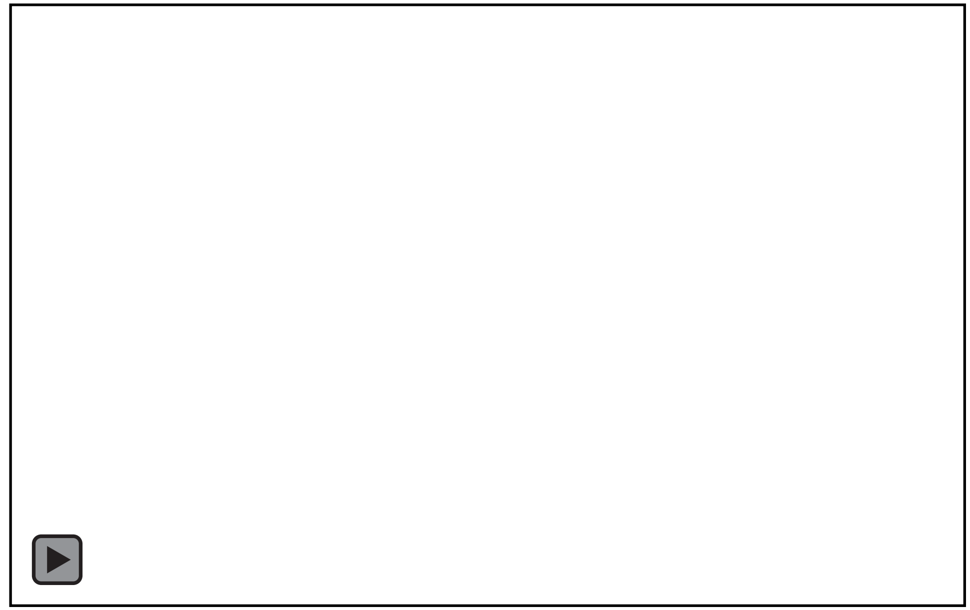


Experiment (top) vs simulation (bottom)

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





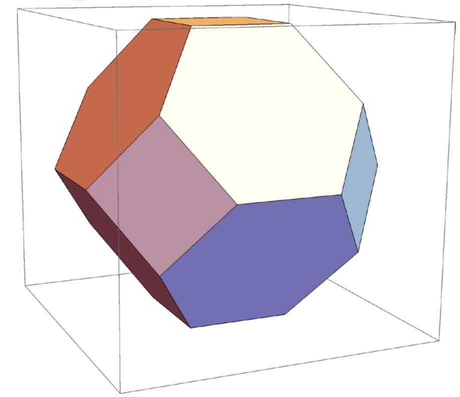
- Dislocation current: $\alpha = b \otimes t \, \mathcal{H}^1 \llcorner \gamma$
- Transport equation: $\dot{\alpha} + \text{curl}\,(\alpha \times v) = 0$
- Dislocation mobility + elastic interaction

