SAND2023-07807C

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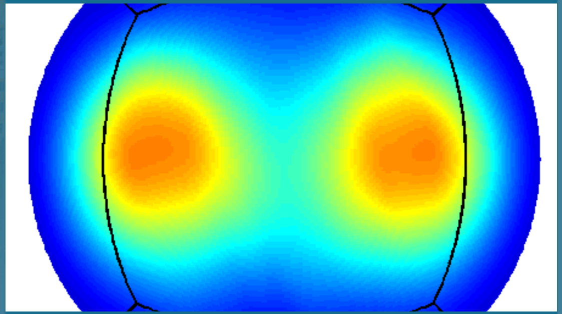
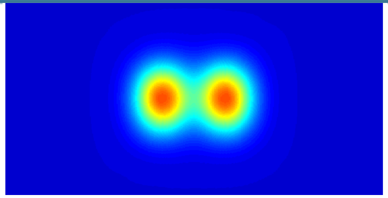
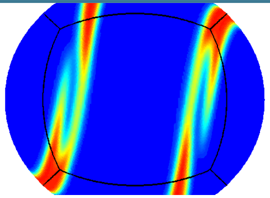
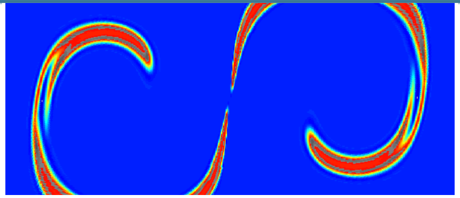
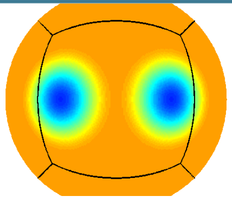
Optimization-based, property-preserving algorithms for passive tracer transport











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Motivation & model problem

Why are transport schemes so important for ESM?

- Atmosphere is the most expensive component of Earth System Models
- Tracer advection is the dominant cost in atmosphere simulations
- With biogeochemistry 100-1000 tracers are needed

Tracer-density system

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{v} = 0 \\ \dfrac{\partial \rho\tau}{\partial t} + \nabla \cdot \rho\tau \boldsymbol{v} = 0 \end{cases} \Rightarrow \quad \frac{D\tau}{Dt} \equiv \frac{\partial \tau}{\partial t} + \boldsymbol{v} \cdot \nabla \tau = 0$$

ρ - Density

τ - Tracer mixing ratio

$\boldsymbol{v}$ - Velocity

Objectives: A numerical transport algorithm for the solution of the tracer transport equations that is

- Accurate
- Efficient
- Works on unstructured grids
- Property preserving

$$\begin{cases} M = \int_\Omega \rho \, dx \qquad Q = \int_\Omega \rho\tau \, dx \\ \rho^{min} \leq \rho \leq \rho^{max} \qquad \tau^{min} \leq \tau \leq \tau^{max} \\ \zeta = a\tau + b \end{cases}$$

← Conservation of **mass** and **total tracer**

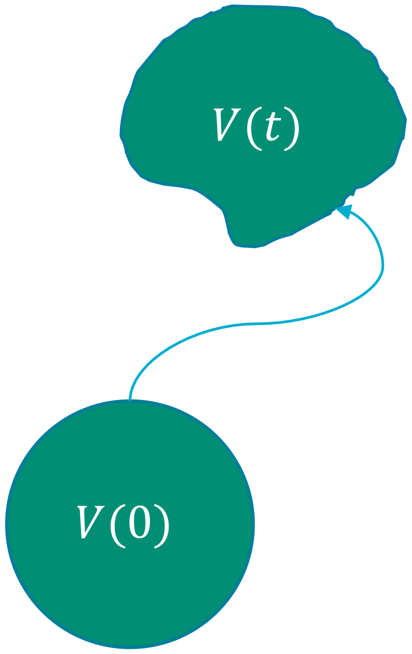
← Preservation of **local bounds**

← Preservation of **tracer correlations**

Background

To develop our method we start with a generic semi-Lagrangian scheme for tracer transport.

- Semi-Lagrangian schemes are popular in the geophysical modeling community because they allow much larger time steps than the CFL- restricted time steps in explicit Eulerian methods.



Lagrangian volume

Nomenclature

$$\mu_{V(t)} = \int_{V(t)} dV \quad \leftarrow \text{Measure of } V(t)$$

$$m_{V(t)} = \int_{V(t)} \rho(\boldsymbol{x},t)dV \quad \leftarrow \text{Mass contained in } V(t)$$

$$q_{V(t)} = \int_{V(t)} \rho(\boldsymbol{x},t)\tau(\boldsymbol{x},t)dV \quad \leftarrow \text{Total tracer in } V(t)$$

$$\overline{\rho}_{V(t)} = \frac{m_{V(t)}}{\mu_{V(t)}} \quad \leftarrow \text{Volume averaged density}$$

$$\overline{\tau}_{V(t)} = \frac{q_{V(t)}}{m_{V(t)}} \quad \leftarrow \text{Density weighted tracer}$$

Mathematical basis for semi-Lagrangian schemes

$$\frac{d}{dt} m_{V(t)} = 0 \longrightarrow \overline{\rho}_{V(t_{n+1})} = \frac{m_{V(t_{n+1})}}{\mu_{V(t_{n+1})}} = \frac{m_{V(t_n)}}{\mu_{V(t_{n+1})}}$$

Mass and total tracer mass are preserved in Lagrangian volumes

$$\frac{d}{dt} q_{V(t)} = 0 \longrightarrow \overline{\tau}_{V(t_{n+1})} = \frac{q_{V(t_{n+1})}}{m_{V(t_{n+1})}} = \frac{q_{V(t_n)}}{m_{V(t_n)}}$$

→ **Lagrangian update formulas for the averaged quantities**

A generic semi-Lagrangian scheme for tracer transport

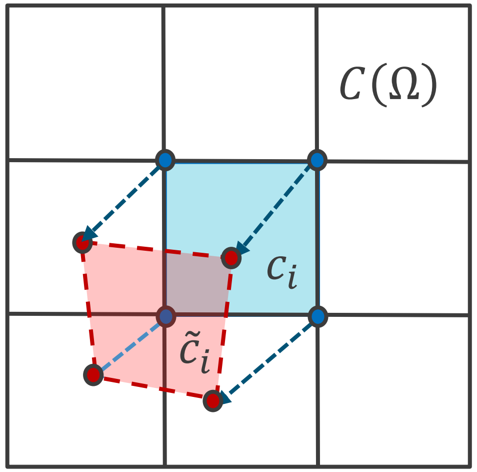
We consider a scheme based on backward incremental remapping

$C(\Omega)$ - Fixed (Eulerian) grid with cells c_i $\quad V(t_k) := c_i \quad \rightarrow \quad \mu_{i,k}, m_{i,k}, q_{i,k}, \overline{\rho}_{i,k}, \overline{\tau}_{i,k}$

$\tilde{C}(\Omega)$ - Deformed (Lagrangian) grid with cells $\tilde{c}_i$ $\quad V(t_k) := \tilde{c}_i \quad \rightarrow \quad \tilde{\mu}_{i,k}, \tilde{m}_{i,k}, \tilde{q}_{i,k}, \tilde{\overline{\rho}}_{i,k}, \tilde{\overline{\tau}}_{i,k}$

$\tilde{C}(\Omega)$= Backward Lagrangian increment: the nodes $\boldsymbol{x}_i$ of $C(\Omega)$ are moved backward in time to positions $\boldsymbol{x}(t-\Delta t)$ by solving for each node

$$\begin{cases} \dot{\boldsymbol{x}}(s) = \boldsymbol{v}(\boldsymbol{x}, s) \\ \boldsymbol{x}(t) = \boldsymbol{x}_j \end{cases}$$



Define the following quantities at the current time t_n:

$$M_n := \sum_{i=1}^{N_C} m_{i,n} = \sum_{i=1}^{N_C} \overline{\rho}_{i,n}\mu_{i,n}$$

$$Q_n := \sum_{i=1}^{N_C} q_{i,n} = \sum_{i=1}^{N_C} \overline{\tau}_{i,n} m_{i,n}$$

