SAND2014-16174PE

Optimization-Based Transport of Passive Tracers

Kara Peterson, Pavel Bochev, and Denis Ridzal

Sandia National Laboratories

International Workshop on Modeling and Simulation of Transport Phenomena

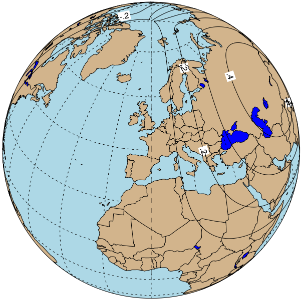
July 29, 2014

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Motivation

Tracers in atmospheric modeling

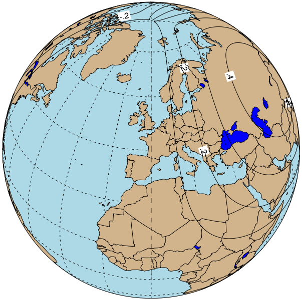
- Typically tracers are chemical species transported with the flow
- In current atmospheric dynamical cores tracer advection accounts for 50% of total cost with 26 tracers
- More detailed biogeochemistry requires 100-1000 tracers



Motivation

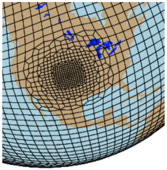
Tracers in atmospheric modeling

- Typically tracers are chemical species transported with the flow
- In current atmospheric dynamical cores tracer advection accounts for 50% of total cost with 26 tracers
- More detailed biogeochemistry requires 100-1000 tracers



Objective:

- Develop computationally efficent tracer advection algorithms that
  - enforce physical tracer bounds
  - exploit the fact that we will be transporting hundreds of species
  - work on unstructured grids



Transport Problem

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

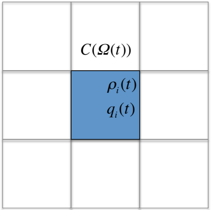
$$\left.\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\ \frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \mathbf{u} = 0\end{aligned}\right\} \rightarrow \frac{Dq}{Dt} = 0$$

Solution methods should satisfy

- conservation of ρq
- monotonicity or bounds preservation of q
- consistency between q and ρ (free stream preserving)
- preservation of linear correlations between tracers ($q_1 = a q_2 + b$)

Incremental Remap for Transport

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 area $\mu_i = \int_{c_i} dV$
- cell average density $\rho_i = \frac{m_i}{\mu_i}$
- cell average tracer concentration

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

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

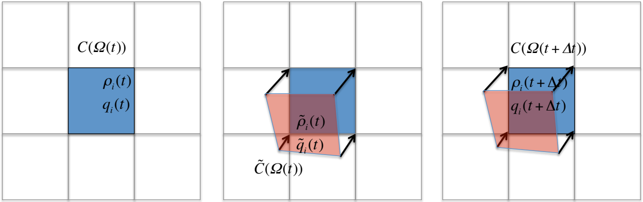
Dukowicz and Baumgardner (2000) *JCP*

For a Lagrangian volume, V_L

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

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

Incremental Remap for Transport



1. Project arrival grid to departure grid: $C(\Omega(t+\Delta t)) \mapsto \widetilde{C}(\Omega(t))$
2. Remap: $\rho(t) \mapsto \tilde{\rho}(t)$, $q(t) \mapsto \widetilde{q}(t)$
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 $\widetilde{m}_i$ and $\widetilde{q}_i$ on the *new* cells $\widetilde{c}_i$ such that:

- Total mass and tracer mass are conserved:

$$\sum_{i=1}^{C} \widetilde{m}_i = \sum_{i=1}^{C} m_i = M \qquad \sum_{i=1}^{C} \widetilde{m}_i \widetilde{q}_i = \sum_{i=1}^{C} m_i q_i = Q \, .$$

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

$$\rho_i^{\text{min}} \leq \widetilde{\rho}_i \leq \rho_i^{\text{max}} \, , \quad i = 1, \ldots, C \, ,$$

$$q_i^{\text{min}} \leq \widetilde{q}_i \leq q_i^{\text{max}} \, , \quad i = 1, \ldots, C \, ,$$

Optimization-Based Remap

Sandia National Laboratories

Objective	Target	Constraints
$\|\widetilde{u} - u^T\|$	$\partial_t u^{\mathsf{T}} = L^h u^{\mathsf{T}}$	$\underline{C} \leq C\widetilde{u} \leq \overline{C}$
minimize the distance between the solution and a suitable target	stable and accurate solution, not required to possess all desired physical properties	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

