Optimization-Based Transport on the Sphere

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Outline

Transport Problem

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \quad \text{on} \quad \Omega \times [0, T]$$

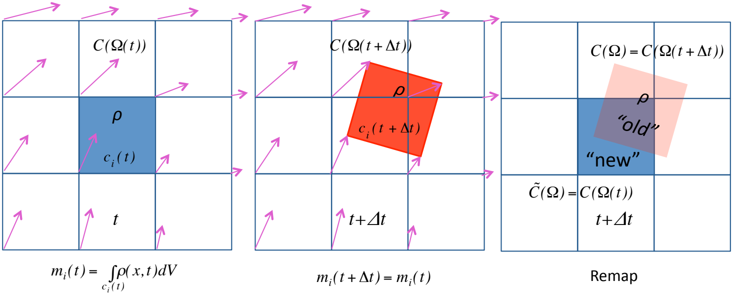
$$\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x})$$

Given a partition $C(\Omega)$ *into cells* $c_i, i = 1, ...C$

- cell mass $m_i = \int_{c_i} \rho(\mathbf{x}, t) dV$
- cell volume $\mu_i = \int_{c_i} dV$
- cell mean density $\rho_i = m_i / \mu_i$
- conservation of mass for Lagrangian volume
  $$\frac{d}{dt} \int_{c_i(t)} \rho(\mathbf{x}, t) d\Omega = 0$$

Incremental Remap for Transport

1. Project depature grid to arrival grid: $C(\Omega(t)) \mapsto C(\Omega(t+\Delta t))$
2. Lagrangian transport: $m_i(t+\Delta t) = m_i(t)$, $\rho_i(t+\Delta t) = m_i(t)/\mu_i(t+\Delta t)$
3. Remap: $m(t+\Delta t) \mapsto \tilde{m}$ and $\rho(t+\Delta t) \mapsto \tilde{\rho}$, for $i = 1, ...C$



Mass-Density Remap

Given mean density values ρ_i on the *old* grid cells c_i, find accurate approximations for the masses $\widetilde{m}_i$ on the *new* cells $\widetilde{c}_i$:

$$\widetilde{m}_i \approx \widetilde{m}_i^{\text{ex}} = \int_{\widetilde{c}_i} \rho(\boldsymbol{x})dV\,, \quad i = 1, \ldots, C \quad \text{such that}$$

- Total mass is conserved: $\sum_{i=1}^{C} \widetilde{m}_i = \sum_{i=1}^{C} m_i = M\,.$
- Mean density approximation on the new cells, $\widetilde{\rho}_i = \frac{\widetilde{m}_i}{\widetilde{\mu}_i}$, satisfies the local bounds
$$\rho_i^{\text{min}} \le \widetilde{\rho}_i \le \rho_i^{\text{max}}\,, \quad i = 1, \ldots, C\,,$$
- If $\rho(\boldsymbol{x})$ is a global linear function on Ω, then the remapped masses are exact:
$$\widetilde{m}_i = \widetilde{m}_i^{\text{ex}} = \int_{\widetilde{c}_i} \rho(\boldsymbol{x})dV\,, \quad i = 1, \ldots, C\,.$$

Remap as Optimization Problem

Objective

$$\|\widehat{u} - u^T\|$$

minimize the distance between the solution and a suitable target

Target

$$\partial_t u^\mathsf{T} = L^h u^\mathsf{T}$$

stable and accurate solution, not required to possess all desired physical properties

Constraints

$$\underline{C} \le C\widehat{u} \le \overline{C}$$

desired physical properties viewed as constraints on the state

Advantages

- Solution is globally optimal with respect to the target and desired physical properties
- Decouples accuracy from enforcement of physical properties
- Enforcement of desired properties as constraints enables feature-preserving methods on arbitrary unstructured grids

Mass-Variable Mass-Target (MVMT) Formulation

Exact mass update

$$\begin{aligned} \widetilde{m}_i^{ex} &= \int_{c_i} \rho(\boldsymbol{x})dV + \left(\int_{\widetilde{c}_i} \rho(\boldsymbol{x})dV - \int_{c_i} \rho(\boldsymbol{x})dV \right) \\ &= \qquad m_i \qquad + \qquad u_i^{ex}, \qquad i = 1, ..., C \end{aligned}$$

