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Continuous Optimization with Response Surfaces for Computationally Expensive Simulation Models Including Environmental Applications

This talk will present an overview of algorithms that employ response surfaces to significantly reduce the computational effort required to solve continuous optimization and uncertainty analysis of nonlinear simulation models that require a substantial amount of CPU time for each simulation. For nonlinear objective functions and simulation models, the resulting optimization problem is usually multimodal and hence requires a global optimization method.

In order to reduce the number of simulations required, we are interested in utilizing information from all previous simulations done as part of an optimization search by building a (radial basis function) multivariate response surface that interpolates these earlier simulations. I will discuss the alternative approaches of direct global optimization search versus using a multistart method in combination with a local optimization method. These different approaches will be illustrated by two global optimization response surface methods to come from our group recently. I will also briefly describe an uncertainty analysis method SOARS that uses derivative-free optimization to help construct a response surface. This approach has been shown to reduce CPU requirements to less than 1/65 of what is required by conventional MCMC uncertainty analysis. I will present examples of the application of these methods to significant environmental problems described by computationally intensive simulation models used worldwide. One model (MODFLOW/MT3D) involves partial differential equation models for groundwater and the second is SWAT, which is used to describe potential pollution of NYC's drinking water. In both cases, the model is applied to data from a specific site.