Total mass and total tracer mass

$$\overline{\rho}_{i,n}^{\min} = \begin{cases} \min\limits_{j\in N(c_i)} \{\overline{\rho}_{j,n}\} & \text{if } c_i \cap \partial\Omega = \emptyset \\ \min\left\{ \min\limits_{j\in N(c_i)} \{\overline{\rho}_{j,n}\}, \min\limits_{\boldsymbol{x}\in N(c_i)\cap\partial\Omega} \rho(\boldsymbol{x}, t_n) \right\} & \text{if } c_i \cap \partial\Omega \neq \emptyset \end{cases}$$

$$\overline{\rho}_{i,n}^{\max} = \begin{cases} \max\limits_{j\in N(c_i)} \{\overline{\rho}_{j,n}\} & \text{if } c_i \cap \partial\Omega = \emptyset \\ \max\left\{ \max\limits_{j\in N(c_i)} \{\overline{\rho}_{j,n}\}, \max\limits_{\boldsymbol{x}\in N(c_i)\cap\partial\Omega} \rho(\boldsymbol{x}, t_n) \right\} & \text{if } c_i \cap \partial\Omega \neq \emptyset \end{cases}$$

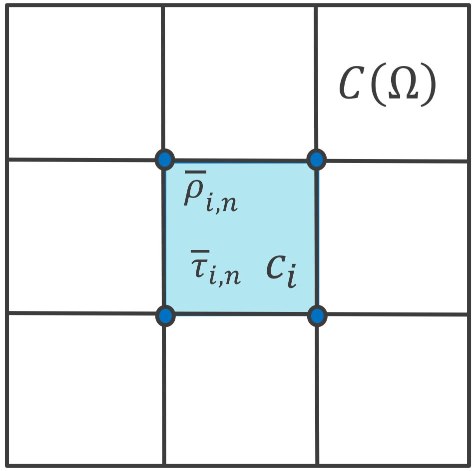
Physically motivated local density bounds (similar for τ)

A generic semi-Lagrangian scheme for tracer transport

Statement of the monotone, conservative and compatible tracer transport problem

Given: $\overline{\rho}_{i,n}$ and $\overline{\tau}_{i,n}$ on the fixed grid $C(\Omega)$ at current time t_n

Find: $\overline{\rho}_{i,n+1}$ and $\overline{\tau}_{i,n+n}$ on the fixed grid $C(\Omega)$ at future time t_{n+1}, satisfying



P1. Monotonicity and compatibility: for all $c_i \in C(\Omega)$

$$\alpha\overline{\rho}_{i,n}^{\min} \le \overline{\rho}_{i,n+1} \le \alpha\overline{\rho}_{i,n}^{\max} \quad \text{and} \quad \overline{\tau}_{i,n}^{\min} \le \overline{\tau}_{i,n+1} \le \overline{\tau}_{i,n}^{\max} \quad \text{where} \quad \alpha = \frac{\widetilde{\mu}_{i,n}}{\mu_{i,n+1}}$$

Note that τ is constant along the characteristics but in general ρ is not. Thus, the local bounds for $\overline{\tau}_{i,n+1}$ are unchanged from those at the current time t_n but the local bounds for $\overline{\rho}_{i,n+1}$ are different!

P2. Conservation of mass and total tracer mass

$$M_{n+1} := \sum_{i=1}^{N_C} m_{i,n+1} = M_n \quad \text{and} \quad Q_{n+1} := \sum_{i=1}^{N_C} q_{i,n+1} = Q_n$$

A generic semi-Lagrangian scheme for tracer transport

Solution: the Lagrangian update formula implies

$$\overline{\rho}_{V(t_{n+1})} = \frac{m_{V(t_{n+1})}}{\mu_{V(t_{n+1})}} = \frac{m_{V(t_n)}}{\mu_{V(t_{n+1})}} \longrightarrow \overline{\rho}_{i,n+1} = \frac{m_{i,n+1}}{\mu_{i,n+1}} = \frac{\widetilde{m}_{i,n}}{\mu_{i,n+1}}$$

$$\overline{\tau}_{V(t_{n+1})} = \frac{q_{V(t_{n+1})}}{m_{V(t_{n+1})}} = \frac{q_{V(t_n)}}{m_{V(t_n)}} \longrightarrow \overline{\tau}_{i,n+1} = \frac{q_{i,n+1}}{m_{i,n+1}} = \frac{\widetilde{q}_{i,n}}{\widetilde{m}_{i,n}}$$

where

$$\widetilde{m}_{i,n} \approx \int_{\tilde{c}_i} \rho(x,t_n)\,dx$$

$$\tilde{q}_{i,n} \approx \int_{\tilde{c}_i} \rho(x,t_n)\tau(x,t_n)\,dx$$

- We need the average mass $\widetilde{m}_{i,n}$ and tracer $\tilde{q}_{i,n}$ on the cells $\tilde{c}_i$ of the deformed mesh $\tilde{C}(\Omega)$.
- However, the solution at current time t_n is given on the cells c_i of the fixed mesh $C(\Omega)$
- Classical schemes use monotone & conservative reconstructions of $\rho(x,t_n)$ and $\tau(x,t_n)$ on the cells c_i of the fixed mesh $C(\Omega)$ to compute the integrals on the cells $\tilde{c}_i$ of the deformed mesh:

$$\rho_n^h(x) \approx \rho(x,t_n) \longrightarrow \rho_{i,n}^h(\boldsymbol{x}) = \overline{\rho}_{i,n} + \mathbf{g}_{\rho,i}\cdot(\boldsymbol{x}-\boldsymbol{x}_{b_i}), \quad \boldsymbol{x}_{b_i} = \frac{\int_{c_i}\boldsymbol{x}dV}{\mu_i}$$

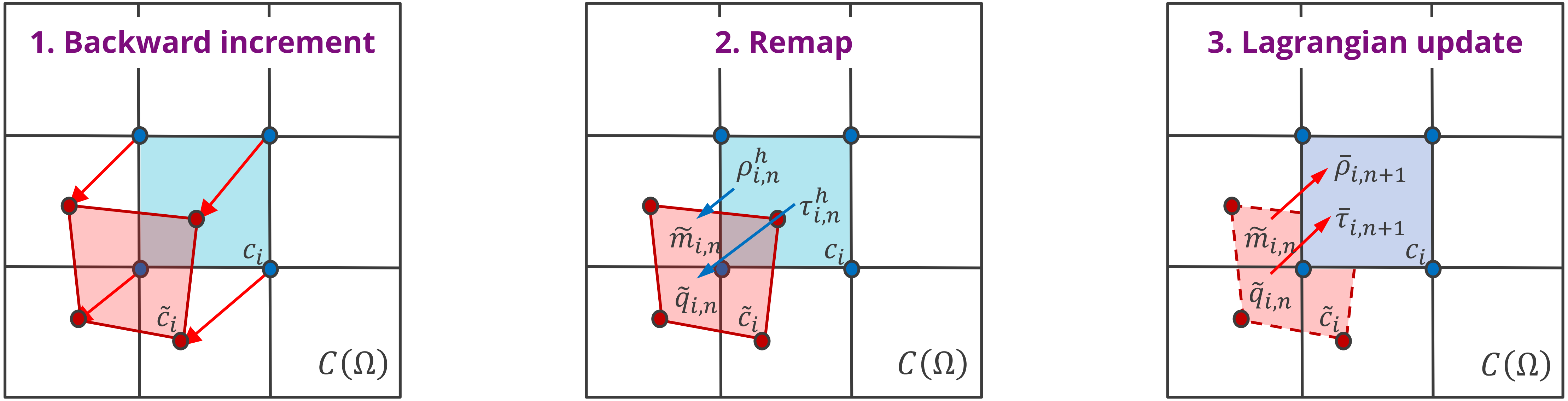
Slope-limited gradient reconstructions

$$\tau_n^h(x) \approx \tau(x,t_n) \longrightarrow \tau_{i,n}^h(\boldsymbol{x}) = \overline{\tau}_{i,n} + \mathbf{g}_{\tau,i}\cdot(\boldsymbol{x}-\boldsymbol{x}_{c_i}), \quad \boldsymbol{x}_{c_i} = \frac{\int_{c_i}\boldsymbol{x}\rho_{i,n}^h(\boldsymbol{x})dV}{\int_{c_i}\rho_{i,n}^h(\boldsymbol{x})dV}$$

➡

- Monotone
- Conservative
- Mean-preserving

We will modify the last two stages of the generic scheme



$$\dot{\boldsymbol{x}}(s) = \boldsymbol{v}(\boldsymbol{x}, s)$$

$$\boldsymbol{x}(t) = \boldsymbol{x}_j$$

$$\widetilde{m}_{i,n} = \int_{\widetilde{c}_i} \rho^h_n(\boldsymbol{x})dV$$

$$\widetilde{q}_{i,n} = \int_{\widetilde{c}_i} \rho^h_n(\boldsymbol{x})\tau^h_n(\boldsymbol{x})dV$$

$$\overline{\rho}_{i,n+1} = \frac{\widetilde{m}_{i,n}}{\mu_{i,n+1}}$$

$$\overline{\tau}_{i,n+1} = \frac{\widetilde{q}_{i,n}}{\widetilde{m}_{i,n}}$$

Monotone reconstruction drawbacks:

- Based on local worst-case scenarios
- Mixes accuracy with preservation of properties
- More difficult to ascertain solution optimality

Our changes separate accuracy from property preservation:

- **Remap stage:** use 2nd order accurate but not monotone and/or conservative reconstruction
- **Lagrangian update stage:** enforce properties by coaching this stage into a constrained optimization problem.

