Uncertainty Quantification and Sensitivity Analysis

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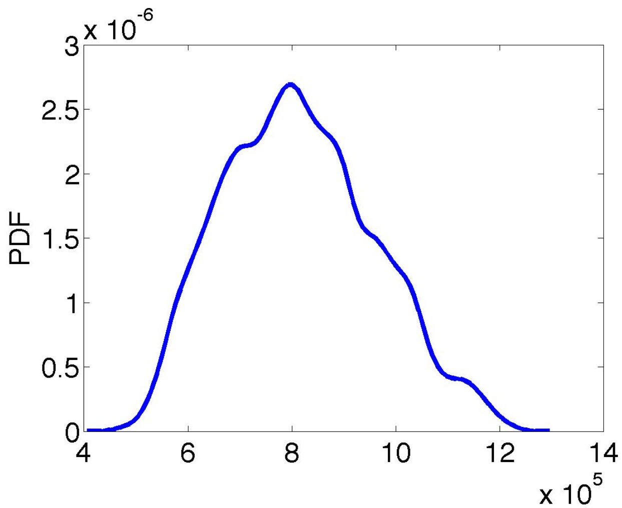
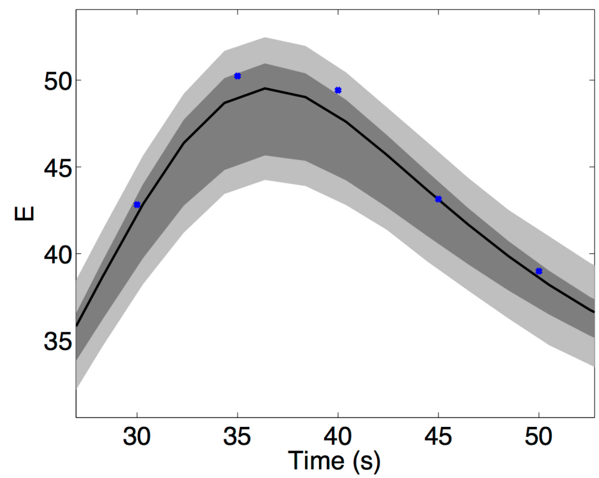
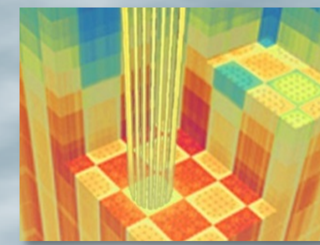
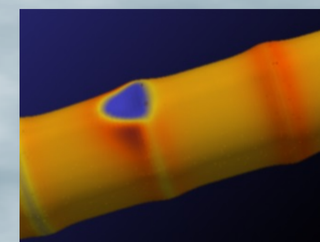


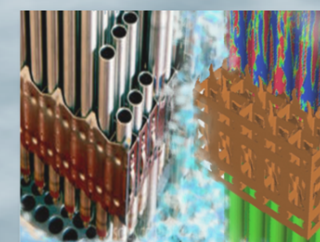


Essentially, all models are wrong, but some are useful, George E.P. Box, Industrial Statistician.

No one trusts a model except the man who wrote it; everyone trusts an observation except the man who made it, Harlow Shapely.





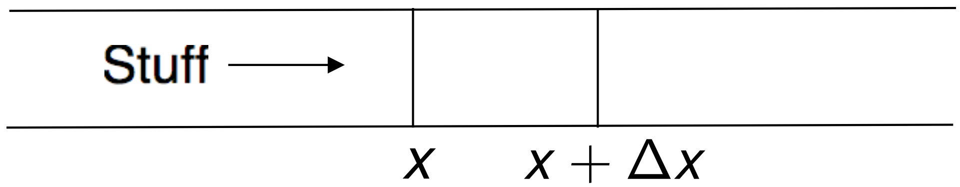


CASL The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

U.S. DEPARTMENT OF ENERGY

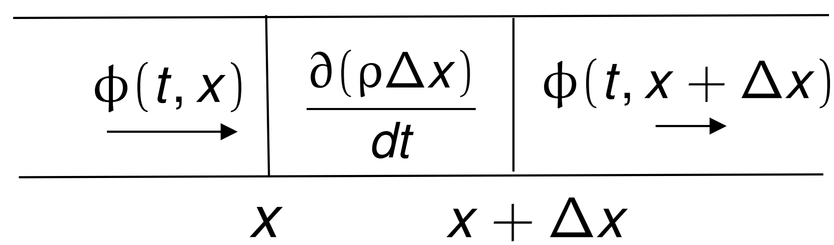
Modeling Strategy

General Strategy: Conservation of stuff



$$\boxed{\frac{dStuff}{dt} = \text{Stuff in - Stuff out + Stuff created - Stuff destroyed}}$$

Continuity Equation:



$$\frac{\partial(\rho \Delta x)}{\partial t} = \phi(t, x) - \phi(t, x + \Delta x)$$

$$\Rightarrow \lim_{\Delta x \to 0} \frac{\partial \rho}{\partial t} = \lim_{\Delta x \to 0} \frac{\phi(t, x) - \phi(t, x + \Delta x)}{\Delta x}$$

$$\boxed{\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = 0}$$

Density: $\rho(t, x)$ - Stuff per unit length or volume

Rate of Flow: $\phi(t, x)$ - Stuff per second

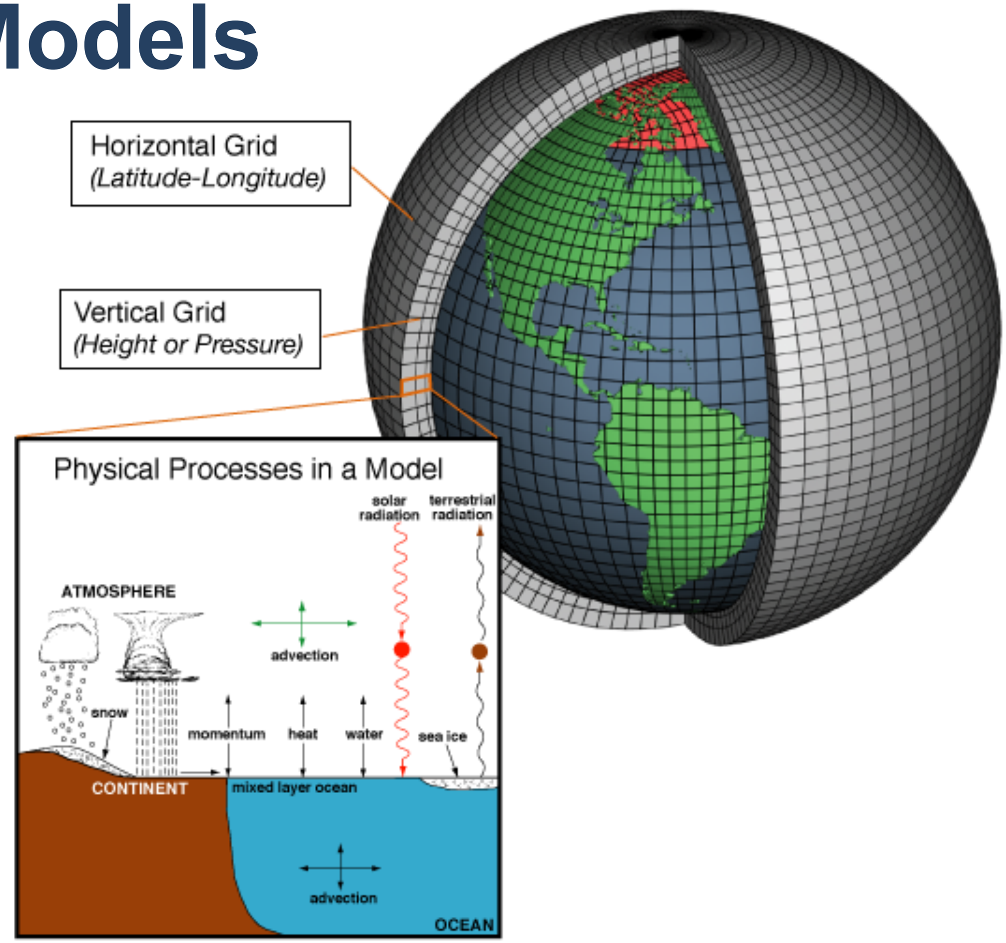
More Generally:

$$\boxed{\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}}$$

Example 1: Weather Models

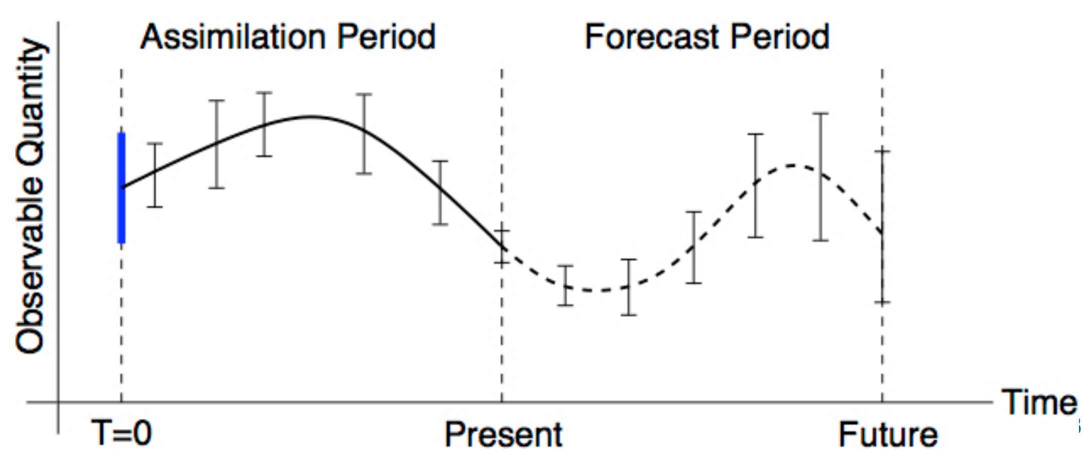
Challenges:

- Coupling between temperature, pressure gradients, precipitation, aerosol, etc.
- Models and inputs contain uncertainties
- Numerical grids necessarily larger than many phenomena; e.g., clouds
- Sensors positions may be uncertain; e.g., weather balloons, ocean buoys.



Goal:

- Assimilate data to quantify uncertain initial conditions and parameters
- Make predictions with quantified uncertainties.



Equations of Atmospheric Physics

Conservation Relations:

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}}$$

Mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

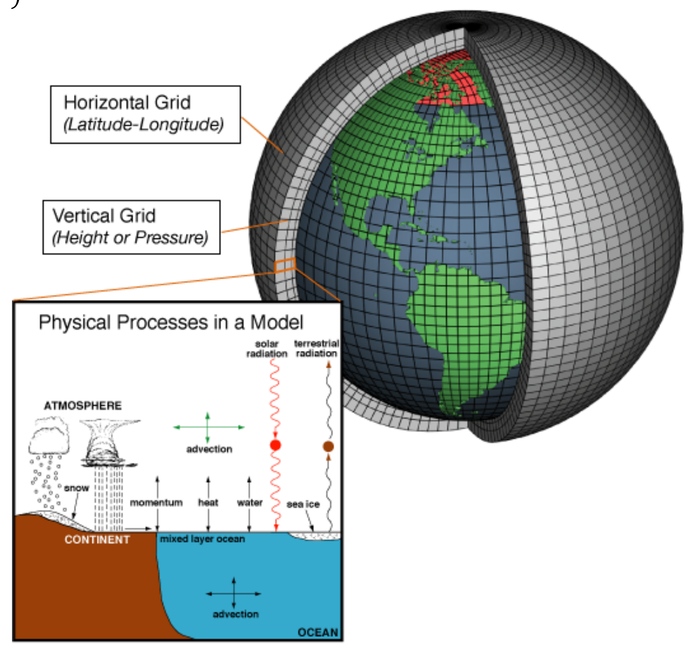
Momentum
$$\frac{\partial v}{\partial t} = -v \cdot \nabla v - \frac{1}{\rho}\nabla p - g\hat{k} - 2\Omega \times v$$

Energy
$$\rho c_V \frac{\partial T}{\partial t} + p\nabla \cdot v = -\nabla \cdot F + \nabla \cdot (k\nabla T) + \rho\dot{q}(T, p, \rho)$$

$$p = \rho R T$$

Water
$$\frac{\partial m_j}{\partial t} = -v \cdot \nabla m_j + S_{m_j}(T, m_j, \chi_j, \rho)\ ,\ j = 1, 2, 3,$$

Aerosol
$$\frac{\partial \chi_j}{\partial t} = -v \cdot \nabla \chi_j + S_{\chi_j}(T, \chi_j, \rho)\ ,\ j = 1, \cdots, J,$$



Constitutive Closure Relations: e.g.,

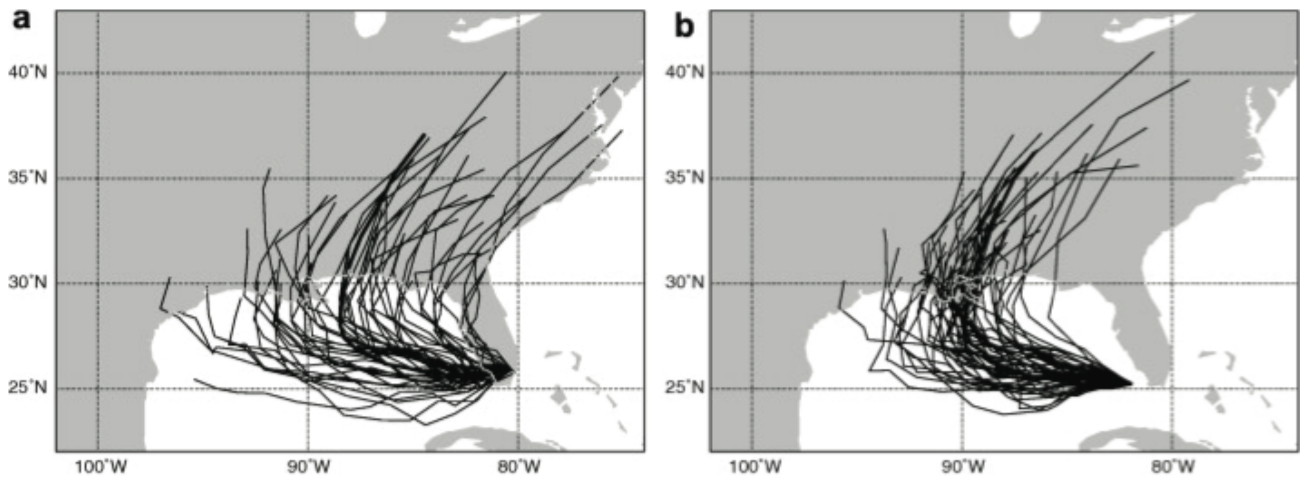
$$S_{m_2} = S_1 + S_2 + S_3 - S_4$$

where

$$S_1 = \bar{\rho}(m_2 - m_2^*)^2 \left[\underline{1.2 \times 10^{-4}} + \left(\underline{1.569 \times 10^{-12}} \frac{n_r}{d_0(m_2 - m_2^*)} \right) \right]^{-1}$$

Ensemble Predictions

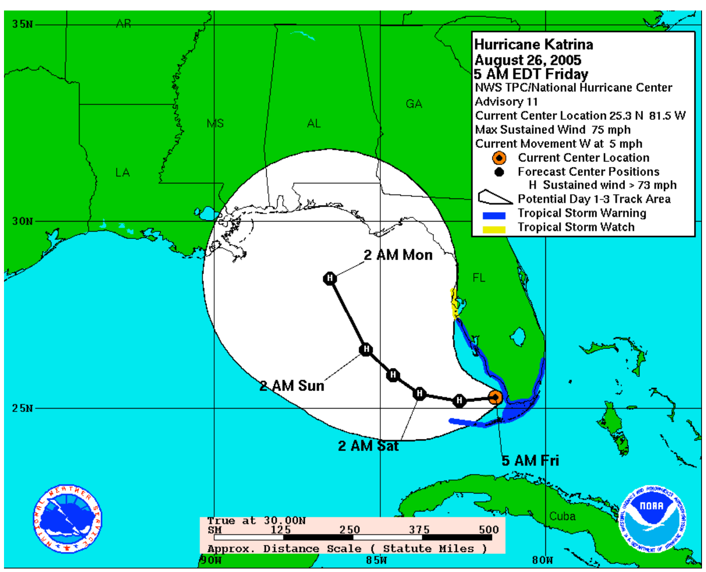
Ensemble Predictions:



00 UTC on August 26, 2005

12 UTC on August 26, 2005

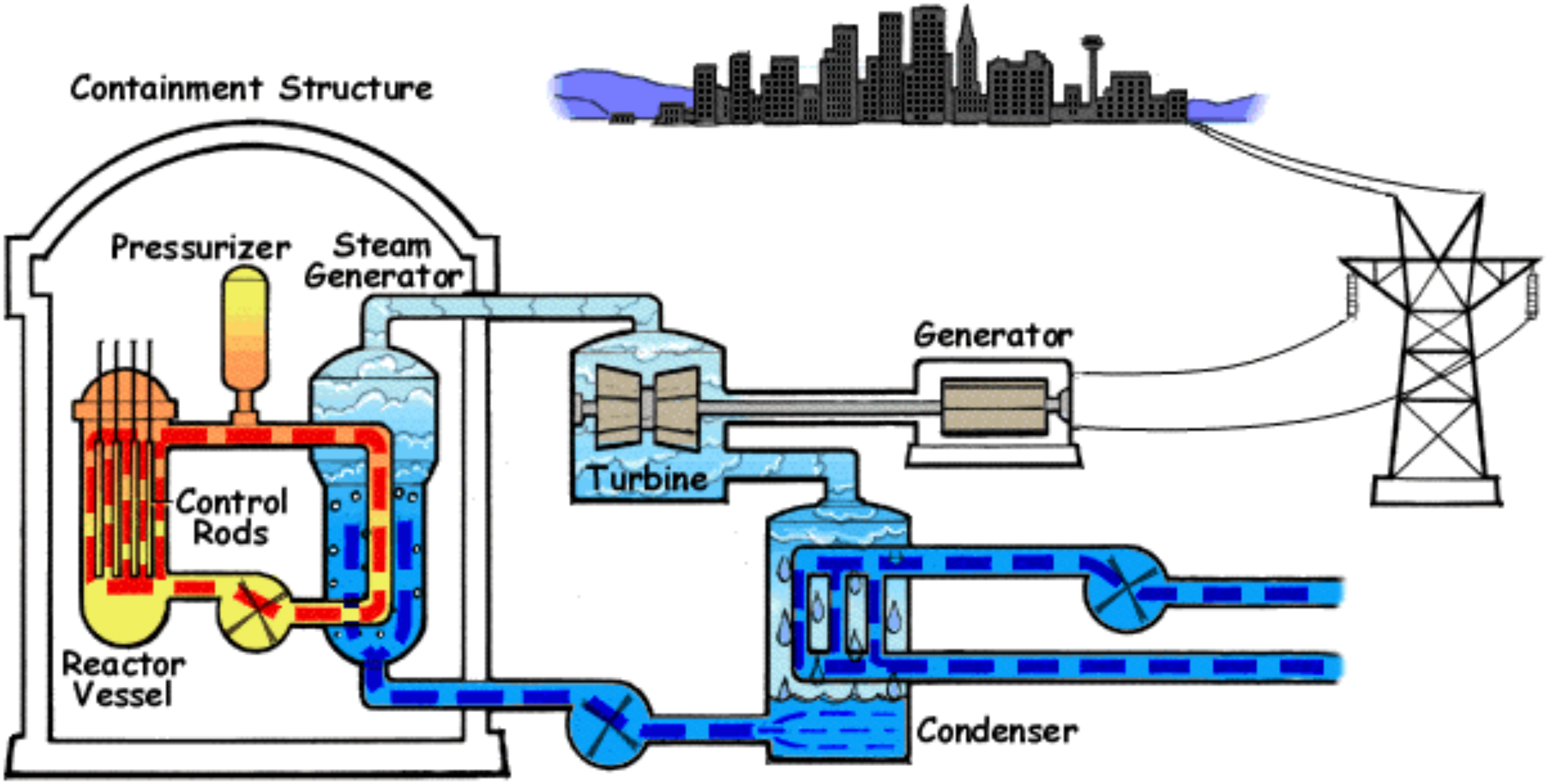
Cone of Uncertainty:



General Questions:

- What is expected rainfall on August 13?
- What is average high temperature?
- Note: Quantities are statistical in nature.

Example 2: Pressurized Water Reactors (PWR)



Models:

- Involve neutron transport, thermal-hydraulics, chemistry, fuels
- Inherently multi-scale, multi-physics.

Example: PWR

3-D Neutron Transport Equations:

$$\frac{1}{|v|}\frac{\partial \varphi}{\partial t} + \Omega \cdot \nabla \varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t)$$

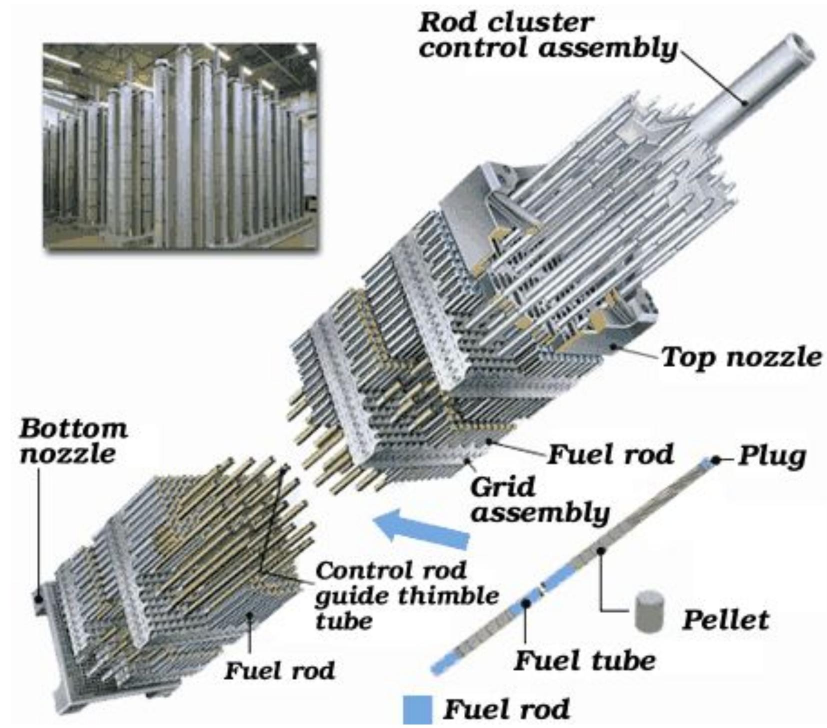
$$= \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(E' \to E, \Omega' \to \Omega)\varphi(r,E',\Omega',t)$$

$$+ \underline{\frac{\chi(E)}{4\pi}} \int_{4\pi} d\Omega' \int_0^\infty dE' \underline{\nu(E')}\,\underline{\Sigma_f(E')}\varphi(r,E',\Omega',t)$$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}}$$

Challenges:

- Very large number of inputs; e.g., 100,000; Active subspace construction critical.
- ORNL Code SCALE: Can take hours to run.
- Numerical errors often difficult to quantify.
- Predicting future requires extrapolatory or out-of-data predictions.



Example: PWR

Thermo-Hydraulic Equations: Mass, momentum and energy balance for fluid

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \nabla \cdot (\alpha_f \rho_f v_f) = -\Gamma$$

$$\alpha_f \rho_f \frac{\partial v_f}{\partial t} + \alpha_f \rho_f v_f \cdot \nabla v_f + \nabla \cdot \sigma_f^R + \alpha_f \nabla \cdot \sigma + \alpha_f \nabla p_f$$
$$= -F^R - F + \Gamma(v_f - v_g)/2 + \alpha_f \rho_f g$$

$$\frac{\partial}{\partial t}(\alpha_f \rho_f e_f) + \nabla \cdot (\alpha_f \rho_f e_f v_f + Th) = (T_g - T_f)H + T_f \Delta_f$$
$$-T_g(H - \alpha_g \nabla \cdot h) + h \cdot \nabla T - \Gamma[e_f + T_f(s^* - s_f)]$$
$$-p_f \left(\frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f v_f) + \frac{\Gamma}{\rho_f} \right)$$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial \phi}{\partial x} = \text{Sources - Sinks}}$$

Notes:

- Similar relations for gas and bubbly phases

Challenges:

- Codes can have 15-30 closure relations and up to 75 parameters.
- Codes and closure relations often ”borrowed” from other physical phenomena; e.g., single phase fluids, airflow over a car (CFD code STAR-CCM+)
- Calibration necessary and closure relations can conflict.

