August 2019

CCSI²

Carbon Capture Simulation for Industry Impact

Maximizing Learning Through Intelligent Test Design

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What is SDoE?

Sequential Design of Experiments (SDoE) is a paradigm of **strategic data collection** that maximizes learning.

One-shot Experiment

Plan → Run Experiment → Analyze

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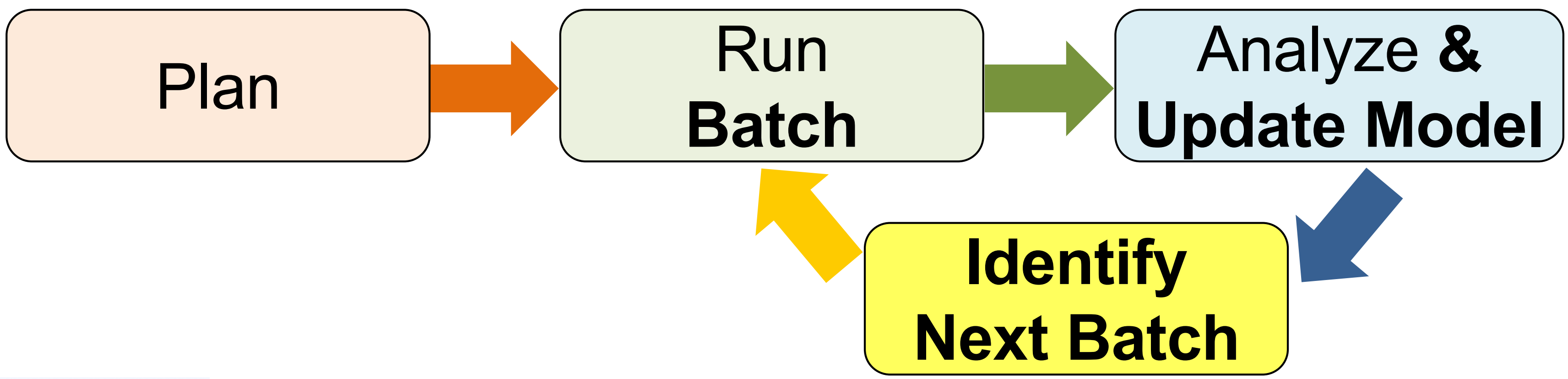
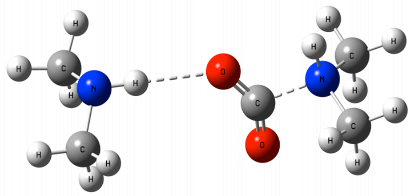
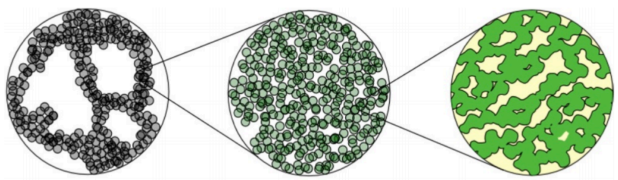
Sequential Experiments

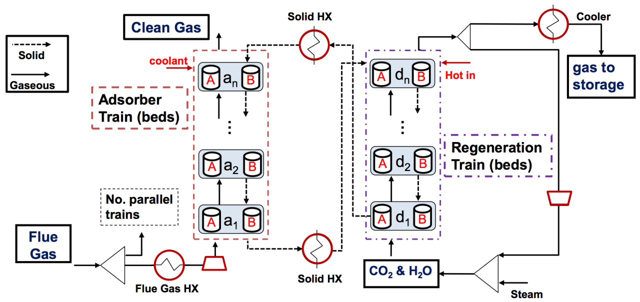


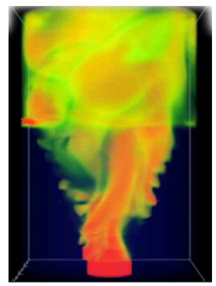
Why is SDoE important?

Development of science & engineering models requires DATA.







