Modeling & Optimization Under Uncertainty

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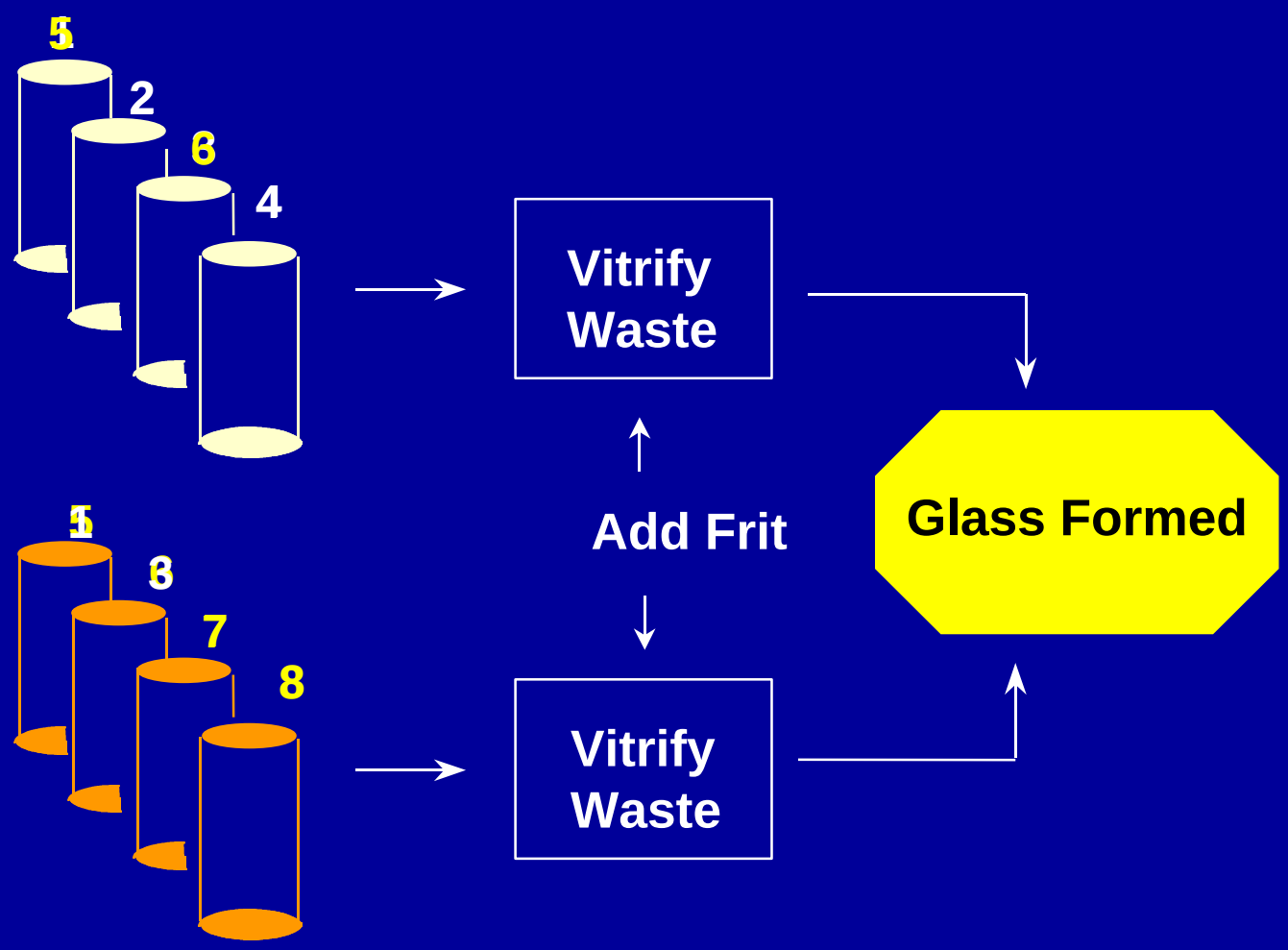
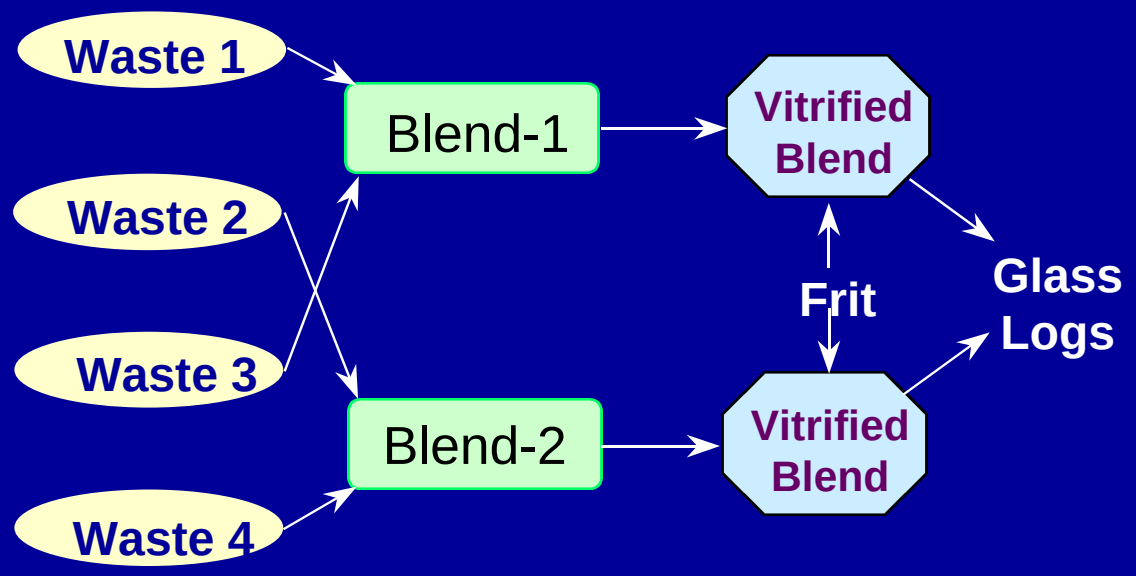
Synthesizing Optimal Waste Blend



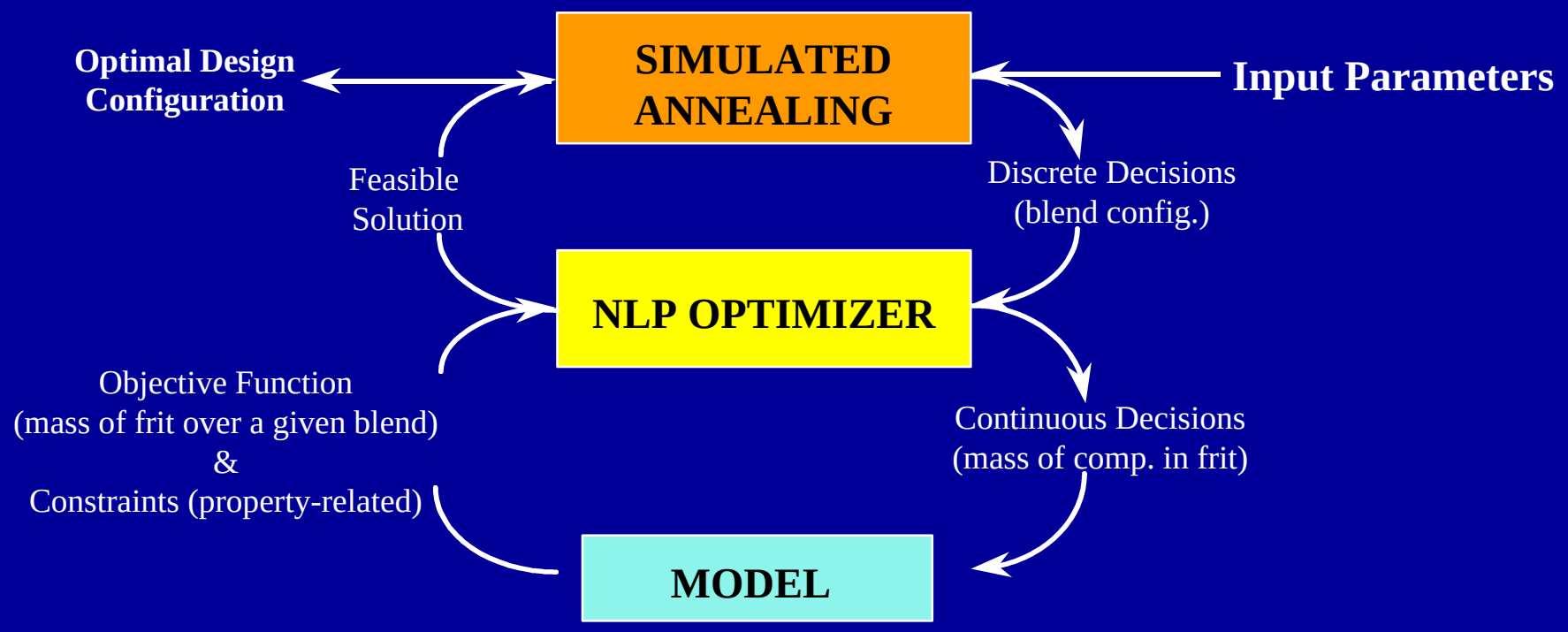
Conversion of Waste to Glass



Objectives: To select the combination of blends so that the total amount frit used is minimized

For 21 tank wastes and 3 blends: 66,512,160 possible combinations

Solution Procedure



"The greatest of all the accomplishments of the 20th-century science has been the discovery of human ignorance"

-- Lewis Thomas

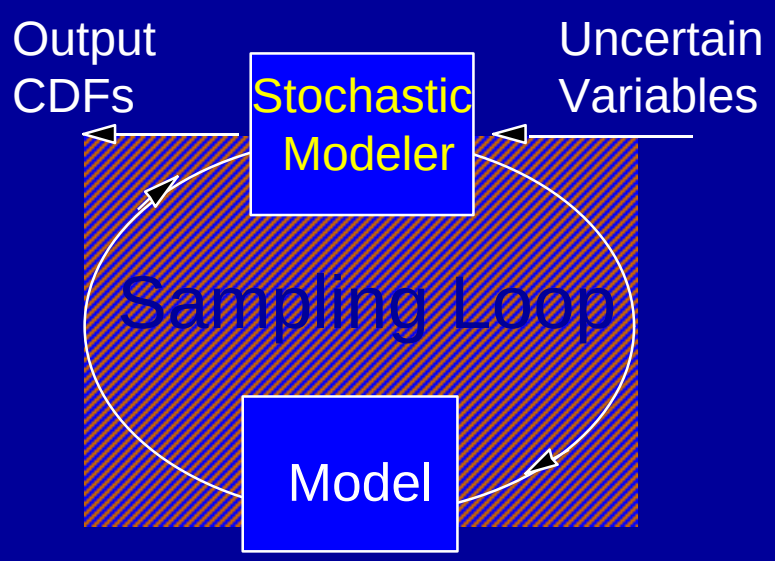
Characterizing Uncertainties in Waste Blends

