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Optimization-Based Tracer Transport on the Sphere

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Transport Problem

A tracer, represented by its mixing ratio q and mass ρq , is transported in the flow with velocity \mathbf{u}

$$\left. \begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} &= 0 \\ \frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \mathbf{u} &= 0 \end{aligned} \right\} \rightarrow \frac{Dq}{Dt} = 0$$

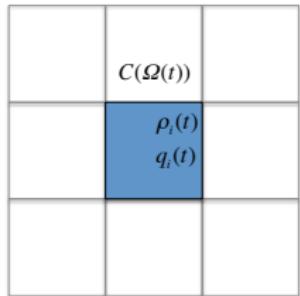
Solution methods should satisfy

- local conservation of ρq
- monotonicity or bounds preservation of q
- consistency between q and ρ (free stream preserving)
- preservation of linear correlations between tracers ($q_1 = aq_2 + b$)

Incremental Remap for Transport

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

- cell mass $m_i = \int_{c_i} \rho(\mathbf{x}, t) dV$
- cell area $\mu_i = \int_{c_i} dV$
- cell average density $\rho_i = \frac{m_i}{\mu_i}$
- cell average tracer concentration



For a Lagrangian volume, V_L

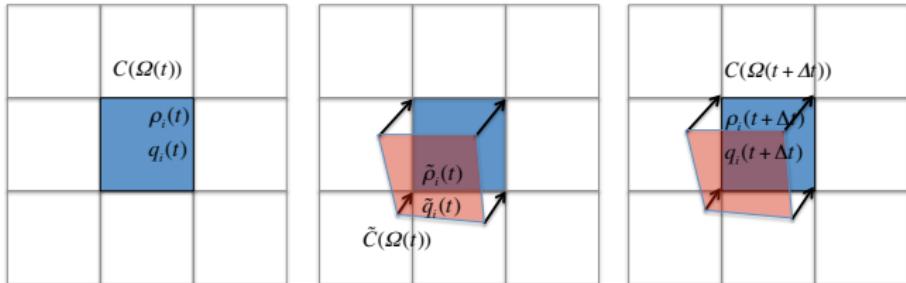
$$q_i = \frac{\int_{c_i} \rho(\mathbf{x}, t) q(\mathbf{x}, t) dV}{\int_{c_i} \rho(\mathbf{x}, t) dV}$$

$$\int_{c_i} \rho(\mathbf{x}, t) q(\mathbf{x}, t) dV = m_i q_i$$

$$\frac{d}{dt} \int_{V_L} \rho(\mathbf{x}, t) dV = 0$$

$$\frac{d}{dt} \int_{V_L} q(\mathbf{x}, t) \rho(\mathbf{x}, t) dV = 0$$

Incremental Remap for Transport



- 1 Project arrival grid to departure grid: $C(\Omega(t + \Delta t)) \mapsto \tilde{C}(\Omega(t))$
- 2 Remap: $\rho(t) \mapsto \tilde{\rho}$, $q(t) \mapsto \tilde{q}(t)$
- 3 Lagrangian update:

$$m_i(t + \Delta t) = \tilde{m}_i(t), \quad \rho_i(t + \Delta t) = \frac{m_i(t + \Delta t)}{\mu_i(t + \Delta t)}, \quad q_i(t + \Delta t) = \tilde{q}_i(t)$$

Dukowicz and Baumgardner (2000) *JCP*

Density and Tracer Remap

Given mean density and tracer values ρ_i, q_i on the *old* grid cells c_i , find accurate approximations for \tilde{m}_i and \tilde{q}_i on the *new* cells \tilde{c}_i such that:

- Total mass is conserved:

$$\sum_{i=1}^C \tilde{m}_i = \sum_{i=1}^C m_i = M \quad \sum_{i=1}^C \tilde{m}_i \tilde{q}_i = \sum_{i=1}^C m_i q_i = Q.$$

