Consistent coupling of finite element advection and finite volume transport

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Galerkin methods with applications in weather and climate forecasting
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Outline

- Comparison: Transport algorithms being implemented in HOMME (dycore package)
  - Eulerian (FE/spectral element)
  - CSLAM (FV with incremental remap)
  - SPELT (FV, with semi-lagrange flux computation)
  - Semi-Lagrange w/optimization

- How to couple flux form FV transport methods to a FE dycore?
  - Use flux formulation to ensure mass/tracer-mass consistency
  - Advect tracers with mean flux from dycore
  - How do we extract fluxes from a FE evolution of density?
Acronyms

- **HOMME**: High-Order Method Modeling Environment
  - Dynamical core package
  - Contains the Spectral Element dynamical core used by CAM

- **CAM**: Community Atmosphere Model used in CESM and ACME

- **CESM**: Community Earth System Model

- **ACME**: Accelerated Climate Modeling for Energy
  - Fork of the CESM being developed by US Department of Energy (DOE) Laboratories
  - Primary focus: high resolution on DOE 100PF systems
Why Tracer Transport?

- In CESM, atmosphere is most expensive (but most scalable) component
- CICE model looks expensive due to poor scaling – improved scaling will make it much cheaper
- Tracer transport is the most expensive kernel in the coupled model
4 types of methods

- **SE**: Native spectral element discretization (locally conservative) of transport equation with monotone limiter.

- **CSLAM**: Incremental remap with conservative and monotone reconstruction
  - Lauritzen et al., *A conservative semi-Lagrangian multi-tracer transport scheme (CSLAM) on the cubed-sphere grid*, JCP 2010

- **SPELT**: Multi-moment FV, with semi-Lagrangian fluxes
  - Erath & Nair, A conservative multi-tracer transport scheme for spectral-element spherical grids, JCP 2013

- **Traditional Semi-Lagrange**
  - Spectral element reconstruction followed by global optimization conservation and monotonicity
  - Bochev et al., *Fast optimization-based conservative remap of scalar fields through aggregate mass transfer*, JCP 2013
CAM-SE “default”

Dynamics: Spectral element dynamics on Gauss-Lobatto nodal values (not quite equally spaced at CAM-SE default 4x4, p=3)

Tracer Advection: Spectral element. Locally conservative and monotone on Gauss-Lobatto nodes

Physics: physics columns computed at Gauss-Lobatto nodal values
CAM-SE physics grid

Dynamics: Spectral element

Tracer Advection: Spectral element.

Physics: physics columns computed with cell averaged data. Physics can use a coarser, identical, or finer resolution grid.
CAM-SE/CSDLAM physics grid

Dynamics: Spectral element

Tracer Advection: CSLAM
Conservative, Semi-Lagrange, multi-tracer efficient algorithm using cell averaged data

Physics: cell averaged data.
Deformational Flow Test Case for the sphere
(Nair & Lauritzen, JCP 2010)
<table>
<thead>
<tr>
<th></th>
<th>SE</th>
<th>CSLAM</th>
<th>SPELT</th>
<th>Semi-Lagrange</th>
</tr>
</thead>
<tbody>
<tr>
<td>Departure Grid</td>
<td>No (Eulerian)</td>
<td>RK 2\textsuperscript{nd} order</td>
<td>RK 2\textsuperscript{nd} order</td>
<td>RK 2\textsuperscript{nd} order</td>
</tr>
<tr>
<td>Reconstruction</td>
<td>No</td>
<td>Yes – mesh intersections. Expensive, but independent of #of tracers (on processor)</td>
<td>FV reconstruction + 3x more degrees of freedom</td>
<td>Yes – use SE basis functions (fast, on processor)</td>
</tr>
<tr>
<td>MPI Bandwidth</td>
<td>Spectral element edge data only</td>
<td>Full spectral element halo</td>
<td>Full spectral element halo</td>
<td>Full spectral element halo</td>
</tr>
<tr>
<td>CFL</td>
<td>0.27 with 3 RK stages</td>
<td>1.0 with 1 element halo</td>
<td>3.0 with 1 SE element halo</td>
<td>3.0 with 1 SE element halo</td>
</tr>
<tr>
<td># of nearest neighbor messages per processor for CFL=1</td>
<td>12</td>
<td>1</td>
<td>.33</td>
<td>.33</td>
</tr>
<tr>
<td>Bandwidth per message</td>
<td>1</td>
<td>3.6</td>
<td>14.4</td>
<td>3.6</td>
</tr>
<tr>
<td>Global Reductions</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>~10 per timestep, each requiring log(NCPU) messages</td>
</tr>
</tbody>
</table>
CSLAM Results in CAM-SE

