Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

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Project 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; and
  - 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.

Research Team

Name	Lab	Science Team	Topic
Pavel B. Bochev	SNL	Atmosphere	Advection
Philip J. Cameron-Smith†	LLNL	Atmosphere	Atm. BGC
Richard C. Easter, Jr.	PNNL	Atmosphere	Aerosols
Scott M. Elliott†	LANL	Ocean	Ocean BGC
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Donald D. Lucas	LLNL	Atmosphere	UQ
Richard T. Mills	ORNL	Comp. Tools & Perf.	Performance
Timothy J. Tautges‡	ANL	Comp. Tools & Perf.	Mesh Tools
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Mariana Vertenstein	NCAR	Comp. Tools & Perf.	SE
Patrick H. Worley†‡	ORNL	Comp. Tools & Perf.	Performance

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Research Team

With over 100 person-years of contributions to CESM, this team

- developed a modal aerosol module and introduced aerosol indirect effects into the CAM;
- introduced fast & super-fast photochemistry into CAM;
- developed a fully coupled sulfur cycle in POP and CAM;
- developed new dynamical cores for CESM;
- improved the computational performance of CLM;
- collaborated on terrestrial biogeochemistry modules in CLM;
- developed and performed Carbon-Land MIP (C-LAMP);
- developed grid tools and methods for structured and unstructured grids;
- applied UQ techniques to global biogeochemical systems; and
- increased scalability of CESM by over a factor of 10 and enabled use of over 200,000 processor cores.

Atmospheric Aerosols

- Current treatment of secondary organic aerosols (SOA) in global models is crude due to a lack of scientific understanding.
- Sources of marine SOA and primary organic aerosols (POA) are often ignored and SOA formation in polluted air is underestimated.
- We will advance 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.

Atmospheric Chemistry

- 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 $CO^{18}O$).

Within the Canopy

- 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 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.

Marine Chemistry

- 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 will add 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.

River Transport and Ocean Coupling

- Riverine chemical fluxes exert strong control on nutrient cycling and biological productivity in coastal waters, influencing climate.
- Tracer transport and reactive chemistry, absent from the River Transport Model (RTM), are needed to represent large mass and energy fluxes.
- We will advance river-to-ocean biogeochemical cycles by
  - collaborating on development of tracer and nutrient transport schemes, building on a new two-way CLM/RTM coupling;
  - adapting ocean ecosystem dynamics to represent coastal zone processes;
  - combining CLM unstructured grid and variable resolution MPAS-Ocean to test river export and coastal zone biogeochemistry; and
  - evaluating model results against observations for the large Mississippi and Amazon basins.

Tracer Advection

- A computationally efficient and accurate tracer advection scheme is critical for supporting large numbers of reactive biogeochemical tracers.
- The backward-trajectory, semi-Lagrangian approach with conservative remapping of the Conservative Semi-Lagrangian Multi-tracer (CSLAM) method and the Characteristic Discontinuous Galerkin (CDG) method applied to unstructured grids offer promising techniques for computationally tractable advection.
- We will develop and test new advection schemes by
  - using the *Mesh-Oriented datABase (MOAB)* library, available through the **Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute**, to extend CSLAM and CDG to unstructured HOMME (CAM-SE) and MPAS grids for CFL > 1, and
  - applying the same MOAB infrastructure for advection in the MPAS-Ocean and MPAS-Atmosphere dynamical cores.

Uncertainty Quantification (UQ)

- Advanced UQ methods are needed to constrain model parameters based on observations and to understand the impacts of uncertainties on model projections.
- We will apply advanced UQ methods to biogeochemical processes by
  - applying targeted schemes and utilizing the *DAKOTA Project tools*, developed by the **SciDAC Institute for Quantification of Uncertainty in Extreme Scale Computations (QUEST)**, to sample parameter spaces,
  - decomposing and analyzing biogeochemical variances,
  - performing dimensionality reductions,
  - constructing statistical surrogate models for biogeochemical processes, and
  - developing a model validation toolkit to optimize biogeochemical parameters using observational data sets (e.g., ARM, NGEE, GoAmazon2014).

Software Engineering

- ACES4BGC will follow software engineering standards for CESM development, coordinating with the head of the CESM Software Engineering Group (CSEG) at NCAR.
- New development will be performed on feature-specific branches in the CESM repository.
- CESM scripting will permit flexible and extensible incorporation of new biogeochemistry features.
- New MOAB-based tracer advection module will be re-usable and integrated into CAM-SE, MPAS-Ocean, and MPAS-Atmosphere dynamical cores.
- Working directly with CSEG staff, ACES4BGC will contribute all new model features to CESM after they are tested, validated, verified, and reviewed.
- New model capabilities that meet with CESM Working Group and Scientific Steering Committee (SSC) approval will be included in future releases of CESM.

Performance Engineering

- The ACES4BGC goal is to significantly enhance the biogeochemical representation within CESM without increasing the computational cost beyond practical limits.
- Development processes must include routine and accurate performance monitoring on relevant HPC systems.
- Partnering with the **SciDAC Institute for Sustained Performance, Energy, and Resilience (SUPER)**, we will monitor and optimize 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; and
  - participating in end-to-end application testing and optimization for the next generation of CESM.

Project Summary

- ACES4BGC is a relatively small project, employing a diverse and multi-disciplinary team in the development of a second generation Earth System Model.
- This model will include
  - new unstructured grid-based semi-Lagrangian advection schemes for large numbers of reactive & non-reactive tracers,
  - treatment of SOA formation and aging,
  - oxidation of VOCs and formation of SOA,
  - representation of the CAS and improved BVOC emissions,
  - representation of marine organic chemistry with VOC and aerosol emissions, and
  - rudimentary river-to-coastal zone biogeochemical cycles.
- Advanced UQ methods, software engineering methodologies, and performance engineering will underlie its development.
- This five-year project is just starting, and we welcome additional collaborators and partners. Follow us on the web at `http://www.aces4bgc.org/`