- Mean density and tracer approximations on the new cells, $\tilde{\rho}_i = \frac{\tilde{m}_i}{\mu_i}$ and \tilde{q}_i satisfy the local bounds

$$\rho_i^{\min} \leq \tilde{\rho}_i \leq \rho_i^{\max}, \quad i = 1, \dots, C,$$

$$q_i^{\min} \leq \tilde{q}_i \leq q_i^{\max}, \quad i = 1, \dots, C,$$

Optimization-Based Remap

Objective

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

minimize the distance
between the solution and a
suitable target

Target

$$\partial_t u^T = L^h u^T$$

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

Constraints

$$\underline{C} \leq C\tilde{u} \leq \overline{C}$$

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

Density Formulation

$$\begin{aligned}\tilde{m}_i &= \int_{c_i} \rho(\mathbf{x}) dV + \left(\int_{\tilde{c}_i} \rho(\mathbf{x}) dV - \int_{c_i} \rho(\mathbf{x}) dV \right) \\ &= m_i + u_i\end{aligned}$$

- *Objective* $\frac{1}{2} \|\tilde{u} - u^\top\|_{\ell_2}^2$
- *Target* $u_i^\top := \int_{\tilde{c}_i} \rho^h(\mathbf{x}) dV - \int_{c_i} \rho^h(\mathbf{x}) dV$
- *Constraints* $\sum_{i=1}^C \tilde{u}_i = 0, \quad \rho_i^{\min} \leq \tilde{\rho}_i \leq \rho_i^{\max}$

Bochev, Ridzal, Shashkov (2013) *JCP*

Tracer Formulation

$$\tilde{q}_i = \frac{\int_{\tilde{c}_i} \rho(\mathbf{x}) q(\mathbf{x}) dV}{\int_{\tilde{c}_i} \rho(\mathbf{x}) dV}$$

- *Objective* $\frac{1}{2} \|\tilde{q} - q^T\|_{\ell_2}^2$
- *Target* $q_i^T := \frac{\int_{\tilde{c}_i} \rho^h(\mathbf{x}) q^h(\mathbf{x}) dV}{\int_{\tilde{c}_i} \rho^h(\mathbf{x}) dV}$
- *Constraints* $\sum_{i=1}^C \tilde{m}_i \tilde{q}_i = Q, \quad q_i^{min} \leq \tilde{q}_i \leq q_i^{max}$

OBR Algorithm

$$\left\{ \begin{array}{l} \text{minimize} \quad \frac{1}{2} \|\tilde{u} - u^\top\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^C \tilde{u}_i = 0, \quad m_i^{\min} \leq m + \tilde{u} \leq m_i^{\max} \end{array} \right.$$

$$\left\{ \begin{array}{l} \text{minimize} \quad \frac{1}{2} \|\tilde{q} - q^\top\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^C \tilde{q}_i = Q, \quad q_i^{\min} \leq \tilde{q} \leq q_i^{\max} \end{array} \right.$$

Singly linearly constrained quadratic programs with simple bounds

- Solve related separable problem (without mass constraint) first, cost $O(C)$
- Satisfy the mass conservation constraint in a few secant iterations

Density and Tracer Reconstructions

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

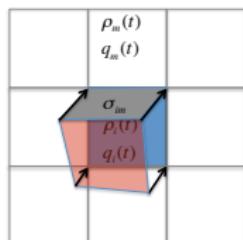
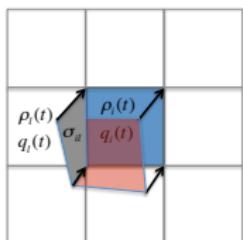
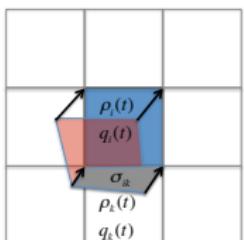
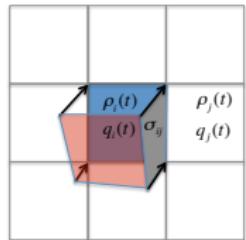
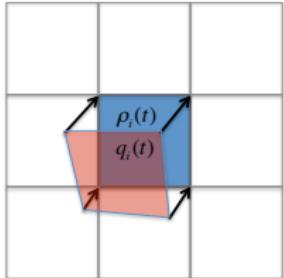
$$q^h(\mathbf{x})|_{c_i} = q_i + \mathbf{g}_i^q \cdot (\mathbf{x} - \mathbf{c}_i)$$

- Approximate gradients ($\mathbf{g}_i^\rho \approx \nabla \rho$, $\mathbf{g}_i^q \approx \nabla q$) computed using least-squares fit with five point stencil
- Cell barycenter $\mathbf{b}_i = \frac{\int_{c_i} \mathbf{x} dV}{\mu_i}$
- Cell center of mass $\mathbf{c}_i = \frac{\int_{c_i} \mathbf{x} \rho_i(\mathbf{x}) dV}{m_i}$
- Mean preserving by construction

$$\frac{1}{\mu_i} \int_{c_i} \rho^h(\mathbf{x}) dV = \rho_i \quad \frac{1}{m_i} \int_{c_i} \rho^h(\mathbf{x}) q^h(\mathbf{x}) dV = q_i$$

