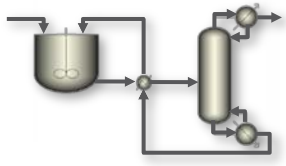
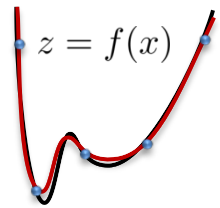




$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

Optimization of Carbon Capture Systems Using Surrogate Models of Simulated Processes

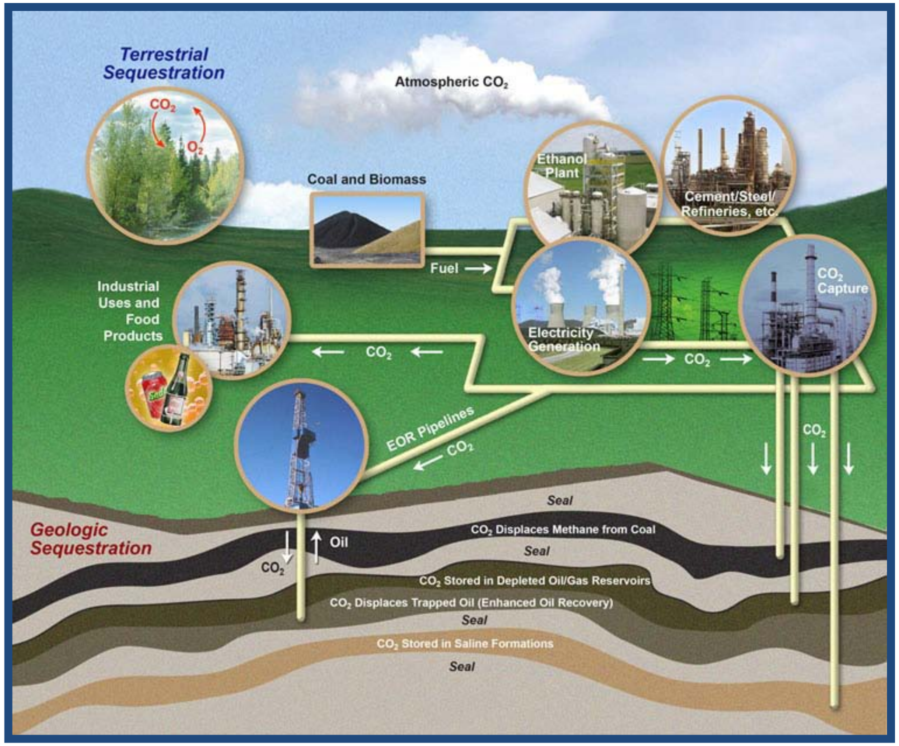
Alison Cozad[1] YoungJung Chang[1] Nick Sahinidis[1] David Miller[2]

[1]Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA

[2]US DOE-National Energy Technology Laboratory, Morgantown, WV

MOTIVATION

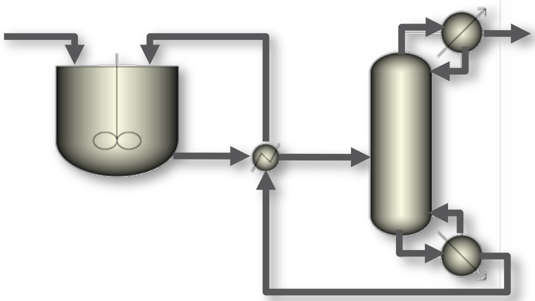
- **One-third of U.S. CO_2 emissions come from power plants and other point sources**
- **Available carbon capture technologies would increase electricity costs**
  - **Pulverized coal plants**
    - ***Currently: 75% increase***
    - ***Goal: <30% increase***



http://www.netl.doe.gov/technologies/carbon_seq/index.html

OBJECTIVE: PROCESS SYNTHESIS

Process simulation



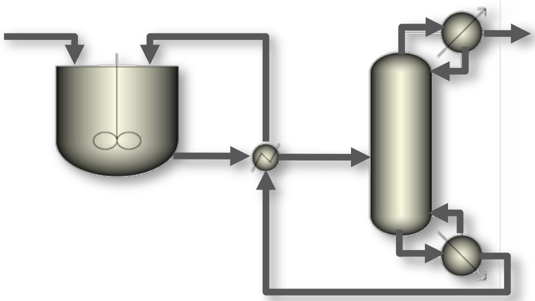
Ideally

Derivative-based optimization

$$\min \quad f(x)$$
$$\text{s.t.} \quad g(x) = 0$$

OBJECTIVE: PROCESS SYNTHESIS

Process simulation



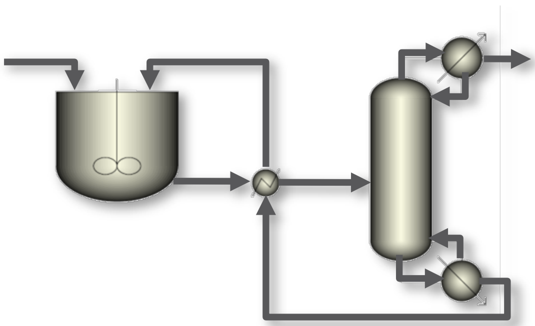
Derivative-based optimization

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

- **Lack of an algebraic models**
- **Computationally costly simulations**
- **Scarcity of fully robust simulations**

OBJECTIVE: PROCESS SYNTHESIS

Process simulation



Ide y

Derivative-based optimization

$$\min \quad f(x)$$
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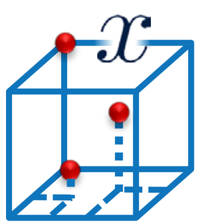
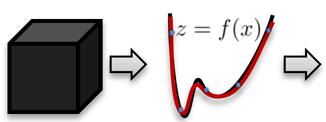


Data

ALAMO

Automated **L**earning of **A**lgebraic **M**odels for **O**ptimization



$$\min \quad f(x)$$
$$\text{s.t.} \quad g(x) = 0$$

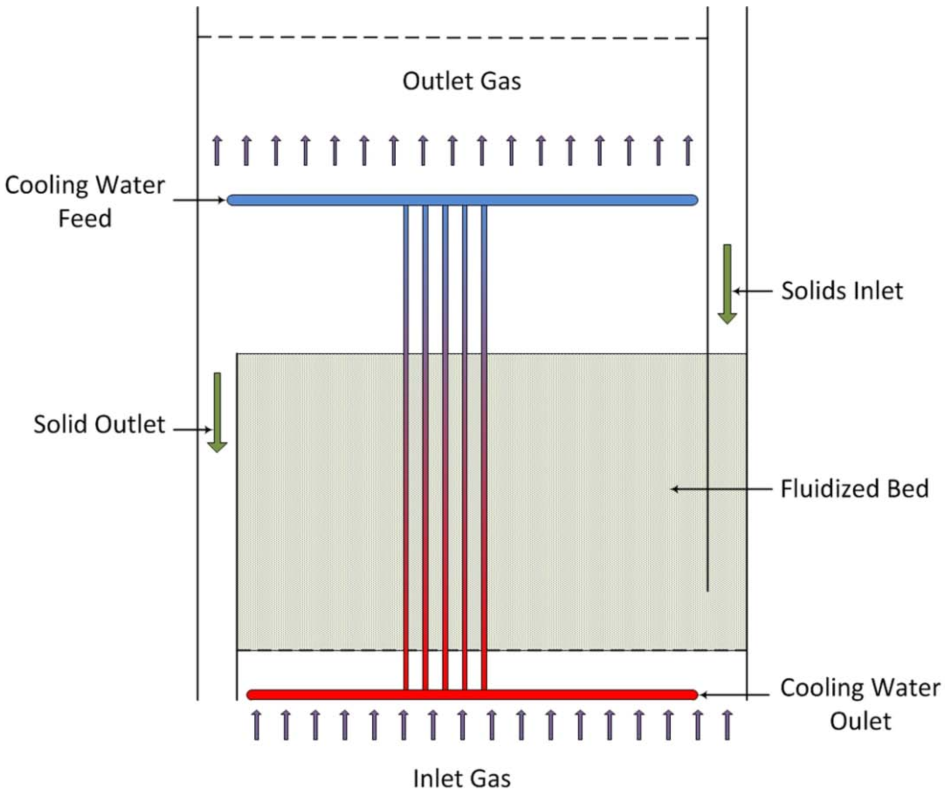
$$z_1 = g_1(x)$$
$$z_2 = g_2(x)$$
$$\dots$$
$$z_k = g_k(x)$$

Models

SOLID SORBENT CARBON CAPTURE

- **Solid sorbent processes**
  - **Fast fluidized bed**
  - **Pneumatic conveyer**
  - **Moving/Fixed bed**
  - **Bubbling fluidized bed**

- **Bubbling fluidized bed**
  - **1D model**
  - **Modeled in Aspen Custom modeler**
  - **Differential model**
  - **Uses Aspen Properties package**



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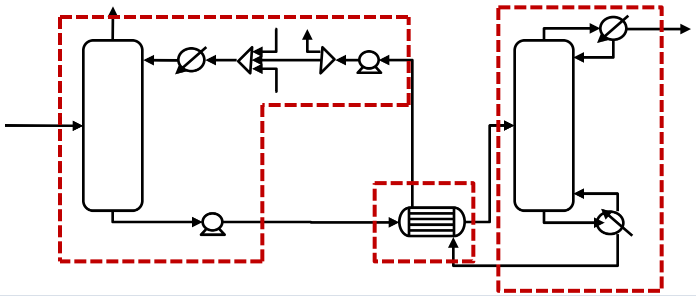
OVERVIEW OF THE METHOD