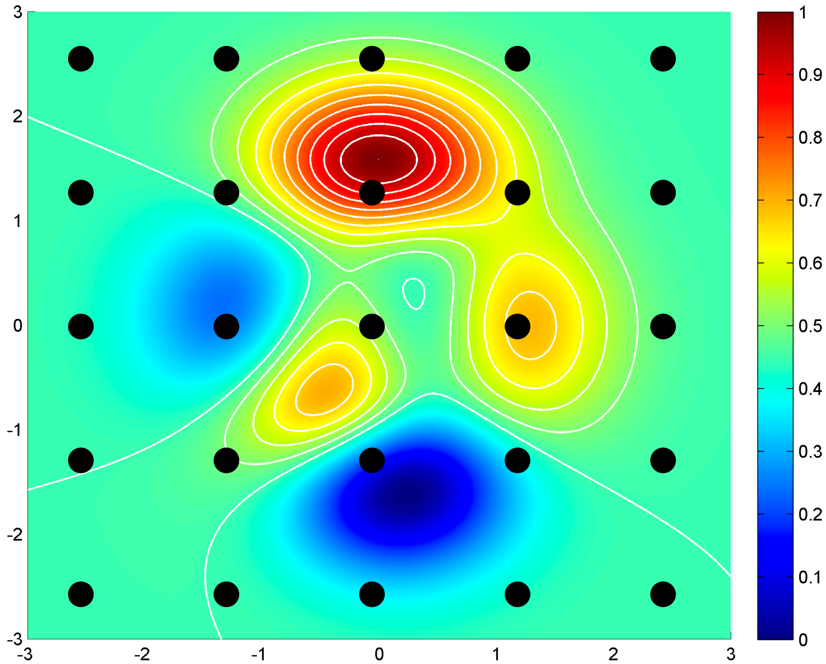


DATA >> RESOURCES

The data needed to adequately train meaningful models will likely exceed the available resources (financial, time, labor) allocated towards experimentation.

Why is SDoE important?

SDoE allows us to make the most out of our resources.



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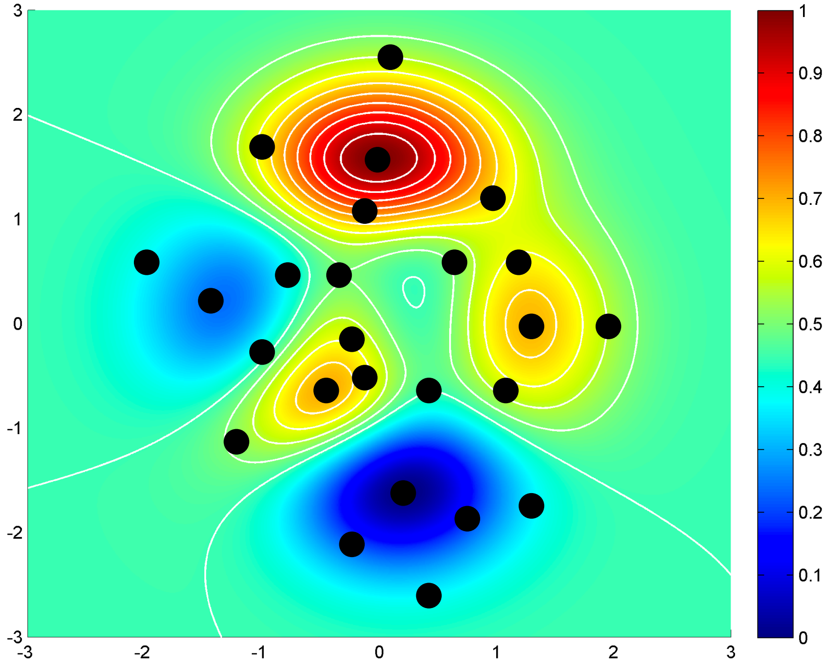

With SDoE, we can…

- ✓ **Be strategic** about collecting the most advantageous data given available resources
- ✓ **Be agile** in our model development to reflect current understanding