- Uncertainties in the glass property models
  - Reduce the feasible range of the applicability of the glass property models
    - Viscosity
    - Electrical conductivity
    - Durability
- Uncertainties in the waste composition
  - Based on the mean and the RSD data available for a particular tank
  - Assume normal probability distributions
  - Sample the distribution (LHS or HSS)
  - Normalize the mass fraction
  - Calculate the mass of each component (from the m.f. and the total mass)

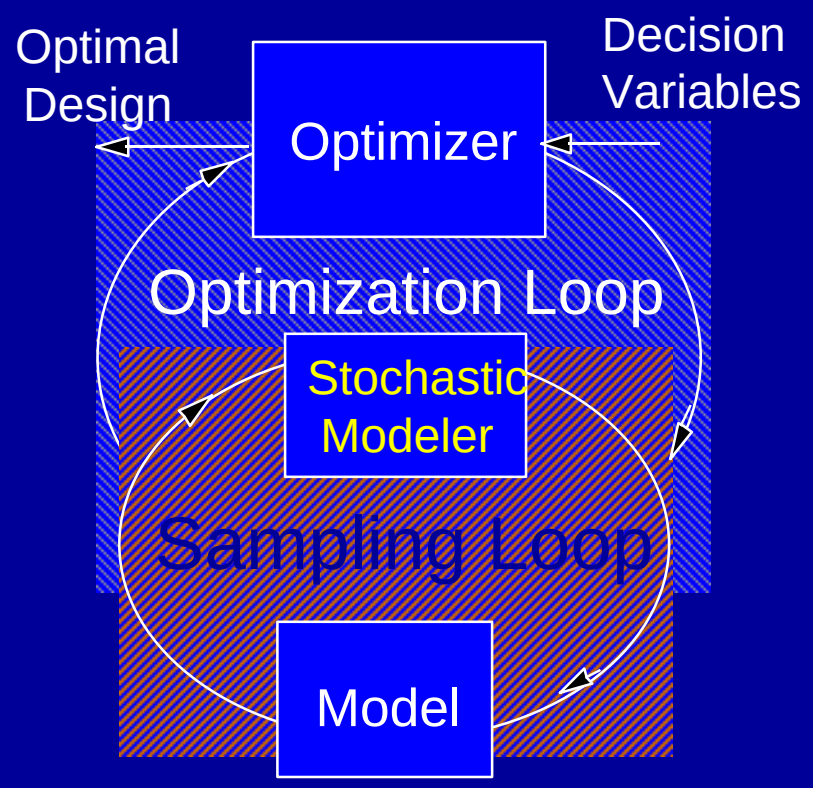
Stochastic Modeling

- Quantifying the uncertainties in key input parameters in terms of probability distributions.
- Sampling the distributions of these key parameters in an iterative fashion.
- Propagating the effects of uncertainties through the flowsheet.
- Applying statistical techniques to analyze the results.

Recursive Loops



Stochastic Modeling



Stochastic Optimization

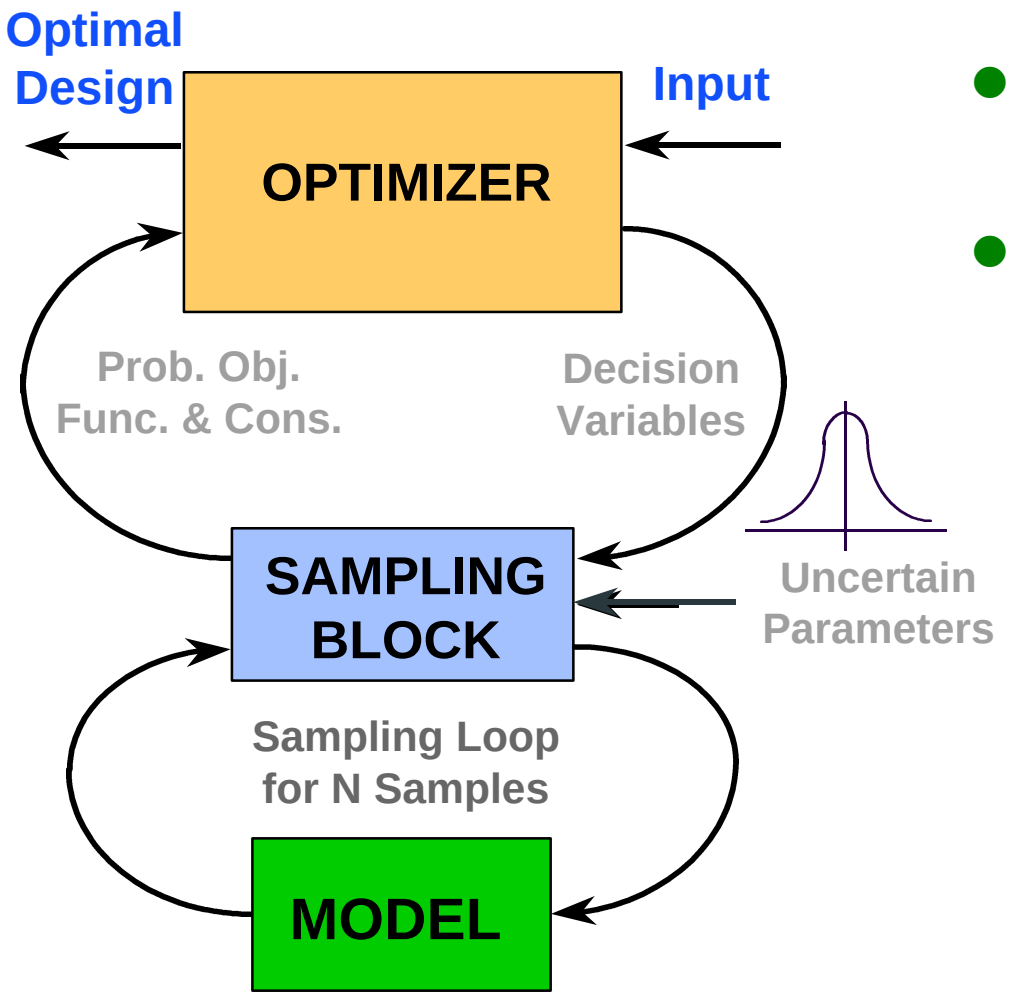
Incorporation of Discrete Decision Variables

Research to date has indicated some potential for solving these problems when conditions such as block-separable recourse……In the most general circumstances, we have some results on extensions of cutting plane methods but practical applications are still limited.

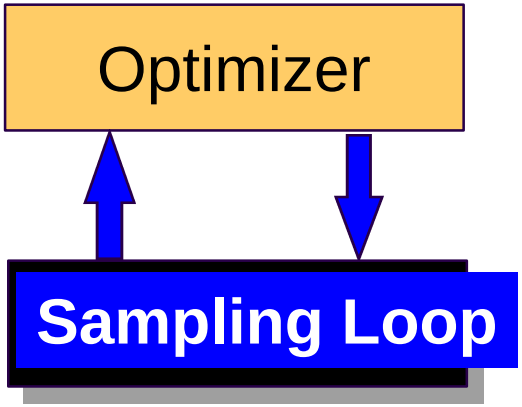
For Broad applicability, stochastic programming methods must include discrete variables in a more comprehensive manner.

- *Birge (1997), Stochastic Programming Computation and Application, Informs Journal of Scientific Computing.*

Framework for Stochastic Optimization



- An efficient sampling methodology
- An efficient interaction between the optimizer and the sampling loop

