An Approach to Optimal Experimental Design for the Analysis of a Complex System

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Phenomenological Sciences LDRD: Methodology for Optimal Selection of Test and/or Simulation Levels for Problems Involving Computational Simulation -- Alvin, Romero, Trucano

MICS predictability of complex phenomena project: Sensitivity Coefficients and Optimal Design of Experiments -- Blackwell

Reliability LDRD: Experimental Design Issues for Reliability Methods for System Analysis -- Robinson, Zimmerman

Computational Sciences LDRD: Uncertainty and Error Assessment in Computational Simulation -- Alvin, Diegert, Oberkampf

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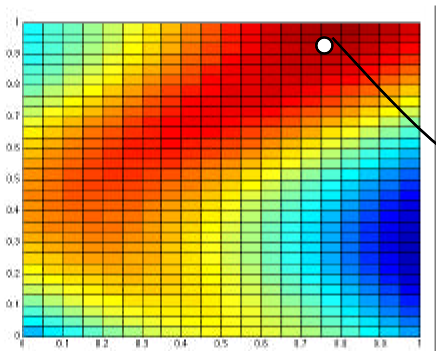
Presentation Outline

- Framework for Analysis
- Important Considerations in Experimental Design for Large Scale Systems
- Resampling Methodology
- Example
- Larger Problems
- Further Applications and Conclusions

In an Ideal (Computing) World

An Optimization Problem

Input x_2

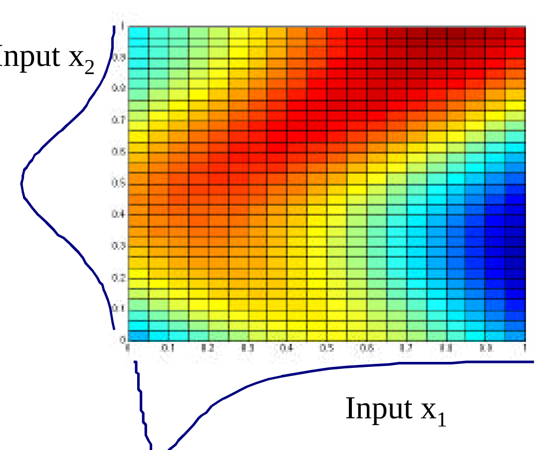


Input x_1

Maximum Value for the Performance Measure at (.75, .92)

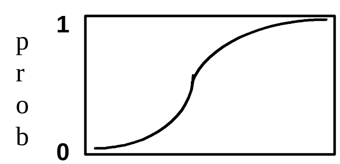
An Uncertainty Problem

Input x_2



Input x_1

Distributed Performance Measure



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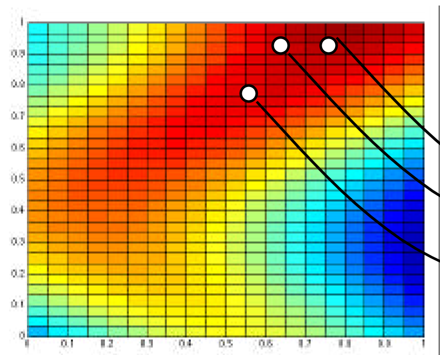
In an (Less) Ideal (Computing) World --

We have to Model the Response with a ‘Response Surface’

An Optimization Problem

Input x_2



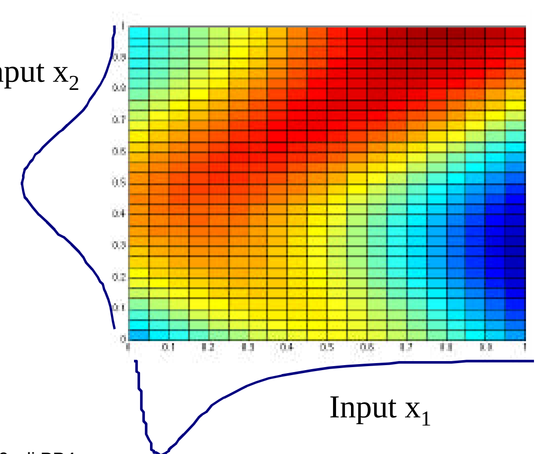
Input x_1

Maximum Value for the Performance Measure at (.75, .92) or (.8, .95) or Maybe at (.65, .79)

(Response Modeling Uncertainty)

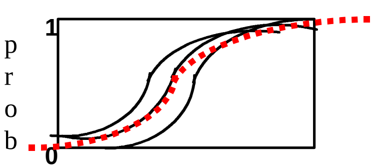
An Uncertainty Problem

Input x_2



Input x_1

Distributed Performance Measure

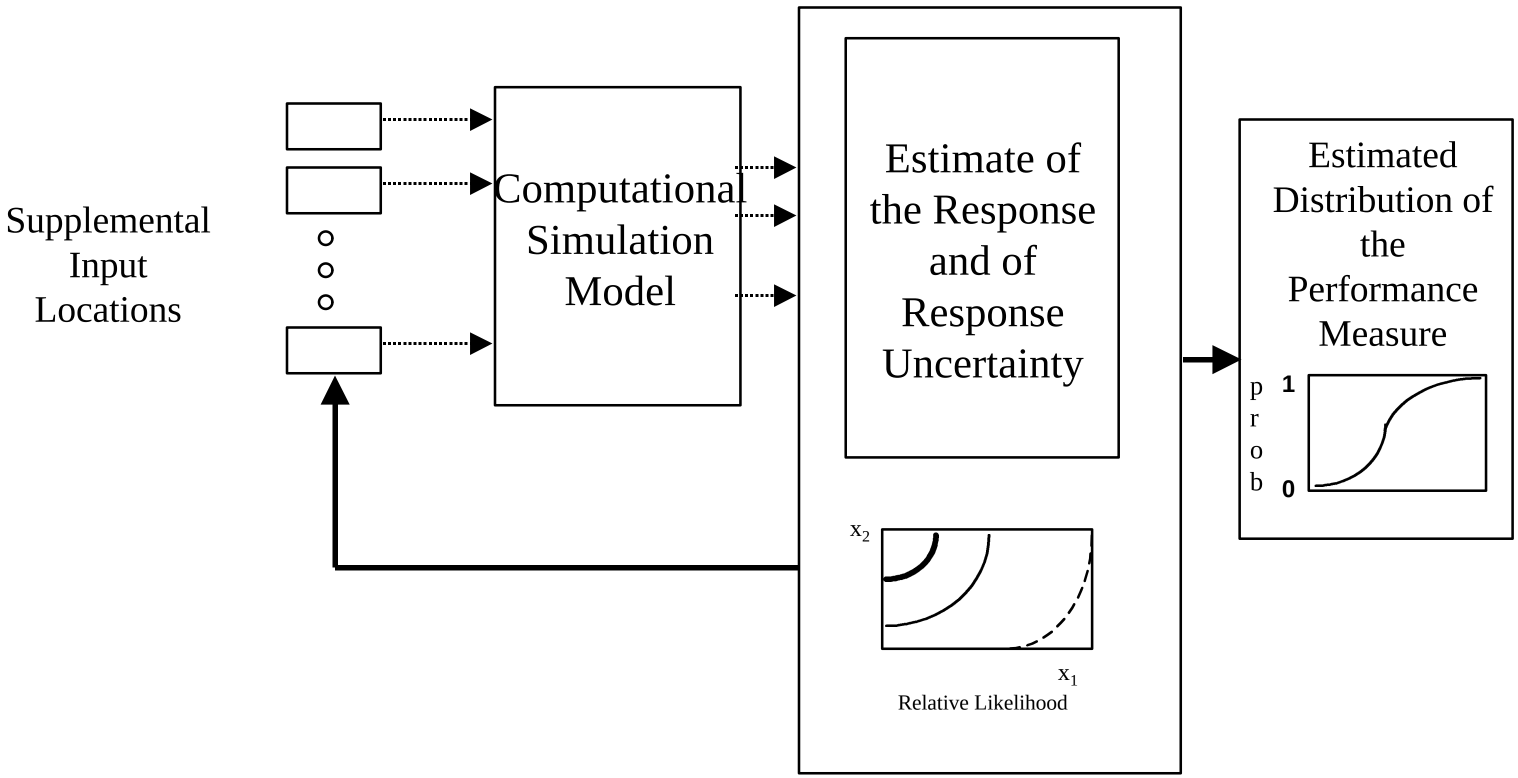


Objective of the Experimental Design

The objective of a good experimental design approach for computer analyses is to select a set simulations that will produce the most relevant information at the least expense. Given well defined project or analysis goals, relevant information can often be expressed in terms of the precision with which performance criterion can be estimated.

