New algorithms and SciDAC tools for scalable monotone transport schemes in the Community Earth System Model

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SciDAC

Scientific Discovery through Advanced Computing

Sandia National Laboratories

ACES4BGC: Applying Computationally Efficient Schemes for BioGeochemical Cycles

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Scott M. Elliott‡	LANL	Ocean	Ocean BGC
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Argonne National Laboratory · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · NCAR National Center for Atmospheric Research · Oak Ridge National Laboratory · Pacific Northwest National Laboratory · Sandia National Laboratories

Outline

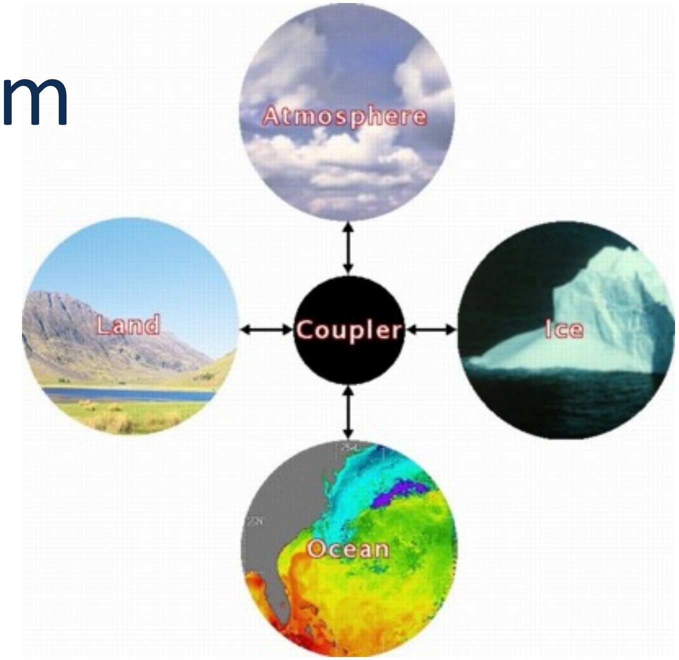
- ACES4BGC Project Overview
- Motivation for multi-tracer transport methods
- Characteristic based algorithms
- FASTMath collaboration: Mesh-Oriented datABase (MOAB)

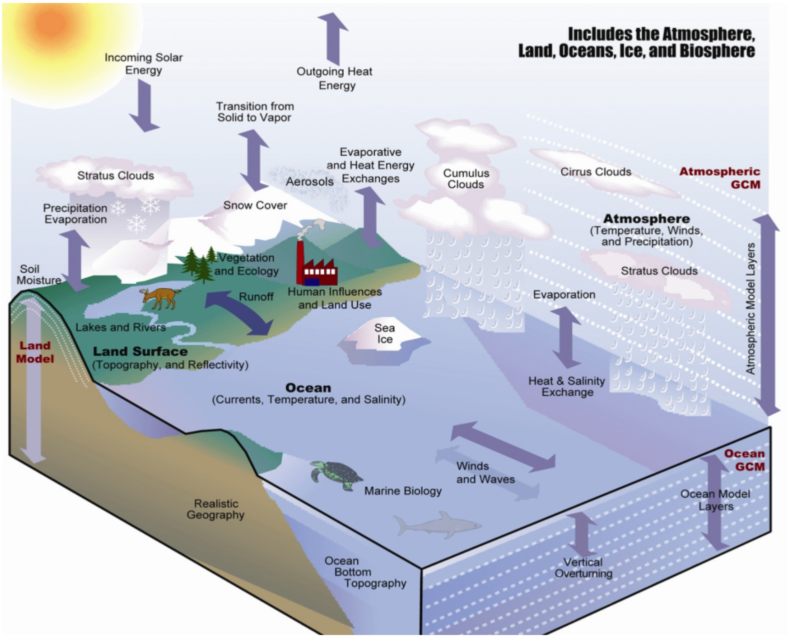
ACES4BGC: Goals and Objective

- Goals: Advance predictive capabilities of Earth System Models (ESMs) by reducing two of the largest sources of uncertainty, *aerosols and biospheric feedbacks*, utilizing a *highly efficient computational approach*.
- ACES4BGC will:
  - implement and optimize new computationally efficient tracer advection algorithms for large numbers of tracer species;
  - add important biogeochemical interactions between the atmosphere, land, and ocean models
  - Apply uncertainty quantification (UQ) techniques to constrain process parameters and evaluate feedback uncertainties.
- Objective: Deliver a second-generation ESM with improved representation of biogeochemical interactions at the canopy-to-atmosphere, river-to-coastal ocean, and open ocean-to-atmosphere interfaces.

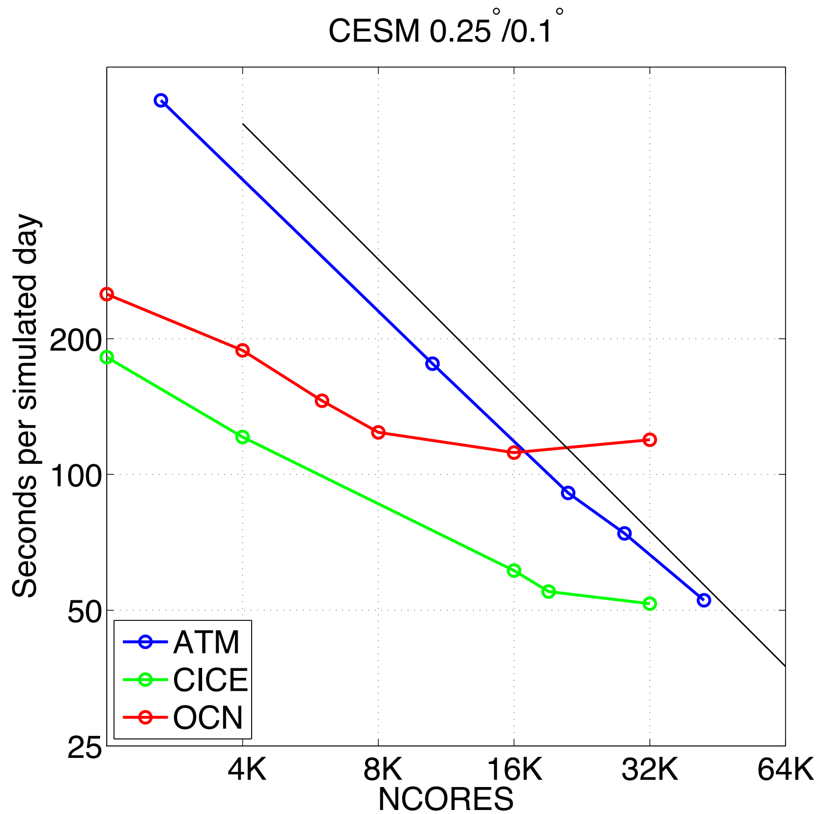
The Community Earth System Model (CESM)

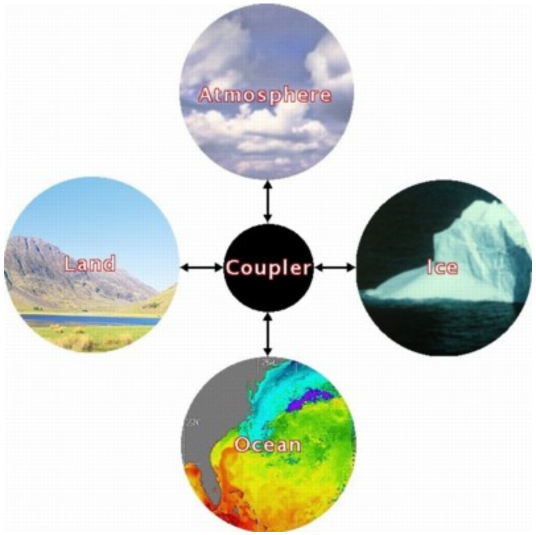
- IPCC-class model developed by NCAR, DOE Labs and Universities
- Atmosphere, Land, Ocean and Sea ice component models
- CAM-SE: Atmosphere component model
- MPAS: future ocean component model