Optimization-based semi-Lagrangian tracer transport

New **remap** stage

$$\widetilde{m}^{\mathsf{T}}_{i,n} = \int_{\widetilde{c}_i} \rho_n^{h,LS}(\boldsymbol{x})dV \longleftarrow \rho_n^{h,LS} = \overline{\rho}_{i,n} + \mathbf{g}^{LS}_{\rho,i}\cdot(\boldsymbol{x} - \boldsymbol{x}_{b_i})$$

$$\widetilde{q}^{\mathsf{T}}_{i,n} = \int_{\widetilde{c}_i} \rho_n^{h,LS}(\boldsymbol{x})\tau_n^{h,LS}(\boldsymbol{x})dV \longleftarrow \tau_n^{h,LS} = \overline{\tau}_{i,n} + \mathbf{g}^{LS}_{\tau,i}\cdot(\boldsymbol{x} - \boldsymbol{x}_{c_i})$$

$\mathbf{g}^{LS}_{\rho,i}$, $\mathbf{g}^{LS}_{\tau,i}$: Least-squares reconstruction of the gradients on cell c_i

- $\widetilde{m}^{\mathsf{T}}_{i,n}$ and $\widetilde{q}^{\mathsf{T}}_{i,n}$ are 2nd order accurate but not guaranteed to be monotone and/or conservative

New **Lagrangian update** stage. Part 1 – definition of targets & local bounds at future time t_{n+1}

$$\overline{\rho}^{\mathsf{T}}_{i,n+1} = \frac{\widetilde{m}^{\mathsf{T}}_{i,n}}{\mu_{i,n+1}} \qquad \overline{\rho}^{\min}_{i,n+1} = \overline{\rho}^{\min}_{i,n}\frac{\widetilde{\mu}_{i,n}}{\mu_{i,n+1}} \qquad \overline{\rho}^{\max}_{i,n+1} = \overline{\rho}^{\max}_{i,n}\frac{\widetilde{\mu}_{i,n}}{\mu_{i,n+1}} \qquad \alpha = \frac{\widetilde{\mu}_{i,n}}{\mu_{i,n+1}}$$

$$\overline{\tau}^{\mathsf{T}}_{i,n+1} = \frac{\widetilde{q}^{\mathsf{T}}_{i,n}}{\widetilde{m}_{i,n}}$$

Tracer is constant along characteristics: reuse bounds from t_n

- $\overline{\rho}^{\mathsf{T}}_{i,n+1}$ and $\overline{\tau}^{\mathsf{T}}_{i,n+1}$ are 2nd order accurate but not guaranteed to be monotone and/or conservative

Optimization-based semi-Lagrangian tracer transport

New Lagrangian update stage. Part 2 – enforce properties at future time t_{n+1}

Density:
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\sum_{i=1}^{N_C} \mu_{i,n+1}^2 (\overline{\rho}_{i,n+1} - \overline{\rho}_{i,n+1}^{\mathsf{T}})^2 \qquad \text{subject to} \\ \sum_{i=1}^{N_C} \overline{\rho}_{i,n+1}\mu_{i,n+1} = M_n \quad \text{and} \quad \overline{\rho}_{i,n+1}^{\min} \le \overline{\rho}_{i,n+1} \le \overline{\rho}_{i,n+1}^{\max}; \quad i = 1, ..., N_C \end{cases}$$

➡ Set
$$\overline{\rho}_{i,n+1} = \overline{\rho}_{i,n+1}^{\mathsf{OPT}}$$
$$m_{i,n+1}^{\mathsf{OPT}} := \overline{\rho}_{i,n+1}^{\mathsf{OPT}}\mu_{i,n+1}$$

Tracer:
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\sum_{i=1}^{N_C} (\overline{\tau}_{i,n+1} - \overline{\tau}_{i,n+1}^{\mathsf{T}})^2 \qquad \text{subject to} \\ \sum_{i=1}^{N_C} \overline{\tau}_{i,n+1} m_{i,n+1}^{\mathsf{OPT}} = Q_n \quad \text{and} \quad \overline{\tau}_{i,n}^{\min} \le \overline{\tau}_{i,n+1} \le \overline{\tau}_{i,n}^{\max}; \quad i = 1, ..., N_C. \end{cases}$$

➡ Set $\overline{\tau}_{i,n+1} = \overline{\tau}_{i,n+1}^{\mathsf{OPT}}$

Theorem 1. Existence & uniqueness

The feasible sets of the optimization problems are non-empty & have unique solutions

Properties

Theorem 2. Global optimality of the optimization-based solution

$$\frac{1}{2}\sum_{i=1}^{N_C} \mu_{i,n+1}^2 (\overline{\rho}_{i,n+1}^{\mathsf{OPT}} - \overline{\rho}_{i,n+1}^{\mathsf{T}})^2 \le \frac{1}{2}\sum_{i=1}^{N_C} \mu_{i,n+1}^2 (\overline{\rho}_{i,n+1}^{\mathsf{G}} - \overline{\rho}_{i,n+1}^{\mathsf{T}})^2$$

$$\frac{1}{2}\sum_{i=1}^{N_C} (\overline{\tau}_{i,n+1}^{\mathsf{OPT}} - \overline{\tau}_{i,n+1}^{\mathsf{T}})^2 \le \frac{1}{2}\sum_{i=1}^{N_C} (\overline{\tau}_{i,n+1}^{\mathsf{G}} - \overline{\tau}_{i,n+1}^{\mathsf{T}})^2$$

Generic scheme

The optimization-based solution is the best possible, with respect to the targets, approximate solution that also satisfies properties P.1–P.2.

Theorem 3. Preservation of tracer correlations

The optimization-based Lagrangian update stage **preserves linear tracer correlations.**

