Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

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Goals and Objectives

- Goals: Advance predictive capabilities of Earth System Models (ESMs) by reducing two of the largest sources of uncertainty, aerosols and biogeochemical 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 ocean-to-atmosphere interfaces.

Research Team

With over 100 person-years of contributions to CESM, this team developed a modular 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 (SOAs) in global models is crude due to a lack of scientific understanding.

- Sources of marine SOA and primary organic aerosols (POA) are often ignored in 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, including ammonia (NH3), which plays a key role in controlling aerosol and cloud droplet pH;
  - calculating the effect of emissions on the concentration of reactive greenhouse gases (CH4, N2O, HFCs) and ozone depleting chemicals, which affect climate and air quality;
  - constraining other model components through comparison with observations of related isotopic tracers (13C, 210Pb, OC, and CO2).

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 is promising techniques for computational tractable advection.

- We will develop and test new advection schemes by:
  - developing the SciDAC Mesh-Oriented dataAbase (MOAD) technology to extend CSLAM and CDG to unstructured grids in CAM-SE; and
  - applying the same MOAD infrastructure for advection in the MPAS-Ocean and MPAS-Atmosphere dynamical cores.

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 directional fluxes of ammonia (NH3);
  - 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.

Research Team

- 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 incorporations of new biogeochemistry features.

- 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.

Software 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 of 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.

Performance Engineering

- The ACES4BGC model 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 computationally efficient 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.

- The project is just starting. Follow us on the web at http://www.climate modeling.org/aces4bgc/