Bochev, Ridzal, Shashkov (2013) *JCP*

Density Formulation

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

- *Objective* $\frac{1}{2}\|\widetilde{u} - u^{\mathsf{T}}\|_{\ell_2}^2$
- *Target* $u_i^{\mathsf{T}} := \int_{\widetilde{c}_i} \rho^h(\boldsymbol{x})dV - \int_{c_i} \rho^h(\boldsymbol{x})dV$
- *Constraints* $\sum_{i=1}^{C} \widetilde{u}_i = 0, \quad \rho_i^{min}\widetilde{\mu}_i \le \widetilde{m}_i \le \rho_i^{max}\widetilde{\mu}_i$

Bochev, Ridzal, Shashkov (2013) *JCP*

Tracer Formulation

$$\widetilde{q}_i = \frac{\int_{\widetilde{c}_i} \rho(\boldsymbol{x}) q(\boldsymbol{x}) dV}{\int_{\widetilde{c}_i} \rho(\boldsymbol{x}) dV}$$

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

OBR Algorithm

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{u} - u^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{C} \widetilde{u}_i = 0, \quad m_i^{\min} \le m_i + \widetilde{u}_i \le m_i^{\max} \end{cases}$$

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{C} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{\min} \le \widetilde{q}_i \le q_i^{\max} \end{cases}$$

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

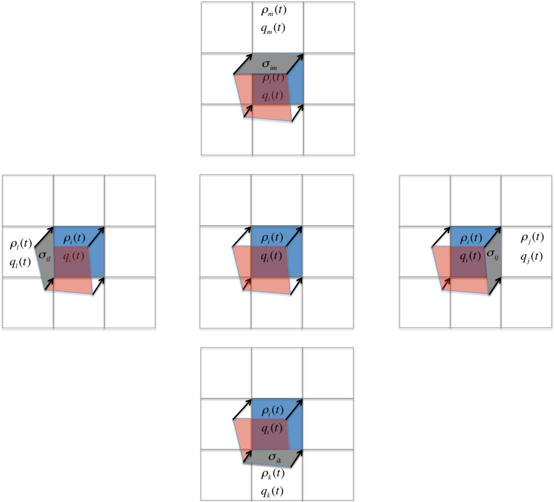
$$\rho^h(\mathbf{x})|_{c_i} = \rho_i + \mathbf{g}_i^\rho \cdot (\mathbf{x} - \mathbf{b}_i)$$

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

- 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 $\mathbf{b}_i = \dfrac{\int_{c_i} \mathbf{x} dV}{\mu_i}$
- Cell center of mass $\mathbf{c}_i = \dfrac{\int_{c_i} \mathbf{x}\rho_i(\mathbf{x}) dV}{m_i}$
- Mean preserving by construction

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

Swept Area Approximation



$$F_{is}^{\rho} = \int_{\sigma_{is}} \rho_{i/s}^{h}(\boldsymbol{x})dV$$

$$F_{is}^{q} = \int_{\sigma_{is}} \rho_{i/s}^{h}(\boldsymbol{x})q_{i/s}^{h}(\boldsymbol{x})dV$$

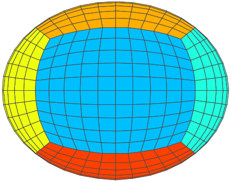
$$u_i^{\mathsf{T}} \approx \sum_s F_{is}^{\rho}$$

$$q_i^{\mathsf{T}} \approx \frac{q_i(t)m_i(t) + \sum_s F_{is}^{q}}{m_i(t) + u_i^{\mathsf{T}}}$$

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

$$x = a \tan\alpha, y = a \tan\beta \quad p = 1, ..., 6$$

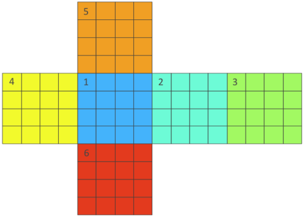


$$\int_V dV = -\int_{\partial V} \frac{1}{1+x^2}\frac{y}{r}dx$$

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

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

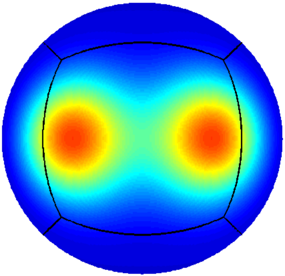
$$r = \sqrt{1+x^2+y^2} \text{ for } a = 1$$