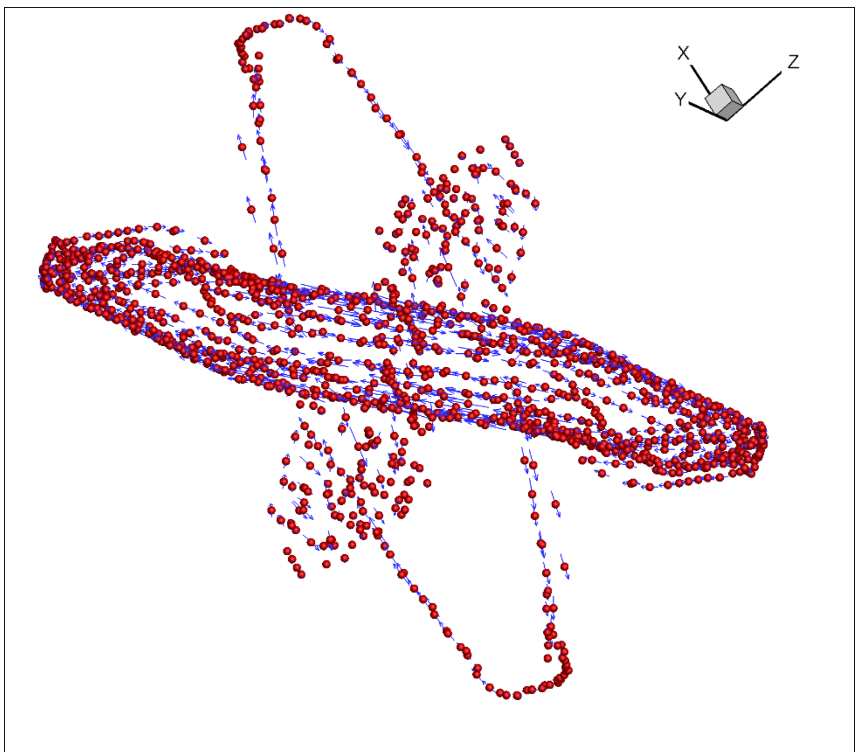
J. Kacher, Materials Science and Engineering, Georgia Tech.

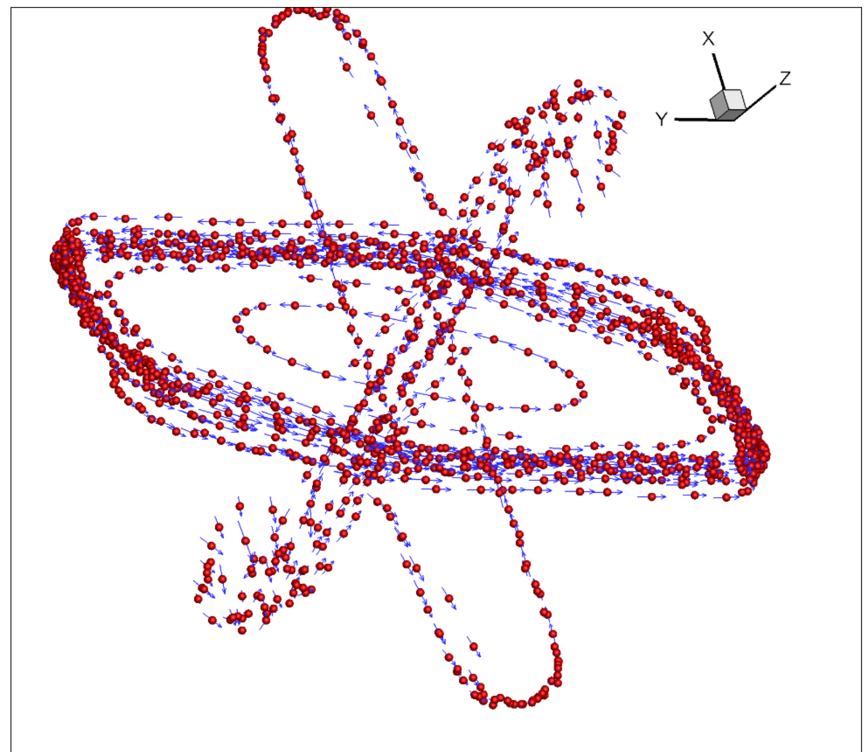
Dislocation transport – BCC grain

- 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.

Analysis

Variational Navier-Stokes

- WED functional for NS, Lagrangian: For $\det(D\varphi(x)) = 1$,

$$F^\epsilon(\varphi) = \int_0^\infty \mathrm{e}^{-t/\epsilon} \int_\Omega \left\{ \frac{\rho}{2} |\ddot\varphi|^2 + \frac{\mu}{\epsilon} |\mathrm{sym}(D\dot\varphi D\varphi^{-1})|^2 \right\} dx\, dt.$$

- WED functional for NS, Eulerian: For $\mathrm{div}\, v(x) = 0$,

$$F^\epsilon(v) = \int_0^\infty \mathrm{e}^{-t/\epsilon} \int_\Omega \left\{ \frac{\rho}{2} |\partial_t v + v\cdot\nabla v|^2 + \frac{\mu}{\epsilon} |\mathrm{sym}\nabla v|^2 \right\} dx\, dt.$$

- Euler-Lagrange equations: Assuming regularity,

$$0 = \rho(\partial_t v + v\cdot\nabla v) - \mu\Delta v + \nabla p + O(\epsilon).$$

- WED: Elliptic regularization of NS!
- WED: Minimum principle! CoV-style existence theory?