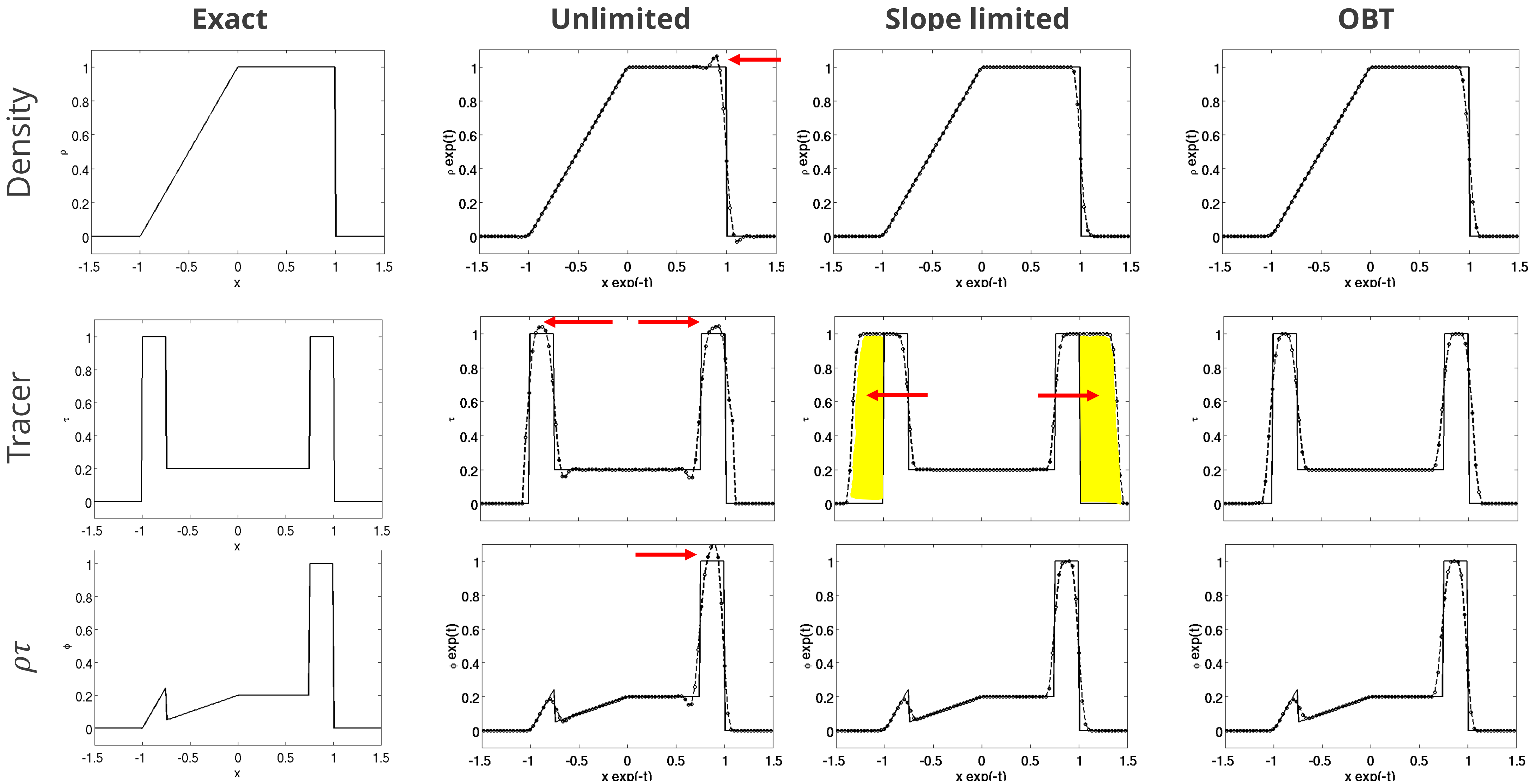
What about the cost?

$$\mathbf{q}_{n+1} = \underset{\mathbf{q}}{\operatorname{argmin}}\, \mathbf{q}^T \mathbf{M} \mathbf{q} + \mathbf{c}^T \mathbf{q} + \mathbf{c}_0 \quad \text{subject to} \quad \begin{cases} \mathbf{w}^T \mathbf{q} = \mathbf{w}^T \mathbf{q}_n & \leftarrow \text{Conservation} \\ \mathbf{q}^{\min} \le \mathbf{q} \le \mathbf{q}^{\max} & \leftarrow \text{Local bounds} \end{cases}$$

☞ A “*singly linearly constrained QP with simple bounds*”

☞ QP structure admits a fast *O(N)* optimization algorithm.

Numerical examples in 1D: Compatibility test



Numerical examples in 2D: Convergence

Tracer profile:

$$\tau = \sin(\pi x)^4 \sin(\pi y)^4 \exp(-\beta(x - x_0)^2 + (y - y_0)^2)$$

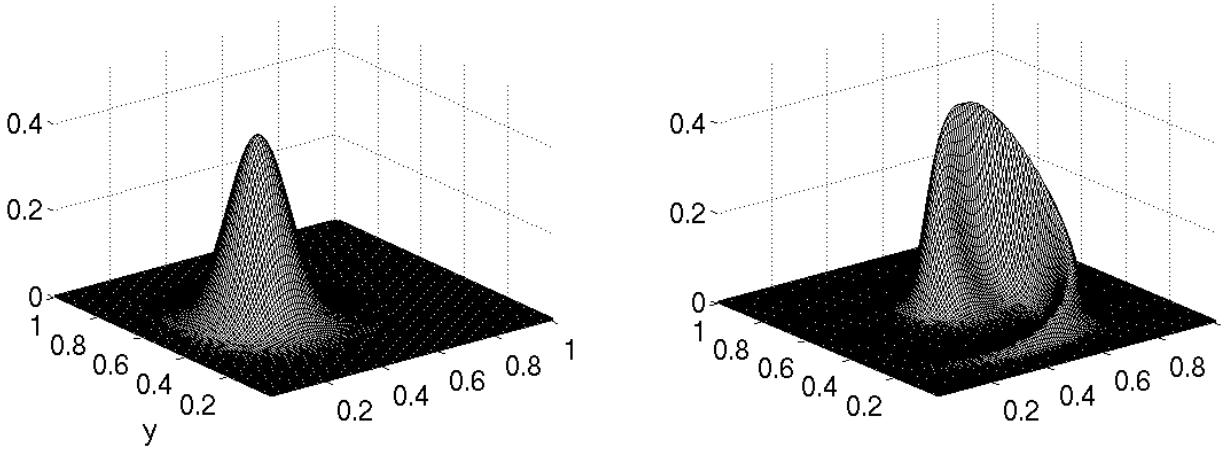
$(x_0, y_0) = (0.25, 0.25)$; $\beta = 40$

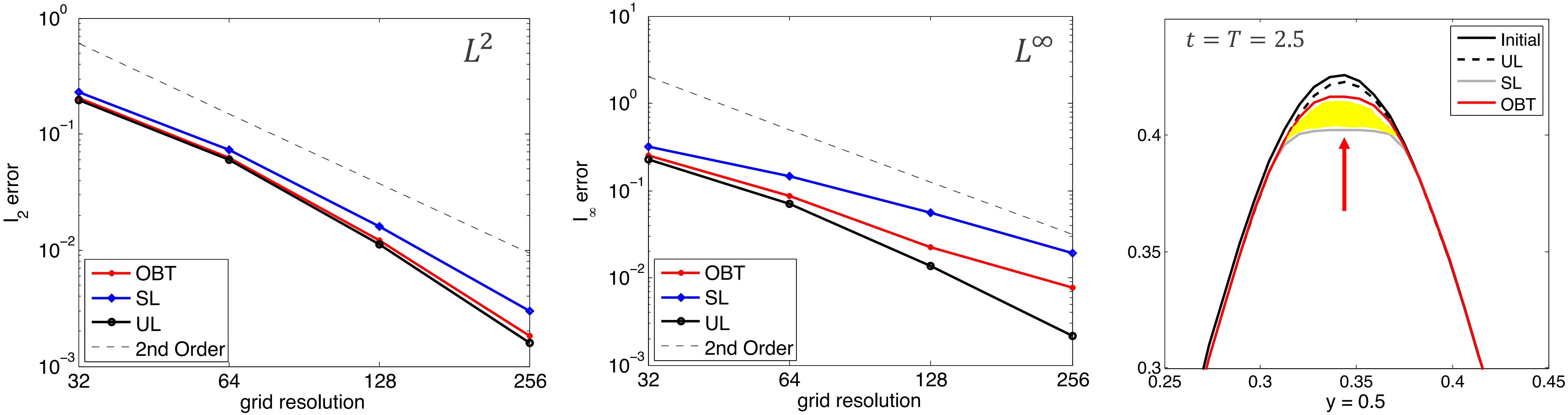
Velocity field*

$$u = \sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T)$$

$$v = -\sin^2(\pi y)\sin(2\pi x)\cos(\pi t/T)$$

$T = 2.5$





(*)R. J. LeVeque, High-resolution conservative algorithms for advection in incompressible flow, SIAM Journal on Numerical Analysis 33 (1996) 627–665.

