SAND2014-15486PE

Transport Methods for the CAM Spectral Element Dynamical Core

Kara Peterson, Mark Taylor

Sandia National Laboratories

SIAM Annual Meeting

MS17 Numerical Methods for the Ocean and Atmosphere

July 7, 2014

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Motivation

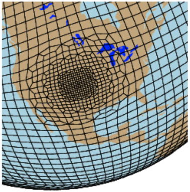
Why are transport schemes so important?

- 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

ACES4BGC
Applying Computationally Efficient Schemes for BioGeochemical Cycles

Objective:

- Implement and optimize new computationally efficent 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

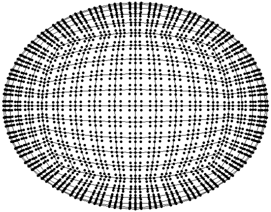
A tracer, represented by its mixing ratio q and mass ρq, is transported in the flow with velocity $\mathbf{u}$

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

Solution methods should satisfy

- local conservation of ρq
- monotonicity or bounds preservation of q
- consistency between q and ρ (free stream preserving)

Spectral Element Dynamical Core



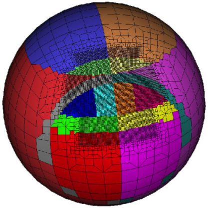
- Continuous Galerkin finite element method using Gauss-Lobatto quadrature
- Generally runs on the cubed sphere grid, but applicable to any unstructured quadrilateral grid on the sphere

Advection using the standard spectral element method with high-degree polynomials is accurate, but expensive due 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 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



Advantages

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

Disadvantages

- Expensive to compute cell intersections
- Requires separate finite volume grid

2. Semi-Lagrangian Spectral Element

- In collaboration P. Bochev, D. Ridzal, J. Overfelt (SNL)
- Nodal Semi-Lagrangian approach to advection
- Combined with optimization approach to maintain bounds and mass conservation

Advantages

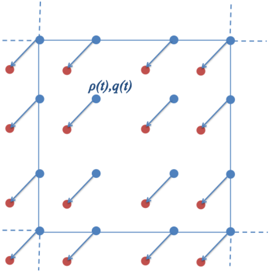
- Allows for long time steps
- Efficient, does not require geometric computations
- Fits naturally with native spectral element method used in CAM-SE

Disadvantages

- Requires optimization or other approach to ensure mass conservation

Semi-Lagrangian Spectral Element Tracer Transport

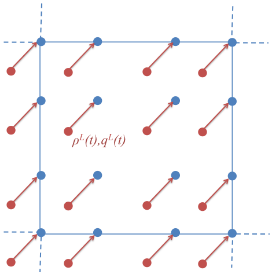
- Consider a cell with density ρ and tracer q values at GLL nodes at time t
- Compute backward Lagrangian trajectories of each node



Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with density ρ and tracer q values at GLL nodes at time t
- Compute backward Lagrangian trajectories of each node
- Map Eulerian nodal values to Lagrangian nodes using spectral element basis

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

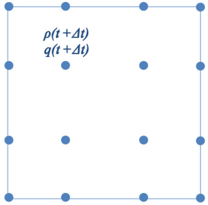


Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with density ρ and tracer q values at GLL nodes at time t
- Compute backward Lagrangian trajectories of each node
- Map Eulerian nodal values to Lagrangian nodes using spectral element basis

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

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



Optimization

Objective

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

minimize the distance between the solution and a suitable target

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

Constraints

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

$$\sum \widetilde{m}_i \widetilde{q}_i = Q$$

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

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

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{\text{min}} \leq \widetilde{q} \leq q_i^{\text{max}} \end{cases}$$

Singly linearly constrained quadratic program with simple bounds

- Solve related separable problem (without mass constraint) first, cost $O(C)$
- Satisfy the mass conservation constraint in a few secant iterations
- In serial, the optimization algorithm is as efficient as standard slope limiting or flux limiting techniques