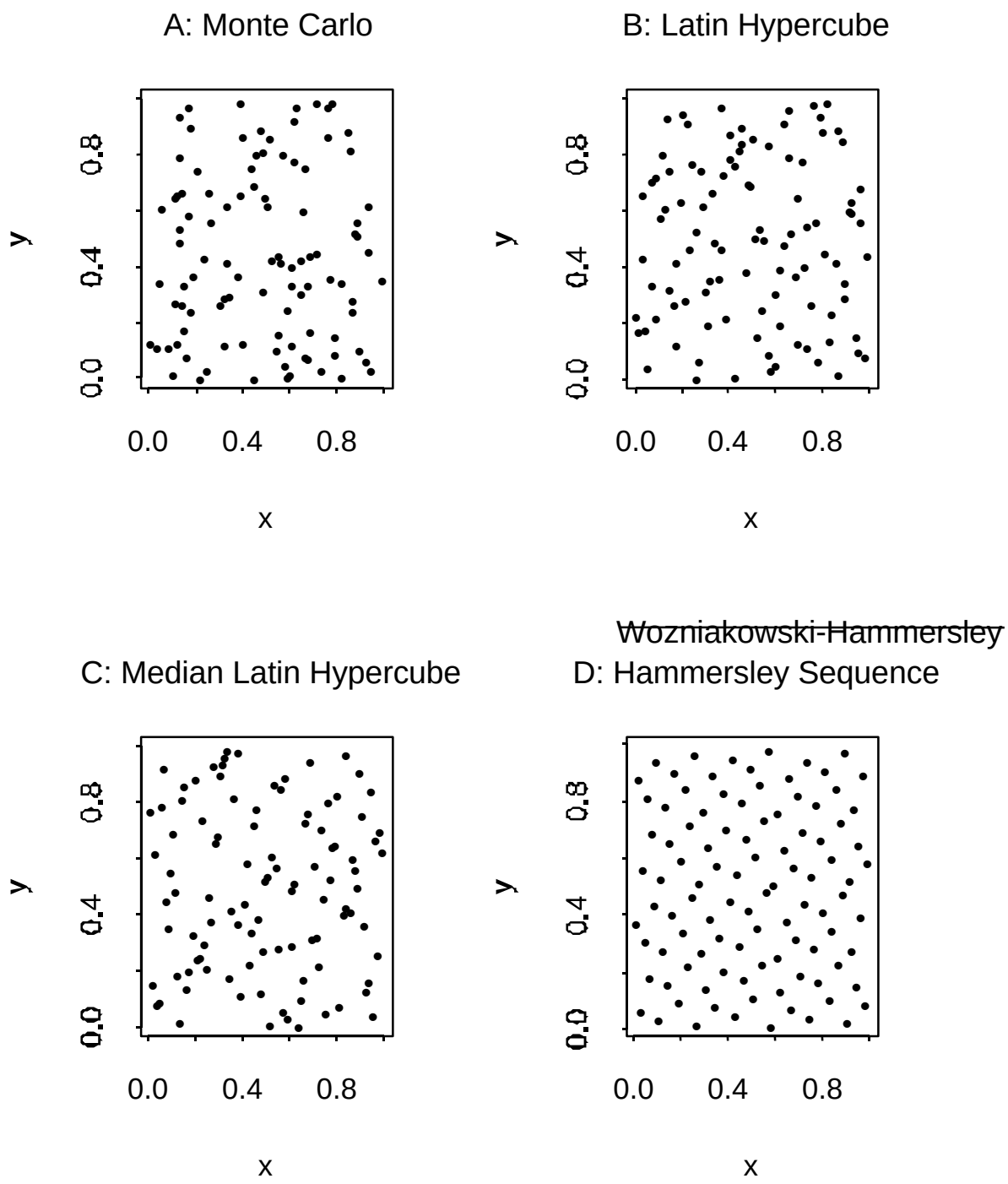


Important Properties of Sampling Techniques

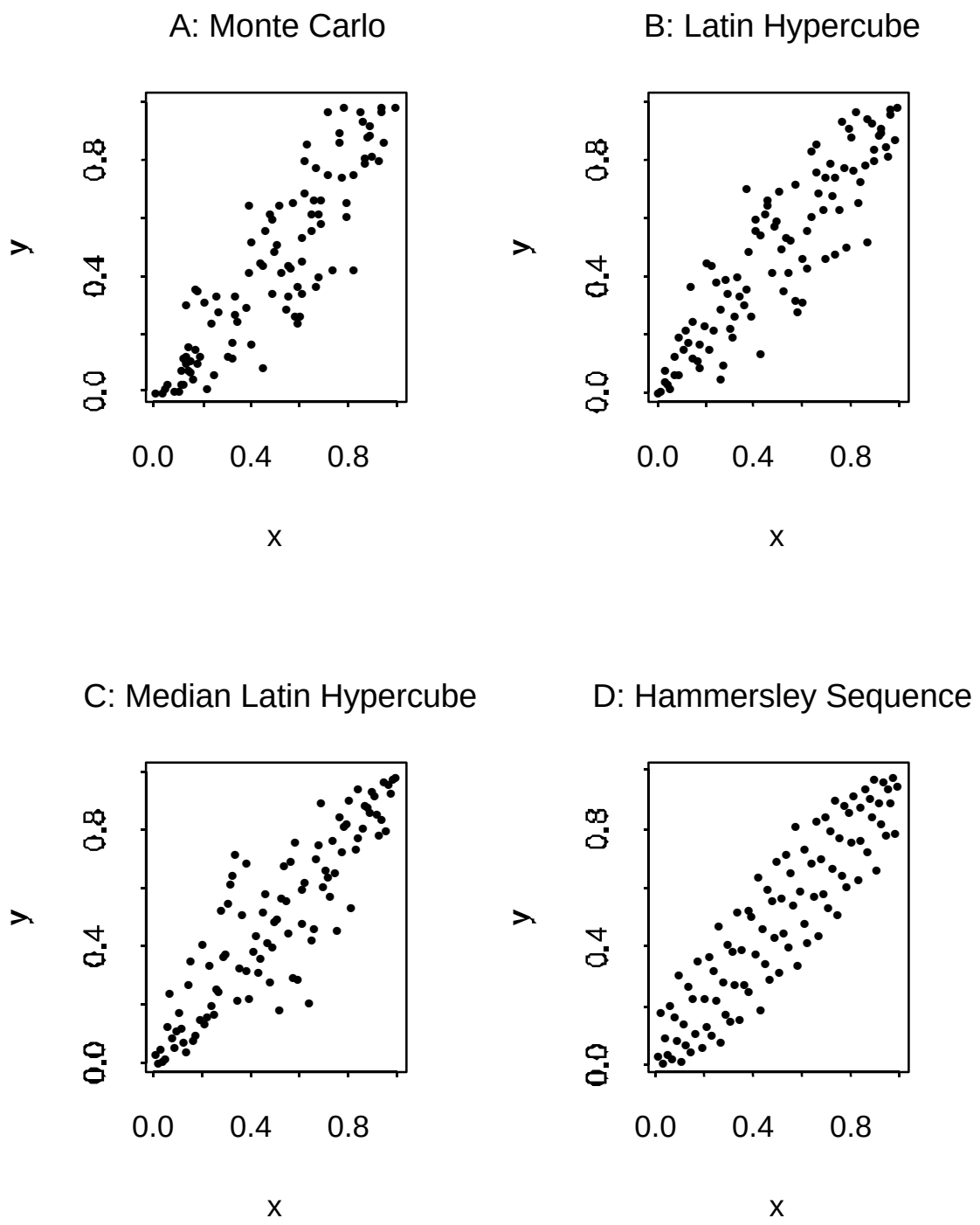
- Independence / Randomness
- Uniformity

In most applications, the actual relationship between successive points in a sample has no physical significance, hence, randomness of the sample for approximating a uniform distribution is not critical (Knuth, 1973).

Once it is apparent that the uniformity properties are critical to the design of sampling techniques, constrained or stratified sampling becomes appealing (Morgan and Henrion, 1990).



~~Wozniakowski-Hammersley~~


A: Monte Carlo
B: Latin Hypercube
C: Median Latin Hypercube
D: Hammersley Sequence
x
y
0.0
0.4
0.8

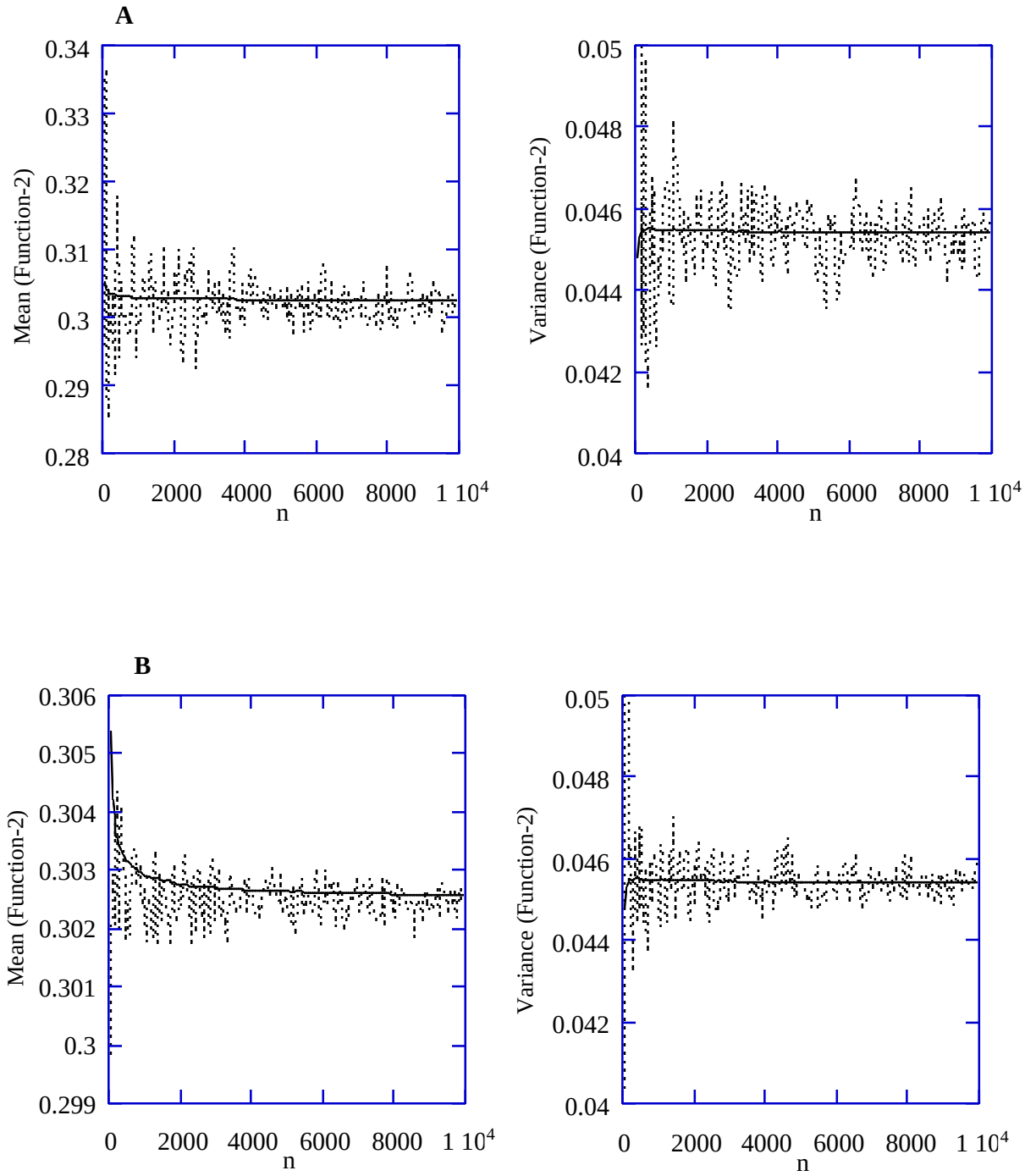
Sample Test Sets

- Five functions
  - Linear additive
  - Multiplicative
  - Quadratic
  - Exponential
  - Logarithmic
- Two to ten input variables
- Four sampling techniques

- Three correlation structures
  - No correlation
  - Correlation = 0.5
  - Correlation = 0.9
- Three types of distributions
  - Uniform
  - Normal
  - Log normal

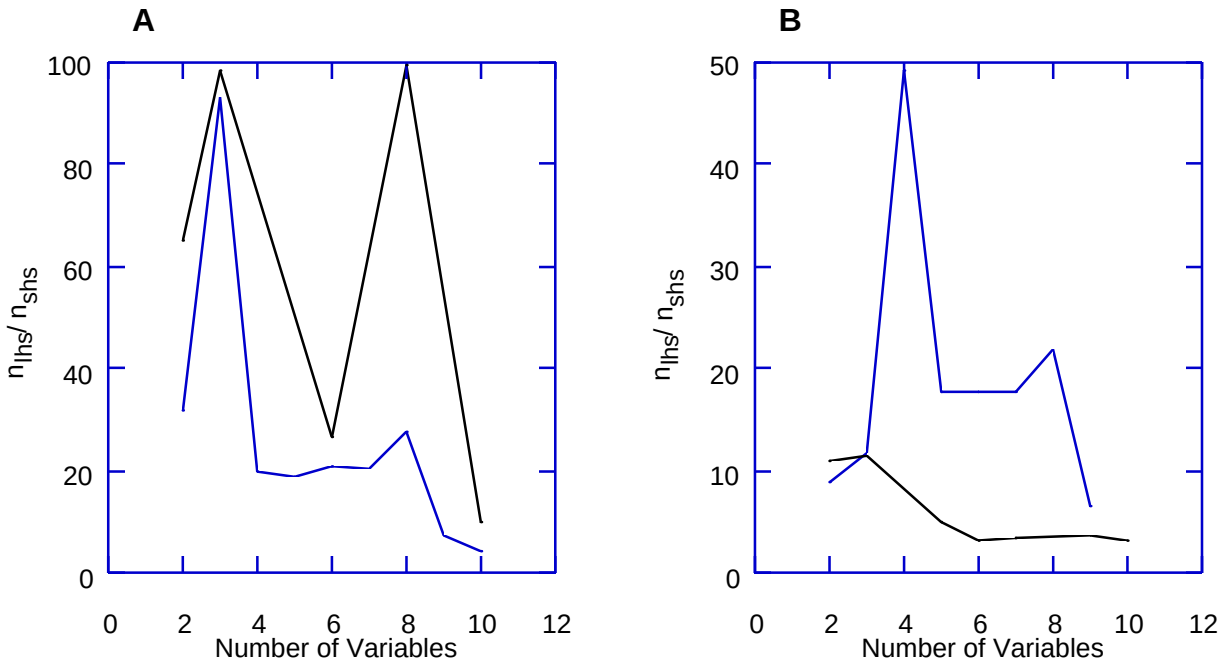
Total > 12000 Data Sets
and
Quality control of CSTR
Taguchi approach to Batch Distillation

