DE-SC0006791: Collaborative Project: Building improved optimized parameter estimation algorithms to improve methane and nitrogen fluxes in a climate model (Cornell PI: Mahowald, co-Is: Shoemaker, Hess, Binder, Duxbury, Yavitt; Collaborator: William Riley, LBLL)

9/15/2011-9/14/2014 (with 2 no cost extensions).

Project Synopsis (from submission)

Soils in natural and managed ecosystems and wetlands are well known sources of methane, nitrous oxides, and reactive nitrogen gases, but the magnitudes of gas flux to the atmosphere are still poorly constrained. Thus, the reasons for the large increases in atmospheric concentrations of methane and nitrous oxide since the preindustrial time period are not well understood. The low atmospheric concentrations of methane and nitrous oxide, despite being more potent greenhouse gases than carbon dioxide, complicate empirical studies to provide explanations. In addition to climate concerns, the emissions of reactive nitrogen gases from soils are important to the changing nitrogen balance in the earth system, subject to human management, and may change substantially in the future. Thus improved modeling of the emission fluxes of these species from the land surface is important. Currently, there are emission modules for methane and some nitrogen species in the Community Earth System Model's Community Land Model (CLM-ME/N); however, there are large uncertainties and problems in the simulations, resulting in coarse estimates. In this proposal, we seek to improve these emission modules by combining state-of-the-art process modules for emissions, available data, and new optimization methods. In earth science problems, we often have substantial data and knowledge of processes in disparate systems, and thus we need to combine data and a general process level understanding into a model for projections of future climate that are as accurate as possible. The best methodologies for optimization of parameters in earth system models are still being developed. In this proposal we will develop and apply surrogate algorithms that a) were especially developed for computationally expensive simulations like CLM-ME/N models; b) were (in the earlier surrogate optimization Stochastic RBF) demonstrated to perform very well on computationally expensive complex partial differential equations in earth science with limited numbers of simulations; and, c) will be (as part of the proposed research) significantly improved both by adding asynchronous parallelism, early truncation of unsuccessful simulations, and the improvement of both serial and parallel performance by the use of derivative and sensitivity information from global and local surrogate approximations $S(x)$. The algorithm development and testing will be focused on the CLM-ME/N model application, but the methods are general and are expected to also perform well on optimization for parameter estimation of other climate models and other classes of continuous multimodal optimization problems arising from complex simulation models. In addition, this proposal will compile available datasets of emissions of methane, nitrous oxides and reactive nitrogen species and develop protocols for site level comparisons with the CLM-ME/N. Once the model parameters are optimized against site level data, the model will be simulated at the global level and compared to atmospheric concentration measurements for the current climate, and future emissions will be estimated using climate change as simulated by the CESM.

This proposal combines experts in earth system modeling, optimization, computer science, and process level understanding of soil gas emissions in an interdisciplinary team in order to improve the modeling of methane and nitrogen gas emissions. This proposal thus meets the requirements of the SciDAC RFP, by integrating state-of-the-art computer science and earth system to build an improved earth system model.

Products:

There were three primary areas of research within this grant, and we describe the resulting papers and improvements in the model development here.

1**. improvement in the methane module of the CESM:**
This work supported work improving and evaluating the representation of methane compared to fluxes [*Meng et al.*, 2012], and looking at how well the model can capture the seasonal cycle and interannual variability using surface concentrations [*Meng et al.*, 2015]. Another manuscript looked at the attribution of changes in natural wetlands since preindustrial [*Paudel et al.*, 2016], which has not previously been considered, and yet is an important question in attributing changes in methane.

2. Improvements in the use of surrogate global optimization algorithms for use within CESM. Three papers were published (Krityarkierne et al., 2015; 2016) and Akhtar et al) describe improvements in the surrogate global optimization algorithms that can be used in model calibration for expensive simulation models including CLM 4.5. Improvements are important since the problem is very difficult given the computational expense and the complexity of the GCMs. Improvements mean we can obtain more accurate answers in less time. The multi objective algorithm can be used to also examine tradeoffs in calibration criteria. An integrated optimization method paper has also been published [*Muller et al.*, 2015], using this global surrogate method with the methane flux model from point 1,showing how the surrogate method changed the resulting flux estimations from the methane module.

3. Improvements in the nitrogen modeling within the CLM.

Problems were identified within the N_2O emissions from the CLM, by looking at the river runoff. Using inverse modeling and atmospheric concentrations, (Nevison et al., 2016) reveal that the CLM spatial distributions (e.g., high Arctic emissions) are incompatible with atmospheric observations, while the strong late spring peak in N_2O emissions in productive agricultural regions receiving large fertilizer inputs are largely consistent with atmospheric observations. The unrealistic features of CLM N_2O were traced to the prescribed potential rates of nitrification, denitrification, immobilization and plant uptake and the sequential way in which plants and the various types of soil microbes compete for mineral N in CLM, and ideas for improvement in the CLM are being developed. This work is described in [Nevison et al., 2016].

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