ACES4BGC

Applying Computationally Efficient Schemes for BioGeochemical Cycles

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Scientific Discovery through Advanced Computing (SciDAC-3)

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The ACES4BGC Project is advancing the predictive capabilities of Earth System Models (ESMs) by reducing two of the largest sources of uncertainty, aerosols and biospheric feedbacks, with a highly efficient computational approach. In particular, this project 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 uncertainties in feedbacks between biogeochemical cycles and the climate system.

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Argonne NATIONAL LABORATORY · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · NCAR NATIONAL CENTER FOR ATMOSPHERIC RESEARCH · Oak Ridge National Laboratory · Pacific Northwest NATIONAL LABORATORY · Sandia National Laboratories

1 Major Accomplishments

Since the project began on April 15, 2012, the ACES4BGC Team has achieved many major accomplishments, which are summarized below.

1.1 Ocean

1.1.1 Organic marine aerosol sources

We have designed and tested, then prepared publications describing, the community's first functionally resolved marine organic chemistry simulator. The concept is to permit ESM simulation of adsorption equilibria, on mixed layer air-water interfaces provided by bubbles and the marine tropospheric interface. These surface chemical relationships determine organic fluxes into sea spray, mediated by global wave-driven bubble breaking. Wave generated particles are a major source of organic material, exerting significant chemical influence on the remote primary aerosol. We have also begun insertion of the new primary organic chemistry scheme into the CAM modal aerosol model, in collaboration with PNNL. At least 6 new ocean biogeochemistry tracers and their reactions are required and must be appended to the relevant ESM modules. In the counterpart atmospheric organic mechanism, several new size modes are required in order to deal with enhanced composition of nascent spray and the evolving remote aerosol system.

1.1.2 Dimethyl Sulfide and OCS

A long-standing DOE marine organosulfur chemistry model has been updated and retested in conjunction with standard BEC ecodynamics, in preparation for global simulations of reduced sulfur flow from the ocean into the atmosphere. Gas phase photochemical reactions then lead to a primary source of OCS, also known as carbonyl sulfide. The molecule is a carbon dioxide analog and tracer of terrestrial photosynthetic uptake. This project follows on earlier SciDAC simulations of the DMS marine aerosol source, but transforms the work into a study of primary production by global vegetation. OCS also happens to be a dominant source of stratospheric sulfate, second only to intermittent volcanic activity.

1.1.3 Citizenship

During the winter Chemistry Climate and Atmospheric Model working groups of CESM, the COSIM ACES4BGC team organized a special session of talks focused on biogenic aerosol sources. The events took place in Boulder Colorado, at the National Center for Atmospheric Research. A joint session summary was presented by COSIM representatives at the invitation of J.F. Lamarque, in order to bring the collected information together for the benefit of the full community. ACES4BGC research was highlighted during this series of meetings.

1.2 Land

1.2.1 Carbonyl sulfide (COS) parameterization

An initial implementation for the biosphere uptake of carbonyl sulfide (COS) was implemented into CLM4. COS provides a potentially powerful tracer for biosphere-atmosphere exchange of CO_2 and a constraint on global gross primary production. This implementation was tested in offline simulations by Wenting Fu during the summer of 2012. Leaf relative uptake (LRU) and ecosystem relative uptake (ERU) were analyzed. The model provided reasonable estimates of global canopy

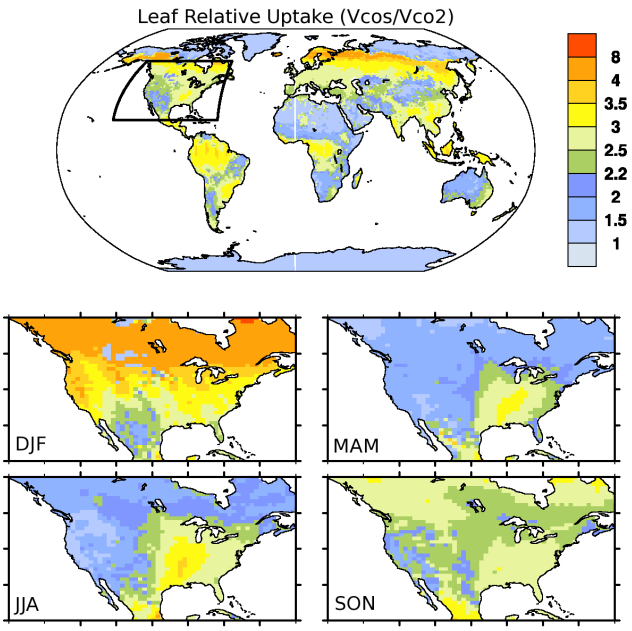

Figure 1: The spatial distribution of leaf relative uptake (LRU), the ratio of the deposition velocities of COS and CO_2, from the initial implementation of COS uptake in CLM4.

and soil uptake of COS as compared to previous studies. The global mean estimation of LRU was 2.28, which compares well with previous model studies (2.2), but differs from chamber studies (1.61 ± 0.26).

1.2.2 Toward an improved photosynthesis model

The photosynthesis model of Farquhar, von Caemmerer and Berry is an important method for predicting the response of plants to climate change. The critical parameters required by the model can be obtained from leaf-level measurements of gas exchange at saturating light conditions, namely the A-C_i curves. To improve the accuracy of A-C_i curve-fitting analysis, we investigated the potential of using multiple A-C_i curves at subsaturating light intensities to more accurately produce important parameter estimates in the over-parameterized photosynthesis model. Mesophyll conductance is not accounted for in the standard model, but has recently been shown to have a statistically significant impact on predictions of terrestrial carbon accumulation under increasing atmospheric CO_2 levels. New curve-fitting methods were tested, accounting for mesophyll conductance, and the resulting parameter sets were tested in simulations of the CLM4.5 photosynthesis algorithm. On-going analyses are being conducted to understand the sensitivity of gross primary production to optimal parameter sets, and constraints on those parameters are being investigated.

1.2.3 CESM1-BGC Simulations

Concentration- and emissions-forced historical (1850–2005) and RCP 8.5 (2006–2100) simulations at $0.9° \times 1.25°$ resolution following the CMIP5 protocol are being performed on Titan at the OLCF using the CESM1-BGC model configuration. These simulations provide an additional ensemble member to complement the single run performed by the CESM Biogeochemistry Working Group (BGCWG) for IPCC AR5, provide a baseline model configuration for testing SUPER performance optimization strategies and from which to compare simulations utilizing improvements

across component models from this project, and provide a set of runs from which feedback sensitivity analyses will be performed in conjunction with collaborators in the RGCM Carbon-Climate Feedbacks Project.

1.2.4 Extended Concentration Pathway (ECP) 8.5 emissions forcing data set

A new emissions forcing data set was developed for use with the CESM1-BGC model configuration for extending the RCP 8.5 simulations from year 2100 to year 2500. In the protocol offered by Meinshausen et al. (2011), the extended RCP 8.5 emissions become constant after 2100, then concentrations become constant after 2250 with a smooth transition of emissions between 2150 and 2250. For ECP 8.5, the atmospheric CO_2 mole fraction reaches 1962 ppm at year 2250 and is held steady thereafter. We developed a $0.9^\circ \times 1.25^\circ$ gridded global monthly fossil CO_2 emissions flux ($\mathrm{kg\,CO_2\,m^{-2}\,s^{-1}}$) data set consistent with this protocol for use in millennial-scale emissions-forced simulations to be conducted by the CESM BGCWG and this project.

1.3 Atmospheric Chemistry and Aerosols

Atmospheric chemistry deals with the fate and transport of chemicals emitted to the atmosphere by both anthropogenic and natural sources. These chemicals can impact the planet through aerosols and reactive greenhouse gases (which may be easier to mitigate than carbon dioxide), and as components of chemical smog, the ozone layer, and acid rain.

Aerosols are tiny particles that float on the winds. They contribute to bad air-quality, and affect climate directly by reflecting sunlight, as well as indirectly by changing cloud properties. Aerosols can either be emitted directly into the atmosphere (primary aerosols), or be created through the action of atmospheric chemistry on precursor gases that are emitted from natural and anthropogenic sources (secondary aerosols).

1.3.1 Coupling atmospheric chemistry to other Earth system components

In the first year and a half of this project:

1. We have merged our super-fast chemistry mechanism with our standard modal aerosol model (MAM3). We have worked with the CESM working groups and the CESM repository gatekeepers, and this is now a standard capability in the CESM model code. It will become generally available with the next CESM release.

2. We have worked to get the LLNL sectional aerosol model (SECT, developed under the Atmospheric Science Research Program) incorporated into the main CESM model version, since it offers a more detailed representation of aerosol processes than the MAM models. The code has been accepted scientifically by the Chemistry-Climate Working Group, and was scheduled to be merged into the main CESM version in two stages, since it involved a large amount of code. The first stage has been successfully implemented, and we are now waiting for a "merge slot" for the second stage to be added to the CESM trunk.

3. We have continued to participate in the Chemistry Climate Modeling Initiative, which is intercomparing the performance and predictions of multiple chemistry climate models, including CESM with our super-fast chemistry mechanism. Such intercomparisons are important for validating our model, and are usually very productive scientifically. The last round involved us in 10 journal publications.

4. We are currently coupling our new superfast-MAM3 atmospheric chemistry-aerosol scheme to the ocean sulfur and aerosol schemes discussed in Section 1.1. This will allow us to study the impact of the sulfur cycle on clouds, as well as simulate carbonyl sulfide (OCS), which we will couple to the land biogeochemical model to constrain the photosynthesis in the model (a key process whose sensitivity is one of the biggest uncertainties in climate predictions). The importance of dimethyl sulfide emissions to climate is illustrated in Figure 2.