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Fundamentals of SDoE

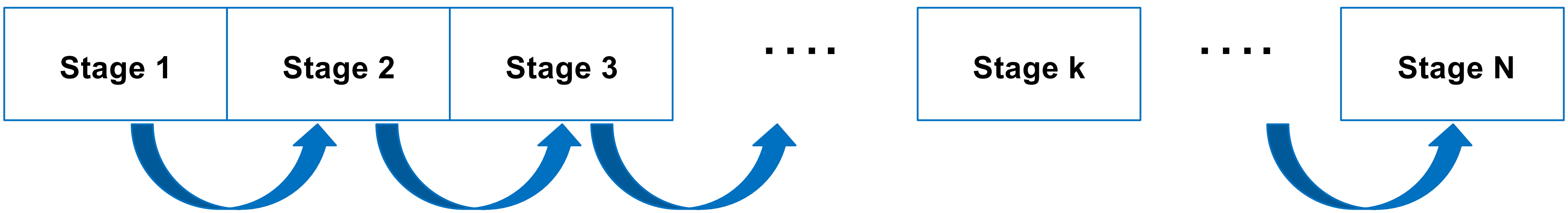
Given an experiment…

Experiment

1) Break the entire experiment into stages

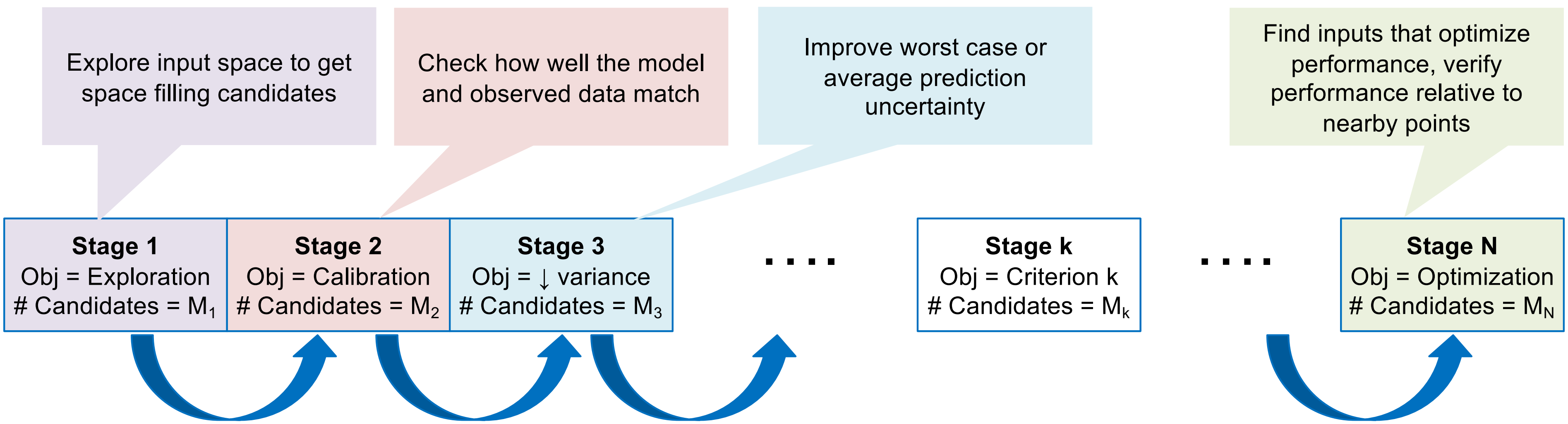
Fundamentals of SDoE

Given an experiment…



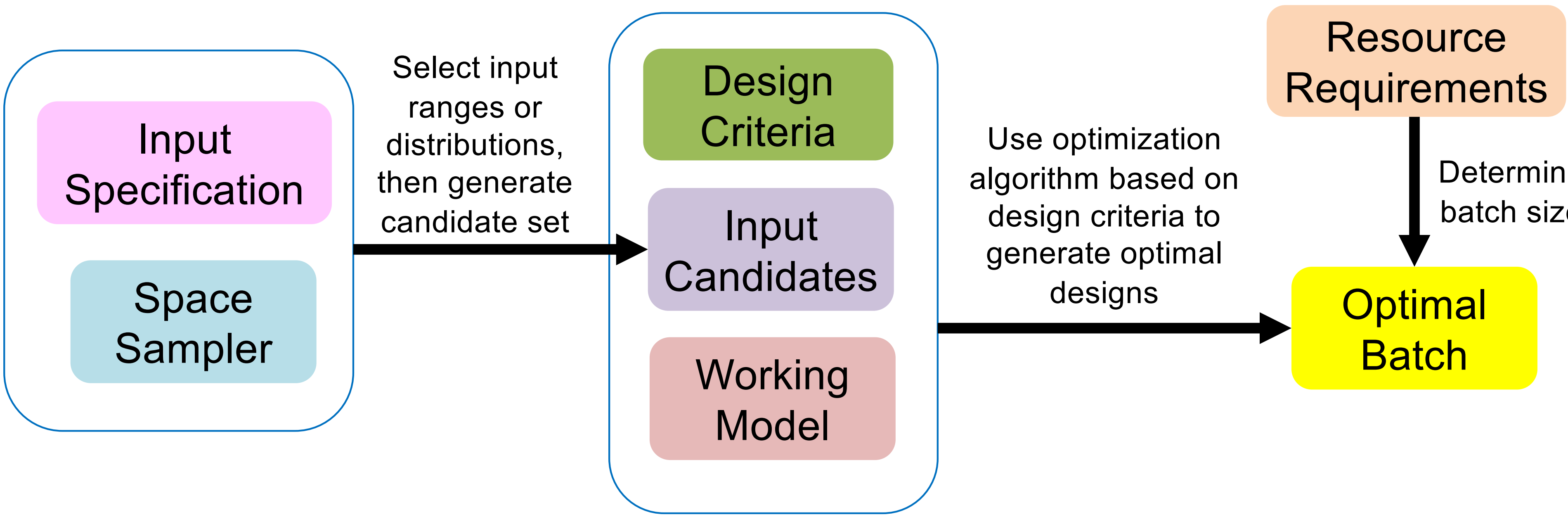
1) Break the entire experiment into stages
