Enhancing Global Biogeochemical Cycles in the Community Earth System Model

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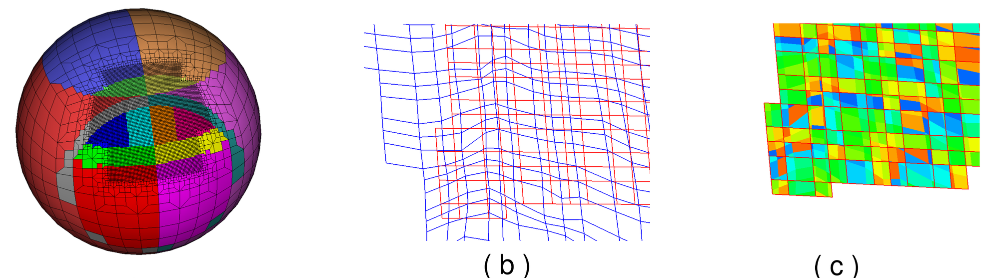
Project Goals and Objectives

- The goal of ACES4BGC is to advance the 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; and
  - apply uncertainty quantification (UQ) techniques to constrain process parameters and evaluate feedback uncertainties.
- The objective of this SciDAC Partnership project is to 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 resulting upgrades to the Community Earth System Model (CESM) will deliver new scientific capabilities, offer unprecedented accuracy in representing biogeochemical interactions, and yield *improved predictive skill and computational performance*.

Advection for Large Numbers of Biogeochemical Tracers
Contact: Timothy J. Tautges (ANL) and Mark A. Taylor (SNL)

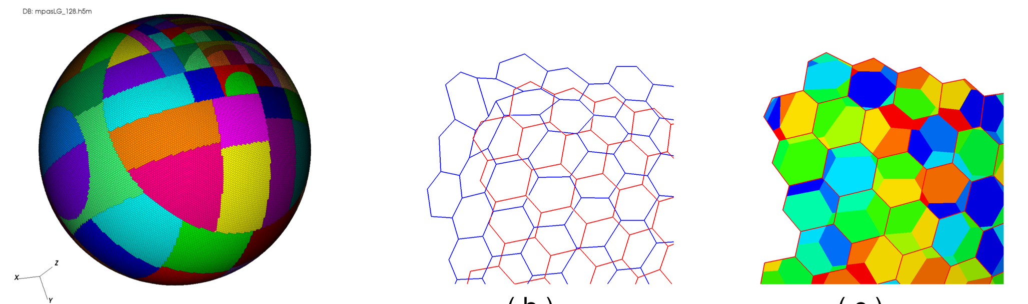
- A computationally efficient and accurate tracer advection scheme is critical for transporting large numbers of reactive biogeochemical tracers throughout all component models of the ESM.
- The Community Earth System Model's atmosphere component, CAM-SE, utilizing the spectral finite element dynamical core from the High Order Method Modeling Environment (HOMME). (Taylor and Fournier, 2010; Evans et al., 2011; Dennis et al., 2011; Worley et al., 2011).



(a) (b) (c)

Figure 1: *(a) An example of an unstructured CAM-SE variable resolution grid. (b) Arrival grid (red) and departure grid (blue) computed from wind velocities (u, v). (c) Intersection of departure grid with arrival grid.*

- The Model for Prediction Across Scales (MPAS) finite volume methods, utilizing Spherical Centroidal Voronoi Tessellations, offer dynamical cores for both future ocean and atmosphere component models (Thuburn et al., 2009; Ringler et al., 2010).



(a) (b) (c)

Figure 2: *(a) An example of an MPAS variable resolution grid. (b) Arrival grid (red) and computed departure grid (blue). (c) Intersection of departure grid with arrival grid.*