Approximate mass update operator

$$\widetilde{m} = L^h(m, u(\rho)) := m + u(\rho)$$

Target is defined as

$$u_i^{\mathsf{T}} := \int_{\widetilde{c}_i} \rho^h(\boldsymbol{x})dV - \int_{c_i} \rho^h(\boldsymbol{x})dV; \ i = 1, \dots, C;$$

Solution $\quad \widehat{u} \in C^h; \quad C^h$ - piecewise constant space with respect to cells

MVMT Formulation

$$\begin{cases} \text{minimize} \quad \dfrac{1}{2}\|\widehat{u} - u^{\mathsf{T}}\|_{\ell_2}^2 \qquad \text{subject to} \\ \widehat{u} \in C^h; \quad \displaystyle\sum_{i=1}^{C} \widehat{u}_i = 0 \quad \text{and} \quad \widetilde{m}^{\mathsf{min}} \leq m + \widehat{u} \leq \widetilde{m}^{\mathsf{max}} \end{cases}$$

- Singly linearly constrained quadratic program with simple bounds
- Related problem without the mass conservation constraint is fully separable
- Solution approach
    - Solve related (separable) problem first, cost $O(C)$
    - Satisfy the mass conservation constraint in a few iterations

MVMT Algorithm

Define Lagrangian functional $\mathcal{L} : \mathbb{R}^C \times \mathbb{R} \times \mathbb{R}^C \times \mathbb{R}^C \to \mathbb{R}$,

$$\mathcal{L}(\widehat{u}, \lambda, \mu_1, \mu_2) = \frac{1}{2} \sum_{i=1}^{C} (\widehat{u}_i - u_i^{\mathsf{T}})^2 - \lambda \sum_{i=1}^{C} \widehat{u}_i -$$

$$\textstyle\sum_{i=1}^{C} \mu_{1,i} \left(\widehat{u}_i - \widetilde{m}_i^{\text{min}} + m_i\right) - \sum_{i=1}^{C} \mu_{2,i} \left(\widetilde{m}_i^{\text{max}} - m_i - \widehat{u}_i\right) \;,$$

where $\widehat{u} \in \mathbb{R}^C$ are the *primal optimization variables*, and $\lambda \in \mathbb{R}$, $\mu_1 \in \mathbb{R}^C$, and $\mu_2 \in \mathbb{R}^C$ are the *Lagrange multipliers*.

Karush-Kuhn-Tucker (KKT) conditions:

$$\begin{aligned}
\widehat{u}_i = u_i^{\mathsf{T}} + \lambda + \mu_{1,i} - \mu_{2,i}; &\quad i = 1, \ldots, C \\
\widetilde{m}_i^{\text{min}} - m_i \leq \widehat{u}_i \leq \widetilde{m}_i^{\text{max}} - m_i; &\quad i = 1, \ldots, C \\
\mu_{1,i} \geq 0\,, \quad \mu_{2,i} \geq 0; &\quad i = 1, \ldots, C \\
\mu_{1,i} \left(\widehat{u}_i - \widetilde{m}_i^{\text{min}} + m_i\right) = 0\,, \quad \mu_{2,i} \left(-\widehat{u}_i + \widetilde{m}_i^{\text{max}} - m_i\right) = 0; &\quad i = 1, \ldots, C \\
\textstyle\sum_{i=1}^{C} \widehat{u}_i = 0
\end{aligned}$$

MVMT Algorithm

Focus on conditions separable in the index i. For any *fixed* value of λ a solution is given by

$$\begin{cases} \widehat{u}_i = u_i^{\mathsf{T}} + \lambda; & \mu_{1,i} = \mu_{2,i} = 0 & \text{if} \quad \widetilde{m}_i^{\mathsf{min}} - m_i \leq u_i^{\mathsf{T}} + \lambda \leq \widetilde{m}_i^{\mathsf{max}} - m_i \\ \widehat{u}_i = \widetilde{m}_i^{\mathsf{min}} - m_i; & \mu_{2,i} = 0,\ \mu_{1,i} = \widehat{u}_i - u_i^{\mathsf{T}} - \lambda & \text{if} \quad u_i^{\mathsf{T}} + \lambda < \widetilde{m}_i^{\mathsf{min}} - m_i \\ \widehat{u}_i = \widetilde{m}_i^{\mathsf{max}} - m_i; & \mu_{1,i} = 0,\ \mu_{2,i} = u_i^{\mathsf{T}} - \widehat{u}_i + \lambda & \text{if} \quad u_i^{\mathsf{T}} + \lambda > \widetilde{m}_i^{\mathsf{max}} - m_i\,, \end{cases}$$

for all $i = 1, \ldots, C$.