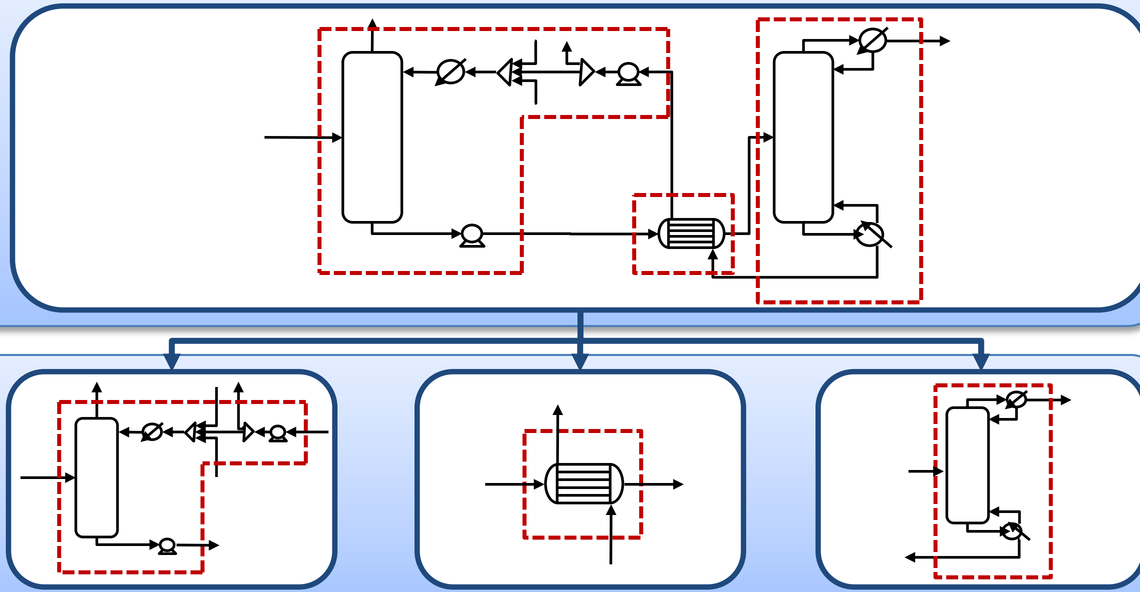
Simulation



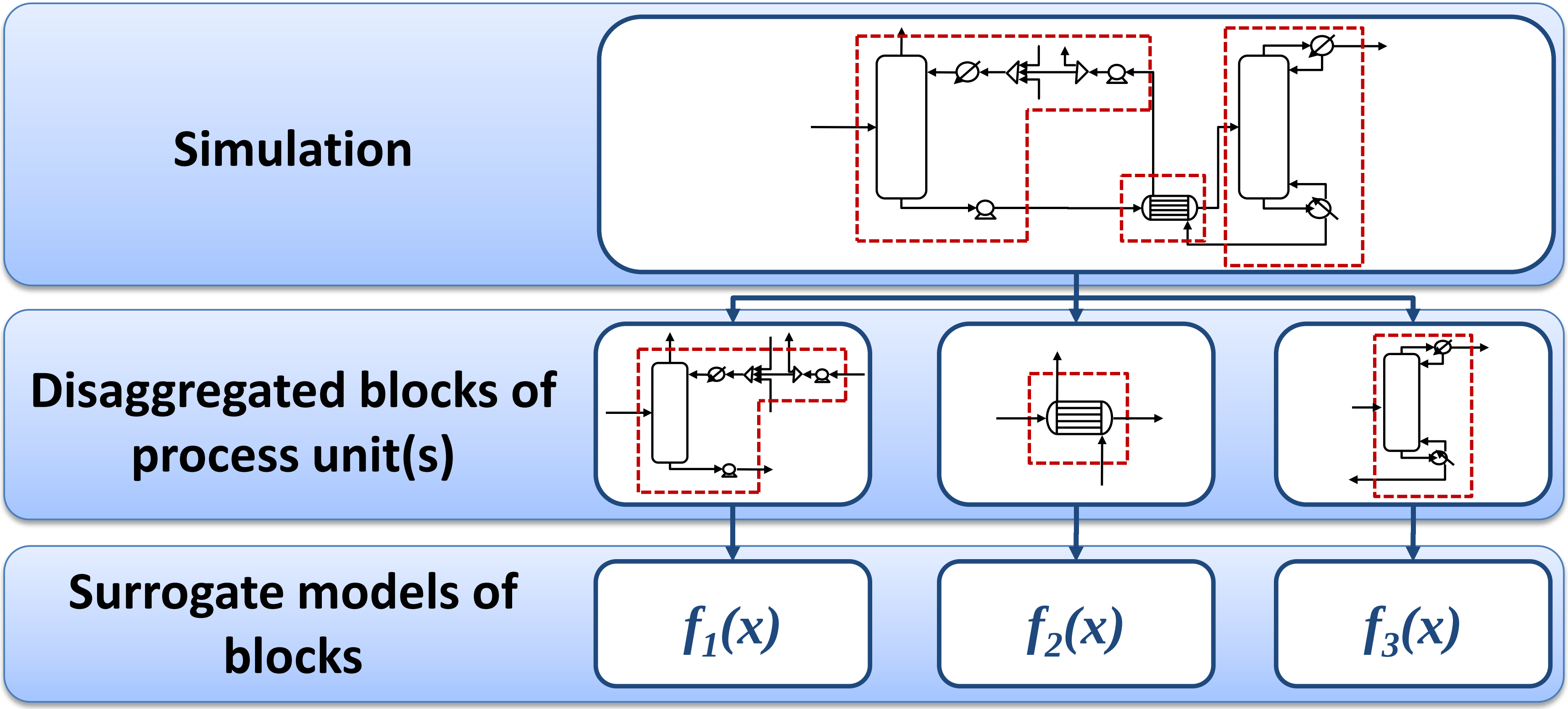
OVERVIEW OF THE METHOD

Simulation

Disaggregated blocks of process unit(s)

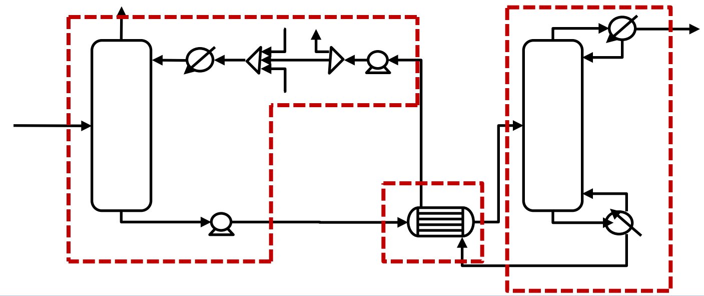


OVERVIEW OF THE METHOD

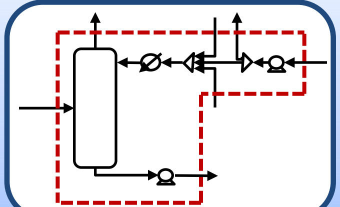


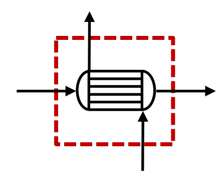
OVERVIEW OF THE METHOD

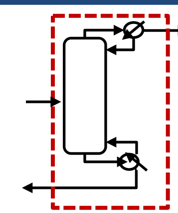
Simulation



Disaggregated blocks of process unit(s)







Surrogate models of blocks

$f_1(x)$ | $f_2(x)$ | $f_3(x)$

Algebraic constraints

Mass balances | Design specs

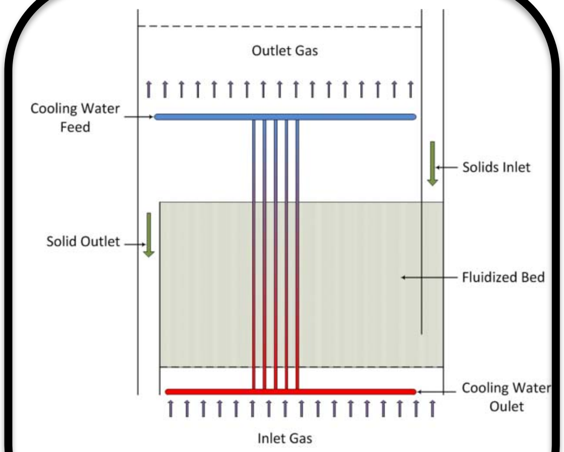
Nonlinear program

Algebraic model for optimization

NOTATION

$$x \in \mathbb{R}^D$$
$$x^l \leq x \leq x^u$$

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \\ \vdots \\ x_D \end{pmatrix}$$



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$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix}$$