Ortiz, M., Schmidt, B. and Stefanelli, U.,
Nonlinearity, **31**(12) (2018) 5664.

Weak (Leray-Hopf) solutions

- Functional framework:
  - $\Omega \subset \mathbb{R}^3$ bounded, open, Lipschitz.
  - $\mathcal{V} = \{v \in C_c^\infty(\Omega; \mathbb{R}^3) \ : \ \mathrm{div}\, v = 0\}$.
  - V_s = closure of $\mathcal{V}$ in $H^s(\Omega; \mathbb{R}^3) \cap H_0^1(\Omega; \mathbb{R}^3)$, $s \geq 1$.
  - H = closure of $\mathcal{V}$ in $L^2(\Omega; \mathbb{R}^3)$.

Definition (Leray-Hopf solutions)

$u \in L^2(0, \infty; V_1)$ is a *Leray-Hopf solution* of NS if $\partial_t u \in L^1(0, \infty; V_1')$,

$$\rho(\partial_t v + v \cdot \nabla v) - \mu \Delta v + \nabla p = 0 \quad \text{in } V_1', \text{ a. e. in } (0, T),$$

$$u(0) = u_0 \quad \text{in } H.$$

- Existence in $L^{8/3}_{\mathrm{loc}}(0, \infty; L^4(\Omega; \mathbb{R}^3))$, weak continuity in time.
- If $u \in L^8_{\mathrm{loc}}(0, \infty; L^4(\Omega; \mathbb{R}^3)) \Rightarrow$ unique, strongly continuous.
- Main result: WED solns converge (weakly) to Leray-Hopf solns!.

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Nonlinearity, **31**(12) (2018) 5664.

Variational existence theory

- Regularized WED functionals for NS: For $\operatorname{div} u = 0$, $F^\epsilon(u) =$

$$\int_0^\infty \mathrm{e}^{-t/\epsilon} \int_\Omega \left\{ \frac{1}{2}|\partial_t u + u \cdot \nabla u|^2 + \frac{\sigma}{2}|u \cdot \nabla u|^2 + \frac{\nu}{2\epsilon}|\nabla u|^2 \right\} dx\, dt.$$

- Admissible set of trajectories:

$$U^\epsilon = \{u \in L^2_{\mathrm{loc}}(0,T;V_1) \,:\, F^\epsilon(u) < +\infty, \quad u(0) = u_0^\epsilon\}$$

Theorem (Existence of minimizers)

Let $\sigma \geq 0$, $u_0 \in H$. Let $u_0^\epsilon \in V_1$ be s.t.

$$u_0^\epsilon \to u_0 \text{ in } H \quad \text{and} \quad \|\nabla u_0^\epsilon\|^2 + \epsilon \|u_0^\epsilon \cdot \nabla u_0^\epsilon\|^2 \leq C\epsilon^{-1}.$$

Then, for every $\epsilon >$ there exists a minimizer u^ϵ of F^ϵ in U^ϵ and $\inf F^\epsilon \leq C\epsilon^{-1}$.

- Remark: If $u_0 \in V_1$ and $u_0 \cdot \nabla u_0 \in H$, then can take constant sequence $u_0^\epsilon = u_0$ (no approximation required).