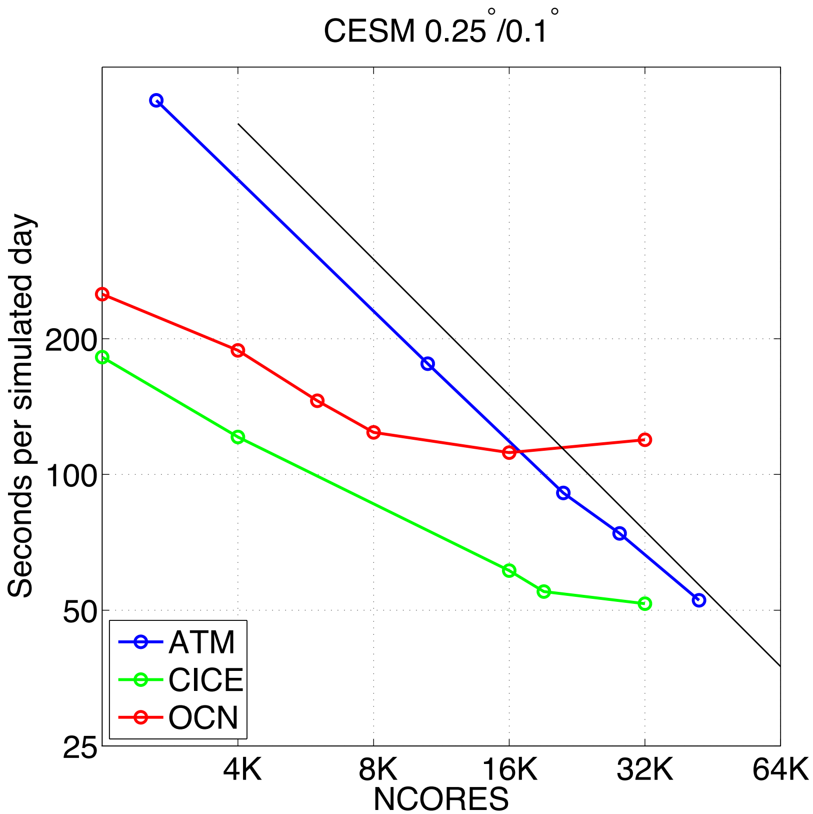
CESM Component Performance

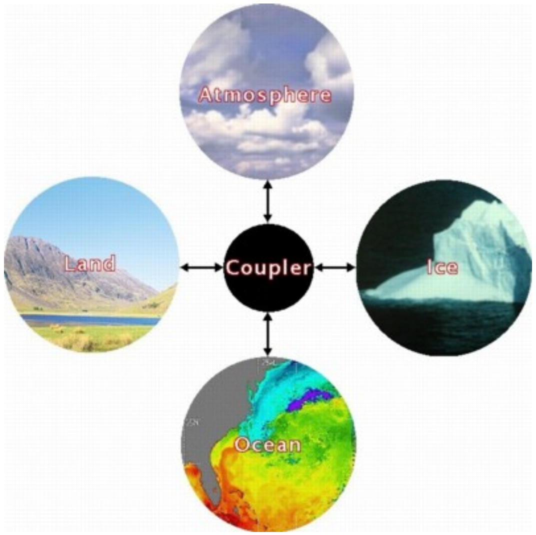




- High-Resolution CESM coupled simulations run on DOE LCF's at about 2 SYPD, ~50K cores.
- LCFs make it possible to perform small ensembles of 30 year simulations, which is a typical use case supporting multiple science objectives.
- Plot shows strong scaling of atmosphere, ocean and sea ice components (land is much faster and is not shown)

CESM Component Performance

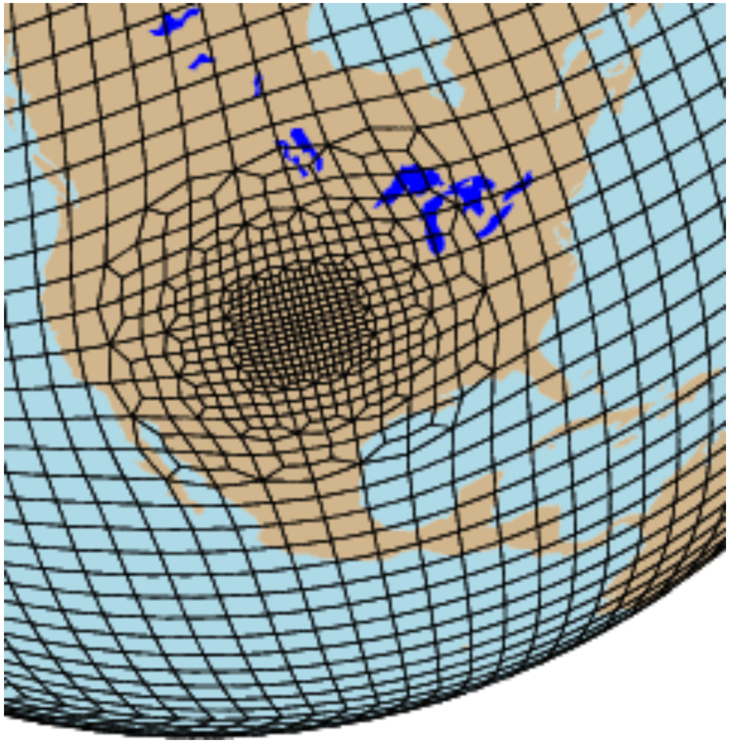


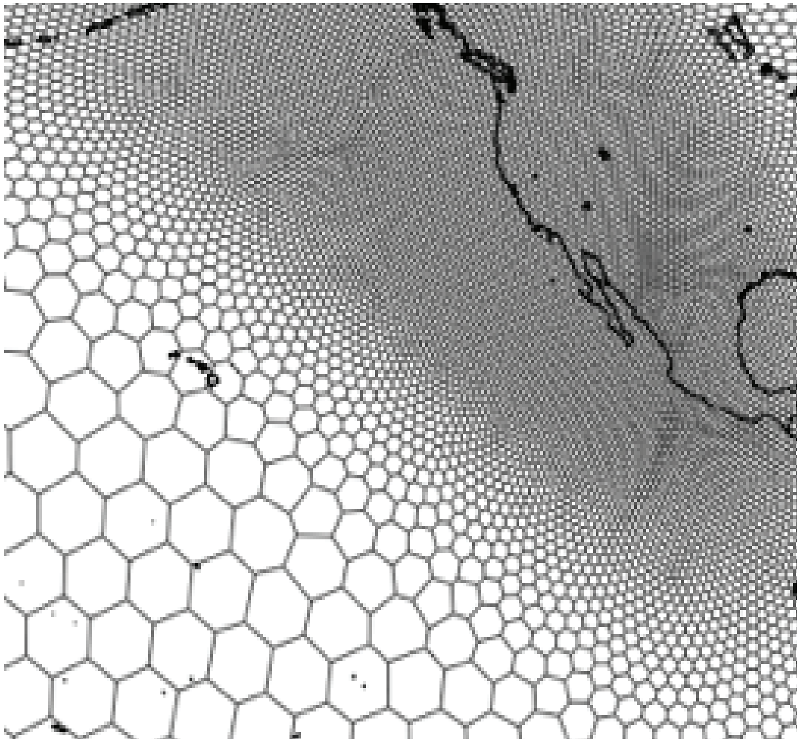


- Atmosphere is the most expensive today w/26 tracers. Within the atmosphere, tracer advection is 50% of the total cost.
- Ocean is the second most expensive component
- With biogeochemistry (needing 100-1000 tracers), cost of both atmosphere and ocean components will be 5-40x more expensive

ACES4BGC Transport R&D

- Faster tracer transport methods for CESM Atmosphere and Ocean components
- Multi-tracer approaches which exploit the fact that we will be transporting hundreds of species
- Accurate on fully unstructured grids supported by next generation CESM





Transport Equations

For each tracer represented by its mixing ratio *q* and tracer mass *ρq*, we transport it in a flow with velocity ***u:***

