

Optimization-based Spectral Element Semi-Lagrangian Tracer Transport

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with

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SIAM CSE

MS296 Recent Advances in High Order Finite Element Methods
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Tracer Transport Problem

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

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

Why are transport schemes so important?

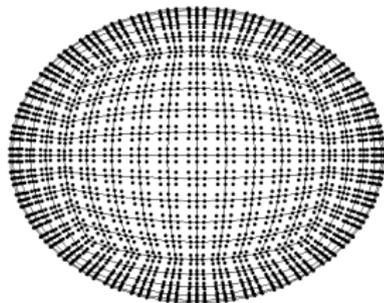
- Biogeochemistry can require 100s of tracers
- Atmosphere is the most expensive component of Earth System Models
- Tracer advection is the dominant cost

We want tracer transport algorithms that are

- conservative (of $\int \rho q$) and bounds preserving (of q)
- free stream preserving (satisfy compatibility between q and ρ)
- capable of running on unstructured grids
- efficient for large numbers of tracers

High-Order Method Modeling Environment (HOMME)

- Spectral element dynamical core used in CESM and ACME
- Continuous Galerkin finite element method using Gauss-Lobatto quadrature
- Generally runs on the cubed sphere grid, but applicable to any unstructured quadrilateral grid on the sphere
- Advection using the standard spectral element method with high-degree polynomials is accurate, but expensive due to time step restrictions



HOMME Tracer Advection Schemes

	SE-Eul ¹	CSLAM ²	Opt-SESL ³
<i>Method</i>	Eulerian spectral element	semi-Lagrangian finite volume	semi-Lagrangian spectral element
<i>Grid type</i>	spectral element	finite volume	spectral element
<i>Unstructured grid</i>	yes	no	yes
<i>Conservative</i>	yes	yes	yes, with optimization
<i>Bounds preserving</i>	yes, with limiter	yes, with limiter	yes, with optimization
<i>Max CFL</i>	0.33 with 3-stage RK	1.0	2.0

¹ Guba *et al.* (2014), Optimization based limiters for the spectral element method, JCP.

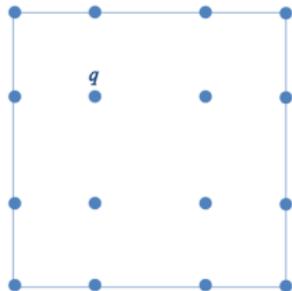
² Lauritzen *et al.* (2010), A conservative semi-Lagrangian multi-tracer transport scheme (CSLAM) on the cubed sphere grid, JCP.

³ Bochev *et al.* (2013), Fast optimization-based conservative remap of scalar fields through aggregate mass transfer, JCP.

Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with tracer q values at GLL nodes at time t

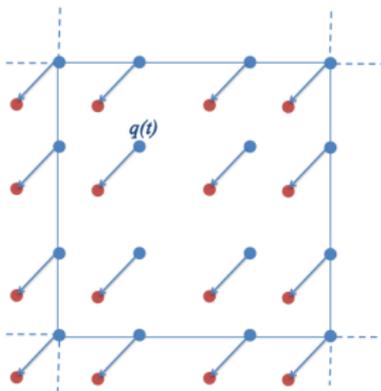
$$\frac{Dq}{Dt} = 0$$



Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with tracer q values at GLL nodes at time t
- Compute backward Lagrangian trajectories of each node

$$\frac{Dq}{Dt} = 0$$

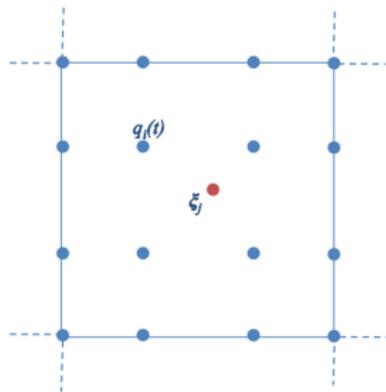


Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with tracer q values at GLL nodes at time t
- Compute backward Lagrangian trajectories of each node
- Locate Lagrangian points on Eulerian mesh $(\xi_1, \xi_2) = F^{-1}(\lambda, \theta)$
- Map Eulerian nodal values to Lagrangian nodes using spectral element basis