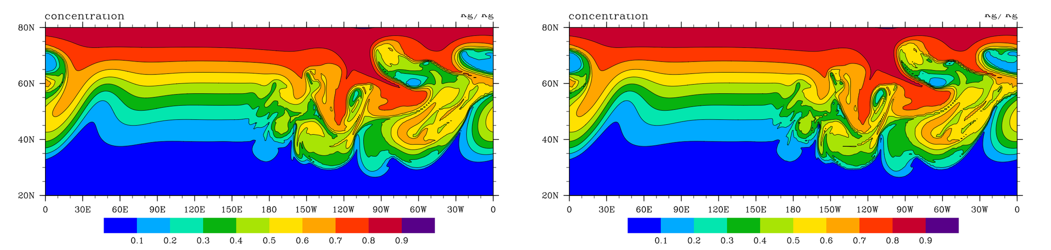
We focus on backward-trajectory characteristic-based transport schemes. These methods allow for very large time steps, but require expensive geometric computation at each time step. However, this cost is independent of the number of tracers and is thus amortized over all the tracers included in the simulation, making these methods ideal for the large numbers of tracers we need for our biogeochemical applications. We are collaborating with the SciDAC3 FASTMath Institute to develop efficient, scalable implementations of these geometry algorithms in FASTMath's **Mesh-Oriented datABase (MOAB)** library:

New MOAB capabilities developed under ACES4BGC:

- Mesh readers for CAM-SE (unstructured quads) and MPAS (Geodesic grids).
- Grid intersection capability for fully unstructured, arbitrary polygonal grids in spherical geometry. Examples: CAM-SE unstructured quadrilateral mesh (Figure 1(c)) and MPAS Geodesic grid (Figure 2(c)).
- Application friendly interface: Given arrival grid and displacements for departure grid: parallel communication to decompose departure and arrival grid into non-overlapping polygons.

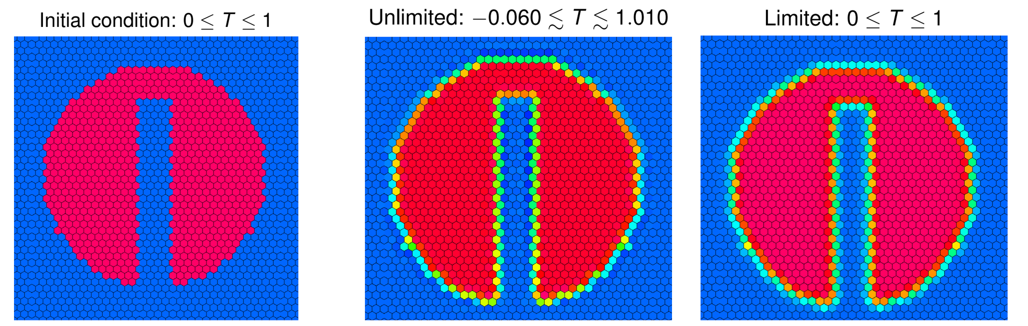
Reconstruction Approaches: Our transport schemes combine MOAB's new mesh intersection capability with monotone conservative reconstruction algorithms. Our initial focus is on two reconstruction techniques, CSLAM and CDG.

- CSLAM: Conservative Semi-Lagrangian Multi-tracer (CSLAM) method (Lauritzen et al., 2010). ACES4BGC (in collaboration with H. Tufo's University SciDAC) has integrated CSLAM into the CAM-SE dynamical core, including the development of a Spectral Element departure grid algorithm and the extension of the method to 3D via a vertically Lagrangian approach. Initial results are shown in Figure 3.
- CGD: The Characteristic Discontinuous Galerkin (CDG) method (Lowrie and Ringler, 2011). ACES4BGC has extended the CDG method to work with unstructured hexagonal (and *n*-gon) meshes. Initial results are shown in Figure 4.



(a) CAM-SE Eulerian (b) CSLAM

Figure 3: *(a) An advected tracer (interpolated to the 850 mb surface) from CAM-SE's existing Eulerian-based advection algorithm. The passive tracer is advected in the three-dimensional wind field produced by a baroclinically unstable jet in the mid-latitudes. (b) The same tracer advected with the CSLAM algorithm. Both algorithms show remarkable agreement.*