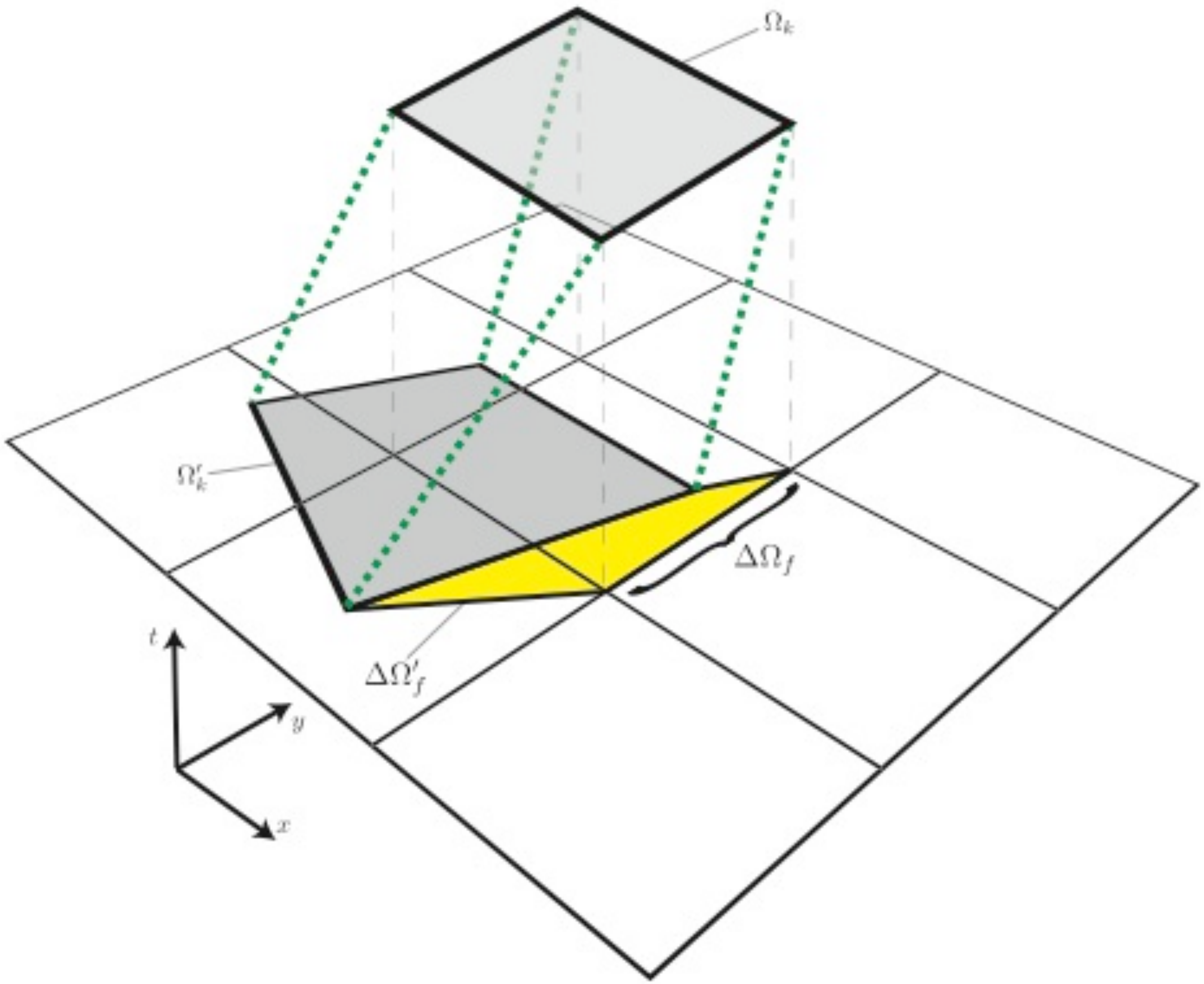
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0$$

$$\frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \vec{u} = 0 \quad \text{OR} \quad \frac{Dq}{Dt} = 0$$

Assume passive tracer for simplicity. Key properties of the transport equations that need to be preserved:

- Local conservation of *ρq*
- Monotonicity or shape-preservation of *q*
- Free stream preserving (*q=1*)

Characteristic Based Methods

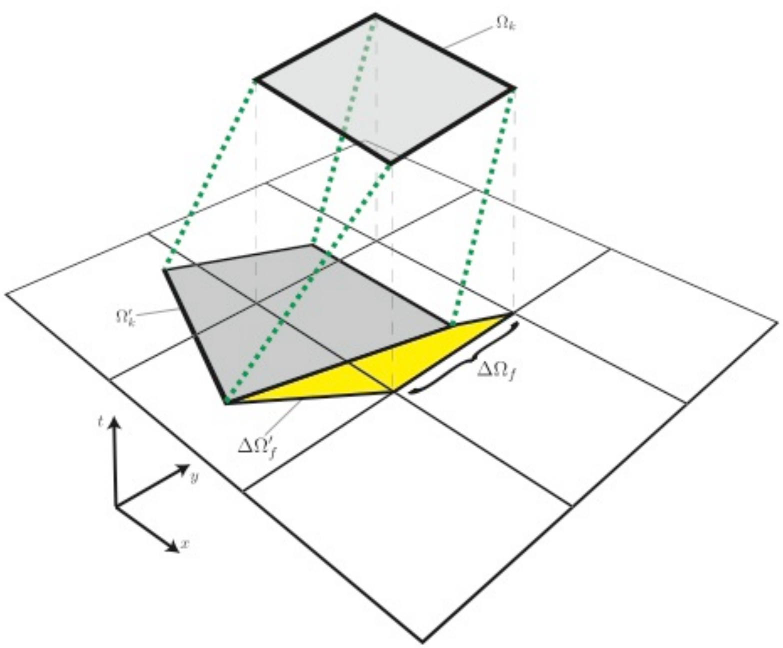


$$\frac{Dq}{Dt} = 0$$

Incremental Remap - Dukowicz & Baumgardner JCP 2000

Characteristic Based Algorithms

- Step 1: Compute *departure grid*
- Step 2: Compute intersections of *departure grid* and *arrival grid*
- Step 3: Compute conservative and monotone *reconstruction* for each tracer
- Step 4: Integrate reconstruction over each sub-polygon

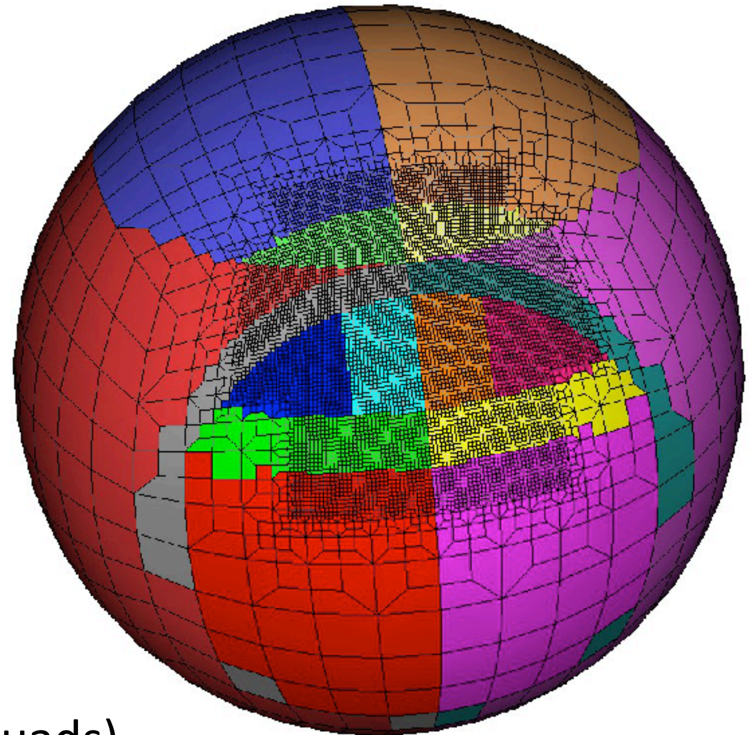


- Assuming you can compute the departure grid, algorithm is unconditionally stable. In practice allows for CFL~5 in the atmosphere.
- Step 2 is Expensive: algorithm is difficult to optimize and parallelize. With CFL>>1, departure grid will often be located in regions belonging to other processors.
- But the cost is independent of the number of tracers

Mesh Intersections in Spherical Geometry

Iulian Grindeanu, Tim Tautges, ANL

- FASTMath's Mesh-Oriented datABase (MOAB)
  - Efficient, distributed & scalable mesh representation
- New capabilities developed under ACES4BGC:
  - Grid intersection capability for fully unstructured, arbitrary polygonal grids in spherical geometry
  - Mesh readers for CAM-SE (unstructured quads) and MPAS (Geodesic grids)
  - Given arrival grid and displacements for departure grid: parallel communication to decompose departure and arrival grid into non-overlapping polygons.



