Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

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Project Goal and Objective

- **Goal:** 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*.

- **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.

- **ACES4BGC** is
  - implementing and optimizing new computationally efficient tracer advection algorithms for large numbers of tracer species;
  - adding important biogeochemical interactions between the atmosphere, land, and ocean models; and
  - applying uncertainty quantification (UQ) techniques to constrain process parameters and evaluate feedback uncertainties.
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†Science Team Lead; ‡SciDAC Institute Liaison
ACES4BGC Tracer Advection Research

Climate Science Needs for Reducing Biogeochemical and Aerosol Feedback Uncertainties

- Faster tracer transport methods for CESM and ACME atmosphere and ocean components
- Accurate on fully unstructured grids needed for next generation models
- Transport hundreds to a thousand of reactive and non-reactive biogeochemical species (trace gases, aerosols, dust, etc.)
A tracer, represented by its mixing ratio $q$ and mass $\rho q$, is transported in the flow with velocity $u$ as

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} &= 0 \\
\frac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \mathbf{u} &= 0
\end{align*}
\]

\[
\frac{Dq}{Dt} = 0.
\]

Solution methods should satisfy

- local conservation of $\rho q$,
- monotonicity or bounds preservation of $q$, and
- consistency between $q$ and $\rho$ (free stream preserving).
The **High-Order Method Modeling Environment (HOMME)** within CAM-SE provides a continuous Galerkin finite element method using Gauss-Lobatto quadrature. Advection using the standard spectral element method with high-degree polynomials is accurate, but expensive due to time step restrictions.

Conservative Semi-LAgrangian Multi-tracer (CSLAM) transport scheme (Lauritzen et al., 2010) offers one approach for improving efficiency for large tracer counts. Stable method for large time steps with CFL $\sim 5$. 

(a) Original CAM-SE mesh  
(b) CSLAM mesh (refined, 2/16 proc)
Early CSLAM Performance

No obvious loss of accuracy.
Erath, Taylor, Lauritzen (SNL & NCAR)
Early CSLAM Performance

► CSLAM is expensive for one tracer, but breaks even with CAM-SE at $\sim 30$ tracers.

► A fast, scalable method for generating grid intersections allowing for CFL $\geq 5$ should improve performance significantly.

Erath, Taylor, Lauritzen (SNL & NCAR)
Eulerian/Lagrangian Grid Intersection

The CSLAM scheme uses an Eulerian arrival grid and integrates backwards to a Lagrangian departure grid. An intersection of these two grids is required to compute the disposition of tracers through time.

The Mesh-Oriented data Base (MOAB) from the FASTMath Institute provides a scalable, parallel algorithm for intersecting arbitrary meshes.

The arrival (red) and departure (blue) meshes are intersected to produce a final set of polygons for reconstruction of all tracer mole fractions.
MOAB Now Coupled to HOMME

Initialization:

- MOAB infrastructure is instanced on every task,
- arrival mesh is initialized from HOMME (CAM-SE and refined CSLAM meshes), and
- parallel infrastructure is established.

At every time step:

- departure point positions are passed to MOAB,
- MOAB computes the intersections (communicating as needed), and
- MOAB returns the intersections to HOMME for reconstruction.

Next Steps:
Complete coupling (return of intersections), verify, and compare results with current CSLAM (cubed-sphere, regular mesh) implementation.
Additional Approaches

- Characteristic Discontinuous-Galerkin (CDG) represents tracers by discontinuous modal expansion within each element. Modal expansion provides compact, numerically efficient high-order reconstruction “built it”, but difficult to impose exact monotonicity (Lowrie and Ringler, 2011).

- Semi-Lagrangian spectral element (SL-SE) algorithm using optimization to enforce mass conservation. Optimization is efficient and works for large time steps on unstructured grids (Peterson and Taylor, 2014).

**Deformational flow, 1.5° resolution**

Mass error = $-3.44 \times 10^{-3}$
Min value = $-0.1070$
Max value = 1.1934

Mass error = $1.69 \times 10^{-11}$
Min value = 0.1
Max value = 0.9979
Terrestrial Biogeochemistry: Carbonyl sulfide (COS)

Objective:

- Add important biogeochemical interactions between the biosphere and atmosphere to the Community Earth System Model (CESM).

New Science:

- Initial parameterization for carbonyl sulfide (COS) uptake by the biosphere tested in the Community Land Model (CLM4) by intern Wenting Fu.

Significance:

- COS provides a potentially powerful tracer for biosphere–atmosphere exchange of CO$_2$ and a constraint on global gross primary production.

ORNL intern Wenting Fu presenting preliminary results from her initial implementation of COS uptake in CLM4.
Volatile Organic Compounds (VOCs)
- Working with Alex Guenther at PNNL to improve VOC emissions factors ($\varepsilon$);
- improving species-specific emissions in MEGAN2 model, initially by adding plant functional types (PFTs) in CLM4; and
- will use GOAmazon2014 observations and UQ to improve model parameters in warm, moist tropical regions.