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Thermo-Hydraulic Equations: Mass, momentum and energy balance for fluid

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Example: Dittus—Boelter Relation

$$Nu = 0.023 Re^{0.8} Pr^{0.4}$$

Nu: Nusselt number
Re: Reynolds number
Pr: Prandtl number

Example: PWR

Example: Shearon Harris outside Raleigh

UQ Questions:

- What is peak operating temperature?
- What is expected level of CRUD buildup?
- What is risk associated with operating regime?
- What is expected profit for new design?

Example 3: Quantum-Informed Continuum Models

Objectives:

- Employ density function theory (DFT) to construct/calibrate continuum energy relations.
  - e.g., Helmholtz energy

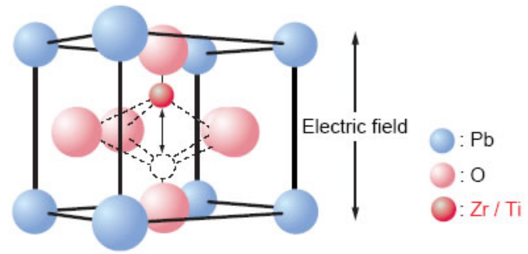
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$

Note:

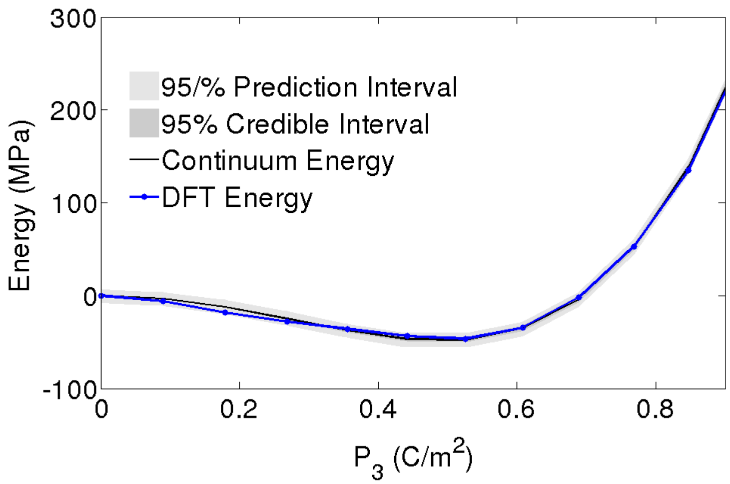
- Linearly parameterized

UQ and SA Issues:

- Is 6^{th} order term required to accurately characterize material behavior?
- **Note:** Determines molecular structure



Lead Titanate Zirconate (PZT)



Helmholtz Energy

Challenge: Terminology and Notation

Terminology:

- Inputs: Parameters, initial conditions, boundary conditions, exogenous forces; e.g., parameters in closure relations, initial conditions in transient models.
- Outputs or Responses: Quantities that we experimentally or numerically measure; e.g., outlet temperature in reactor.
- Quantities of Interest (QoI): Statistical quantity that we want to compute; e.g., average CRUD buildup, expected profit for a given design.

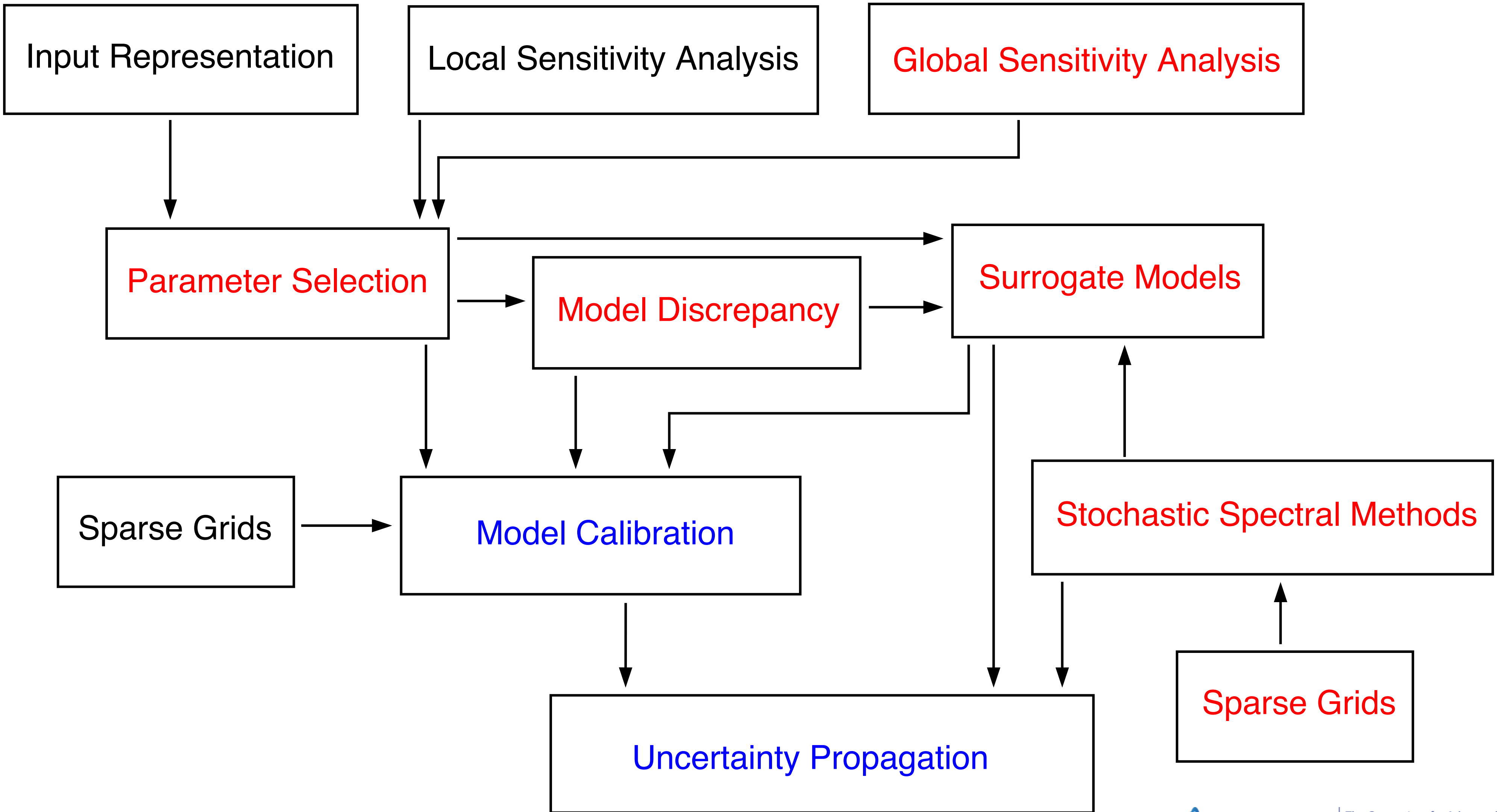
Input Notation: Can vary even within disciplines!

- Math Control Community: $q = [q_1, \ldots, q_p]$
- Math Reduced-Order Community: $p = [p_1, \ldots, p_q]$
- Statistics: $\theta = [\theta_1, \ldots, \theta_d]$
- Nuclear Engineering: $\alpha = [\alpha_1, \ldots, \alpha_k]$
- Active subspace community: $x = [x_1, \ldots, x_p]$

Note: Same variability in notation for outputs and quantities of interest

Steps in Uncertainty Quantification

Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



Deterministic Model Calibration

Example: Helmholtz energy $\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$

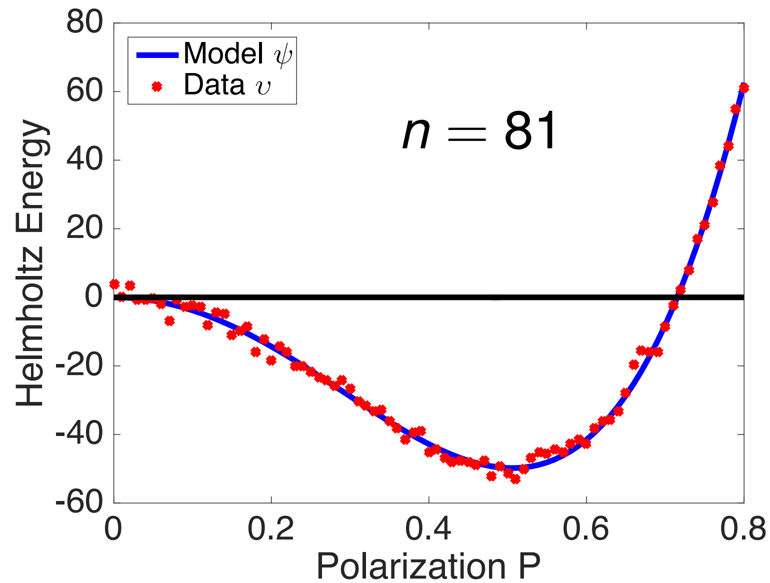
$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

Statistical Model: Describes observation process

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \quad , \; i = 1, \dots, n$$

Point Estimates: Ordinary least squares

$$q^0 = \arg\min_q \frac{1}{2} \sum_{j=1}^{n} [\upsilon_i - \psi(P_i, q)]^2$$



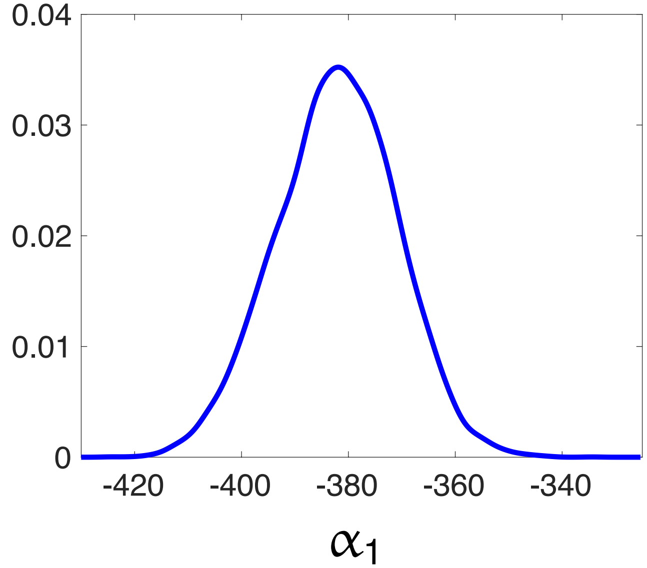
Note: Provides point estimates but no quantification of uncertainty in:

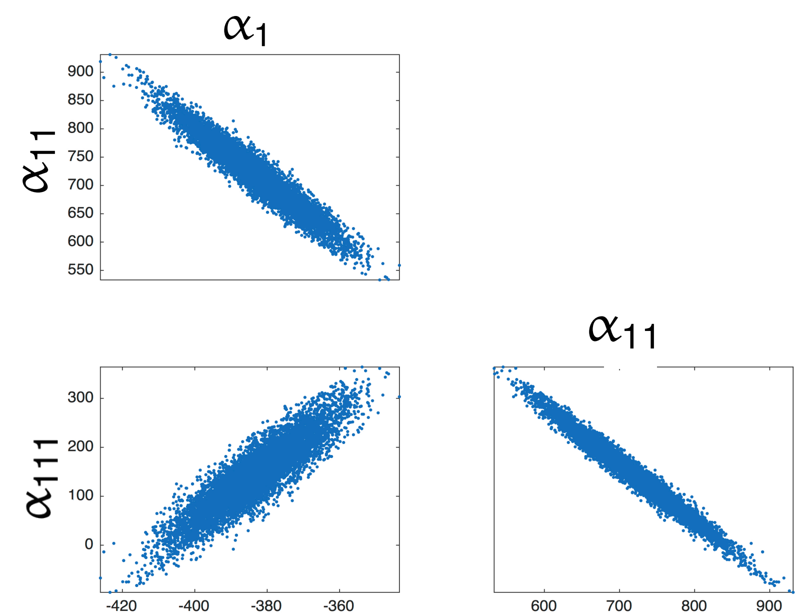
- Model
- Parameters
- Data

Objectives for Uncertainty Quantification

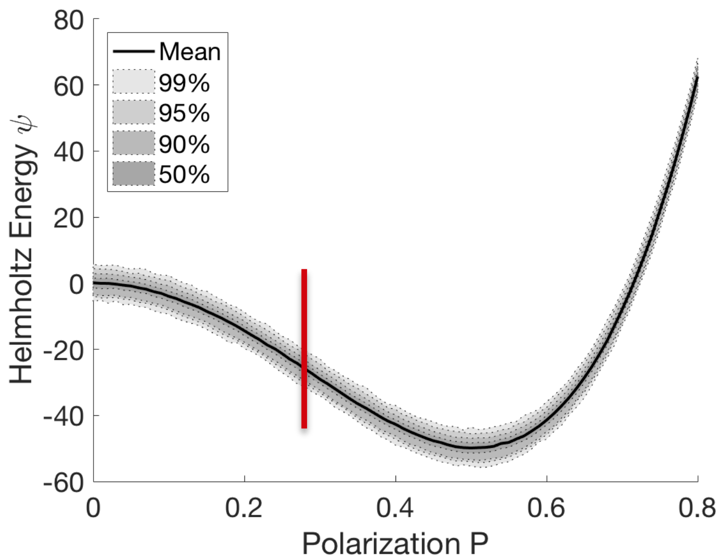
Goal: Replace point estimates with distributions or credible intervals

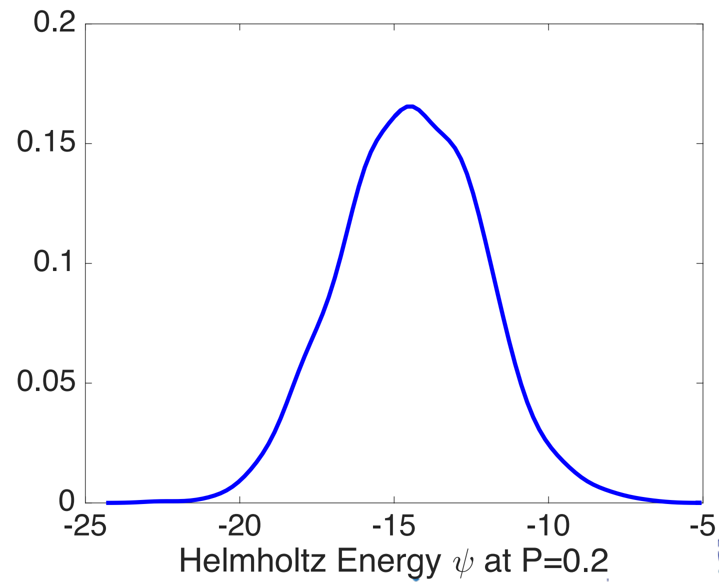
E.g., Parameter Densities





E.g., Response Intervals





Objectives for Uncertainty Quantification

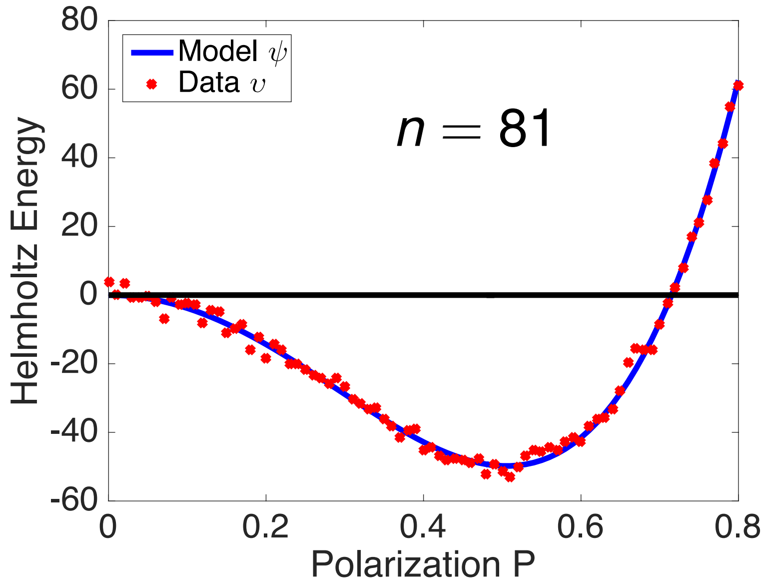
Example: Helmholtz energy $\psi(P, q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$

Statistical Model: Describes observation process

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \quad , \; i = 1, \ldots, n$$

Common Assumption: $\varepsilon_i \sim N(0, \sigma^2)$

UQ Goals: Quantify parameter and response uncertainties



Strategy 1: Perform Experiments

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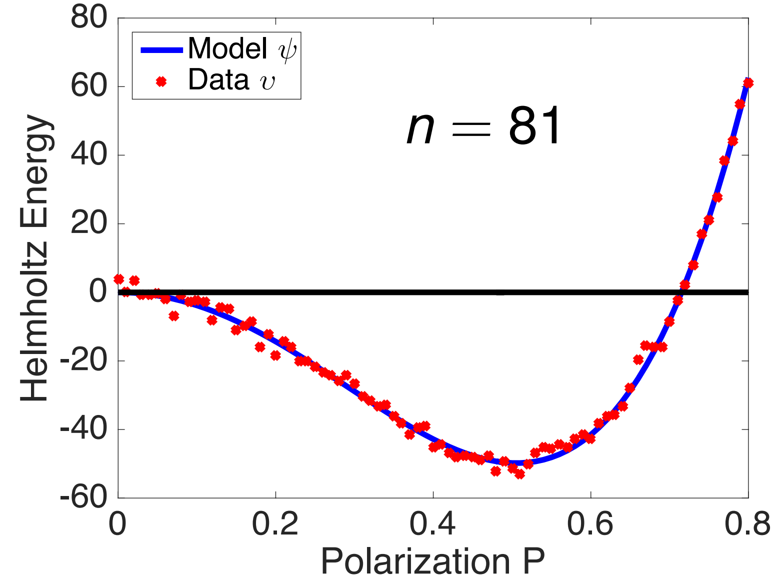

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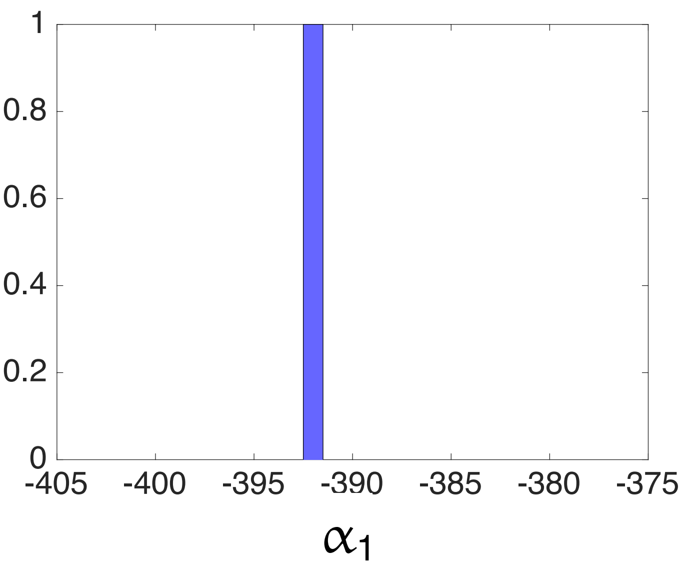

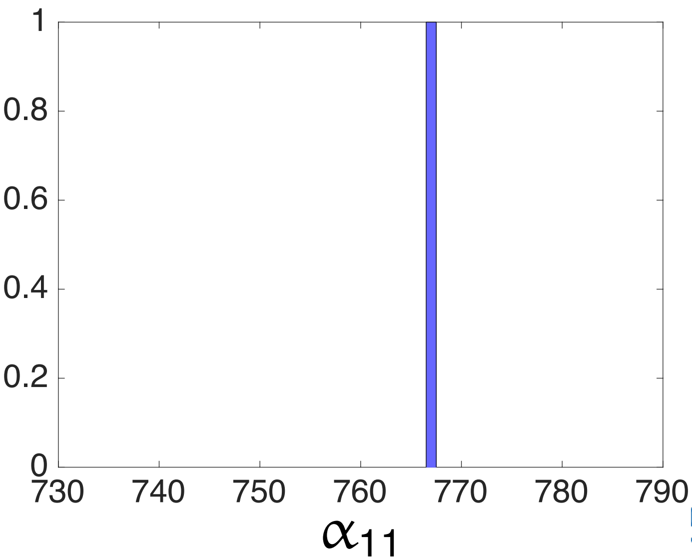

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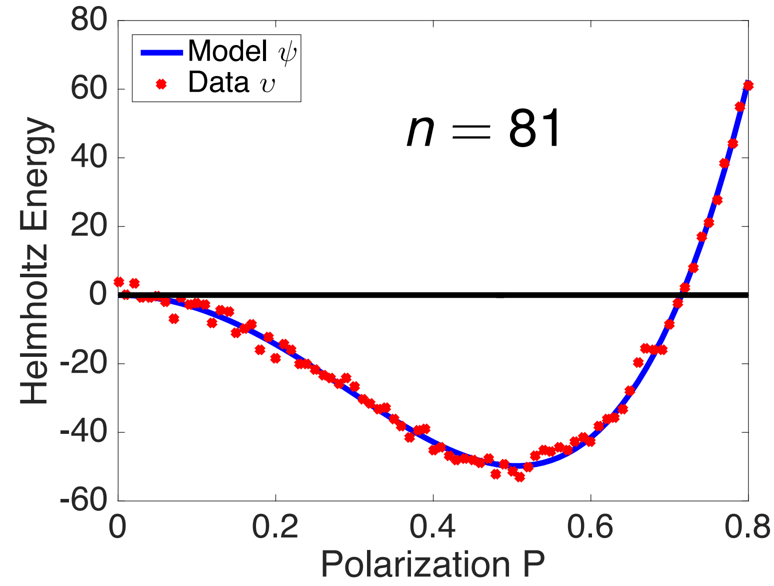

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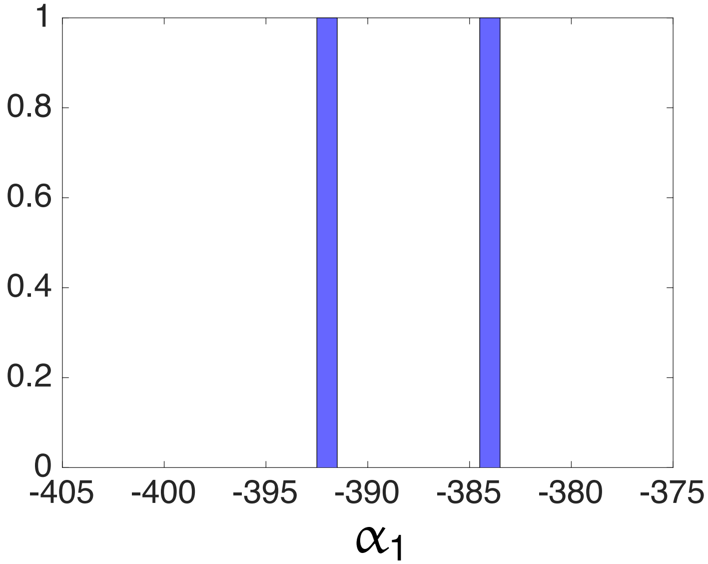

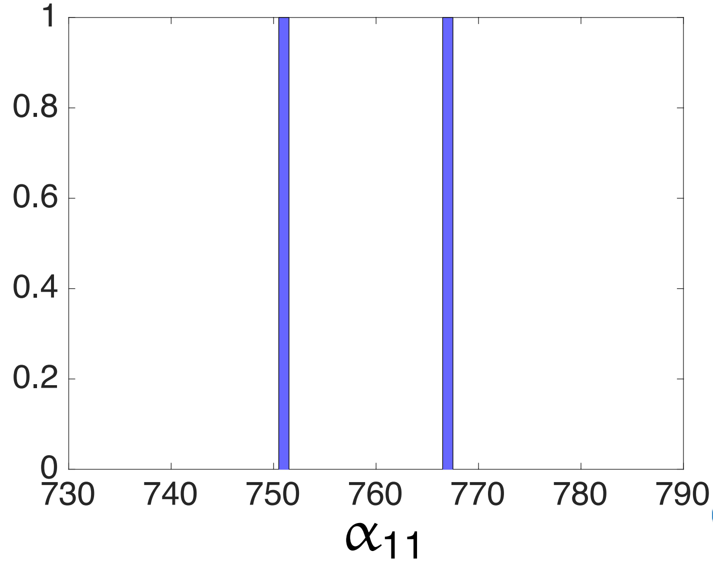

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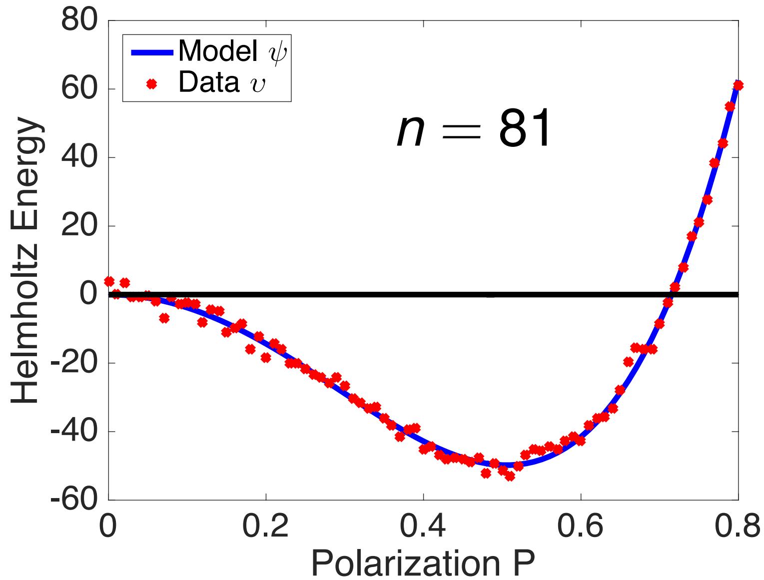