In terms of the previous slides, a good experimental design will reduce the impact of response modeling uncertainty on performance measure precision as much as possible for a fixed number of computer runs.

Experimental Design Process



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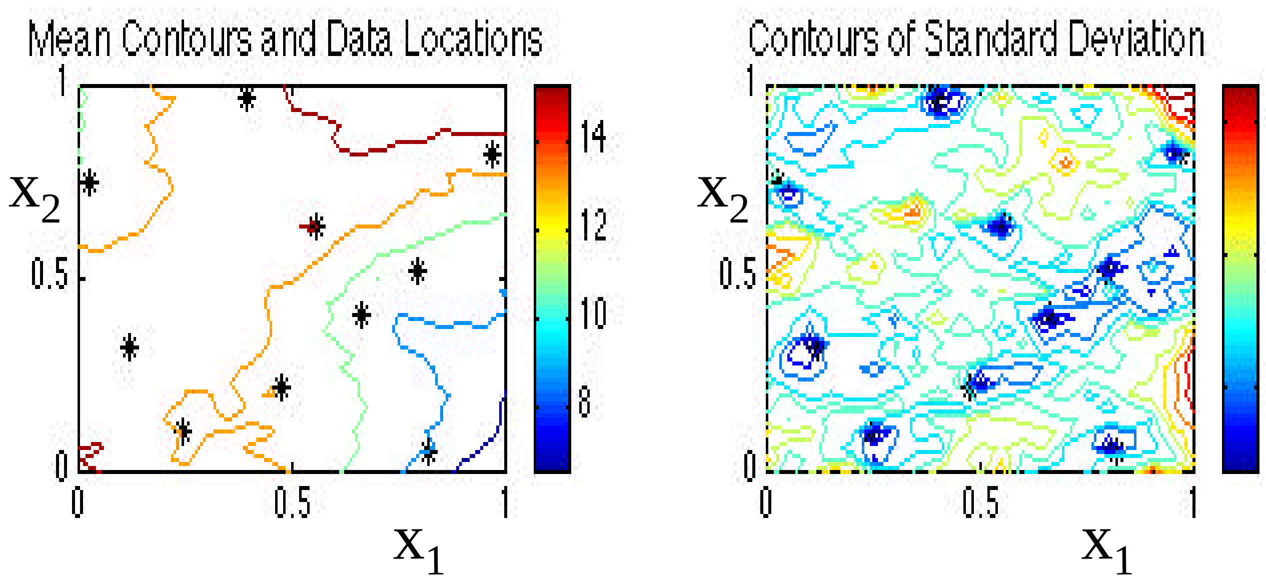
Estimate of the Response and Response Uncertainty



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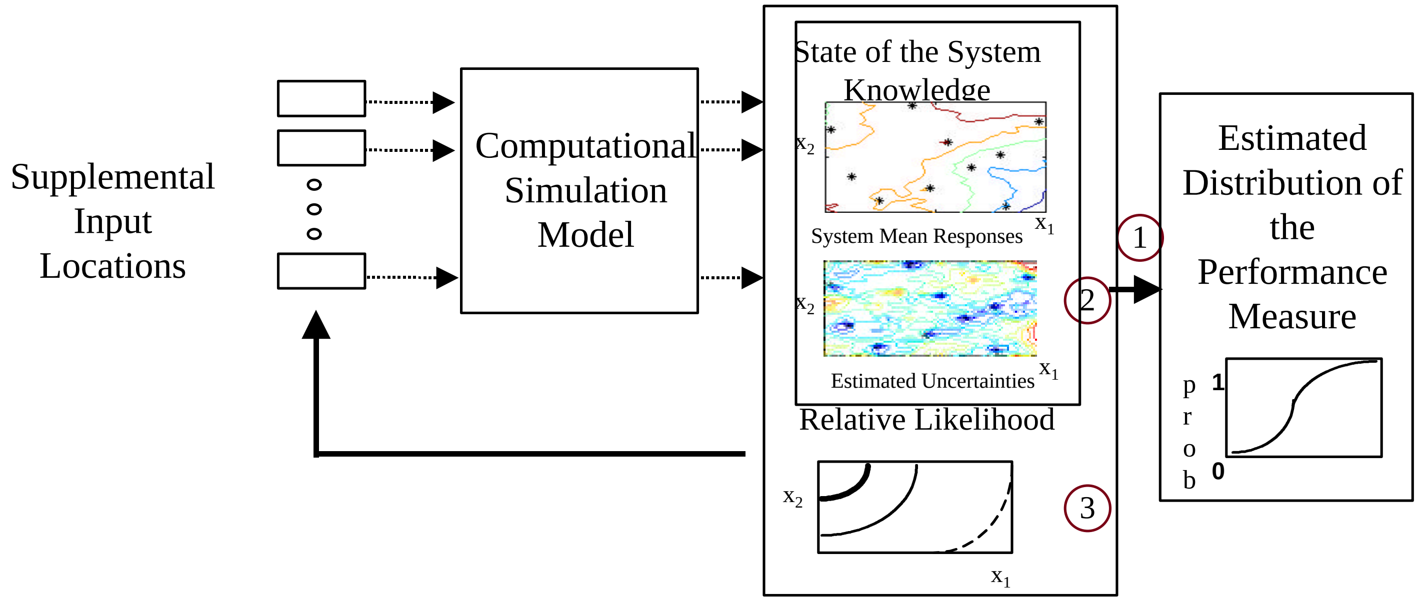
Important Considerations in Experimental Design for Large Scale Systems



At any test location:

1. Is the response of any consequence to the performance measure?
2. How well are the responses at this location already known?
3. How likely is this set of inputs?

Other Approaches to Selecting Runs

Method	Input Uncertainty	Response Uncertainty	Performance Uncertainty
SAMPLING			
Monte Carlo	Yes	No	No
Latin Hypercube	Yes	Yes	No
Importance Sampling	No	No	Yes
RESPONSE SURFACE			
RSM	Not Generally	Yes	No
Stochastic Surfaces	Not Generally	Yes	No
OTHER			
Analytical or Reliability	Yes	No	Yes

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Approach for the Proposed Methodology

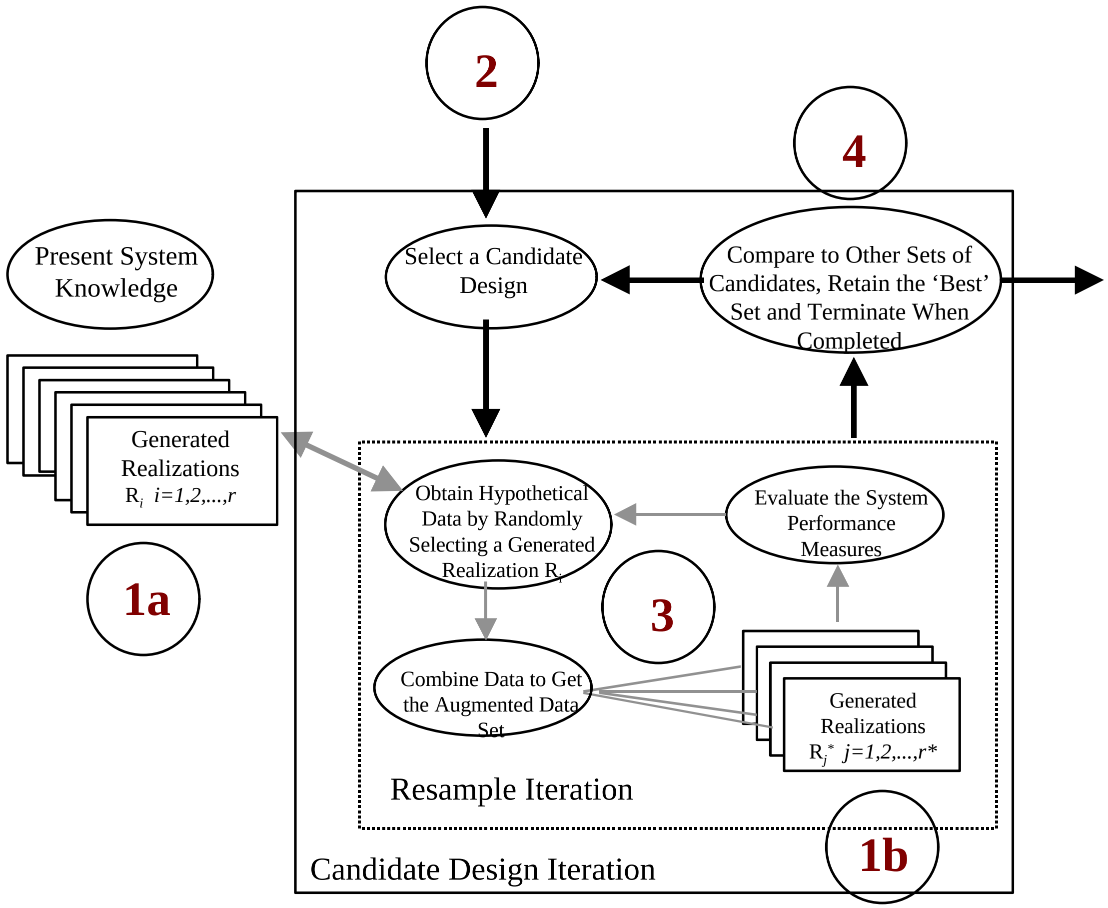
1 Construct a probabilistic representation of the response (stochastic simulation)