Dukowicz and Baumgardner (2000) *JCP*

Swept Area Approximation



$$F_{ij}^{\rho} = \int_{\sigma_{ij}} \rho_i^h(\mathbf{x}) dV$$

$$F_{ij}^q = \int_{\sigma_{ij}} \rho_i^h(\mathbf{x}) q_i^h(\mathbf{x}) dV$$

$$F_{ik}^{\rho} = \int_{\sigma_{ik}} \rho_k^h(\mathbf{x}) dV$$

$$F_{ik}^q = \int_{\sigma_{ik}} \rho_k^h(\mathbf{x}) q_k^h(\mathbf{x}) dV$$

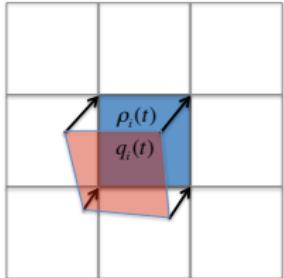
$$F_{il}^{\rho} = \int_{\sigma_{il}} \rho_l^h(\mathbf{x}) dV$$

$$F_{il}^q = \int_{\sigma_{il}} \rho_l^h(\mathbf{x}) q_l^h(\mathbf{x}) dV$$

$$F_{im}^{\rho} = \int_{\sigma_{im}} \rho_i^h(\mathbf{x}) dV$$

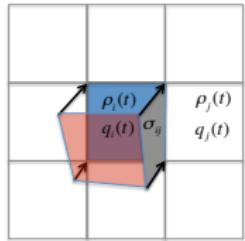
$$F_{im}^q = \int_{\sigma_{im}} \rho_i^h(\mathbf{x}) q_i^h(\mathbf{x}) dV$$

Swept Area Approximation



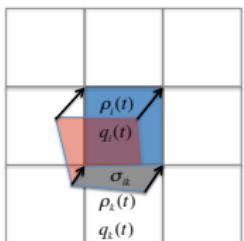
$$u_i^T = \int_{\tilde{c}_i} \rho^h(\mathbf{x}) dV - \int_{c_i} \rho^h(\mathbf{x}) dV \approx \sum_s F_{is}^T$$

$$q_i^T = \frac{\int_{\tilde{c}_i} \rho^h(\mathbf{x}) q^h(\mathbf{x}) dV}{\int_{\tilde{c}_i} \rho^h(\mathbf{x}) dV} \approx \frac{q_i(t) m_i(t) + \sum_s F_{is}^T}{m_i(t) + u_i^T}$$



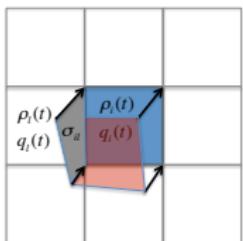
$$F_{ij}^{\rho} = \int_{\sigma_{ij}} \rho_i^h(\mathbf{x}) dV$$

$$F_{ij}^q = \int_{\sigma_{ij}} \rho_i^h(\mathbf{x}) q_i^h(\mathbf{x}) dV$$



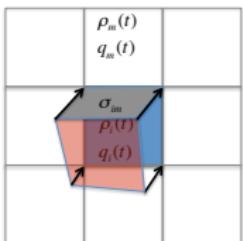
$$F_{ik}^{\rho} = \int_{\sigma_{ik}} \rho_k^h(\mathbf{x}) dV$$

$$F_{ik}^q = \int_{\sigma_{ik}} \rho_k^h(\mathbf{x}) q_k^h(\mathbf{x}) dV$$



$$F_{il}^{\rho} = \int_{\sigma_{il}} \rho_l^h(\mathbf{x}) dV$$

$$F_{il}^q = \int_{\sigma_{il}} \rho_l^h(\mathbf{x}) q_l^h(\mathbf{x}) dV$$

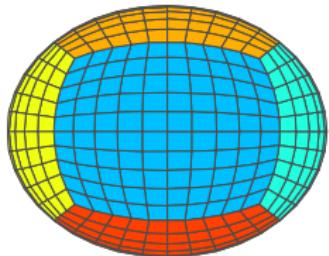


$$F_{im}^{\rho} = \int_{\sigma_{im}} \rho_i^h(\mathbf{x}) dV$$

$$F_{im}^q = \int_{\sigma_{im}} \rho_i^h(\mathbf{x}) q_i^h(\mathbf{x}) dV$$

Cubed Sphere Grid

- Six faces of cube projected onto surface of sphere
- Equiangular gnomonic projection with central angles, $\alpha, \beta \in [-\pi/4, \pi/4]$
- Local coordinates
 $x = a \tan \alpha, y = a \tan \beta \quad p = 1, \dots, 6$

