Sequential Design of Experiment (SDoE) for FOQUS

CCSI² Carbon Capture Simulation for Industry Impact

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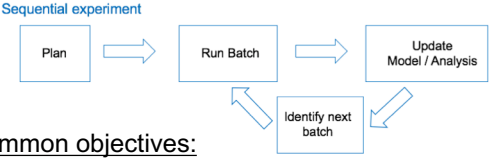
Design of Experiments

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

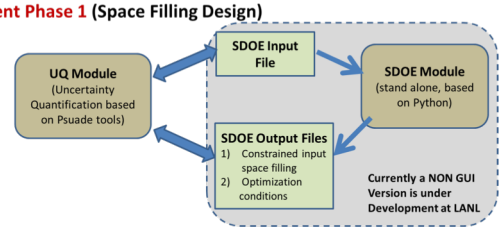
1. Identify criteria
2. Develop a working model of the process.
3. Define the inputs (with their ranges).
4. Identify candidate input factor combinations.
5. Identify the initial batch of experiments
6. Develop a working model of the process able to receive data and update
7. Determine feasible size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

During Experiment

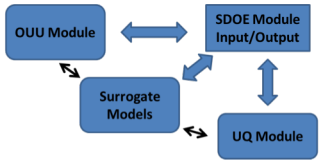
8. Run the first batch & update the model.
9. Select the next batch of experimental runs.
10. Repeat steps 8-9 for subsequent batches.

Development Plan

Current Phase 1 (Space Filling Design)



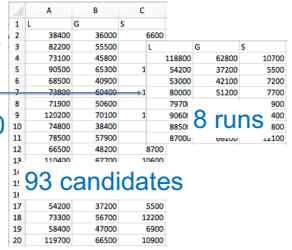
Future Phase 2 (Connect to surrogate models & other modules)



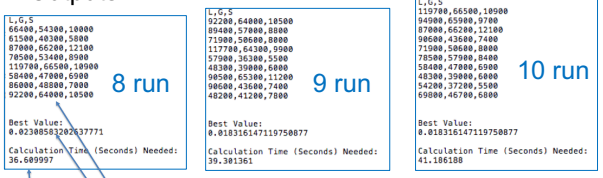
Phase-1 Example:

Inputs:

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



Outputs:



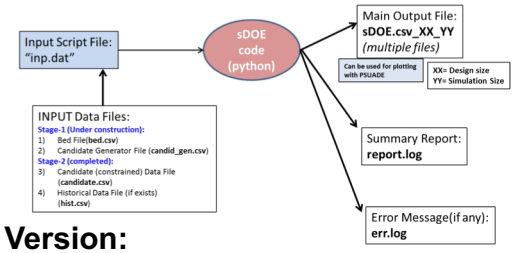
Which runs to use

Design criteria

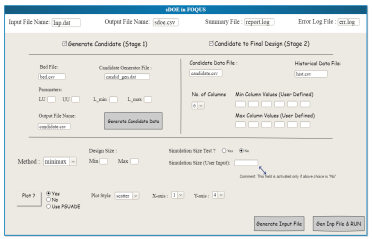
Time to generate solution

Ability to consider multiple solutions, allows exploration of best use of resources

Work Flow in SDoE Program

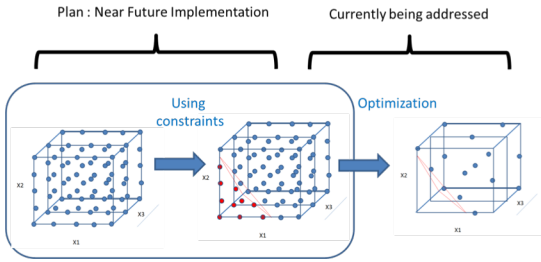


GUI Version: ***(Under Construction)***



Next Step:

Generalized Constrained Space-Filling:



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

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