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

Convergence Test - Solid Body Rotation

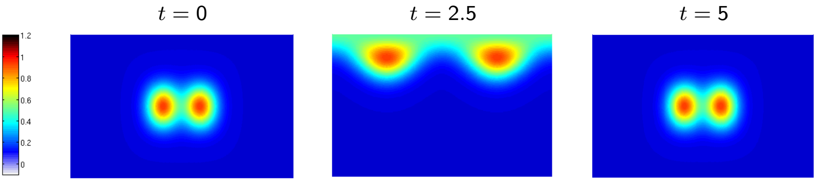
- Initial density distribution set to one everywhere
- Initial tracer distribution two smooth Gaussian hills centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent rotational flow field, $\alpha = \pi/4$:



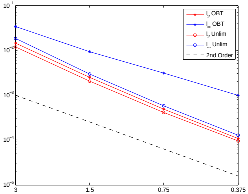
$$u(\lambda, \theta) = 2\pi \left(\cos(\theta)\cos(\alpha) + \cos(\lambda)\sin(\theta)\sin(\alpha)\right)$$

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

Convergence Test - Solid Body Rotation



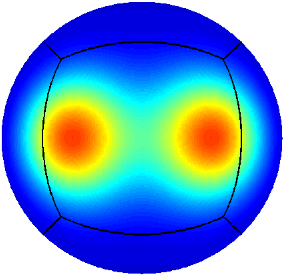
		OBT*		Unlimited	
mesh	steps	l_2	l_∞	l_2	l_∞
3.0°	600	0.0145	0.0338	0.0120	0.0185
1.5°	1200	0.00247	0.00934	0.00203	0.00296
0.75°	2400	0.000486	0.00308	0.000412	0.000412
0.375°	4800	0.000108	0.000997	0.0000958	0.000127
	Rate	*2.36*	*1.68*	*2.43*	*2.51*



* Optimization-based transport

Convergence Test - Deformational Flow

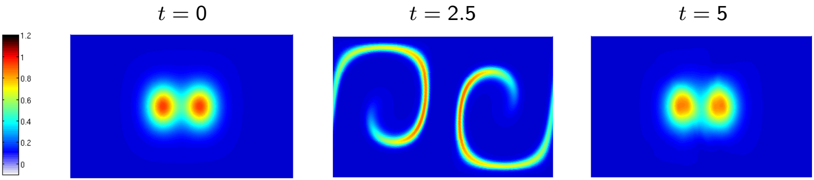
- Initial density distribution set to one everywhere
- Initial tracer distribution two smooth Guassian hills centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent deformational flow field, $T = 5$:



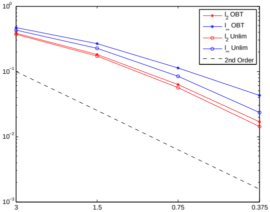
$$u(\lambda, \theta, t) = 2\sin^2(\lambda - 2\pi t/T)\sin(2\theta)\cos(\pi t/T) + 2\pi\cos(\theta)/T$$

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

Convergence Test - Deformational Flow



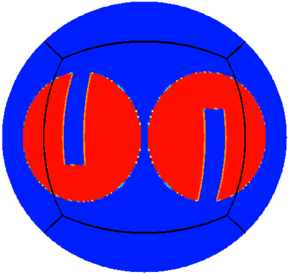
		OBT*		Unlimited	
mesh	steps	l_2	l_∞	l_2	l_∞
3.0°	600	0.386	0.465	0.368	0.425
1.5°	1200	0.182	0.268	0.172	0.225
0.75°	2400	0.0626	0.113	0.0559	0.0843
0.375°	4800	0.0167	0.0425	0.0144	0.0233
	Rate	*1.51*	*1.16*	*1.56*	*1.40*



* Optimization-based transport

Discontinuous Tracer Test

- Initial density distribution set to one everywhere
- Initial tracer distribution two notched cylinders centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- Nondivergent deformational flow field, $T = 5$:

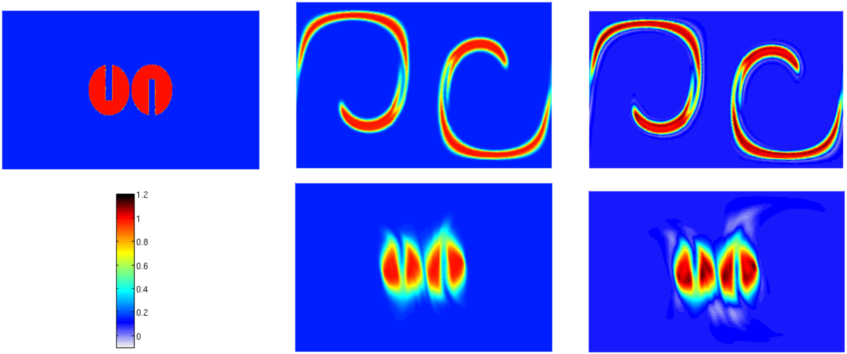


$$u(\lambda, \theta, t) = 2\sin^2(\lambda - 2\pi t/T)\sin(2\theta)\cos(\pi t/T) + 2\pi\cos(\theta)/T$$