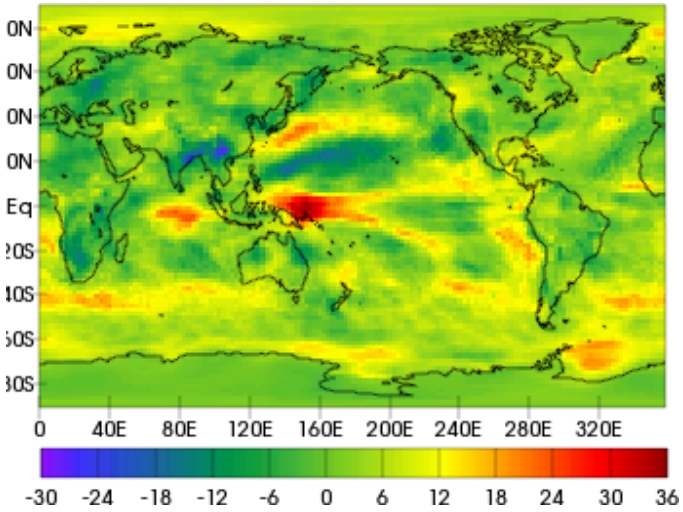

Figure 2: The impact of dimethyl sulfide on the annual mean amount of solar energy reaching the surface of the Earth in W/m^2, as calculated by our model. The global mean difference is 3.5 W/m^2 of cooling, most of which is the result of indirect effects of the sulfate aerosols on clouds. This is comparable to the radiative forcing of all the greenhouse gases combined, in spite of the fact that the other aerosol types are included and will compete with sulfate as cloud condensation nuclei. NOTE: This result is only illustrative, since it is the difference between the present-day climate and the same simulation without any DMS, which is not a plausible state. Nonetheless, our previous work (Cameron-Smith, et al., GRL 2011) has shown that regional changes in DMS emissions can be large, and we will be able to calculate the actual climate impact once the coupling to the ocean is validated.

Because of the computational cost of advecting the tracers for atmospheric chemicals and aerosols, especially at high resolution, the new advection scheme being developed by this project (Section 1.4) is critical to future progress. It is also critical that the advection scheme conserves tracer mass without producing spikes in tracer concentrations, so we are working with the advection development team to ensure this is satisfied. To help explore and constrain the many uncertainties in the chemical and aerosol system, we are also working closely with the UQ team on their recent simulations (Section 1.7).

1.3.2 Representation of secondary organic aerosols (SOA) using the VBS-MAM approach in CAM5

We implemented a new modeling framework using the modified volatility basis set (VBS-MAM) approach coupled to the modal aerosol module with three log-normal modes (MAM3) to improve SOA treatment within the CESM model. In this work, we replaced the previous crude treatment of SOA with an advanced SOA parameterization that includes 174 advected chemical tracers including 68 SOA gas and particle tracers. We quantified SOA formation from three different source

categories: fossil (anthropogenic), biomass burning, and biogenic emission. We implemented daily fire emissions in CAM5 using the Global Fire Emissions Database version 3.1 (GFED3.1) and constrained the model towards observed meteorological states (re-analysis) using the nudging method. This VBS-MAM approach is flexible enough for addition of new SOA species, and represents multi-generational gas-phase chemistry of organic precursors including both functionalization reactions (reducing volatility) and fragmentation reactions (increasing volatility). Results show large changes in the horizontal and vertical distribution of SOA loadings compared to the previous crude SOA treatment in MAM. The improved treatment better resolves the natural vs. human sources of SOA formation and is essential to understand the aerosol effects on clouds and global biogeochemical cycles. Simulation results will be evaluated with organic aerosol (OA) measurements using the Aerosol Mass Spectrometer (AMS) at different locations representative of each of the three major source categories (e.g., Manaus, Brazil, characterized by strong biogenic SOA formation, and Welgegund, Africa, characterized by large biomass burning sources).

1.3.3 Implementation of two new marine organic modes to represent marine organic aerosols

Collaborating with Scott Elliott, we have been implementing two new marine organic modes (MOM) on top of the 7-mode version of MAM (MAM7) to represent the marine organic aerosols in the Aitken- and accumulation-mode size range. There are five primary organic compounds in each MOM: polysaccharide, protein, lipid, humics, and fulvic acid, which generally have lower hygroscopicities than sea salt. By the aerosol microphysics (condensation and coagulation) these marine organic compounds will be transferred to the other modes in MAM7 (i.e., Aitken, accumulation and primary carbon mode). We are planning to examine the effects of the MOM on clouds and climate.

1.3.4 Anthropogenic warming exacerbated by the decrease of global dimethyl sulphide (DMS) emissions

In Six et al. (2013), we found that global dimethyl sulphide (DMS) emissions decrease by about 18($\pm$3)% in 2100 compared with pre-industrial times as a result of the combined effects of ocean acidification and climate change. This study indicates that ocean acidification has the potential to exacerbate anthropogenic warming in the future. We are currently preparing a manuscript describing the new SOA treatments using the VBS-MAM approach.

1.4 Atmosphere and Ocean Advection

Our advection work focuses on multi-tracer efficient characteristic-based methods in both the atmosphere and ocean on fully unstructured grids in spherical geometry. We are considering both incremental remap and optimization based reconstructions.

1.4.1 Mesh tools for advection support

In the first year, as part of upgrading the advection schemes used in atmospheric and ocean components, CAM-SE and MPAS, developments were made in the common infrastructure related to the computations of the backward trajectories and the intersection of the unstructured meshes on the sphere. CAM-SE refers to CAM running with the spectral finite element dynamical core from the High Order Method Modeling Environment (HOMME), and MPAS refers to both the atmosphere and ocean models developed by the Model for Prediction Across Scales collaboration.

Cell integrated semi-Lagrangian transport methods need a deformation step, where an Eulerian grid is tracked upstream to a departure (source) grid, and a remapping step, where tracer fields are remapped onto the source grid to give the updated tracers in each cell.

The infrastructure for remapping involves intersection of departure and arrival meshes and an integration/normalization step. The intersection of arbitrary meshes on a sphere or in a plane was fully implemented in the MOAB library. It supports different element types, triangle, quads or polygons, and it is designed to allow CFL numbers greater than 1.

Support for fully unstructured variable resolution grids was extended for loading, querying, and communicating meshes and related data in parallel. Efficient processing in parallel was demonstrated on MPAS data files with 65M cells and 130M vertices, using repartitioning and renumbering of mesh entities to achieve a better data locality. The intersection algorithm was run on this model on 1024 processes on a Leadership Class machine (fusion.lcrc.anl.gov) and it showed good scalability. Figure 3 shows a typical partition in an MPAS model, and the result of the intersection algorithm on one of the partitions.

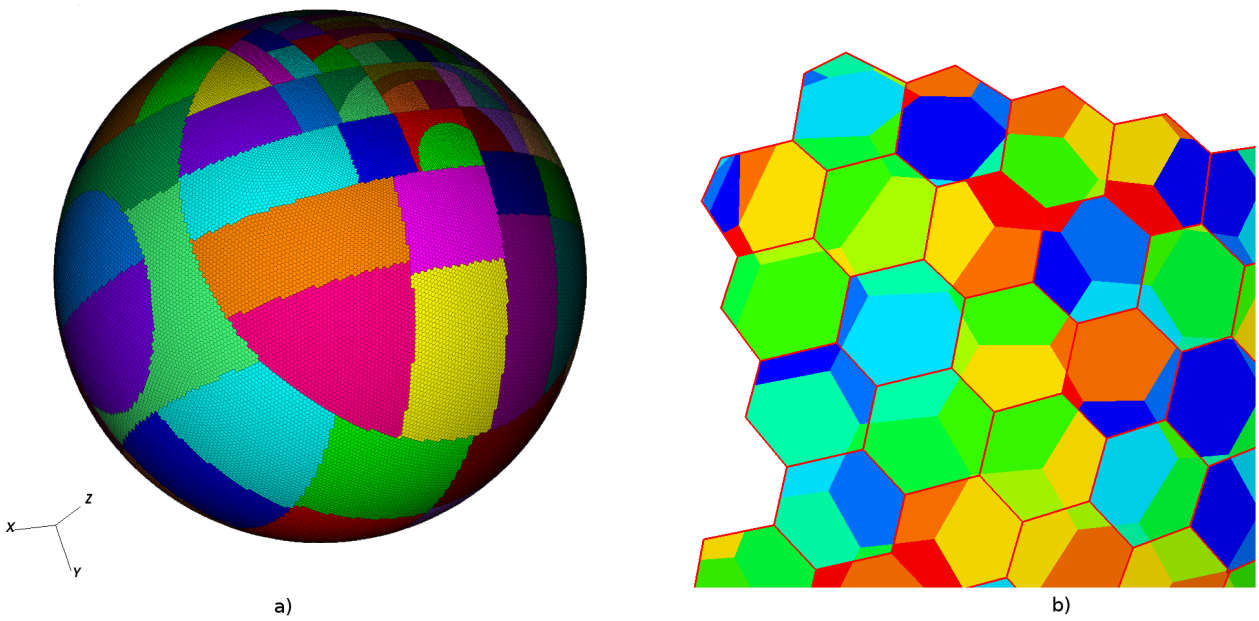

Figure 3: (a) An example of a MPAS variable resolution grid, partitioned; (b) Intersection of departure and arrival grids.