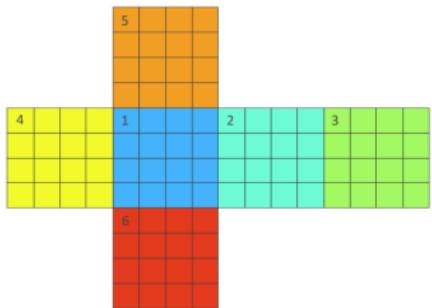


$$\int_V dV = - \int_{\partial V} \frac{1}{1+x^2} \frac{y}{r} dx$$

$$\int_V x dV = - \int_{\partial V} \frac{1}{1+x^2} \frac{xy}{r} dx$$

$$\int_V y dV = \int_{\partial V} \frac{1}{r} dx$$

$$r = \sqrt{1 + x^2 + y^2} \text{ for } a = 1$$



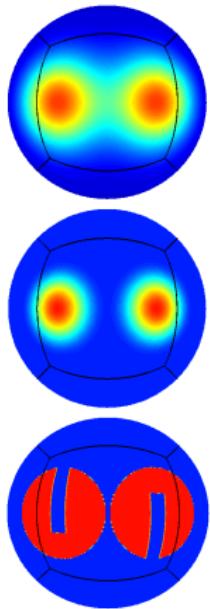
See Ullrich *et al.* (2009) Monthly Weather Review, Lauritzen *et al.* (2010) JCP.

Computational Examples

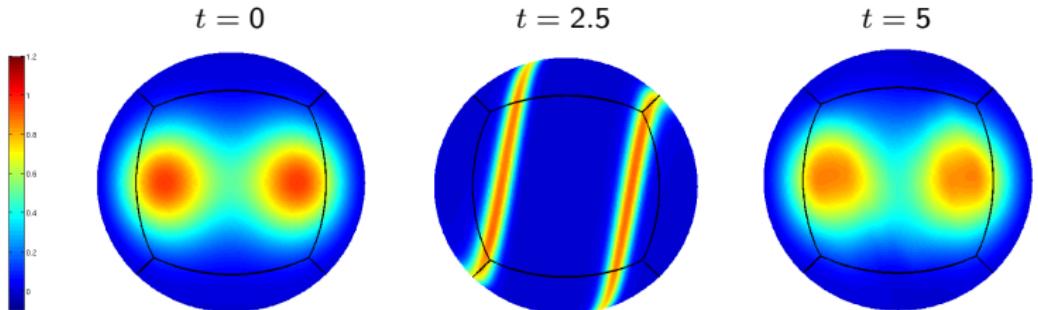
- Test cases from Lauritzen *et al.* (2012) Geosci. Model Dev.
- Initial density distribution set to one everywhere
- Three types of tracer distributions
 - Smooth Gaussian hills
 - Cosine bells
 - Notched cylinders
- Initial tracer distributions centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent deformational flow field, $T = 5$:

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

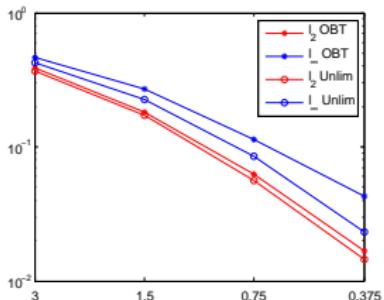
$$v(\lambda, \theta, t) = 2 \sin(2(\lambda - 2\pi t/T)) \cos(\theta) \cos(\pi t/T)$$