   - Data from each stage is analyzed to inform what data to collect at the next stage.

Fundamentals of SDoE



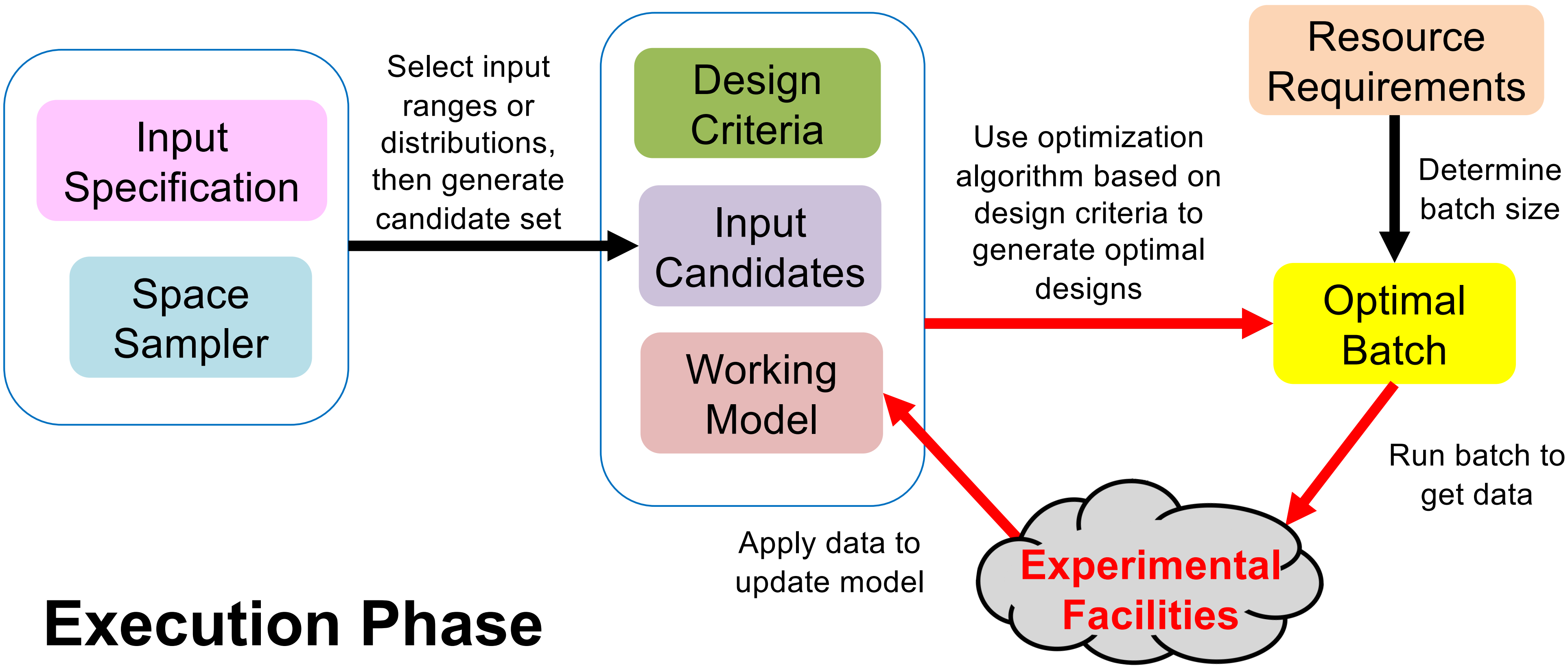
1) Break the entire experiment into stages
   - Data from each stage is analyzed to inform what data to collect at the next stage.
2) Customize each stage based on its objective and budget.