The departure points can be found by back-tracing the velocity characteristics of the vertices of each cell in the mesh, over the prescribed time step. A simple one step Taylor approximation was implemented as part of MOAB, while the interface to allow user-calculated departure points was put in place: the client can specify departure points by defining a tag on the arrival mesh.

Example drivers for mesh intersection and advection were demonstrated for benchmark problems for which an analytical solution was known, and for which the departure mesh can be computed exactly too.

The library allows support for larger CFL numbers, limited only by solver convergence considerations.

1.4.2 HOMME/CSLAM on unstructured grids

We have completed this initial integration of CSLAM into HOMME. This work was in partnership with the University-lead SciDAC project, *Chemistry in CESM-SE: Evaluation, performance and optimization,* (PI J. F. Lamarque). That project integrated the CSLAM reconstruction algorithm for the cubed-sphere grid into HOMME, while we developed a spectral element based departure grid algorithm. The combination of these two technologies allows us to run the CSLAM algorithm in HOMME for CFL < 1. Our departure grid algorithm is based on a Runge-Kutta / Taylor series approach. This new approach avoids the iterative nature of typical departure grid algorithms and instead makes use of the high-order spectral element representation of the velocities. Given the spectral element representation of the velocity at individual timesteps, we use Taylor series to approximate the velocity at arbitrary points in space and time, coupled to a RK2 algorithm to march backwards in time from the arrival grid in order to determine the departure grid. Our next steps will be to couple this algorithm with MOAB to allow for CFL > 1, and then to extend the CSLAM reconstruction algorithm to support unstructured grids.

To use these algorithms in CAM, we also need mass / tracer mass *consistency*, meaning that a tracer that is initialized the same as the atmosphere density (i.e., a mixing ratio of 1), should remain equal to the density as the flow evolves in the absence of sources or sinks. We are pursing two approaches for achieving consistency: the first is converting CSLAM to flux form, and then if the tracers are advected with the mean flux from the dynamics they will be consistent. The second approach is to add a small flux correction to either the tracers of the dynamical evolution of density which will maintain consistency.

1.4.3 Optimization-based Transport

We are also pursing an optimization based approach to transport. This is a relatively new approach which has not yet been tried for atmospheric or oceanic flows. It is promising because it avoids the need to compute mesh intersections, but at the expense of introducing iterative algorithms which require global reductions.

The optimization-based strategy for advection utilizes optimization and control ideas to formulate conservative and bound-preserving solutions to the transport equation. To apply this strategy we first define a target that is a stable and accurate solution to the advection equation, but which may not satisfy local bounds or conservation. We then minimize the distance between the target and the final solution in a suitable norm and enforce bounds and conservation through the optimization constraints. This procedure ensures that the solution is globally optimal with respect to the target and possesses the desired physical properties.

The strategy has been further developed in two directions this year. First, a new semi-Lagrangian spectral element optimization-based transport scheme has been implemented in HOMME. In this scheme the target solution is defined by mapping nodal values to points determined by Lagrangian backward trajectories using the high-order spectral element basis. This solution can be computed very efficiently, but is not conservative or bounds preserving. The optimization strategy is then used to determine the best fit solution that satisfies conservation and bounds constraints. Initial evaluation of the scheme for standard advection tests has begun. Additionally, a prototype incremental remap and optimization-based transport scheme for multiple tracers has been developed. In this scheme, the target solution is computed by integrating a linear tracer reconstruction over swept regions defined by Lagrangian nodal trajectories.

1.5 Computational Tools and Performance

Enhanced performance data collection and archive logic for production runs of the Community Earth System Model (CESM), co-developed with the SciDAC3 SUPER Institute, was implemented in versions of the CESM being used for production runs on the Cray XK7 (Titan) at the Oak Ridge Leadership Computing Facility (OLCF). The same performance data collection capability is also available for runs on the Cray XC30 (Edison) and the Cray XE6 (Hopper) at the National Energy Research Scientific Computing Center (NERSC) and on the BG/Q (Mira) in the Argonne Leadership Computing Facility (ALCF).

Based on the data collected and on further experimentation it was determined how to improve performance on Titan by a factor of 1.6 at the cost of only 1.1 times more processors for a long running suite of production runs, resulting in a savings in allocation and an increase in productivity.

We also evaluated performance of other relevant configurations of the CESM on Edison, Hopper, and Titan. In particular, we collected performance baselines for the Community Atmosphere Model (CAM) using the CAM5 physics and the spectral element dynamical core in preparation for evaluating the capabilities of the new tracer advection schemes under development.

In joint work with SUPER, kernels from MOAB used in the development of the new tracer advection capability were provided to SUPER for further investigation, and performance analysis of some preliminary algorithm options conducted.

1.6 Software Engineering

The software engineering tasks, led by partners at NCAR, focused on aerosol model implementation, build system and script changes, coupler enhancements for biogeochemical tracers, and a series of improvements to the Community Land Model (CLM) code and testing as described below.

1.6.1 Aerosol model

We updated the LLNL sectional aerosol code to a recent version of the CAM trunk, and checked it in to a branch of the CESM Subversion repository. We have attempted to reduce the numerous CPP directives used to embed the aerosol model specific code. In addition, the code has undergone initial code reviews by CAM software engineers. These reviews have identified the need for a cleaner interface between CAM chemistry and aerosol models, which should be implemented in the future.

We began work with Xiaohong Liu (formerly at PNNL) to implement a new 4-modal version of the modal aerosol module (MAM4) for CAM. MAM4 adds a new primary carbon mode to the default aerosol scheme in CESM1 to better treat the aging of organic aerosol and black carbon from sources to remote areas. In the future, NCAR scientists and software engineers will provide a generic interface for aerosol optical properties for MAM4.

1.6.2 CESM Build system and scripts

We enhanced the CESM build system in a number of ways that will contribute to this project. First, we have made it easier to bring in C++ code. Second, we have made it easier to bring in external libraries, especially those written in C++. And third, we have added capabilities to facilitate performance tuning on LCF platforms.

We refactored the CESM scripts to be able to address the growing complexity of the model system and thereby facilitate adding new model configurations (component sets) and new model grids (including new statically refined grids).

1.6.3 Coupler enhancements for tracers

We finalized enhancements to the CESM coupler that make it easier to add new tracers that are exchanged between components. New tracers can now be added as namelist items, without having to change any coupler code. Previously, coupler code needed to be modified any time a new exchange of fields between components was introduced.

1.6.4 Land model improvements

We separated the River Transport Model (RTM) component from CLM and introduced it as a separate component at the driver level. This will facilitate the introduction of new parameterizations of surface flow and transport of chemical species, which is a key need for this project. It will also permit for the first time testing different river transport schemes with a data land model, something that was not possible when the RTM was embedded in CLM.

We fixed a number of threading bugs in the CLM code, which had prevented the latest CLM version (CLM4.5) from running multi-threaded. In addition, we developed and applied coding conventions that will help ensure that CLM continues to work properly in a threaded environment. These fixes will enable better coupled model performance than was previously possible.

We introduced the first unit tests into the CLM source code. We are now gradually expanding the set of modules covered by unit tests, complementing the existing CESM system tests. This unit test framework will allow bringing in new code with greater confidence and fewer bugs.

We introduced the capability to regrid CLM initial conditions at runtime. Previously, the procedure for interpolating CLM initial conditions to the resolution of interest confused many users. Now this can be done much more simply, through a single CLM namelist setting. This capability will also facilitate online regridding capabilities in the future.

1.7 Uncertainty Quantification

The application of UQ to biogeochemistry in the CESM presents a number of unique challenges, including the complexities of conducting statistical analyses in very high dimensional UQ spaces (i.e., 100 or more dimensions) and the added computational burden of simulating biogeochemical cycles. To overcome these challenges, we have developed a UQ ensemble framework (SCAM-UQ) that runs large numbers of concurrent single column CAM simulations on high performance computers, and that uses Monte Carlo-based schemes to propagate uncertainties from biogeochemical and physical processes through the system. We have run preliminary ensembles using SCAM-UQ with active MOZART chemistry and CAM5 physics to test the effects of two classes of model uncertainties (physical and biogeochemical parameters) on the vertical distribution of chemical tracers. The preliminary ensembles account for uncertainties in the relative humidity threshold for low level clouds (*rhminl*), the deep convection precipitation efficiency (*ke*), and the A-factor and activation energy of the rate constant for the chemical reaction $O + O_3 \rightarrow 2\ O_2$. The results from the preliminary ensembles are promising. The right hand side in Fig. 4 shows the distribution of vertical profiles of ozone simulated using a 50-member Latin Hypercube ensemble that sampled uncertainties in *rhminl* and *ke*. Uncertainties in these parameters alone induce a 10% spread in the simulated O_3 mole fraction. We fully expect that the uncertainty in O_3 and other tracers will increase significantly as additional sources of model uncertainty are added. Toward this goal, we have since implemented many new UQ parameters in the system, bringing the total, so far, to 75 parameters (64 parameters for 32 reactions in the MOZART chemical mechanism, and 11 parameters in various CAM5 physics packages). Using this newly-developed capability, we will run massive SCAM-UQ ensembles with $\sim 10^4$ ensemble members to quantify uncertainties in the production

and loss of pollutants and aerosols (see Fig. 4), and to test new methods for high dimensional UQ systems under development by QUEST.