Comparison of (Top) MCS versus HSS
(bottom) LHS Versus HSS



Comparison of LHS Versus HSS

(left) Uniform Distribution (right) Lognormal Distribution



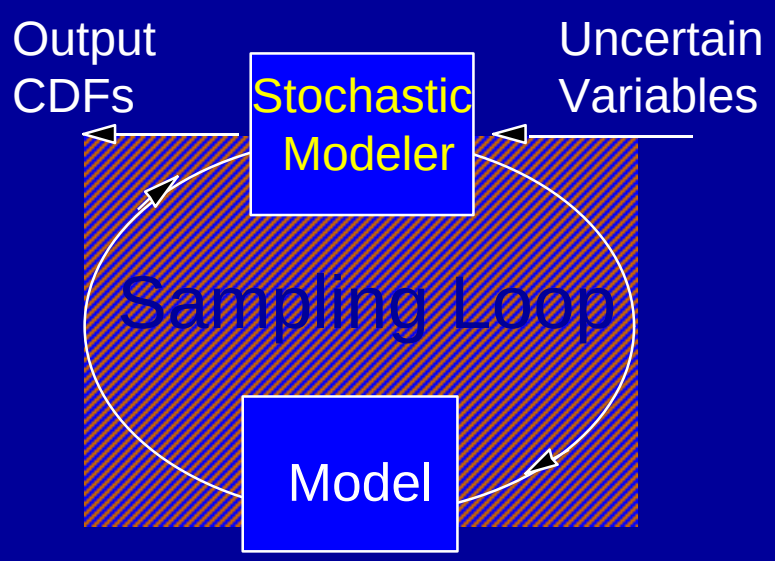
New Sampling Technique

HSS shows better uniformity than LHS or MCS.

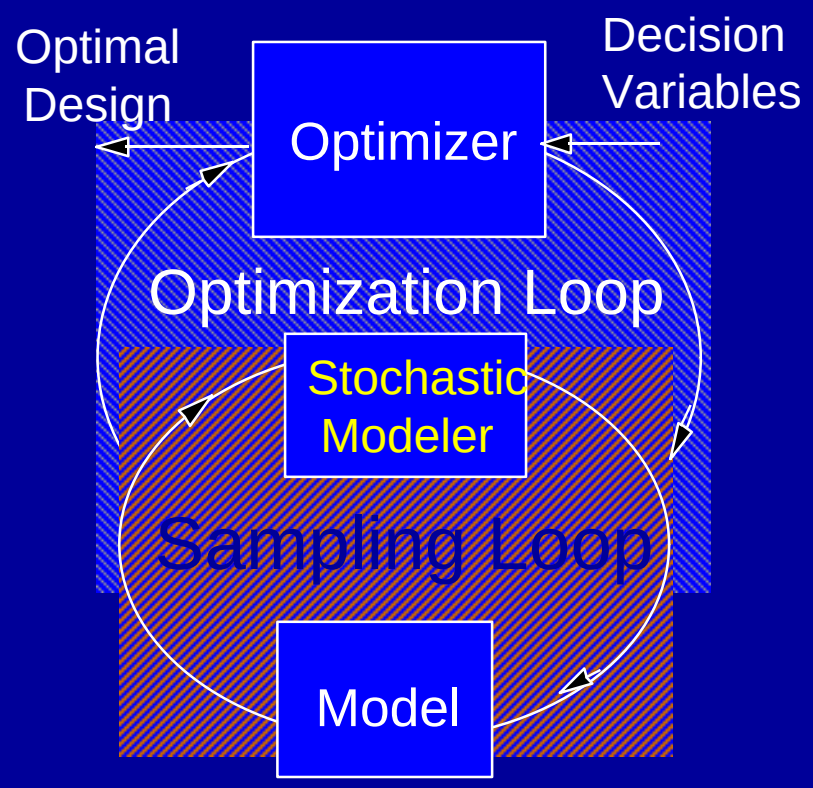
HSS sampling is at least 3 to 100 times faster than LHS or MCS.

HSS is preferred sampling for stochastic modeling and/or stochastic optimization.

Recursive Loops

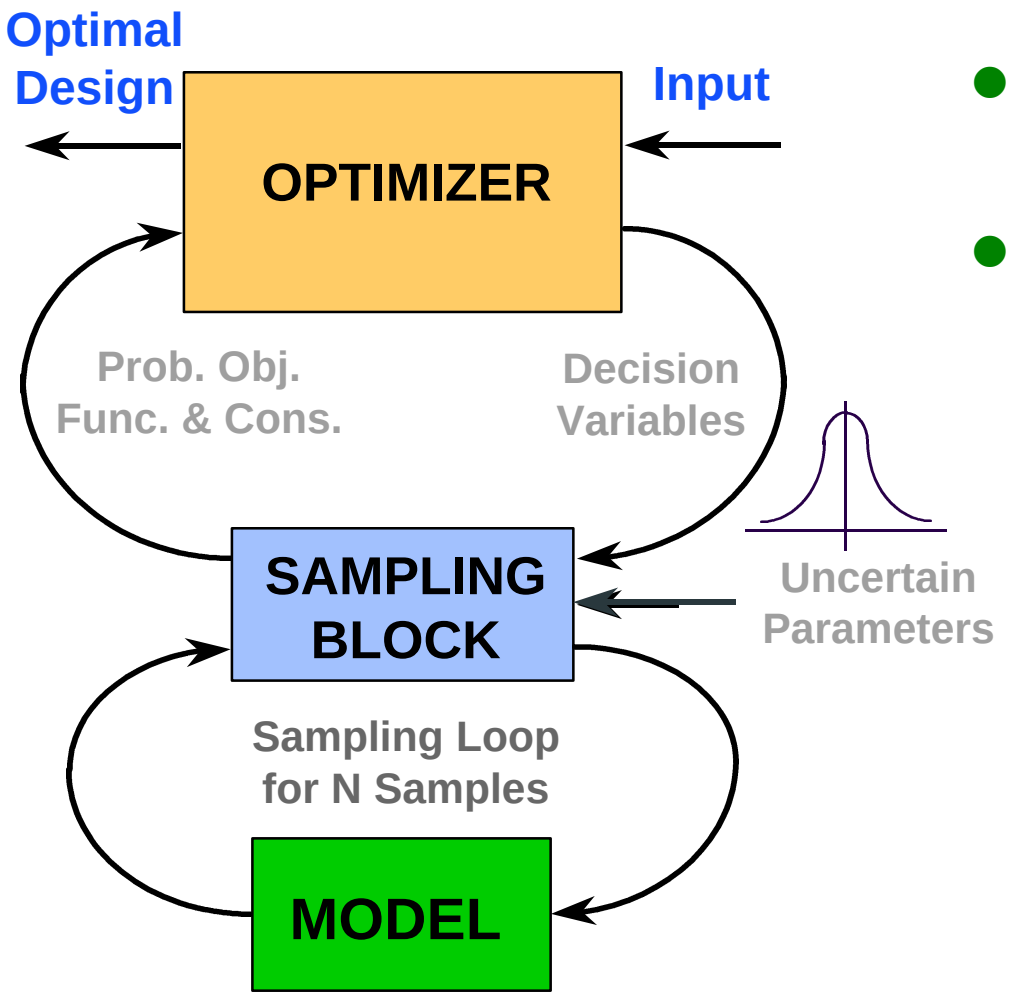


Stochastic Modeling



Stochastic Optimization

Framework for Stochastic Optimization



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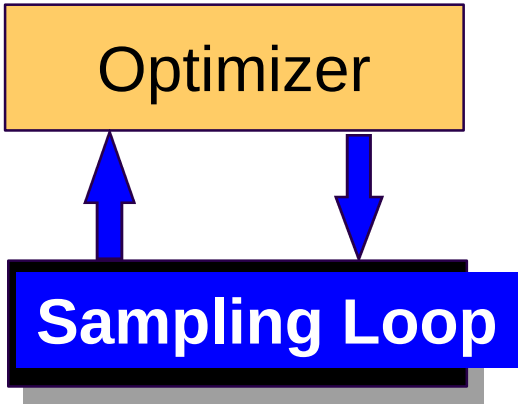
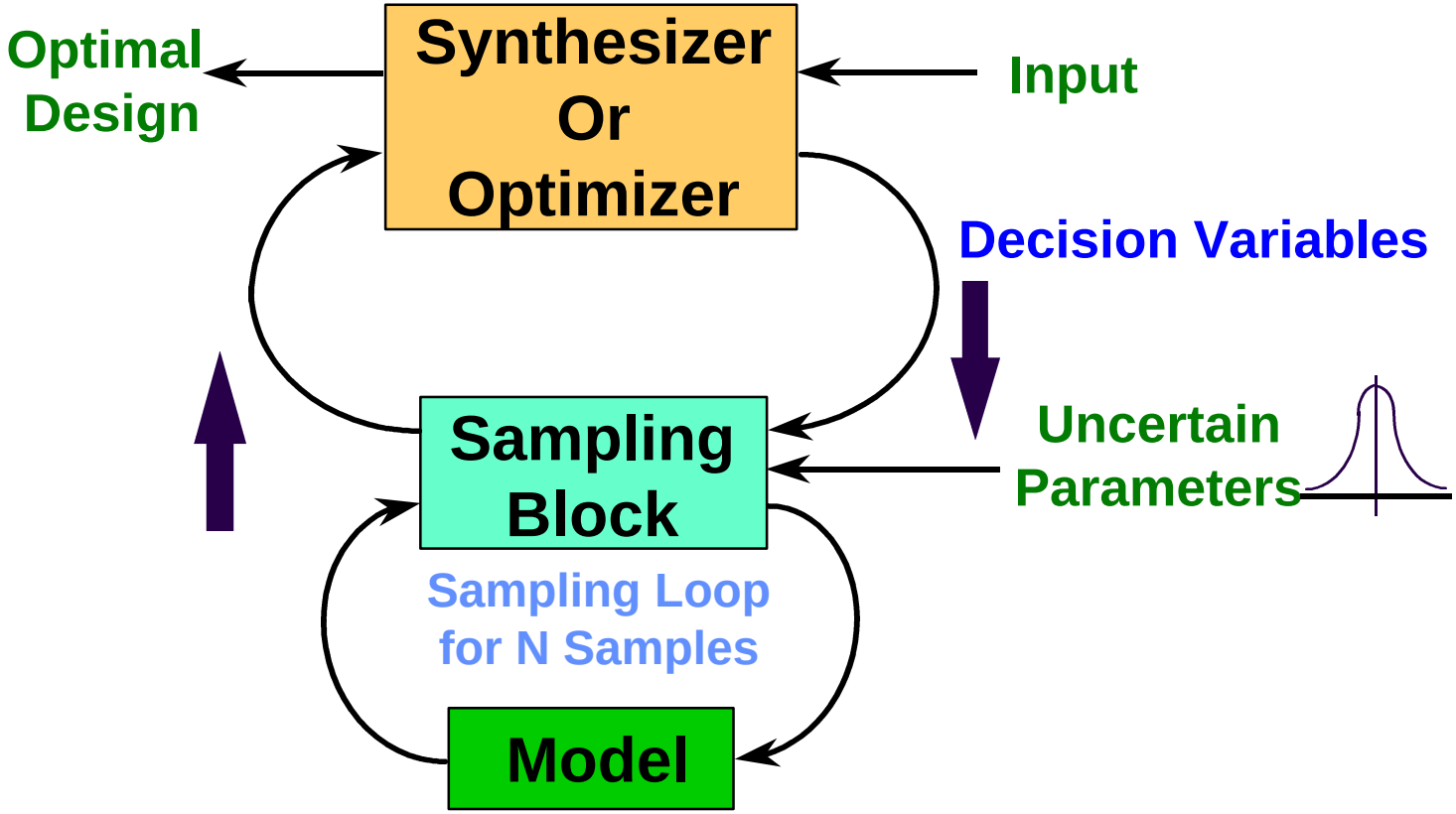