2 Select and compare candidate designs for their 'potential relevant information'

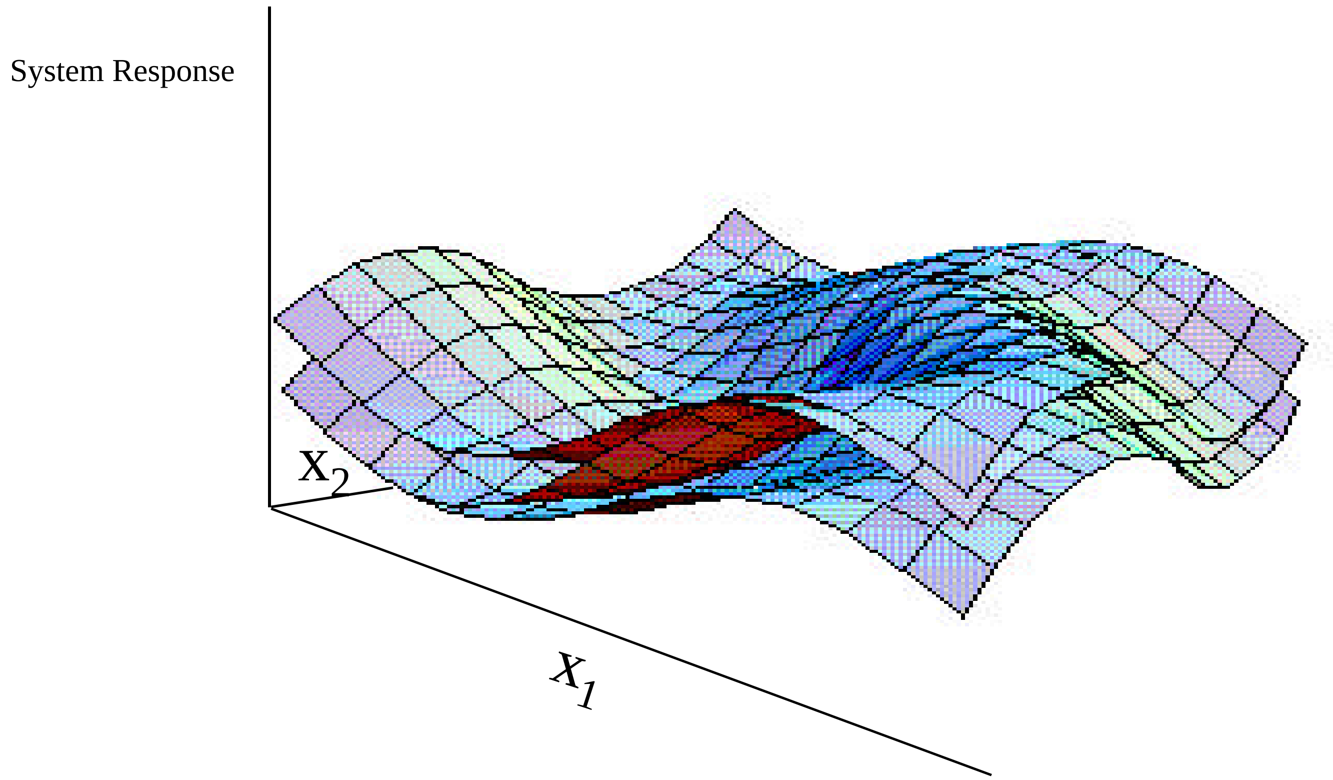
3 Use this representation to evaluate the relevant information that might be gained for a specific 'candidate design'

4 Choose the design that indicates the highest potential for reducing the modeling uncertainty

Flow Diagram for the Proposed Approach



‘Stochastic Simulation’ #1



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Stochastic Simulation (continued)

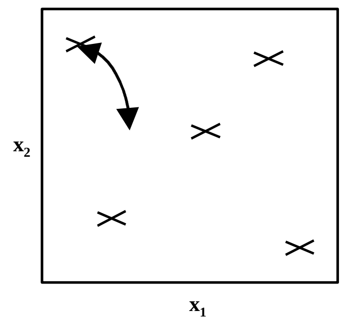
An ensemble of realizations constructed through stochastic simulation provides a discrete approximation to a probability measure over the response surface -- much as a histogram might represent a probability density.

One way it might be used is to estimate the performance criterion using one realization at a time. This provides a means of segregating modeling uncertainty from variability that can be attributed to non-deterministic inputs.

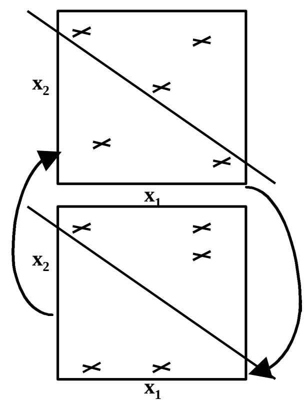
It will be used in another way as well for the proposed approach