Ignoring μ_1 and μ_2 and treating $\widehat{u}_i$ as a function of λ yields

$$\widehat{u}_i(\lambda) = \mathsf{median}(\widetilde{m}_i^{\mathsf{min}} - m_i,\ u_i^{\mathsf{T}} + \lambda,\ \widetilde{m}_i^{\mathsf{max}} - m_i)\,, \qquad i = 1, \ldots, C\,.$$

Adjust λ in outer iteration to satisfy $\sum_{i=1}^{C} \widehat{u}_i(\lambda) = 0$.

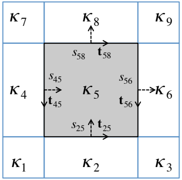
In all our examples, the algorithm requires ≤ 5 outer secant iterations

Defining the Target

Mean preserving density reconstruction

$$\rho^h(\mathbf{x})|_{c_i} = \rho_i + \mathbf{g}_i \cdot (\mathbf{x} - \mathbf{b}_i)$$

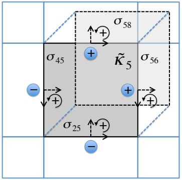
$$\mathbf{g}_i \approx \nabla\rho \qquad \text{and} \qquad \mathbf{b}_i = \frac{\int_{c_i} \mathbf{x}\, dV}{\mu_i}$$



Target mass increment

$$u^{\mathsf{T}} = \int_{\tilde{c}_i} \rho^h(\mathbf{x})dV - \int_{c_i} \rho^h(\mathbf{x})dV$$

$$= \sum_{j \in N'(c_i)} \int_{\tilde{c}_i \cap c_j} \rho_j^h(\mathbf{x})dV - \int_{c_i} \rho_i^h(\mathbf{x})dV$$



Integrate over swept areas σ using Green's theorem

$$\int_\sigma dV = \int_{d\sigma} x dy, \quad \int_\sigma x dV = \int_{\partial\sigma} \frac{x^2}{2} dy, \quad \int_\sigma y dV = \int_{\partial\sigma} \frac{y^2}{2} dx,$$

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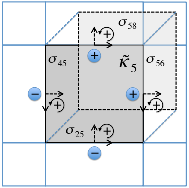
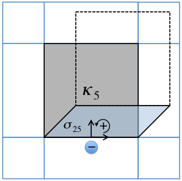
Swept Region Approximation



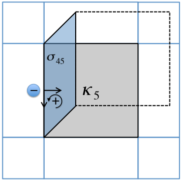
$$u^{\mathsf{T}} = \sum_{j \in N'(\kappa_i)} F_{ij}^{\mathsf{T}}$$

$$F_{ij}^{\mathsf{T}} = \begin{cases} \int_{\sigma_{ij}} \rho_i^h(\boldsymbol{x})dV & \text{if } \mu^\star(\sigma_{ij})d_{i,ij} < 0 \\ \int_{\sigma_{ij}} \rho_j^h(\boldsymbol{x})dV & \text{if } \mu^\star(\sigma_{ij})d_{i,ij} > 0 \end{cases}$$

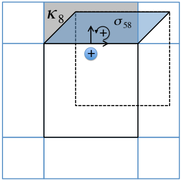
$d_{i,ij}$ - elements of cell to side incidence matrix, corresponding to signs in blue circles



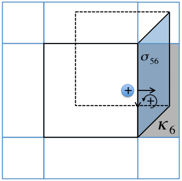
$\mu^\star(\sigma_{ij})d_{i,ij} < 0$



$\mu^\star(\sigma_{ij})d_{i,ij} > 0$



$\mu^\star(\sigma_{ij})d_{i,ij} > 0$



$\mu^\star(\sigma_{ij})d_{i,ij} < 0$

Adaptable Target

Mean preserving density reconstruction

$$\rho^h(\mathbf{x})|_{c_i} = \rho_i + \mathbf{g}_i \cdot (\mathbf{x} - \mathbf{b}_i), \quad \mathbf{g}_i \approx \nabla\rho \qquad \text{and} \qquad \mathbf{b}_i = \frac{\int_{c_i} \mathbf{x} dV}{\mu_i}$$