Prognostic Canopy Air Space
- Initially implementing single-layer canopy air space scheme of Vidale and Stöckli (2005) and
- extending to a multiple-layer CAS to improve representation of canopy trace gas exchange.

Ammonia
- Focusing on canopy exchange and
- adding soil and agricultural emissions (cattle, hogs, fertilizer).
Marine Biogeochemistry

(Stefels et al., 2007)
Organic ocean emissions are sources of primary organic aerosols.
Ozone concentration differences for simulations of enhanced Arctic Ocean methane released due to clathrate destabilization on continental slopes → complex HO$_x$/NO$_x$ chemistry.
Volatility basis set (VBS) representation for secondary organic aerosol (SOA) precursors

(Shrivastava et al., 2013)
A very simplified volatility basis set (VBS) is used for current climate models, with only 8 tracers.
Ozone tracer emitted uniformly at surface with 90-day exponential decay.

(Prather et al., 2011)
ACE4BGC Uncertainty Quantification

Vertical profile (days 5–10)
191 simulations

Time evolution (level 887 hPa)

Effects of parameter changes (days 5–10, lev 887)

Don Lucas (LLNL)
MOZART Ozone Example

- Implemented PDFs for 100 photochemical parameters in the MOZART mechanism.
- Ran $\sim 10^4$ ensemble SCAM simulations using Latin hypercube sampling.
- Analyzing ensemble variance using new UQ methods in collaboration with QUEST Institute.

Second order decomposition of the variance of daily mean $O_3$ concentration in the middle troposphere is dominated by 10 laboratory rate constant parameters.
How do we pull together all these individual science components?

- Combine code onto a single ACES4BGC branch of ACMEv0.
- Perform new science simulations, turning on new biogeochemical and aerosol processes incrementally.
- Develop a science and computational performance baseline before switching to CSLAM on unstructured grids.
- Validate and use a GPU-enabled version of the existing finite volume tracer advection scheme with large numbers of tracers.

Enabled by **SUPER Institute** collaboration and the Oak Ridge Leadership Computing Facility (OLCF) Director’s Discretion Project: **ACES4BGC SciDAC-3 Partnership Project Gen2ESM Foundry**

- Titan: 6M core-hours; Rhea: 6K core-hours
ACES4BGC Benefitting from SciDAC Institute Partnerships

▶ **FASTMath Institute** – Development and implementation of MOAB by Iulian Grindeanu and Vijay Mahadevan (ANL) will provide a significant advance to enable new science.

▶ **SUPER Institute** – Critically important performance tracking and optimization by Pat Worley (ORNL) continues to enable more science in less time and fewer computing resources and supporting performance portability across new architectures.

▶ **QUEST Institute** – Uncertainty quantification tools and methods being used by Don Lucas (LLNL) to develop framework for biogeochemistry sensitivity studies.

▶ **SDAV Institute** – Began after our project, but we are starting a conversation with Rob Ross (ANL) about *in situ* analysis, parallel I/O, and tracer visualization.
Intersection of Distributed Meshes for Multi-Tracer Transport Schemes

Iulian Grindeanu†, Kara Petersonβ, Timothy J. Tautges, Mark A. Taylor‡ and Patrick H. Worley§
†Argonne National Laboratory, §Oak Ridge National Laboratory, and §Sandia National Laboratories

One of the important goals of ACES4BGC project is to implement and optimize new computationally efficient advection algorithms for large number of tracer species.

The transport problem is related to a challenging problem in the Lagrangian mesh movement is presented (Laursen et al., 2013).

The transport problem can be solved in Eulerian or Lagrangian—Lagrangian—Eulerian form. One popular variant is semi-Lagrangian method, run in Lagrangian mode for one-time step and then interpolated back to Eulerian mesh (Stoffelen and Cole, 1991).

A tracer, represented by its mixing ratio, is transported in the flow with (Jones, 1999) and the method was extended for regular lat-lon into line-integrals. This approach has been applied for up to second-order static grid-to-grid remapping in (Jones, 1999).

The semi-Lagrangian approach involves interpolating quantities from a distorted Lagrangian mesh to a regular Eulerian mesh or vice versa, depending on the tracer. Each time-step, the transport problem is resolved by a semi-Lagrangian approach which is based on the method of characteristics (Moore and Recker, 1966).

The resulting upgrades to the Community Earth System Model (CESM) will deliver mass conserving and free stream preserving. The method is stable for large time steps and in practice performs well with up to second-order accuracy (Jones, 1999).

The transport field is cast in Eulerian, Lagrangian or Arbitrary Lagrangian—Eulerian (ALE) form, and the translation of the MOAB mesh topology is handled using a semi-Lagrangian approach which is based on the method of characteristics (Moore and Recker, 1966).

Semi-Lagrangian Remap Algorithm for Transport

The transport field is cast in Eulerian, Lagrangian or Arbitrary Lagrangian—Eulerian (ALE) form, and the translation of the MOAB mesh topology is handled using a semi-Lagrangian approach which is based on the method of characteristics (Moore and Recker, 1966). By using a search tree, this will constitute the seed of the front. Advancing in both directions, the algorithm will be able to handle intersections of arbitrary topology.

