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Optimization-Based Semi-Lagrangian Tracer Transport

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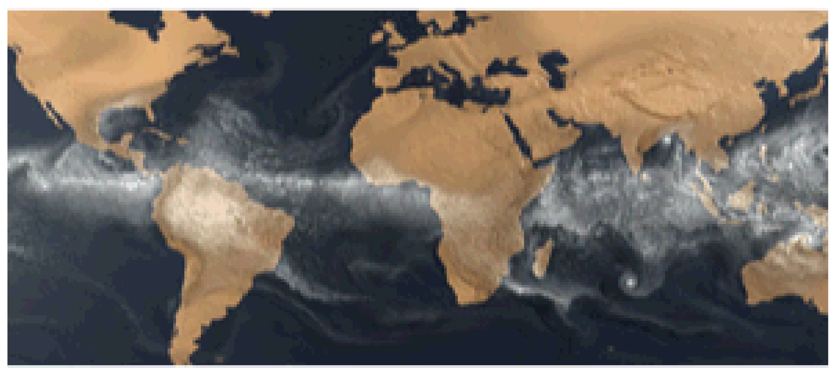
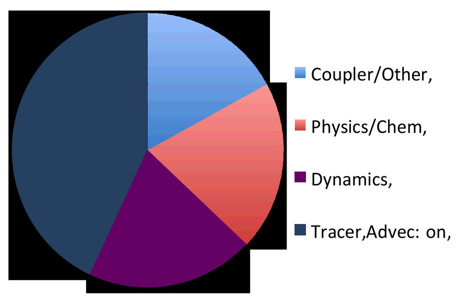
Problem



Numerical transport algorithms are critical for modeling many physical systems particularly the atmosphere in Earth System Models (ESM).

The atmosphere is the most expensive component of an ESM and tracer advection is the dominant cost requiring an efficient numerical solution of the tracer transport equations:

CESM atmosphere cost breakdown



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

ρ - Density
q - Tracer mixing ratio
$\mathbf{u}$ - Velocity

While ensuring accuracy and

- Bounds preservation $\quad q^{\min} \le q \le q^{\max}$
- Mass conservation $\quad \int_\Omega \rho q\, dx = Q$
- Preservation of tracer correlations

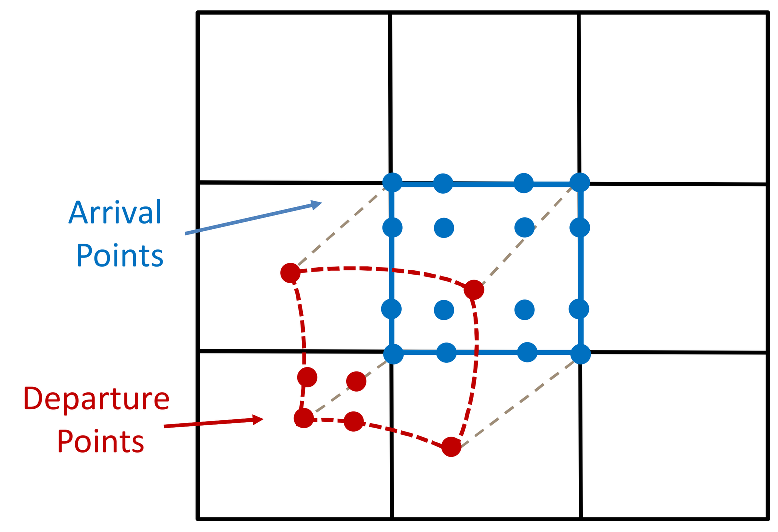
Traditional semi-Lagrangian finite volume schemes require expensive mesh intersection algorithms, while Eulerian methods are limited to small time steps due to stability constraints.

Approach

We develop an efficient atmospheric tracer transport method by combining a high-order spectral element semi-Lagrangian (SESL) scheme with optimization to enforce conservation and preservation of physically motivated local solution bounds.

Spectral Element Semi-Lagrangian (SESL)Transport

1. Compute departure points $(\tilde{\mathbf{p}})$
$$\frac{dx}{dt} = \mathbf{v}(x(t),t), \quad \mathbf{x}(t^{n+1}) = \mathbf{p}$$
2. Interpolate tracer mixing ratio from arrival to departure grid using spectral element basis
$$q(\tilde{\mathbf{p}}^n, t^n) = \sum_i q_i^n \varphi(\tilde{\mathbf{p}}^n)$$
3. Update tracer
$$q(\mathbf{p}, t^{n+1}) = q(\tilde{\mathbf{p}}, t^n)$$



Optimization-Based Transport Formulation (OBT)

Divide and conquer alternative to traditional property-preserving methods, e.g., limiters. OBT has 3 key ingredients:

q^{T} Numerical scheme generating optimally accurate target
Q, q^{max}, q^{min} Operator describing desired physical properties
$\|q - q^{\mathsf{T}}\|$ Measure of target to state misfit