Define reconstruction residual

$$r_i = \sum_{j \in N(c_i)} |\rho_j - \rho_i^h(\mathbf{b_j})|$$

$$r_i = 0 \quad \text{if} \quad \rho_i^h(\mathbf{b}_j) = \rho(\mathbf{b}_j) = \rho_j$$

Adaptable density reconstruction

$$\alpha_i(\xi) \geq 1 \quad \text{and} \quad \alpha_i(0) = 1$$

$$\rho^A(\mathbf{x})|_{c_i} = \rho_i + \alpha_i(r_i)\mathbf{g}_i \cdot (\mathbf{x} - \mathbf{b}_i),$$

- Residual measures deviation of mean density from global linear function
- Solution remains exact for linears
- Performs better than slope-limited reconstructions for problems combining "smooth" and "sharp" features

Extension of Formulation to Spherical Coordinates

Lat-Lon Coordinates $\theta \in [-\pi/2, \pi/2], \quad \lambda \in [0, 2\pi]$

Mean Preserving density reconstruction

$$\rho^h(\boldsymbol{s})|_{c_i} = \rho_i + \left(g_i^\theta\right)(\theta - \boldsymbol{b}_{\theta,i}) + \left(g_i^\lambda\right)(\lambda \cos\theta - \boldsymbol{b}_{\lambda,i}).$$

$$g_i^\lambda \approx \frac{1}{\cos\theta}\frac{\partial \rho}{\partial \lambda} \quad g_i^\theta \approx \frac{\partial \rho}{\partial \theta} \quad \boldsymbol{b}_{\lambda,i} = \frac{\int_{c_i} \lambda \cos\theta dV}{\mu_i} \quad \boldsymbol{b}_{\theta,i} = \frac{\int_{c_i} \theta dV}{\mu_i}$$

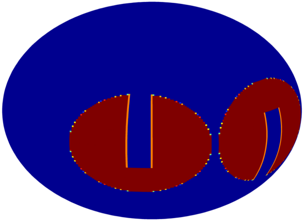
Integrate over swept areas σ using Green's theorem

$$\int_\sigma dV = -\int_{\partial\sigma} \sin\theta d\lambda, \quad \int_\sigma \theta dV = -\int_{\partial\sigma} (\cos\theta + \theta \sin\theta) d\lambda$$

$$\int_\sigma \lambda \cos\theta dV = -\int_{\partial\sigma} \frac{\lambda}{2}\left(\cos\theta \sin\theta + \theta\right) d\lambda$$

Spherical transport

Initial Data



Nair and Lauritzen (2010) *JCP*

Deformational Flow:

$$u(\lambda, \theta, t) = 2\sin^2(\lambda)\sin(2\theta)\cos(\pi t/T)$$

$$v(\lambda, \theta, t) = 2\sin(2\lambda)\cos(\theta)\cos(\pi t/T)$$

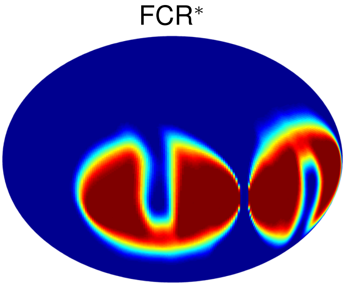
Zonal Flow:

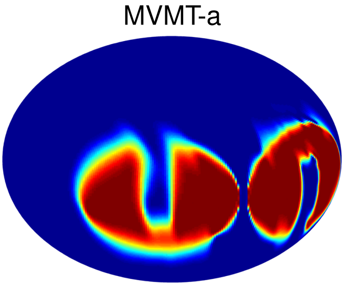
$$u(\lambda, \theta) = 2\pi\left(\cos(\theta)\cos(\alpha) + \cos(\lambda)\sin(\theta)\sin(\alpha)\right)$$

