Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

Forrest M. Hoffmanγδ, Pavel B. Bochevβ, Philip J. Cameron-Smith‡δ, Richard C. Easter, Jr.α, Scott M. Elliot*δ, Xiaohong Liuα, Robert B. Lowrie*, Donald D. Lucas‡, Richard T. Mills§, Timothy J. Tautges†ɛ, Mark A. Taylorβ, Mariana Vertenstein¶, and Patrick H. Worley§δɛ

†Argonne National Laboratory, ‡Lawrence Livermore National Laboratory, *Los Alamos National Laboratory, ¶National Center for Atmospheric Research, §Oak Ridge National Laboratory, αPacific Northwest National Laboratory, and βSandia National Laboratories;
γPrincipal Investigator, δScience Team Member, and ɛSciDAC Institute Liaison

SciDAC-3 Principal Investigators Meeting ● Rockville, Maryland, USA
September 10, 2012
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

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†Science Team Lead  
‡SciDAC Institute Liaison
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$_2$O, 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.
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.
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.
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/