Optimization Algorithm

Define Lagrangian functional $\mathcal{L} : \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$,

$$\mathcal{L}(\widetilde{q}, \lambda, \mu_1, \mu_2) = \frac{1}{2} \sum_{i=1}^{N} (\widetilde{q}_i - q_i^{\mathsf{T}})^2 - \lambda \sum_{i=1}^{N} \widetilde{q}_i -$$

$$\textstyle\sum_{i=1}^{N} \mu_{1,i} \left(\widetilde{q}_i - q_i^{min}\right) - \sum_{i=1}^{N} \mu_{2,i} \left(q_i^{max} - \widetilde{q}_i\right) \,,$$

where $\widetilde{q} \in \mathbb{R}^C$ are the *primal optimization variables*, and $\lambda \in \mathbb{R}$, $\mu_1 \in \mathbb{R}^C$, and $\mu_2 \in \mathbb{R}^C$ are the *Lagrange multipliers*.

Karush-Kuhn-Tucker (KKT) conditions:

$$\begin{aligned} \widetilde{q}_i = q_i^{\mathsf{T}} + \lambda + \mu_{1,i} - \mu_{2,i}; &\quad i = 1, \ldots, N \\ q_i^{min} \le \widetilde{q}_i \le q_i^{max}; &\quad i = 1, \ldots, N \\ \mu_{1,i} \ge 0 \,, \quad \mu_{2,i} \ge 0; &\quad i = 1, \ldots, N \\ \mu_{1,i} \left(\widetilde{q}_i - q_i^{min}\right) = 0 \,, \quad \mu_{2,i} \left(-\widetilde{q}_i + q_i^{max}\right) = 0; &\quad i = 1, \ldots, N \\ \textstyle\sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i = Q & \end{aligned}$$

Optimization Algorithm

Focus on conditions separable in the index i. For any *fixed* value of λ a solution is given by

$$\begin{cases} \widetilde{q}_i = q_i^{\mathsf{T}} + \lambda; & \mu_{1,i} = \mu_{2,i} = 0 & \text{if} \quad q_i^{min} \le q_i^{\mathsf{T}} + \lambda \le q_i^{max} \\ \widetilde{q}_i = q_i^{min}; & \mu_{2,i} = 0,\ \mu_{1,i} = \widetilde{q}_i - q_i^{\mathsf{T}} - \lambda & \text{if} \quad q_i^{\mathsf{T}} + \lambda < q_i^{min} \\ \widetilde{q}_i = q_i^{max}; & \mu_{1,i} = 0,\ \mu_{2,i} = q_i^{\mathsf{T}} - \widetilde{q}_i + \lambda & \text{if} \quad q_i^{\mathsf{T}} + \lambda > q_i^{max}\ , \end{cases}$$

for all $i = 1, \ldots, N$.

Ignoring μ_1 and μ_2 and treating $\widetilde{q}_i$ as a function of λ yields

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

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

The algorithm generally requires ≤ 5 outer secant iterations

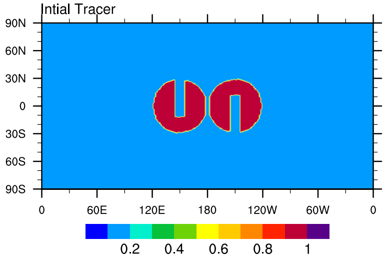
Computational Examples

- Velocity fields
  - Solid body rotation
  - Nondivergent deformational flow field, $T = 5$

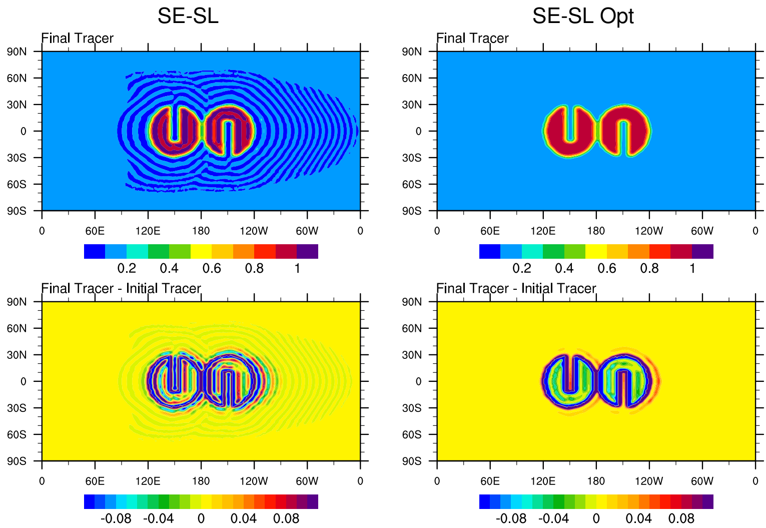
$$u(\lambda, \theta, t) = 2\sin^2(\lambda)\sin(2\theta)\cos(\pi t/T)$$