Mesh Intersections in Spherical Geometry

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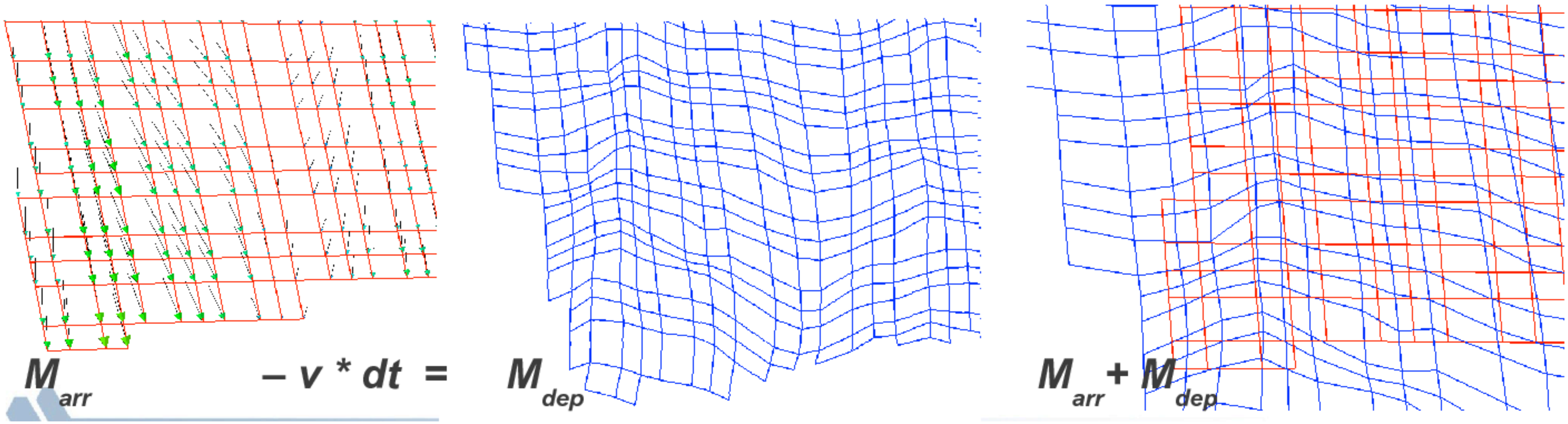

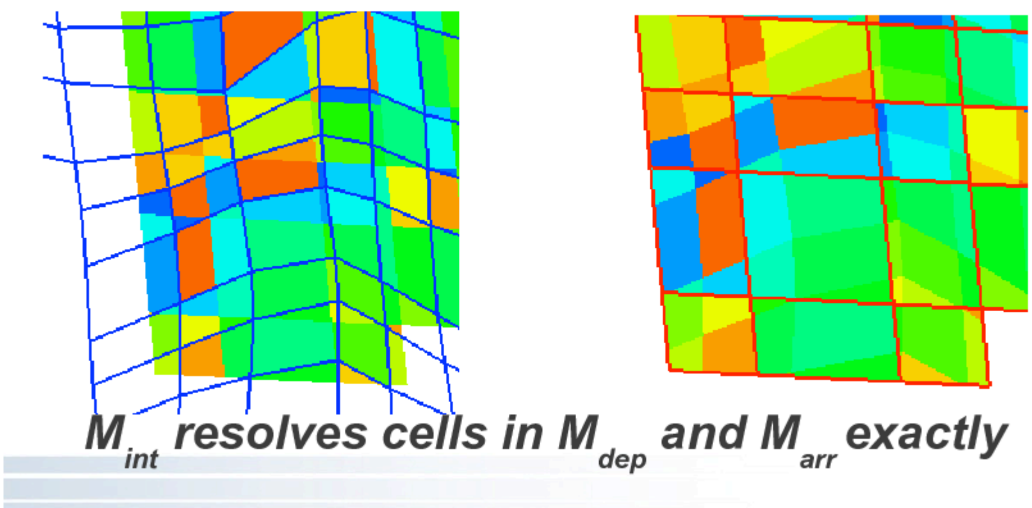

Updated mass in arrival cell given by the mass in the multiple polygons which decompose the arrival cell.

Mesh Intersections in Spherical Geometry

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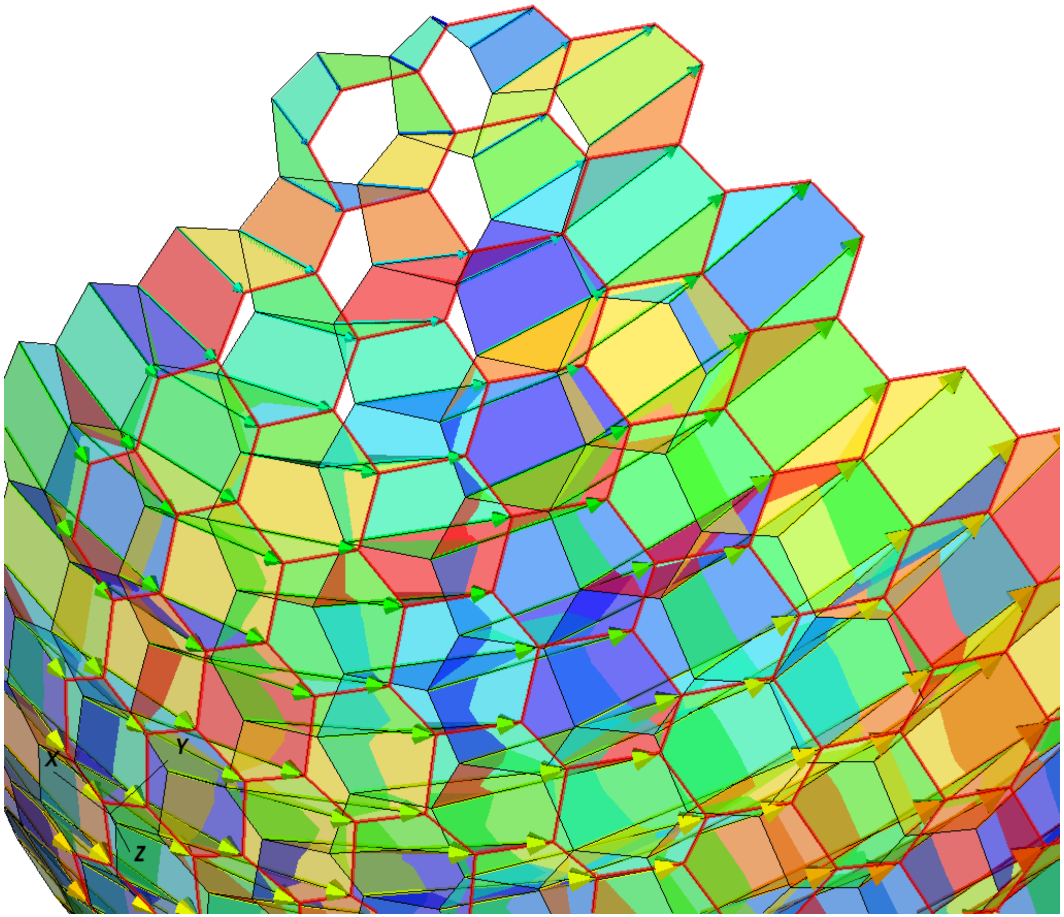


Example from geodesic/voronoi gird. This example shows flux-form, where polygons represent mass fluxed through each arrival cell edge during the timestep.

