

*RIPS 2007 / LLNL Project Proposal:
Computer Experiments for Function Approximations*

With the advent of high performance computing, computational models are increasingly used for scientific discovery. Mathematically, we can think of a simulation capability as a (for simplicity, deterministic) mapping $F : X \rightarrow Y$ where $X \in \mathfrak{R}^m$ and $Y \in \mathfrak{R}^n$ are vectors of independent and dependent variables, respectively. Oftentimes we would want to explore the parameter space (independent variables) for purposes of studying uncertainties, sensitivities, or extremums. Since evaluating this function may be expensive, response surface (also called surrogate model, meta-model, or emulator) methods are often used to create a surrogate function closely approximating the original function. This requires the evaluations of the models at a limited number of evaluation points in the parameter space and the use of the results to construct an approximate representation of the function.

Response surface methodology is a collection of techniques for the design of computer experiments, data analysis, and data interpolation. The major challenges for response surface methods are efficiency and accuracy. Efficiency is measured by the number of function evaluations needed to construct an adequate response surface. Various design of computer experiment (DOE) techniques have been developed to efficiently sample the parameter space. There is, however, much room for improvements. One aspect of this project is to investigate intelligent and adaptive sampling design techniques that yield optimal information for the construction of response surfaces. Once the experimental design has been created, it is propagated via multiple simulation runs. Data analysis and maybe more sampling designs are then used to build an approximate function that is sufficiently accurate for the entire parameter space.

The objective of this project is two-fold:

1. investigate and develop intelligent sampling methods
2. investigate effective function approximation methods

The deliverables include:

1. a prototype software implementing your best experimental design and your corresponding function approximation schemes,
2. an evaluation of your methodologies on a selected set of test problems (to be provided by LLNL), and

3. a technical report detailing your approaches and results.

References

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- [5] A. B. Owen, *Orthogonal Arrays for Computer Experiments, integration, and visualization*, *Statist. Sinica* 2, pp. 439-452, 1992.
- [6] B. Tang, *Orthogonal Array-based Latin Hypercubes*, *J. Amer. Statist. Assn.* 88, 1392-1397, 1993.