$$z \in \mathbb{R}^K$$
$$z = f(x)$$

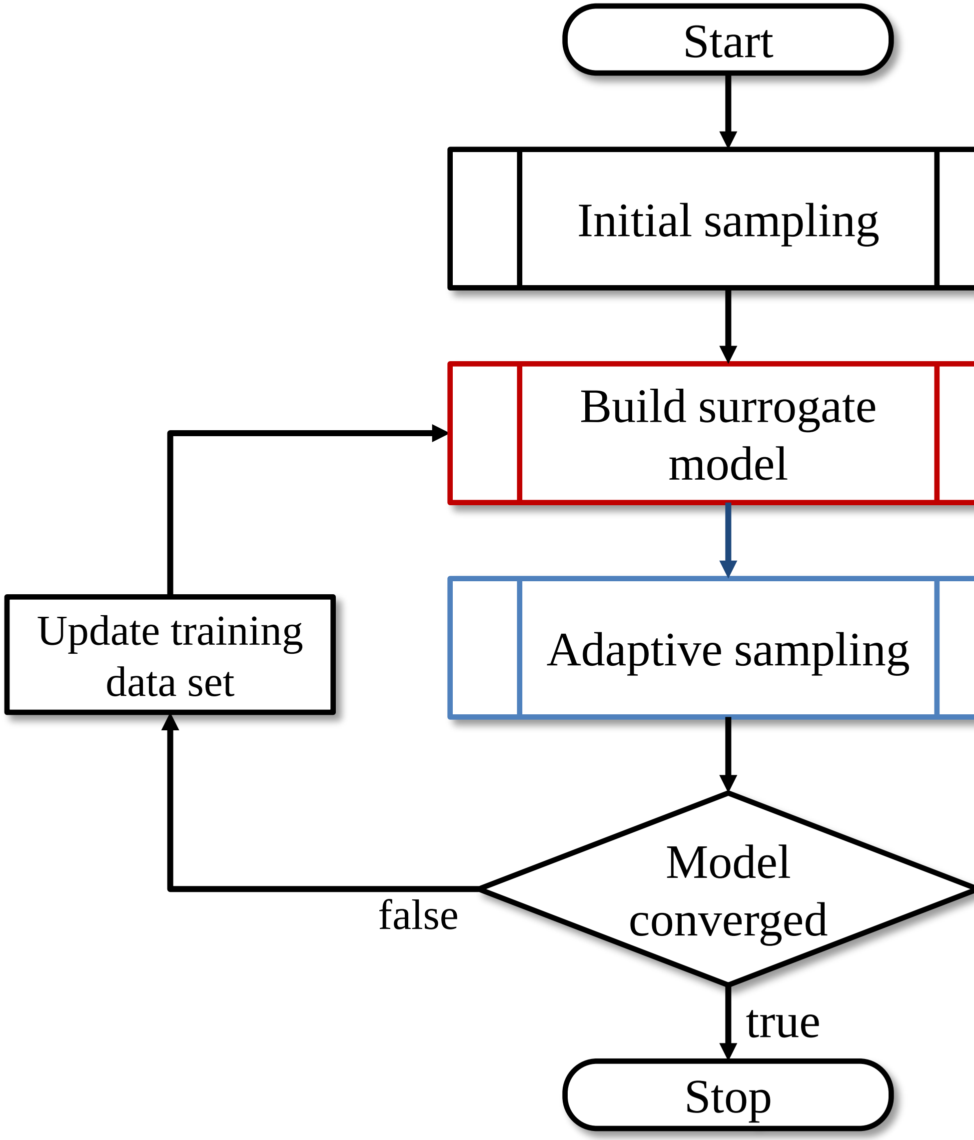
Independent variables, x

- Geometry
- Operating conditions
- Inlet flow conditions

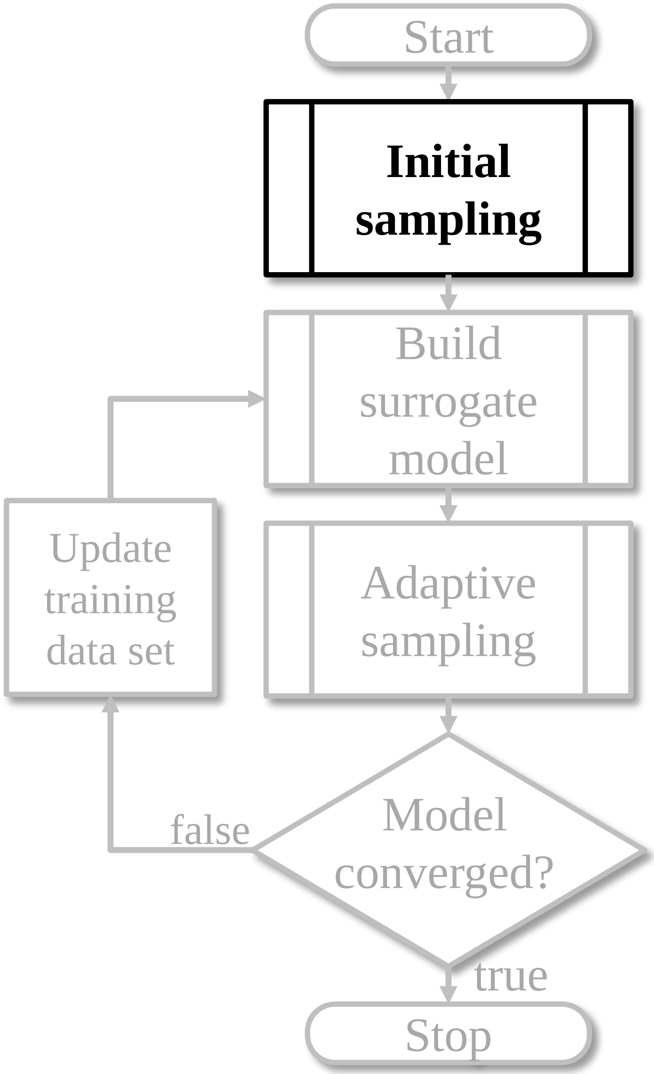
Dependent variables, z

- Geometry required
- Operating condition required
- Outlet flow conditions
- Design constraints

SURROGATE MODEL GENERATION

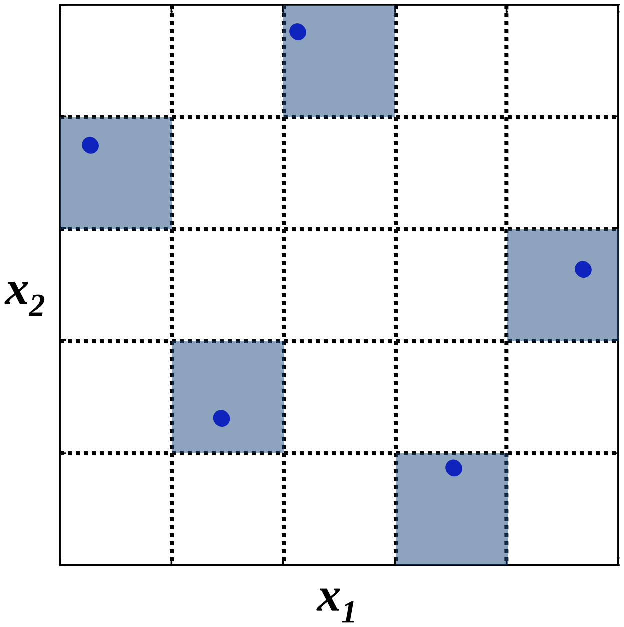


SAMPLE PROBLEM SPACE

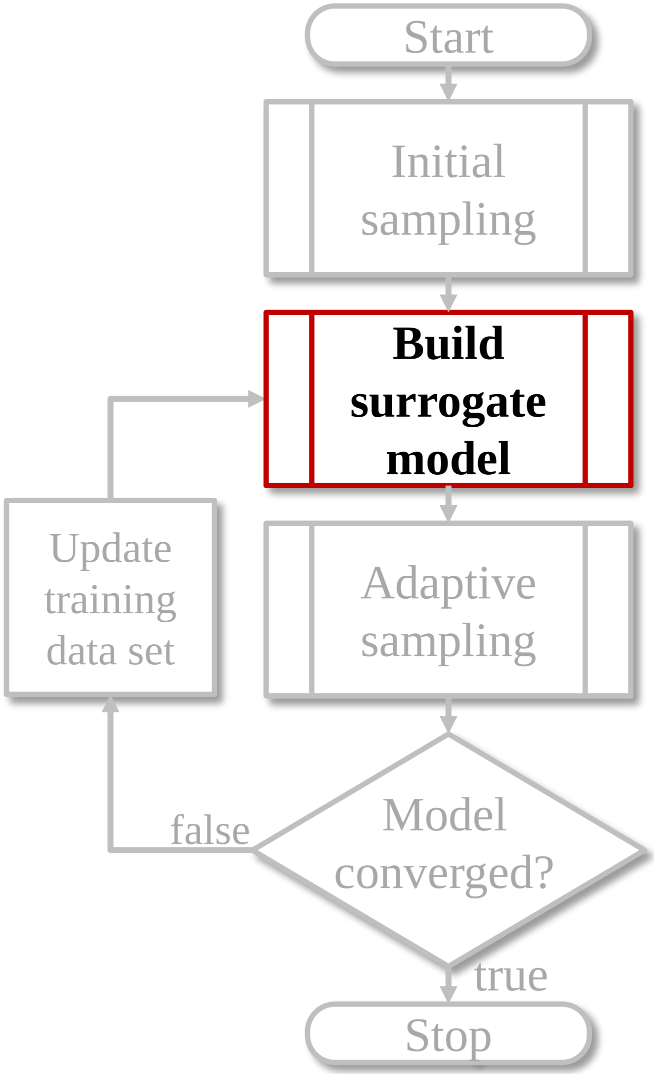


Design of experiments

1. Random points sampling
2. Factorial design
3. Latin hypercube design
   - *Space-filling design*



MODEL BUILDING



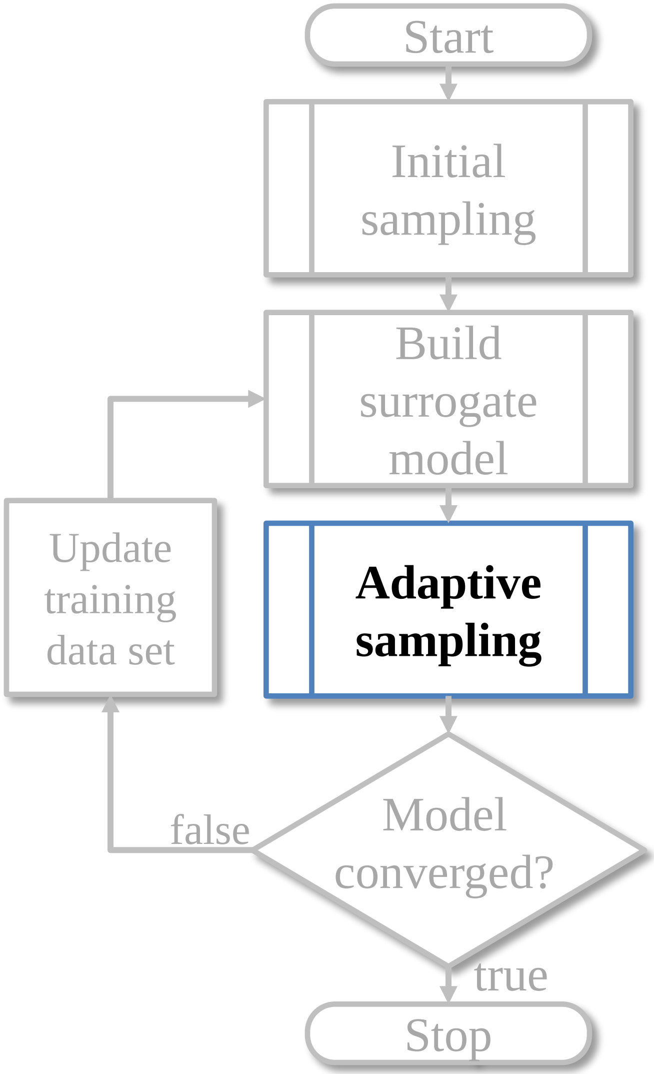
- **Identify the functional form and complexity of the surrogate models**

$$z = f(x)$$

- **Functional form:**
  - **Combine simple basis functions**

Category	Basis function
Polynomial	$(x_d)^\alpha$
Multinomial	$\prod_{d=1}^{m} (x_d)^{\alpha_d}$, for $m = 1, 2, \ldots$
Exponential and logarithmic forms	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha$, $\log\left(\frac{x_d}{\gamma}\right)^\alpha$
Expected bases	From experience, simple inspection, etc.