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

Discontinuous Tracer Test

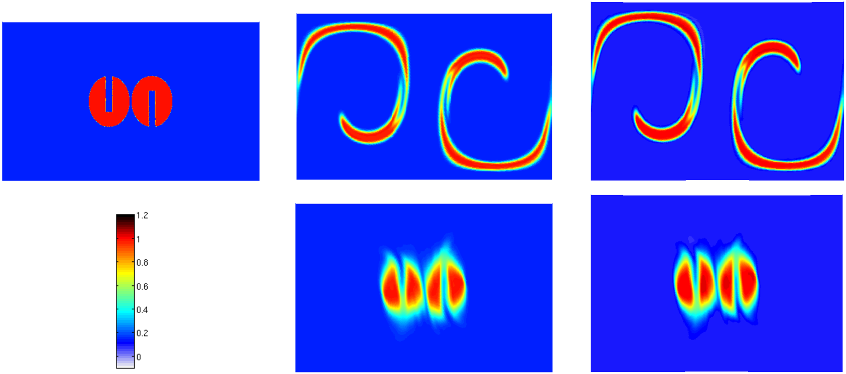
Initial | OBT | Unlimited



Initial	OBT	Unlimited
min = 0.1	min = 0.10	min = -0.020
max = 1.0	max = 1.00	max = 1.14

Discontinuous Tracer Test

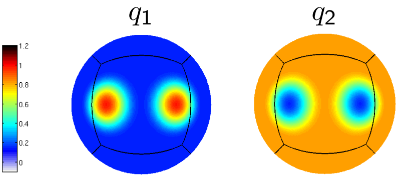
Initial	OBT	Slope Limited

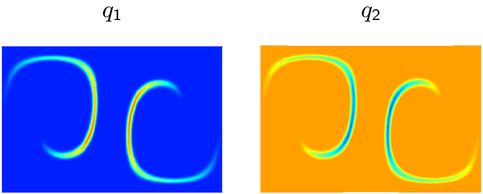


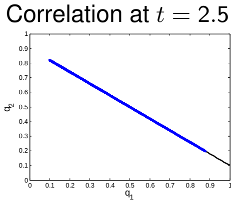
Initial	OBT	Slope Limited
min = 0.1	min = 0.10	min = 0.078
max = 1.0	max = 1.00	max = 1.030

Linear Tracer Correlation Test

- Initial density distribution set to one
- Initial tracer distributions two cosine bells centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$
- q_1 has min = 0.1 and max = 1.0
- $q_2 = -0.8q_1 + 0.9$
- Nondivergent deformational flow



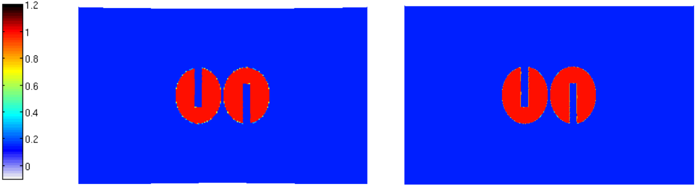




Locality Test - Initial Conditions

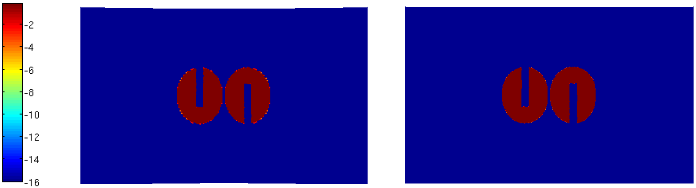
Tracer (q)

1.5° 0.75°



$log(q - 0.1)$

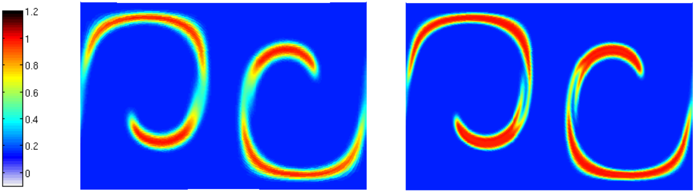
1.5° 0.75°



Locality Test - Deformational Flow

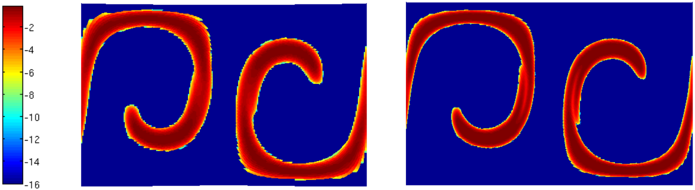
Tracer (q)