Numerical examples in 2D: Solid body rotation

Tracer profile:

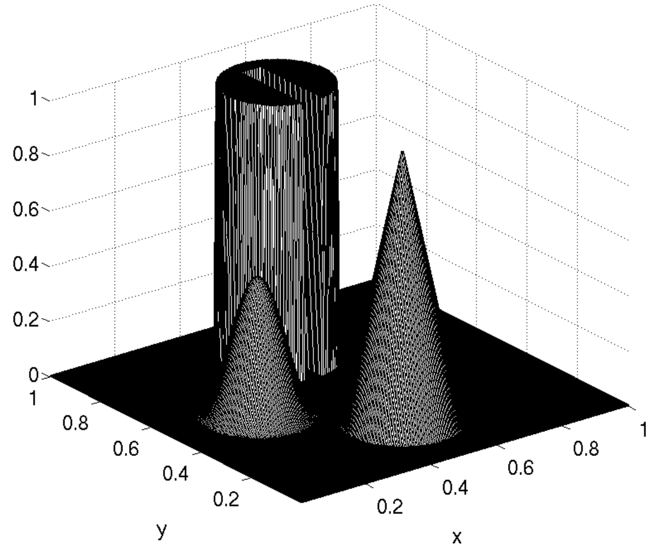
- Zalesak cylinder +
- cone +
- Gaussian hump

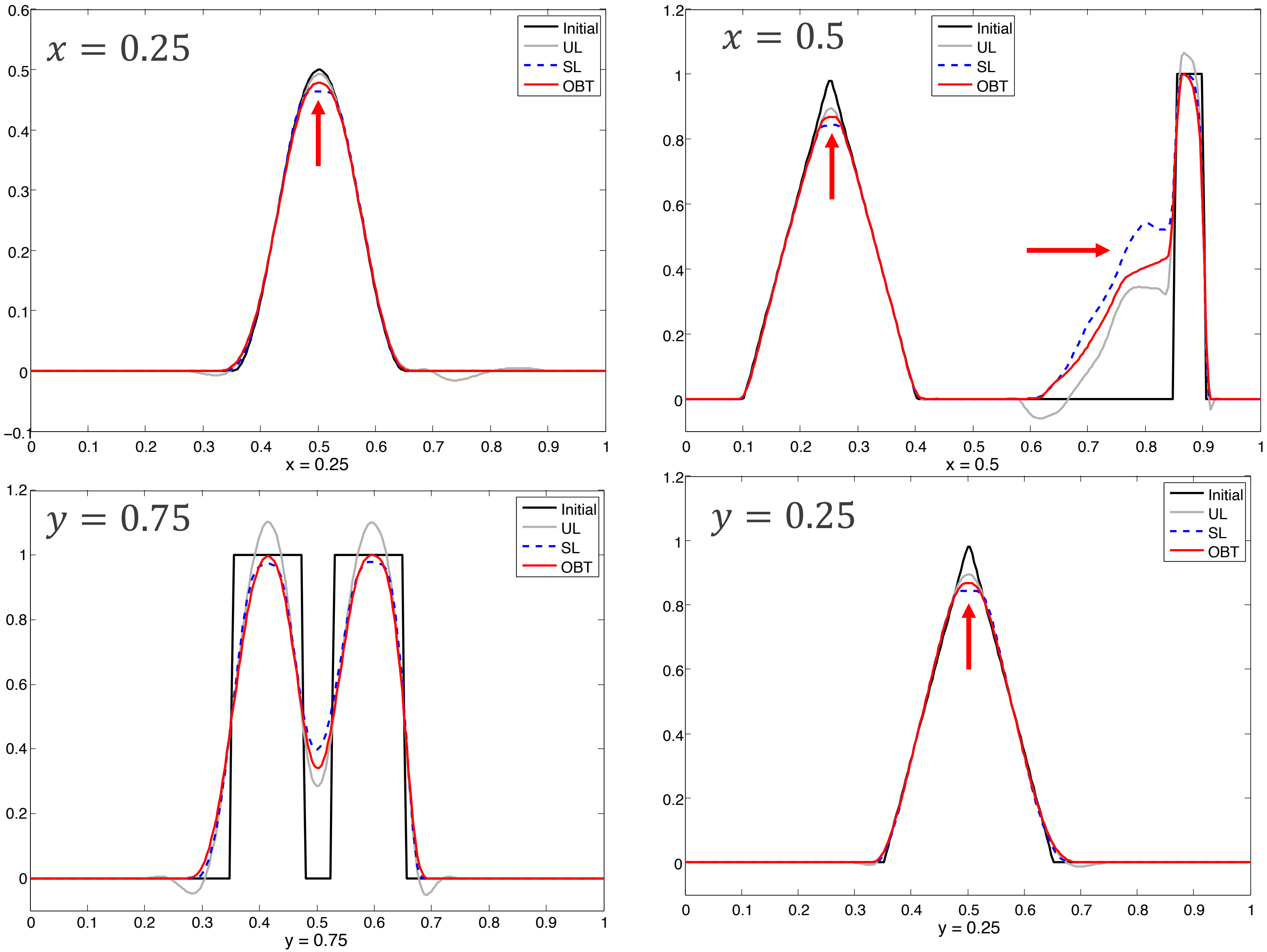
Velocity field*

$$u = \sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T)$$

$$v = -\sin^2(\pi y)\sin(2\pi x)\cos(\pi t/T)$$

$$T = 2.5$$





(*)R. J. LeVeque, High-resolution conservative algorithms for advection in incompressible flow, SIAM Journal on Numerical Analysis 33 (1996) 627–665.

Numerical examples in 2D: Linear tracer correlation

Tracers profile:

$$\tau = 0.4\big(1 + \cos\big(\pi r(x,y)\big)\big)$$

$$\xi = -1.2\tau + 1$$

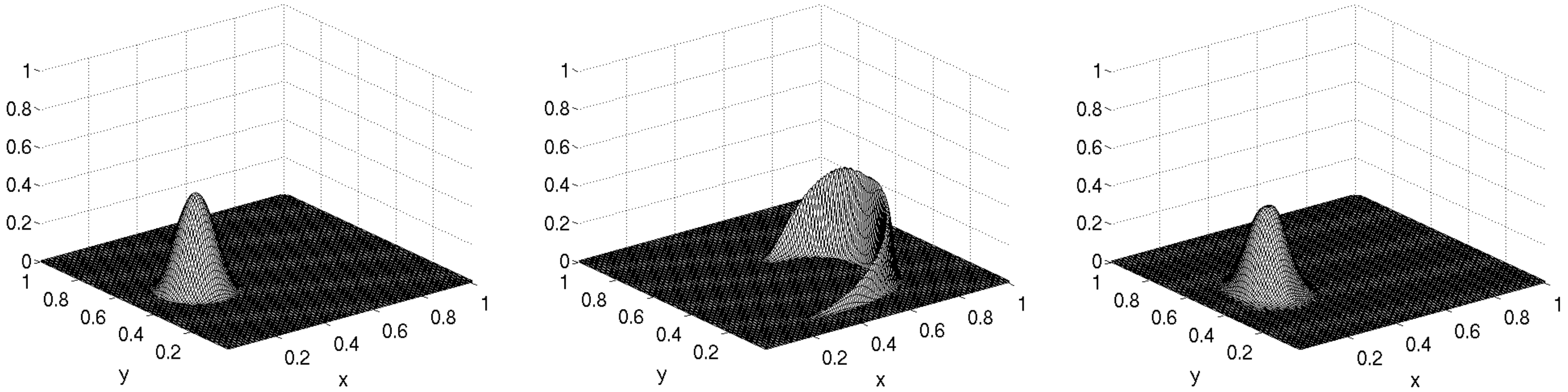
$$r(x,y) = \min\{\|\boldsymbol{x} - \boldsymbol{x}_0\|, r_0\}/r_0$$

Velocity field*

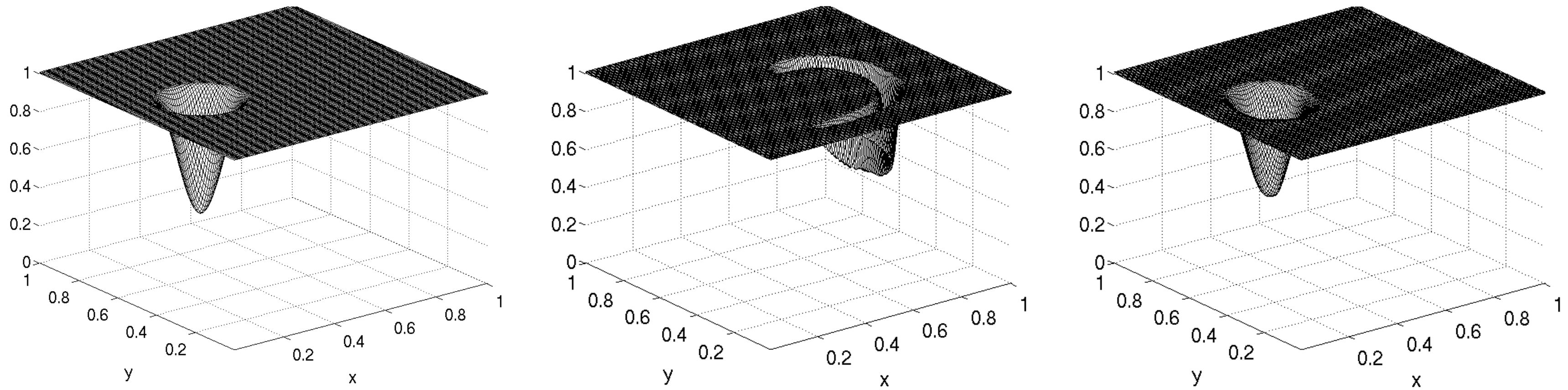
$$u = \sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T)$$