The SDoE Process



Planning Phase

The SDoE Process



Execution Phase

The SDoE Process

Select input ranges or

Design Criteria

Use optimization

Resource Requirements

Input

Stay tuned for the next talk on

"Application of Sequential Design of Experiments (SDoE) to Solvent-Based CO_2 Capture Systems at Multiple Scales"

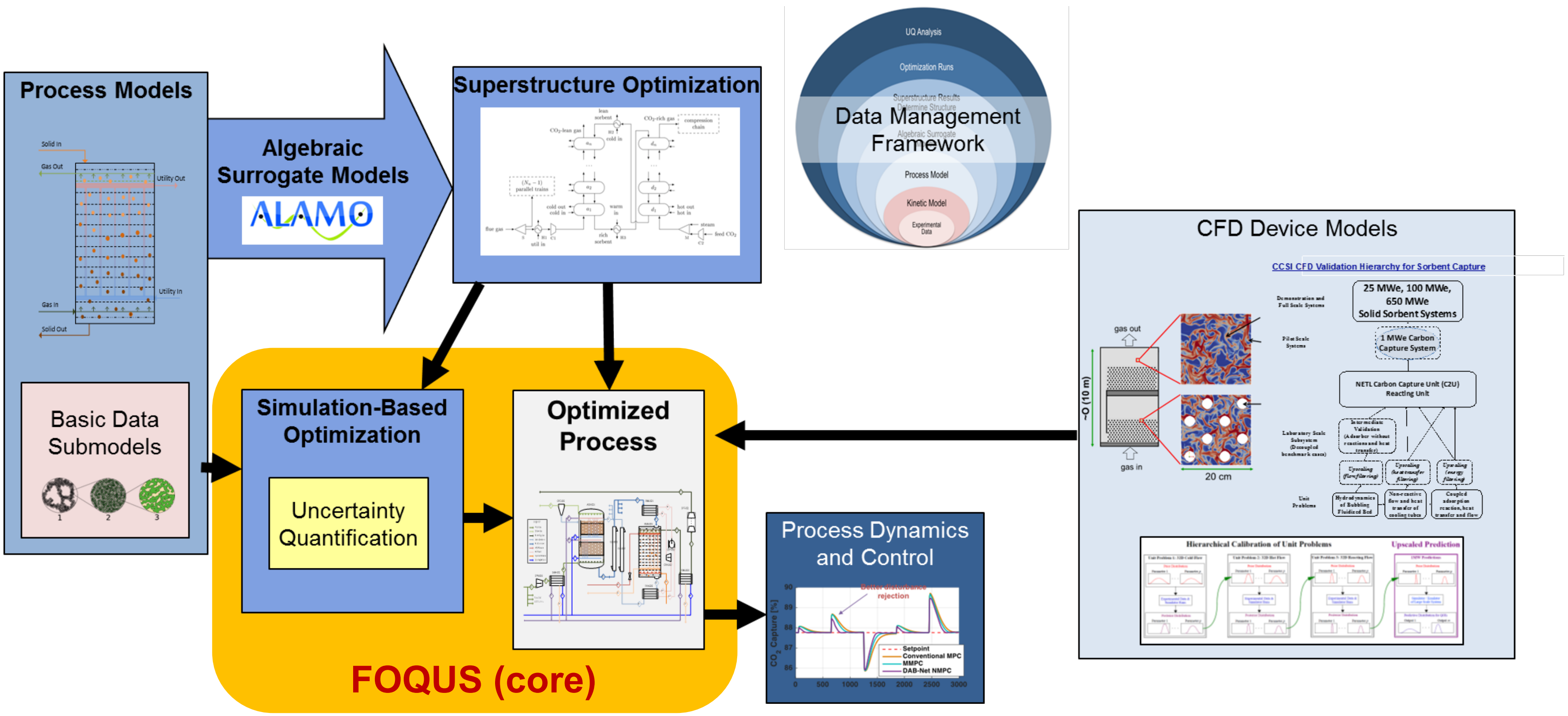
Batch

Working Model