Selecting Candidate Designs #2

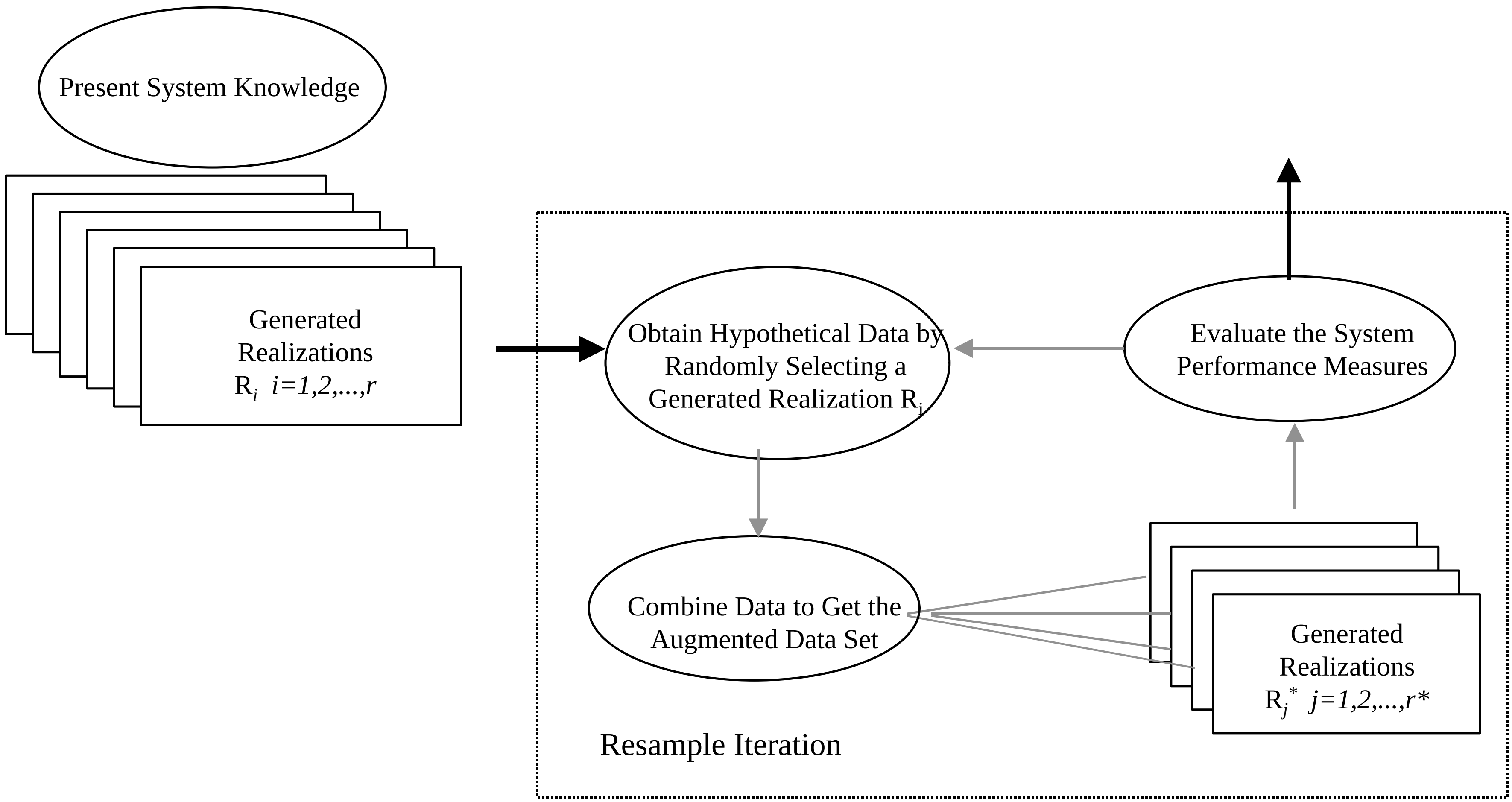
Simulated annealing



Evolutionary algorithms



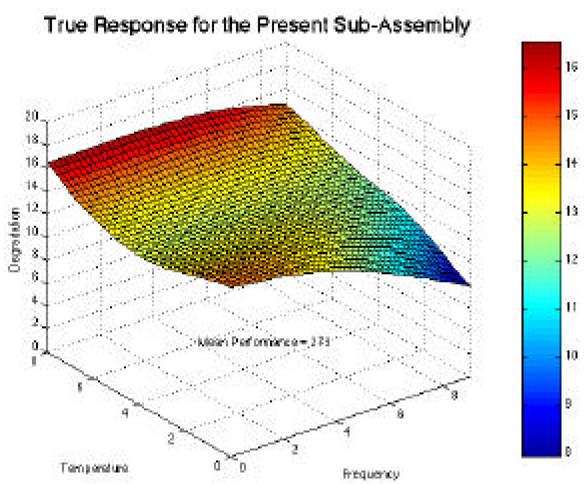
Evaluating Candidate Designs #3

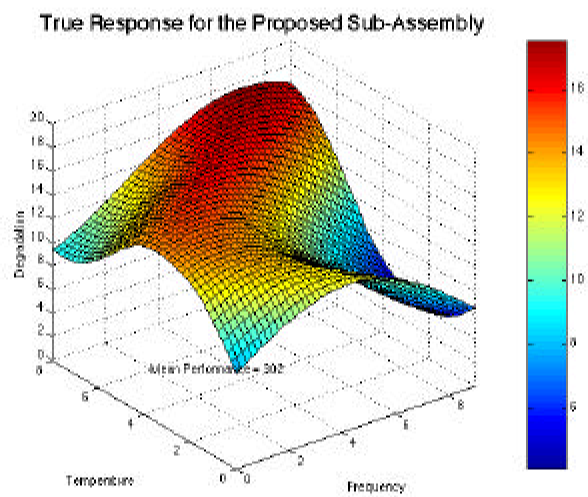


Comparing Candidate Designs #4

- No general approach established yet
- For the uncertainty problem, choose to maximize the ratio s_b^2 / s_w^2
- For optimization, a similar metric has been used

Example


True Response for the Present Sub-Assembly
Degradation
Temperature
Frequency


True Response for the Proposed Sub-Assembly
Degradation
Temperature
Frequency

Example (base-case)

- Objective for the base-case analysis is to determine whether or not to replace the present sub-assembly with a new design based on the expected degradation during re-entry
- The temperature is assumed to be 'uniformily distributed' throughout the specified range
- The frequencies are expected to occur in approximately equal proportion throughout the specified range
- The distribution of degradation is computed as:

$$p(z) = \int I\left(z, \int I\left(r(x_1, x_2), T\right)\left(r(x_1, x_2) - T\right)^c dx_1\right) dF_{x_2}(x_2)$$

Where c=2, T=10 and $I(v_1,v_2)=\{1 \quad \text{if} \quad v_1 > v_2\ ; \quad 0 \text{ otherwise}\}$.

Example (other cases)

1 Change the temperature (x_2) distribution to a truncated normal

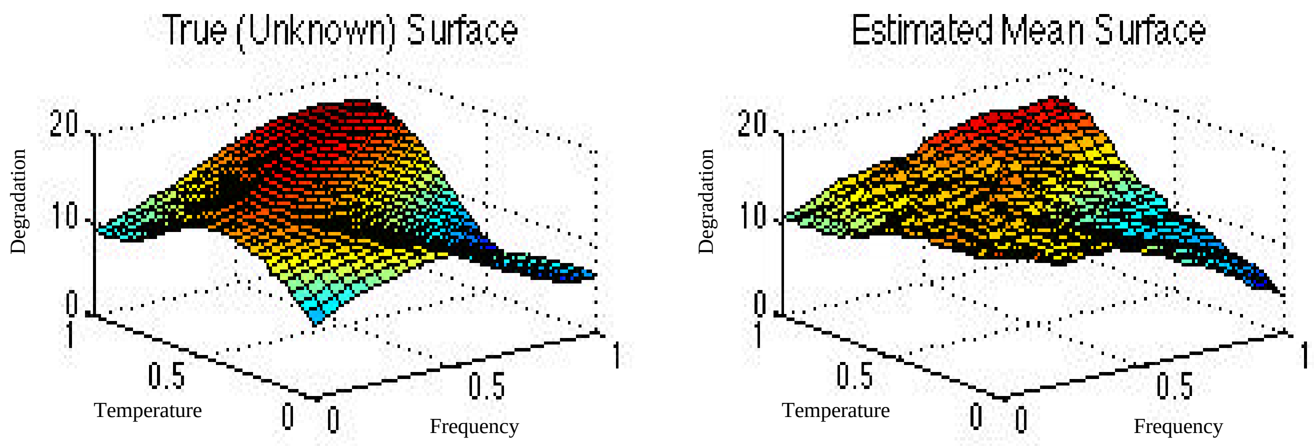
2 Change the degradation parameters to c=2, T=12

3 Change the problem to finding an ideal temperature level

4 Change the design size to 5 (additional) samples

5 Change the form of the response model

Response Modeling



Estimate Made using the Response Model:

$$r'(x_1, x_2) = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_1 x_2 + b_4 x_1^2 + b_5 x_2^2 + e(x_1, x_2)$$

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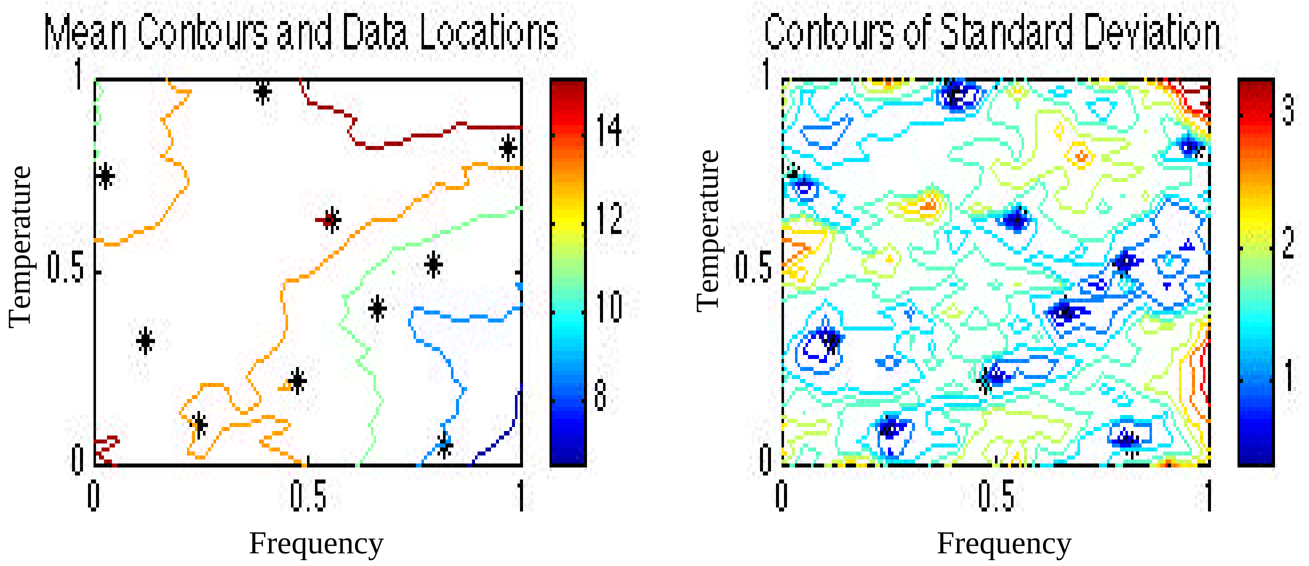
Contours of Mean and Standard Deviation