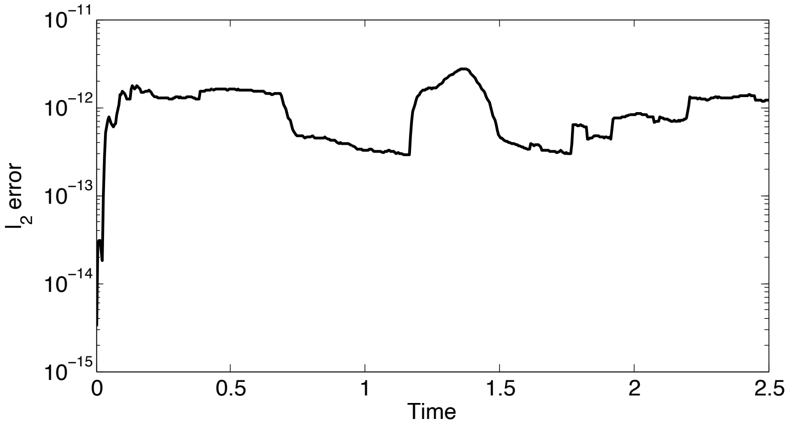
$$v = -\sin^2(\pi y)\sin(2\pi x)\cos(\pi t/T)$$

$$T = 2.5$$



$t = 0$ $t = 1.25$ $t = 2.5$





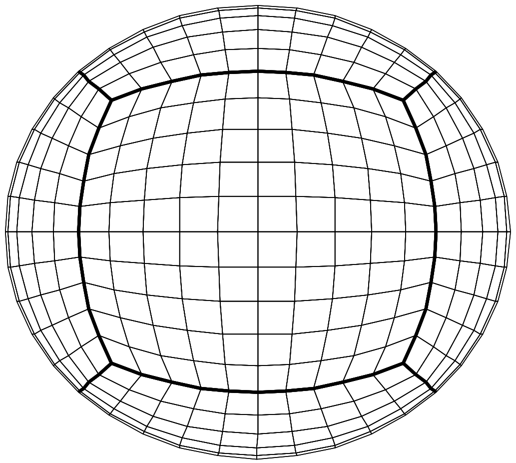
(*)R. J. LeVeque, High-resolution conservative algorithms for advection in incompressible flow, SIAM Journal on Numerical Analysis 33 (1996) 627–665.

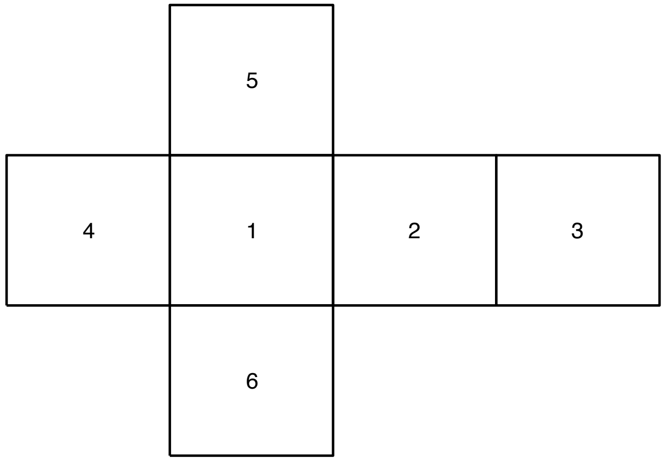
Tracer transport on a sphere: setup and convergence

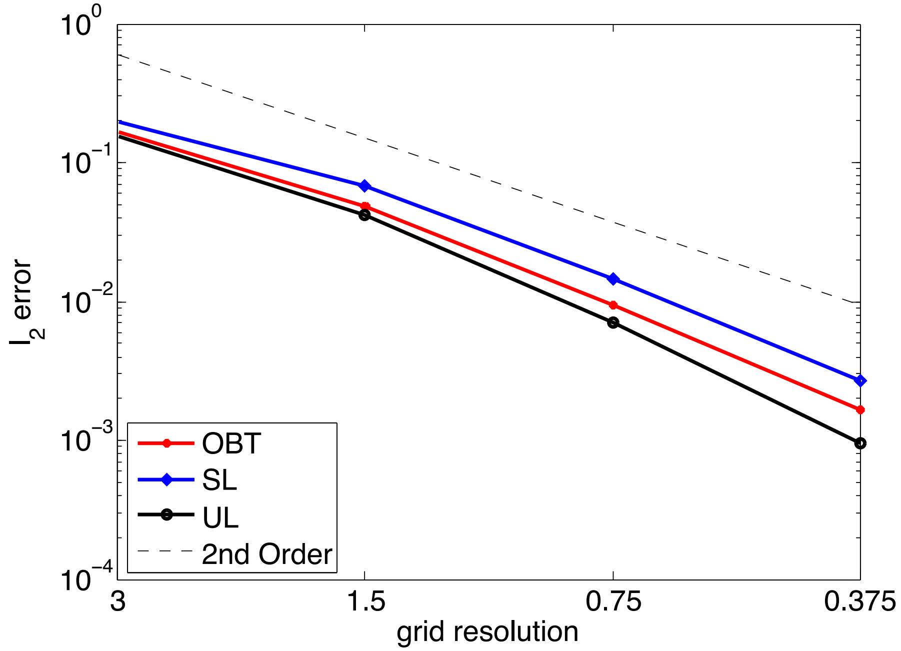
Tracer profile - 2 Gaussian hills

Velocity field* - deformational, div-free field

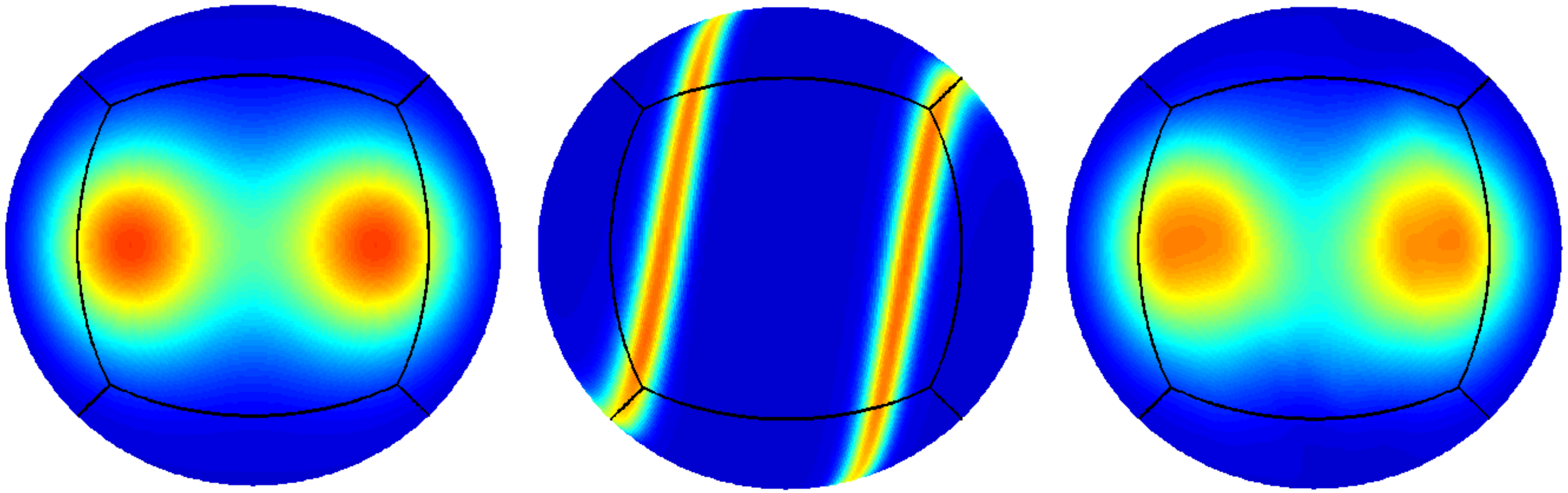
$$u(\lambda, \theta, t) = 2\sin^2(\lambda)\sin(2\theta)\cos(\pi t/T)$$
$$v(\lambda, \theta, t) = 2\sin(2(\lambda))\cos(\theta)\cos(\pi t/T)$$