Reconstruction Approaches

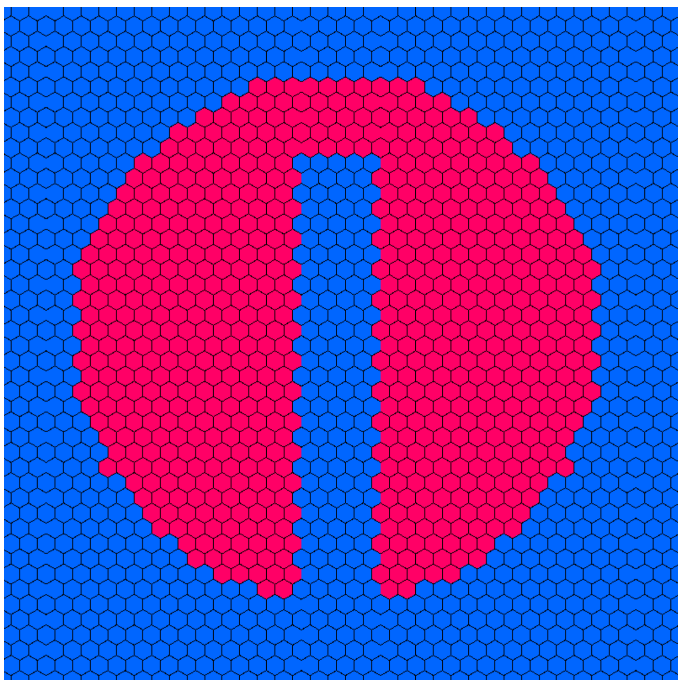
- CSLAM (Conservative Semi-Lagrangian Multi-tracer)
  - FV approach where the tracer is represented by cell averages. CSLAM reconstruction for cubed sphere grid relies on PPM. FV approach makes it relatively easy to build accurate monotone reconstructions but requires large halo regions. (Lauritzen et al., 2010)
  - ACES4BGC working with University SciDAC projects (J.F. Lemarque/NCAR and H. Tufo/CU Boulder) to integrate CSLAM into the CESM. (Erath et al., 2012).
  - CSLAM's uses cubed-sphere grids. ACES4BGC is developing new reconstructions to extend CLSAM to unstructured grids.
- CDG: Characteristic Discontinuous-Galerkin:
  - Tracers are represented by discontinuous modal expansion within each element. Modal expansion provides compact, numerically efficient high-order reconstruction "built in", but more difficult to impose exact monotonicity. (Lowrie & Ringler, 2011)

CDG Results (Rob Lowrie, LANL)

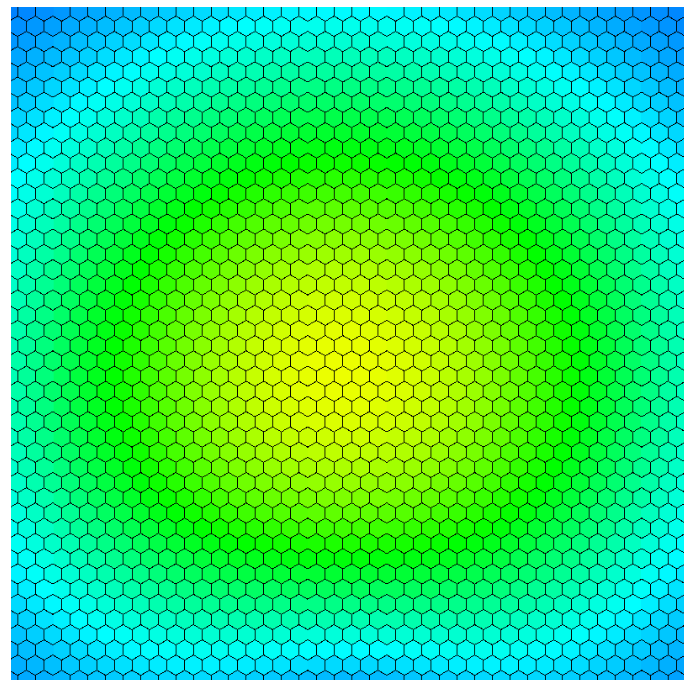
Extend CDG approach to unstructered Voronoi meshes. Initial evaluation using solid-body rotation of a slotted cylinder, following Zalesak JCP 1979

Piecewise-constant in each cell; generalized Godunov method

Initial condition: $0 \leq T \leq 1$



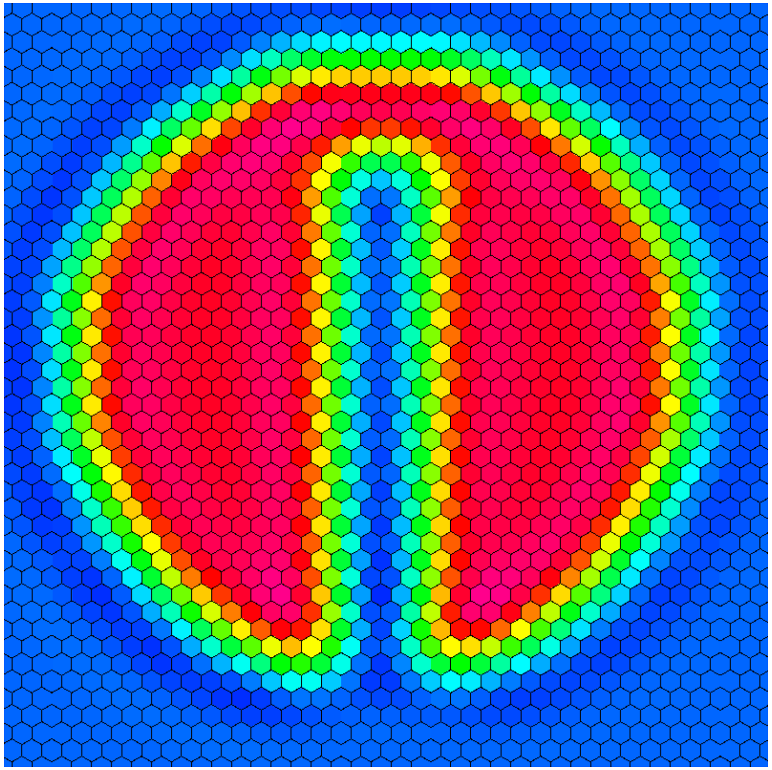
CDG(0): $0 \leq T \lesssim 0.632$



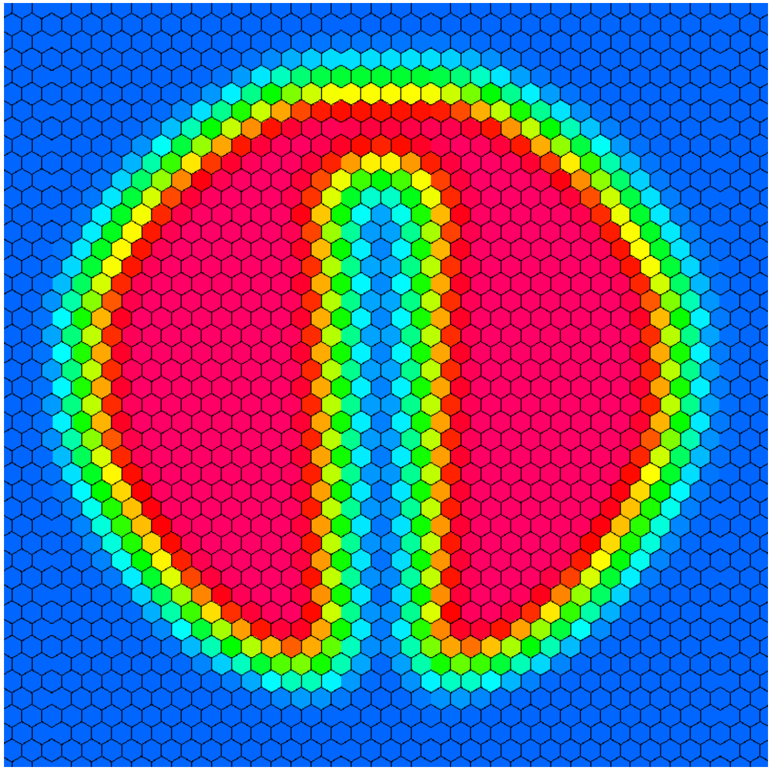
CDG Results (Rob Lowrie, LANL)