ADAPTIVE SAMPLING



- **Goal: Search the problem space for areas of model inconsistency or model mismatch**
- **More succinctly, we are trying to find points that maximize the model error with respect to the independent variables**

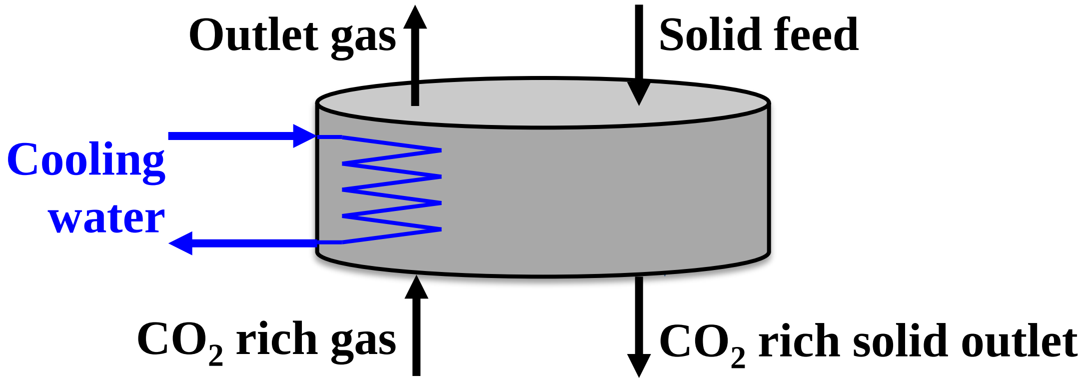
Surrogate model

$$\max_{x}\left(\frac{z(x)-\hat{z}(x)}{z(x)}\right)^{2}$$

  - **Maximize the relative model error using a derivative-free solver (SNOBFIT):**

BUBBLING FLUIDIZED BED

Bubbling fluidized bed adsorber diagram

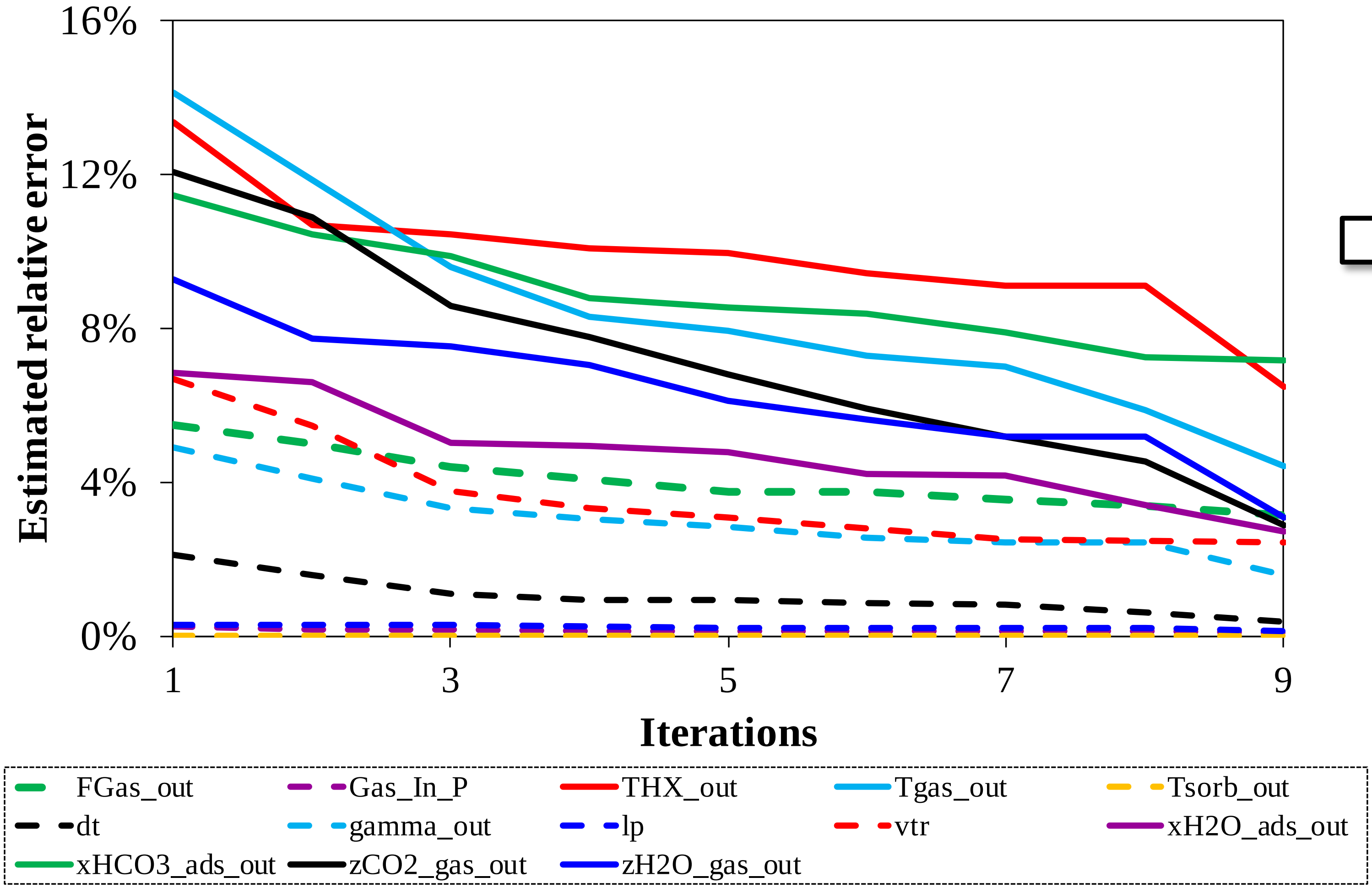


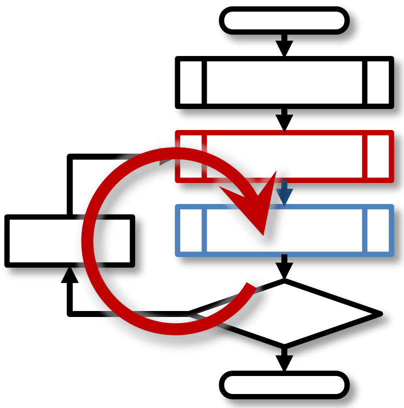
- **Model inputs (14 total)**
  - Geometry (3)
  - Operating conditions (4)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (4)

- **Model outputs (13 total)**
  - Geometry required (2)
  - Operating condition required (1)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (2)
  - Outlet temperatures (3)
  - Design constraint (1)