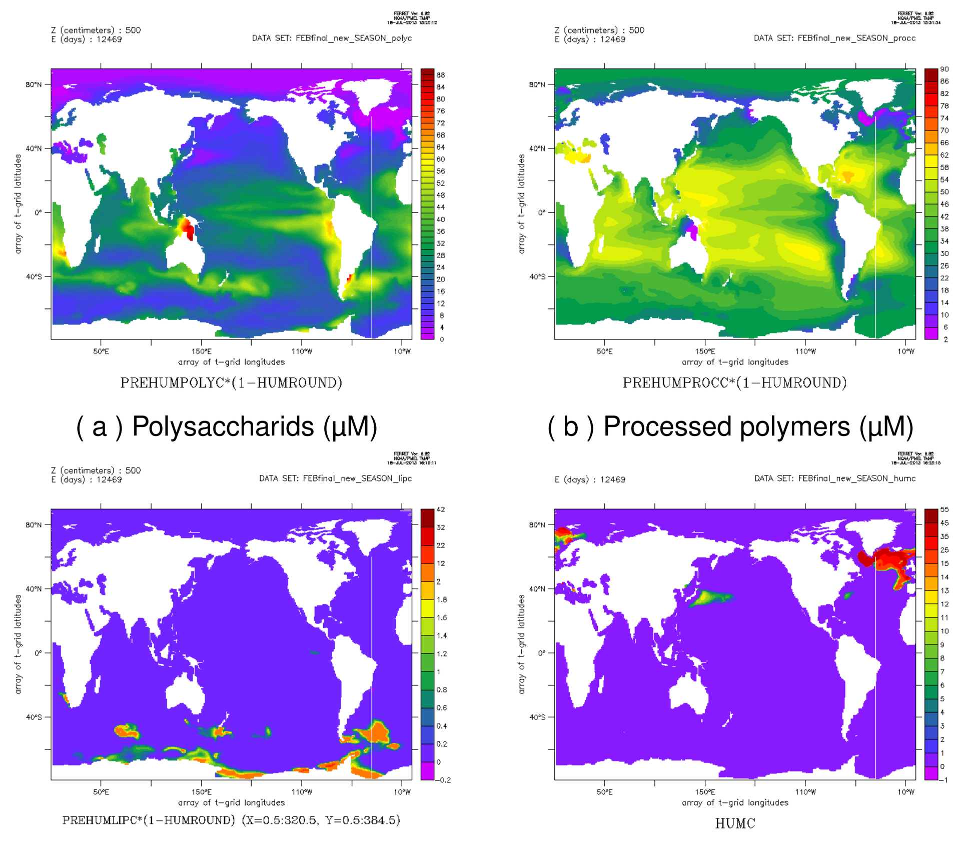


(a) Initial Condition (b) CDG Results

Figure 4: *Advection of a 2D slotted cylinder by ridged body rotation in a periodic domain (following Zalesak (1979)). Results show the successful extension of the CGD method to hexagonal meshes. (a) Initial condition. (b) Results from the CDG method after one rotation, with (right panel) and without (left panel) a limiter.*

Marine Chemistry
Contact: Scott M. Elliott

- Organic enhancement to aerosols over oceans may be locally significant to radiative forcing.
- Recently developed organic sulfur processing concepts are extensible to representation of mixed layer organics that lead to atmospheric aerosols.
- We are adding representation of marine organic chemistry by
  - identifying major classes of dissolved and particulate matter, and mapping compounds onto atmospheric species;
  - simulating dynamic distributions of chemical species across the surface ocean (due to grazing, ballasting, upwelling, photochemistry, heterotrophy, etc.);
  - providing OCS, NH_3, VOC, and aerosol emissions to the atmosphere; and
  - evaluating model performance using relevant data sets and traditional atmosphere-based kappa sensitivities.



(a) Polysaccharids (µM) (b) Processed polymers (µM)

(c) Lipids (µM) (d) Humics (µM)

Figure 5: *Dissolved organic macromolecules are simulated in the ocean mixed layer in the Parallel Ocean Program (POP) model. Simulated and analyzed by O. Ogunro, O. Wingenter, S. Burrows, and S. Elliott.*

Terrestrial Emissions
Contact: Forrest M. Hoffman (ORNL)

- As vertical resolutions improve, it becomes necessary to represent the finite size and storage capacity of the canopy.
- With the addition of biogenic VOC (BVOC) and soil emissions into CLM, an interactive canopy air space (CAS) scheme is needed.
- We will improve the representation of biogenic emissions by
  - developing a canopy air space scheme supporting emissions of BVOCs, carbonyl sulfide (COS), and bi-directional fluxes of ammonia (NH_3);
  - developing and testing methods for reducing the range of uncertainty in BVOC emission factors, initially adding plant functional types (PFTs); and
  - evaluating emissions from dense woody vegetation against GOAmazon2014 observations under pristine and industrially polluted conditions.