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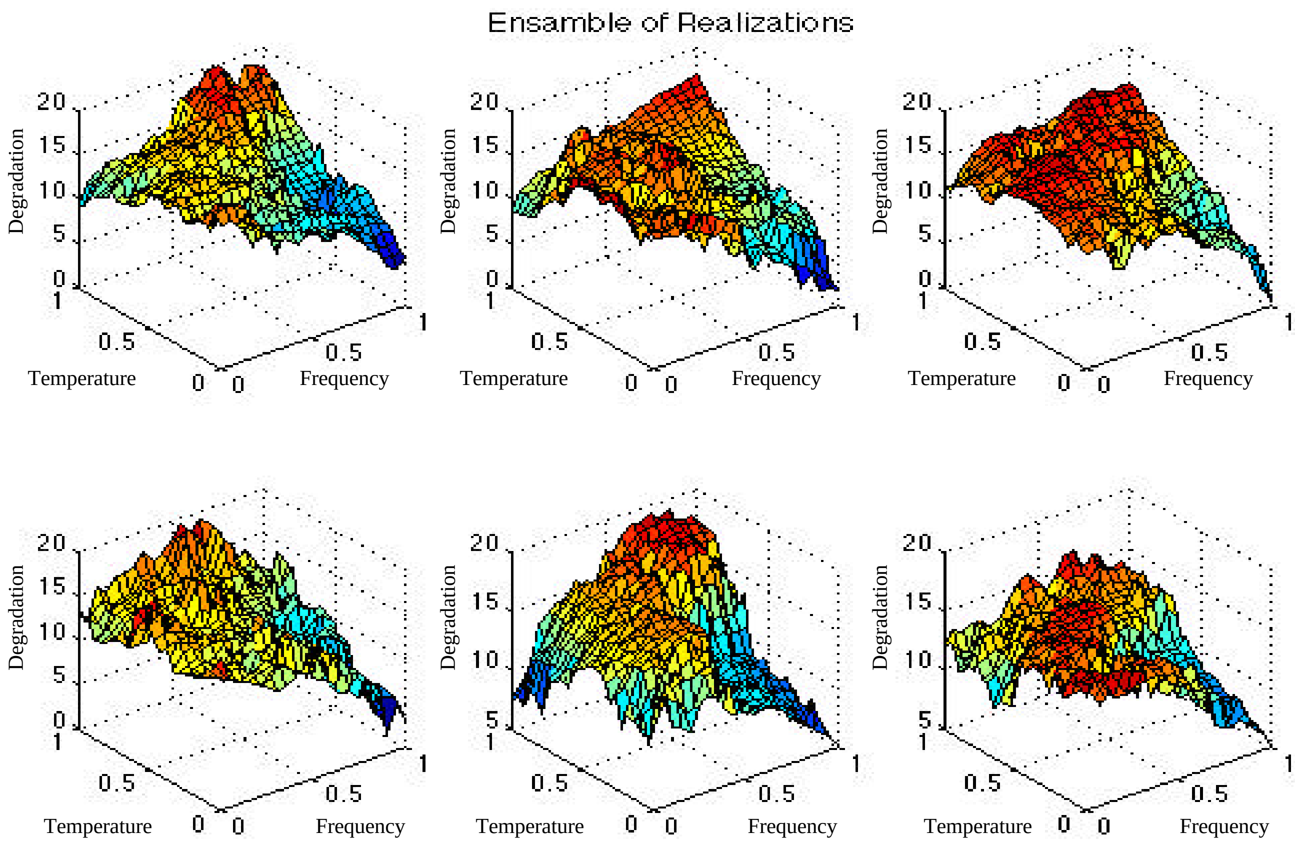
Some of the Possible Responses



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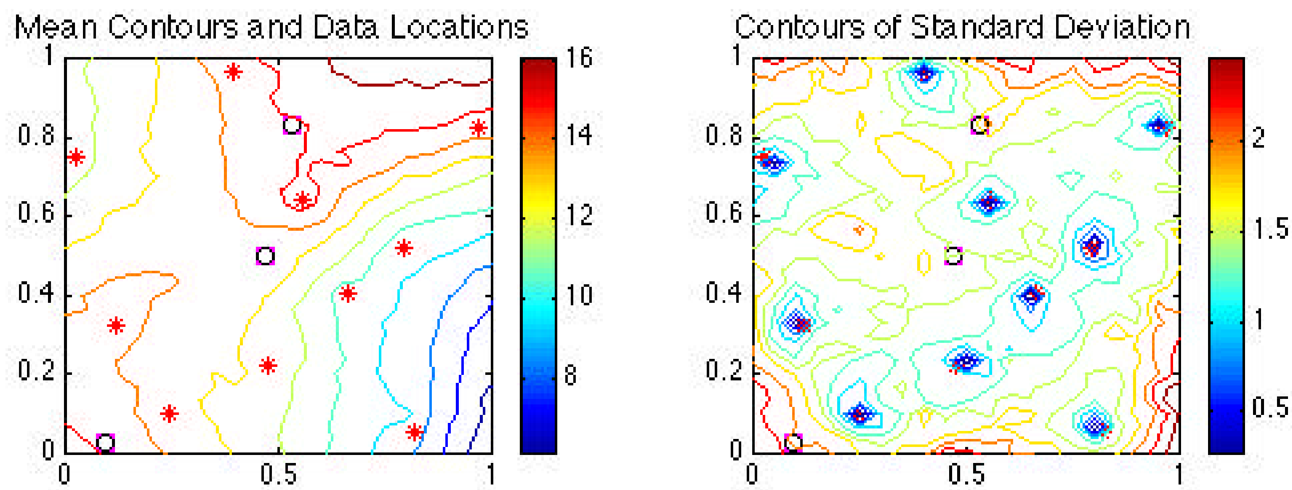
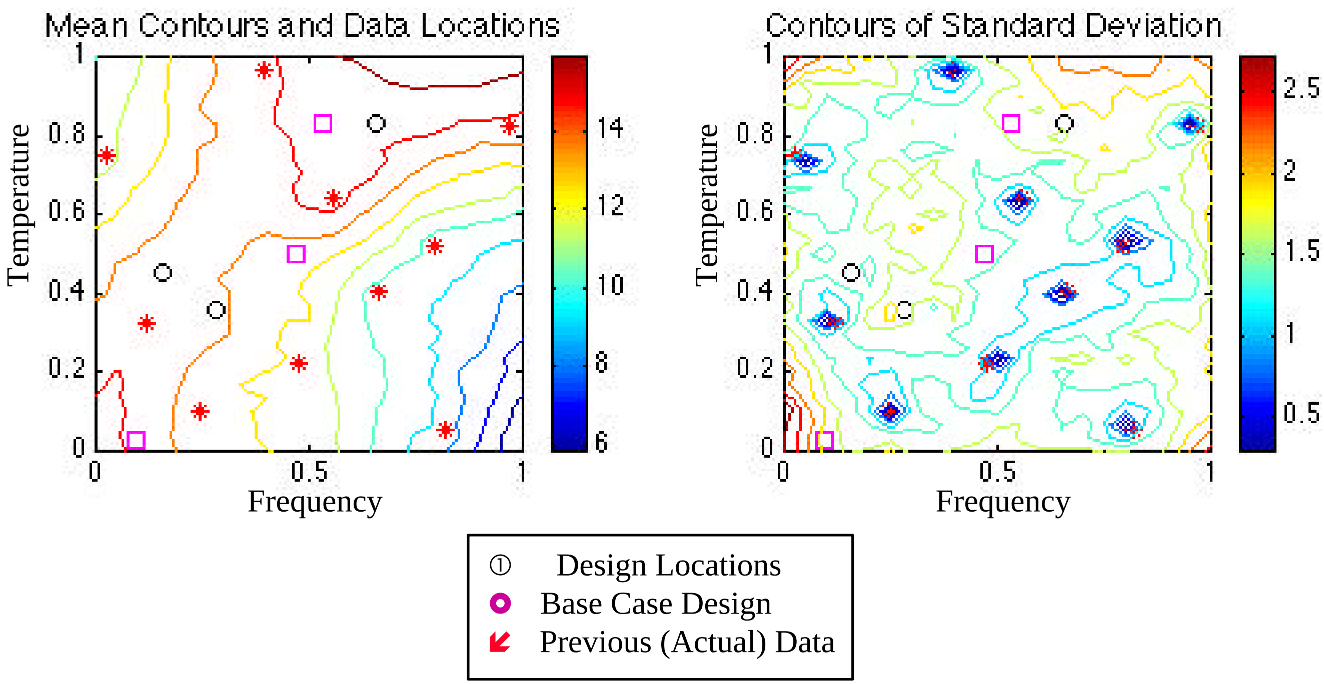
Base Case Analysis