ADAPTIVE SAMPLING

Progression of mean error through the algorithm

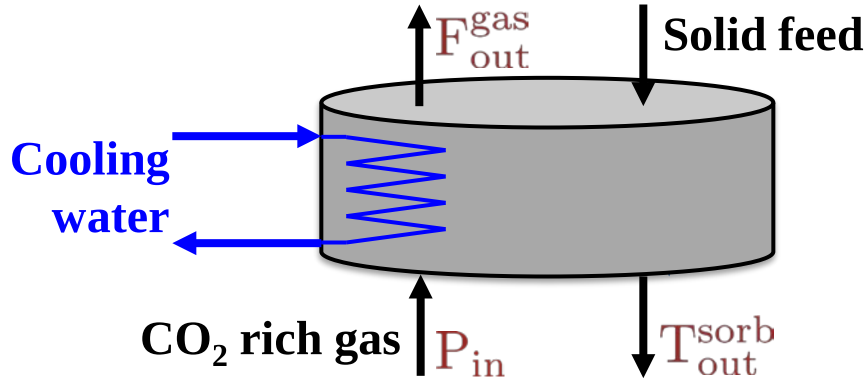




Initial data set: 137 pts

Final data set: 261

EXAMPLE MODELS

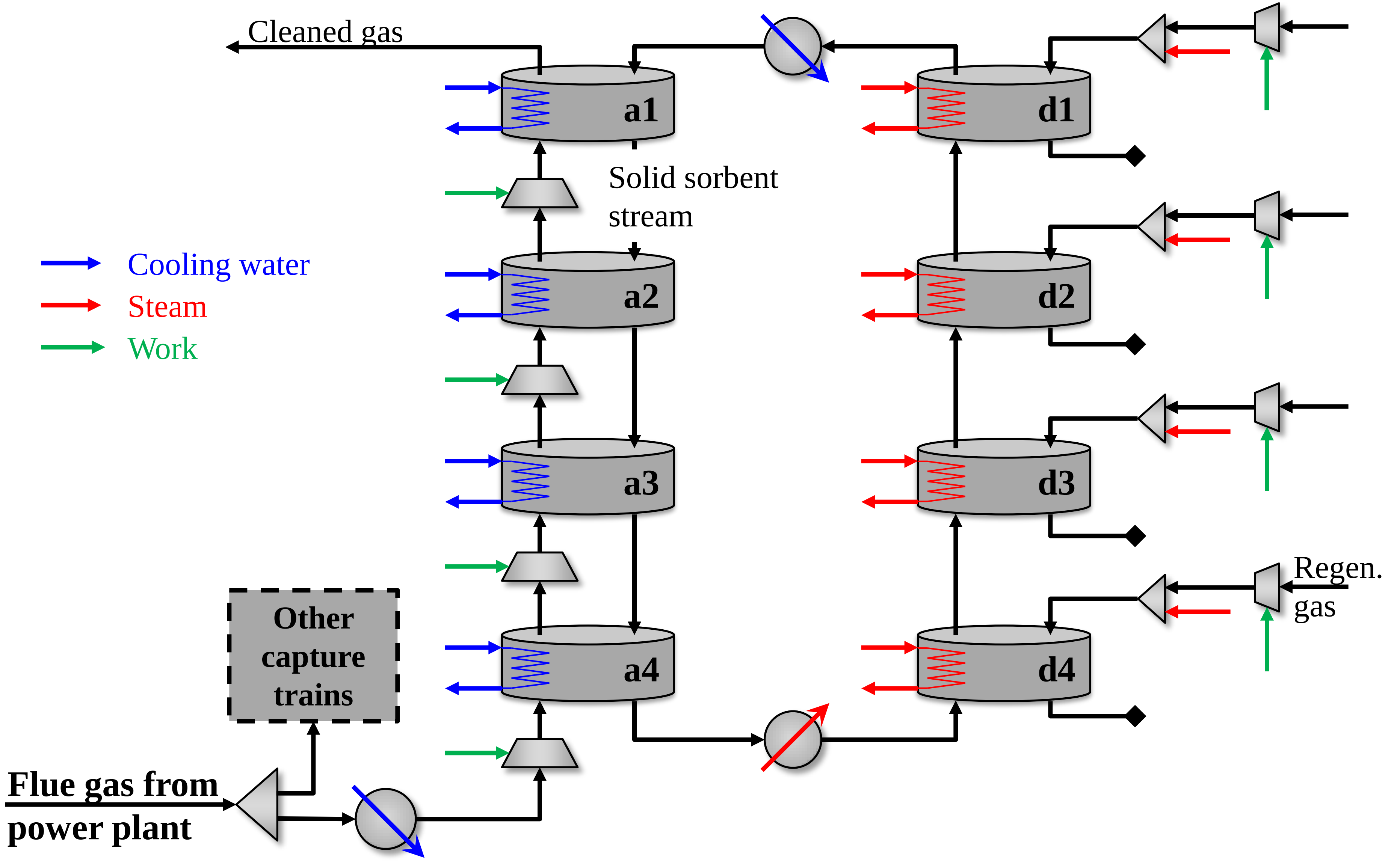


$$P_{in} = 1.0\,P_{out} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,v_{gi}) - \frac{51.1\,xHCO3^{ads}_{in}}{F^{gas}_{in}}$$

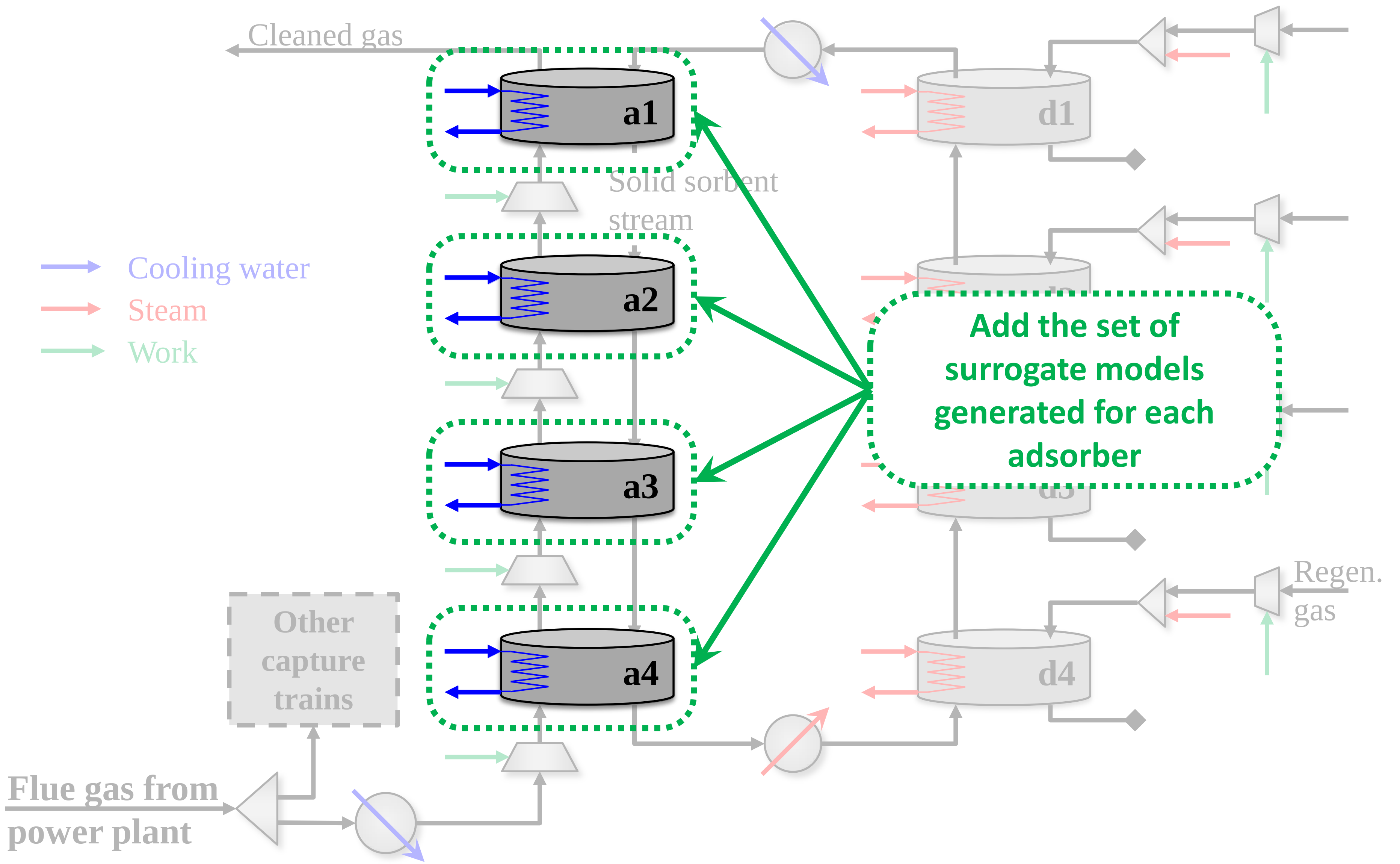
$$T^{sorb}_{out} = 1.0\,T^{gas}_{in} - \frac{\left(1.77 \cdot 10^{-10}\right)\,NX^2}{\gamma^2} - \frac{3.46}{NX\,T^{gas}_{in}\,T^{sorb}_{in}} + \frac{1.17 \cdot 10^4}{F^{sorb}\,NX\,xH2O^{ads}_{in}}$$

$$F^{gas}_{out} = 0.797\,F^{gas}_{in} - \frac{9.75\,T^{sorb}_{in}}{\gamma} - 0.77\,F^{gas}_{in}\,xCO2^{gas}_{in} + 0.00465\,F^{gas}_{in}\,T^{sorb}_{in} - 0.0181\,F^{gas}_{in}\,T^{sorb}_{in}\,xH2O^{gas}_{in}$$