- Evaluate in CAM-SE (Community Atmosphere Model with HOMME’s Spectral Element dynamical core)
- 3D: Use vertically Lagrangian approach (S.J. Lin, 2004): CSLAM used in horizontal directions on floating lagrangian levels with occasional 1D vertical remap back to reference levels
- Runge-Kutta/Taylor Series (interpolation free, SE based) departure grid algorithm
- Tracers advected using model winds and density (Jablonowski & Williamson baroclinic instability test case)
Transport in an idealized baroclinic instability flow

- Initial zonally symmetric tracer after 13 days.
- CAM-SE Eulerian advection and CSLAM are remarkably identical, even at fine scales.
- CSLAM running with a CFL=1. One (large) communication step and expensive geometry step.
- CAM-SE uses CFL=0.3 with RK-3. Three (small) communication steps, dense matvecs for all computations.
SE vs. CSLAM as a function of tracer count

- Moderate resolution on a moderate number of cores
- For 1 tracer, CSLAM is quite expensive
- Breakeven with SE at 29 tracers
- Significantly faster at 100+ tracers
Strong parallel scaling: SE vs Semi-Lagrange

- High Resolution (1/4 degree) cubed-sphere mesh has 86K elements
- SE scheme has excellent scaling out to 1 element per core
- Semi-Lagrange algorithm is faster except at the limit of scalability
- Semi-Lagrange algorithm without optimization (and hence non conservative) is very efficient
Transport Mass/Mass consistency

For each tracer represented by its mixing ratio \( q \) and tracer mass \( \rho q \), we transport it in a flow with velocity \( u \):

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad \text{Dynamics}
\]

\[
\frac{\partial \rho q}{\partial t} + \nabla \cdot (\rho q \vec{u}) = 0 \quad \text{Tracer scheme}
\]

Consistency: If tracer mixing ratio \( q=1 \), then tracer scheme should match results produced by dynamics:

- **Advect \((\rho q)\)**: At end of timestep, will \((\rho q)/\rho_{\text{dyn}}\) be monotone?
- **Advect \( q \)**: At end of tracer timestep, will \( \rho_{\text{dyn}} q \) be conserved?
Transport Mass/Mass consistency

• Several approaches in the literature involving some type of implicitness: iterate on departure grid or flux correction so that implied density from tracer scheme matches prescribed density
• Use flux form: advect tracers with a mean flux from the dynamics.
  • Need fluxes from the spectral element method at all the FV “subcells”
Spectral element subcell flux

• For each FV “subcell”, define the density within each subcell via integration of the spectral element shape function
• Compute this subcell mass before and after the spectral element dynamics update
• Can the change in the subcell mass be given by fluxes defined on each subcell edge?
Spectral elements: weak form

Consider advection/diffusion equation (with mixing)

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = \nabla \cdot \tau \nabla \Delta \rho
\]

Generic notation in terms of flux term $F$ and mixing term $G$

\[
\frac{\partial \rho}{\partial t} = F + \nabla \cdot G
\]
Spectral elements: weak form

Spectral element weak formulation uses GLL quadrature approximation.

