Transport Methods for the CAM Spectral Element Dynamical Core

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Motivation

Why are transport schemes so important?

- Atmosphere is the most expensive component of CESM
- Tracer advection is 50% of total cost for 26 tracers
- With biogeochemistry 100-1000 tracers are needed

Objective:

- Implement and optimize new computationally efficient tracer advection algorithms for large numbers of tracer species that
  - work on fully unstructured grids
  - exploit the fact that we will be transporting hundreds of species
Transport Problem

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0$$

$$\frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q u = 0$$

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

Solution methods should satisfy

- local conservation of $\rho q$
- monotonicity or bounds preservation of $q$
- consistency between $q$ and $\rho$ (free stream preserving)
Spectral Element Dynamical Core

- 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, and results can be quite oscillatory

We are pursuing two different approaches for advection that will work for large time steps on unstructured grids
1. Extension of CSLAM\(^1\) with Exact Cell Intersections

- In collaboration with I. Grindeanu (ANL)
- Semi-Lagrangian finite volume approach to advection
- Intersections for unstructured polygonal grids in spherical geometry from MOAB\(^2\)

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**Advantages**
- Allows for long time steps
- Tracer mass conserving and free stream preserving
- Geometric quantities are only computed once so cost is independent of number of tracers

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**Advantages**
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**Disadvantages**
- Expensive to compute cell intersections
- Requires separate finite volume grid

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- Fits naturally with native spectral element method used in CAM-SE
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**Advantages**
- Allows for long time steps
- Efficient, does not require geometric computations
- Fits naturally with native spectral element method used in CAM-SE

**Disadvantages**
- Requires optimization or other approach to ensure mass conservation
Semi-Lagrangian Spectral Element Tracer Transport

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

![Diagram showing GLL nodes and Lagrangian points on an Eulerian mesh]
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

\[
q_j^L(t) = \sum_{i=1}^{n\text{Nodes}} q_i \phi_i(\xi_j^L)
\]
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  \[
  q^L_j(t) = \sum_{i=1}^{nNodes} q_i \phi_i(\xi^L_j)
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- Lagrangian update of tracer values
  \[
  q^T(t + \Delta t) = q^L(t)
  \]
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- Perform optimization step
Optimization

<table>
<thead>
<tr>
<th>Objective</th>
<th>Target</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|\tilde{q} - q^T|$</td>
<td>$\partial_t q^T + u \cdot \nabla q^T = 0$</td>
<td>$q_{min} \leq \tilde{q} \leq q_{max}$</td>
</tr>
<tr>
<td>minimize the distance between the solution and a suitable target</td>
<td>stable and accurate solution, not required to possess all desired physical properties</td>
<td>$\sum \tilde{m}_i \tilde{q}_i = Q$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>desired physical properties viewed as constraints</td>
</tr>
</tbody>
</table>

**Advantages**

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

\[
\begin{aligned}
\text{minimize} & \quad \frac{1}{2} \| \tilde{q} - q^T \|_2^2 \\
\text{subject to} & \quad \sum_{i=1}^{N} \tilde{m}_i \tilde{q}_i = Q, \quad q_i^{\text{min}} \leq \tilde{q} \leq q_i^{\text{max}}
\end{aligned}
\]

Lagrangian functional \( \mathcal{L} : \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R} \)

\[
\mathcal{L}(\tilde{q}, \lambda, \mu_1, \mu_2) = \frac{1}{2} \sum_{i=1}^{N} (\tilde{q}_i - q_i^T)^2 - \lambda \sum_{i=1}^{N} \tilde{q}_i - \\
\sum_{i=1}^{N} \mu_{1,i} (\tilde{q}_i - q_i^{\text{min}}) - \sum_{i=1}^{N} \mu_{2,i} (q_i^{\text{max}} - \tilde{q}_i),
\]

where \( \tilde{q} \in \mathbb{R}^N \) are the optimization variables, and \( \lambda \in \mathbb{R}, \mu_1 \in \mathbb{R}^N, \) and \( \mu_2 \in \mathbb{R}^N \) are the Lagrange multipliers

\(^1\) Based on the Optimization-Based Remap Algorithm (Bochev, Ridzal, Shashkov, JCP 2013)
Optimization Algorithm

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} \| \tilde{q} - q^T \|_{\ell_2}^2 \\
\text{subject to} & \quad \sum_{i=1}^{N} \tilde{m}_i \tilde{q}_i = Q, \quad q_i^{\text{min}} \leq \tilde{q} \leq q_i^{\text{max}}
\end{align*}
\]