Run batch to get data

Apply data to update model

Framework for Optimization & Quantification of Uncertainty and Surrogates



2016 R&D 100 Award Recipient

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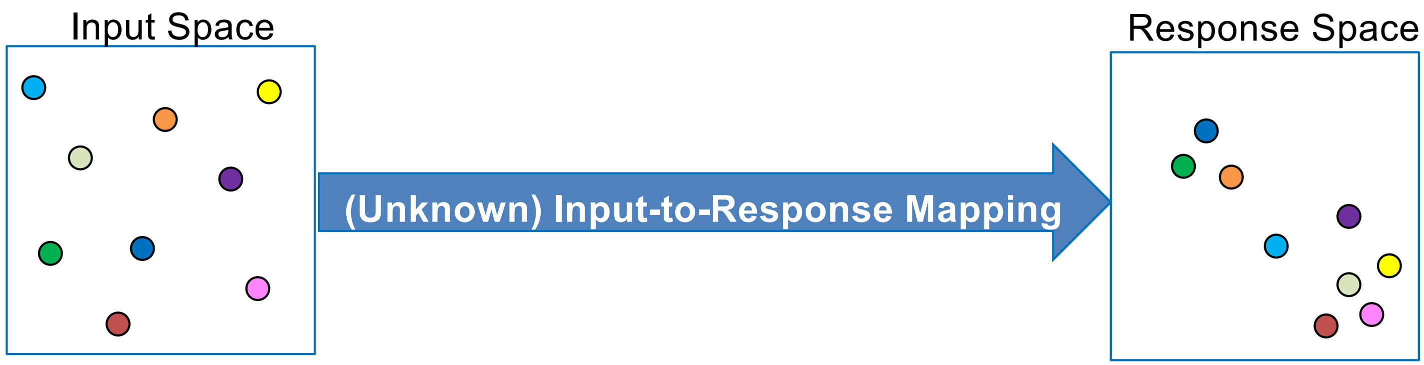
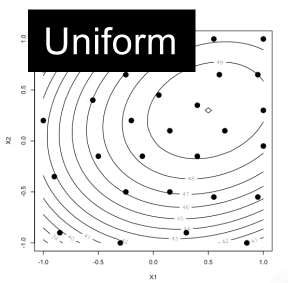
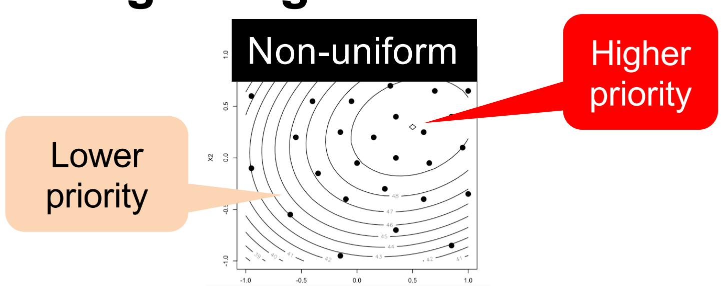
Space Filling Designs in FOQUS (Current)