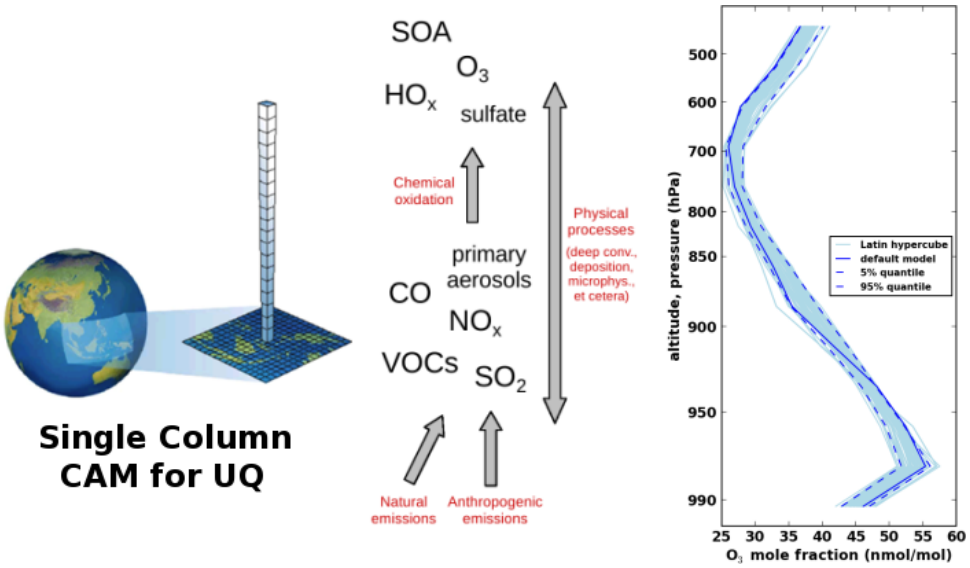

Figure 4: An ensemble-based single column atmosphere model framework (SCAM-UQ) with active MOZART chemistry and CAM5 physics has been developed to quantify uncertainties in high dimensional biogeochemical cycles.

2 Publications, Presentations, and Symposia

2.1 Journal Papers

Ogunro, O., S. Burrows, **S. Elliott**, A. Frossard, R. Letscher, J. K. Moore, L. M. Russell and O. Wingenter, Distribution and surface activity of macromolecules in offline simulations of marine organic chemistry, *Adv. Meteorol.*, to be submitted February 2014.

Burrows, S., O. Ogunro, P. Rasch and **S. Elliott**, A framework for modeling organic fractionation of the sea spray aerosol, *Atmos. Chem. Phys.*, submitted January 2014.

P. Lauritzen et al. (including **M. A. Taylor**) (2014), A standard test case suite for two-dimensional linear transport on the sphere: results from a collection of state-of-the-art schemes, *Geosci. Model Dev.*, to appear.

O. Guba, **M. A. Taylor**, A. St.Cyr (2014), Optimization based limiters for the spectral element method, *J. Comput. Phys.*, in review.

Elliott, S., S. Burrows, C. Deal, **X. Liu**, O. Ogunro and L. M. Russell, Prospects for the simulation of surfactant chemistry in Marine Systems Models, *Environ. Res. Lett.*, submitted August 2013.

Hoffman, Forrest M., James T. Randerson, Vivek K. Arora, Qing Bao, Katharina D. Six, Patricia Cadule, Duoying Ji, Chris D. Jones, Michio Kawamiya, Samar Khatiwala, Keith Lindsay, Atsushi Obata, Elena Shevliakova, Jerry F. Tjiputra, Evgeny M. Volodin, and Tongwen Wu (2013), Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, *J. Geophys. Res. Biogeosci.*, in press. DOI:10.1002/2013JG002381.

P. Bochev, D. Ridzal, K. Peterson (2014) Optimization-based remap and transport: a divide and conquer strategy for feature-preserving discretizations, *J. Comput. Phys.*, 257(Part B):1113–1139. DOI:10.1016/j.jcp.2013.03.057.

Eyring, V., I. Cionni, J. Arblaster, J. Sedlacek, J. Perlwitz, P. Young, S. Bekki, **D. Bergmann**, **P. Cameron-Smith**, W. Collins, G. Faluvegi, K.-D. Gottschaldt, L. Horowitz, D. Kinnison, J.-F. Lamarque, D. R. Marsh, D. Saint-Martin, D. Shindell, K. Sudo, S. Szopa, S. Watanabe (2013), Long-term changes in tropospheric and stratospheric ozone and associated climate impacts in CMIP5 simulations, *J. Geophys. Res.*, 118(10), 5029–5060, DOI:10.1002/jgrd.50316.

Meskhidze, N., with **S. Elliott** and 42 others (2013), Production mechanisms, number concentration, size distribution chemical composition and optical properties of sea spray aerosols, *Atmos. Sci. Lett.*, in press.

Keppel-Aleks, Gretchen, James T. Randerson, Keith Lindsay, Britton B. Stephens, J. Keith Moore, Scott C. Doney, Peter E. Thornton, Natalie M. Mahowald, **Forrest M. Hoffman**, Colm Sweeney, Pieter P. Tans, Paul O. Wennberg, and Steven C. Wofsy (2013), Atmospheric Carbon Dioxide Variability in the Community Earth System Model: Evaluation and Transient Dynamics During the Twentieth and Twenty-First Centuries. *J. Clim.*, 26(13):4447–4475. DOI:10.1175/JCLI-D-12-00589.1.

Mann G. et al. (including **X. Liu**) (2013), Intercomparison and evaluation of aerosol microphysical properties among AeroCom global models of a range of complexity, *Atmos. Chem. Phys. Disc.*, 13, 30841–30928. DOI:10.5194/acpd-13-30841-2013.

Mao, J., X. Shi, P. E. Thornton, **F. M. Hoffman**, Z. Zhu, and R. B. Myneni (2013), Global Latitudinal-Asymmetric Vegetation Growth Trends and Their Driving Mechanisms: 1982–2009, *Remote Sens.*, 5(3):1484–1497. DOI:10.3390/rs5031484.

Jiao, C., et al. (including **X. Liu**) (2013), An AeroCom assessment of black carbon in Arctic snow and sea ice, *Atmos. Chem. Phys. Disc.*, 13, 26217–26267, DOI:10.5194/acpd-13-26217-2013.

Hu, N., and **X. Liu** (2013), A modeling study of the effect of anthropogenic aerosols on drought in the late spring of south China, *Acta Meteorologica Sinica*, 27(5):701–715, DOI:10.1007/s13351-013-0506-z.

Todd-Brown, K. E. O., J. T. Randerson, W. M. Post, **F. M. Hoffman**, C. Tarnocai, E. A. G. Schuur, and S. D. Allison (2013), Causes of Variation in Soil Carbon Simulations from CMIP5 Earth System Models and Comparison with Observations, *Biogeosci.*, 10(3):1717–1736. DOI:10.5194/bg-10-1717-2013.

Jiang, Y., **X. Liu**, X.-Q. Yang, and M. Wang (2013), Effects of anthropogenic aerosols on East Asian summer clouds and precipitation with Community Atmospheric Model version 5, *Atmos. Environ.*, 70, 51–63, DOI:10.1016/j.atmosenv.2012.12.039.

Long, M. S., W. C. Keene, **R. Easter**, R. Sander, A. Kerkweg, D. Erickson, **X. Liu**, and S. J. Ghan (2013), Implementation of the chemistry module MECCA (v2.5) in the modal aerosol version of the Community Atmosphere Model component (v3.6.33) of the Community Earth System Model, *Geosci. Model Dev.*, 6, 255–262, DOI:10.5194/gmd-6-255-2013.

Samset, B. H., Myhre, G., Schulz, M., Balkanski, Y., Bauer, S., Berntsen, T. K., Bian, H., Bellouin, N., Diehl, T., **Easter, R. C.**, Ghan, S. J., Iversen, T., Kinne, S., Kirkevåg, A., Lamarque,

J.-F., Lin, G., **X. Liu**, Penner, J., Seland, Ø., Skeie, R.B., Stier, P., Takemura, T., Tsigaridis, K., and Zhang, K. (2013), Black carbon vertical profiles strongly affect its radiative forcing uncertainty, *Atmos. Chem. Phys.*, 12, 2423–2434, DOI:10.5194/acp-13-2423-2013.

Shindell, D. T., Lamarque, J.-F., Schulz, M., Flanner, M., Jiao, C., Chin, M., Young, P., Lee, Y. H., Rotstayn, L., Milly, G., Faluvegi, G., Balkanski, Y., Collins, W. J., Conley, A. J., Dalsoren, S., **Easter, R.**, Ghan, S., Horowitz, L., **X. Liu**, Myhre, G., Nagashima, T., Naik, V., Rumbold, S., Skeie, R., Sudo, K., Szopa, S., Takemura, T., Voulgarakis, A., and Yoon, J.-H. (2013), Radiative forcing in the ACCMIP historical and future climate simulations, *Atmos. Chem. Phys.*, 13, 2939–2974, DOI:10.5194/acp-13-2939-2013.

Myhre, G., et al. (including **X. Liu**) (2013), Radiative forcing of the direct aerosol effect from AeroCom Phase II simulations, *Atmos. Chem. Phys.*, 13, 1853–1877, DOI:10.5194/acp-13-1853-2013.

