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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 for Atmospheric Sciences

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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?

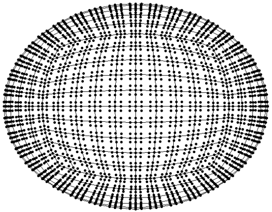
- Biogeochemistry can require 100s of tracers
- Atmosphere is the most expensive component of Earth System Models
- Tracer advection is the dominant cost

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]
Method	Eulerian spectral element	semi-Lagrangian finite volume	semi-Lagrangian spectral element
Grid type	spectral element	finite volume	spectral element
Unstructured grid	yes	no	yes
Conservative	yes	yes	yes, with optimization
Bounds preserving	yes, with limiter	yes, with limiter	yes, with optmization
Max CFL	0.33 with 3-stage RK	1.0	2.0

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

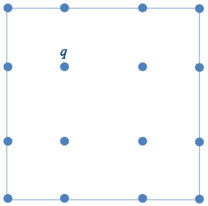
[2] Lauritzen *et al.* (2010), A conservative semi-Lagrangian multi-tracer transport scheme (CSLAM) on the cubed sphere grid, JCP.

[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

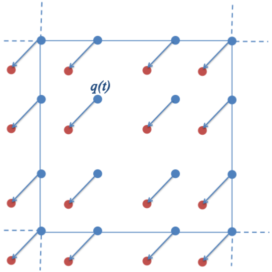
$$\frac{Dq}{Dt} = 0$$



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

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

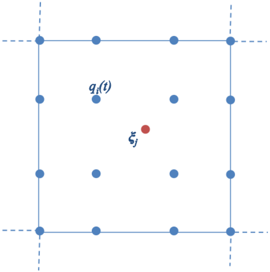


Semi-Lagrangian Spectral Element Tracer Transport

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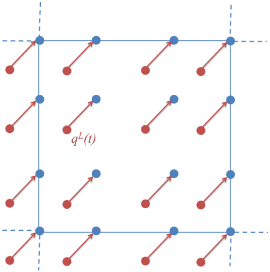
$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i(t)\phi_i(\xi_j^L)$$

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

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



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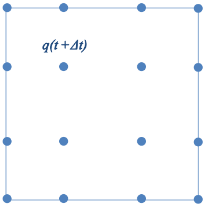
- Lagrangian update of tracer values $q(t + \Delta t) = q^L(t)$
- Perform optimization step

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



Optimization

Target

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

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

Objective

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

minimize the distance between the solution and a suitable target

Constraints

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

$$\int \rho q = Q$$

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

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$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \int \rho q = Q, \qquad q^{\text{min}} \le \widetilde{q} \le q^{\text{max}} \end{cases}$$

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

$$\int \rho q \approx \sum_i \rho_i m_i q_i$$

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

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

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

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

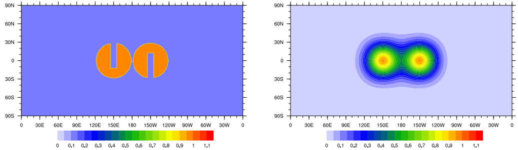
2-D Advection Tests

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

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

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

- 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 $(\lambda_2,\theta_2) = (7\pi/6, 0)$

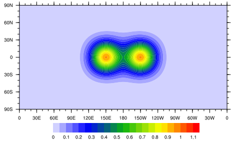


- Run Opt SESL with CFL = 2, corresponding to $dt = 720s$ for 0.75° resolution

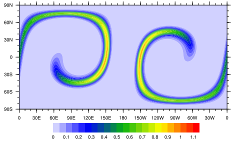
Lauritzen *et al.* (2012) A standard test case suite for two-dimensional linear transport on the sphere, Geosci. Model Dev.

2-D Advection Tests: Convergence

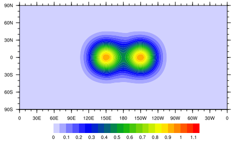
Initial

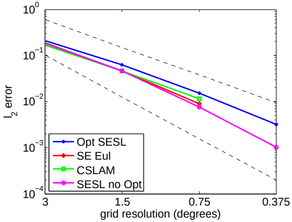


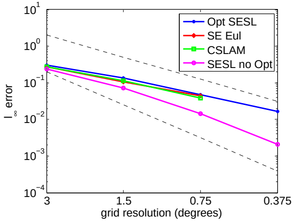
Midpoint



Final



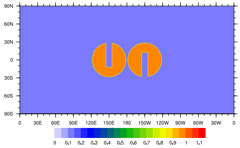




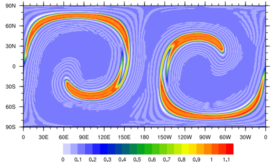
Opt-SESL is competitive with Eulerian SE transport and CSLAM in terms of accuracy and much more efficient for this simple example