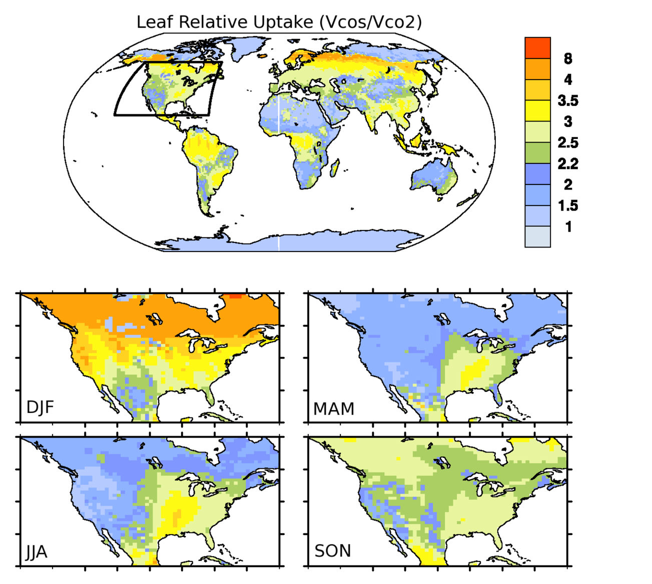


Figure 6: *Leaf relative uptake from simulation testing COS uptake in CLM (Fu et al., in prep.).*

Atmospheric Aerosols
Contact: Xiaohong Liu (PNNL)

- Current treatment of secondary organic aerosols (SOA) in global models is crude due to a lack of scientific understand.
- Sources of marine SOA and primary organic aerosols (POA) are often ignored and SOA formation in polluted air is underestimated.
- We are advancing the representation of SOA in CESM by
  - improving the treatment of SOA formation and aging based on the latest mechanistic understanding and evaluate against observation data (GOAmazon2014, GVAX, IMPROVE network, and the CAPT-aerosol capability);
  - implementing new mechanistic schemes for emission of volatile organic compounds (VOCs), POA, and other species;
  - apply UQ techniques to new schemes for OA to understand sensitivities and reduce uncertainties related to organics.