Long, M. S., W. C. Keene, **R. C. Easter**, R. Sander, **X. Liu**, A. Kerkweg, and D. Erickson (2013), Sensitivity of tropospheric chemical composition to halogen-radical chemistry using a fully coupled size-resolved multiphase chemistry/global climate system I: Halogen distributions, aerosol composition, and sensitivity of climate-relevant gases, *Atmos. Chem. Phys. Discuss.*, 13, 6067–6129. DOI:10.5194/acpd-13-6067-2013.

Six K. D., S. Kloster, T. Ilyina, S. D. Archer, **K. Zhang**, and E. Maier-Reimer (2013), Global warming amplified by reduced sulfur fluxes as a result of ocean acidification, *Nature Climate Change*, 3(11):975–978.DOI:10.1038/NCLIMATE1981.

Lucas, D. D., Klein, R., Tannahill, J., Ivanova, D., Brandon, S., Domyancic, D., and Zhang, Y. (2013), Failure analysis of parameter-induced simulation crashes in climate models, *Geosci. Model Dev.*, 6, 1157-1171, DOI:10.5194/gmd-6-1157-2013.

B. D. Santer , J. Painter, C. Mears, C. Doutriaux, P. Caldwell, J. M. Arblaster, **P. Cameron-Smith**, N. P. Gillett, P. J. Gleckler, J. R. Lanzante, J. Perlwitz, S. Solomon, P. A. Stott, K. E. Taylor, P. W. Thorne, M. F. Wehner, F. J. Wentz, T. M. L. Wigley, and C.-Z. Zou (2013), Identifying human influences on atmospheric temperature, *Proc. Nat. Acad. Sci.*, 110(1):26–33. DOI:10.1073/pnas.1210514109.

Luo, Y. Q., J. T. Randerson, G. Abramowitz, C. Bacour, E. Blyth, N. Carvalhais, P. Ciais, D. Dalmonech, J. B. Fisher, R. Fisher, P. Friedlingstein, K. Hibbard, **F. Hoffman**, D. Huntzinger, C. D. Jones, C. Koven, D. Lawrence, D. J. Li, M. Mahecha, S. L. Niu, R. Norby, S. L. Piao, X. Qi, P. Peylin, I. C. Prentice, W. Riley, M. Reichstein, C. Schwalm, Y. P. Wang, J. Y. Xia, S. Zaehle, and X. H. Zhou (2012), A Framework for Benchmarking Land Models, *Biogeosci.*, 9(10):3857–3874. DOI:10.5194/bg-9-3857-2012.

P. H. Lauritzen, W. C. Skamarock, M. J. Prather, **M. A. Taylor** (2012), A standard test case suite for two-dimensional linear transport on the sphere, *Geosci. Model Dev.*, **5**:887–901.

2.2 Reports

M. A. Taylor and P. Ullrich (2014), *Spectral Element Subcell Flux*, Sandia National Laboratory Technical Report, SAND no. (to be assigned).

2.3 Presentations

- **Elliott, S.**, et al., Distribution and surface activity of macromolecules in offline simulations of marine organic chemistry, Chemistry Department seminar (January 2014), New Mexico Institute of Mining and Technology, Socorro NM, USA.

- Wang, Yingping, et. al., (including **Forrest M. Hoffman**), Theoretical analysis of the global land carbon cycle: what determines the trajectory of future carbon uptake? 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract B51L-02.

- Mu, Mingquan, **Forrest M. Hoffman**, et al., Design and development of a community carbon cycle benchmarking system for CMIP5 models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract H33B-1356.

- Hargrove, William W., Jitendra Kumar, Kevin M. Potter, and **Forret M. Hoffman**, Global Tree Range Shifts Under Forecasts from Two Alternative GCMs Using Two Future Scenarios, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract B32D-06.

- Lawrence, David M., et al. (including **Forrest M. Hoffman**), Development and application of a benchmarking system for land models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract H32G-01. *Invited.*

- Mills, Richard T., et al. (including **Forrest M. Hoffman**), Development of a Process-Rich Modeling Framework for Arctic Ecohydrology Using the Open-Source PFLOTRAN and CLM models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract DI31A-2207.

- **Hoffman, Forrest M.**, et al., Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract B13M-07. *Invited.*

- Fu, Wenting, Lianhong Gu, and **Forrest M. Hoffman**, Advantages of estimating parameters of photosynthesis model by fitting A-C_i curves at multiple subsaturating light intensities, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA. Abstract B13D-0543.

- **Taylor, M. A.**, The spectral element dynamical core in the Community Atmosphere Model, 66th Annual Meeting of the APS Division of Fluid Dynamics (November 2013), Pittsburgh, Pennsylvania, USA. *Invited.*

- **Taylor, M. A.**, The Spectral Finite Element Dynamical Core in The Community Atmosphere Model, 2013 KIAPS International Symposium and Science Advisory Committee Meeting (October 2013), Seoul, Korea. *Invited.*

- **Elliott, S.**, et al., Should the CESM ocean resolve marine biogenics? Pacific Northwest National Laboratory (invitation declined), Pacific Northwest National Laboratory (August 2013), Richland WA, USA.

- **Hoffman, Forrest M.**, Pavel B. Bochev, Philip J. Cameron-Smith, Richard C. Easter, Jr., Scott M. Elliott, Iulian Grindeanu, Oksana Guba, Xiaohong Liu, Robert B. Lowrie,

Donald D. Lucas, Richard T. Mills, William J. Sacks, Timothy J. Tautges, Mark A. Taylor, Mariana Vertenstein, and Patrick H. Worley, Enhancing Global Biogeochemical Cycles in the Community Earth System Model, Scientific Discovery through Advanced Computing (SciDAC-3) Principal Investigators Meeting (July 24–26, 2013), Rockville, Maryland, USA.

- **Taylor, M. A.**, et al., New algorithms and SciDAC tools for scalable monotone transport schemes in the Community Earth System Model, DOE SciDAC-3 PI Meeting (July 2013), Rockville, Maryland, USA. *Invited.*

- **Liu, X.**, and **K. Zhang**, Assessing Aerosol Indirect Effect Through Ice Clouds with Two Global Climate Models, Asia Oceania Geosciences Society (AOGS) 10^{th} Annual Meeting (June 24–28, 2013), Brisbane, Australia.

- Burrows, S. with **S. Elliott**, **X. Liu**, et al., A framework for modeling organic fractionation of the sea spray aerosol, 18^{th} CESM Workshop (June 17–20, 2013), Breckenridge, Colorado, USA.

- Ogunro, O. with **S. Elliott**, S. Burrows, et al., Distribution and surface activity of macromolecules in offline simulations of marine organic chemistry, SOLAS annual summer meeting (June 2013), Xiamen, PRC.

- **Hoffman, Forrest M.**, et al., Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, oral presentation at the 9^{th} International Carbon Dioxide Conference (ICDC9) (June 3–7, 2013), Beijing International Conference Center, Beijing, China.

- **Hoffman, Forrest M.**, et al., Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, poster presentation #285 at the 9^{th} International Carbon Dioxide Conference (ICDC9) (June 3–7, 2013), Beijing International Conference Center, Beijing, China.

- **Peterson, K.**, P. Bochev, D. Ridzal, Optimization-based conservative transport on the cubed-sphere grid (June 2013), 9th International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria.

- **Elliott, S.** et al., Should the CESM ocean resolve marine biogenics? Presented at Scripps Institute of Oceanography (April 2013), La Jolla CA, USA. *Invited.*

- **Hoffman, F. M.**, et al., The Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, Climate 2013: Next Generation Climate Models and Knowledge Discoveries through Extreme High-Performance Simulations and Big Data Workshop (March 20–22, 2013), Lawrence Berkeley National Laboratory, Berkeley, California, USA.

- **Taylor, M. A.**, et al., The Community Atmosphere Model's cubed-sphere spectral-element configuration, SIAM CS&E (February 2013), Boston, MA, USA.

- **Taylor, M. A.**, et al., CAM-SE Development Updates, Atmosphere Model Working Group (February 2013), National Center for Atmospheric Research, Boulder, Colorado, USA.

- **Philip Cameron-Smith, Don Lucas, ACES4BGC team**, Applying Computational Efficient Schemes for Biogeochemistry (ACES4BGC), CESM Chemistry-Climate Working Group

Winter Meeting (February 2013) National Center for Atmospheric Research, Boulder, Colorado, USA. `http://www.cesm.ucar.edu/working_groups/Chemistry/Presentations/2013/cameronsmith1.pdf`

- **Elliott, S. M.**, et al., Developing Primary Organic Aerosol Emissions from POP, CESM Chemistry-Climate Working Group Winter Meeting (February 2013), National Center for Atmospheric Research, Boulder, Colorado, USA.

- **Elliott, S. M.**, et al., Overview of the CESM Aerosol Symposium, Joint Chemistry-Climate / Atmosphere Model / Polar Climate Working Groups Winter Meeting (February 2013), National Center for Atmospheric Research, Boulder, Colorado, USA.

- **Hoffman, F. M.**, et al., The Causes and Implications of Persistent Atmospheric Carbon Dioxide Biases in Earth System Models, Community Earth System Model (CESM) Joint Land Model Working Group and Biogeochemistry Working Group Meeting (February 19–22, 2013), National Center for Atmospheric Research (NCAR), Boulder, Colorado, USA.

- **Liu, X.**, et al., Simulations of Global Impact of Dust Speciation on Mixed-Phase Clouds Through Ice Nucleation, Fifth Symposium on Aerosol-Cloud-Climate Interactions, AMS 93rd Annual Meeting (January 6–10, 2013), Austin, Texas, USA.

