

Computational Bayesian Framework for Quantification and Reduction of Predictive Uncertainty in Climate Modeling and Groundwater Reactive Transport Modeling

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In the first two years of the project, we have developed a computational Bayesian framework for uncertainty quantification and reduction in environmental modeling. The framework is mathematically and computationally general, and can be applied to a wide range of environmental problems.

In the third year of the project, we have applied the computational Bayesian framework to both climate change modeling and subsurface reactive transport modeling. The application to climate change modeling is focused on understanding the mechanisms of soil microbial respiration behind the Birch effect, i.e., pulsed wetting causes a dramatic increase in soil respiration after a period of drought. We examined five models with different levels of complexity, evolving from an existing four-carbon-pool model to models with additional carbon pools and explicit representations of soil moisture controls on carbon degradation and microbial update rates. By evaluating structural uncertainty of the models, our Bayesian framework identified the best model, and helped gain insights for understanding why the model outperforms the other models. To facilitate the model identification, we developed a new statistical metric called relative model score, which is evaluated using the results of Bayesian computation of the framework. In addition, by considering eight formal likelihood functions for the soil respiration models, we investigated a fundamental question in Bayesian inference, i.e., how the likelihood functions affect the results of Bayesian inference. This analysis provided a number of insights and guidelines for calculating soil respiration models and for improving predictive capability of the models.

The computational Bayesian framework has also been applied to evaluate the data-worth of geophysical, hydraulic, and transport observations for reducing predictive uncertainty. This study was conducted by collaborating with scientists at the Pacific Northwest National Laboratory for the Hanford 300 Area, where a large amount of field data have been collected in the past. A new method has been developed to use ensemble Kalman filter and level set methods for reducing uncertainty in constructing hydrogeological facies. We are conducting research to evaluate this method using the data available at the 300 Area.

We have also continued on theoretical research to develop new sparse grid collocation methods for computationally efficient implementation of the framework. We proposed a new method to construct sparse grid surrogate for system state variables (e.g., hydraulic head and concentration). The new method has been evaluated for a groundwater flow problem, and we will further evaluate the method for reactive transport problems.