Optimization and Uncertainty

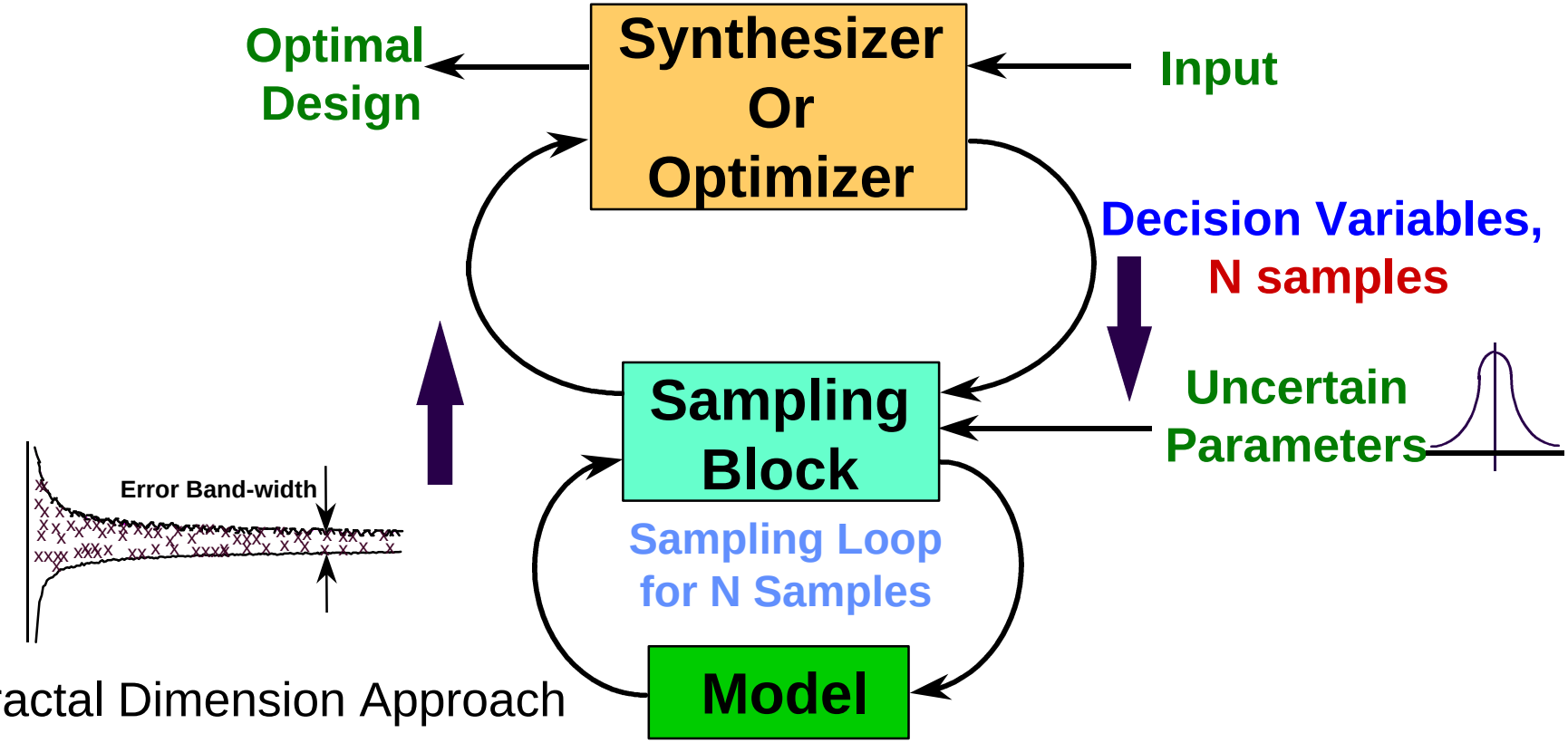
Uncertainty surface changes at each optimization iteration

Number of samples needed for each iteration is different.

