Sequential Design of Experiment (SDoE) for FOQUS

T. Ahmed, C. Anderson-Cook, LANL  candcook@lanl.gov, atowfiq@lanl.gov

Design of Experiments

Statistical Design of Experiments is a way to accelerate learning by collecting a strategic sample of data:
- Reach required precision or understanding faster
- Learn more with a fixed set of resources

Common objectives:
1. Exploration: Space-filling designs
2. Model Calibration: Data to check how well the model and observed data match
3. Improving the quality of prediction: Using a measure of prediction precision, seek to reduce prediction uncertainty
4. Optimization of response value: Find the location in the input space to optimize performance

Process for SDoE

Planning Phase
1. Identify criteria
2. Develop a working model of the process.
3. Define the inputs (with their ranges).
4. Identify candidate input factor combinations.
5. Identify the initial batch of experiments
6. Develop a working model of the process able to receive data and update
7. Determine feasible size of batches.

During Experiment
8. Run the first batch & update the model.
9. Select the next batch of experimental runs.
10. Repeat steps 8-9 for subsequent batches.

Development Plan

Current Phase 1 (Space Filling Design)
- UQ Module (Uncertainty Quantification based on Plausso tools)
- SDoE Input File
- SDoE Module (stand-alone, based on Python)
- SDoE Output Files
  1. Constrained input space filling
  2. Optimization conditions

Future Phase 2 (Connect to surrogate models & other modules)
- GUI Module
- SDoE Module Input/Output
- Surrogate Models
- UQ Module

Phase-1 Example:

Inputs:
- Candidate runs
- Historical runs
- Desired design size 8-10
- Space-filling criterion: (minimax or maximin)
- Simulation size 100000

Outputs:

8 runs
93 candidates

Which runs to use
Design criteria
Time to generate solution
Ability to consider multiple solutions, allows exploration of best use of resources

Work Flow in SDoE Program

Main Output File
SDoE code (Python)

GUI Version: (Under Construction)

Next Step: Generalized Constrained Space-Filling:

Plan: Near Future Implementation
Currently being addressed

Goal: allow the straightforward generation of candidates sets that accommodate simple and complex input and output constraints to define the feasible region of interest.

Design of experiments is a powerful tool to accelerate learning, by targeting maximally helpful input combinations for the experiment goals Sequential DoE allows for near real-time incorporation of information from an experiment as it is being run.