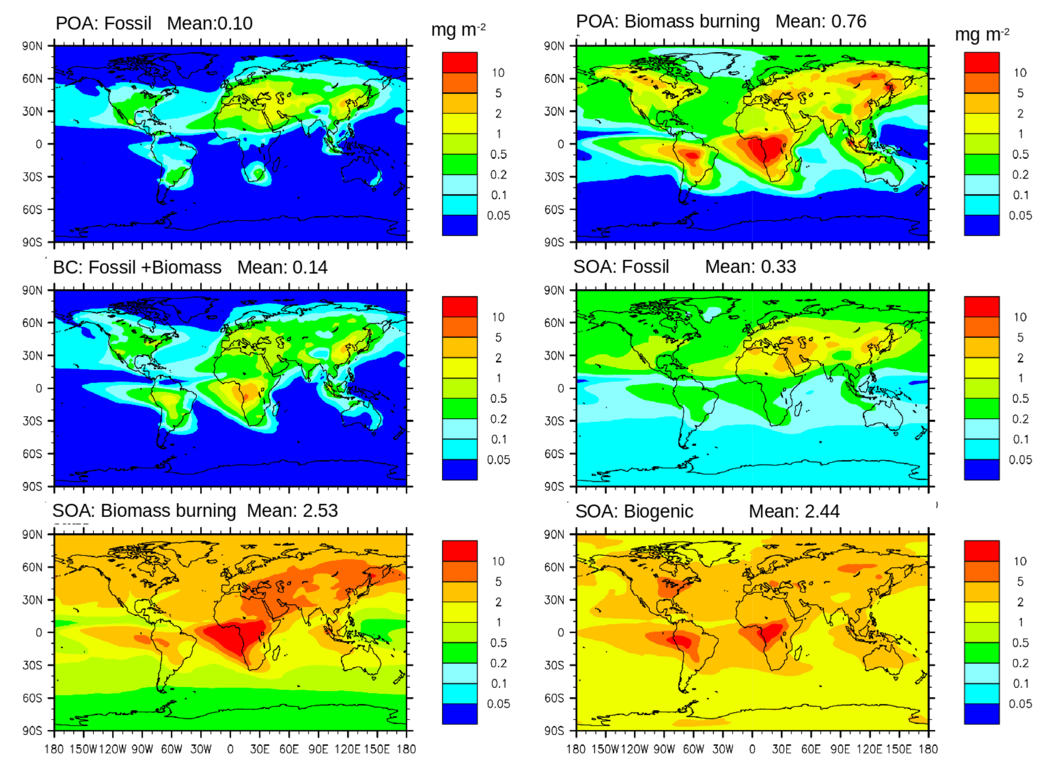


Figure 7: *July 5-year average column burdens of primary and secondary organic aerosols and black carbon from fossil and biomass sources. The SOA treatment was improved in these simulations using the volatility basis set (VBS) approach in CAM5.*

Atmospheric Chemistry
Contact: Philip J. Cameron-Smith (LLNL)

- The *fast* and *super-fast* mechanisms developed in the previous project offer reduced computational burdens for chemistry.
- Explicit representation of complex organic chemistry is absent.
- We will improve the representation of organic chemistry by
  - calculating the rate of oxidation of VOCs into the condensable chemicals that form SOAs, which plays a key role in controlling aerosol and cloud droplet pH;
  - adding ammonia (NH_3), which plays a key role in controlling pH of aerosols and cloud droplets;
  - calculating the effect of emissions on the concentration of reactive greenhouse gases (CH_4, N_2O, HCFCs) and ozone depleting chemicals, which affect climate and air quality; and
  - constraining other model components through comparison with observations of related isotopic tracers (SF_6, ^{222}Rn, ^{210}Pb, OCS, and $CO^{18}O$).

Verification, Validation & Uncertainty Quantification (UQ)
Contact: Donald D. Lucas (LLNL)

- **UQ Goal** – Quantify sensitivities and uncertainties of atmospheric chemistry and biosphere-atmosphere interactions in support of GOAmazon2014 (O_3, NO_x, VOCs, SOA formation)
- **UQ Challenge** – With well over 100 uncertain parameters, chemical oxidation in the Amazon basin is an extremely high dimensional UQ problem ("curse of dimensionality")!
- **UQ Approach** – Apply Latin hypercube sampling to parameters in CAM5 physics and MOZART chemistry and run ensembles of the single column model (SCAM)