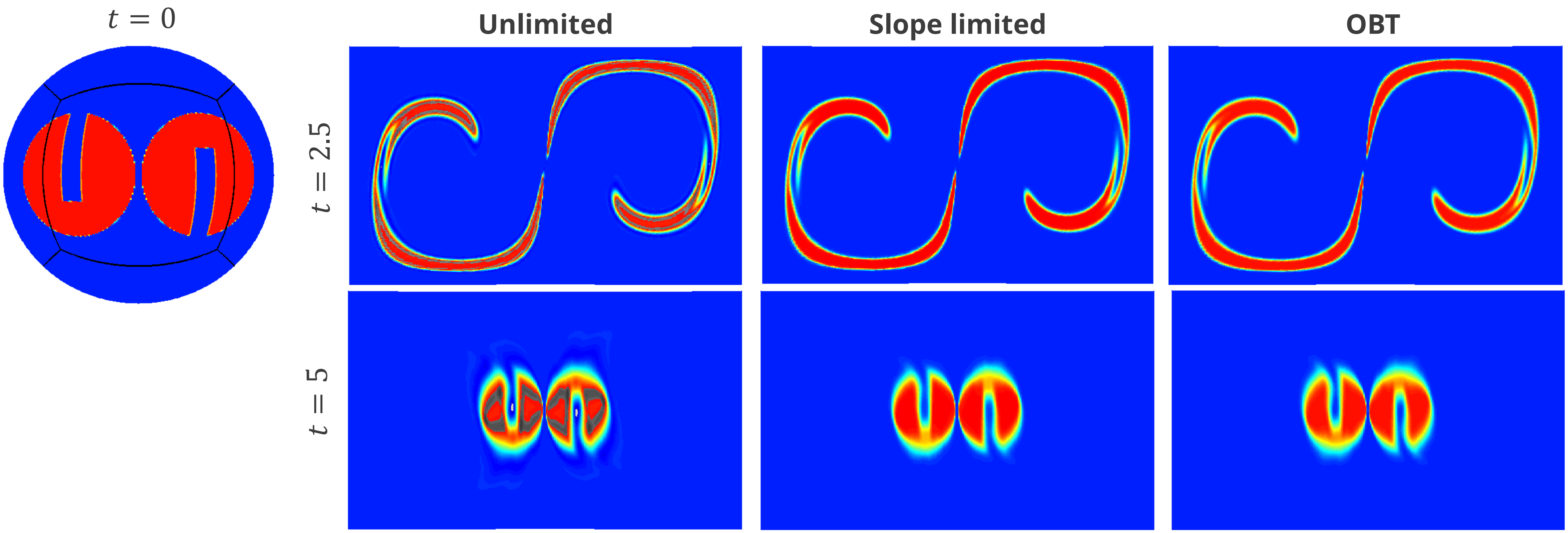
Grid resolution: 0.75°



$t = 0$ $t = 2.5$ $t = 5$

(*)R. D. Nair, P. H. Lauritzen, A class of deformational flow test cases for linear transport problems on the sphere, J. Comp. Phys. 229 (2010) 8868 – 8887.

Tracer transport on a sphere: 2 notched cylinders

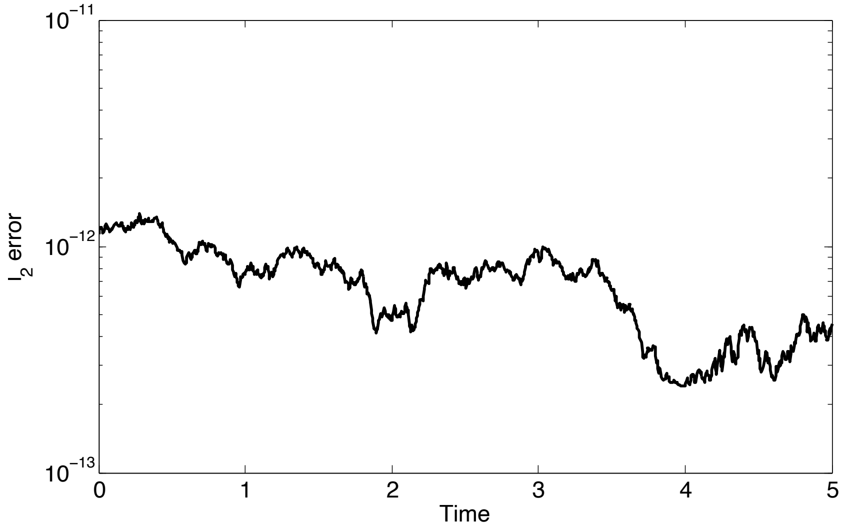


Unlimited	Slope limited	OBT
$\min = -0.020$	$\min = 0.100$	$\min = 0.100$
$\max = 1.140$	$\max = 0.999$	$\max = 1.000$

Latitude-longitude projection used for better representation of the results

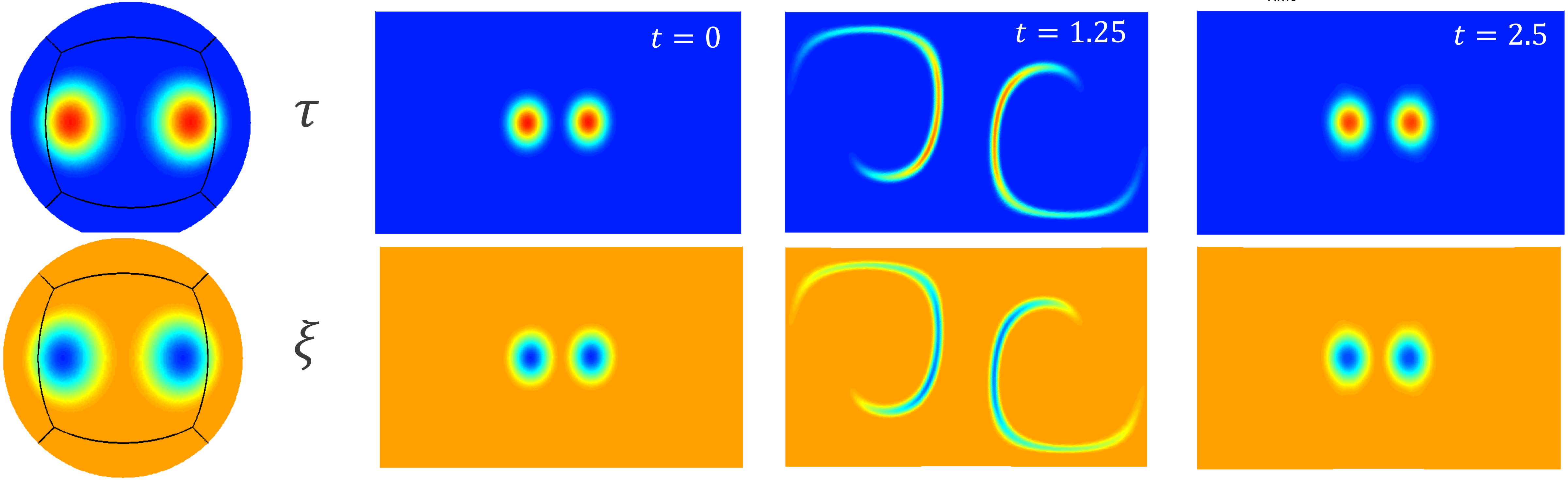
Tracer transport on a sphere: tracer correlations

Grid resolution: 0.75°



Tracers profile: two cosine bells

$$\tau = \begin{cases} 0.5(1+\cos(\pi r_i/r)) & \text{if } r_i < r, i = 1{,}2 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad \xi = -0.8\tau + 0.9$$



How much does it cost?

