

Poster #XXX

Computational Bayesian Framework for Quantification of Predictive Uncertainty in Environmental Modeling

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A computational Bayesian framework has been developed for quantification and reduction of uncertainty in environmental modeling. In this year of the project, we have collaborated with scientists at the Oak Ridge National Laboratory (ORNL) and Pacific Northwest National Laboratory to apply our computational methods to several problems of interest to DOE. The collaboration with Xingyuan Chen at PNNL is focused on developing a Bayesian network that can incorporate uncertainty in model parameters, structures, and scenarios in a flexible manner. This Bayesian network has been used for a sensitivity analysis to determine important model parameters and processes at the 300 Area of the Hanford Site. The collaboration with the ORNL is for mercury modeling and for leaf modeling. The collaborative research with Scott Brooks at ORNL on mercury modeling has produced a model that integrates the mercury complexation model (WHAM Model VII) into the PHREEQC framework. The on-going research is to use the PHREEQC VII model for addressing uncertainty in equilibrium coefficients of mercury reactions. Different ways of addressing the parametric uncertainty reported in literature are compared to explore the appropriate way of addressing the uncertainty. The collaborative research with Anthony Walker at ORNL on leaf modeling is to integrate our research of multi-models sensitivity analysis and his multi-hypotheses leaf photosynthesis modeling, and the goal is to identify the processes important to leaf photosynthesis. Our contribution is to develop a theoretical framework for the identification. A computationally efficient method has been developed for implementing the framework.

We have also made progress on computational evaluation of Bayesian evidence, which is critical for evaluating relative plausibility of multiple models (a more plausible model has larger Bayesian evidence). We have evaluated several state-of-the-art methods for evaluating the Bayesian evidence, and they are the thermodynamics integration, stepping-stone, and nested sampling methods. Our research of this year is focused on the nested sampling method by improving its sampling efficiency. To reduce the computational cost, the sparse grid methods are used to build cheap-to-evaluate surrogates of computationally demanding models. Using the surrogates, we compared several methods of evaluating the Bayesian evidence, including an improved nested sampling method. We plan to develop a public domain software so that our computational methods can be used by other scientists who may not be an experts on computational science but are interested in exploring model structure uncertainty.