Bi-Linear representation within each hexagon

Unlimited: $-0.060 \lesssim T \lesssim 1.038$



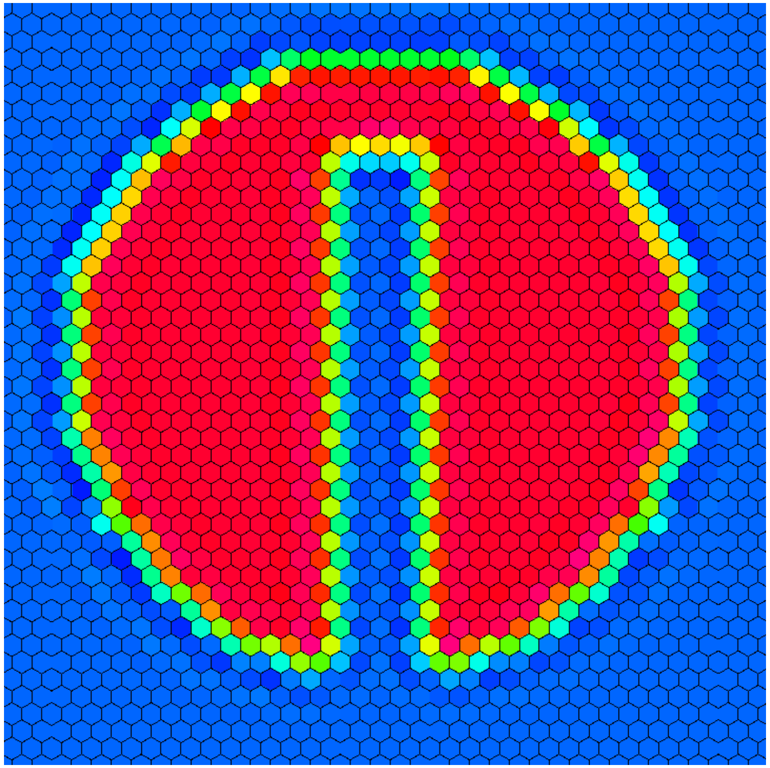
Limited: $0 \leq T \leq 1$



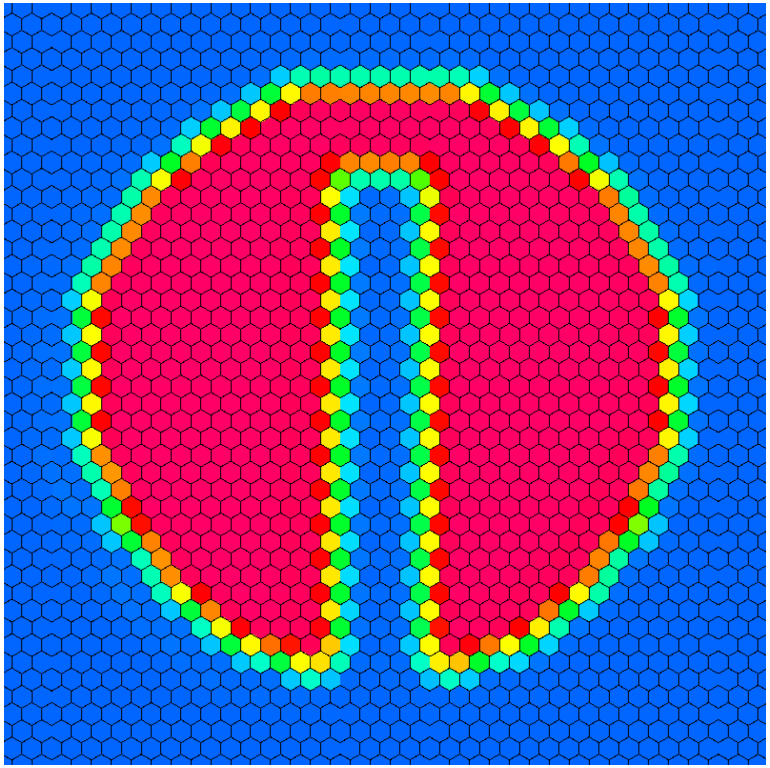
CDG Results (Rob Lowrie, LANL)

Bi-quadratic representation within each hexagon

Unlimited: $-0.075 \lesssim T \lesssim 1.027$



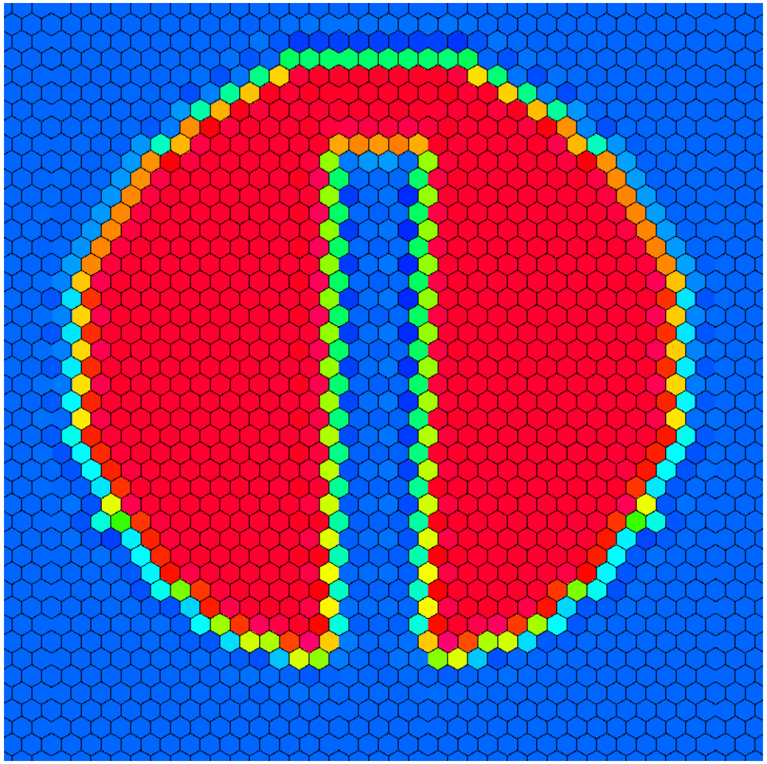
Limited: $0 \leq T \leq 1$



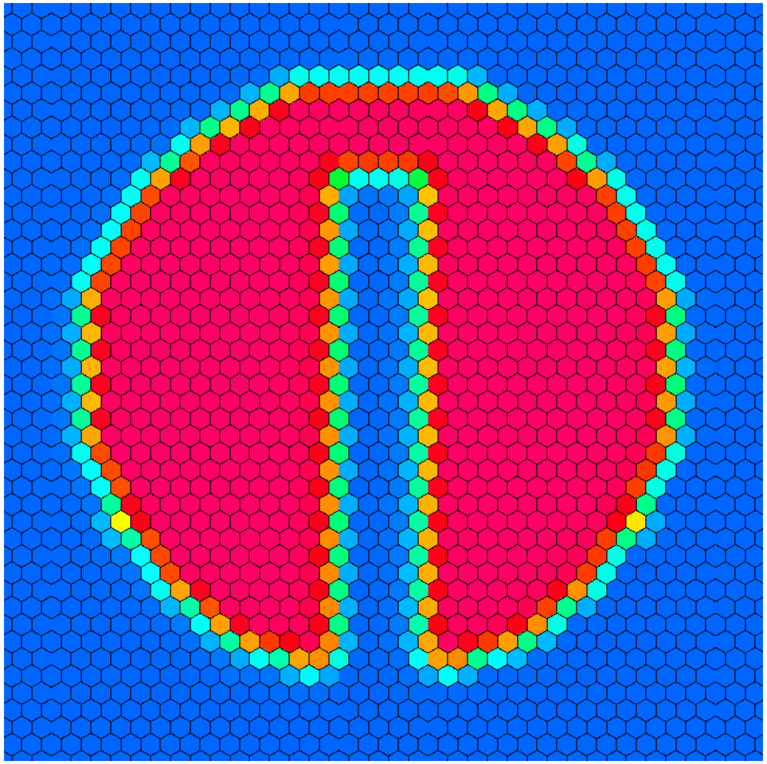
CDG Results (Rob Lowrie, LANL)