Stochastic Optimization

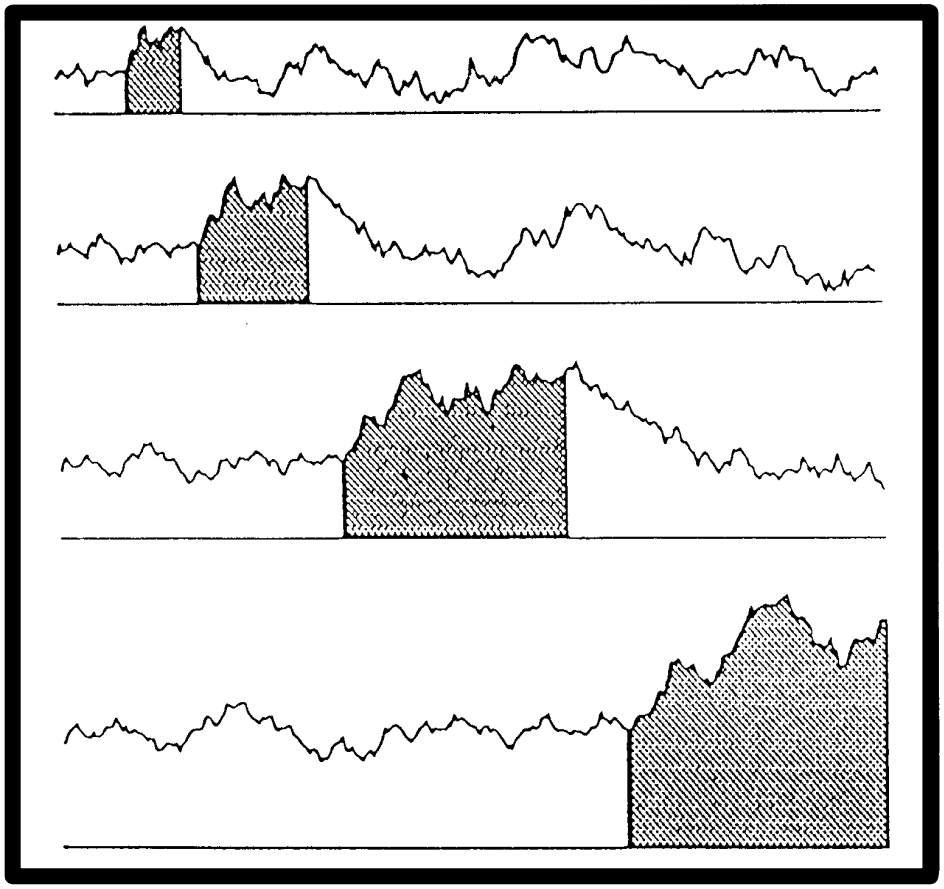


Stochastic Annealing



Fractal Dimension Approach

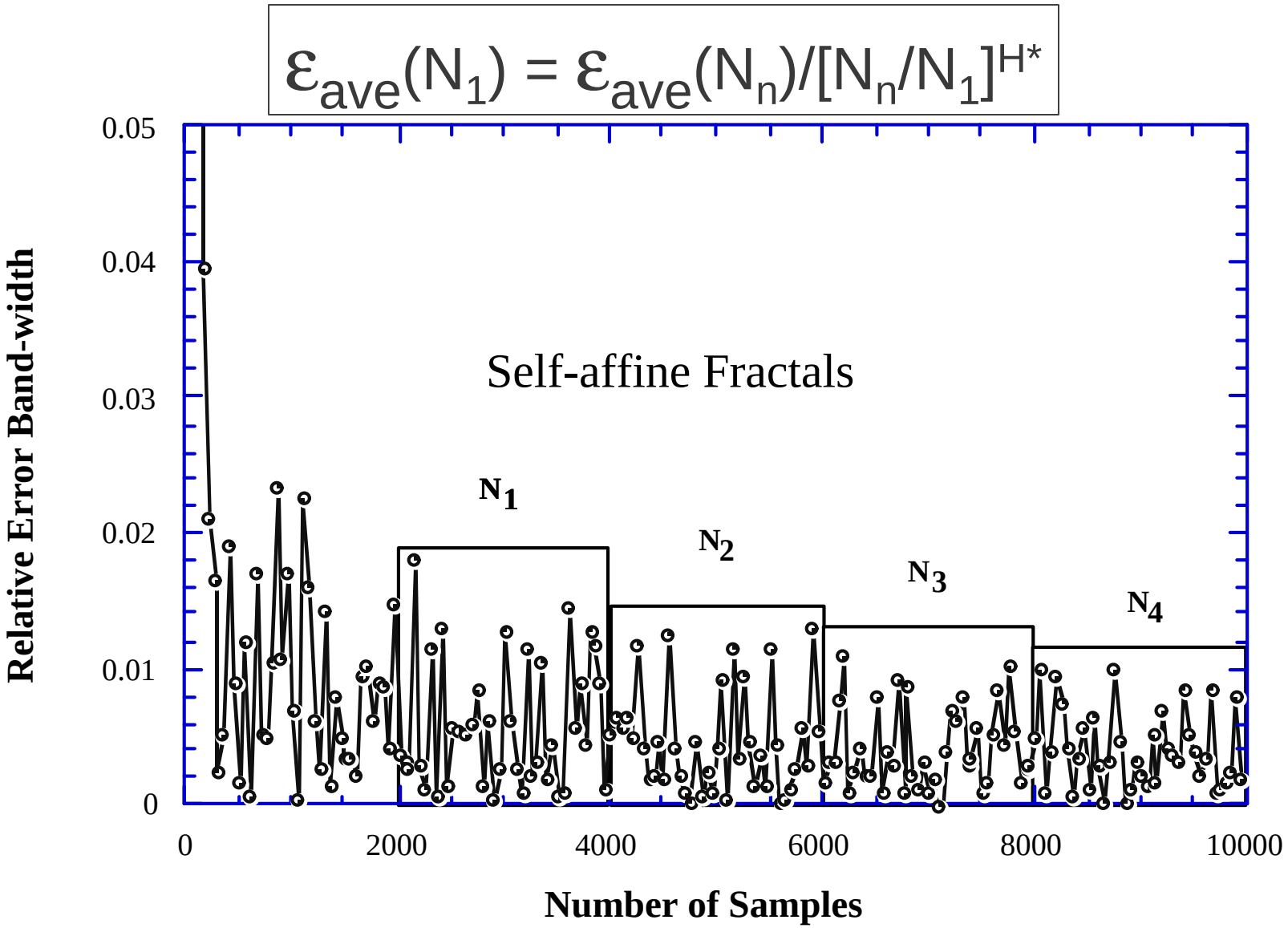
Brownian Motion as Self Affine Fractals



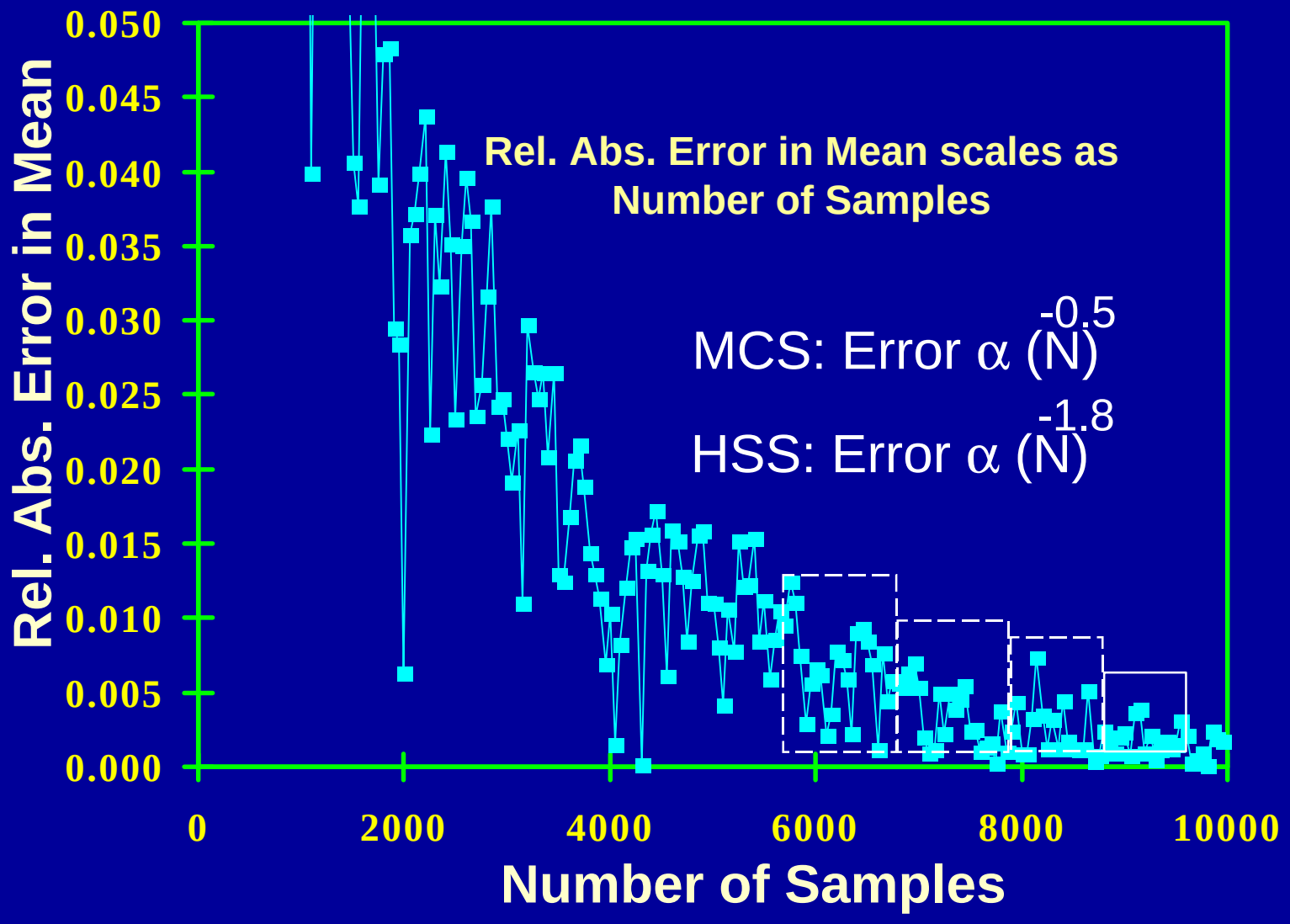
Scaling the Brownian motion with horizontal scaling factor of 2 and vertical scaling factor $r = 2^{0.5}$.

0.5 is the Hurst Exponent

The curves are statistically equivalent, the shaded region shows the shape properly scaled for different stages.


$\varepsilon_{ave}(N_1) = \varepsilon_{ave}(N_n)/[N_n/N_1]^{H*}$
Self-affine Fractals
N_1
N_2
N_3
N_4
Relative Error Band-width
0.05
0.04
0.03
0.02
0.01
0
0
2000
4000
6000
8000
10000
Number of Samples

The Fractal Model - Approach



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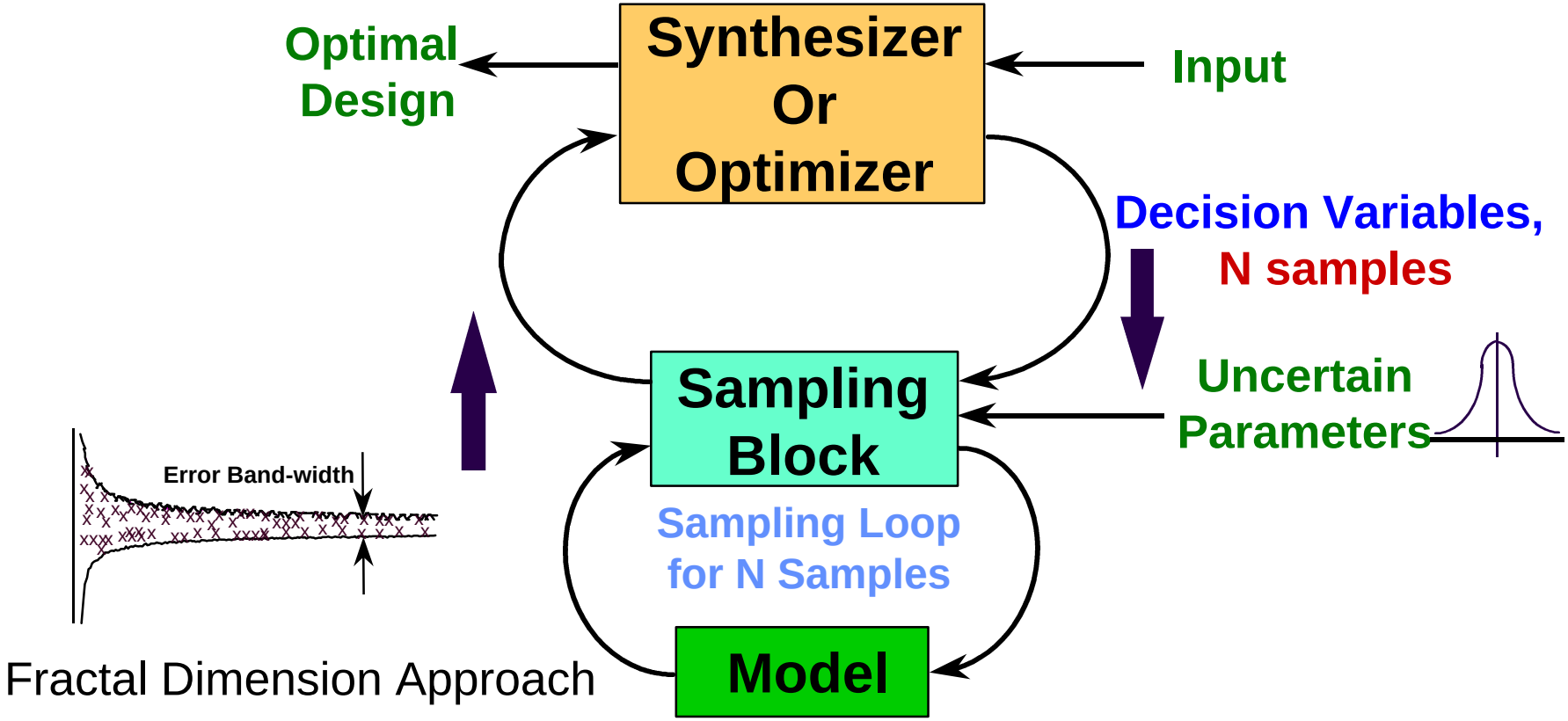
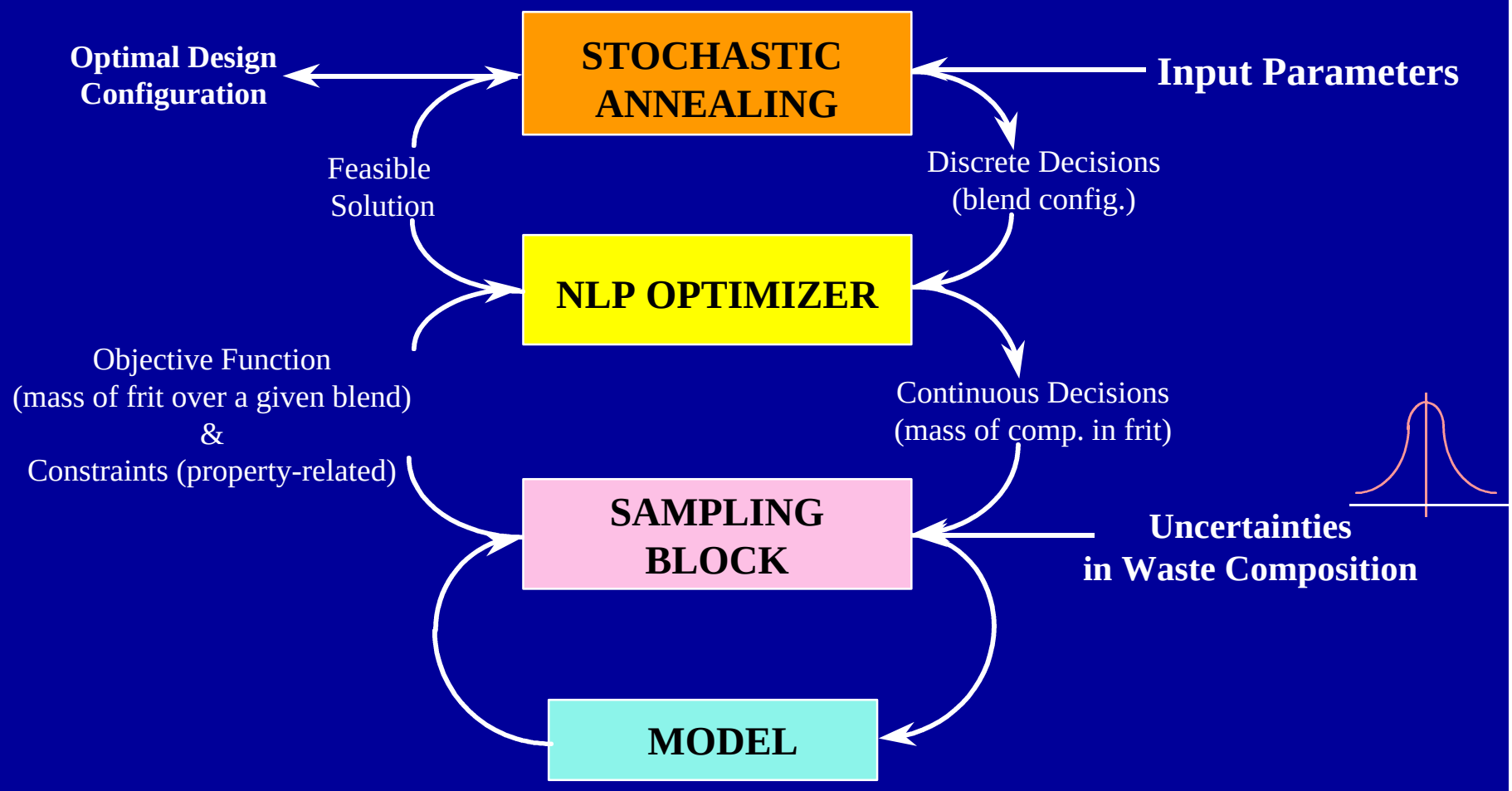