$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i(t) \phi_i(\xi_j^L)$$

$$\frac{Dq}{Dt} = 0$$



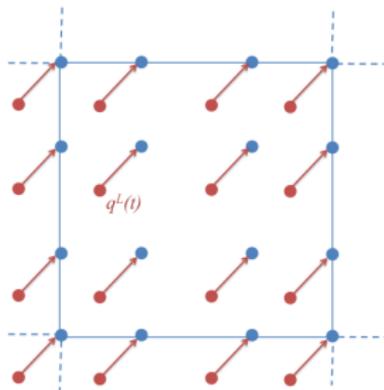
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$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i(t) \phi_i(\xi_j^L)$$

- Lagrangian update of tracer values $q(t + \Delta t) = q^L(t)$

$$\frac{Dq}{Dt} = 0$$



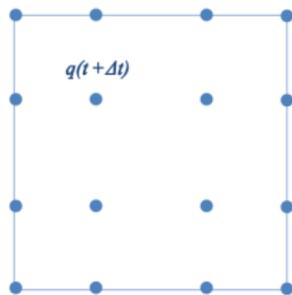
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- Lagrangian update of tracer values $q(t + \Delta t) = q^L(t)$
- Perform optimization step

$$\frac{Dq}{Dt} = 0$$



Optimization

Target

$$\partial_t q^T + \mathbf{u} \cdot \nabla q^T = 0$$

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

Objective

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

minimize the distance
between the solution and a
suitable target

Constraints

$$q^{min} \leq \tilde{q} \leq q^{max}$$

$$\int \rho q = Q$$

desired physical properties
viewed as constraints

Advantages

- Solution is globally optimal with respect to the target and desired physical properties
- Decouples accuracy from enforcement of physical properties

Optimization Algorithm

$$\left\{ \begin{array}{l} \text{minimize } \frac{1}{2} \|\tilde{q} - q^T\|_{\ell_2}^2 \quad \text{subject to} \\ \int \rho q = Q, \quad q^{\min} \leq \tilde{q} \leq q^{\max} \end{array} \right.$$

- Use local bounds over element where interpolation is done $q_i^{\min} \leq \tilde{q}_i \leq q_i^{\max}$
- Total tracer mass where m_i are elements of diagonal mass matrix

$$\int \rho q \approx \sum_i m_i q_i = Q$$

- Use secant method for Lagrange multiplier λ
- Optimal solution satisfies

$$\tilde{q}_i(\lambda) = \text{median}(q_i^{\min}, q_i^T + m_i \lambda, q_i^{\max}), \quad i = 1, \dots, N$$

$$\text{and } \left(\sum_{i=1}^N m_i \tilde{q}_i(\lambda) \right) - Q = 0$$

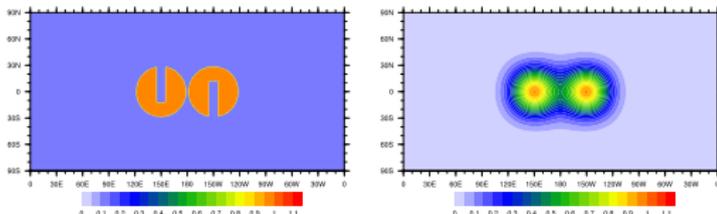
The algorithm generally requires ≈ 5 secant iterations. In serial, it is as efficient as standard slope limiting or flux limiting techniques.