Bi-cubic representation within each element

Unlimited: $-0.060 \lesssim T \lesssim 1.010$



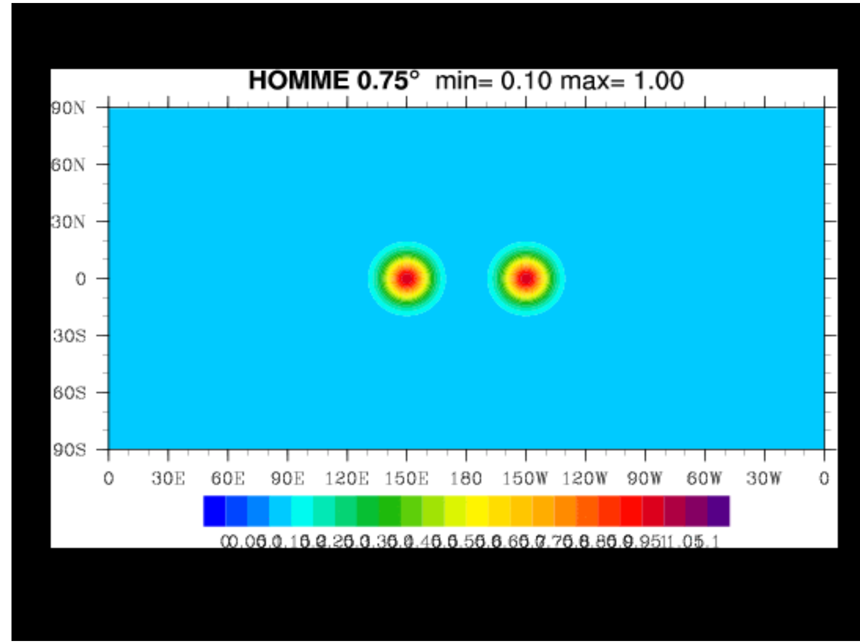
Limited: $0 \leq T \leq 1$

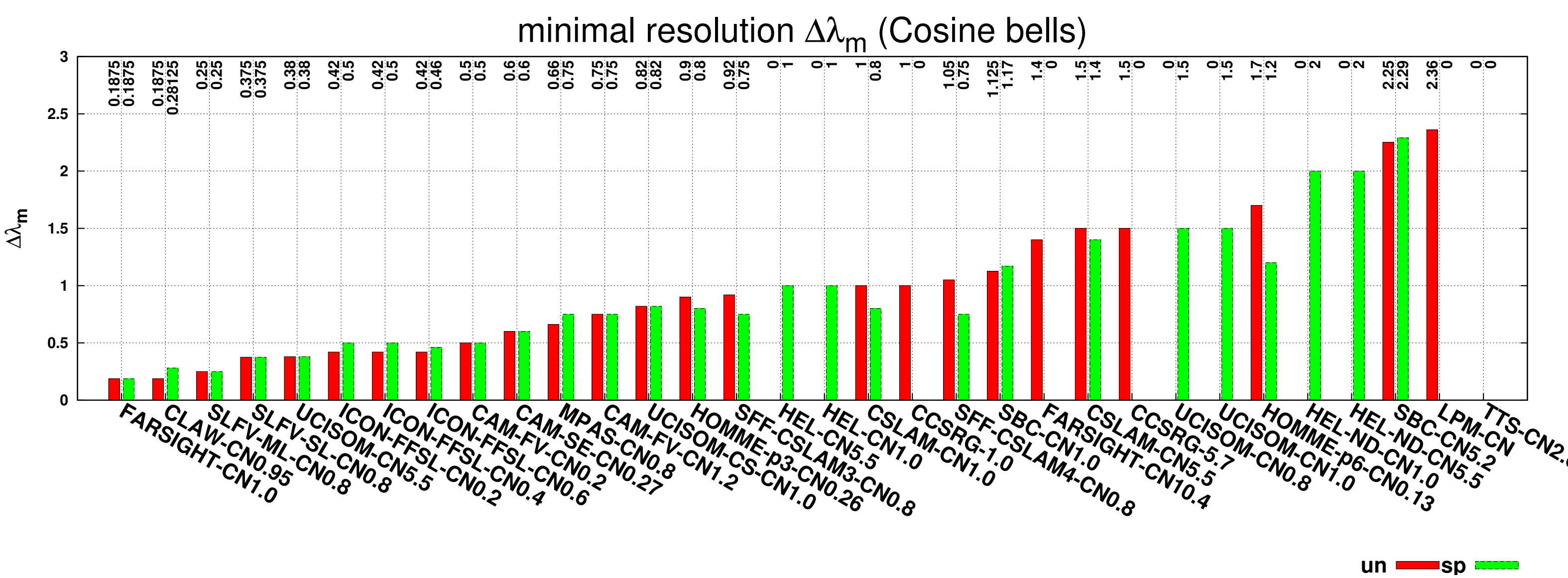


CSLAM Results in CAM-SE

Erath, Taylor, Lauritzen (NCAR & SNL)

- CSLAM and a host of other transport schemes have been been extensively evaluated in 2D spherical geometry. See Lauritzen + 21 authors: *A standard test case suite for two-dimensional linear transport on the sphere, in review, GMD*

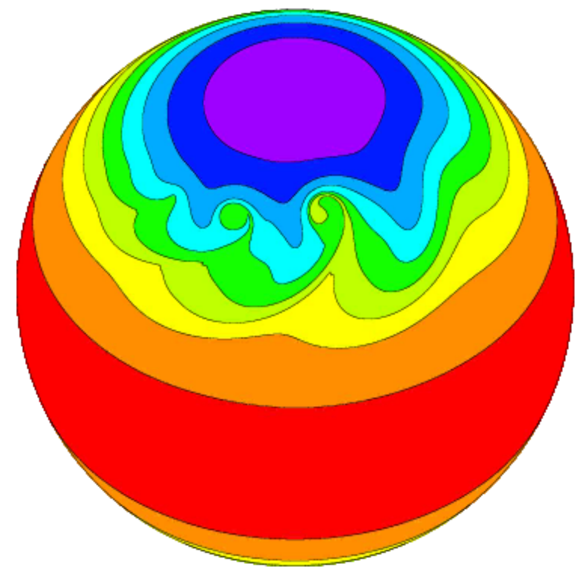


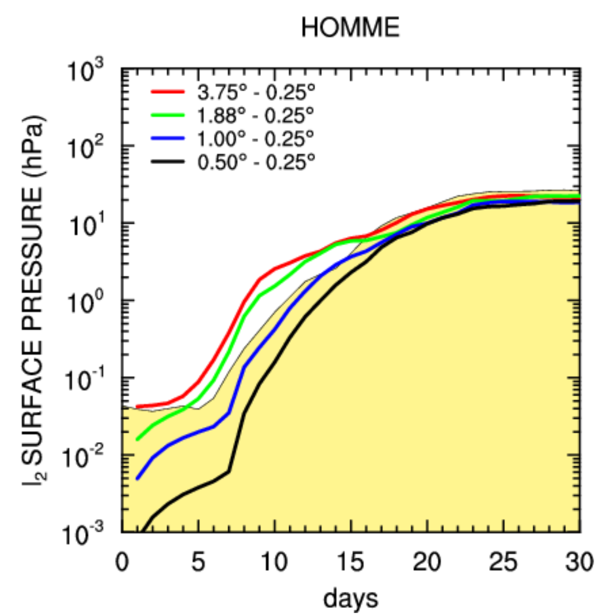


CSLAM Results in CAM-SE

Erath, Taylor, Lauritzen (NCAR & SNL)