- **Hoffman, F. M.**, et al., The International Land Model Benchmarking (ILAMB) Project, 93rd American Meteorological Society (AMS) Annual Meeting (January 6–10, 2013), Austin, Texas, USA. *Invited.*

- **Hoffman, F. M.**, et al., The Causes and Implications of Persistent Atmospheric CO_2 Biases in Earth System Models, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B41C-0290.

- Randerson, J. T., **F. M. Hoffman**, et al., Evaluation of the Seasonal Dynamics of Photosynthesis and Drought Stress in CMIP5 Models, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B34B-02. *Invited.*

- Keppel-Aleks, G., **F. M. Hoffman**, et al., Evaluating Carbon Dioxide Variability in the Community Earth System Model Against Atmospheric Observations, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract A32A-08.

- Mei, R., **F. M. Hoffman**, et al., Do High-resolution Global Models Add Value to Climate Model Predictions? Results from a Cluster Analysis, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract IN21C-1488.

- **Fu, W.**, R. E. Dickinson, L. Gu, and **F. M. Hoffman**, Estimation of Terrestrial COS Uptake From a Global Carbon Cycle Model (CLM-4.0), 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B21B-0354.

- Shi, X., **F. M. Hoffman**, et al., Spatiotemporal Pattern of CLM4 Simulated Evapotranspiration in Response to Multifactor Environmental Changes, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B13B-0507.

- Mao, J., **F. M. Hoffman**, et al., Global Latitudinal-asymmetric Vegetation Growth Trends and Their Driving Mechanisms Over the Past Three Decades, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B13B-0506.

- Bauerle, W., et al. (including **F. M. Hoffman**), Seasonal Patterns of Photosynthetic Capacity: Photoperiodic Control and Its Carbon Cycling Implications, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract B13B-0486.

- **Lucas, D.** et al., Good Models Gone Bad: Quantifying and Predicting Parameter-Induced Climate Model Simulation Failures, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA. Abstract GC43E-1073.

- **Hoffman, F. M.**, et al., Measurements to Models: ILAMB and Representativeness/Scaling, Heterotrophic Respiration (R_H) Workshop (October 30–November 1, 2012), H. J. Andrews Experimental Forest, Blue River, Oregon, USA. *Invited*.

- **Hoffman, F. M.**, et al., Using Remotely-sensed Data Sets for Model Evaluation and Benchmarking, ForestSAT 2012 (September 11–14, 2012), Oregon State University, Corvallis, Oregon, USA. *Invited*.

- **Hoffman, F. M.**, et al., Computational Challenges of the Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC) Project, Scientific Discovery through Advanced Computing (SciDAC3) Principal Investigators Meeting (September 10–12, 2012), Rockville, Maryland, USA.

- **Hoffman, F. M.**, et al., Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC), Scientific Discovery through Advanced Computing (SciDAC3) Principal Investigators Meeting (September 10–12, 2012), Rockville, Maryland, USA.

- **Liu, X.**, et al., Dust Speciation and Global Impacts on Mixed-Phase Clouds Through Ice Nucleation, Session on Asian Dust and Air Pollution: Climate Impact and Biogeochemical Feedbacks Over the Pacific Ocean, Asian Oceania Geosciences Society (AOGS) – American Geophysical Union (AGU) (WPGM) Joint Assembly (August 13–17, 2012), Singapore. *Invited*.

- **P. Cameron-Smith**, Chem-Aersol plans, CESM Chemistry-Climate Working Group Meeting, 17$^{\text{th}}$ Annual Community Earth System Model (CESM) Workshop (June 18–21, 2012), Breckenridge, Colorado, USA.

- **Hoffman, F. M.**, et al., Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC), Software Engineering Working Group Meeting, 17$^{\text{th}}$ Annual Community Earth System Model (CESM) Workshop (June 18–21, 2012), Breckenridge, Colorado, USA. *Invited*.

- **Hoffman, F. M.**, et al., Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC), 17$^{\text{th}}$ Annual Community Earth System Model (CESM) Workshop (June 18–21, 2012), Breckenridge, Colorado, USA.

- **Elliot, S. M.**, et al., Overview of Biogeochemistry, DOE-BER Cloud Cryosphere Project (May 2012), Lawrence Berkeley National Laboratory, Berkeley, California, USA.

- **Elliot, S. M.**, et al., CESM Marine Organic Emissions, Scripps Institute of Oceanography (May 2012), La Jolla, California, USA. *Invited.*

2.4 Workshops, Symposia, and Special Sessions Organized

- **Hoffman, F. M.**, Co-convener and co-chair, Big Data in the Geosciences: New Analytic Methods and Parallel Algorithms, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, New Mechanisms, Feedbacks, and Approaches for Improving Predictions of the Global Carbon Cycle in Earth System Models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Phenology as Both Forcing and Response: Integrating Measurements and Models Across Terrestrial and Aquatic Ecosystems, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Best Practices in Model Verification and Uncertainty Analysis across Earth's Dynamic Systems, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA.

- **Lucas, D.**, Co-convener and co-chair, Session on Uncertainty Quantification of Climate Change, Earth System, and Integrated Assessment Models, 2013 American Geophysical Union (AGU) Fall Meeting (December 9–13, 2013), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Session on Phenology, 28$^{\text{th}}$ Annual U.S.-International Association for Landscape Ecology (US-IALE) Symposium (April 14–18, 2013), Austin, Texas, USA.

- **Hoffman, F. M.**, Co-chair, Session on Earth System Modeling, Climate 2013: Next Generation Climate Models and Knowledge Discoveries through Extreme High-Performance Simulations and Big Data Workshop (March 20–22, 2013), Lawrence Berkeley National Laboratory, Berkeley, California, USA.

- **Elliott, S. M.**, Convener, Symposium on Marine Aerosols, CESM Chemistry-Climate Working Group Winter Meeting (February 2013), National Center for Atmospheric Research, Boulder, Colorado, USA.

- **Liu, X.**, Co-convener and co-chair, Session on Cloud Condensation Nuclei (CCN) and Ice Nuclei (IN) Properties of Aerosol: Measurement, Modeling and Impacts on Clouds, 5$^{\text{th}}$ Symposium on Aerosol-Cloud-Climate Interactions, 93$^{\text{rd}}$ AMS Annual Meeting (January 6–10, 2013), Austin, Texas, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Session on Phenology Responses and Feedbacks to Biogeophysics, Disturbance, and Climate Change, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Session on New Mechanisms, Feedbacks, and Approaches for Improving Predictions of the Global Carbon Cycle in Earth System Models,

2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA.

- **Hoffman, F. M.**, Co-convener and co-chair, Session on Large-Scale Data Analytics in Earth System Science, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA.
- **Hoffman, F. M.**, Co-convener and co-chair, Session on Quantifying Heterogeneity of Landscapes and Ecosystems in Earth System Models, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA.
- **Lucas, D.**, Co-convener and co-chair, Session on Uncertainty Quantification and Climate Change, 2012 American Geophysical Union (AGU) Fall Meeting (December 3–7, 2012), San Francisco, California, USA.
- **Liu, X.**, Co-convener and co-chair, Session on Asian Aerosols and Their Impacts on Regional and Global Climate, Asian Oceania Geosciences Society (AOGS) – American Geophysical Union (AGU) (WPGM) Joint Assembly (August 13–17, 2012), Singapore.
- **Lucas, D.**, Co-convener and co-chair, Session on Climate Uncertainty Quantification, 2012 Society for Industrial and Applied Mathematics (SIAM) UQ12 Meeting (April 2012), Rayleigh, North Carolina, USA.

3 Milestones

3.1 Ocean

Major milestones to date for the ocean model are the development of a marine organic chemistry simulator and the addition of OCS as a marine source gas. Both of these developments are on track. The organic chemistry simulator has been designed and tested. The marine organosulfur chemistry code has been updated and retested with the BEC module for future simulations, tracking sulfur flow from the ocean to the atmosphere.

3.2 Land

To date the major milestones for the land model were development of a COS parameterization and the addition of PFTs for improving the VOC emissions factors in MEGAN2. An initial COS parameterization has been implemented and tested, and additional flux data are being collected to further constrain model parameters. The MEGAN2 improvements have been delayed by the relocation of collaborator Alex Guenther from NCAR to PNNL, but we expect this move will enhance our collaboration since Alex is now at a partner Laboratory.

3.3 Atmospheric Chemistry and Aerosols

After 1.5 years, we are generally on track with our milestones, as rescoped to fit the revised budget at the time the project was awarded. However, we did choose to delay the implementation of the ^{222}Rn, ^{210}Pb, and SF_6 tracer test suite, since the chemistry-aerosol interface has been undergoing changes. The other milestones to date for atmospheric chemistry and aerosols have been covered by the accomplishments listed in Section 1.3.

Several months ago, there were a couple of personnel changes that have significantly affected the project:

- The abrupt retirement in 2013 of Daniel Bergmann (a computer scientist at LLNL with great experience in atmospheric chemistry models), significantly slowed progress on the LLNL parts of this project. In collaboration with the other program leaders at LLNL, we are working to replace the capabilities provided by Dan and other recent retirees, and the situation is improving.

- Xiaohong Liu left PNNL for an academic position at U. Wyoming. He has now been replaced on the project by other aerosol modelers at PNNL.