2-D Advection Tests

- Implemented in HOMME shallow water code
- Use prescribed nondivergent deformational flow field, $T = 5$

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

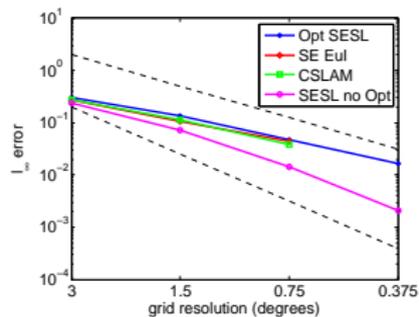
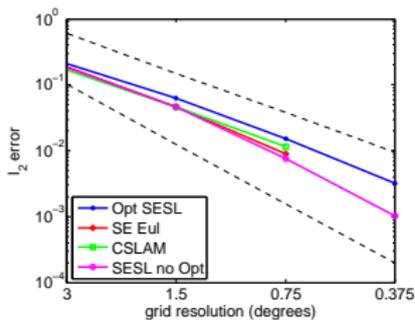
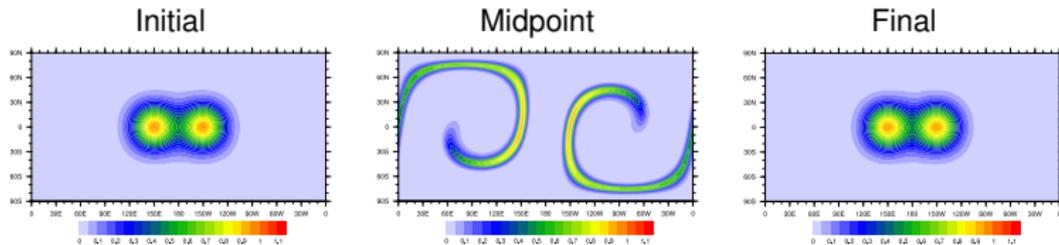
$$v(\lambda, \theta, t) = 2 \sin(2(\lambda - 2\pi t/T)) \cos(\theta) \cos(\pi t/T)$$
- Departure points computed using Taylor series approach and analytic velocity field
- Initial tracer distributions are notched cylinders and Gaussian hills centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$



- Run Opt SESL with CFL = 2, corresponding to $dt = 720s$ for 0.75° resolution

Lauritzen *et al.* (2012) A standard test case suite for two-dimensional linear transport on the sphere, Geosci. Model Dev.

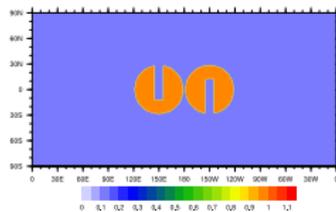
2-D Advection Tests: Convergence



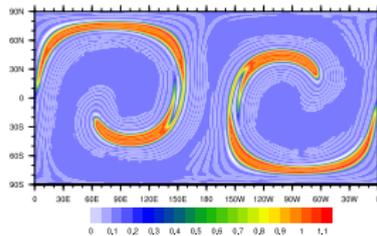
Opt-SESL is competitive with Eulerian SE transport and CSLAM in terms of accuracy and much more efficient for this simple example

2-D Advection Tests: Discontinuous Distribution

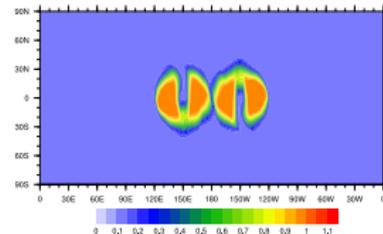
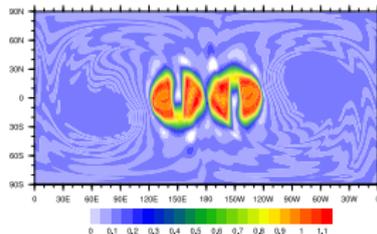
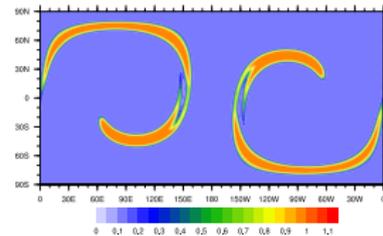
Initial Condition