1.5°　　　　　　　　0.75°

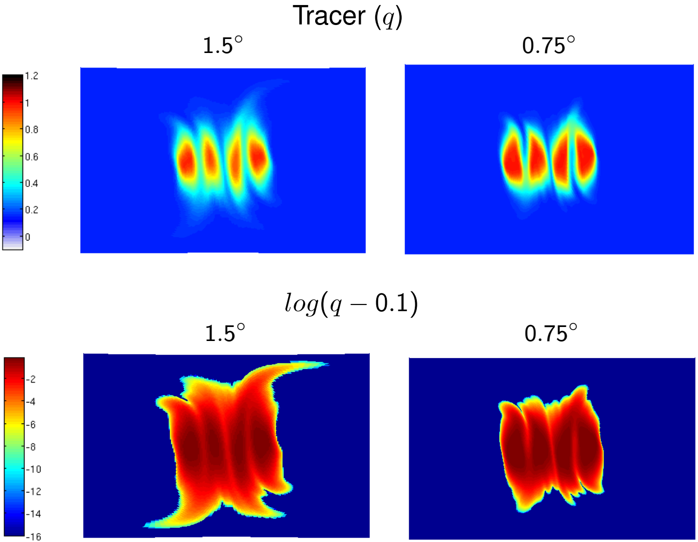


$log(q - 0.1)$

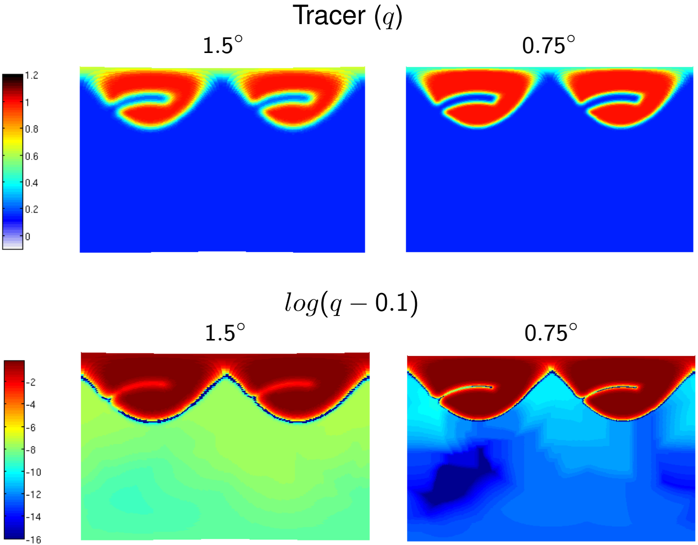
1.5°　　　　　　　　0.75°



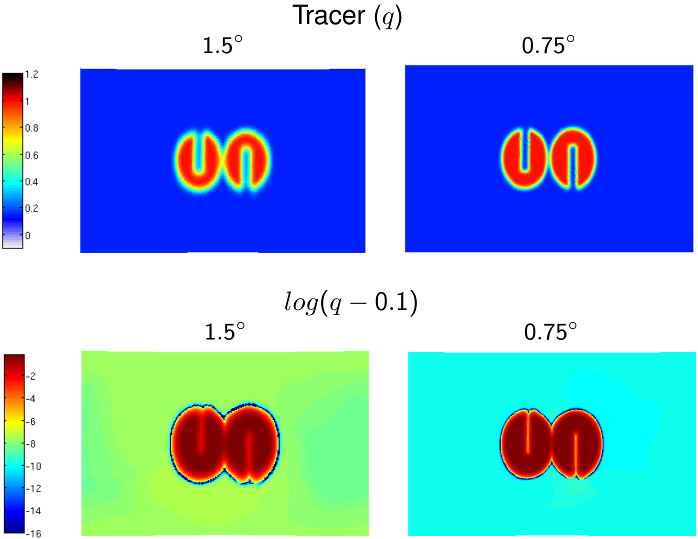
Locality Test - Deformational Flow



Locality Test - Solid Body Rotation



Locality Test - Solid Body Rotation



Conclusions

- Optimization-based transport using incremental remapping offers a robust and flexible alternative to standard transport techniques
  - Solution is globally mass conserving and bounds preserving
  - Optimization algorithm is efficient and computationally competitive with standard slope limiting
  - Swept area integrals are computed once per time step are used for multiple tracers
- Future work
  - Continue to investigate the behavior of algorithm in regards to global versus local mass conservation
  - Developing optimization-based limiting for nodal spectral element semi-Lagrangian tracer transport