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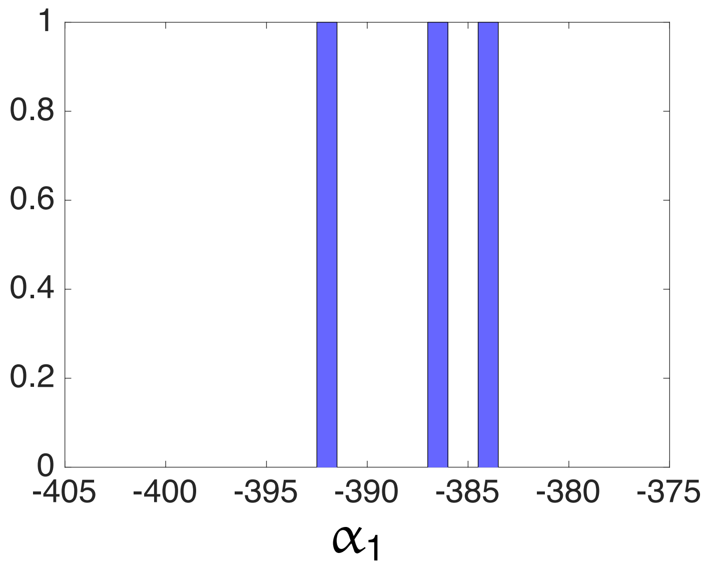

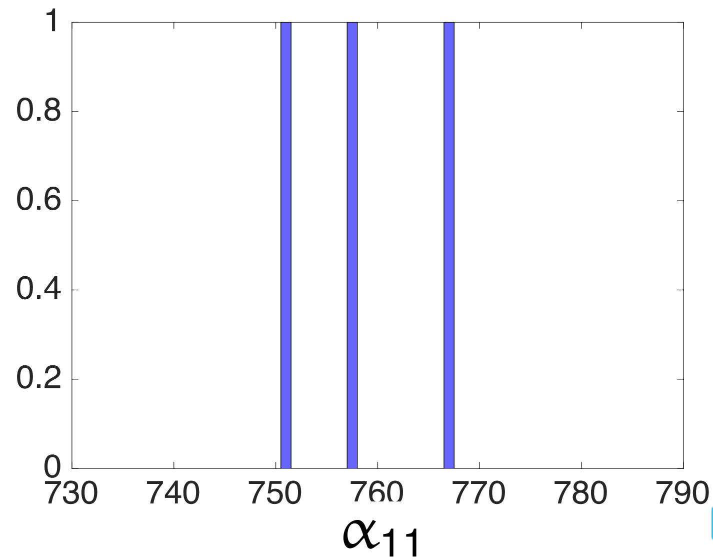

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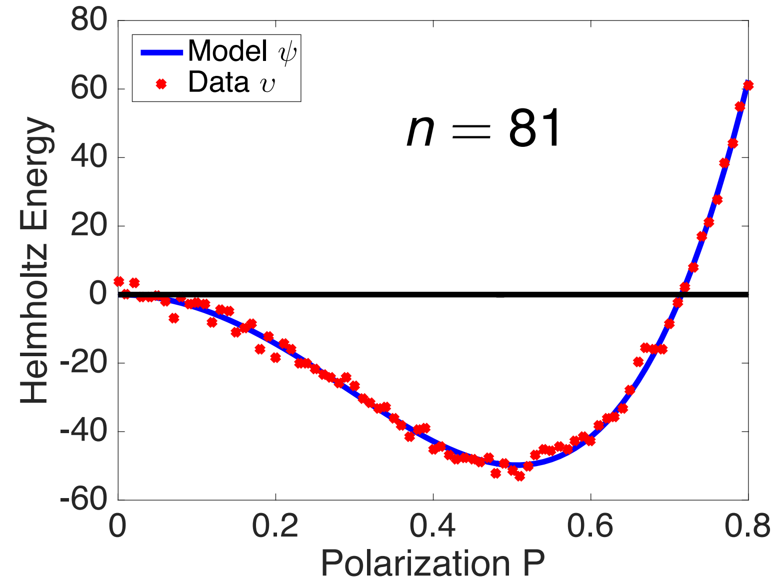
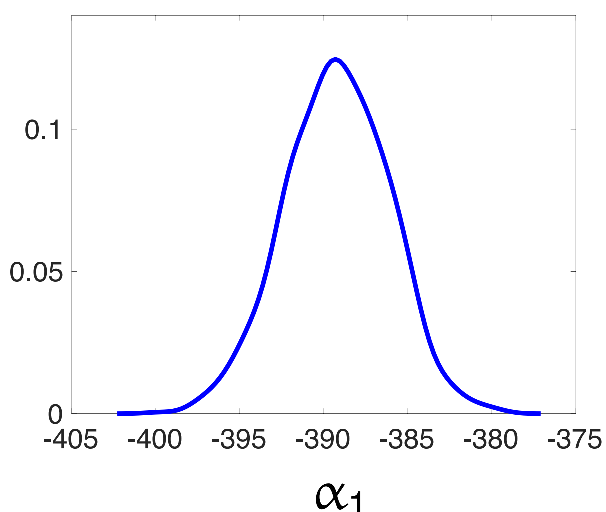
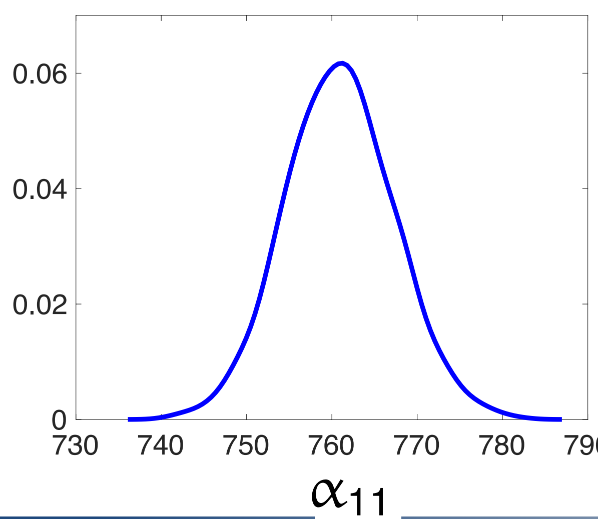
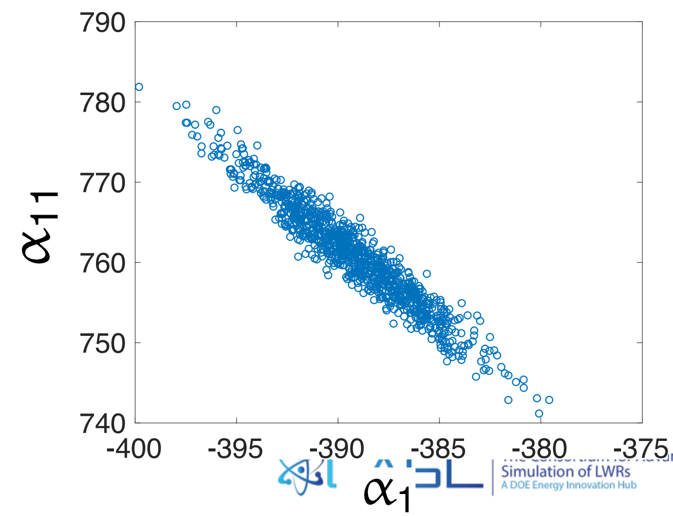


Strategy 1: Perform many experiments; e.g., 1000







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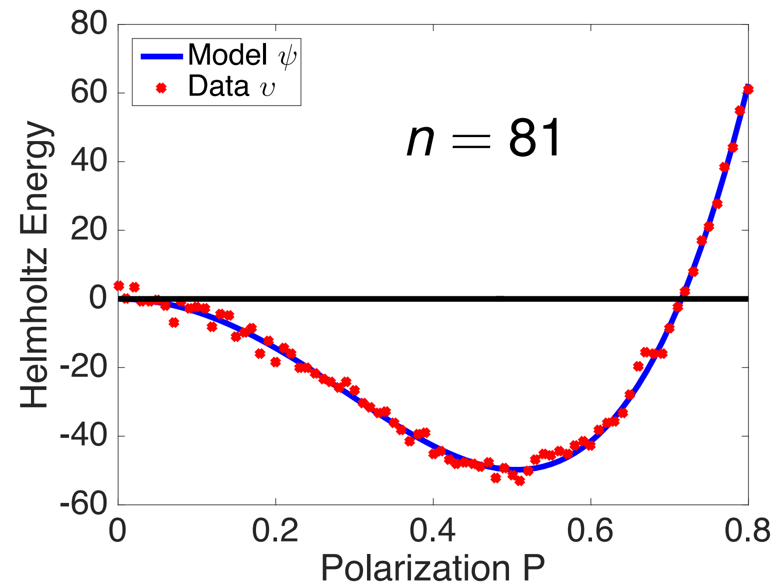

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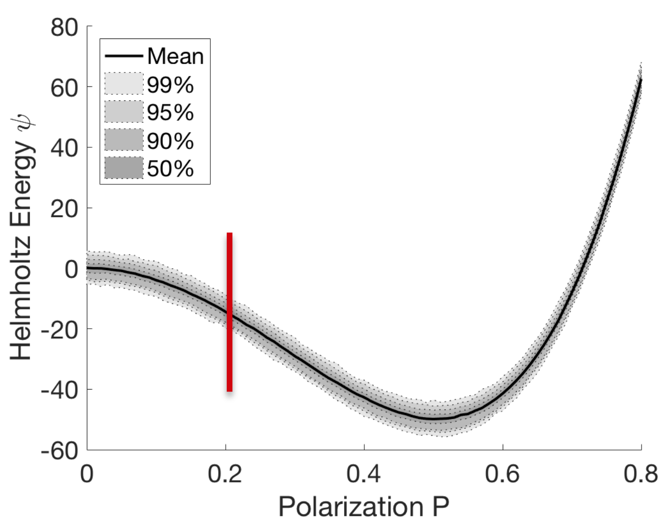

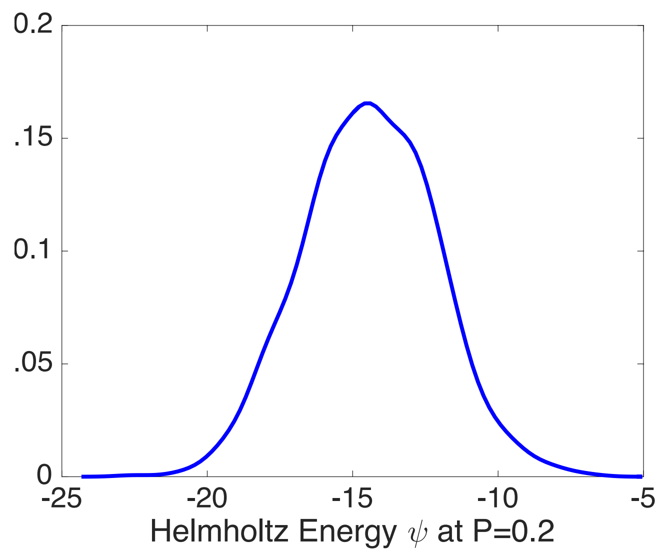

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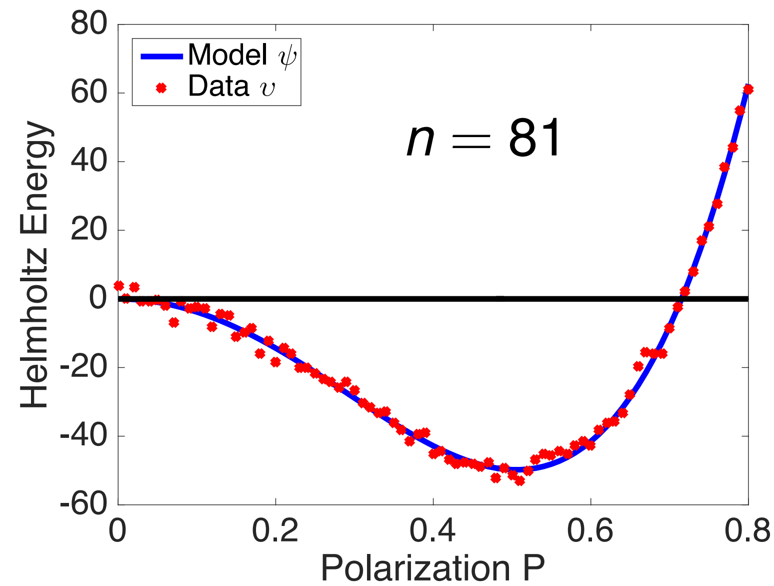
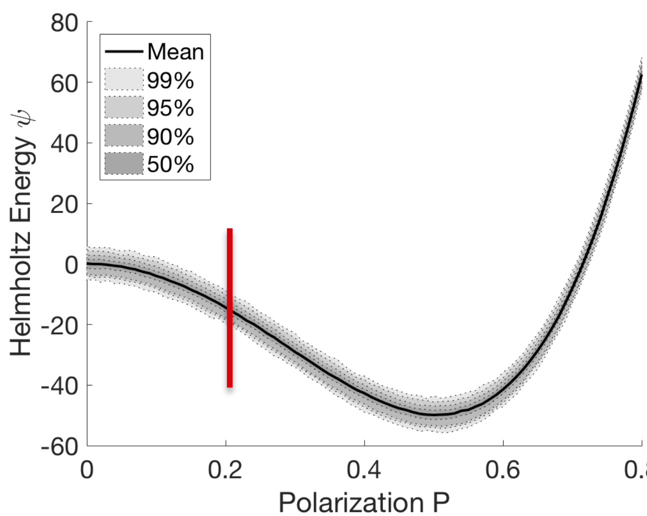
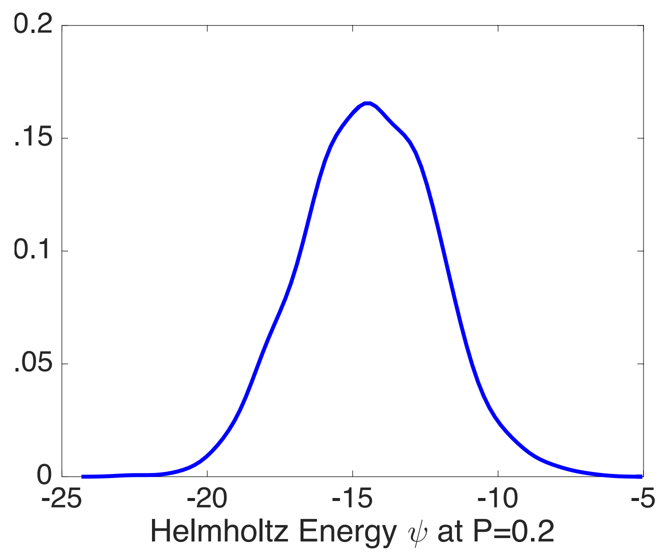


Strategy 1: Perform many experiments; e.g., 1000





Problem: Often cannot perform required number of experiments or high-fidelity simulations.

Solution: Statistical inference

Polarization Example

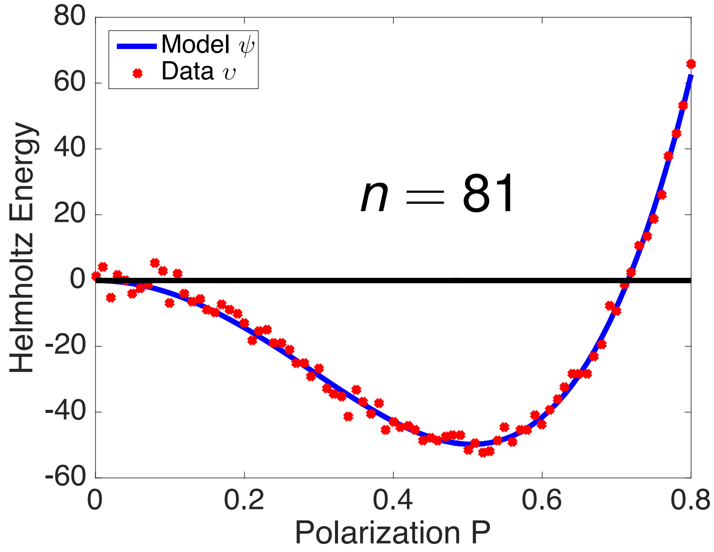
Statistical Model: For i = 1, …, n

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$

$$= \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i$$

$$\Rightarrow \begin{bmatrix} \upsilon_i \end{bmatrix} = \begin{bmatrix} P_i^2 & P_i^4 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_{11} \end{bmatrix} + \begin{bmatrix} \varepsilon_i \end{bmatrix}$$

$$\Rightarrow \upsilon = Xq + \varepsilon$$



Statistical Quantities:

$$q = (X^T X)^{-1} X^T \upsilon$$

Polarization Example

Statistical Model: For i = 1, …, n

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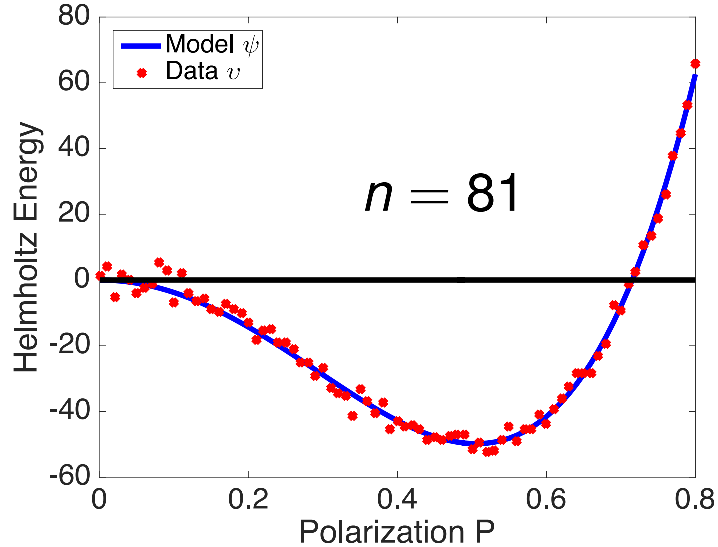

Statistical Quantities:

$$q = (X^T X)^{-1} X^T \upsilon$$

Note: $\mathbb{E}(q) = \mathbb{E}[(X^T X)^{-1} X^T \upsilon]$

$$= (X^T X)^{-1} X^T \mathbb{E}(\upsilon)$$

$$= q_0$$

$$\upsilon = Xq_0 + \varepsilon$$

Polarization Example

Statistical Model: For i = 1, …, n

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$
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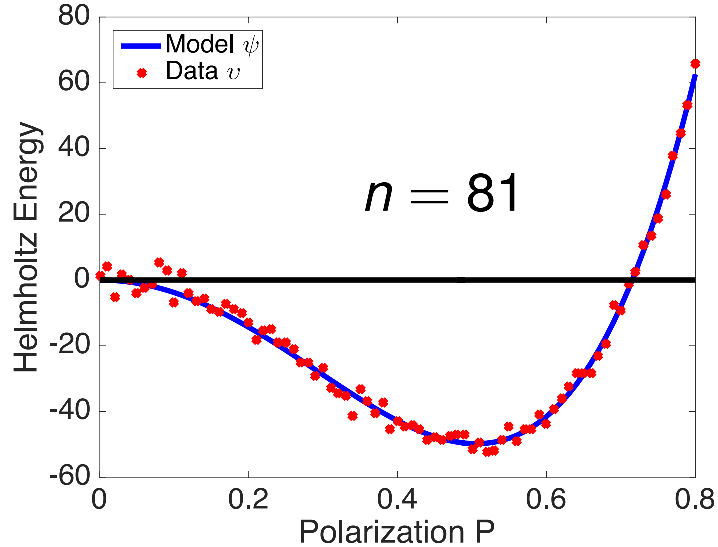

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$$= (X^T X)^{-1} X^T \mathbb{E}(\upsilon)$$
$$= q_0$$

$$\upsilon = Xq_0 + \varepsilon$$

And: Let $A = (X^T X)^{-1} X^T$

$$\begin{aligned} V(q) &= \mathbb{E}[(q - q_0)(q - q_0)^T] \\ &= \mathbb{E}[(q_0 + A\varepsilon - q_0)(q_0 + A\varepsilon - q_0)^T] \ \text{since } q = A\Upsilon = A(Xq_0 + \varepsilon) \\ &= A\mathbb{E}(\varepsilon\varepsilon^T)A^T \\ &= \sigma^2 (X^T X)^{-1} \end{aligned}$$

Polarization Example

Statistical Model: For i = 1, …, n

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$

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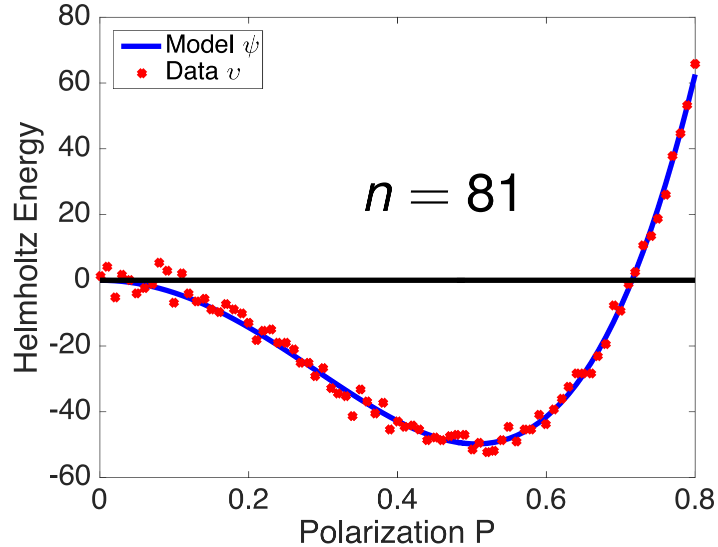
$$\Rightarrow \upsilon = Xq + \varepsilon$$



Statistical Quantities:

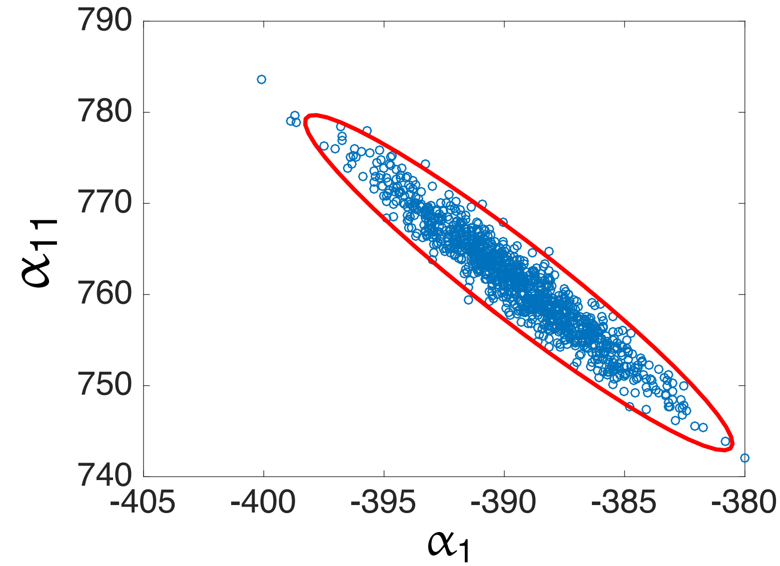
$$q = (X^T X)^{-1} X^T \upsilon$$

$$V = \sigma^2 (X^T X)^{-1} = \begin{bmatrix} 8.8 & -17.4 \\ -17.4 & 37.6 \end{bmatrix}$$

var(α_1)

cov(α_1, α_{11})

var(α_{11})



Note: Covariance matrix incorporates "geometry"

Goal: Employ Bayesian inference for UQ

Statistical Inference

Goal: The goal in statistical inference is to make conclusions about a phenomenon based on observed data.