SESL



Opt-SESL



Mass error = $5.52e-4$

Min value = -0.0902

Max value = 1.158

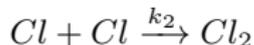
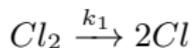
Mass error = $1.51e-11$

Min value = 0.1

Max value = 0.9997

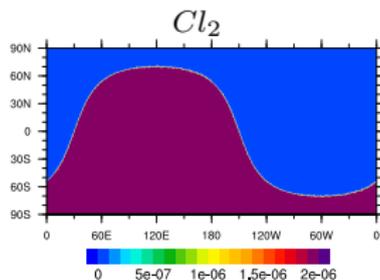
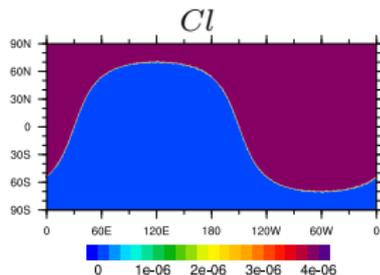
Terminator Test

- Idealized chemistry test



- Track two species: Cl and Cl_2 , total should remain constant
 $Cl_y = Cl + 2.0Cl_2$
- Use deformational velocity field from 2-D passive tracer tests
- Results shown here using 0.75° grid resolution
- Limiting methods that preserve linear relationships between tracers should be able to preserve Cl_y as constant

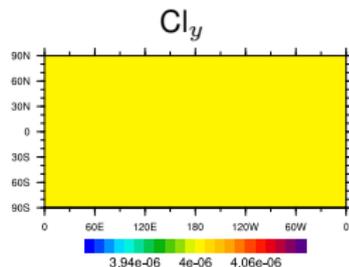
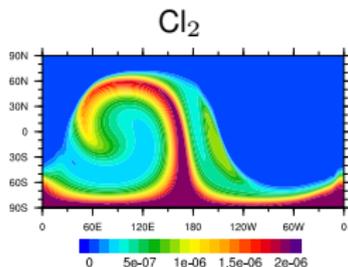
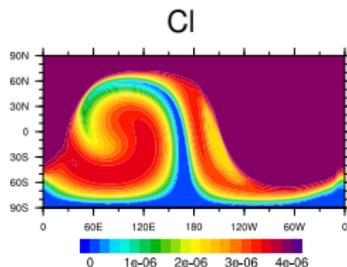
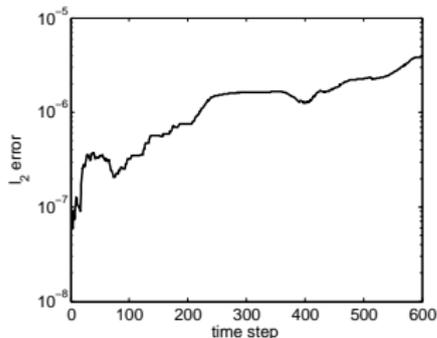
Initial Conditions:



Lauritzen *et al.* (2014) The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes, Geosci. Model Dev.

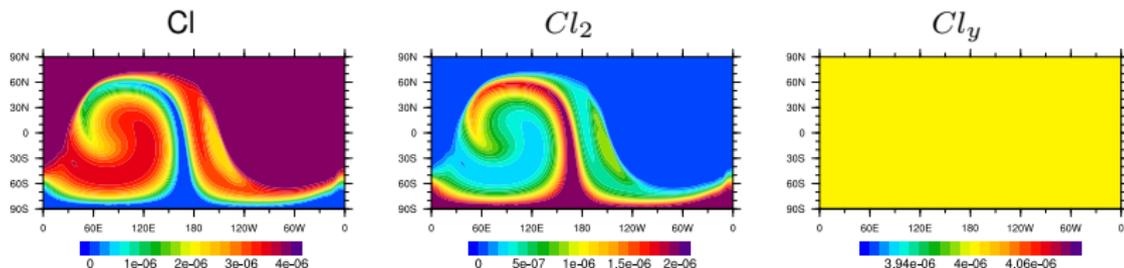
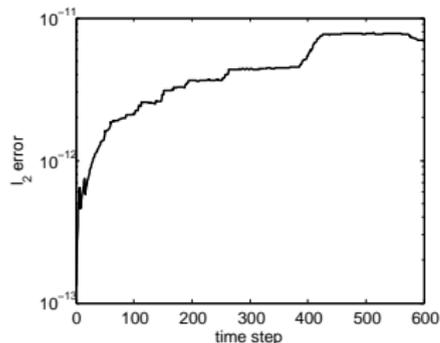
Terminator Test