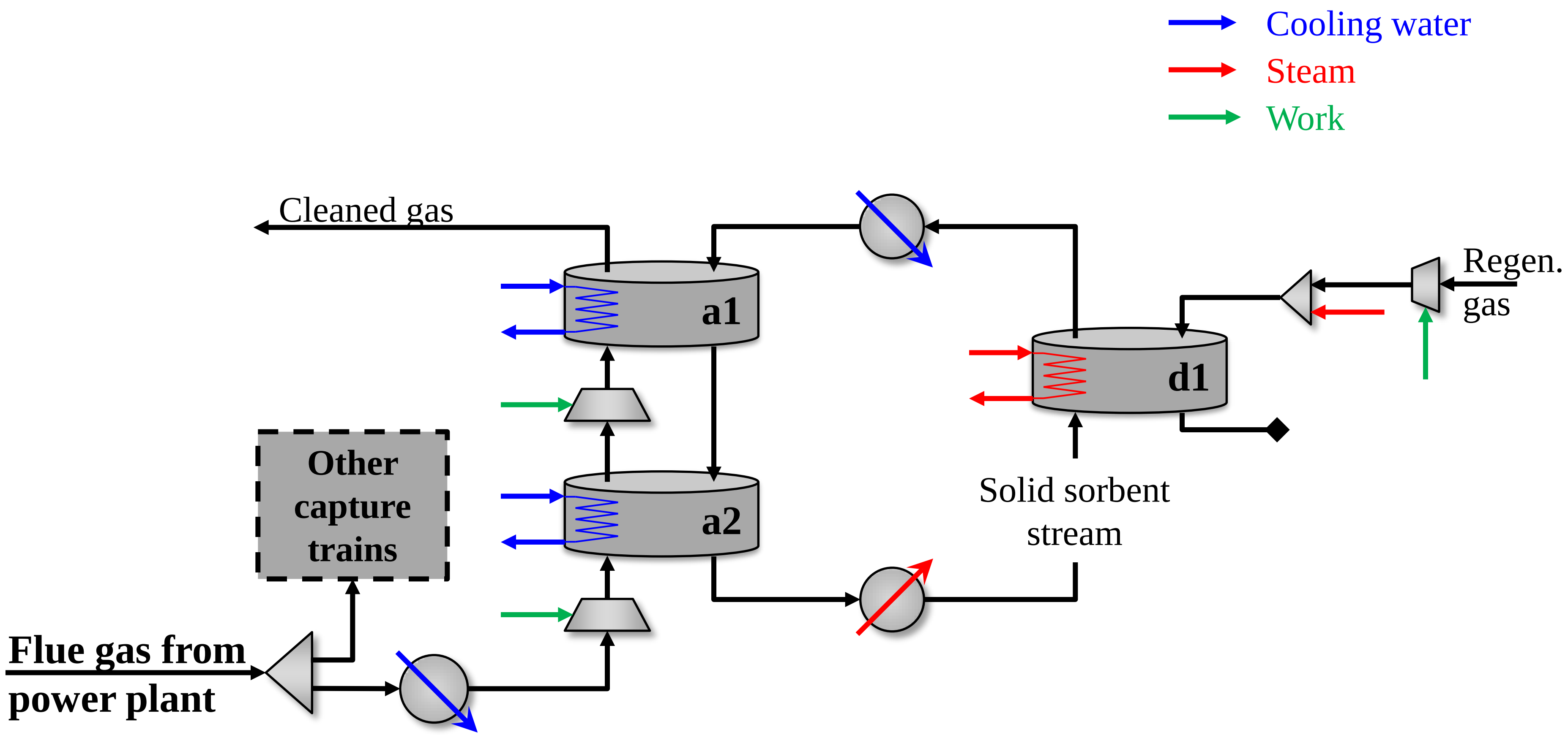
SUPERSTRUCTURE FLOWSHEET



SUPERSTRUCTURE FLOWSHEET



PRELIMINARY RESULTS



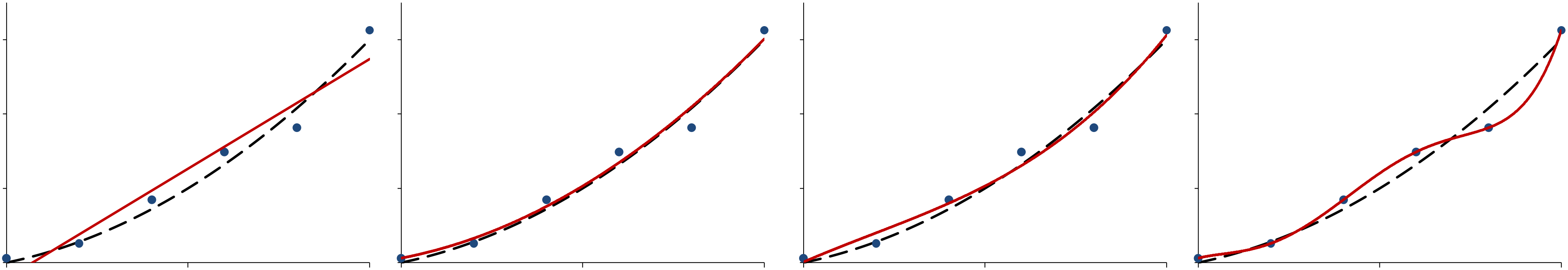
CONCLUSIONS

- **Using the our method, we were able to link detailed simulations of solid sorbent carbon capture processes with advanced derivative-based optimization software**
- **The resulting set of surrogates have been used to define a superstructure model that suggests a series of two adsorbers**

- For more information about,
  - The effort by the Carbon Capture and Simulation Initiative (CCSI) recently formed by the Department of Energy
    - *Synthesis of Optimal Adsorptive Carbon Capture Processes*. Y. Chang, et al (Given by D. Miller)
    - *Tuesday, October 18, 2011: 1:20 PM,   209 A/B*
  - The algorithm used to generate surrogate models
    - *Learning Surrogate Models of Processes From Experiments or Simulations.* A. Cozad, N. Sahinidis, D. Miller
    - *Thursday, October 20, 2011: 12:30 PM,   101 I*

AVOID OVERFITTING THE DATA

Increasing model complexity



Linear | **Quadratic** | **Cubic** | **5th Order**

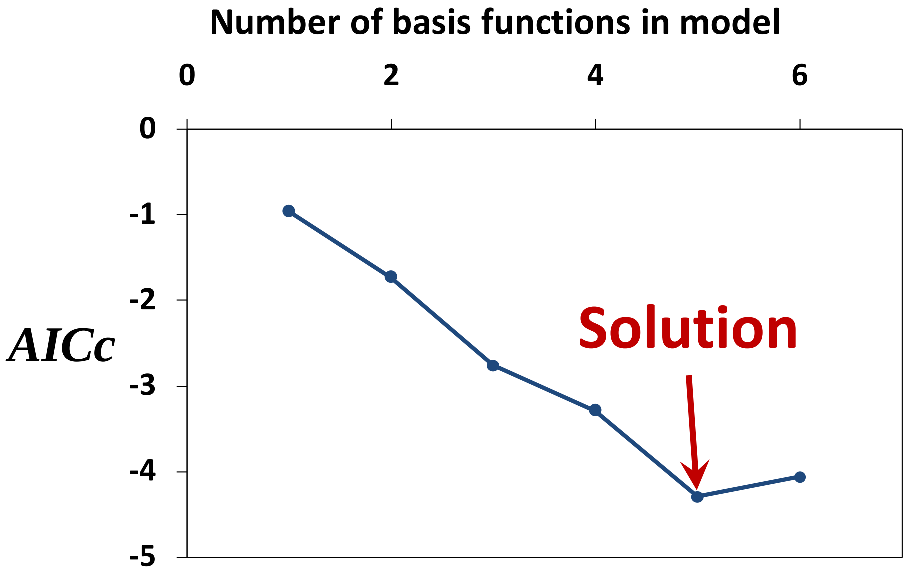
— True Function
• Data Points
— Model

HOW TO PICK THE BEST SUBSET

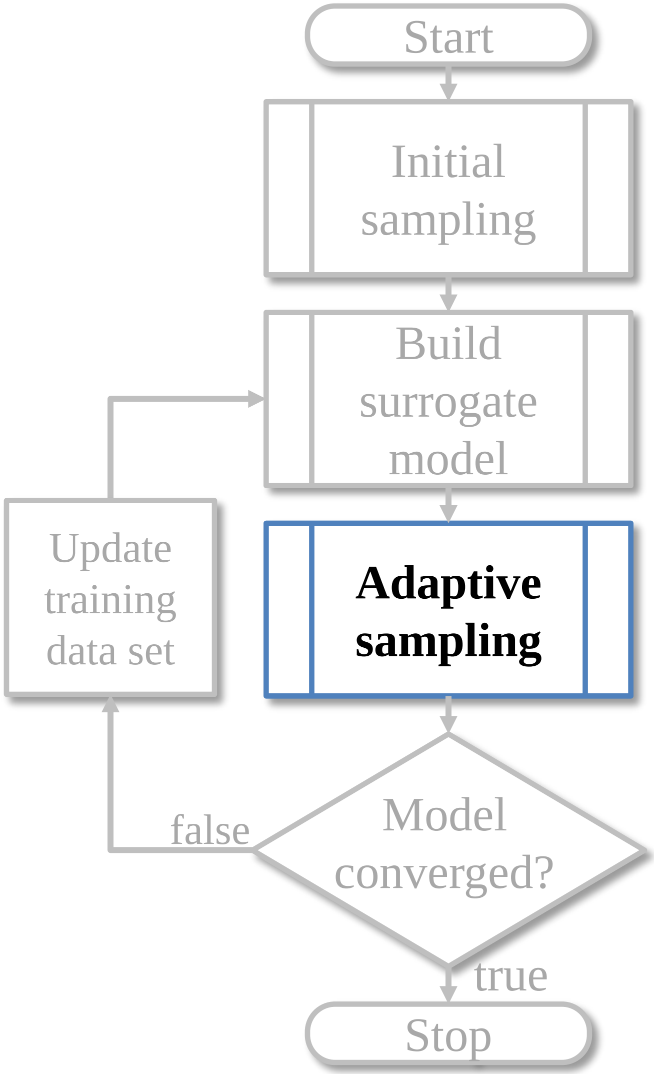
- **Corrected Akaike Information Criterion (*AICc*)**
  - **Gives an estimate of the difference between a model and the true function**

$$AICc = \underbrace{N \log\left(\frac{SSE}{N}\right)}_{\text{Accuracy}} + \underbrace{2T + \frac{2T\,(T+1)}{N-T-1}}_{\text{Complexity}}$$