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

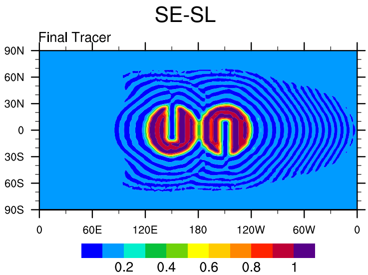
- Tracer distribution: notched cylinders centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$



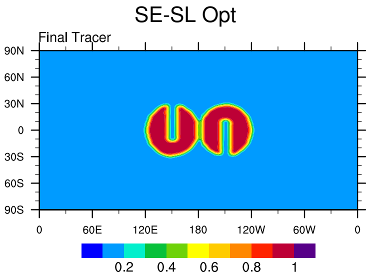
Solid Body Rotation, 1.5° resolution



Solid Body Rotation, 1.5° resolution

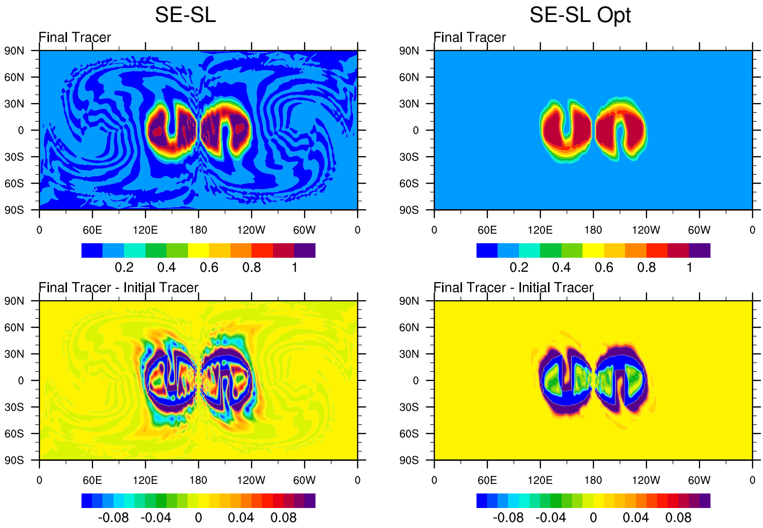


Mass error = -3.14e-3
Min value = -0.1223
Max value = 1.2472



Mass error = 1.4e-13
Min value = 0.1
Max value = 1.0

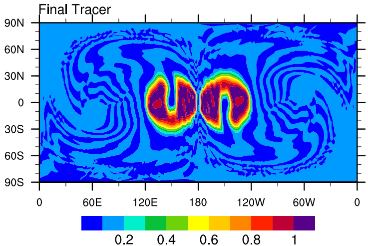
Deformational flow, 1.5° resolution



Sandia National Laboratories

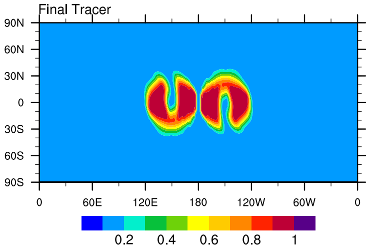
Deformational flow, 1.5° resolution

SE-SL



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

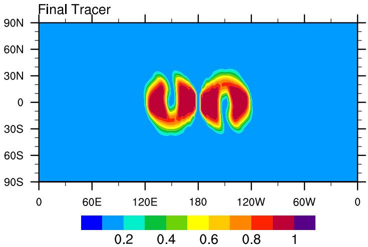
SE-SL Opt



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

Sandia National Laboratories

- 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
- The SL-SE algorithm looks promising
  - Efficient, works for large time steps
  - Applicable to unstructured grids
  - Optimization algorithm succesfully conserves mass and enforces bounds