$$v(\lambda, \theta) = 2\pi\sin(\lambda)\sin(\alpha)$$

In the following examples: $T = 5$, $\alpha = 0$, *and radius of sphere = 1.*

Spherical transport: Deformation



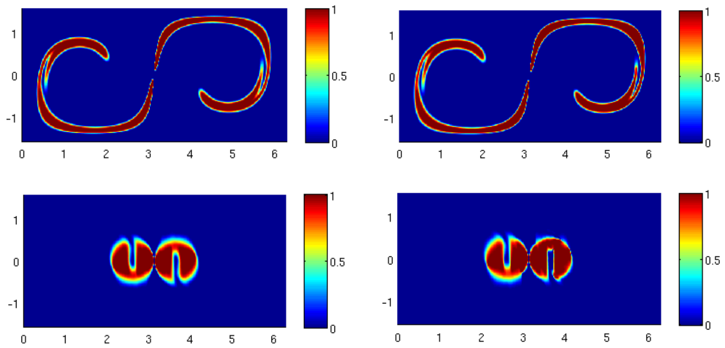


Transport results for the deformational flow test on the sphere at a final time $T = 5$ after 2400 time steps on a 0.75° mesh.

* Flux Corrected Remap

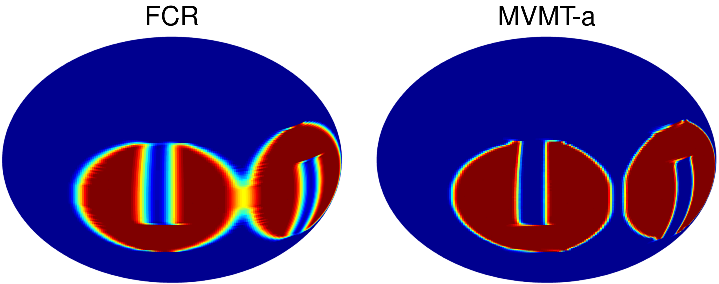
Spherical transport: Deformation

FCR MVMT-a



mesh	steps	**FCR** time(sec)	**MVMT-a** time(sec)	ratio	**FCR** L_1 error	rate	**MVMT-a** L_1 error	rate
3°	600	23.0	24.2	**1.1**	4.34e-2	—	3.60e-2	—
1.5°	1200	187.7	190.0	**1.0**	2.85e-2	0.61	2.27e-2	0.66
0.75°	2400	1644.4	1717.7	**1.0**	1.67e-2	0.69	1.40e-2	0.68

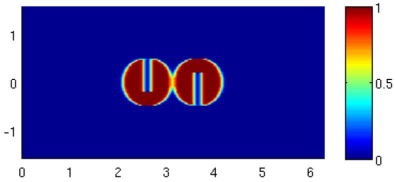
Spherical transport: Rotation



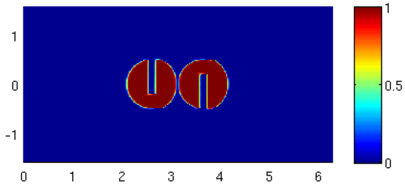
Transport results for the solid-body rotation test on the sphere, for two revolutions, left to right and back (1920 time steps) on a 0.75° mesh.

Spherical transport: Rotation

FCR



MVMT-a



mesh	steps	**FCR** time(sec)	**MVMT-a** time(sec)	ratio	**FCR** L_1 error	rate	**MVMT-a** L_1 error	rate
3°	480	17.4	18.2	**1.0**	3.25e-2	—	2.79e-2	—
1.5°	960	132.5	151.6	**1.1**	1.99e-2	0.78	1.36e-3	1.04
0.75°	1920	1184.5	1379.0	**1.2**	1.10e-2	0.78	5.41e-3	1.18

Conclusions

- Optimization-based transport offers a robust and accurate alternative to standard transport algorithms
- The MVMT algorithm is as fast as flux-corrected remap (FCR) and is easily paralellizable
- Separating accuracy from feature preservation allows extension to arbitrary cells, *e.g.* polygons

More details in:

Bochev, Ridzal, Scovazzi, Shashkov (2011) "Formulation, analysis and numerical study of an optimization-based conservative interpolation (remap) of scalar fields for arbitrary lagrangian-eulerian methods", *JCP*

Bochev, Ridzal, Shashkov (2012) "Fast optimization-based conservative remap of scalar fields through aggregate mass transfer", *JCP*

Bochev, Ridzal, Peterson (2012) "Optimization-based remap and transport: a divide and conquer strategy for feature-preserving discretizations", *JCP*, submitted