Design Locations
Previous (Actual) Data

Normally Distributed Temperature



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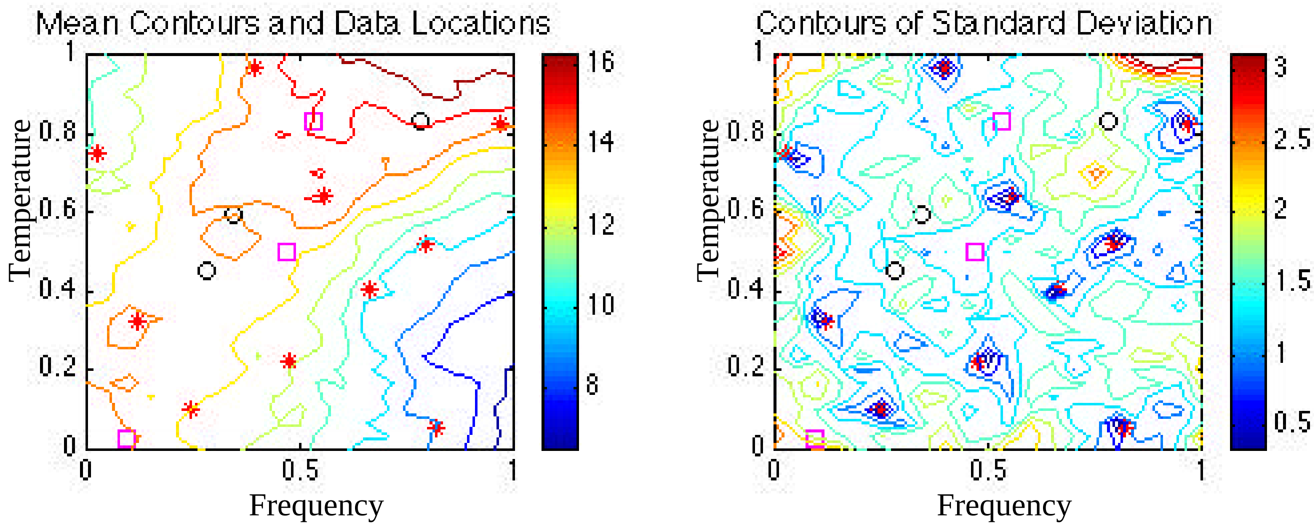
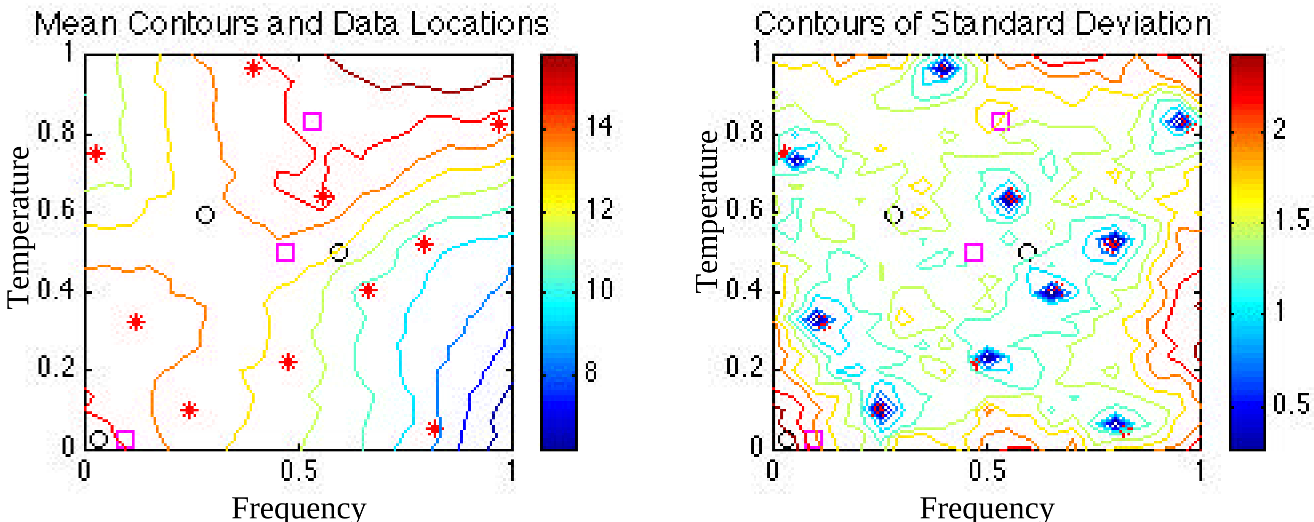
More ‘Harsh’ Degradation Parameters



① Design Locations
Base Case Design
Previous (Actual) Data

Minimization Problem



① Design Locations
Base Case Design
Previous (Actual) Data

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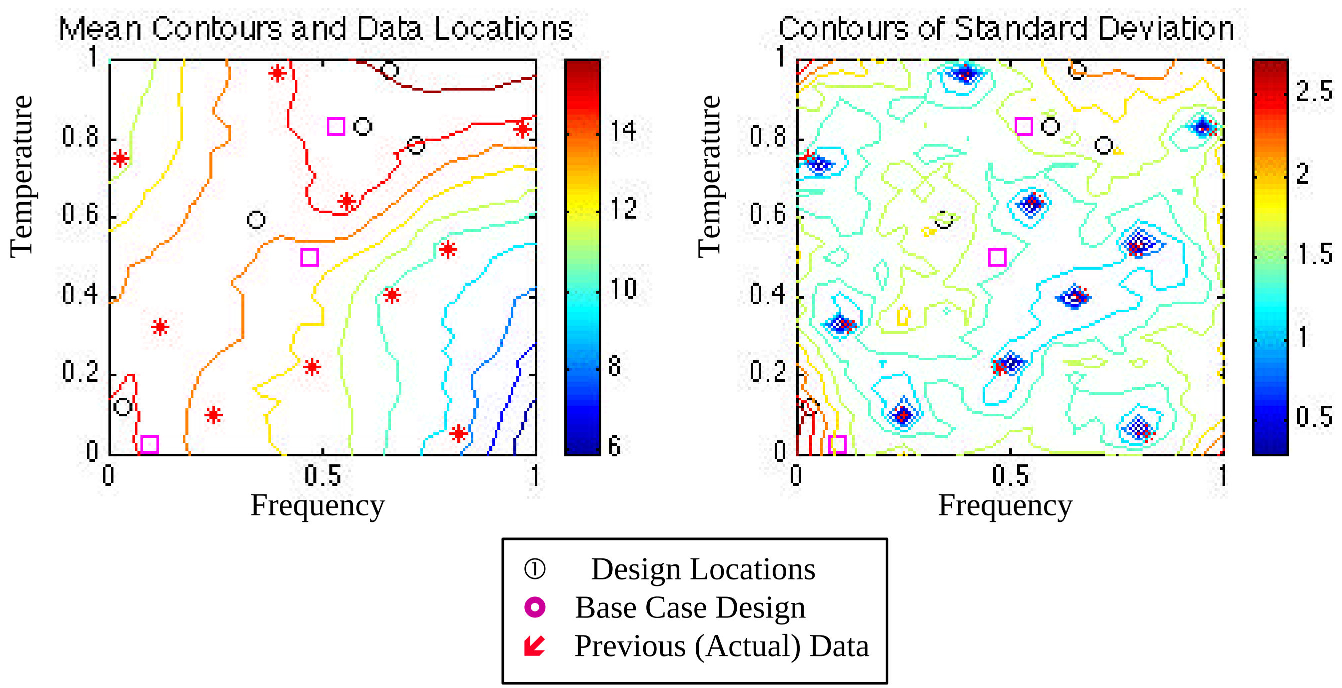
5 Design Points