- Naive implementation
- Max difference $|Cl_y - 4.0 \times 10^{-6}| = 2.83 \times 10^{-11}$
- Final l_2 error in $Cl_y = 3.90 \times 10^{-6}$



Terminator Test

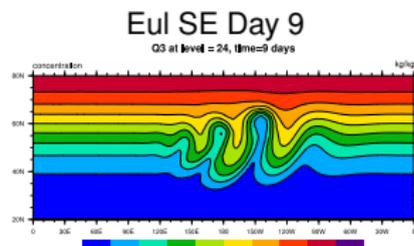
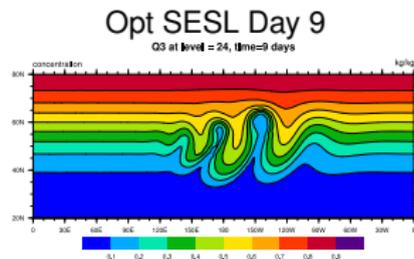
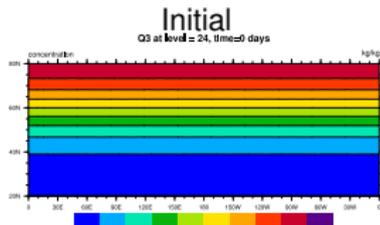
- Scale Cl and Cl_2 by 4.0×10^{-6} before transport algorithm
- Max difference $|Cl_y - 4.0 \times 10^{-6}| = 6.78 \times 10^{-17}$
- Final l_2 error in $Cl_y = 6.94 \times 10^{-12}$



Opt-SESL maintains linear relationships between tracers even with simple chemistry

Baroclinic Instability Test Case

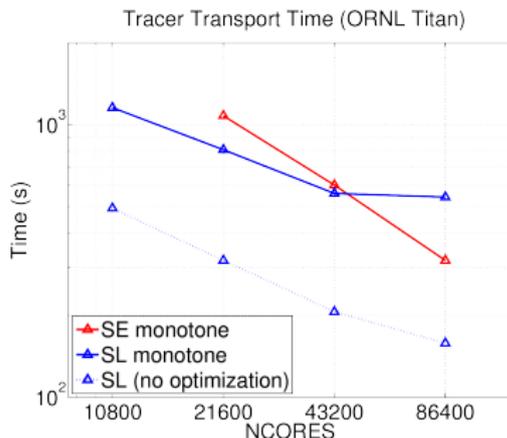
- 2 ° degree grid resolution
- Tracers transported using model velocity
- Runge-Kutta/Taylor series approach for departure points
- 1D vertical remap



Opt-SESL results are comparable to Eulerian SE solution

Preliminary Parallel Scaling Results

- Opt-SESL implemented in HOMME primitive equations
- 1/4 degree cubed-sphere mesh with 86K elements
- Eulerian SE scheme has excellent scaling out to 1 element per core
- Opt-SESL algorithm is faster except at the limit of scalability
- SESL algorithm without optimization is very efficient, but not conservative



Conclusions

- Opt-SESL algorithm looks promising
 - Optimization algorithm successfully conserves mass and enforces bounds
 - Efficient, can be run with large time steps
 - Preserves linear relationships between tracers
- Future Work
 - Continue to investigate parallel efficiency
 - Testing with large numbers of tracers
 - More testing of 3-D examples