Input Space Filling Designs

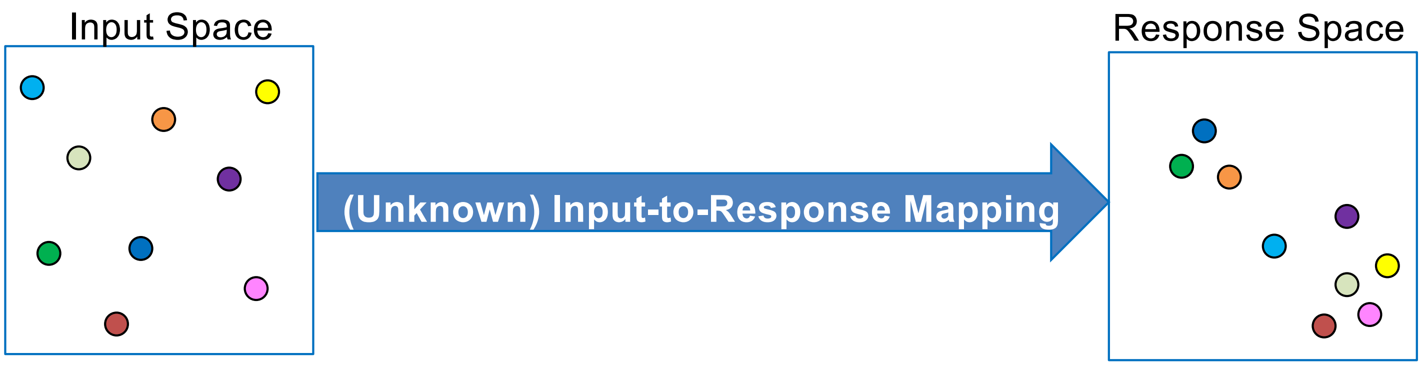


Industry standard for input space exploration



Allows control over density of points, based on optimizing response or reducing uncertainty

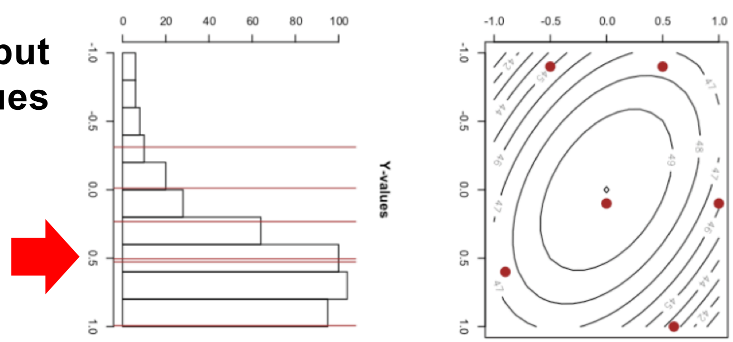
Space Filling Designs in FOQUS (Planned)



Input Space Filling Designs

Output values

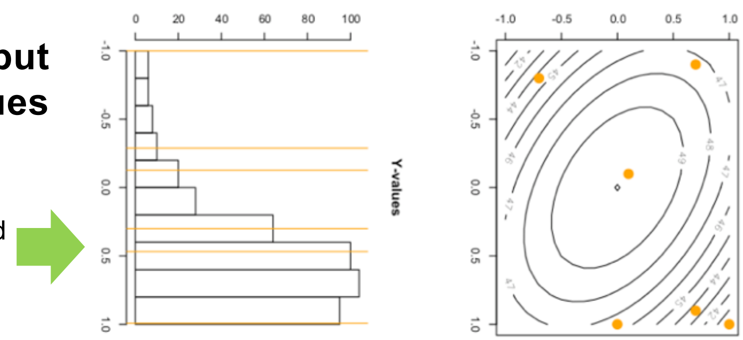
Poor spread



Input-Response Filling Designs

Output values

Improved spread



Allows good spread in both input & response spaces

SDoE Capabilities in FOQUS

- **Version 1 – already released (March 2019) with documentation**
  - **Uniform space filling designs**
    - ✓ Candidates can be read from file or sampled based on input ranges/PDFs

