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Efficient Methods for Bayesian Uncertainty Analysis and Global Optimization of Computationally Expensive Environmental Models

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Models of complex environmental systems can be computationally expensive in order to describe the dynamic interactions of the many components over a sizeable time period. Diagnostics of these systems can include forward simulations of calibrated models under uncertainty and analysis of alternatives of systems management. This discussion will focus on applications of new surrogate optimization and uncertainty analysis methods to environmental models that can enhance our ability to extract information and understanding. For complex models, optimization and especially uncertainty analysis can require a large number of model simulations, which is not feasible for computationally expensive models. Surrogate response surfaces can be used in Global Optimization and Uncertainty methods to obtain accurate answers with far fewer model evaluations, which made the methods practical for computationally expensive models for which conventional methods are not feasible. In this paper we will discuss the application of the SOARS surrogate method for estimating Bayesian posterior density functions for model parameters for a TOUGH2 model of geologic carbon sequestration. We will also briefly discuss new parallel surrogate global optimization algorithm applied to two groundwater remediation sites that was implemented on a supercomputer with up to 64 processors. The applications will illustrate the use of these methods to predict the impact of monitoring and management on subsurface contaminants.