3.4 Atmosphere and Ocean Advection

We are on track for all the CAM-SE/HOMME milestones. We have developed a departure grid algorithm for spectra elements and now have working transport algorithms using both incremental remap and optimization approaches. These algorithms run in the HOMME primitive equation dynamical core. We are making steady progress on interfacing with the MOAB meshing library to enable CFL > 1 calculations. We have initiated work on tracer consistency and expect this to be wrapped up in year 2.

3.5 Computational Tools and Performance

Both Year 1 and Year 2 performance-related milestones have been addressed:

> Year 1: Do project-specific performance evaluation on initial target systems.
>
> Year 2: Port and evaluate performance of existing software on initial target systems; do project-specific performance evaluation of secondary target systems.

In particular, representative performance evaluations have been conducted on the primary shared systems: Hopper, Edison, and Titan, and studies with the most recent version of the CESM have begun on Mira.

We have not yet captured performance data for all code versions and configurations used within ACES4BGC, as some researchers are using frozen versions of the code and of the configurations, or are running only on local systems. Instead we focused primarily on the needs of future experiments. As researchers move to new versions of the CESM and when there is an opportunity for performance evaluation and optimization before new suites of experiments begin, we will be including these configurations in future evaluations.

3.6 Software Engineering

Software engineering milestones include 1) incorporation of sectional aerosol and modal aerosol modules into the CESM repository, 2) coupler enhancements to simplify adding new biogeochemical tracers, 3) isolation of the RTM as a separate model component, and 4) development of a model testing framework and unit testing for CLM. The aerosol modules have been brought into the repository, RTM is now running as a separate model component, and the coupler modifications for an arbitrary number of tracers have been completed. The CLM testing framework is on track, and unit tests are being added.

3.7 Uncertainty Quantification

The major UQ milestones to date for ACES4BGC have been to (1) identify and compile a list of biogeochemical parameters for in-depth UQ analysis, (2) run preliminary factorial sampling studies over the selected biogeochemical parameters, and (3) perform an initial dimensional reduction by downselecting the important parameters from the complete set. We achieved the first milestone by incorporating two different classes of model parameters into our single column CAM ensemble UQ system (SCAM-UQ). These parameters are uncertain and can affect the vertical distribution of chemical tracers in SCAM-UQ. The first class of parameters is associated with physical processes (e.g., cloud formation, deep convection, boundary layer turbulence), and were selected based on their rankings in other UQ studies. The second class of UQ parameters is associated with chemical reaction rate constants in the MOZART mechanism, with uncertainties specified using values published in the NASA JPL photochemical tables. Toward the second milestone, we conducted two sets of preliminary SCAM-UQ ensembles using a Latin Hypercube sampling method, one for each class of parameters (physical and chemical). The ensembles demonstrate the sensitivity of the vertical distribution of ozone, carbon monoxide, peroxyacetyl nitrate, and other tracers to the values of the parameters. Given the computational efficiency of the SCAM-UQ system, there is not a pressing need to perform an immediate parameter downselect, as noted in milestone 3. The downselect will occur after including additional parameters related to MAM aerosol processes and running ensembles that sample jointly over the three classes of parameters. Postponing this milestone will also present an opportunity to test and utilize new UQ methods developed under QUEST to deal with very high dimensional UQ problems (e.g., compressive sensing).

4 Plans for the Coming Year

4.1 Ocean

We will incorporate additional new tracers in the marine organic simulations in order to represent distinct classes of surfactant macromolecules of the surface ocean. Special attention will be paid to aminosugars produced by autotrophic and heterotrophic bacteria. Examples include chitin, peptidoglycan and their oligomeric and monosugar decay products. We will seek improved proxy compounds for the representation of generalized Langmuir isothermal behavior along the air-water interface. We will work with university colleagues to test our concepts in the laboratory and the field. Specifically, we will measure real adsorption processes for representative macromolecules along with their temperature, salt and kinetic dependencies. We will complete the linkages from ocean organic carbon distributions through bubble driven spray generation to chemistry of the modal aerosol in CAM. With regard to the dimethyl sulfide simulations and cycling, we will finalize our current update of the ocean organosulfur simulator with optimization to the most recent data base. We will then conduct coupled (ocean emission) to (atmospheric photochemical) simulations leading to the product species OCS. These results will be handed off to our ACES4BGC collaborators at LLNL, who will interpret them in the analogy with photosynthetic uptake of carbon dioxide. This latter work is a close collaboration with the University of California at Merced.

4.2 Land

Over the coming year, we will further test and improve the initial COS implementation, test improvements to the MEGAN2 model within CLM4.5 by incorporating a larger class of plant functional types (PFTs), and perform offline and coupled experiments to investigate the climate impacts of improved volatile organic compound (VOC) emissions and associated biogeochemical

feedbacks. Engagement with Alex Guenther, a key collaborator and author of the MEGAN model, was interrupted by his departure from NCAR, but we expect to work more closely on the terrestrial VOC sources for secondary organic aerosols now that he is established at PNNL. In addition, we have initiated a collaboration with Joe Wright from the Smithsonian Tropical Research Institute to improve the representation of tropical vegetation and processes in CLM. We will investigate the impact of additional tropical PFTs or trait-based productivity schemes in CLM. Pending availability of computational resources, we will perform a series of coupled ECP 8.5 simulations to investigate long term effects increasing atmospheric CO_2 on the biosphere.

4.3 Atmospheric Chemistry and Aerosols

In the coming year, we will work to finish coupling the atmospheric sulfur cycle to the ocean, and then carryout various simulations with the model to validate the model and study the sulfur cycle, including the feedbacks between DMS and climate. We also hope to start coupling the OCS cycle to the land model.

We also plan to participate in the Chemistry Climate Model Intercomparison (CCMI) if computational resources become available.

We will incorporate the role of SOA and other organics (e.g., amines) in new particle nucleation and growth. This work will leverage the advanced SOA treatment for MAM described above. An ultrafine mode will be added to MAM to improve the numerical representation of new particle growth to Aitken mode size. We will collaborate with BNL researchers to utilize recent laboratory and field estimates of uncertain physical parameters relating to new particle formation and growth.

We will investigate how CESM model predictions of the direct and indirect radiative forcing of climate change due to the more complex SOA treatment and improved representation of new particle formation and growth that include the role of organics.

4.4 Atmosphere and Ocean Advection

4.4.1 Mesh Tools for Advection

Currently, tracers are averaged over an arrival cell. We will integrate mesh intersection code with higher order reconstruction schemes, to conservatively transfer tracer species between departure and arrival meshes.

4.4.2 Transport in CAM-SE/HOMME

Our highest priority in year 2 will be to integrate the MOAB meshing algorithms into HOMME. We will then initiate work on generalizations of the CSLAM reconstruction that is appropriate for unstructured grids. We will continue our work on mass / tracer mass consistency algorithms and decide on the best approach. It is anticipated this will require us to use a flux form of the incremental remap algorithms, so this will also require us to add a flux form to the MOAB intersections algorithm. This is identical to the existing intersection technology, but the intersections will now be done using the region swept out by the motion from the departure grid to the arrival grid instead of intersecting the departure grid with the reference grid.

Development of the optimization-based transport schemes will continue. We will compare these schemes to existing approaches for standard advection tests.

4.5 Computational Tools and Performance

Performance engineering activities will primarily be reactive in the coming year. We will continue to track and evaluate performance of jobs that already include the enhanced performance data collection logic, including supporting moving these jobs to new platforms if needed. As more ACES4BGC researchers move from their current "frozen" versions of the CESM to more recent versions, we will work with them to add the new instrumentation logic and to begin to analyze, optimize, and track performance.

As the new tracer advection scheme development matures, we will work with the developers to evaluate performance, especially in the context of relevant full CESM runs. We will also track the development of the communication optimization tools under development within SUPER and FASTMath, and will evaluate these for ACES4BGC production runs.

Finally, the SUPER institute is focusing significant resources on the new ocean code MPAS-Ocean that is scheduled to replace POP in the CESM. We will track this activity, to determine the impact (and importance) of using the new ocean model within ACES4BGC.

4.6 Software Engineering

The software engineering team at NCAR will continue providing support for incorporation of new capabilities into the CESM repository, enhance the coupler capabilities as needed, and support the framework for routine testing of CLM.

4.7 Uncertainty Quantification

Our near-term UQ efforts will focus on propagating a large number of uncertainties from $\sim$100 or so parameters in MOZART chemistry and CAM5 physics through ensemble simulations of SCAM-UQ. To sample an uncertainty volume this large, we plan to run an ensemble with at least 10^5–10^6 members. Our preliminary UQ simulations suggest that some simulations may crash because the parameter perturbations may push them into regions not handled by numerical algorithms and solvers. If these situations arise, we will apply fault-tolerant or preemptive UQ methods developed by QUEST or other SciDAC team members. The analysis of our high dimensional ensemble will also require new UQ methods, for example compressive sensing, that are under development under SciDAC. Once completed, we will prepare a manuscript describing the results of the MOZART-CAM5 ensemble. This activity will be followed up with work to incorporate uncertainties in MAM aerosols into SCAM-UQ.

5 SciDAC Institute Engagement

5.1 Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath)

Mesh intersection algorithms leveraging parallel infrastructure and functionality have been developed as part of the FASTMath Institute. Integration of improved parallel readers, especially for unstructured meshes, take advantage of the Zoltan Partitioning Tool. We are also considering the deployment of Zoltan2, in collaboration with Karen Devine, from the FASTMath Institute.