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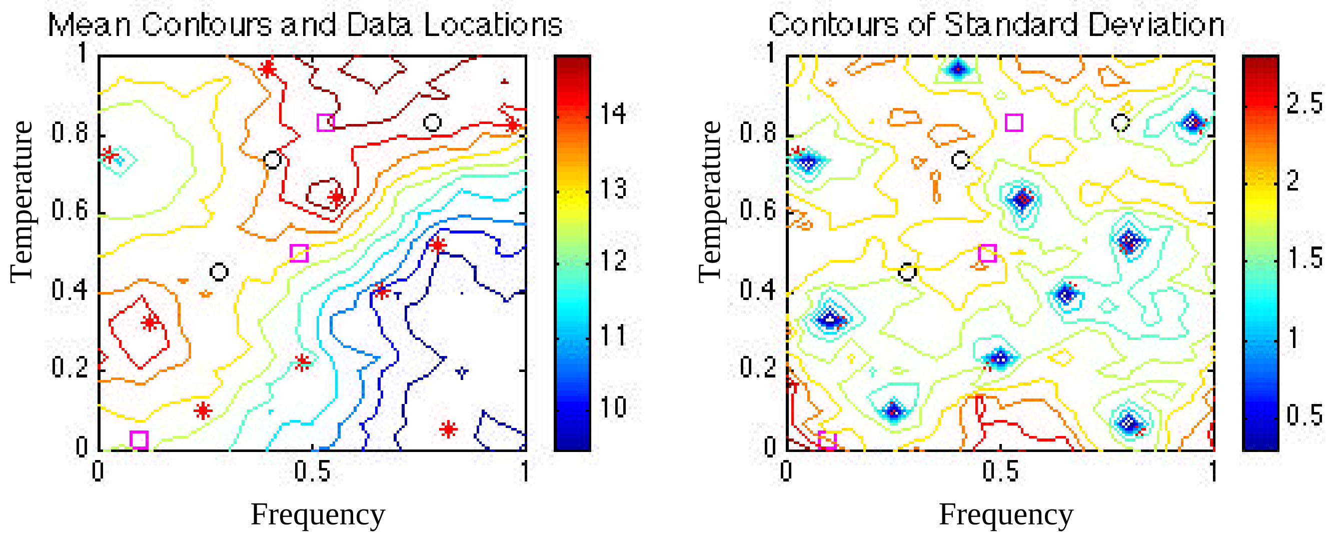
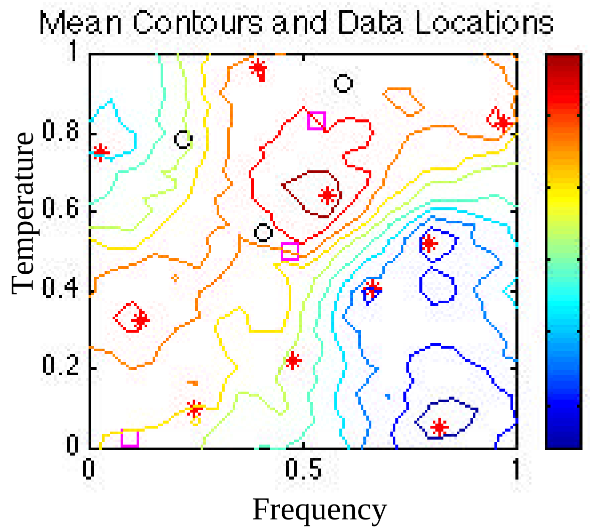
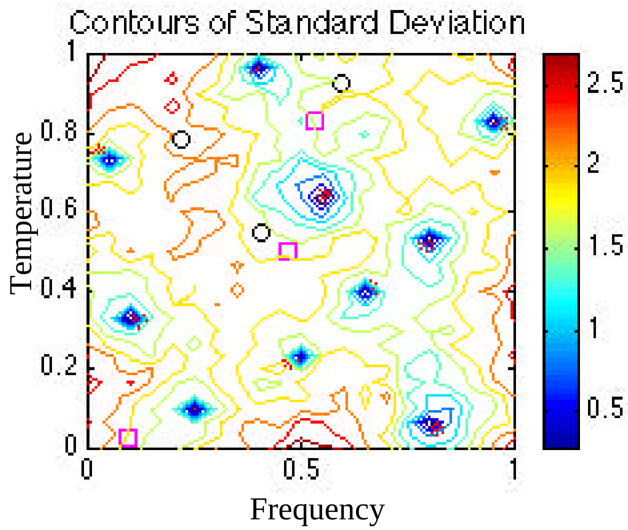
Alternative Model (Linear)



①	Design Locations
o	Base Case Design
↙	Previous (Actual) Data

Alternative Model (Kriging)



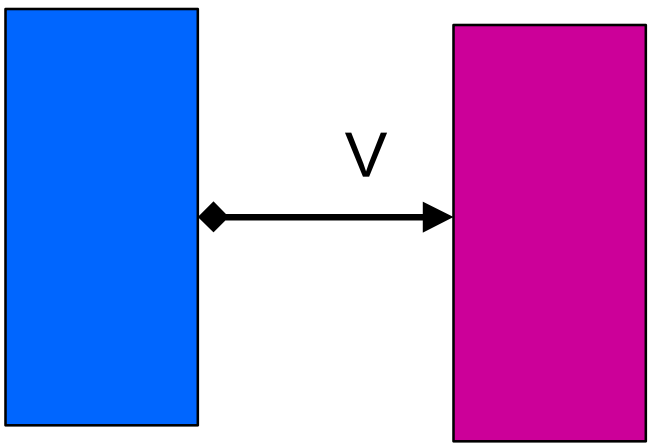


① Design Locations
Base Case Design
Previous (Actual) Data

Shock Wave Physics

Consider the following shock wave experiment, which can be performed with explosive configurations, or gas guns, or other controlled means of acceleration.

V = Impact Velocity



“Impactor” “Target”

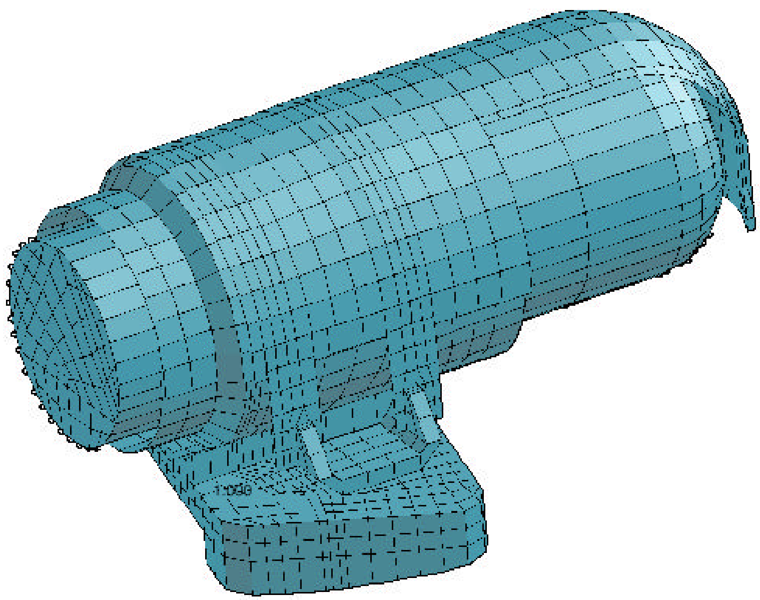
Inputs:

1) Numerical Parameters
2) Impactor Material Parameters
3) Target Material Parameters

Outputs:

1) Shock Velocity
2) Particle Velocity
3) Parameters of the empirical relationship above

Neutron Generator Application



Inputs:

1) Center of Gravity

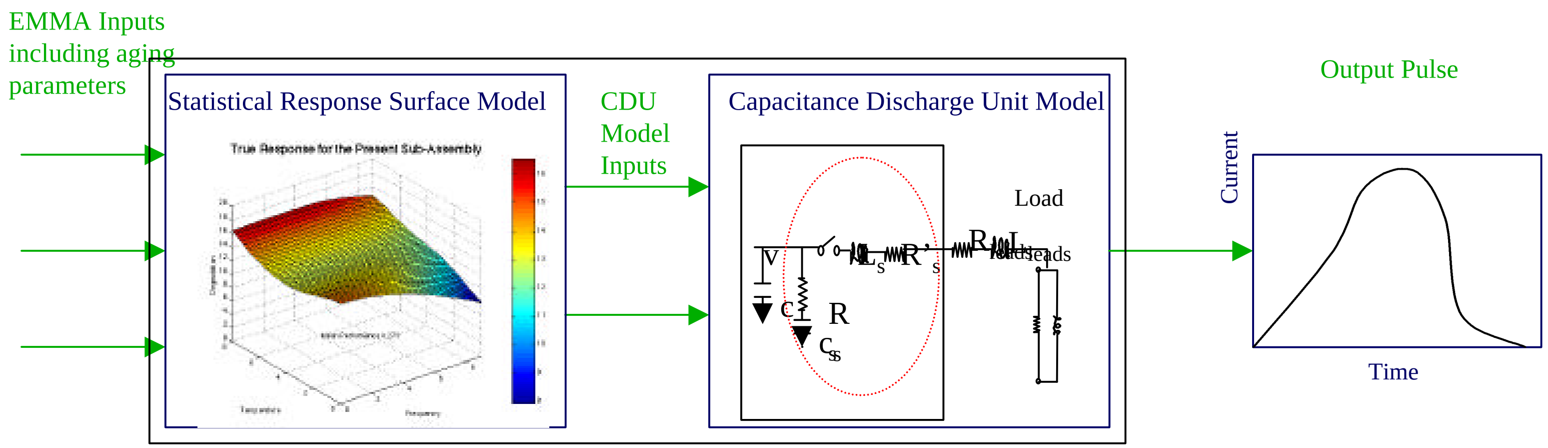
2) Bolt Tightness

3) Foam Composition

Outputs:

1) Response to Shock

Firing Set Behavioral Model Application



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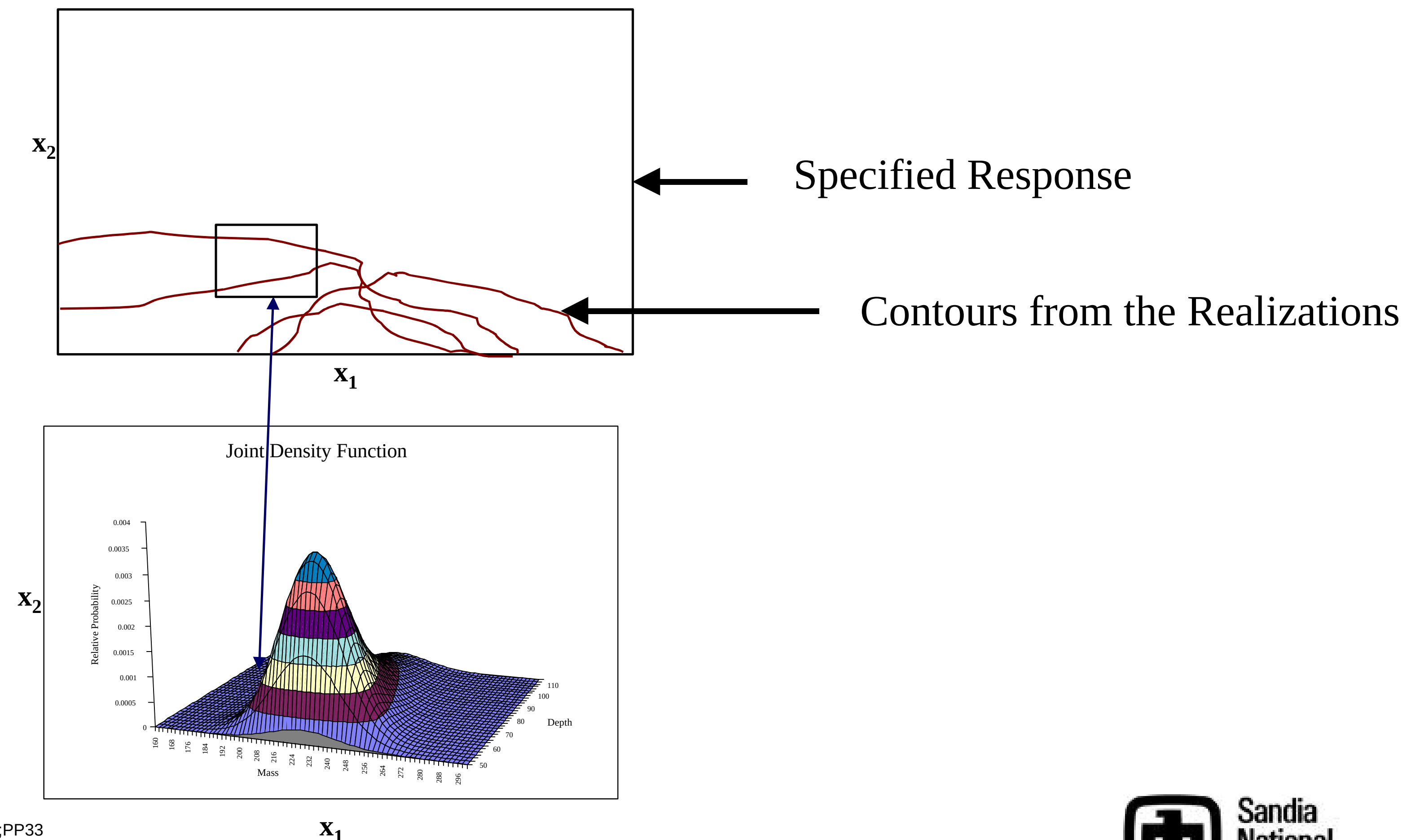
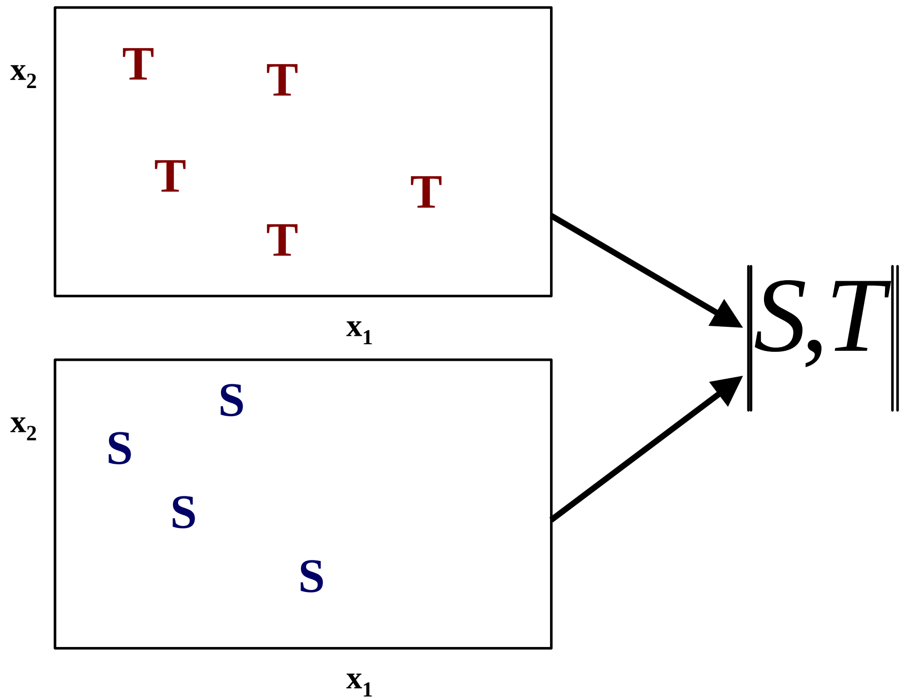
The Inverse Problem



Model Validation



Candidate designs now include cost, error

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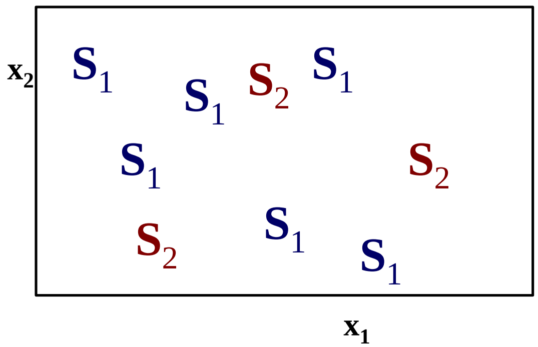
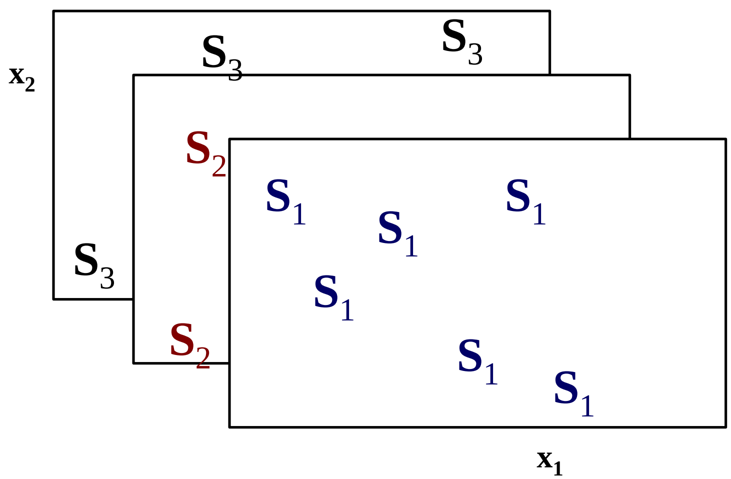
Applications Involving different Modeling Assumptions



Responses are based on data from simulations using models of differing fidelity



Responses are based on alternative conceptual or mathematical models

$$\mathbf{R}_T=\mathbf{W}_1\mathbf{R}_1+\mathbf{W}_2\mathbf{R}_2+\mathbf{W}_3\mathbf{R}_3$$

Summary

- A good computer experimental design can reduce costs substantially by minimizing response modeling uncertainty
- The proposed approach accomplishes this task for very general types of computer analyses
- Testing for low-dimensional problems has provided promising results; Work on higher dimensional problems is in progress.