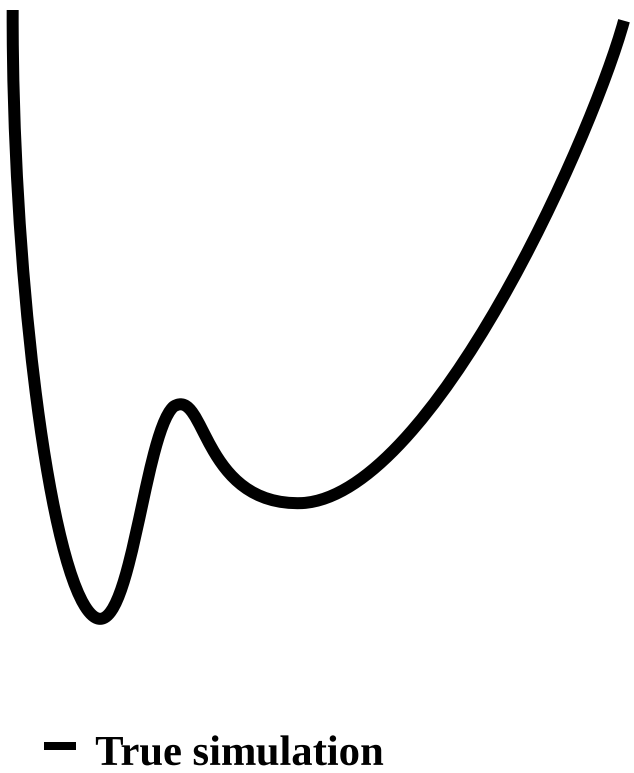
Accuracy + Complexity



ADAPTIVE SAMPLING



- **Illustrative example:**



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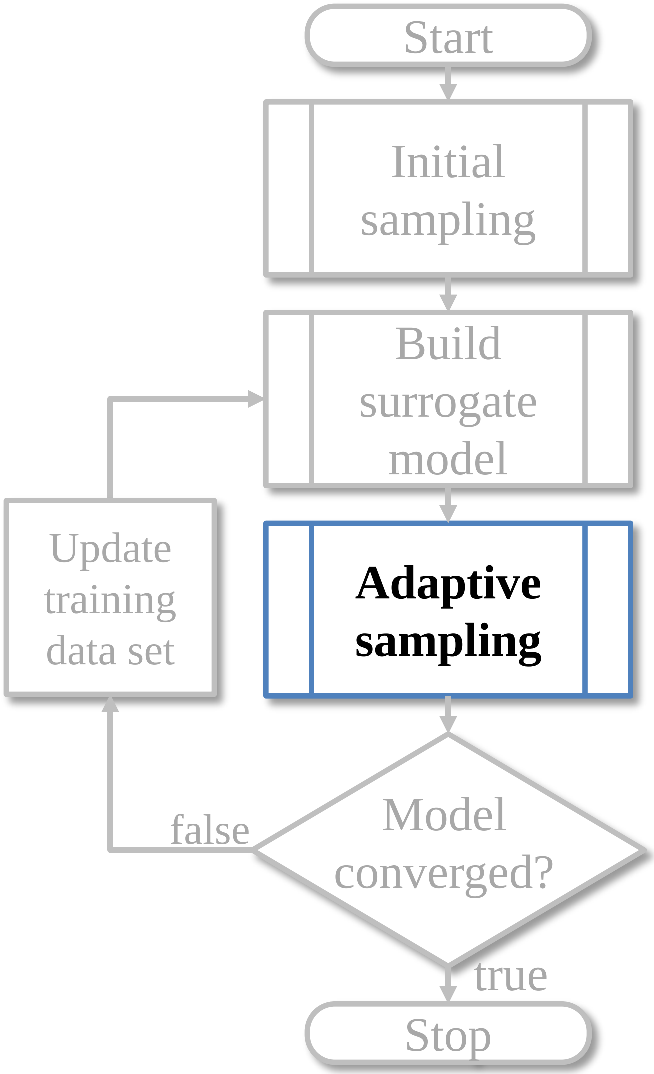

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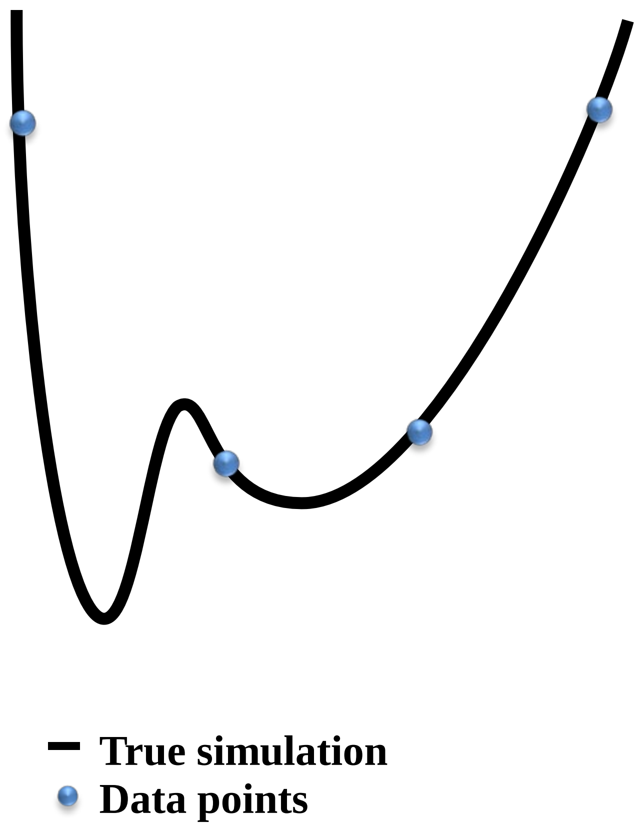

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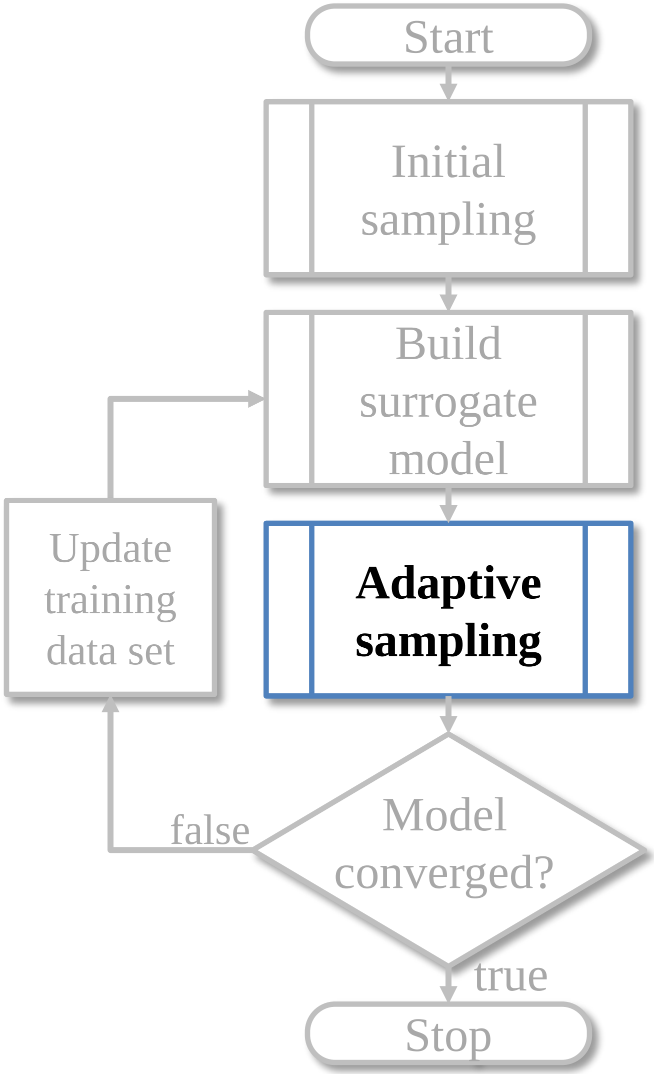

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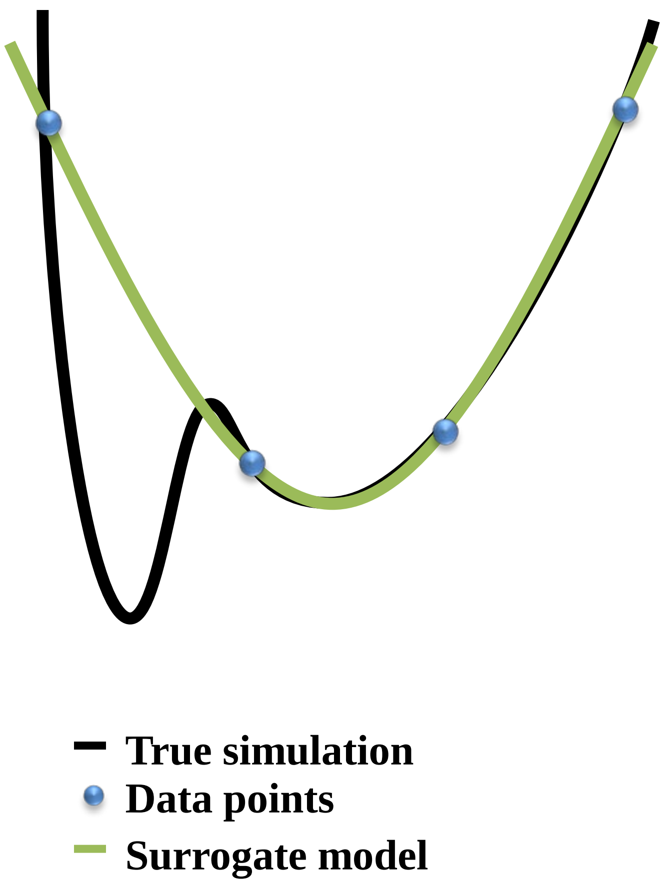

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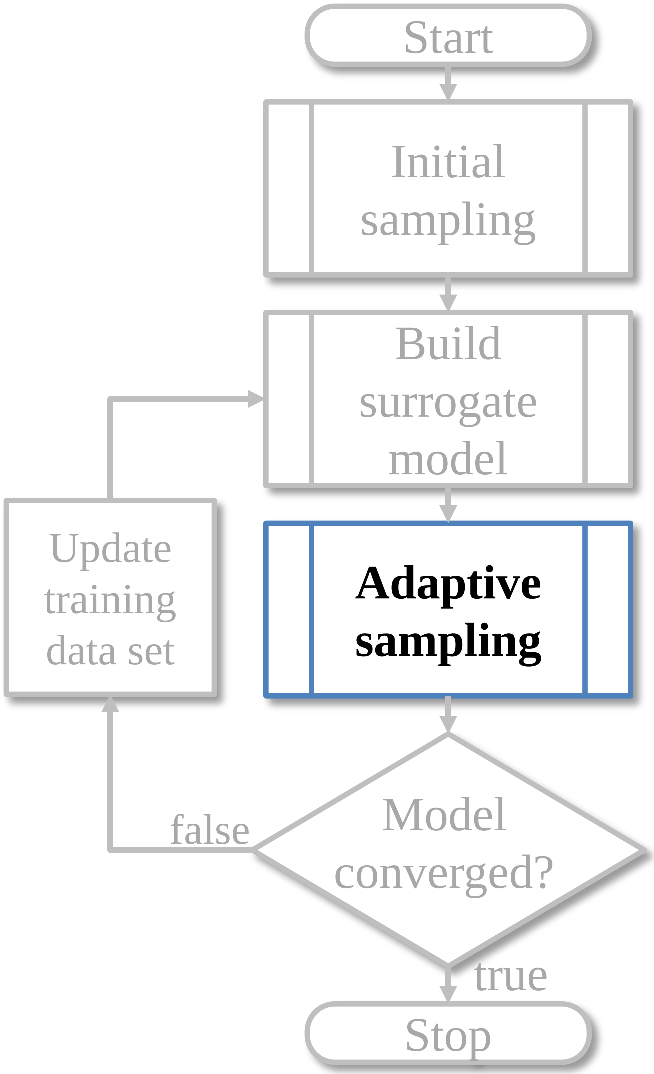