Notation (single element:)

\[
\langle f, g \rangle = \sum_{i,j} w_{i,j} f(x_i, y_j) g(x_i, y_j) \sim \iint f g \, dA
\]
Spectral elements: weak form solution

1. solve weak formulation in each element, for all test functions $\phi$. (Local element update)
2. projection / DSS / assembly / inverse mass matrix step. (Or, for DG, replace step 2 by flux calculation)

$$\left\langle \phi, \frac{\rho^* - \rho^t}{\Delta t} \right\rangle = \left\langle \phi, F \right\rangle + \left\langle \nabla \phi, G \right\rangle$$

$$\rho^{t+1} = \text{DSS}(\rho^*)$$
Spectral elements: weak form solution

If we define

\[ D = \frac{\text{DSS}(\rho^*) - \rho^*}{\Delta t} \]

The SE solution satisfies:

\[ \frac{\langle \phi, \rho^{t+1} \rangle - \langle \phi, \rho^t \rangle}{\Delta t} = \langle \phi, F \rangle + \langle \nabla \phi, G \rangle + \langle \phi, D \rangle \]

Taking \( \phi=1 \), this gives us the change in element mass from 1 dynamics timestep. Taking other choices of test functions \( \phi \) can give us the change in subcell mass.
Subcell Mass in terms of $\langle , \rangle$

- Define the subcell mass by integration over the subcell of the shape function representation of $\rho$
- This is a linear map from GLL nodal values of $\rho$ to a scalar
- **Riesz Representation Theorem**: for every subcell $(m,n)$, there is a polynomial $\phi^{m,n}$ in our space of test functions where the subcell mass is given by:

\[ \langle \phi^{m,n}, \rho \rangle \]

**Formula for subcell mass using the same inner product as weak form equations.**
Spectral elements: weak form solution

Spectral element solution $\rho$ satisfies for all $\phi$

$$
\frac{\langle \phi, \rho^{t+1} \rangle - \langle \phi, \rho^t \rangle}{\Delta t} = \langle \phi, F \rangle + \langle \nabla \phi, G \rangle + \langle \phi, D \rangle
$$

Take $\phi = \phi^{m,n}$

$$
\frac{\langle \phi^{m,n}, \rho^{t+1} \rangle - \langle \phi^{m,n}, \rho^t \rangle}{\Delta t} = \langle \phi^{m,n}, F \rangle + \langle \nabla \phi^{m,n}, G \rangle + \langle \phi^{m,n}, D \rangle
$$

Change in subcell mass given as sum of 3 terms. Each must be expressed as edge fluxes
Term by term analysis

Flux term: $\langle \phi^{m,n}, F \rangle$

Very physical: Using that $F$ is a divergence, can derive fluxes that are discrete integrals along subcell edges.
Term by term analysis

Mixing term: \( \langle \nabla \phi^{m,n}, G \rangle \)

Weak form operator hard to interpret physically.

- In 1D: there exists a unique set of continuous fluxes which give the correct change in subcell mass.
- 2D: Non-unique. Use tensor product of unique 1D result
Term by term analysis

DSS/Projection term: $\langle \phi^m, n, D \rangle$

Exchanges mass between elements. Changes GLL nodal values only on the boundary, but this changes mass in all subcells:

- In 1D: there exists a unique set of continuous fluxes which give the correct change in subcell mass.
- 2D: Non-unique. Use tensor product of unique 1D result
Results:

- One can derive subcell edge fluxes consistent with SE evolution of density
- Implemented in HOMME (99% done)
- Initial results: tracers are identical in the eyeball norm
Conclusions

- HOMME dycore package supports research in a variety of transport schemes spanning a range of tradeoffs between:
  - Floating point intensity
  - Structured array access vs indirect addressing
  - Bandwidth
  - Latency

- Transport schemes cast in flux form can be made consistent with HOMME’s spectral element (or DG) dycores:
  - “Subcell” flux can be defined on any square subcell within the spectral element
  - Result would apply to any FE method, if the inverse mass matrix procedure is conservative and local
  - Taylor, Overfelt, and Ullrich, in preparation