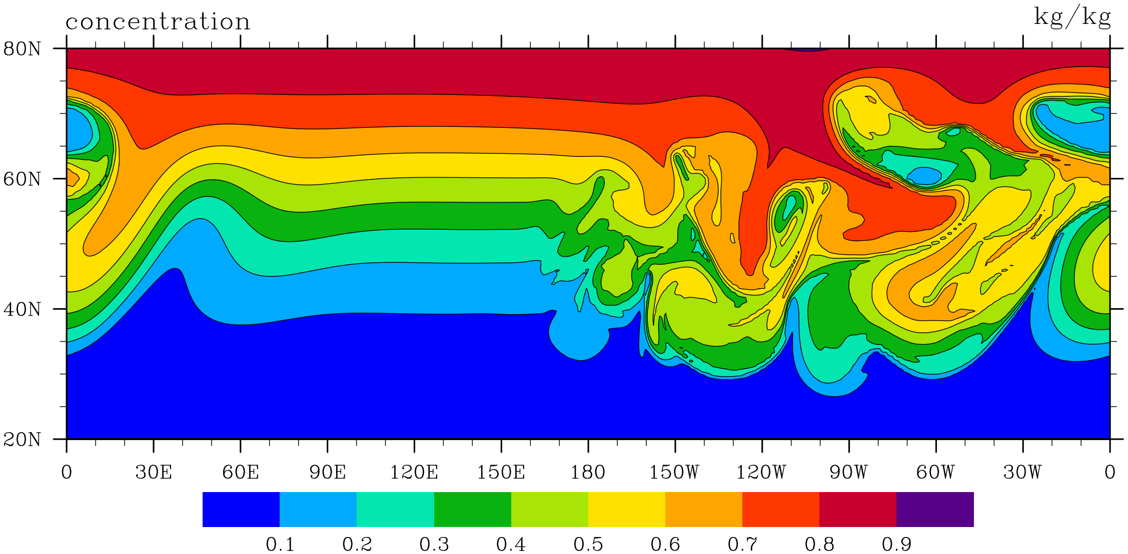
- Evaluate in CAM-SE (Community Atmosphere Model with HOMME's Spectral Element dynamical core)
- 3D: Use vertically Lagrangian approach (S.J. Lin, 2004): CSLAM used in horizontal directions on floating lagrangian levels with occasional 1D vertical remap back to reference levels
- Runge-Kutta/Taylor Series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

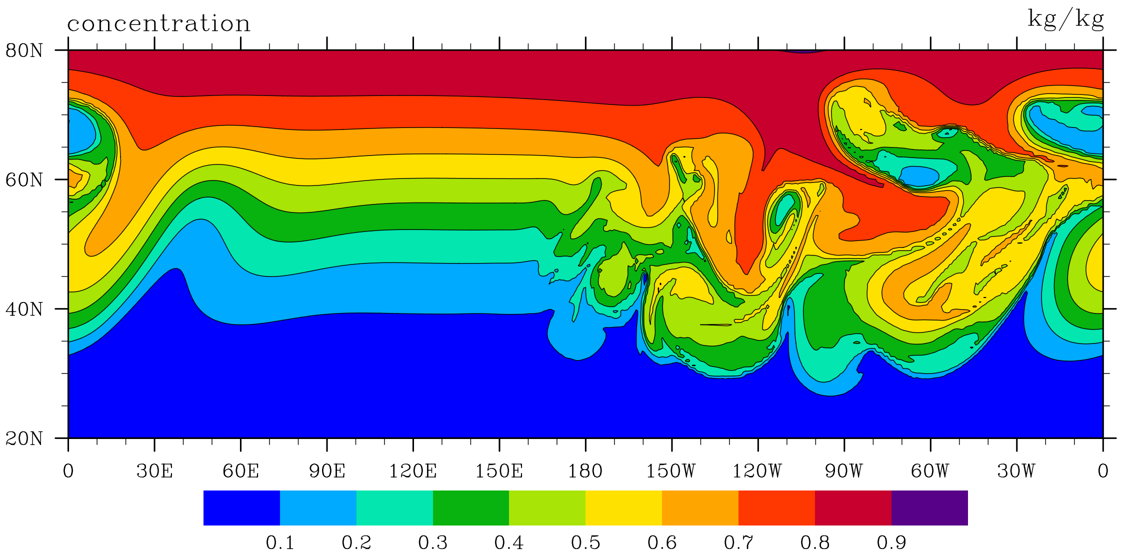




CSLAM Results in CAM-SE

Erath, Taylor, Lauritzen (NCAR & SNL)

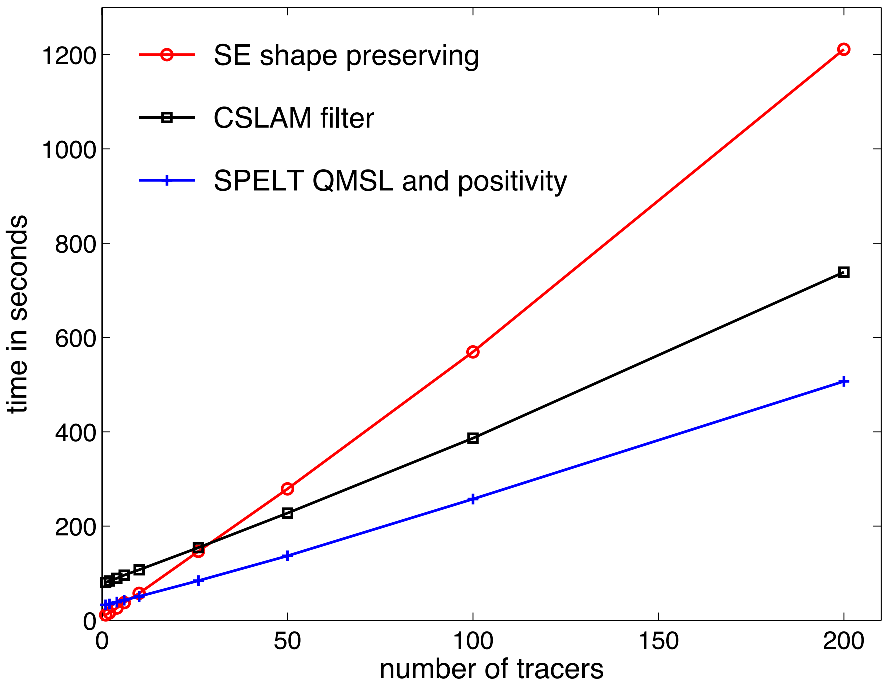


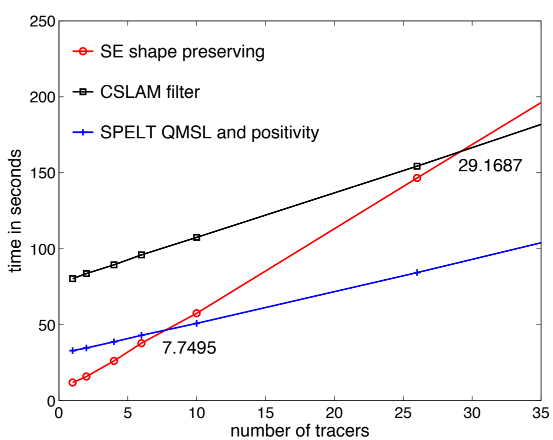


- Initial zonally symmetric tracer after 13 days.
- CAM-SE Eulerian advection and CSLAM are remarkably identical, even at fine scales.
- CSLAM running with a CFL=1. One (large) communication step and expensive geometry step
- CAM-SE uses CFL=0.3 with RK-3. Three (small) communication steps, dense matvecs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

CSLAM Results in CAM-SE

Erath, Taylor, Lauritzen (NCAR & SNL)





- For 1 tracer, CSLAM is quite expensive
- Breakeven with CAM-SE Eulerian at 29 tracers
- Significantly faster at 100+ tracers
- Using internal (CFL<1) intersection algorithm. Additional improvements expected with MOAB and CFL>5

Conclusions

- New grid intersection capability in MOAB
- Key functionality for high-CFL conservative & monotone transport methods. Also useful for other grid transfer/remap applications.
- Shared by next-generation CESM atmosphere and ocean components.
- CDG approach extended to unstructured hexagon (and n-gon) meshes.
- CSLAM integrated into CAM-SE dynamical core with SE departure algorithm and extension to three-dimensions.