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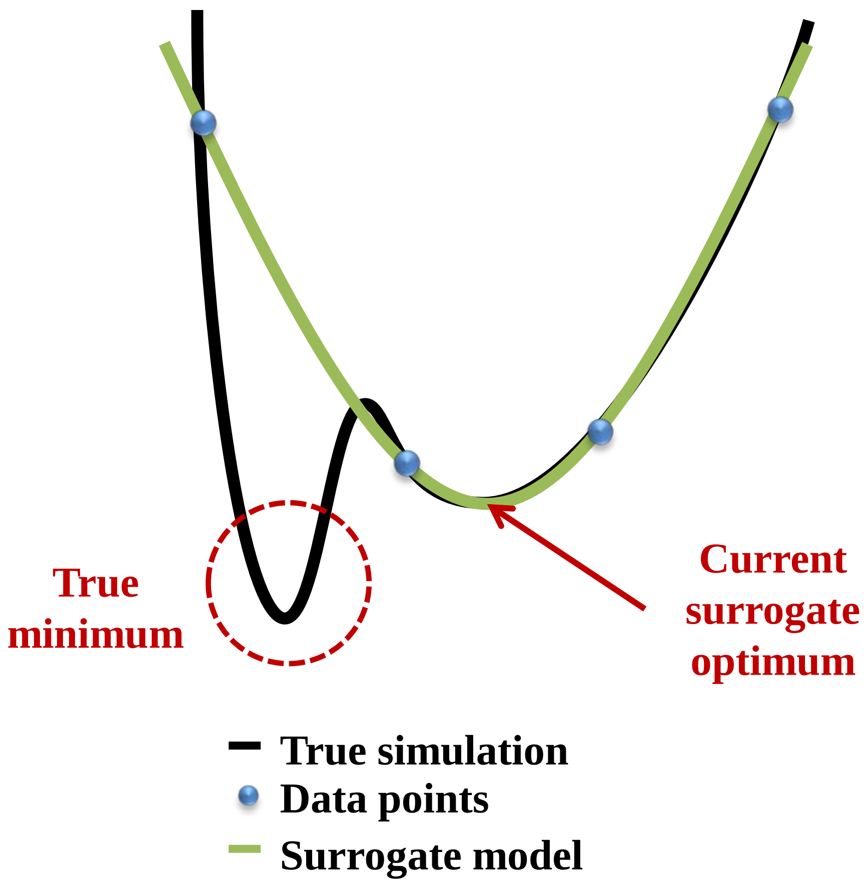

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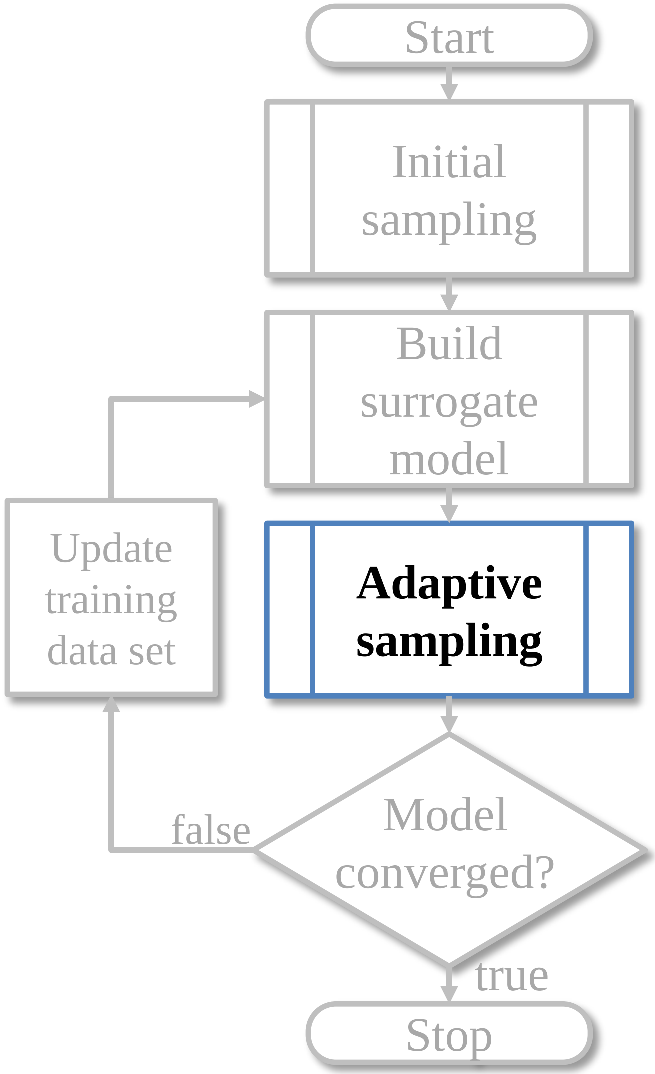

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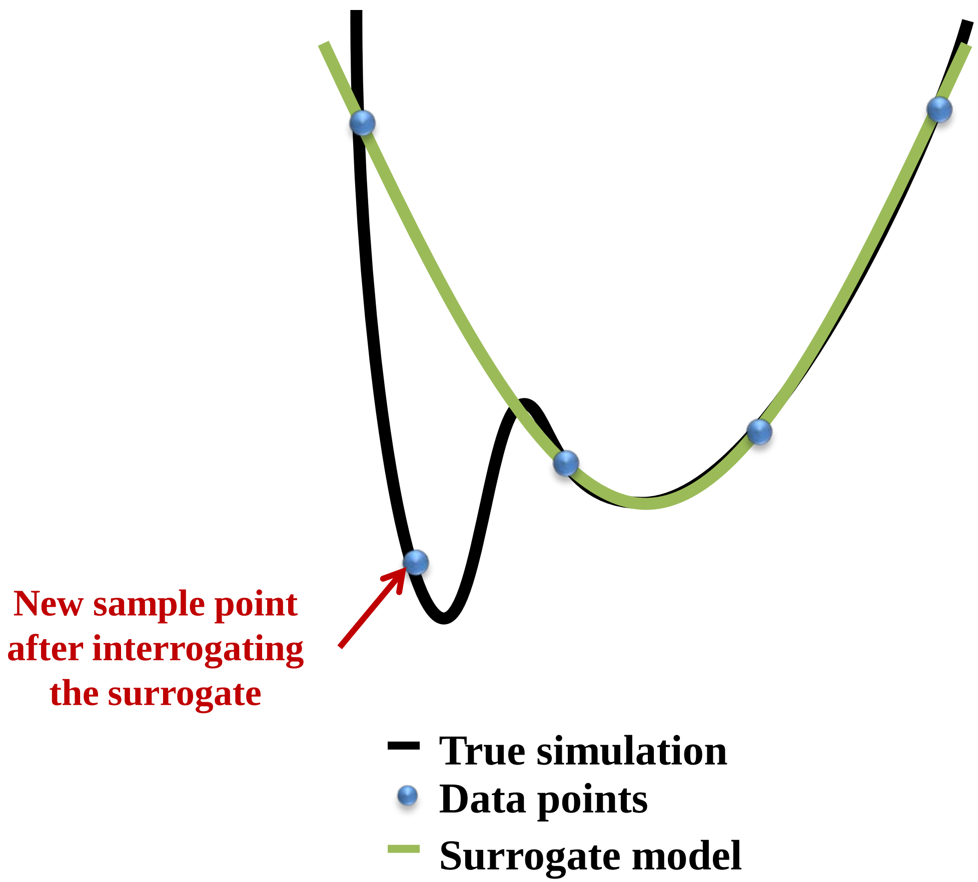

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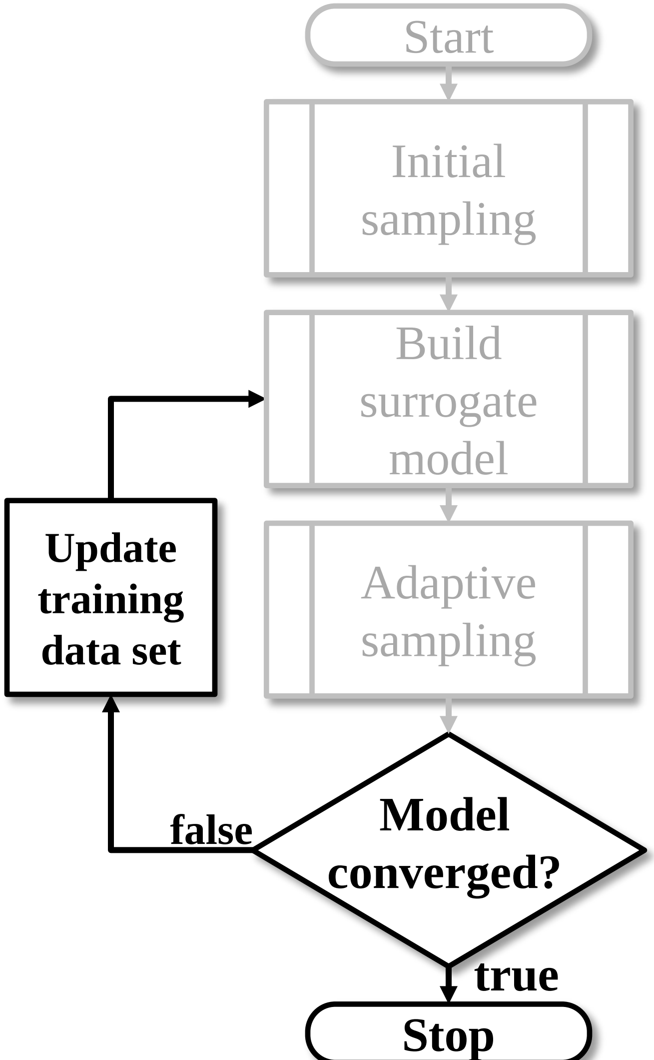

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