Convergence Test



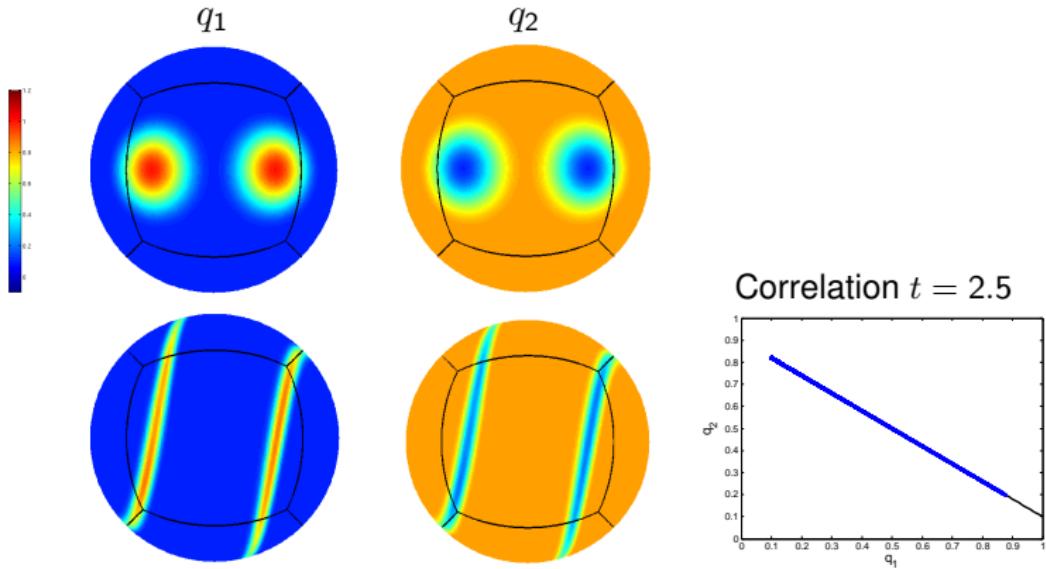
mesh	steps	OBT*		Unlimited	
		l_2	l_∞	l_2	l_∞
3°	600	0.386	0.465	0.368	0.425
1.5°	1200	0.182	0.268	0.172	0.225
0.75°	2400	0.0626	0.113	0.0559	0.0843
0.375°	4800	0.0167	0.0425	0.0144	0.0233
<i>Rate</i>		1.51	1.16	1.56	1.40



* Optimization-based transport

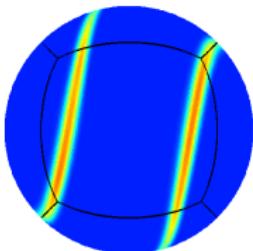
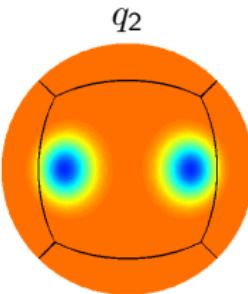
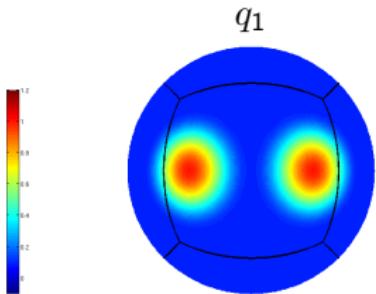
Linear Tracer Correlation Test

Two tracers with initial distributions linearly correlated cosine bells,
 q_1 has min = 0.1 and max = 1.0, $q_2 = -0.8q_1 + 0.9$.



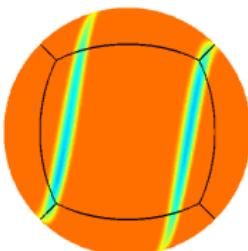
NonLinear Tracer Correlation Test

Two tracers with initial distributions nonlinearly correlated cosine bells,
 q_1 has min = 0.1 and max = 1.0, $q_2 = -0.8(q_1)^2 + 0.9$
 with min = 0.1 and max = 0.892.