5.2 Institute for Sustained Performance, Energy and Resilience (SUPER)

Responsibility for performance engineering is shared between internally-funded activities and collaborative activity with SUPER, the SciDAC-3 Institute for Sustained Performance, Energy, and Resilience. Since the beginning of the project, SUPER has contributed directly in three ways: (a) development of enhanced performance instrumentation and data archive infrastructure for use with production runs of the Community Earth System Model (CESM), (b) performance analysis of a MOAB kernel, resolving a performance issue that arose in the development ACES4BGC-specific MOAB work, and (c) collaboration with ACES4BGC on performance evaluation studies on the Cray XK7 (Titan) at the Oak Ridge Leadership Computing Facility (OLCF) and on the Cray XC30 (Edison) at the National Energy Research Scientific Computing Center (NERSC). ACES4BGC implemented the enhanced performance data collection and archive capability in relevant versions of the CESM and this is being used in some of the production runs on Titan and on the XE6 at NERSC (Hopper), and is available for production runs on Edison and on the BG/Q (Mira) in the Argonne Leadership Computing Facility (ALCF). As indicated in the accomplishments section, these data were then used to improve performance for a suite of important production runs by a factor of 1.6.

Within SUPER the CESM performance data collected by ACES4BGC (and by other projects using the CESM) was used to characterize the role of process placement and interference from other running jobs in performance degradation and variability. Based on this, new research activities have recently begun on optimizing process placement to minimize communication cost when the physical topology of allocated nodes is not known until runtime, both evaluating proposed solutions in the literature and implementing and evaluating new schemes motivated by the CESM performance data. Results from this SUPER crosscutting activity will then be applied to the CESM, and to ACES4BGC production runs at the ALCF, NERSC, and OLCF in particular.

5.3 Quantification of Uncertainty in Extreme Scale Computations (QUEST)

Don Lucas and Philip Cameron-Smith initially engaged QUEST by attending the multi-day training course run by the QUEST institute on their various UQ toolkits. The workshop afforded an opportunity to assess the status of UQ methods that are currently available and under development. Through a discussion with QUEST's M. Eldred, we made a request to support the probabilistic collocation sampling method for our activities. This method is now available in the DAKOTA package, and will be used as a sampling engine for our upcoming SCAM-UQ ensembles. We will engage QUEST on one or two more activities. The ensemble represents a very high dimensional problem that will be severly undersampled. We will work with QUEST to apply their compressive sensing tools to this problem. We also expect high failure rates in our ensemble, which may benefit from the fault tolerant UQ methods being explored by QUEST.

6 Management

Since the inception of the project, we have held 10 project-wide conference calls, averaging one every other month. In addition, individual team members frequently hold their own conference calls. We have convened four project-wide meetings, held jointly with the CESM Workshops in Breckenridge and the AGU Fall Meetings in San Francisco in 2012 and 2013, to reduce travel costs. The meeting in Breckenridge in 2013 was held in conjunction with the other two BER Lab SciDAC projects. To facilitate project-wide communication, we operate a mailing list (aces4bgc@aces4bgc.org) and an internal website for sharing documents and repositories.

As new component model capabilities are implemented, the project will require more frequent communication and coordination to plan for coupled simulations, analysis, and paper writing. To facilitate this, ACES4BGC is moving to holding monthly conference calls in 2014, where every other call will include a scientific presentation by a team member or group. The alternate meetings will focus on model development, simulations, and analysis. A dedicated, day-long, project-wide meeting is scheduled for February 14 in Boulder, Colorado, following the Atmosphere Model, Whole Atmosphere, and Chemistry-Climate Working Group Meetings to be held February 10–13. Since new model capabilities are expected to be available in the coupled modeling system this year, we are planning to conduct at least two modeling experiments, which will require use of DOE Leadership Computing Facility resources. We are presently developing an ASCR Leadership Computing Challenge (ALCC) proposal to meet this need.

Over the past year, ACES4BGC team members have contributed to the development of the ACME SFA Proposal. In some cases, partial support for this project development has come from the ACES4BGC project. Taylor serves on the Council, and Ghan, Hoffman, Tautges, and Worley serve on the Leadership Team. These individuals, who provide critical links between ACES4BGC and ACME, have attended a number of meetings to plan for this new SFA activity.

7 Personnel

Table 1 contains a list of key project personnel, their institutions, full time equivalent (FTE) levels of effort, and major tasks.

Table 1: Key project personnel and major tasks for ACES4BGC.

Name	**Institute**	**FTE**	**Major Tasks**
Dan Bergmann	LLNL	0.12	Computer scientist contributing to atmospheric chemistry and aerosols
Philip J. Cameron-Smith	LLNL	0.48	Atmospheric chemistry and aerosol tasks
Scott M. Elliott	LANL	0.25	Ocean biogeochemistry modeling and analysis
Steven Ghan	PNNL	0.05	Lead aerosol model development
Iulian Grindeanu	ANL	0.20	Mesh Algorithms and Tools
Oksana Guba	SNL	0.50	Transport algorithm development & implementation
Forrest M. Hoffman	ORNL	0.40	Project management, land model development & evaluation
Manish Shrivastava	PNNL	0.15	Aerosol model development and testing
Robert B. Lowrie	LANL	0.25	Ocean transport algorithm development & implementation
Donald D. Lucas	LLNL	0.15	UQ and QUEST Institute liaison
William J. Sacks	NCAR	0.15	Coordinate integration into CESM repository; land model software engineering
Timothy J. Tautges	ANL	0.10	MOAB developer & FASTMath Institute liaison
Mark A. Taylor	SNL	0.20	Transport algorithm development & implementation
Mariana Vertenstein	NCAR	0.00	Oversee integration into CESM repository
Patrick H. Worley	ORNL	0.20	Performance optimization & SUPER Institute liaison

A Project Highlights

Improve the treatment of secondary organic aerosols (SOA)

Pacific Northwest NATIONAL LABORATORY
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Motivation

- SOA is a major submicron aerosol species and has an important impact on climate, which is under-represented in global climate models

Objective

- Implement a new modeling framework using the modified volatility basis set (VBS) to improve SOA treatment within the CESM model

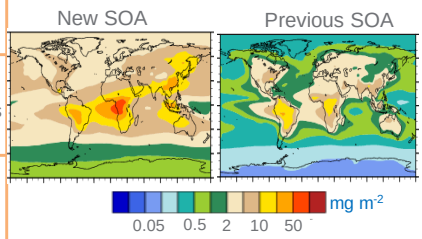
Accomplishments

- Replaced the previous crude treatment of SOA by our most advanced SOA parameterization using 174 advected tracers (including 68 SOA gas and particle phase tracers)
- Quantified SOA formation from three different source categories: fossil (anthropogenic), biomass burning and biogenic
- Represented multi-generational gas-phase chemistry of organic precursors in each of the three source categories
- Implemented an approach to treat the semi-solid (glassy) nature of SOA based on latest experimental findings

Impact

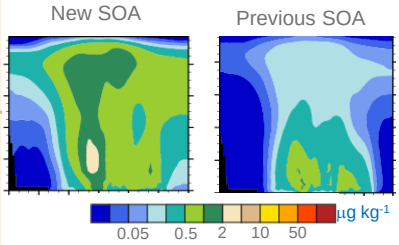
- Results in large changes in the horizontal and vertical distribution of SOA with implications for changes in direct and indirect forcing
- Better resolves the human vs. natural sources of SOA
- Essential tool to better understand the effects of aerosols and clouds affecting the global biogeochemical cycle processes

Annual burden



New treatment increases SOA burdens over most of the domain including oceans

Zonal annual mean



New treatment increases SOA loadings at higher vertical levels

Parallel Mesh Intersection For Tracer Transport in Atmospheric Modeling

Timothy J. Tautges & Iulian Grindeanu, Argonne National Laboratory

Objectives

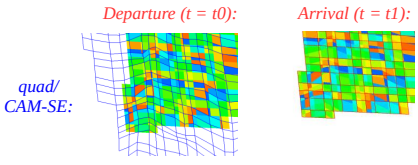
- Develop parallel mesh back-tracing and intersection capability to support semi-Lagrange tracer advection
  - Support transport CFL > 1
  - Allow application-specified discretization approach, departure point calculation
  - Support multiple mesh types (quad, polygons)
  - Implement as software module for use in multiple dynamical cores

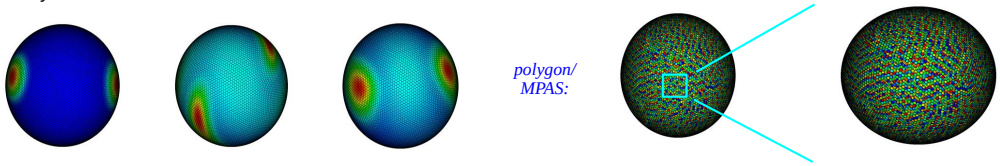
Impact

- Scalability limits current tracer transport to 100s of tracer species
  - New approach should allow 1000s of tracer species to be used, yielding much greater accuracy in biogeochemistry
- Reusable mesh intersection module will support multiple climate dynamical cores (e.g. CAM-SE, MPAS-O, etc.)

Accomplishments

- Developed MOAB-based tool for parallel mesh intersection
  - Edge-based algorithm supports both quad (CAM-SE) and SCVT (MPAS) grids, easily extensible to other grid types
  - Uses scalable off-processor communication, so not limited by CFL number





Advection test, MPAS grid

Intersection between departure and original/arrival meshes

U.S. DEPARTMENT OF ENERGY | Office of Science

Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC)

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