Frequentist: Observations made in the past are analyzed with a specified model. Result is regarded as confidence about state of real world.

• Probabilities defined as frequencies with which an event occurs if experiment is repeated several times.

• Parameter Estimation:

o Relies on estimators derived from different data sets and a specific sampling distribution.

o Parameters may be unknown but are fixed and deterministic.

Bayesian: Interpretation of probability is subjective and can be updated with new data.

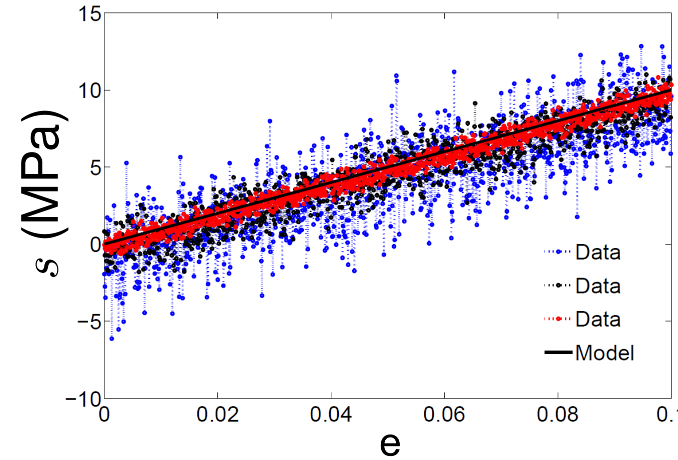
• Parameter Estimation: Parameters are considered to be random variables having associated densities.

Bayesian Inference: Simpler Example

Example: Displacement-force relation (Hooke's Law)

$$s_i = Ee_i + \varepsilon_i \ , \ i = 1, \ldots, N$$

$$\varepsilon_i \sim N(0, \sigma^2)$$



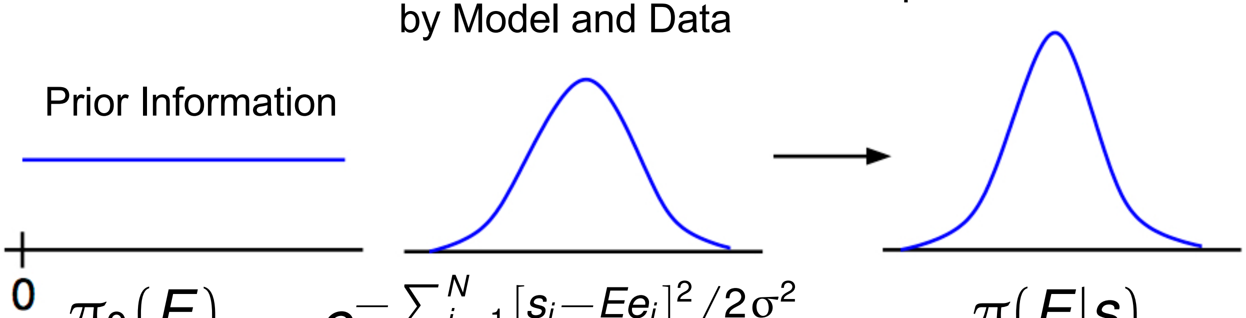
Parameter: Stiffness E

Strategy: Use model fit to data to update prior information

Prior Information

Information Provided by Model and Data

Updated Information



$\pi_0(E)$ $\qquad e^{-\sum_{i=1}^N [s_i - Ee_i]^2/2\sigma^2}$ $\qquad \pi(E|s)$

Data $\qquad$ Model

Non-normalized Bayes' Relation:

$$\pi(E|s) = e^{-\sum_{i=1}^N [s_i - Ee_i]^2/2\sigma^2} \pi_0(E)$$

Bayesian Inference

Bayes' Relation: Specifies posterior in terms of likelihood and prior

Likelihood: $e^{-\sum_{i=1}^{N}[s_i - Ee_i]^2/2\sigma^2}$, $q = E$

$\upsilon = [s_1, \ldots, s_N]$

Posterior Distribution

$$\boxed{\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}}$$

Prior Distribution

Normalization Constant

- Prior Distribution: Quantifies prior knowledge of parameter values
- Likelihood: Probability of observing a data given set of parameter values.
- Posterior Distribution: Conditional distribution of parameters given observed data.

Problem: Can require high-dimensional integration

- e.g., Thermal-hydraulics and chemistry codes: p = 5-20!
- Solution: Sampling-based Markov Chain Monte Carlo (MCMC) algorithms.
- Metropolis algorithms first used by nuclear physicists during Manhattan Project in 1940's to understand particle movement underlying first atomic bomb.

Bayesian Model Calibration

Bayes' Relation:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Bayesian Model Calibration:

- Parameters assumed to be random variables

$$\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}$$

Example: Coin Flip

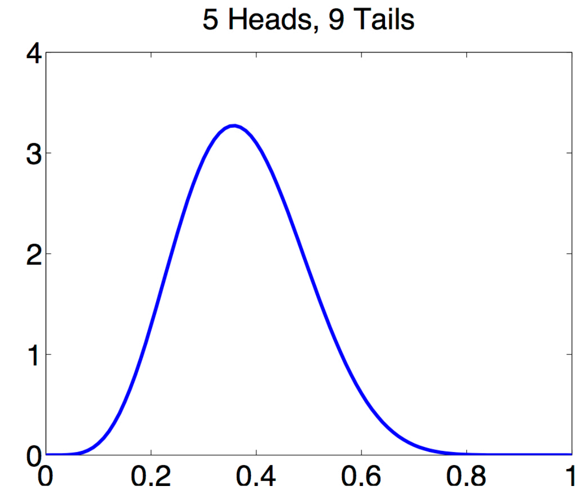
$$\Upsilon_i(\omega) = \begin{cases} 0 & , \quad \omega = T \\ 1 & , \quad \omega = H \end{cases}$$

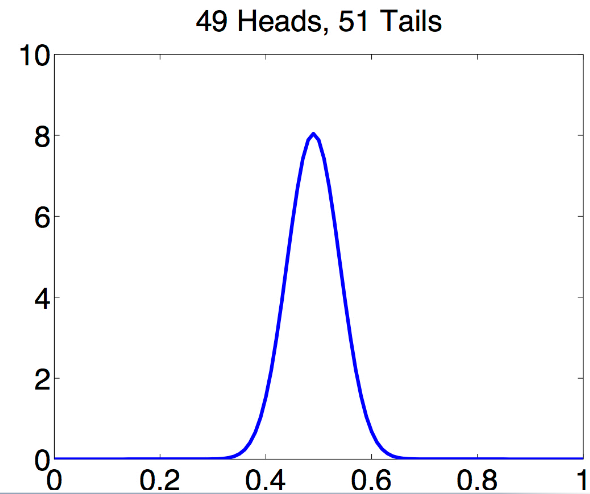
Likelihood:

$$\begin{aligned} \pi(\upsilon|q) &= \prod_{i=1}^{N} q^{\upsilon_i}(1-q)^{1-\upsilon_i} \\ &= q^{N_1}(1-q)^{N_0} \end{aligned}$$

Posterior with Noninformative Prior: $\pi_0(q) = 1$

$$\pi(q|\upsilon) = \frac{q^{N_1}(1-q)^{N_0}}{\int_0^1 q^{N_1}(1-q)^{N_0}dq} = \frac{(N+1)!}{N_0!N_1!} q^{N_1}(1-q)^{N_0}$$



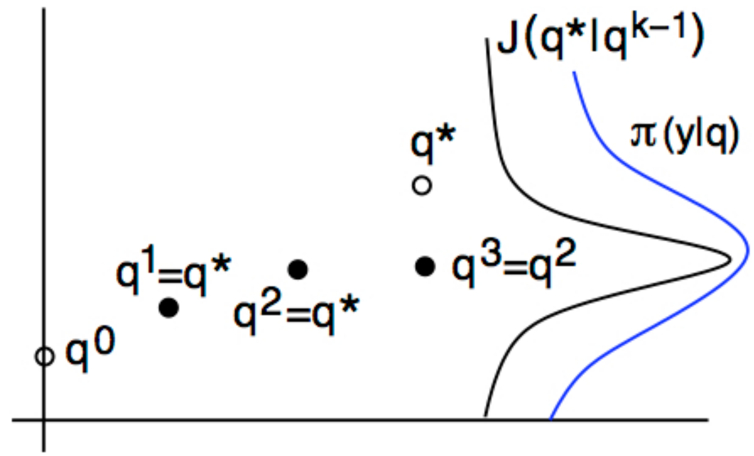


Bayesian Model Calibration

Bayesian Model Calibration:

• Parameters considered to be random variables with associated densities.

$$\pi(q|\upsilon) = \frac{\pi(\upsilon|q)\pi_0(q)}{\int_{\mathbb{R}^p} \pi(\upsilon|q)\pi_0(q)dq}$$



Problem:

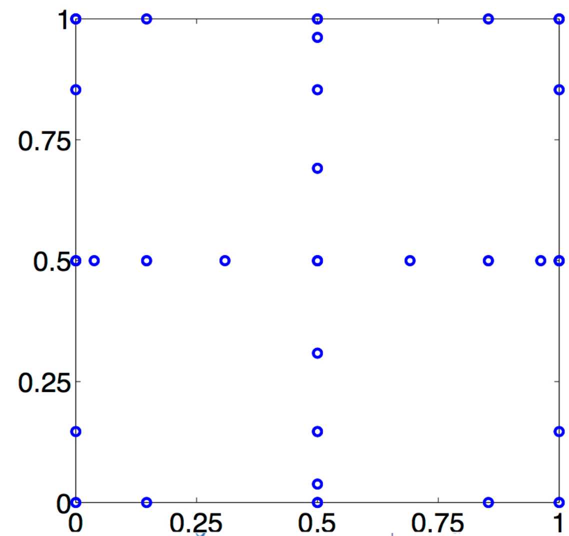
• Often requires high dimensional integration;

  ○ p = hundreds to thousands for some models

Strategies:

• Sampling methods

• Sparse grid quadrature techniques



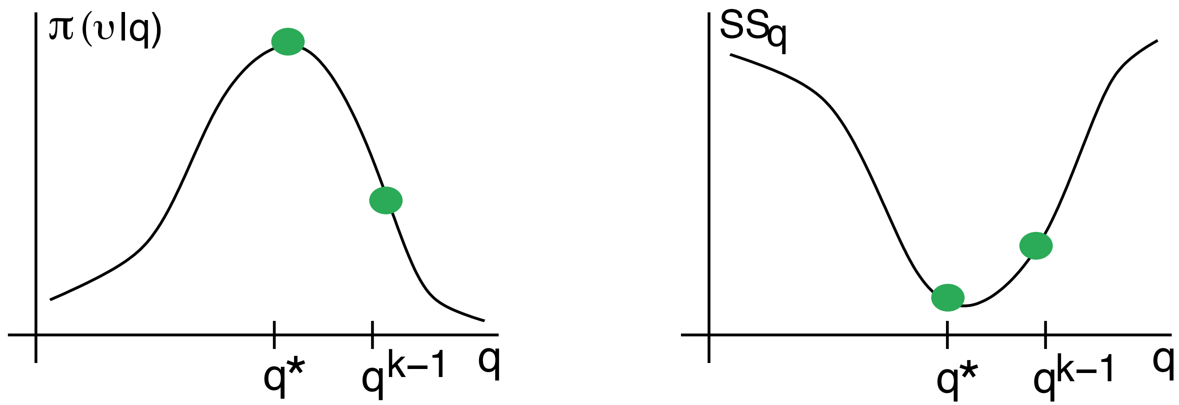
Markov Chain Monte Carlo Methods

Strategy:

- Sample values from proposal distribution $J(q^*|q^{k-1})$ that reflects geometry of posterior distribution
- Compute $r(q^*|q^{k-1}) = \frac{\pi(\upsilon|q^*)\pi_0(q^*)}{\pi(\upsilon|q^{k-1})\pi_0(q^{k-1})}$
  - $*$ If $r \geqslant 1$, accept with probability $\alpha = 1$
  - $*$ If $r < 1$, accept with probability $\alpha = r$

Intuition: Consider flat prior $\pi_0(q) = 1$ and Gaussian observation model

$$\pi(\upsilon|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2} \qquad SS_q = \sum_{i=1}^{N} [\upsilon_i - f(t_i, q)]^2$$



Delayed Rejection Adaptive Metropolis (DRAM)

Algorithm: [Haario et al., 2006] – MATLAB, Python, R

1. Determine $q^0 = \arg\min_q \sum_{i=1}^{N} [\upsilon_i - \psi(P_i, q)]^2]$

Example: Helmholtz energy

$$\upsilon_i = \psi(P_i, q) + \varepsilon_i \longleftarrow \varepsilon_i \sim N(0, \sigma^2)$$

$$= \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i$$

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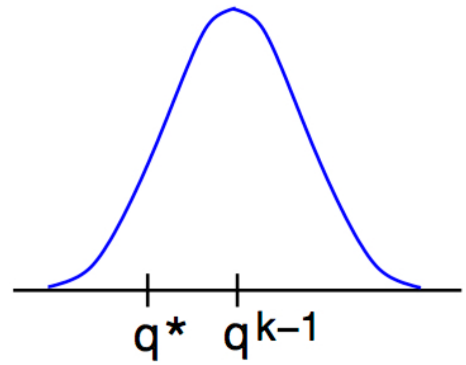

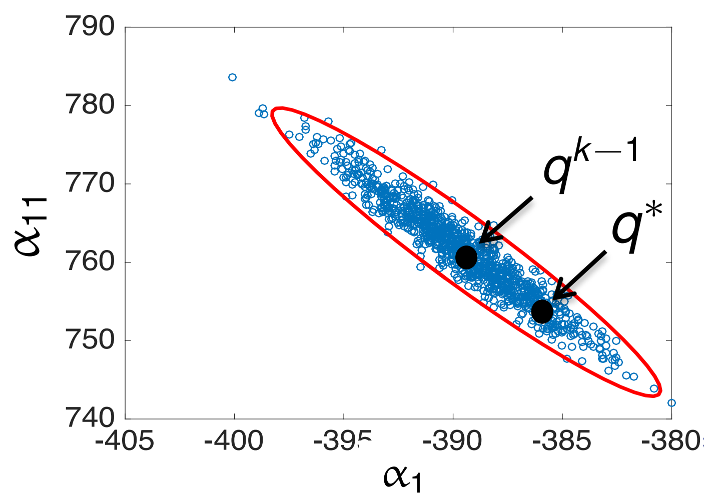

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Recall: Covariance V incorporates geometry

Delayed Rejection Adaptive Metropolis

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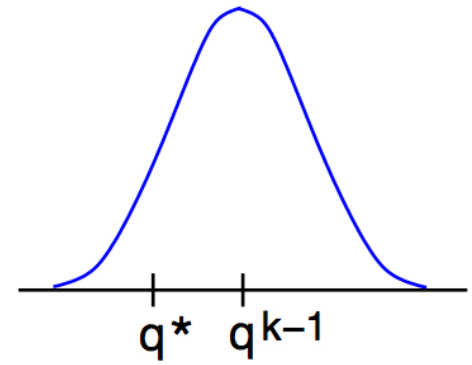

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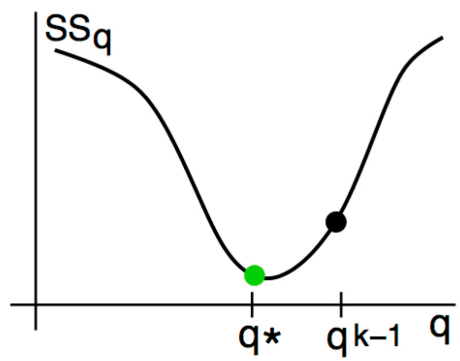

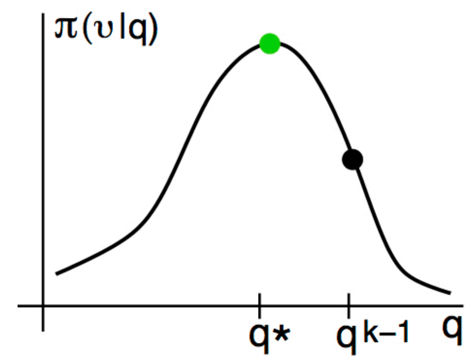

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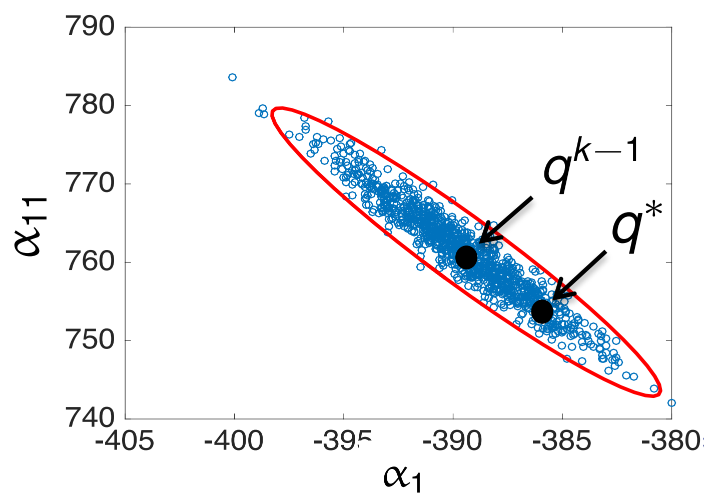

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Delayed Rejection Adaptive Metropolis

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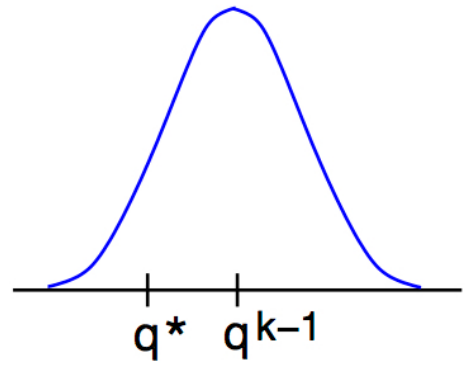

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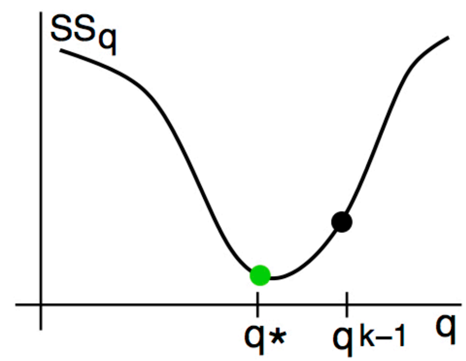

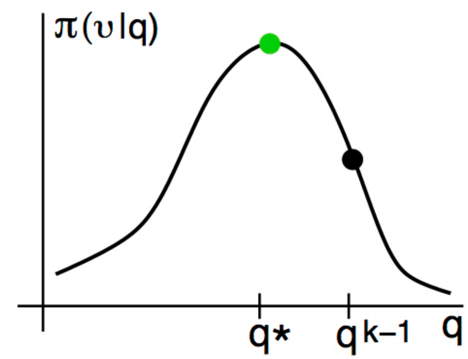

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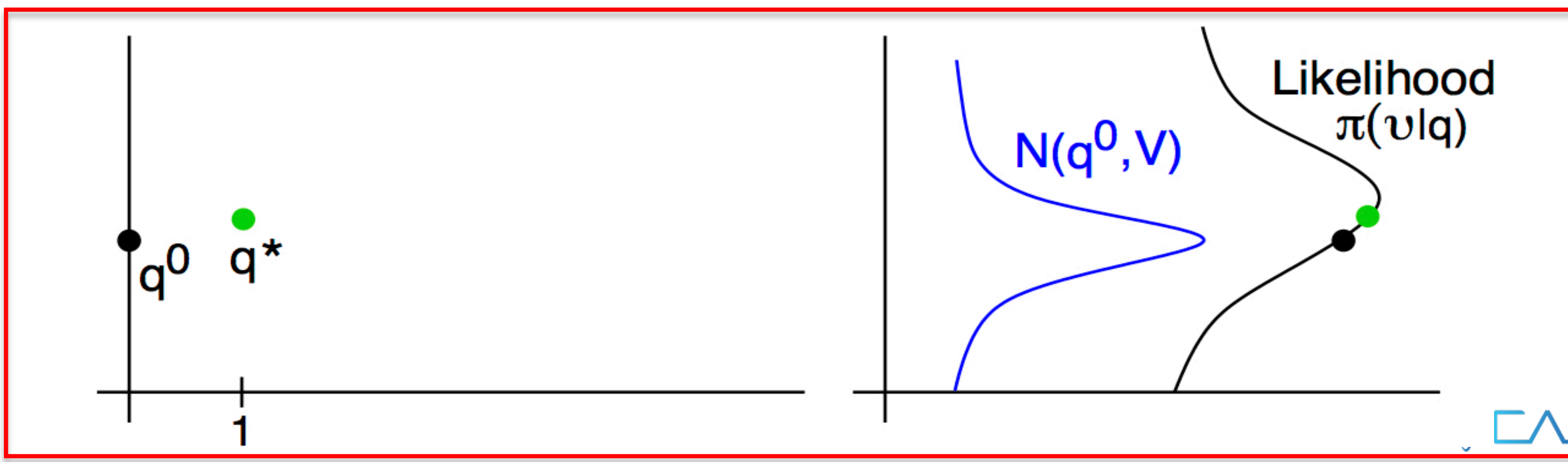

Delayed Rejection Adaptive Metropolis

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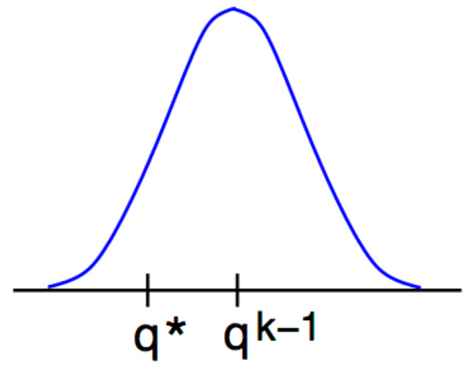

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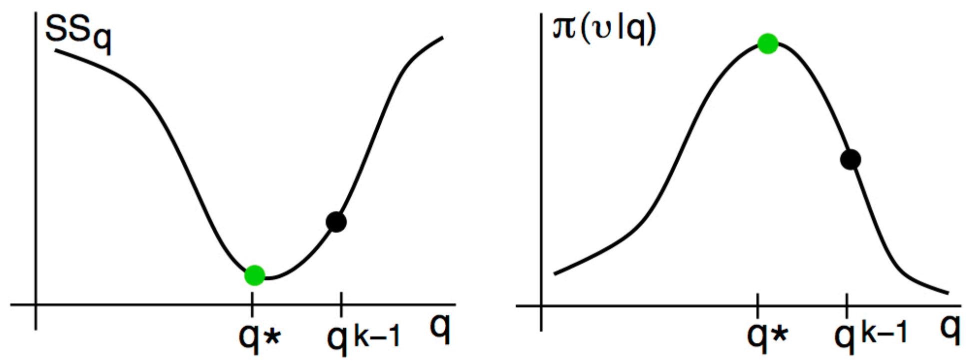

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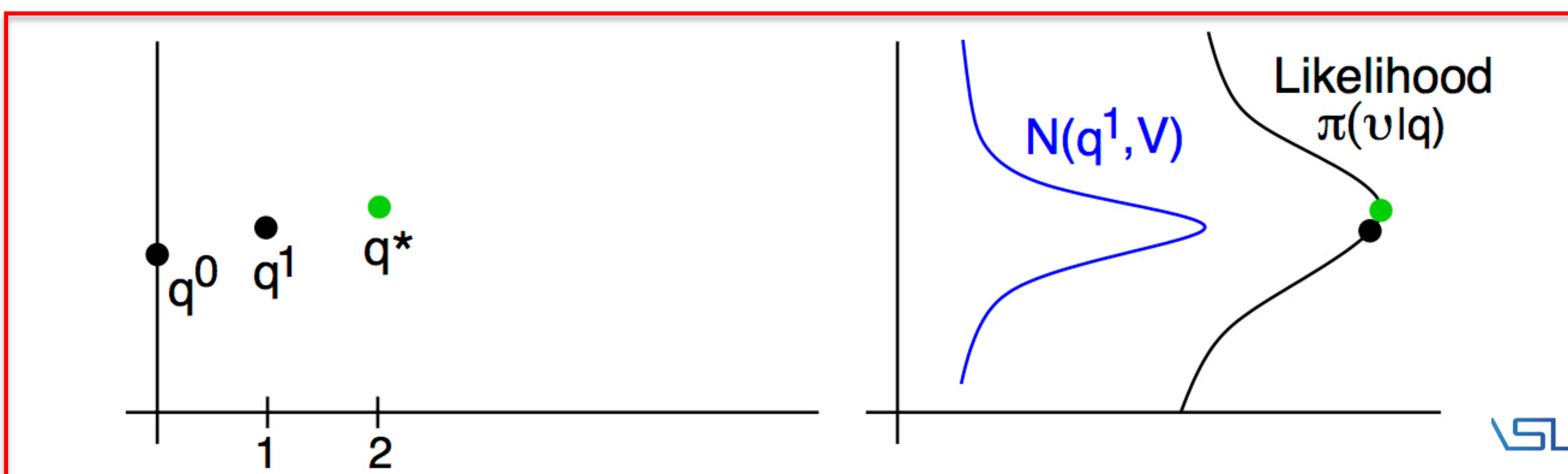