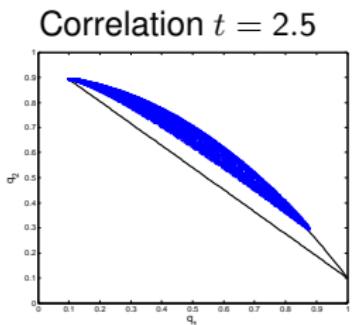


min/max

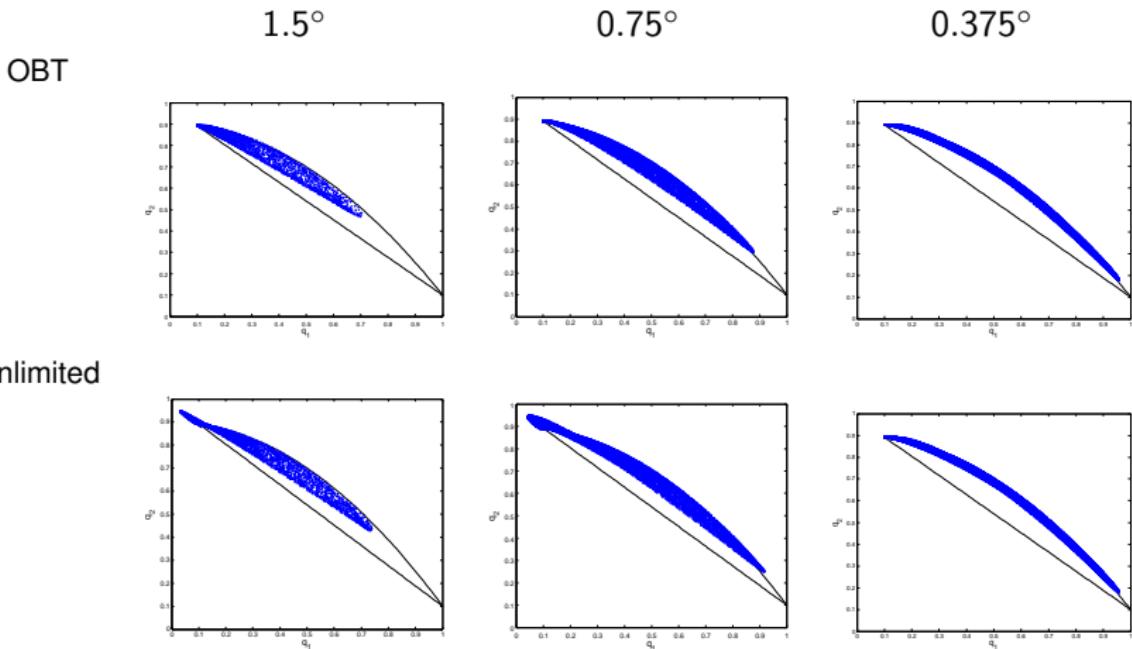
0.1/0.878



0.292/0.892



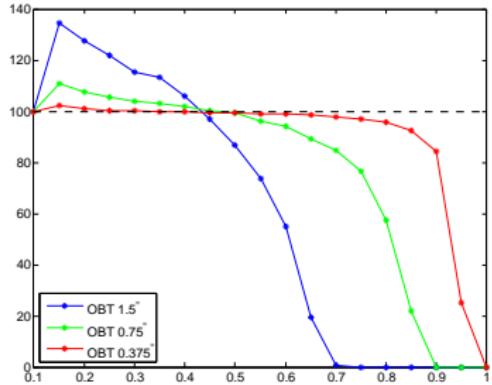
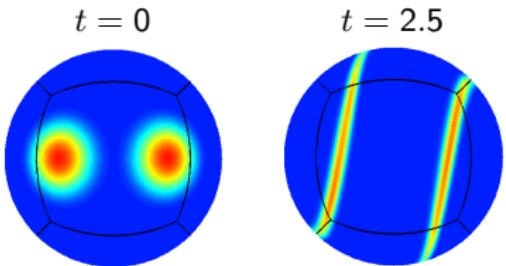
Nonlinear Tracer Correlation Test