- **Version 2 – planned release (target date: December 2019)**
  - **Non-uniform space filling designs**
    - ✓ Allows experimenter to emphasize some regions of input space

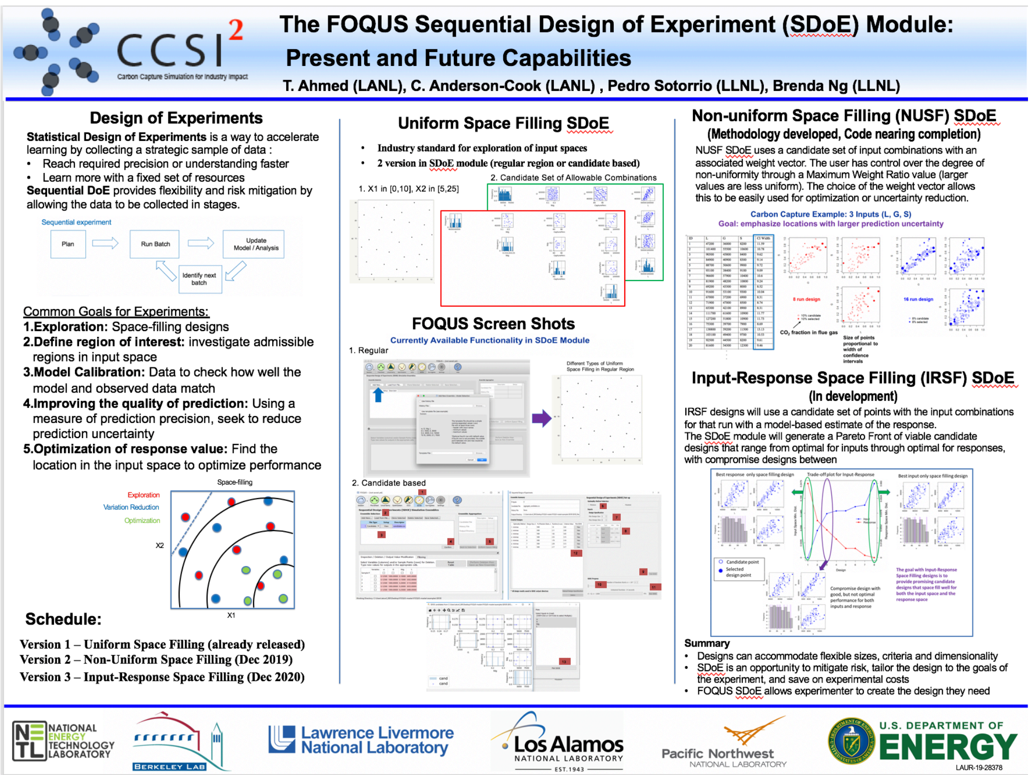
- **Version 3 – planned release (target date: December 2020)**
  - **Input-response space filling designs**
    - ✓ Allows experimenters to achieve balance between space filling in input space AND good range of response values

Summary

- **SDoE is a powerful tool to accelerate learning**, by incorporating (in near real time) empirical information from an experiment as it is being run.
- **SDoE targets maximally helpful input combinations** for experiment goals.
- Innovations in SDOE allow for:
  - **Risk reduction**: by breaking the experiment into stages, knowledge gained from earlier stages can be leveraged to refine data collection in later stages
  - **Customization**: experimenter may tune the sample density using NUSF
  - **Improved optimization**: input-response space filling designs incorporates good spread in both input and output space
- **FOQUS SDoE module currently supports uniform and non-uniform space-filling designs, with or without historical data.**

To learn more, check out our poster and demo!

Poster presented by Towfiq Ahmed (LANL)



Demo presented by Brenda Ng (LLNL)