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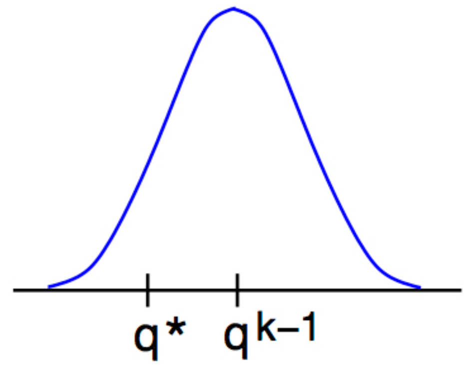

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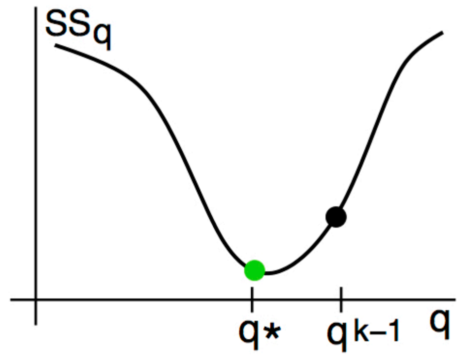

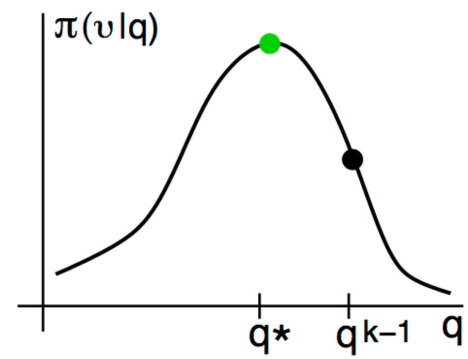

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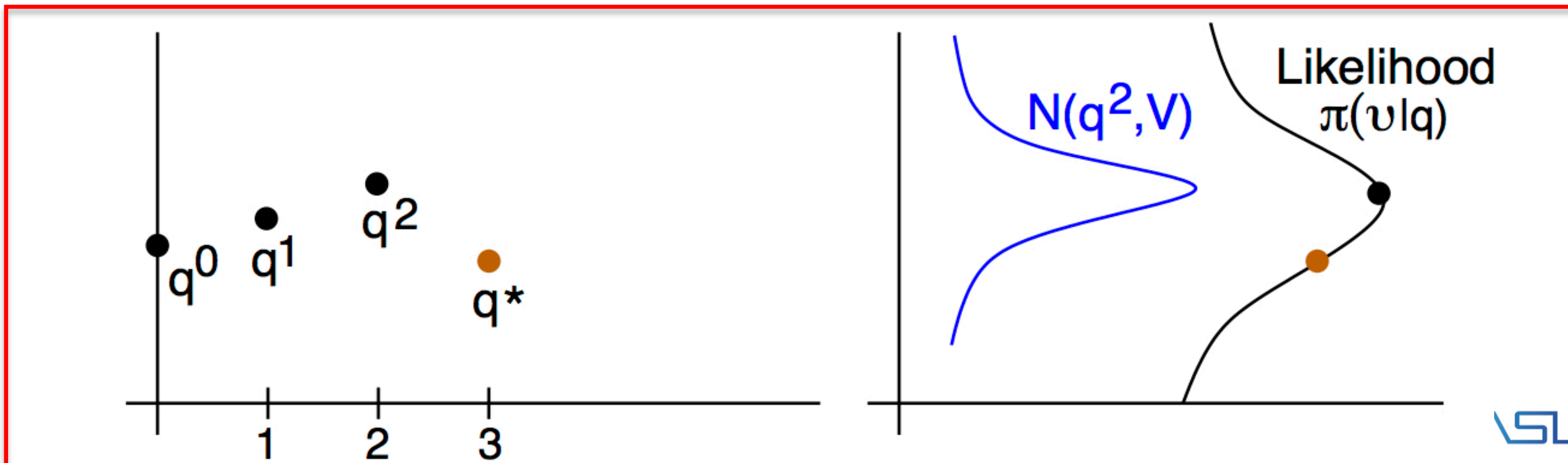

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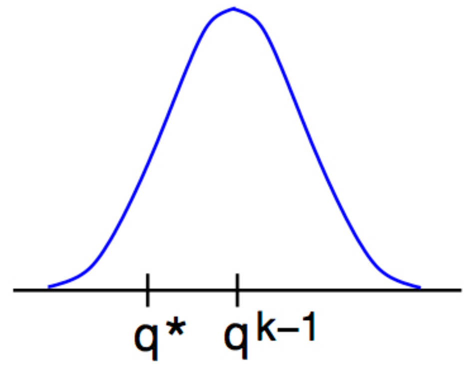

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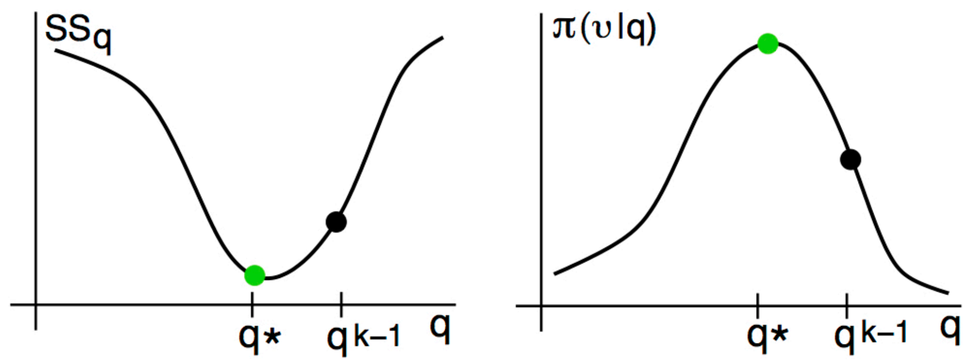

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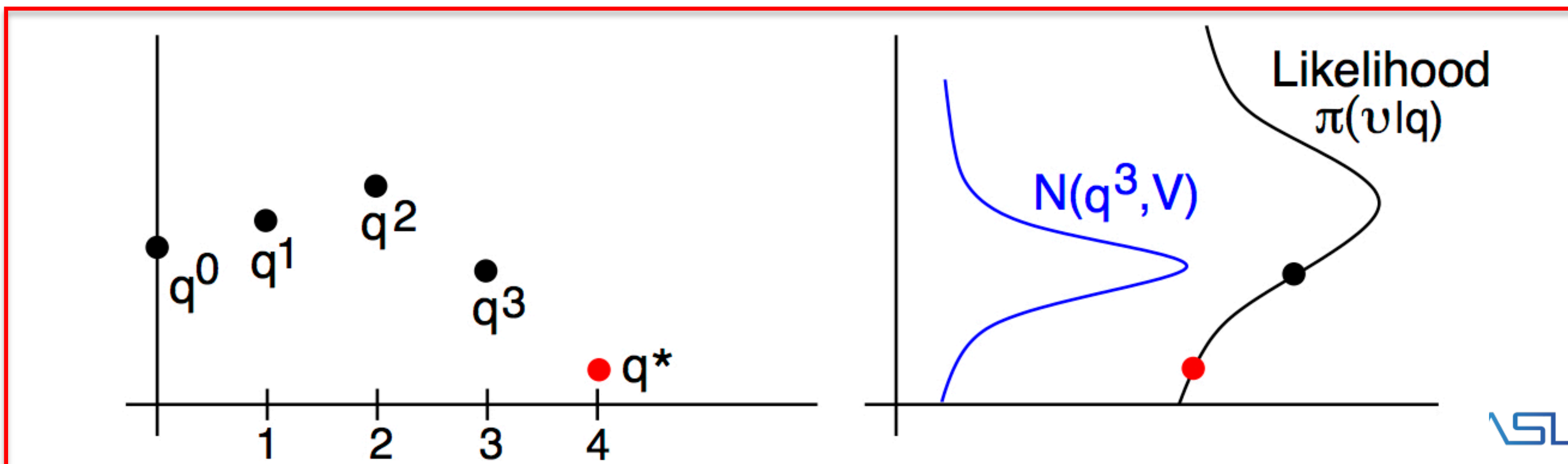

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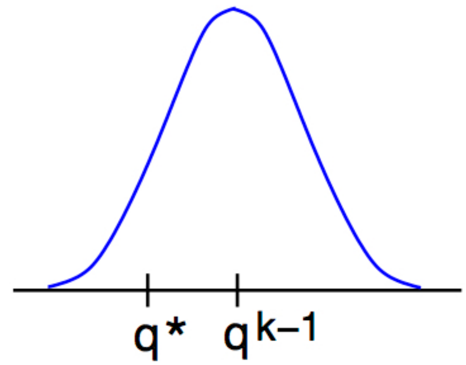

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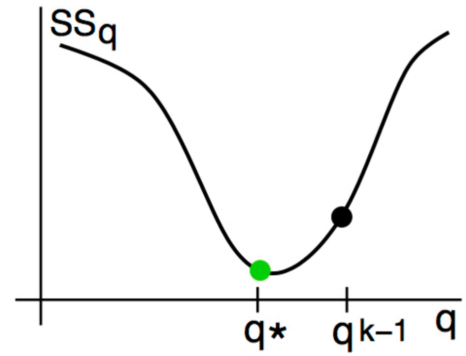
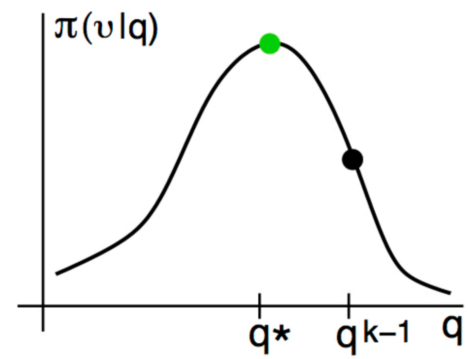
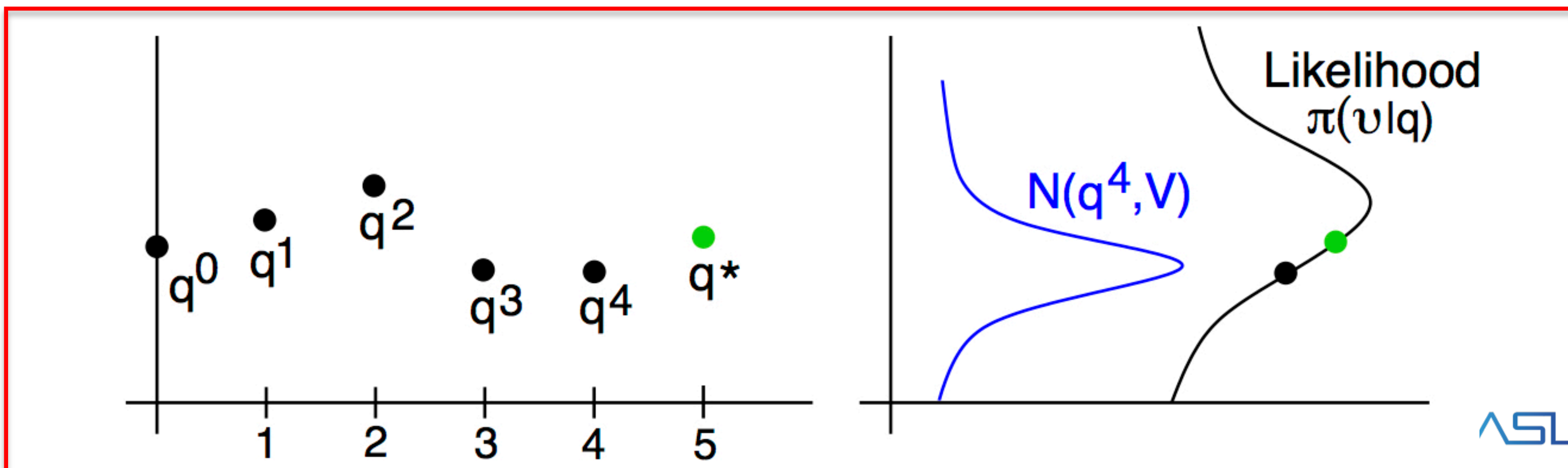




   (c) Accept q^* with probability dictated by likelihood



Delayed Rejection Adaptive Metropolis

Algorithm: [Haario et al., 2006] – MATLAB, Python, R

1. Determine $q^0 = \arg\min_q \sum_{i=1}^{N} [\upsilon_i - \psi(P_i, q)]^2]$

2. For $k = 1, \ldots, M$

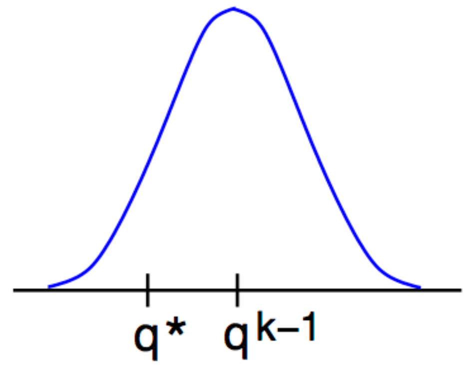
   (a) Construct candidate $q^* \sim N(q^{k-1}, V)$

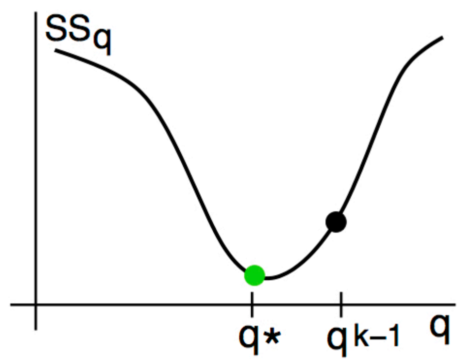
   (b) Compute likelihood

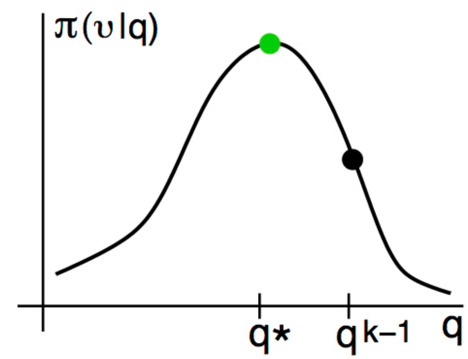
$$SS_{q^*} = \sum_{i=1}^{N} \upsilon_i - \psi(P_i, q^*)]^2$$

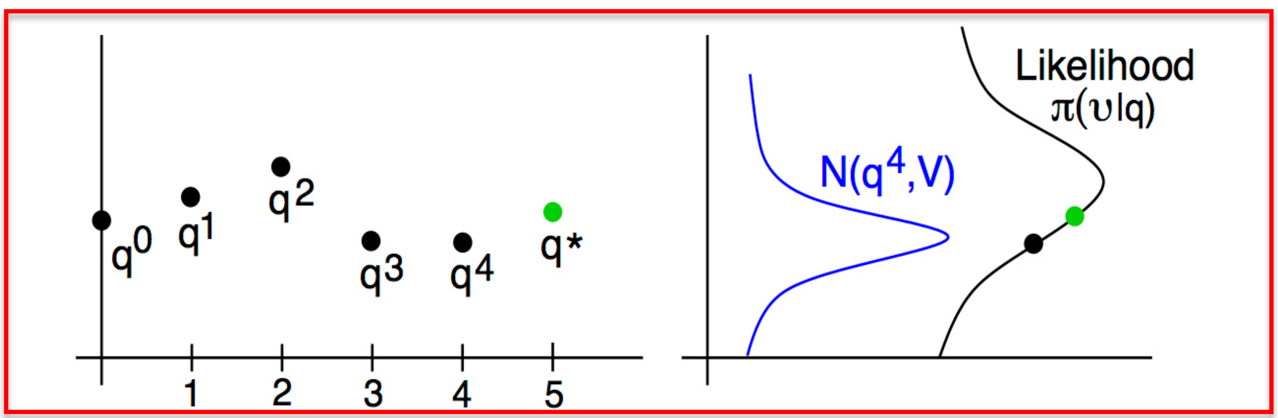
$$\pi(\upsilon|q) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-SS_q/2\sigma^2}$$

   (c) Accept q^* with probability dictated by likelihood









Note:

- Delayed Rejection: Shrink proposal: γV
- Adaptive Metropolis: Update proposal as samples are accepted

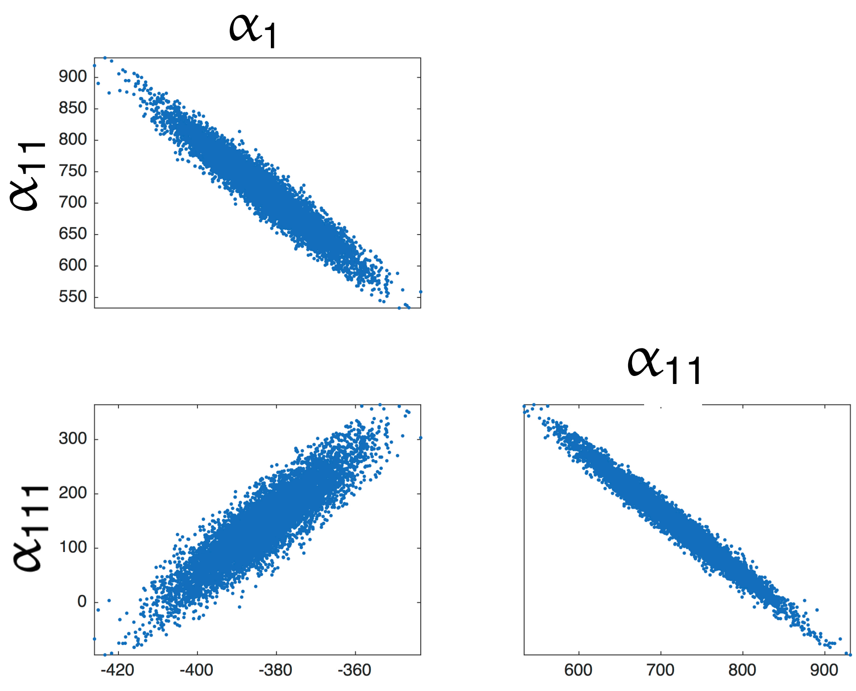
Delayed Rejection Adaptive Metropolis

Example: Helmholtz energy with 3 parameters

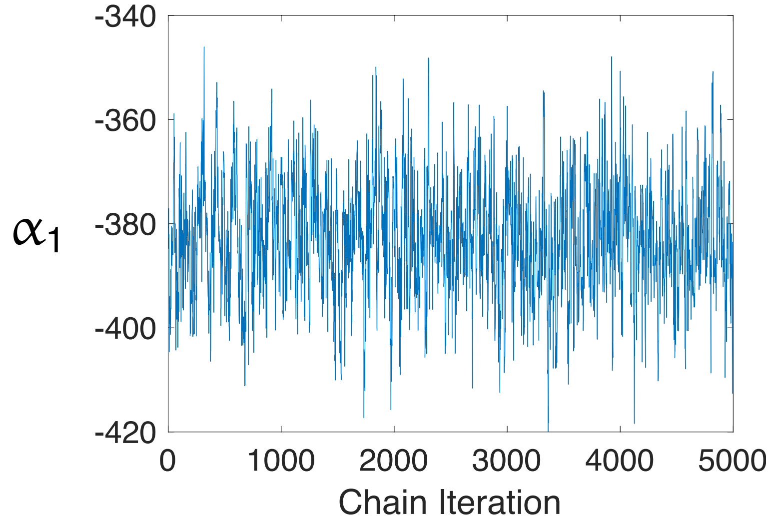
$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Note: Similar results for α_{11} and α_{111}

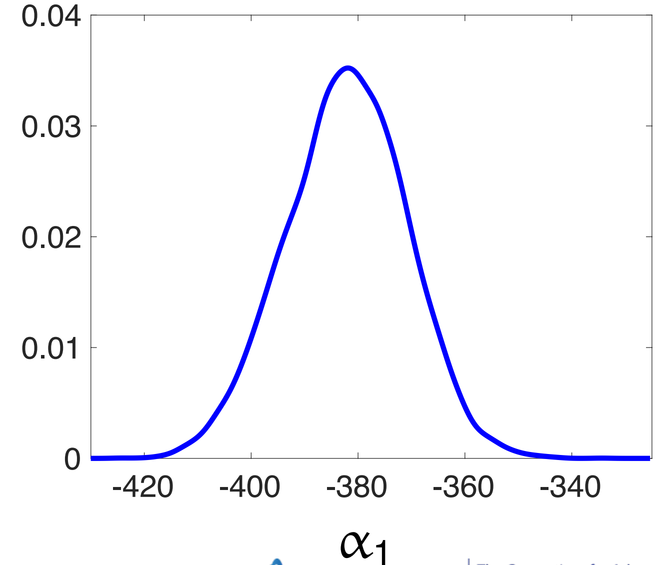
Pairwise Plots: Quantify correlation



Chain for α_1 with 5000 samples



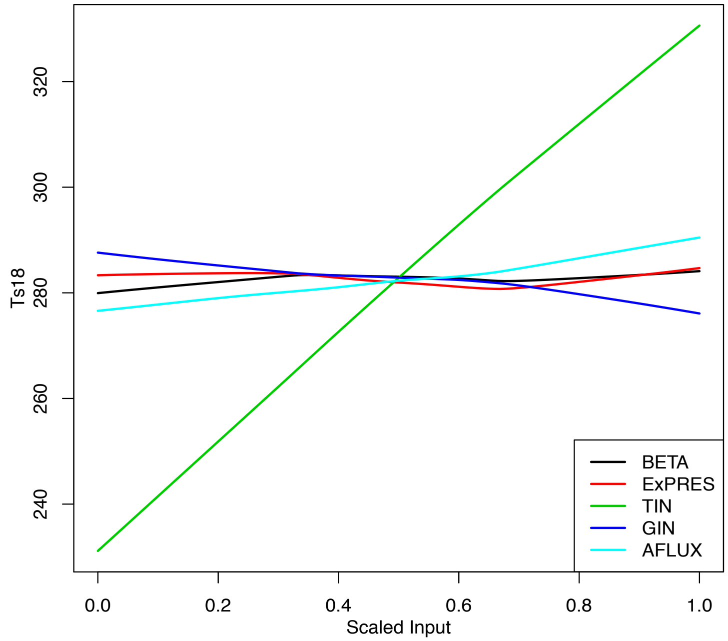
Marginal density for α_1



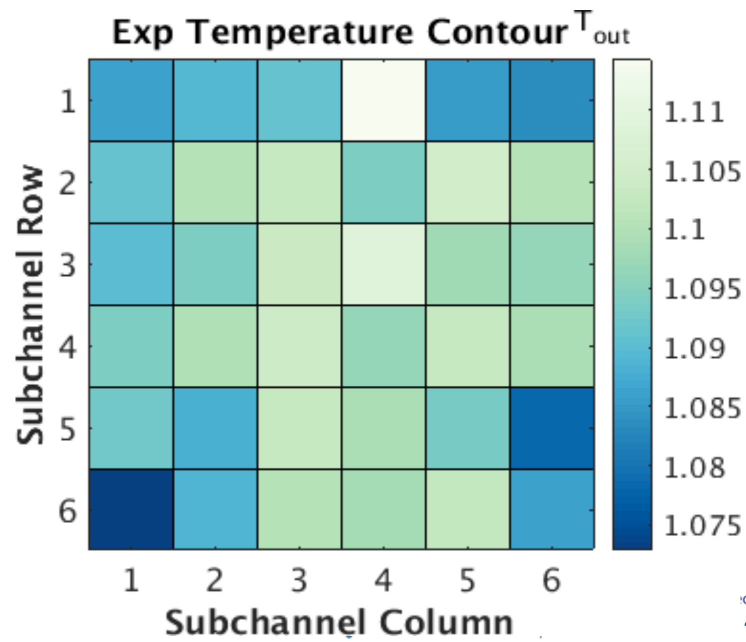
Bayesian Calibration: Beta in CTF

Problem Setup:

- Configuration (Design) Variables in STAR
  - ExPRES: Initial pressure of fluid domain
  - TIN: Initial temperature in fluid domain
  - GIN: Inlet mass flow rate
  - AFLUX: Average linear heat rate per rod



- Calibration Variable in CTF
  - BETA: Turbulent mixing factor
- Experimental Data from WEC
  - 21 tests each of which produce 36 outlet temperatures



Surrogate Construction for CTF

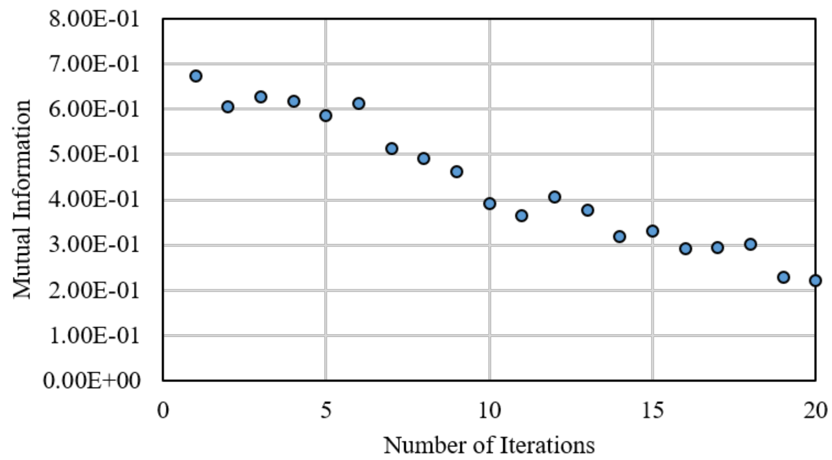
Bayesian Inference:

- MCMC with 20% burn-in removed and subsampling rate of 3 requires minimum of 18,750 iterations.
- Mutual information computation requires 5000 independent samples.
- Each CTF takes approximately 5 minutes.
- This necessitates construction and verification of fast surrogate for CTF – will discuss later
- Gaussian process (GP) surrogate trained and verified for all 36 subchannels.
  - 1000 LHS samples used to compute surrogate, 300 LHS used for verification.
  - Difference between surrogate and CTF-computed outlet temperatures within 1.8%.
  - Surrogate runs in seconds.