Filament Preservation Test

$$l_f(\tau, t) = 100.0 \times \frac{A(\tau, t)}{A(\tau, 0)}$$

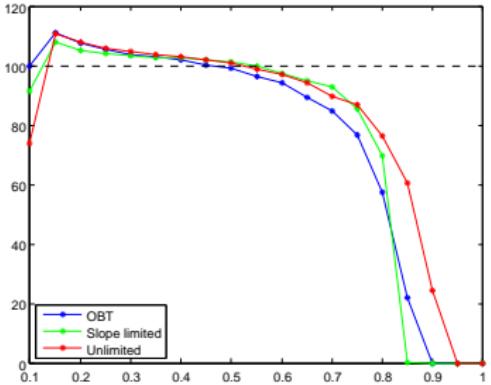
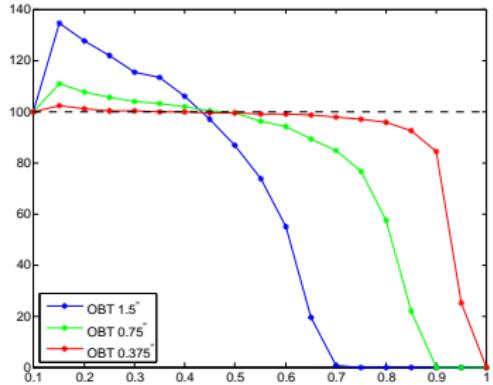
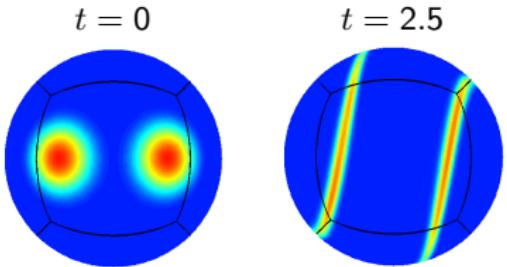
where $A(\tau, t)$ is the total area for which $q \geq \tau$.



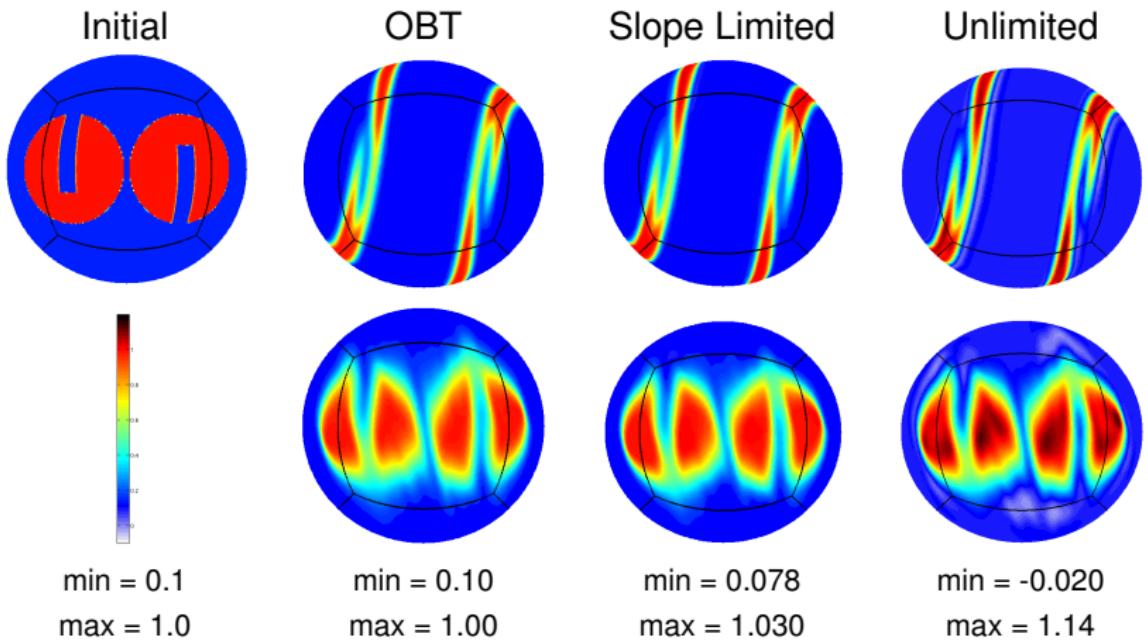
Filament Preservation Test

$$l_f(\tau, t) = 100.0 \times \frac{A(\tau, t)}{A(\tau, 0)}$$

where $A(\tau, t)$ is the total area for which $q \geq \tau$.



Discontinuous Tracer Test



Conclusions

- Optimization-based transport offers a robust and flexible alternative to standard transport techniques
- Solution is mass conserving, bounds preserving, and free stream preserving.
- Optimization algorithm is efficient and computationally competitive with standard slope limiting in these examples.

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 (2013) "Fast optimization-based conservative remap of scalar fields through aggregate mass transfer", *JCP*

Bochev, Ridzal, Peterson (2014) "Optimization-based remap and transport: a divide and conquer strategy for feature-preserving discretizations", *JCP*

Peterson, Bochev, Ridzal (2014) "Optimization-based transport on the cubed sphere grid", *Proceedings of LSSC13*.