# Sequential Designs for Computer Experiments

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**DEREK BINGHAM**, Simon Fraser University
*An Application of Sequential Design for Multi-fidelity Computer Models*

The design and analysis of experiments on simulators of physical systems have become common practice in many physics-based applications. For many of these applications, the computer model can be run in different levels of fidelity. The question of how one should allocate the experimental resources is one of primary importance. It turns out that sequentially allocating the trials can improve the predictive ability of the final model. In this work, we consider an application where experimenters have a multi-fidelity simulator of radiative shocks and also real-world experimenters to consider. Allocating the simulator and experimental trials are the main issues.

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**JASON LOEPPKY**, University of British Columbia, Okanagan
*Gaussian Process Models for Mixture Experiments*

Computer models are often used to simulate outputs of complex physical systems when physical experiments are not possible. In many areas of science the input variables are expressed as a percentage contribution to a total amount of material, resulting in a mixture experiment. In such situations the input variables are correlated because they must sum to one. In the context of a deterministic computer model additional care must be used in building an emulator. We propose use of a Gaussian process with transformed input variables and illustrate the resulting methodology on a chemical compositional simulator and a physical experiment.

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**ROBERT B GRAMACY**, University of Chicago
*Optimization under Unknown Constraints*

We consider optimization for computer experiments under unknown constraints, i.e., when simulation is required to determine real-valued responses and check constraints. We develop GP surrogates to approximate both simulator outputs. A new integrated improvement criterion recognizes that responses that violate the constraint are still informative about the function, and thus potentially useful in the optimization. We illustrate our approach on a problem from health care policy.