Bayesian Calibration of Beta

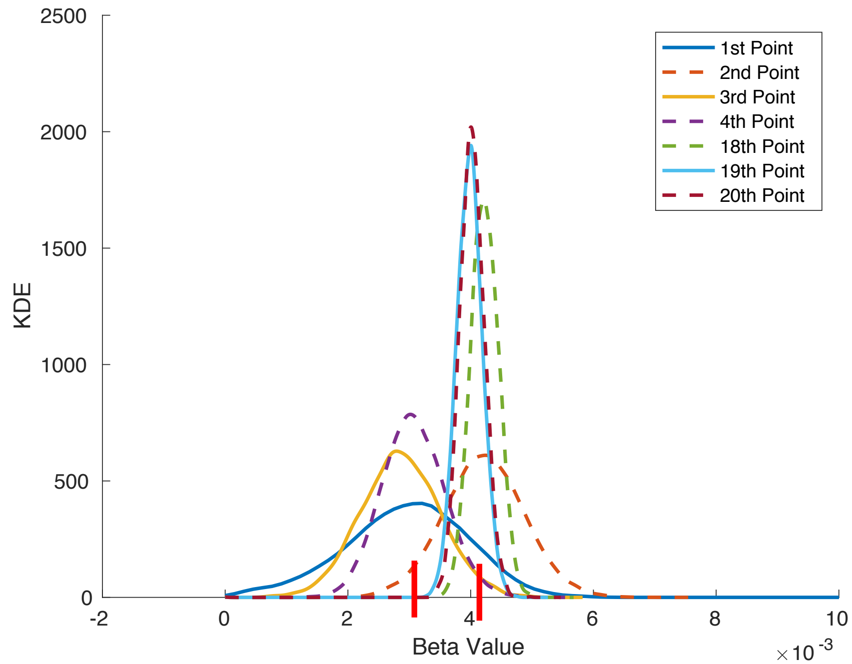
Hi2Lo Workflow and Results:

- Calibrate Beta to initial simulation and/or experiment.
- Performed Hi2Lo calibration using both experimental data and STAR simulations.
- Estimate MI between Beta samples and HiFi predictions at each candidate. Select candidate with largest MI.
- Repeat until MI is sufficiently small or design budget is exhausted.



Results:

- Mean Beta value increased from 0.0028 to 0.004 with *reduced uncertainty*.



Bayesian Inference

Advantages:

• Advantageous over frequentist inference when data is limited.

• Directly provides parameter densities, which can subsequently be propagated to construct response uncertainties.

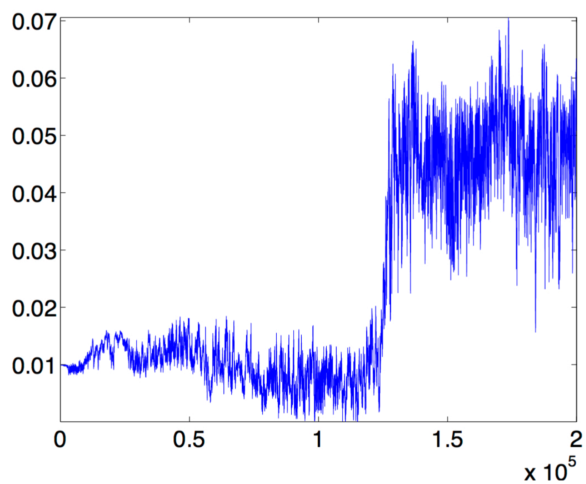
• Can be used to infer non-identifiable parameters if priors are tight.

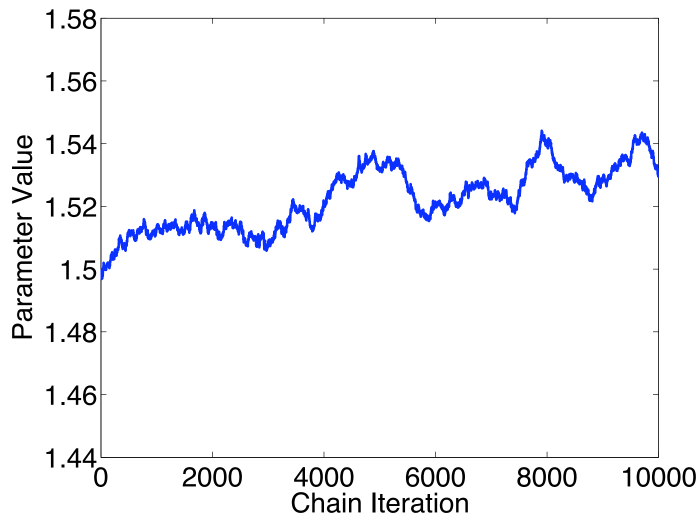
• Provides natural framework for experimental design.

Disadvantages:

• More computationally intense than frequentist inference.

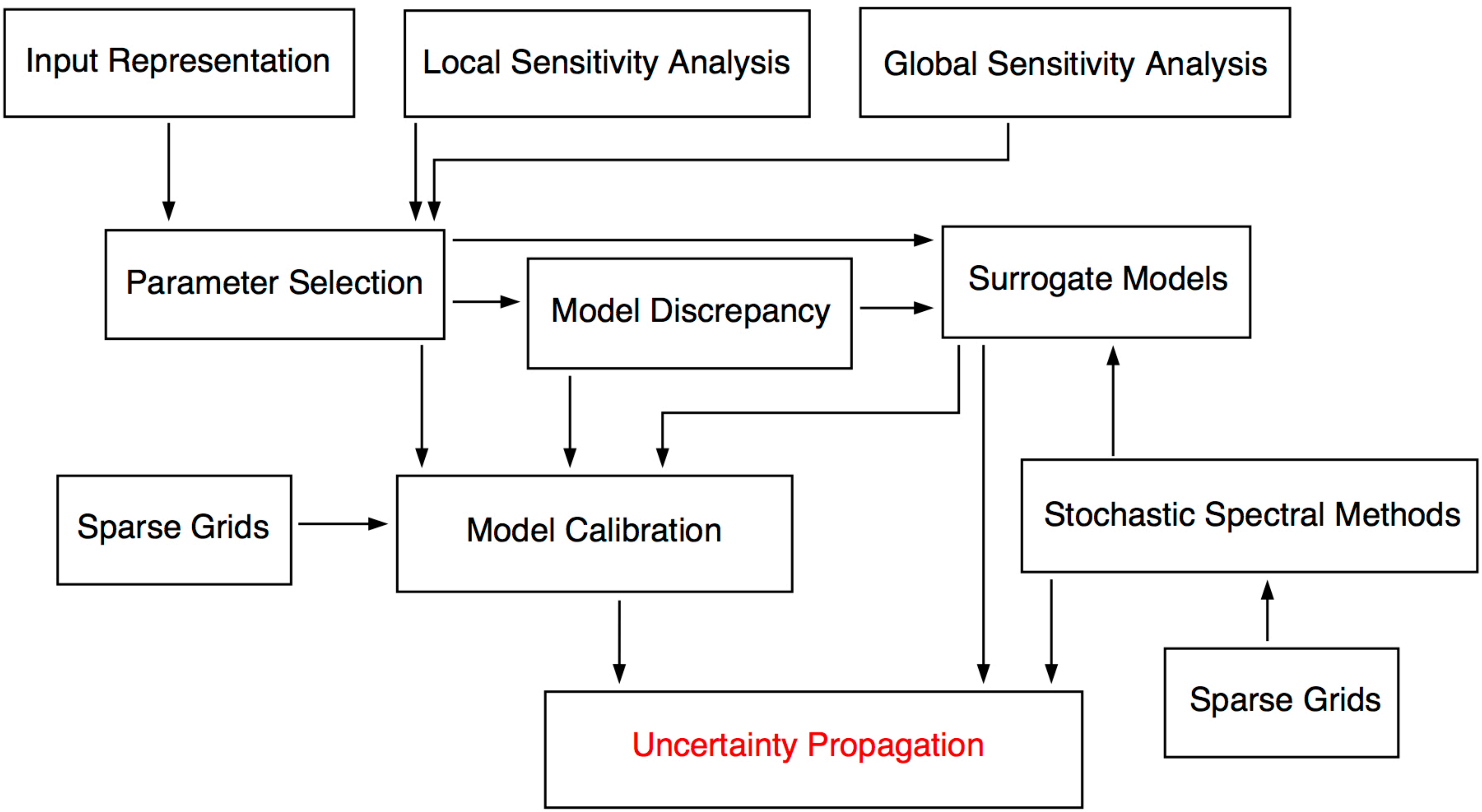
• Can be difficult to confirm that chains have burned-in or converged.





Steps in Uncertainty Quantification

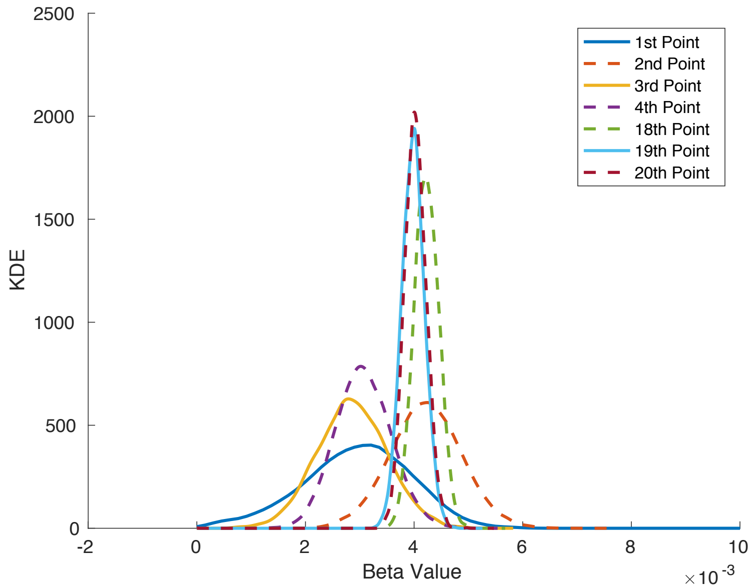
Note: Uncertainty quantification requires synergy between statistics, mathematics and application area.



Uncertainty Propagation

Setting:

- We assume that we have determined distributions for parameters
    - e.g., Bayesian inference, prior experiments, expert opinion



Goal: Construct statistics for quantities of interest (QoI)

- e.g., Void fraction, peak clad temperature, total pressure drop
- Note: Often involves moderate to high-dimensional integration

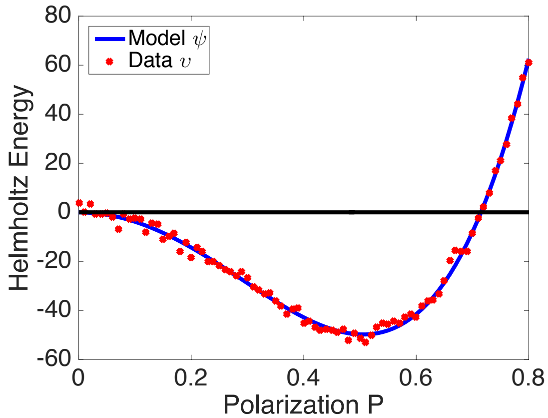
$$\mathbb{E}[u(t,x)] = \int_{\mathbb{R}^p} u(t,x,q)\rho(q)dq$$

Uncertainty Propagation: Linear Models

Note: Analytic mean and variance relations

Example: Helmholtz energy

$$\Upsilon_i = \alpha_1 P_i^2 + \alpha_{11} P_i^4 + \varepsilon_i \; , \; \text{var}[\varepsilon_i] = \sigma^2$$



Model Statistics:

Let $\overline{\alpha}_1, \overline{\alpha}_{11}$ and $\text{var}(\alpha_1), \text{var}(\alpha_{11})$ denote parameter means and variance. Then

$$\mathbb{E}[\alpha_1 P_i^2 + \alpha_{11} P_i^4] = \overline{\alpha}_1 P_i^2 + \overline{\alpha}_{11} P_i^4$$

$$\text{var}[\alpha_1 P_i^2 + \alpha_{11} P_i^4] = P_i^4 \text{var}[\alpha_1] + P_i^8 \text{var}[\alpha_{11}] + 2P_i^6 \text{cov}[\alpha_1, \alpha_{11}]$$

Response Statistics: Assume measurement errors uncorrelated from model response.

$$\mathbb{E}[\Upsilon] = \overline{\alpha}_1 P_i^2 + \overline{\alpha}_{11} P_i^4$$

$$\text{var}[\Upsilon] = P_i^4 \text{var}[\alpha_1] + P_i^8 \text{var}[\alpha_{11}] + 2P_i^6 \text{cov}[\alpha_1, \alpha_{11}] + \sigma^2$$

Problem: Models almost always nonlinearly parameterized

Uncertainty Propagation: Sampling Methods

Strategy 1: Randomly sample from parameter and measurement error distributions and propagate through model to quantify response uncertainty.

Advantages:

- Applicable to nonlinear models.
- Parameters can be correlated and non-Gaussian.
- Straight-forward to apply and convergence rate is independent of number of parameters.
- Can directly incorporate both parameter and measurement uncertainties.

Disadvantages:

- Very slow convergence rate: $\mathcal{O}(1/\sqrt{M})$ where M is the number of samples.
- 100-fold more evaluations required to gain additional place of accuracy.
- This motivates numerical analysis techniques.

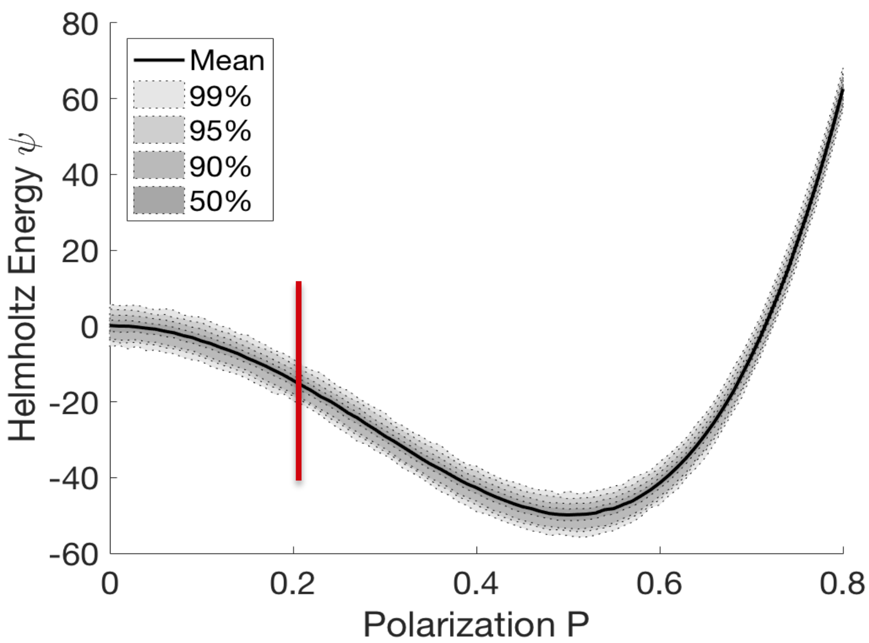
Strategy 2: Employ numerical surrogate representations to analytically propagate uncertainties.

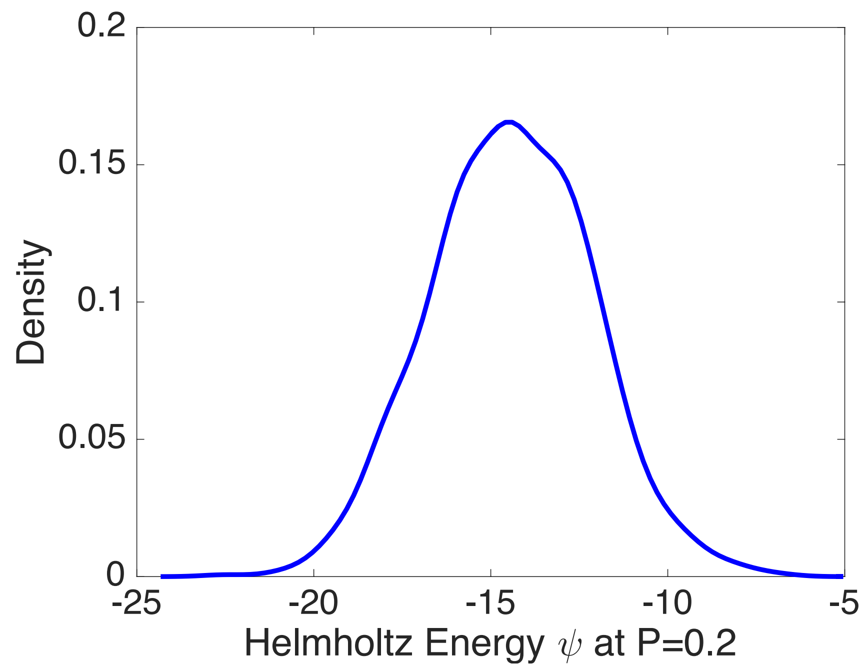
Prediction Intervals

Note:

- We now know how to compute the mean response for the QoI.
- Sample to compute prediction intervals.

Example: Helmholtz energy $\psi(P,q) = \alpha_1 P^2 + \alpha_{11} P^4$, $q = [\alpha_1, \alpha_{11}]$

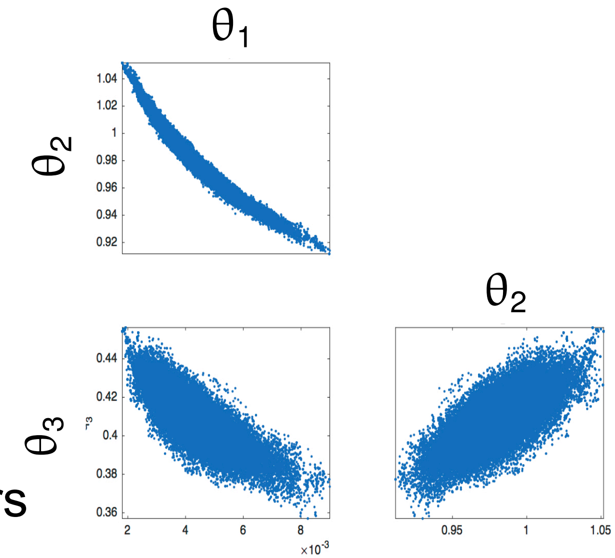




Bayesian Calibration: CASL Application

Example: Dittus—Boelter Relation

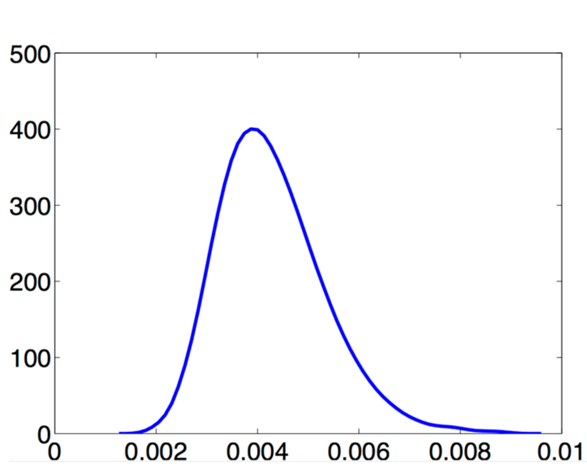
$$Nu = 0.023 Re^{0.8} Pr^{0.4}$$



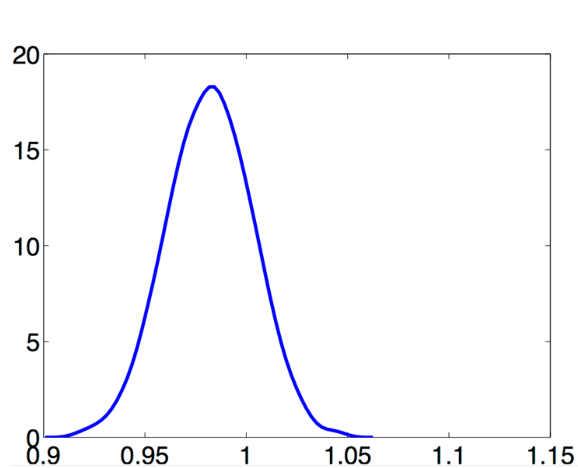
Industry Standard: Conservative, uniform, bounds

i.e., [0, 0.046], [0, 1.6], [0,0.8]

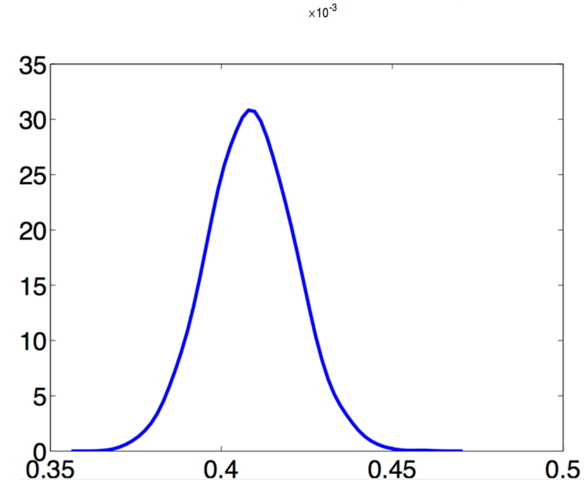
Bayesian Analysis: Employ conservative bounds as priors



$2\sigma \approx 0.0035$



$2\sigma \approx 0.06$



$2\sigma \approx 0.03$

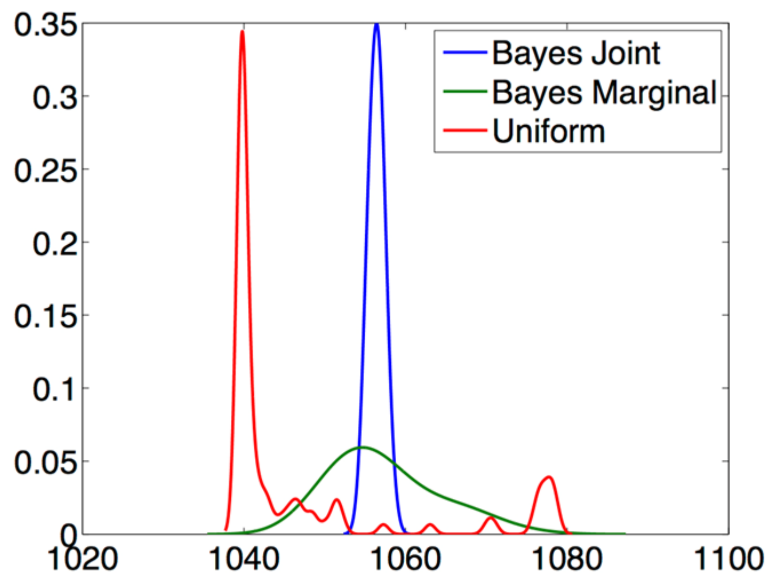
Note:

- Substantial reduction in parameter uncertainty
- Quantifies correlation between parameters

The Consortium for Advanced Simulation of LWRs
A DOE Energy Innovation Hub

Use of Prediction Intervals: CASL

Strategy: Propagate parameter uncertainties through COBRA-TF to determine uncertainty in maximum fuel temperature



Ramifications:

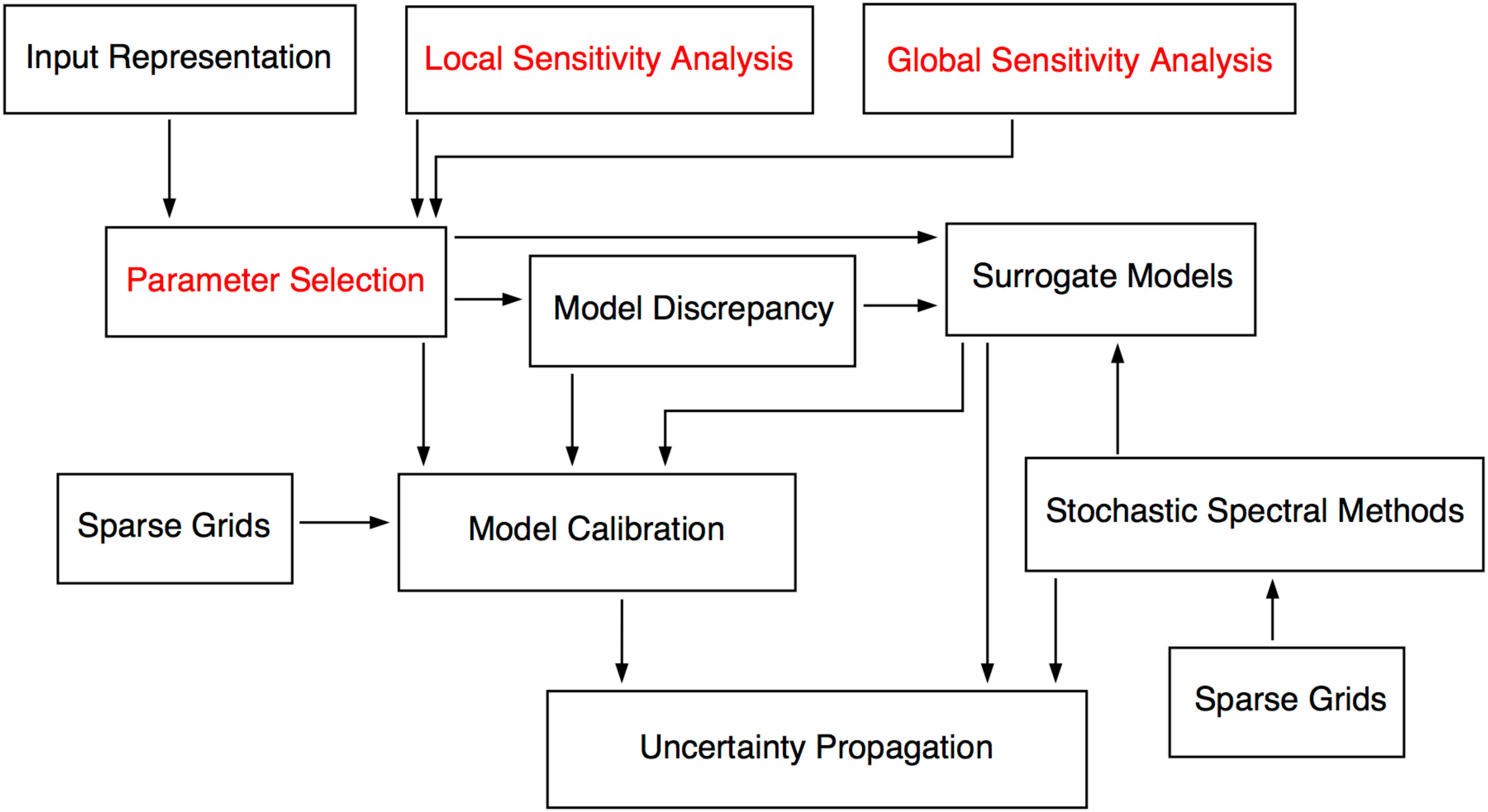
- Temperature uncertainty reduced from 40 degrees to 5 degrees.
- Can run plant 20 degrees hotter, which significantly improves efficiency.
- Warranted continued calibration of closure relations.
- Accommodates disparate data sets.

Potential Ramification: Savings of 10 billion dollars per year for US power plants

Issues:

- We considered only one of many closure relations
- Nuclear regulatory commission takes years to change requirements and codes

Steps in Uncertainty Quantification



Parameter Selection: Required for models with unidentifiable or noninfluential inputs

- e.g., Many closure relations, thermal-hydraulics

Parameter Subset/Subspace Selection

First Issue: Parameters often not *identifiable* in the sense that they are not uniquely determined by the data.

Example 1: Spring model

$$m\frac{dy}{dt^2} + ky = 0$$

$$y(0) = y_0 \, , \; \frac{dy}{dt}(0) = 0$$

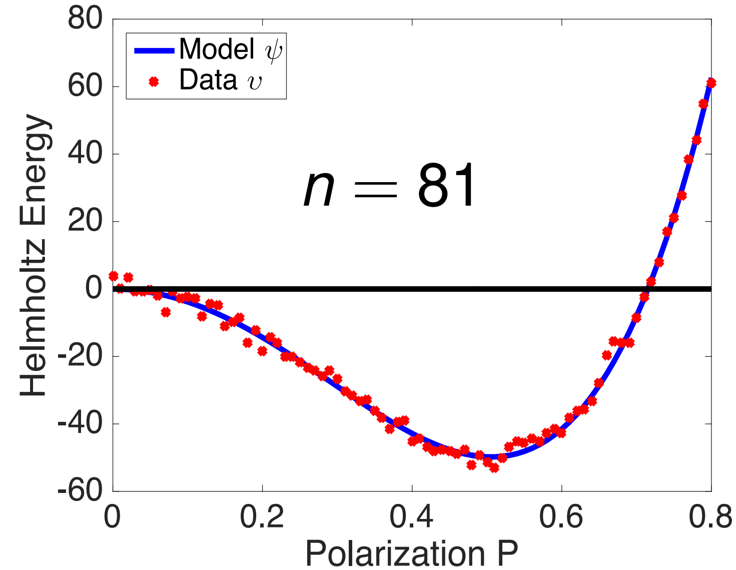
Solution: $y(t,q) = y_0 \cos\left(\sqrt{k/m} \cdot t\right)$

Note: q = [k,m] not jointly identifiable

Example 2: Helmholtz energy

$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$

Question: Are $q = [\alpha_1, \alpha_{11}, \alpha_{111}]$ identifiable for $P \in [0, 0.8]$?



Techniques:

- Global Sensitivity analysis
- Parameter subset selection
- Active subspace techniques (SVD,QR)

Parameter Subset/Subspace Selection

Second Issue: Models can have thousands to millions of parameters

3-D Neutron Transport Equations:

$$
\begin{aligned}
&\frac{1}{|v|}\frac{\partial \varphi}{\partial t} + \Omega \cdot \nabla \varphi + \Sigma_t(r,E)\varphi(r,E,\Omega,t) \\
&\quad = \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(E' \to E, \Omega' \to \Omega)\varphi(r,E',\Omega',t) \\
&\quad + \underline{\frac{\chi(E)}{4\pi}} \int_{4\pi} d\Omega' \int_0^\infty dE' \underline{\nu(E')}\,\underline{\Sigma_f(E')}\varphi(r,E',\Omega',t)
\end{aligned}
$$

Challenges:

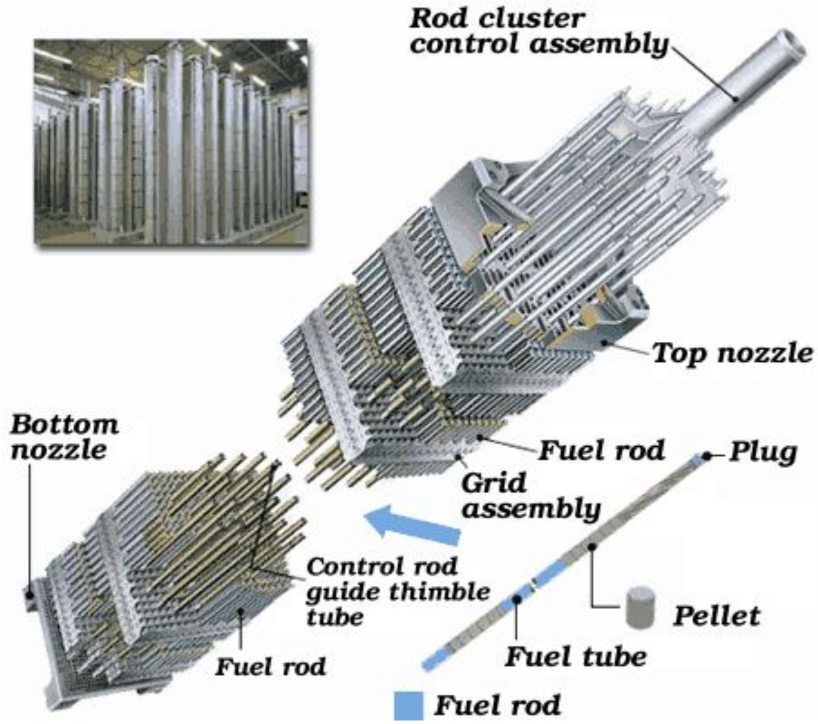
- Very large number of inputs; e.g., 100,000;
Active subspace construction critical.

- ORNL Code SCALE: Can take hours to run

Techniques for General Models:

- Identifiability and sensitivity analysis

- Active Subspaces



Sensitivity Analysis: Motivation

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100,\ c = 0.1,\ e = 0.001,\ \frac{de}{dt} = 0.1$

Question: To which parameter E or c is stress most sensitive?

Local Sensitivity Analysis:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\boxed{\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1}$$

Conclusion: Model most sensitive to damping parameter c

Limitations:

- Does not accommodate potential uncertainty in parameters.
- Does not accommodate potential correlation between parameters.
- Sensitive to units and magnitudes of parameters.

Global Sensitivity Analysis

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100,\ c = 0.1$

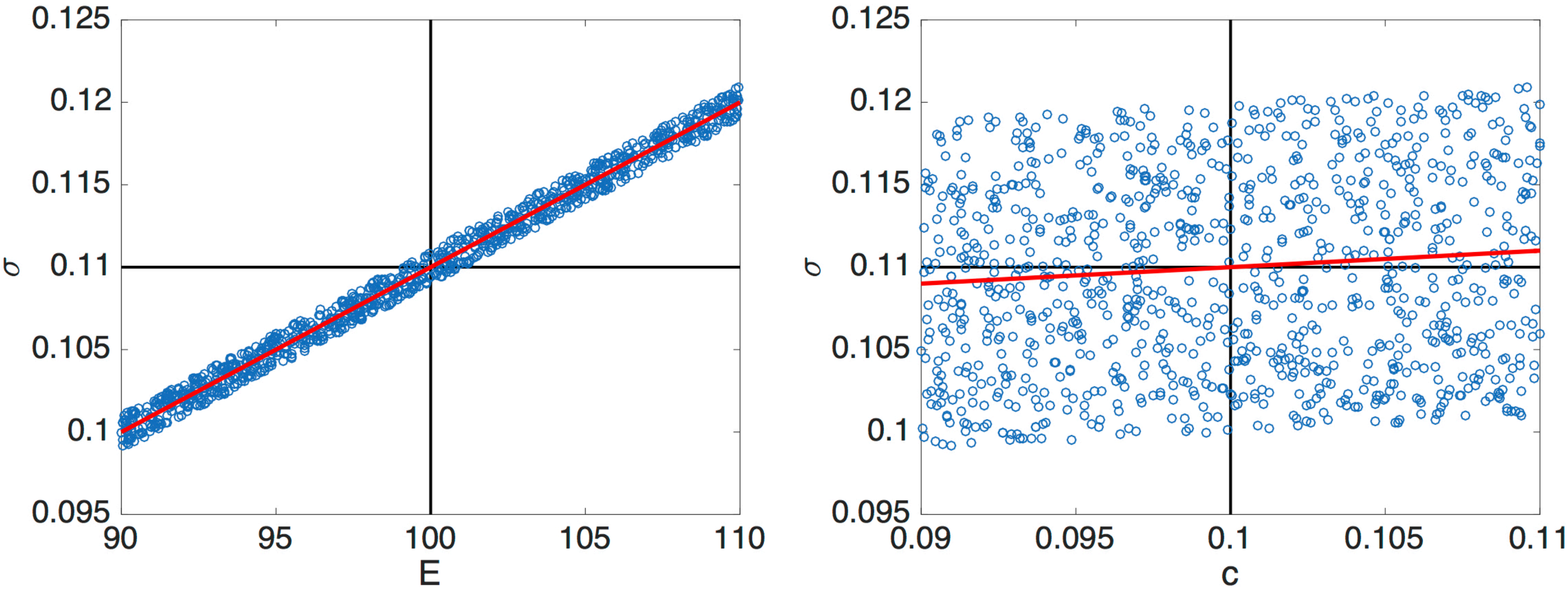
Uncertainty: 10% of nominal values

$$E \sim \mathcal{U}(90, 110)\ ,\ \ c \sim \mathcal{U}(0.09, 0.11)$$

Local Sensitivities:

$$\frac{\partial \sigma}{\partial E} = e = 0.001$$

$$\frac{\partial \sigma}{\partial c} = \frac{de}{dt} = 0.1$$



Global Sensitivity: E is more influential

Global Sensitivity Analysis

Example: Linear elastic constitute relation

$$\sigma = Ee + c\frac{de}{dt}$$

Nominal Values: $E = 100, \; c = 0.1$

Uncertainty: 10% of nominal values

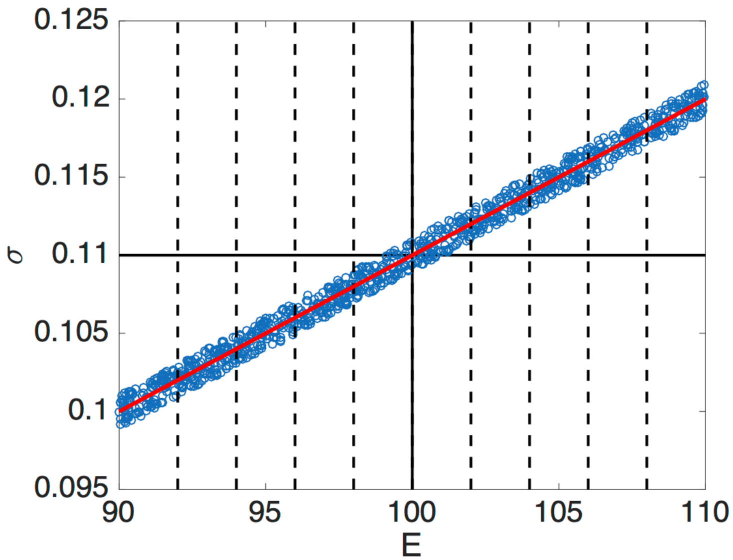
$$E \sim \mathcal{U}(90, 110)\;, \; c \sim \mathcal{U}(0.09, 0.11)$$

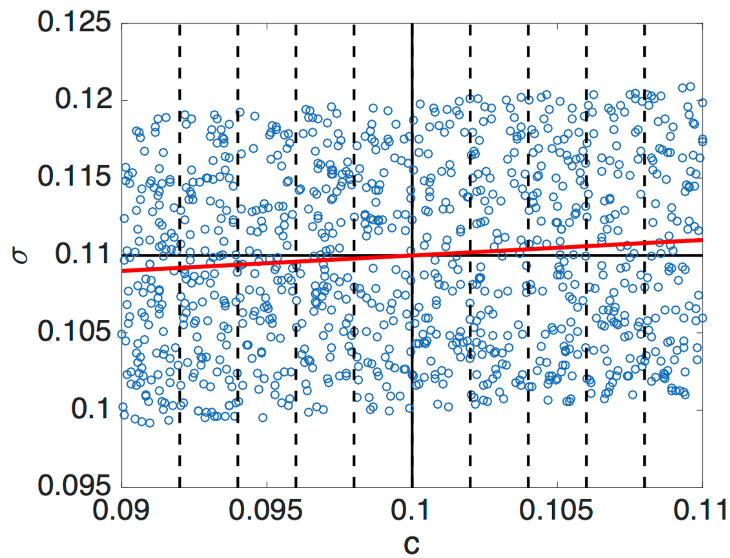
Assumption: Mutually independent parameters

Statistical Interpretation:

$$D_i = \mathrm{var}[\mathbb{E}(Y|q_i)]$$

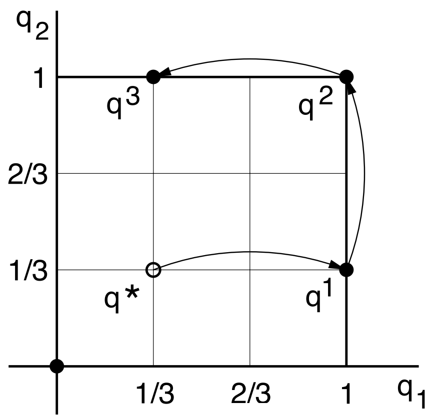
$$S_i = \frac{\mathrm{var}[\mathbb{E}(Y|q_i)]}{\mathrm{var}(Y)}$$

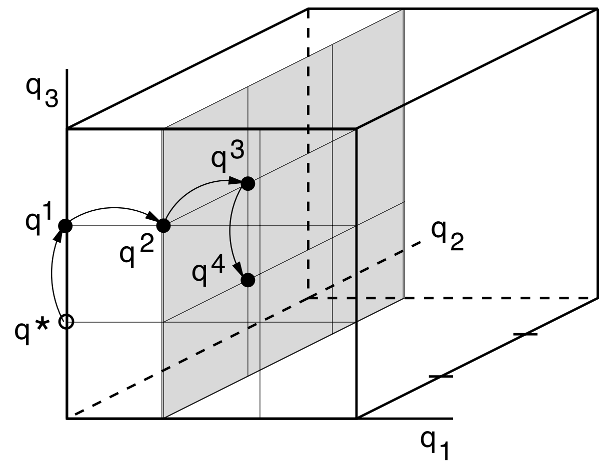




Global Sensitivity Analysis: Morris

Example: Consider independent uniformly distributed parameters on $\Gamma = [0,1]^p$





Elementary Effect:

$$d_i^j = \frac{f(q^j + \Delta e_i) - F(q^j)}{\Delta}$$, i^{th} parameter , j^{th} sample

Global Sensitivity Measures: r samples

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r} |d_i^j(q)|$$

$$\sigma_i^2 = \frac{1}{r-1}\sum_{j=1}^{r}\left(d_i^j(q) - \mu_i\right)^2 \quad , \quad \mu_i = \frac{1}{r}\sum_{j=1}^{r} d_i^j(q)$$

Global Sensitivity Analysis: CASL

Subchannel Code (COBRA-TF): numerous closure relation and parameters

parameter	partial correlation	simple correlation	morris main	morris interaction	CPS variation
k_eta	0.07	0.03			
k_gama	-0.03	0.04			
k_sent	-0.03	-0.02			
k_sdent	-0.07	-0.01			
k_tmasv	-0.03	0.00			
k_tmasl	0.11	0.00	6.48E-05	2.28E-05	medium
k_tmasg	-0.19	-0.01			
k_tmomv	-0.12	-0.01			
k_tmome	0.02	0.00			
k_tmoml	0.02	-0.02	2.23E-04	1.30E-04	medium
k_xk	0.08	-0.02			
k_xkes	-0.05	0.00			
k_xkge	-0.07	0.01			
k_xkl	0.04	-0.01			
k_xkle	-0.03	0.00			
k_xkvls	0.11	-0.01			
k_xkwvw	-0.10	0.01			
k_xkwlw	0.14	0.01			
k_xkwew	-0.01	0.03			
k_qvapl	-0.09	-0.01			
k_tnrgv	-0.03	0.00			
k_tnrgl	-0.01	0.03	9.00E-06	9.49E-06	low
k_rodqq	0.02	-0.01			
k_qradd	-0.02	0.00			
k_qradv	-0.01	0.00			
k_qliht	-0.01	0.00			
k_sphts	-0.05	0.03			
k_cond	-0.04	0.00			
k_xkwvx	0.03	-0.02			
k_xkwlx	1.00	0.88	1.80E-01	7.07E-03	high
k_cd	1.00	0.46	9.59E-02	7.88E-03	high
k_cdfb	-0.02	-0.01			
k_wkr	0.02	0.02			

5 Identified Active Inputs:

k_cd: Pressure loss coefficient of space in sub-channel

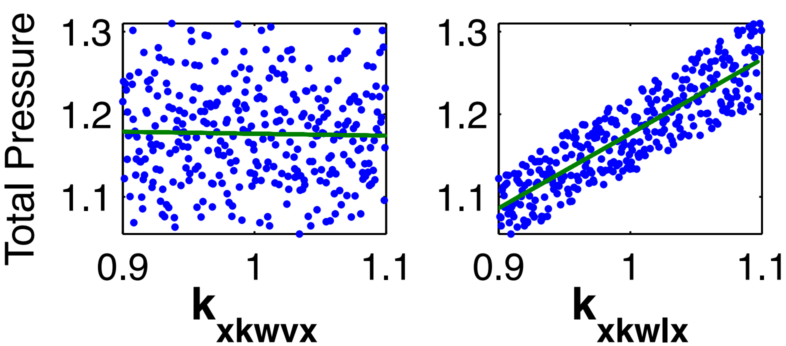
k_xkwlx: Vertical liquid wall drag coefficient

k_tmasl: Loss of liquid mass due to mixing and void drift

k_tmoml: Loss of liquid momentum due to mixing and void drift

k_tnrgl: Loss of liquid enthalpy due to mixing and void drift

Partial Correlation:



Note: 33 initial parameters reduced to 5 via sensitivity analysis

Global Sensitivity Analysis

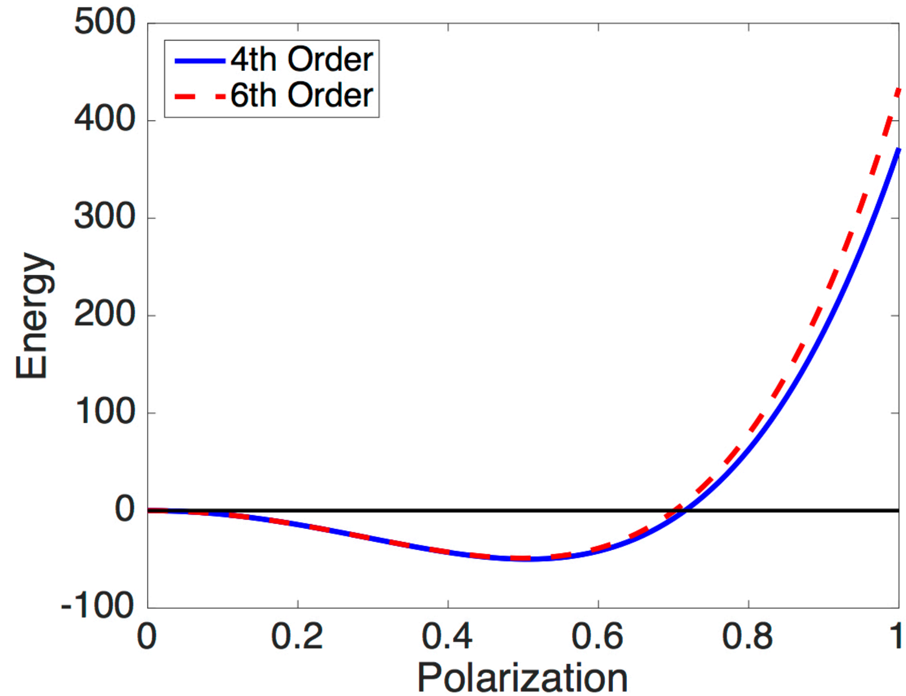
Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$



Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03

Conclusion: α_{111} insignificant and can be fixed

Global Sensitivity Analysis

Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

$$\psi(P,q) = \underline{\alpha_1} P^2 + \underline{\alpha_{11}} P^4 + \underline{\alpha_{111}} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