- Achieves trade-off between accuracy and computational efficiency
- Computational efficiency up to 90%

Solution Procedure



Optimal Waste Blend Configuration

	•Det. Case •(SA-NLP)	•Stoch. Case •(STA-NLP, C.S.)	•Stoch. Case •(STA-NLP, F.D.)
•Blend-1	•3,4,5,6,8,9,20	•7,13,14,17,18,19,21	•7,13,14,17,18,19,21
•Blend-2	•1,10,11,12,16,19,21	•4,5,6,8,9,16,20	•4,5,6,8,9,16,20
•Blend-3	•2,7,13,14,15,17,18	•1,2,3,10,11,12,15	•1,2,3,10,11,12,15
•Min. Frit (Kgs.)	**•11,028 (12,022 w/unc)**	**•11,307**	**•11,307**
•CPU time (secs)	**•45 mins**	**•4 days**	**•18 hours**

Observations:

- Uncertainties affect the optimal blend configuration
- Estimated time for stochastic synthesis with fixed sample framework 20 days

Summary

- An efficient sampling technique for uncertainty analysis
- A faster algorithm for stochastic optimization
- Fractal dimension approach for error characterization
- Application to large scale problems

Contributors

- Jayant Kalagnanam, IBM Watson Laboratory
- Laura Painton, Sandia National Laboratories
- Prosenjit Chaudhuri, BOC Group
- Venkatesh Narayan, Avery Denison
- Mark Hoza, Pacific Northwest Laboratories

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- Morgantown Energy Technology Center
- Pacific Northwest Laboratory
- Amoco Corporation
- Ben Franklin Research Center

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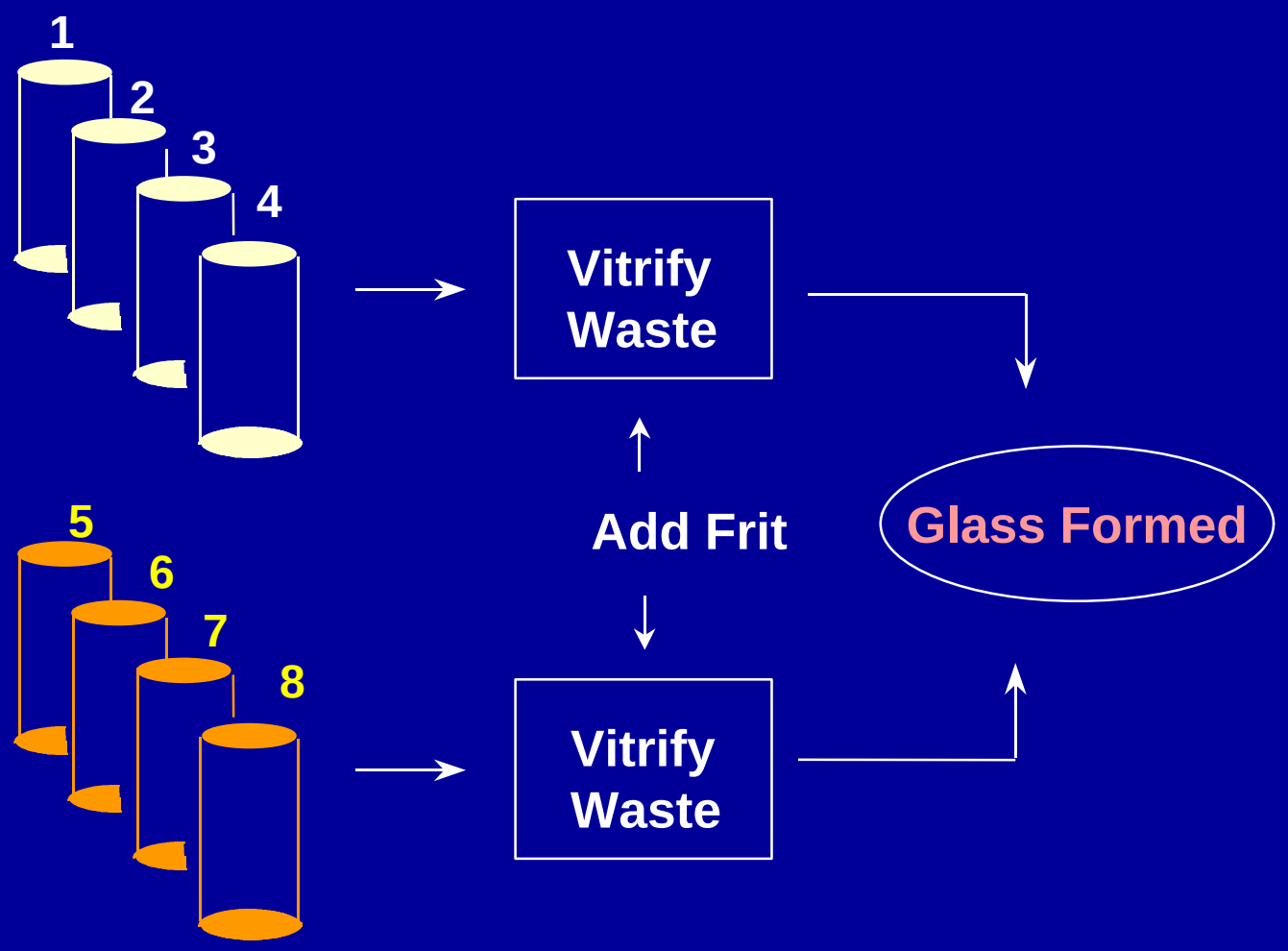


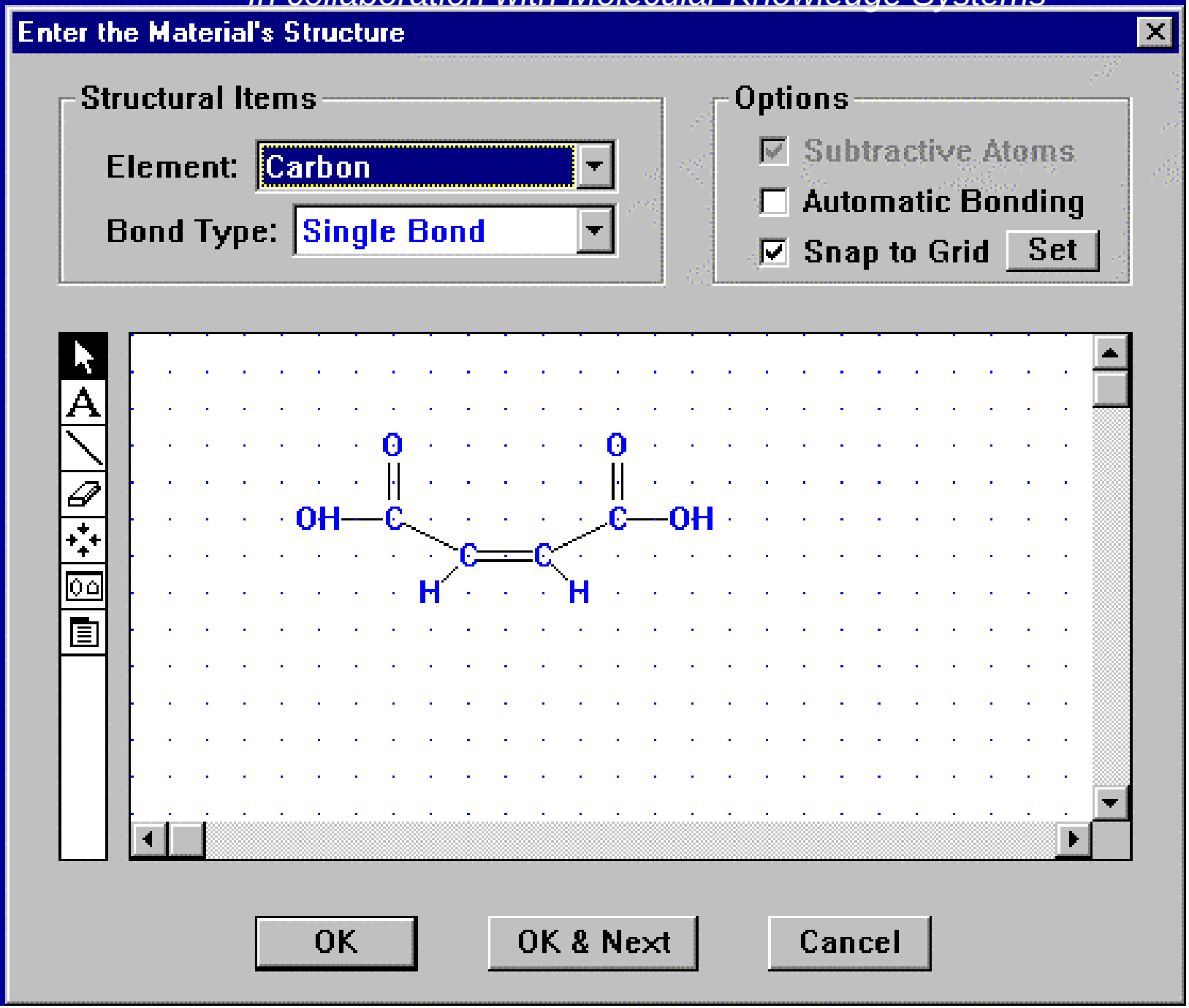
The Value of Research: Stochastic Optimization as a Policy Tool

- To minimize expected value of the objective function (conventional objective in optimization under uncertainty)
- To minimize variance--constraint violation-- a proxy for robustness
- To minimize time devoted to research:

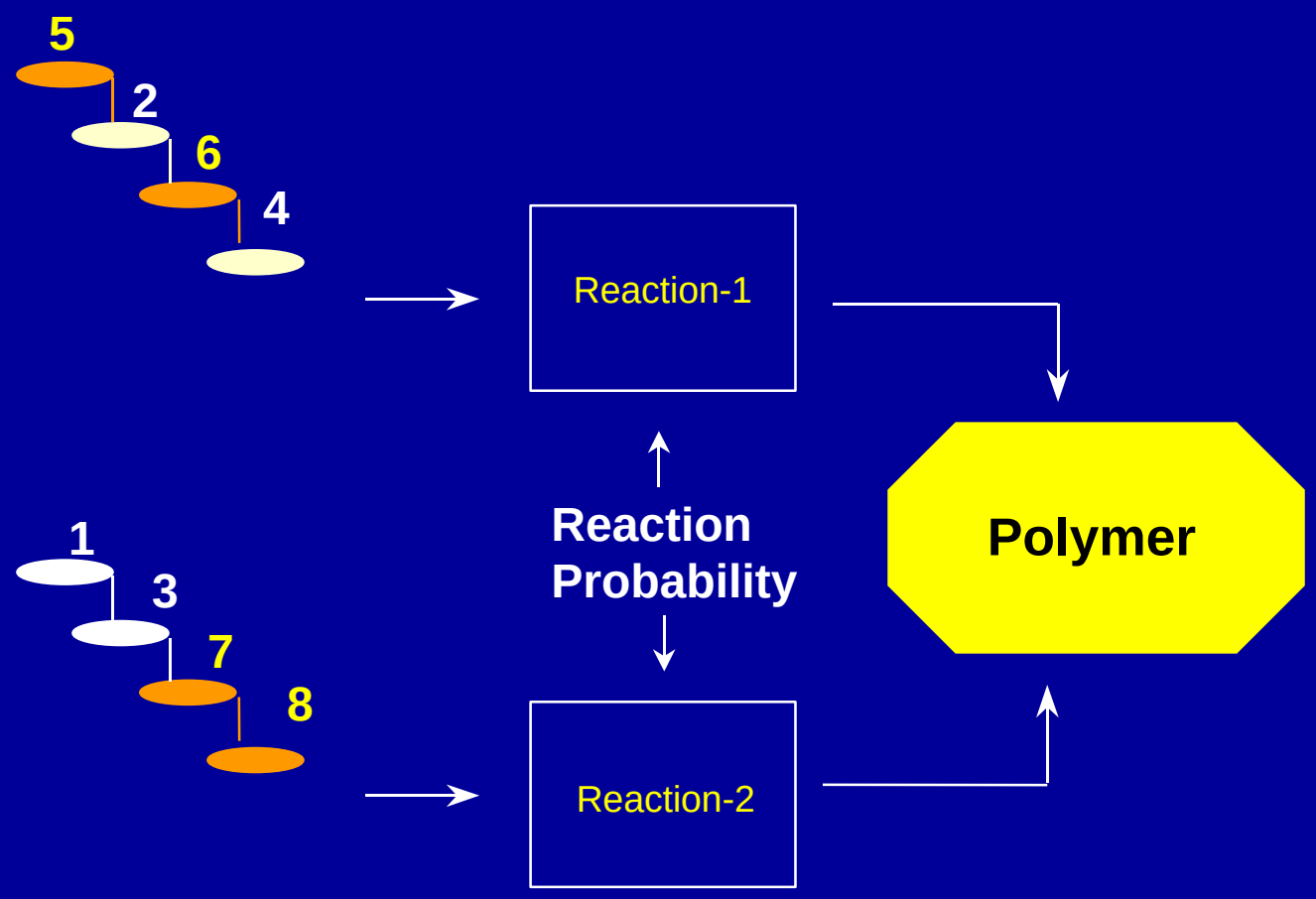
Time devoted for research increases understanding, and therefore decreases the variation (uncertainties) in quantitative estimates derived from this knowledge. Qualitative function to capture research has diminishing marginal returns as uncertainty declines with time spent on research

Molecular Designs with Uncertainties - Manish Tayal

In collaboration with Molecular Knowledge Systems



Molecular Design Under Uncertainty



Environmental

Operations Research

NOx Reduction

Renewable Energy

Modeling New Environmental Control Technologies

Nuclear Waste Management

Solvent Selection & Recycling

Efficient Algorithms

Uncertainty Analysis

Optimization Under Uncertainty

Efficient and Generalized Methods and Tools

Fractal Dimension Approach

Multi-objective Optimization

AI & Optimization

Batch Distillation: Design, Optimization, & Optimal Control; Synthesis; Feasibility; Efficiency.

Dynamic and Steady-state Models for Chemical & Physical Phenomena

Molecular Design Under Uncertainty

Multi-criteria Decision Analysis

New Decision Analysis Criteria

Value of Research

Chemical

Policy

Modeling & Optimization Under Uncertainty

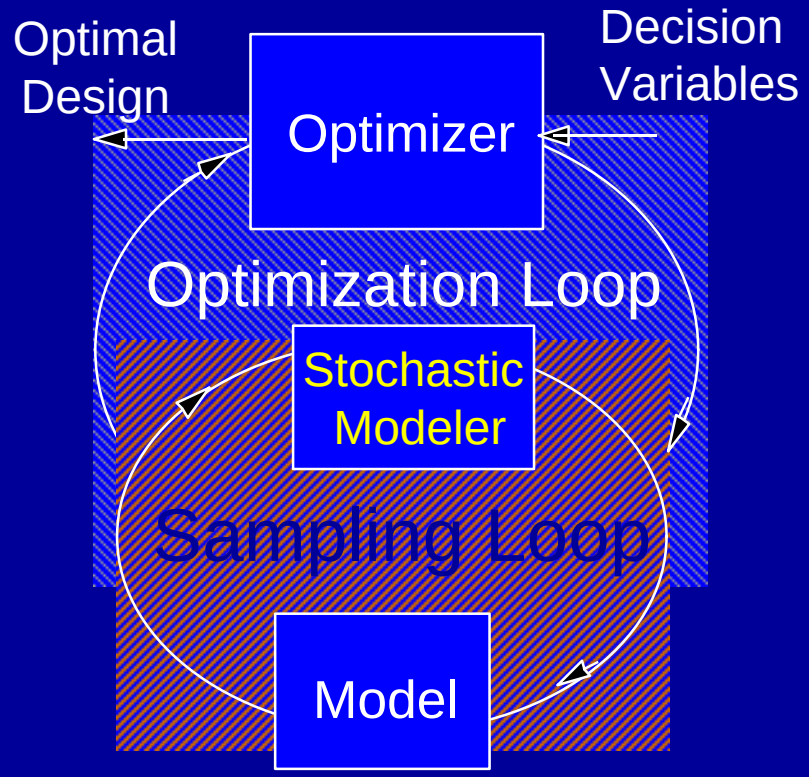
EPP/OM Program

A Multi-disciplinary Ph.D Program

between College of Engineering &

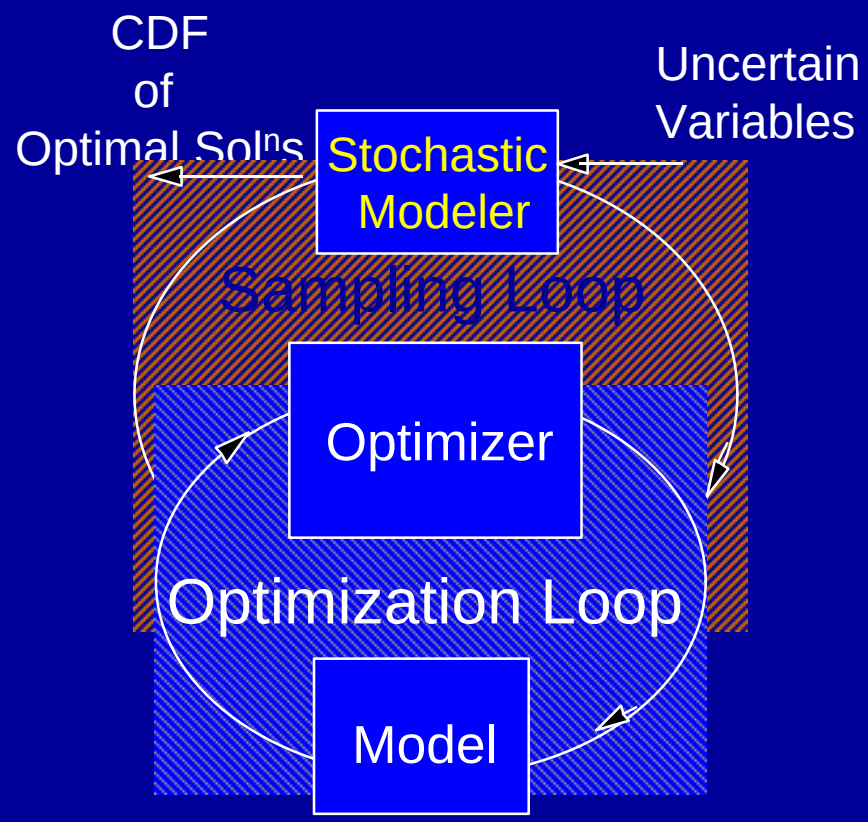
School of Business

Stochastic Optimization



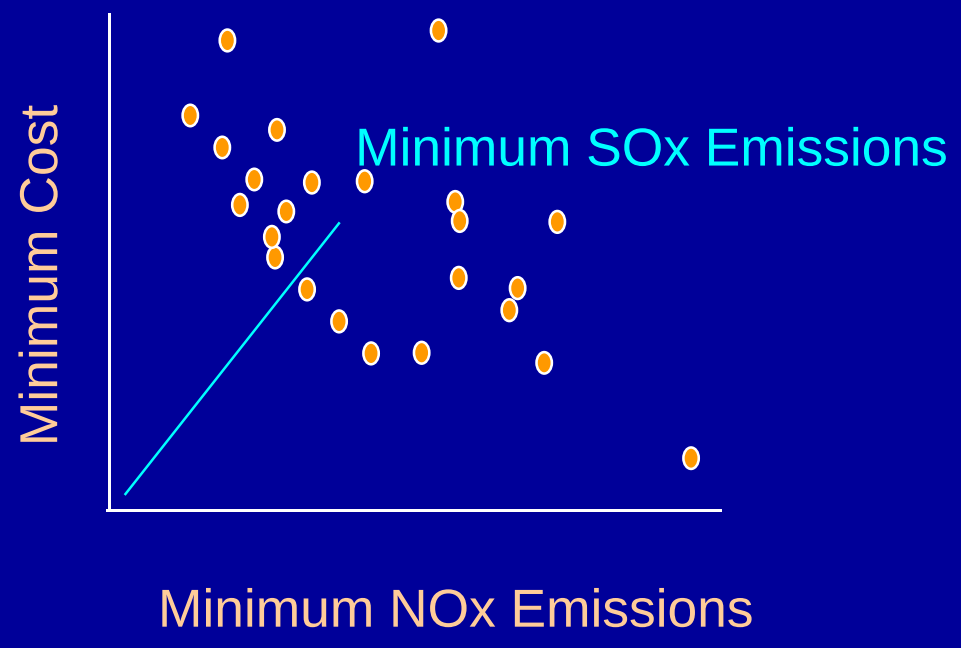
Here and Now
Chance Constrained
Optimal Flexibility Design
Taguchi's Quality Control

Stochastic Programming



Wait and See
Flexibility Index
Multi-period Optimization

Multi-objective Optimization



"Statistics in the hands of an engineer are like a lamppost to a drunk. They're used more for support than illumination."

--Bill Sangster