Karush-Kuhn-Tucker (KKT) conditions:

\[
\tilde{q}_i = q_i^T + \lambda + \mu_{1,i} - \mu_{2,i}; \quad i = 1, \ldots, N
\]

\[
q_i^{\text{min}} \leq \tilde{q}_i \leq q_i^{\text{max}}; \quad i = 1, \ldots, N
\]

\[
\mu_{1,i} \geq 0, \quad \mu_{2,i} \geq 0; \quad i = 1, \ldots, N
\]

\[
\mu_{1,i} (\tilde{q}_i - q_i^{\text{min}}) = 0, \quad \mu_{2,i} (-\tilde{q}_i + q_i^{\text{max}}) = 0; \quad i = 1, \ldots, N
\]

\[
\sum_{i=1}^{N} \tilde{m}_i \tilde{q}_i = Q
\]

\(^1\)Based on the Optimization-Based Remap Algorithm (Bochev, Ridzal, Shashkov, JCP 2013)
Optimization Algorithm

For any fixed value of \( \lambda \) a solution is given by

\[
\begin{cases}
\tilde{q}_i = q_i^T + \lambda; & \mu_1,i = \mu_2,i = 0 \\
\tilde{q}_i = q_i^{min}; & \mu_2,i = 0, \mu_1,i = \tilde{q}_i - q_i^T - \lambda \\
\tilde{q}_i = q_i^{max}; & \mu_1,i = 0, \mu_2,i = q_i^T - \tilde{q}_i + \lambda
\end{cases}
\]

if \( q_i^{min} \leq q_i^T + \lambda \leq q_i^{max} \)

if \( q_i^T + \lambda < q_i^{min} \)

if \( q_i^T + \lambda > q_i^{max} \),

for all \( i = 1, \ldots, N \).

Ignoring \( \mu_1 \) and \( \mu_2 \) and treating \( \tilde{q}_i \) as a function of \( \lambda \) yields

\[
\tilde{q}_i(\lambda) = \text{median}(q_i^{min}, q_i^T + \lambda, q_i^{max}), \quad i = 1, \ldots, N.
\]

Adjust \( \lambda \) in outer iteration to satisfy \( \sum_{i=1}^{N} \tilde{m}_i \tilde{q}_i(\lambda) = Q \).

The algorithm generally requires \( \leq 5 \) outer secant iterations. In serial, it is as efficient as standard slope limiting or flux limiting techniques.
Computational Examples

- Velocity fields
  - Solid body rotation
  - Nondivergent deformational flow field, $T = 5$
    \[
    u(\lambda, \theta, t) = 2 \sin^2 (\lambda) \sin(2\theta) \cos \left( \frac{\pi t}{T} \right)
    \]
    \[
    v(\lambda, \theta, t) = 2 \sin (2\lambda) \cos(\theta) \cos \left( \frac{\pi t}{T} \right)
    \]
  - Tracer distribution: notched cylinders centered at $\left(\lambda_1, \theta_1\right) = \left(\frac{5\pi}{6}, 0\right)$ and $\left(\lambda_2, \theta_2\right) = \left(\frac{7\pi}{6}, 0\right)$
Solid Body Rotation, 1.5° resolution
Solid Body Rotation, 1.5° resolution
Solid Body Rotation, 1.5° resolution

Mass error = -3.14e-3
Min value = -0.1223
Max value = 1.2472

Mass error = 1.4e-13
Min value = 0.1
Max value = 1.0
Deformational flow, 1.5° resolution
Deformational flow, 1.5° resolution
Deformational flow, 1.5° resolution

SE-SL

Final Tracer

Mass error = -3.44e-3
Min value = -0.1070
Max value = 1.1934

SE-SL Opt

Final Tracer

Mass error = 1.69e-11
Min value = 0.1
Max value = 0.9979
Open Questions

- How to define bounds for optimization? All DOFs in surrounding cells? Nearest neighbor DOFs?
- Can we modify the target to improve the final solution using smoothness indicators?
- How will the method scale on many processors? Will the global sum for each secant iteration be problematic?
Conclusions

- Pursuing two approaches to tracer transport in CAM-SE
  - CSLAM-based algorithm using cell intersections computed with MOAB
  - Semi-Lagrangian spectral element (SL-SE) algorithm using optimization to enforce mass conservation
- SL-SE algorithm looks promising
  - Efficient, works for large time steps
  - Applicable to unstructured grids
  - Optimization algorithm successfully conserves mass and enforces bounds
- Future Work
  - Complete implementation of new advection methods in HOMME/CAM-SE
  - Compare parallel efficiency and accuracy