Variational existence theory

- Regularized WED functionals for NS: For $\operatorname{div} u = 0$, $F^\epsilon(u) =$

$$\int_0^\infty e^{-t/\epsilon} \int_\Omega \left\{ \frac{1}{2}|\partial_t u + u\cdot\nabla u|^2 + \frac{\sigma}{2}|u\cdot\nabla u|^2 + \frac{\nu}{2\epsilon}|\nabla u|^2 \right\} dx\, dt.$$

Theorem (Variational approach to Navier-Stokes)

Let $\sigma > 1/8$ and let $u^\epsilon \in U^\epsilon$ be a minimizer of F^ϵ. Then, there exists a subsequence (not relabeled) such that

$$u^\epsilon \rightharpoonup u \quad \text{in } L^2(0,\infty;V_1), \quad \partial_t u^\epsilon \rightharpoonup \partial_t u \quad \text{in } L^2(0,\infty;V_s'),$$

$s > 5/2$, and $u \in L^2(0,\infty;V_1) \cap L^\infty(0,\infty;H)$ is a Leray-Hopf solution with $\partial_t u \in L^2(0,\infty;V_s')$ and $u(0) = u_0$. Moreover, for a. e. $T > 0$,

$$\|u(T)\|^2 + 2\nu \int_0^T \|\nabla u(t)\|^2\, dt \le \|u_0\|^2.$$

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Nonlinearity, **31**(12) (2018) 5664.

Sketch of proof.

- Let u^ϵ be minimizer of F^ϵ, $\epsilon \downarrow 0$.
- *A priori* estimates (from minimality, EL equations): For $\sigma > 1/8$,

$$\|u^\epsilon(T)\|^2 + 2\nu \int_0^T (1 - \mathrm{e}^{-t/\epsilon}) \|\nabla u^\epsilon(t)\|^2 \, dt \leq \|u_0^\epsilon\|^2, \; T > 0.$$

$$\|\partial_t u^\epsilon\|_{L^2(0,\infty;V_s')} + \|u^\epsilon \cdot \nabla u^\epsilon\|_{L^2(0,\infty;V_s')} \leq C, \; s > 5/2.$$

- Compactness, $s > 5/2$, $\exists u \in L^2(0,\infty;V) \cap L^\infty(0,\infty;H)$ s. t.

$$u^\epsilon \rightharpoonup u \quad \text{in } L^2(0,\infty;V), \qquad u^\epsilon \overset{*}{\rightharpoonup} u \quad \text{in } L^\infty(0,\infty;H),$$

$$\partial_t u^\epsilon \rightharpoonup \partial_t u \quad \text{in } L^2(0,\infty;V_s'), \qquad \Delta u^\epsilon \rightharpoonup \Delta u \quad \text{in } L^2(0,\infty;V_s')$$

- Aubin-Lions: $u^\epsilon \to u$ in $L^2_{\mathrm{loc}}(0,\infty;H) \Rightarrow u^\epsilon \cdot \nabla u^\epsilon \rightharpoonup u \cdot \nabla u$ in $L^2(0,\infty;V_s')$.
- Passing to the causal limit $\epsilon \downarrow 0$, for all $\varphi \in C_c^\infty((0,\infty);V_s)$,

$$\int_0^\infty \int_\Omega \Big(\partial_t u + u \cdot \nabla u - \nu \Delta u \Big) \varphi \, dx \, dt = 0 \qquad \text{(QED)}$$

Dismount

Concluding Remarks

- *Transport problems* are formulated naturally in the framework of *geometric measure theory*
- *Weighted Energy-Dissipation (WED)* functionals (both kinetics and dynamics) supply a *minimum principle for the entire trajectory* of the system
- WED functionals bring *Calculus of Variations* to bear on time-dependent evolution problems
- Approximation by restriction (*à la Galerkin*):
  - *Wasserstein-type metrics (action, dissipation…)*
  - *Push-forward operations (exact geometrical updates)*
  - *Transport maps (updated Lagrangian formulation)*
- Powerful tools of analysis (*weak convergence*, compactness, lower-semicontinuity…)

Adopt a measure

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