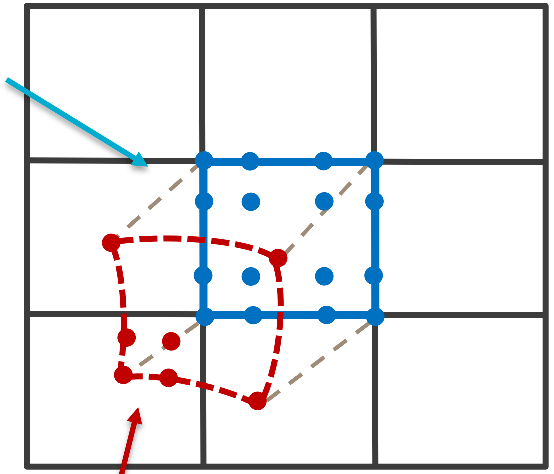
Scheme	Mesh	Relative time	ℓ_2 error	Min	Max	Exact max
Unlimited (benchmark)	32×32	1.00	1.958e-01	-0.054	0.340	0.42585
	64×64	1.00	5.954e-02	-0.079	0.402	
	128×128	1.00	1.1132e-02	-0.105	0.423	
	256×256	1.00	1.6020e-03	-0.105	0.426	
Slope Limited	32×32	**1.05**	2.3030e-01	**0**	0.281	0.42585
	64×64	**1.06**	7.3340e-02	**0**	0.362	
	128×128	1.11	1.5930e-02	**0**	0.402	
	256×256	1.19	2.9830e-03	**0**	0.418	
OBT	32×32	1.10	**2.0540e-01**	**0**	**0.323**	0.42585
	64×64	1.08	**6.2220e-02**	**0**	**0.391**	
	128×128	**1.07**	**1.2120e-02**	**0**	**0.416**	
	256×256	**1.14**	**1.8360e-03**	**0**	**0.423**	

Red = best result

Extensions: semi-Lagrangian spectral element scheme

Start with a generic SE+SL (SESL) scheme:

1. Determine GL departure points → $\tilde{\mathbf{p}}_{ij} = x(t_n)$
2. Determine solution at arrival points → $\rho_h(\mathbf{p}_{ij}, t_{n+1}) = \rho(t_{n+1})$ and $q_h(\mathbf{p}_{ij}, t_{n+1}) = q(t_{n+1})$



Then proceed as follows to find the tracer at t_{n+1} (density is similar)

3. Set optimization target to SE+SL solution: $\hat{q} := q_h(\mathbf{p}_{ij}, t_{n+1})$
4. Determine local solution bounds: $q_{ij}^{\min} \le q(\mathbf{p}_{ij}, t_{n+1}) \le q_{ij}^{\max}$
5. Set solution at the new time step by solving

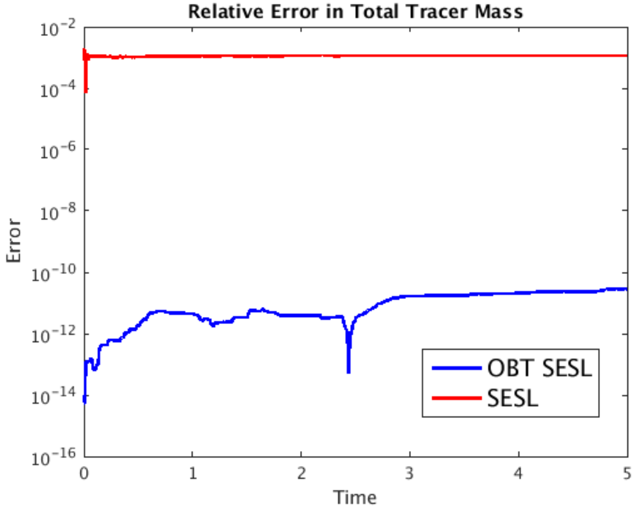
$$q_{n+1}^{*} = \underset{q \in Q^r}{\operatorname{argmin}} \|q - \hat{q}\|_0^2 \quad \text{subject to} \quad \begin{cases} \int_\Omega q\,dx = \int_\Omega q_n\,dx & \leftarrow \text{Conservation} \\ q_{ij}^{\min} \le q_{ij} \le q_{ij}^{\max} & \leftarrow \text{Local bounds} \end{cases}$$

The structure of the optimization problem is identical to the one before!

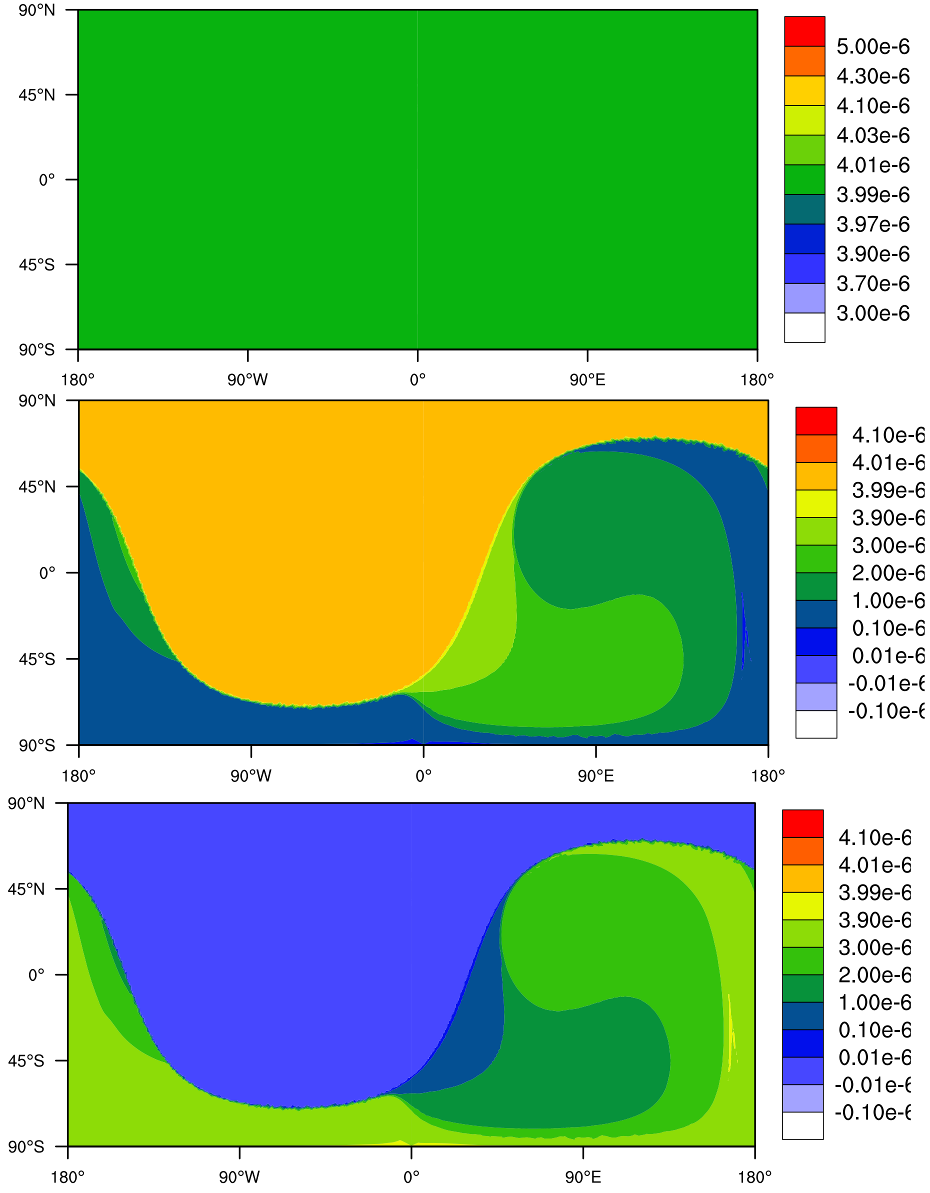
☞QP structure admits a fast *O(N)* optimization algorithm.

Numerical examples

Mass conservation



For the same tracer distribution and flow field, the error in total tracer mass reveals the lack of mass conservation in the underlying SESL scheme and the recovery of conservation by the OBT approach



Linear correlation

OBT SESL performs well on challenging idealized chemistry test where total sum of species should remain constant as long as advection scheme preserves linear relationships.

$$X_2 \xrightarrow{k_1} 2X$$

$$X + X \xrightarrow{k_2} X_2$$

Conclusions

Optimization-based tracer transport offers a robust and flexible alternative to traditional limiter-based transport techniques.

- Ensures global mass conservation and bounds preservation,
- Provably preserves linear tracer correlations,
- Robust and efficient (cost similar to conventional slope limiters),
- Formulation applicable to finite volume, finite element, and spectral element discretizations.
- Spectral element optimization-based transport has been implemented in the High-Order Method Modeling Environment (HOMME), the code on which DOE's E3SM dynamical core is based.