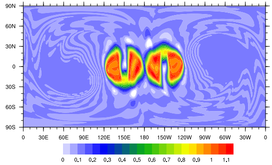
2-D Advection Tests: Discontinuous Distribution

Initial Condition



SESL



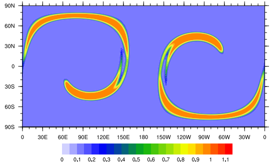


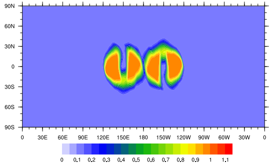
Mass error = 5.52e-4

Min value = -0.0902

Max value = 1.158

Opt-SESL





Mass error = 1.51e-11

Min value = 0.1

Max value = 0.9997

Terminator Test

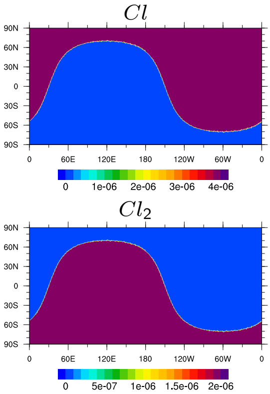
- Idealized chemistry test

$$Cl_2 \xrightarrow{k_1} 2Cl$$

$$Cl + Cl \xrightarrow{k_2} Cl_2$$

- 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

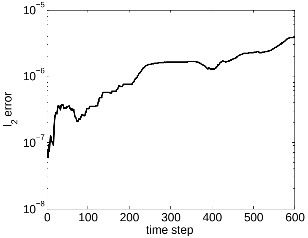
Initial Conditions:

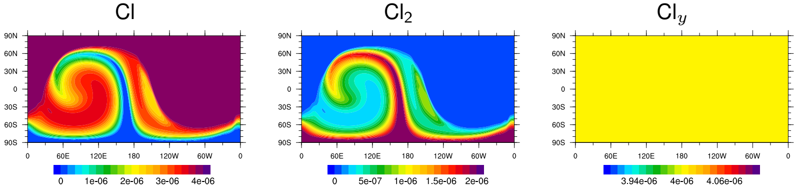


Lauritzen *et al.* (2014) The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes, Geosci. Model Dev.

Terminator Test

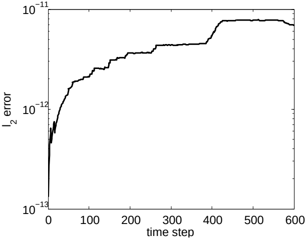
- Naive implementation
- Max difference $|Cl_y - 4.0 \times 10^{-6}|$ = 2.83 $\times 10^{-11}$
- Final l_2 error in $Cl_y = 3.90 \times 10^{-6}$

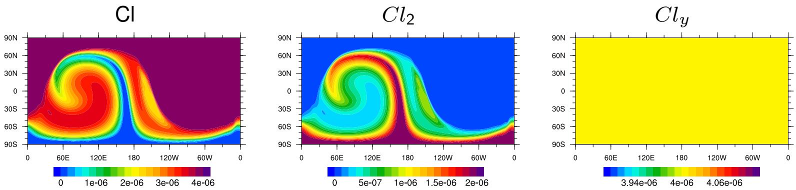




Terminator Test

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



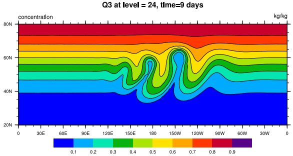


Opt-SESL maintains linear relationships between tracers even with simple chemistry

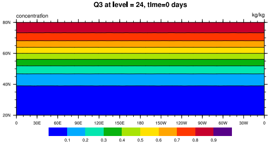
Baroclinic Instability Test Case

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

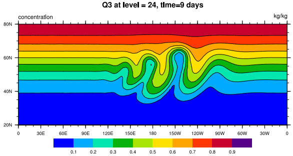
Opt SESL Day 9



Initial



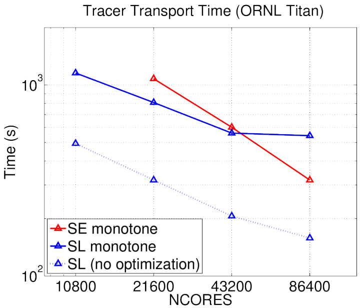
Eul SE Day 9



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 succesfully conserves mass and enforces bounds
  - Efficient, can be run with large time steps
  - Preserves linear relationships between tracers
  - Applicable to unstructured grids
- Future Work
  - Continue to investigate parallel efficiency
  - Testing with large numbers of tracers
  - More testing of 3-D examples