Figure 8: Results of a transport simulation in the Modular Ocean Model (MOM) using the semi-Lagrangian remap algorithm. (a) Initial tracer field. (b) Velocity field. (c) Final tracer field. (d) Positive (red) and negative (blue) tracer concentrations.

References

An efficient interpolation algorithm for distributed unstructured meshes has been developed and is currently being integrated into the Community Earth System Model (CESM). This interpolation algorithm will provide CESM with the ability to perform efficient tracer transport on fully unstructured, quadrilateral meshes in the sphere. The infrastructure and methodology will be leveraged for MPAS framework, too.

Conclusions

Figure 6 shows the results of a transport simulation in the Modular Ocean Model (MOM) using the semi-Lagrangian remap algorithm. (a) Initial tracer field. (b) Velocity field. (c) Final tracer field. (d) Positive (red) and negative (blue) tracer concentrations.

Acknowledgments

This research was supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

Figure 7 shows the results of the algorithm up to 64,000 tracer species transported on a MPAS model on 64 processors. The simulation was run on Mira at Argonne National Laboratory (ANL), which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

At every time-step, the semi-Lagrangian approach involves interpolating quantities from a distorted Lagrangian mesh to a regular Eulerian mesh or vice versa, depending on the transport. Each time-step, the transport problem is resolved by the semi-Lagrangian approach which is based on the method of characteristics (Moore and Recker, 1966).

The semi-Lagrangian approach involves interpolating quantities from a distorted Lagrangian mesh to a regular Eulerian mesh or vice versa, depending on the transport. Each time-step, the transport problem is resolved by the semi-Lagrangian approach which is based on the method of characteristics (Moore and Recker, 1966). By using a search tree, this will constitute the seed of the front. Advancing in both directions, the algorithm will be able to handle intersections of arbitrary topology.

Figure 8: Results of a transport simulation in as in (Nair and Lauritzen, 2010), the course does not change and any downstream flow. The transported scalar field follows complex topologies and undergoes severe deformation during the simulation, but it re-emerges its course halfway through and returns to the initial position by the end of the simulation. If there would be no error in the simulation, the initial and final result should be the same. The picture shows how the clear transport constant in our approximation is not sufficient, higher polynomial order is mandatory.

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Biological emissions affect climate and air-quality

**Ocean ecosystem is the source of many gases and aerosols to the atmosphere**

- **Decrease in soar surface heating due to d-methyl sulfide produced in the ocean**
  - Global mean = 3.5 W/m²
  - Organic chemicals in atmosphere oxidize into aerosols

**Land ecosystem is source of CO₂ and hydrocarbons**

- **Carbonyl sulfide (OCS) is a natural tracer that is similar to CO₂, and can be used to quantify the difference between photosynthesis and respiration.**

Tracers can answer: who, what, where, why?

**Natural tracers can validate unmeasurable processes**

- Radon affected by convective mixing
- CH₄ tracks uplift from oceans.
- SF₆ quantifies interhemispheric exchange rate.

**Natural tracers can constrain stratospheric motion and fossil CO₂**

- TC tracks wind motion & fossil CO₂
- Tract SF₆ tracks stratospheric air in troposphere

**Idealized tracers can unambiguously identify tropical mixing barrier atmospheric equator**

**Tracers emitted north and south with 90° day decay.**

**Tracers can be tagged in model to quantify contribution from source region or plant type**

- Atmosphere is a key to understanding the Earth System Modeling program of the Earth System Model of the Department of Energy. This work was performed under the auspices of the Office of Science of the Department of Energy under Contract No. DE-AC02-05CH11231, the National Center for Computational Sciences and Argonne National Laboratory, which is supported by the Office of Science of the Department of Energy under Contract DE-AC02-06CH11357. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science (BER) of the U.S. Department of Energy.
Earth system modeling is entering a new era as the climate community transitions to extreme-scale computing and as the need for more capable models becomes increasingly evident in the face of “no-analogs” climate regimes emergent under global warming. We invite presentations at the frontiers of climate simulation that address the prospects, early development, and proof-of-principle experiments with the next generation of Earth System Models (ESMs). We seek talks and posters demonstrating how to best exploit recent advances in theory, applied mathematics, computational science, process-scale modeling, uncertainty quantification, and observational assimilation to make ESMs more accurate, robust, scalable, and extensible. These more robust ESMs are characterized by increasing reliance on more mechanistic, and more computationally intensive, treatments of core climate processes. Examples include global cloud resolving models, regional large eddy simulation models, full physics, high-resolution land ice models, and high-throughput treatments of chemical and biogeochemical transport across the climate system.

Invited speakers:

▶ Omar Ghattas, Univ. of Texas at Austin (next-generation ice sheet models)
▶ Peter Lauritzen, NCAR (atmospheric transport)
▶ Charlotte DeMott, Colorado State University (cloud/turbulence interactions)
▶ Hisashi Yashiro, RIKEN (non-hydrostatic global cloud-resolving models)

Abstracts are due August 6, 2014 at http://fallmeeting.agu.org/2014/
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