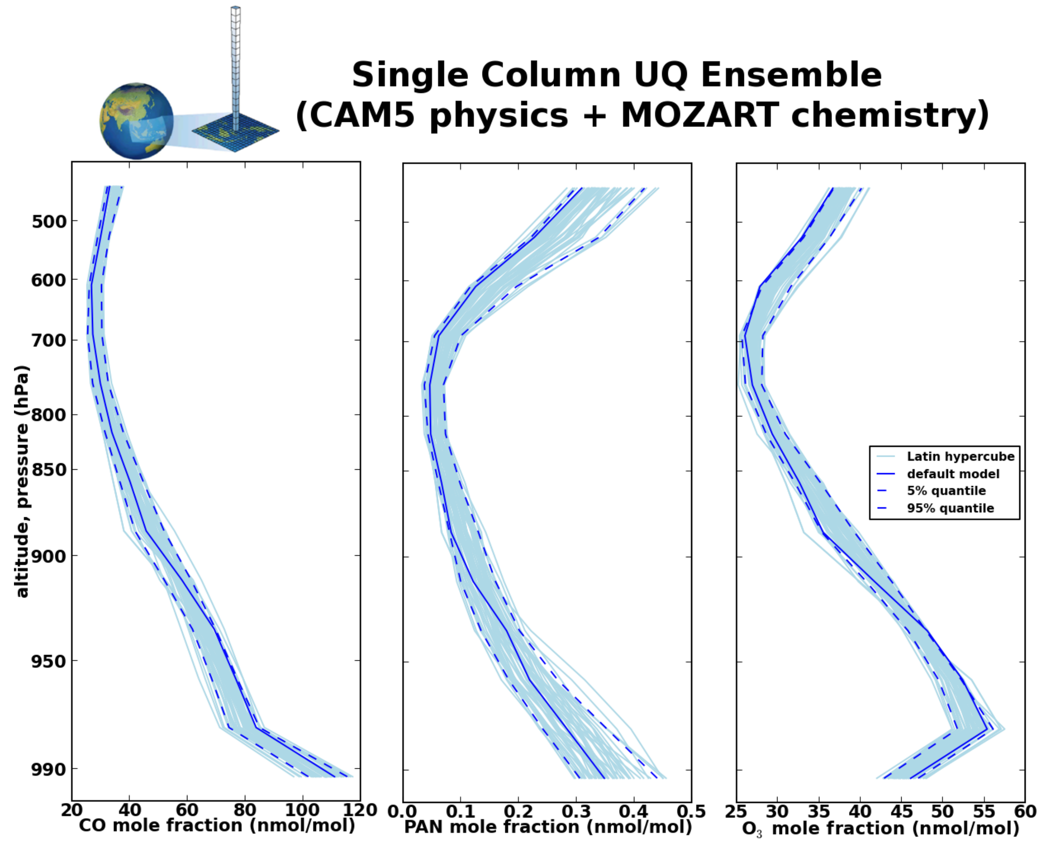


Figure 8: *Variations in the vertical profiles of carbon monoxide (CO), peroxyacetyl nitrate (PAN), and ozone using a 50-member SCAM ensemble with MOZART chemistry using QUEST's Latin hypercube sampling method* **nond**. *We sampled two uncertain physical parameters (RH threshold for low clouds, entrainment rate in deep convection). Chemical uncertainties have been implemented, but not yet sampled.*

Performance Engineering
Contact: Patrick H. Worley (ORNL)

- ACES4BGC is leveraging computer performance tools and technologies from the **SciDAC Institute for Sustained Performance, Energy, and Resilience (SUPER)**.
- We are monitoring and optimizing performance by
  - instrumenting code, deploying performance data bases and analysis tools, and establishing procedures for performance tracking;
  - routinely testing and tracking performance of new algorithms and model configurations;
  - developing optimized communications algorithms for new tracer schemes, particularly motivated by the expected large core count per compute node in the target systems; and
  - participating in end-to-end application testing and optimization for the next generation of CESM.

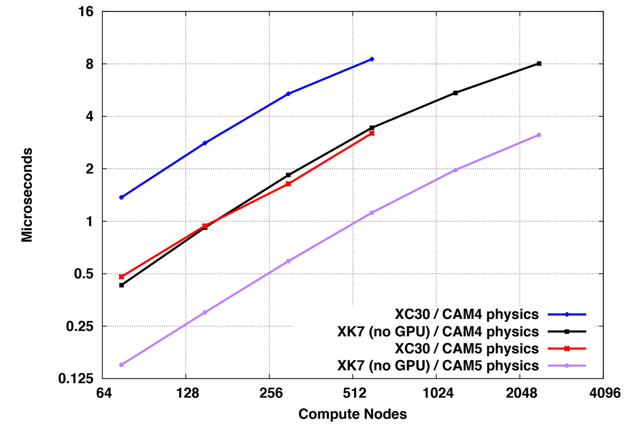


Figure 9: *CAM-SE performance on a 5-day simulation without generating restart files on Titan (Cray XK7 without GPUs) and Edison (Cray XC30).*

Software Engineering
Contact: Bill Sacks and Mariana Vertenstein (NCAR)

- ACES4BGC is following the established software engineering standards for CESM development, coordinating with NCAR's CESM Software Engineering Group.
- New development will be performed on feature-specific code branches.
- CESM scripting will permit flexible incorporation of new biogeochemistry features, simplify testing of model configurations, and support many UQ simulations.
- ACES4BGC is contributing all new model features to the CESM research community after they are tested, verified, validated, and reviewed.

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