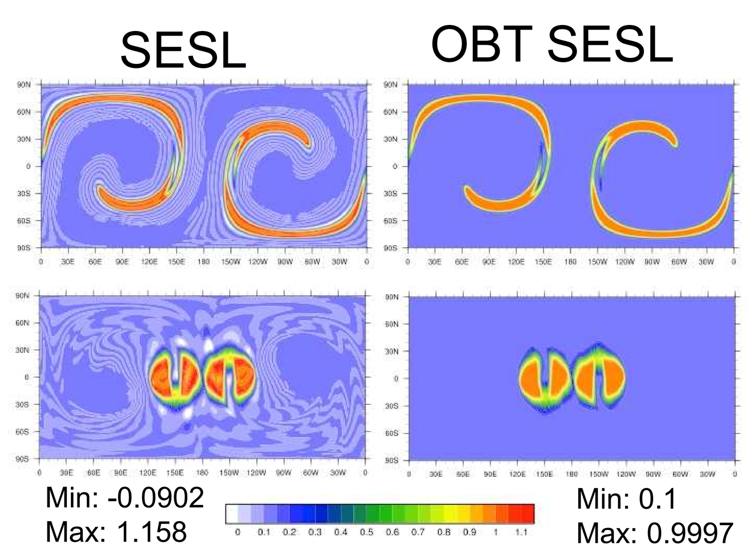
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|q - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \int_\Omega \rho q\, dx = Q \quad \text{and} \quad q^{\min} \le q \le q^{\max} \end{cases}$$

Separates property preservation from accuracy considerations.

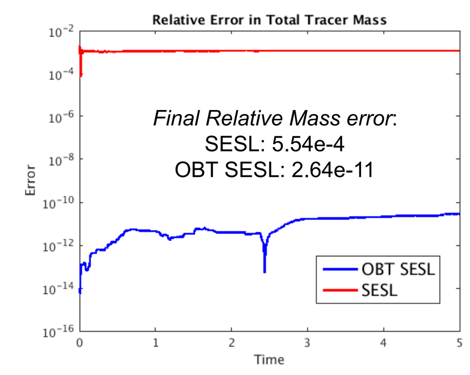
Results

Preserves Bounds

Transport of notched cylinders tracer distribution on the sphere in a rotating, strongly deformational flow field at the midpoint (top) and final time (bottom). The SESL solution violates physical solution bounds (0.1,1.0), but OBT SESL effectively recovers a solution that satisfies bounds.



Conserves Mass



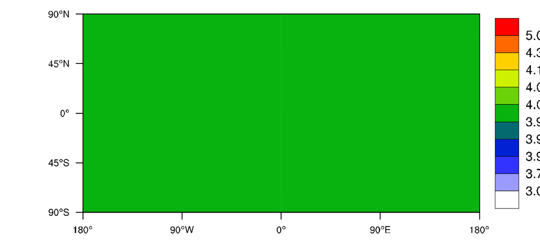
For the same tracer distribution and flow field, the error in total tracer mass reveals the lack of mass conservation in the underlying SESL scheme and the recovery of conservation by the OBT approach.

Preserves Linear Correlations

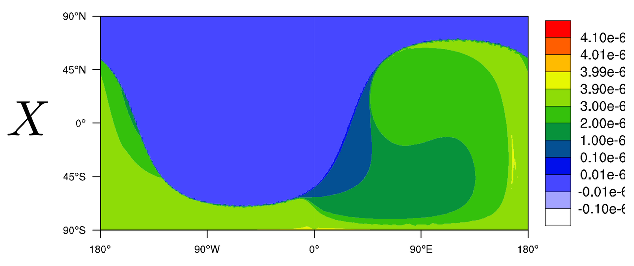
OBT SESL performs well on challenging idealized chemistry test where total sum of species should remain constant as long as advection scheme preserves linear relationships.

$$X_2 \xrightarrow{k_1} 2X$$
$$X + X \xrightarrow{k_2} X_2$$

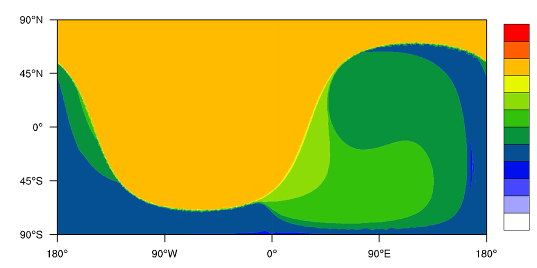
$$\text{Total} \; = 2X_2 + X$$



X



X_2

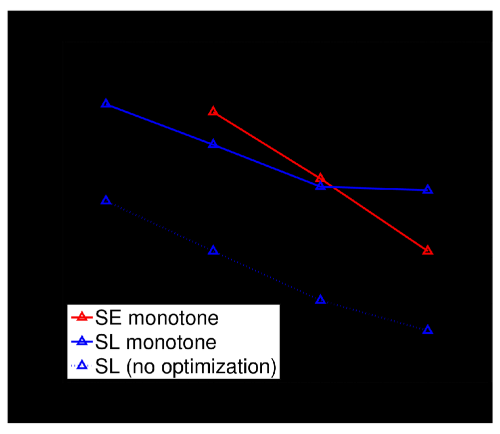


Significance

Developed an efficient new strategy for tracer advection that utilizes optimization and control ideas to formulate conservative and bound-preserving solutions to the transport equation.

SESL Transport with Optimization

- Implemented in HOMME, the spectral element dynamical core for ACME
- Allows a 18x increase in timestep per communication over Eulerian spectral element transport



Optimization-Based Transport

- 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

References

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