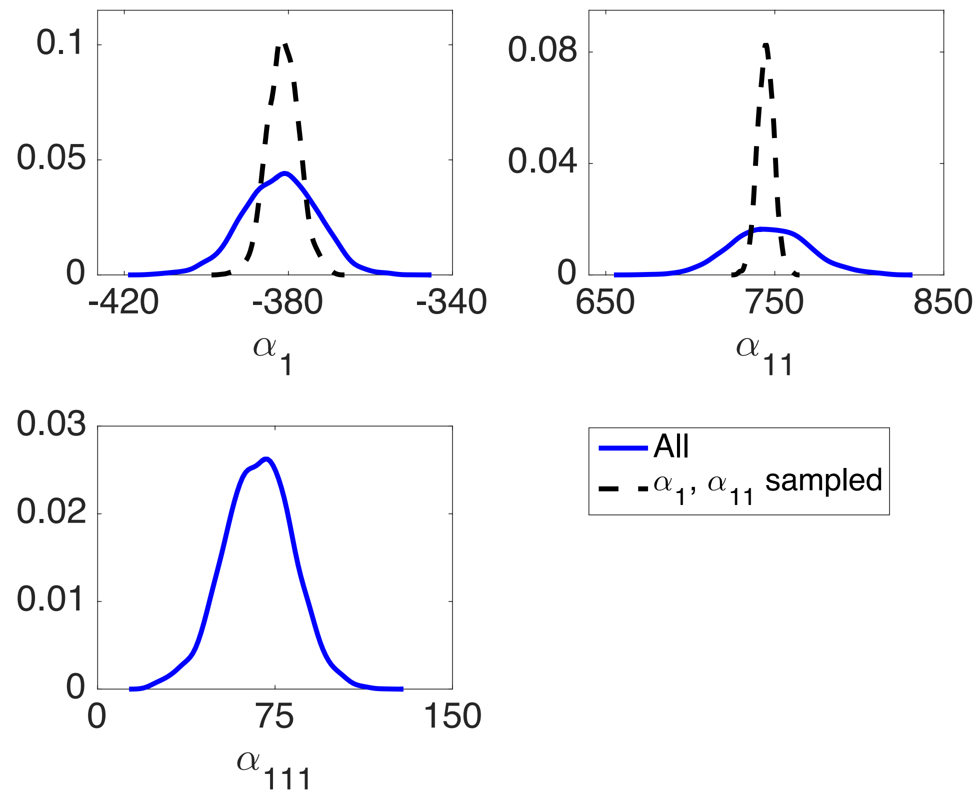
Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_i	0.62	0.39	0.01
S_{T_i}	0.66	0.38	0.06
μ_i^*	0.17	0.07	0.03

Conclusion:

α_{111} insignificant and can be fixed

Problem: We obtain different distributions when we perform Bayesian inference with fixed non-influential parameters



Global Sensitivity Analysis

Example: Quantum-informed continuum model

Question: Do we use 4th or 6th-order Landau energy?

$$\psi(P,q) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$

Parameters:

$$q = [\alpha_1, \alpha_{11}, \alpha_{111}]$$

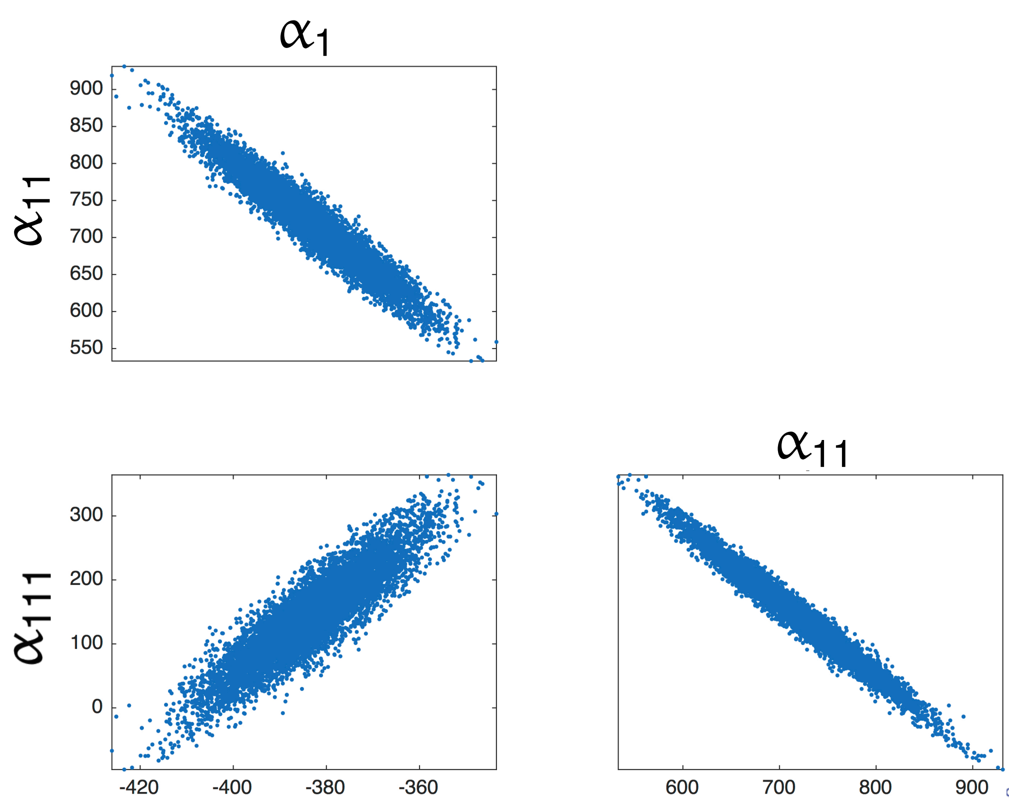
Global Sensitivity Analysis:

	α_1	α_{11}	α_{111}
S_k	0.62	0.39	0.01
T_k	0.66	0.38	0.06
μ_k^*	0.17	0.07	0.03

Note: Must accommodate correlation

Problem:

- Parameters correlated
- Cannot fix α_{111}



Parameter Subset Selection

Consider

$$\psi(P_i, q) \approx \psi(P_i, q^*) + \nabla_q \psi(P_i, q^*)\Delta q$$

where

$$\nabla_q \psi(P_i, q^*) = \left[\frac{\partial \psi}{\partial \alpha_1}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{11}}(P_i, q^*)\ ,\ \frac{\partial \psi}{\partial \alpha_{111}}(P_i, q^*) \right]$$

Functional: Since $\upsilon_i \approx \psi(P_i, q^*)$

$$\begin{aligned} J(q) &= \frac{1}{n}\sum_{i=1}^{n} [\upsilon_i - \psi(P_i, q)]]^2 \\ &\approx \frac{1}{n}\sum_{i=1}^{n} [\nabla_q \psi(P_i, q^*) \cdot \Delta q]^2 \\ &= \frac{1}{n}(\chi \Delta q)^T (\chi \Delta q) \end{aligned}$$

Sensitivity Matrix:

$$\chi(q^*) = \begin{bmatrix} \frac{\partial \psi}{\partial \alpha_1}(P_1, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_1, q^*) \\ \vdots & \cdots & \vdots \\ \frac{\partial \psi}{\partial \alpha_1}(P_n, q^*) & & \frac{\partial \psi}{\partial \alpha_{111}}(P_n, q^*) \end{bmatrix}$$

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n}\Delta q^T \chi^T \chi \Delta q$$

Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

Strategy: Take Δq to be eigenvector of $\boxed{\chi^T \chi}$ Fisher Information

$$\Rightarrow \chi^T \chi \Delta q = \lambda \Delta q$$

$$\Rightarrow J(q^* + \Delta q) \approx \frac{\lambda}{n} \|\Delta q\|_2^2$$

Note: $\lambda \approx 0 \Rightarrow$ Perturbations $J(q^* + \Delta q) \approx 0$

$\Rightarrow$ Nonidentifiable

Note: Estimator for covariance matrix

$$V = s^2 \left[\chi^T \chi\right]^{-1} = \begin{bmatrix} \mathrm{var}(q_1) & \mathrm{cov}(q_1, q_2) & \cdots & \mathrm{cov}(q_1, q_n) \\ \mathrm{cov}(q_2, q_1) & \mathrm{var}(q_2) & \mathrm{cov}(q_2, q_3) & \\ \vdots & & & \vdots \\ \mathrm{cov}(q_n, q_1) & \cdots & \cdots & \mathrm{var}(q_n) \end{bmatrix}$$

Parameter Subset Selection

Note:

$$J(q^* + \Delta q) \approx \frac{1}{n} \Delta q^T \chi^T \chi \Delta q$$

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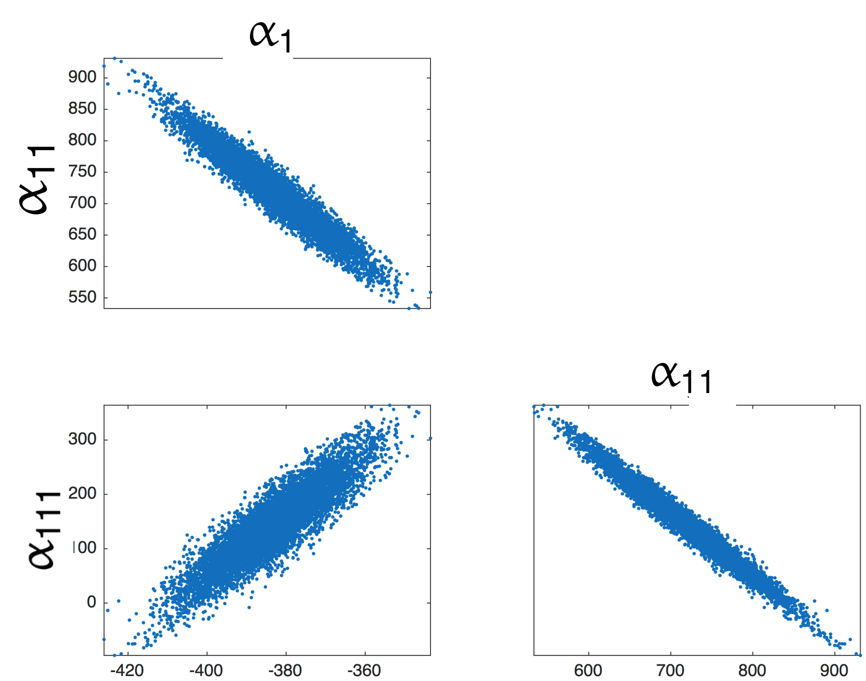


Result: rank($\chi^T \chi$) = 3 so all parameters identifiable

Active Subspaces

Note:

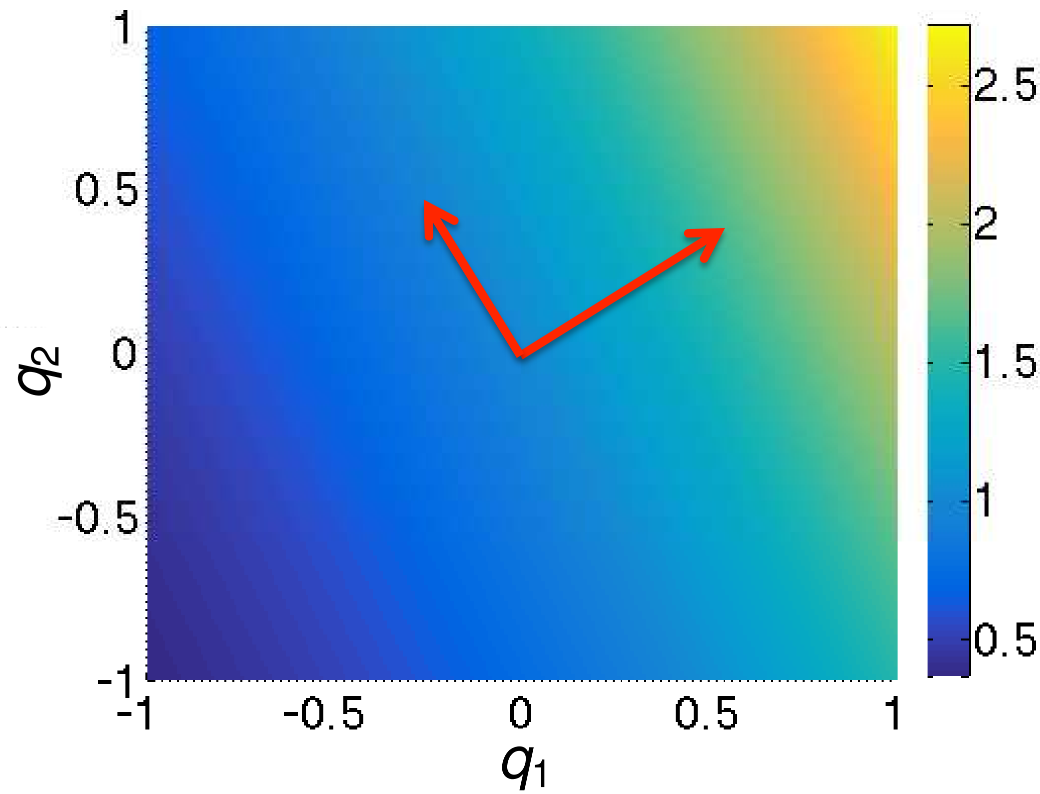
- Functions may vary significantly in only a few directions
- “Active” directions may be linear combination of inputs

Example: $y = \exp(0.7q_1 + 0.3q_2)$

- Varies most in [0.7, 0.3] direction
- No variation in orthogonal direction

Strategy:

- *Linearly parameterized problems:* Employ SVD or QR decomposition.
- *Nonlinear problems:* Construct approximate gradient matrix and employ SVD or QR.



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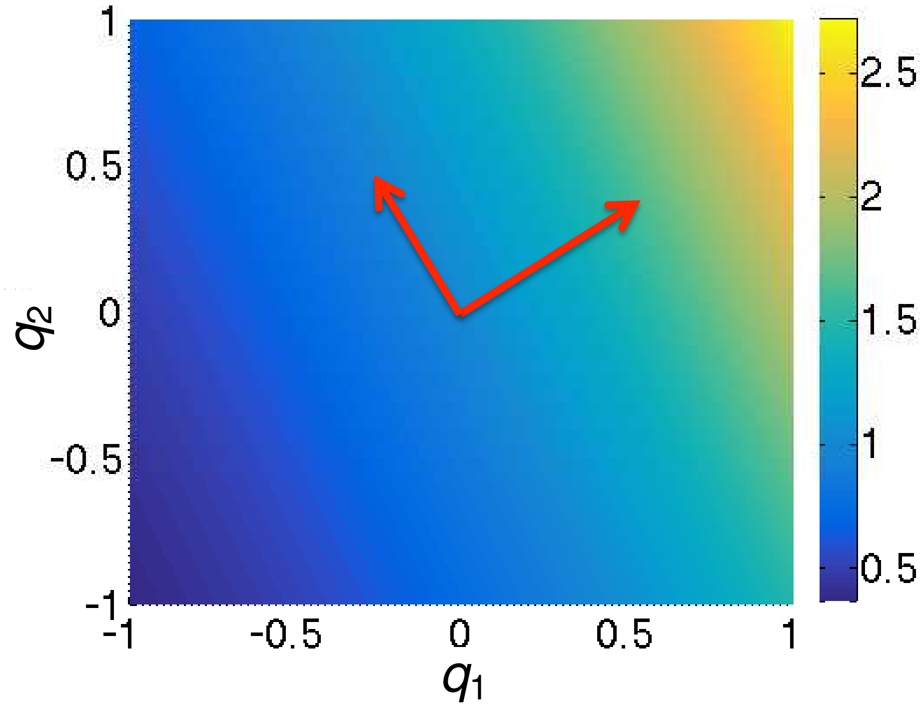

A Bit of History:

- Often attributed to Russi (2010).
- Concept same as *identifiable subspaces* from systems and control; e.g., Reid (1977).
- For linearly parameterized problems, active subspace given by SVD or QR; Beltrami (1873), Jordan (1874), Sylvester (1889), Schmidt (1907), Weyl (1912). See 1993 *SIAM Review* paper by Stewart.

Linear Problems

Second Issue: Models depends on very large number of parameters – e.g., millions – but only a few are "significant".

Linear Algebra Techniques: Linearly parameterized problems

$$y = Aq \ , \ q \in \mathbb{R}^p \ , \ y \in \mathbb{R}^m$$

Singular Value Decomposition (SVD):

$$A = U\Sigma V^T \ , \ \Sigma = [S \quad 0]$$

$$S = \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & 0 \end{bmatrix} \ , \ \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq \varepsilon$$

Rank Revealing QR Decomposition: $A^T P = QR$

Problem: Neither is directly applicable when m or p are very large; e.g., millions.

Solution: Random range finding algorithms.

Active Subspaces

Note:

- Functions may vary significantly in only a few directions
- "Active" directions may be linear combination of inputs

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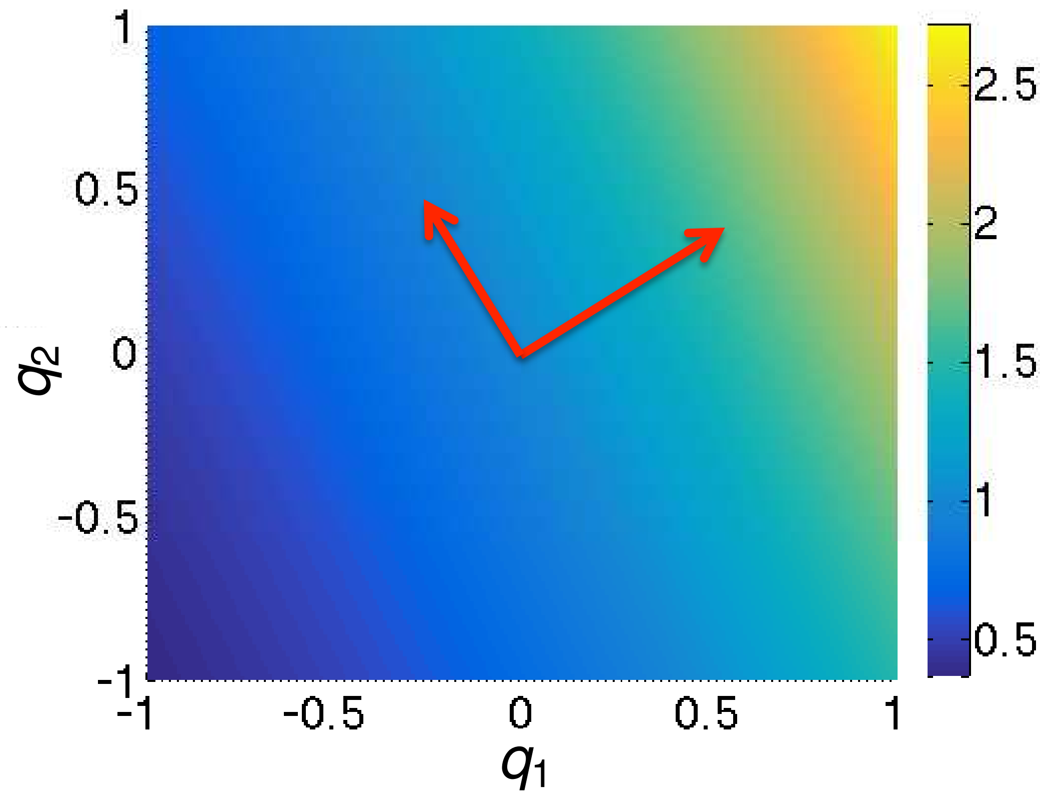


Strategy:

- *Linearly parameterized problems:* Employ SVD or QR decomposition.
- *Nonlinear problems:* Construct approximate gradient matrix and employ SVD or QR.

Gradient-Based Active Subspace

Active Subspace: Consider

$$f = f(q)\ ,\, q \in \mathcal{Q} \subseteq \mathbb{R}^p$$

- E.g., see [Constantine, SIAM, 2015; Stoyanov & Webster, *IJUQ*, 2015]

and

$$\nabla_q f(q) = \left[\frac{\partial f}{\partial q_1}, \cdots, \frac{\partial f}{\partial q_p}\right]^T$$

Construct outer product

$\rho(q)$: Distribution of input parameters q

$$C = \int (\nabla_q f)(\nabla_q f)^T \rho dq$$

Question: How sensitive are results to distribution, which is typically not known?

Partition eigenvalues: $C = W \Lambda W^T$

$$\Lambda = \begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix}\ ,\quad W = [W_1 \quad W_2]$$

Rotated Coordinates:

$$y = W_1^T q \in \mathbb{R}^n \quad \text{and} \quad z = W_2^T q \in \mathbb{R}^{p-n}$$

Active Variables

Active Subspace: Range of eigenvectors in W_1

Gradient-Based Active Subspace

Active Subspace: Construction based on random sampling

1. Draw M independent samples $\{q^j\}$ from ρ

2. Evaluate $\nabla_q f_j = \nabla_q f(q^j)$

3. Approximate outer product

$$C \approx \widetilde{C} = \frac{1}{M} \sum_{j=1}^{M} (\nabla_q f_j)(\nabla_q f_j)^T$$ Monte Carlo Quadrature

Note: $\widetilde{C} = GG^T$ where $G = \frac{1}{\sqrt{M}}[\nabla_q f_1, \ldots, \nabla_q f_M]$

4. Take SVD of $G = W\sqrt{\Lambda}V^T$

- Active subspace of dimension n is first n columns of W

Current Research: Develop efficient algorithms for codes that do not have adjoint capabilities

Note: Finite difference approximations tempting but not very effective

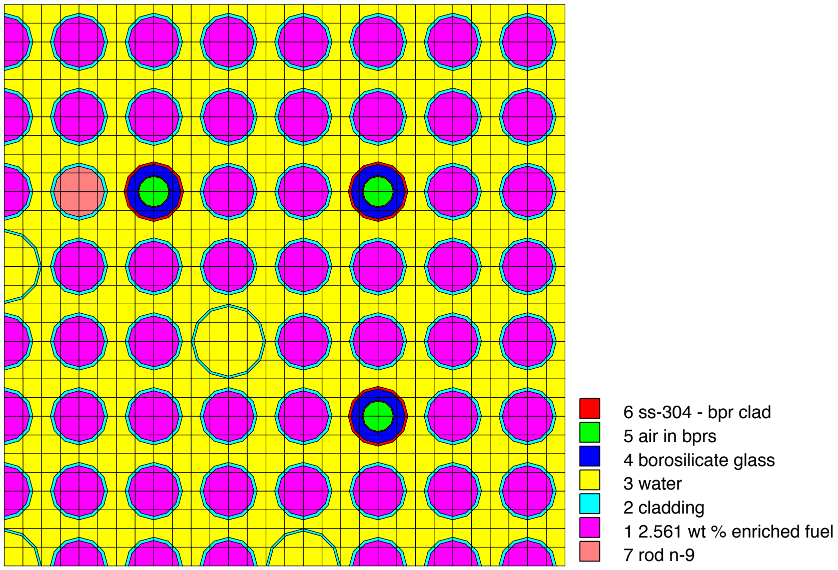
Strategy: Algorithm based on initialized adaptive Morris indices

SCALE6.1: High-Dimensional Example

Setup: Cross-section computations SCALE6.1

- Input Dimension: 7700
- Output k_{eff}

Materials			Reactions	
$^{234}_{92}\mathrm{U}$	$^{10}_{5}\mathrm{B}$	$^{31}_{15}\mathrm{P}$	Σ_t	$n \rightarrow \gamma$
$^{235}_{92}\mathrm{U}$	$^{11}_{5}\mathrm{B}$	$^{55}_{25}\mathrm{Mn}$	Σ_e	$n \rightarrow p$
$^{236}_{92}\mathrm{U}$	$^{14}_{7}\mathrm{N}$	$_{26}\mathrm{Fe}$	Σ_f	$n \rightarrow d$
$^{238}_{92}\mathrm{U}$	$^{15}_{7}\mathrm{N}$	$^{116}_{50}\mathrm{Sn}$	Σ_c	$n \rightarrow t$
$^{1}_{1}\mathrm{H}$	$^{23}_{11}\mathrm{Na}$	$^{120}_{50}\mathrm{Sn}$	$\bar{\nu}$	$n \rightarrow {}^{3}\mathrm{He}$
$^{16}_{8}\mathrm{O}$	$^{27}_{13}\mathrm{Al}$	$_{40}\mathrm{Zr}$	χ	$n \rightarrow \alpha$
$_{6}\mathrm{C}$	$_{14}\mathrm{Si}$	$_{19}\mathrm{K}$	$n \rightarrow n'$	$n \rightarrow 2n$



PWR Quarter Fuel Lattice

Note: Requires efficient initialization algorithm.

SCALE6.1: High-Dimensional Example

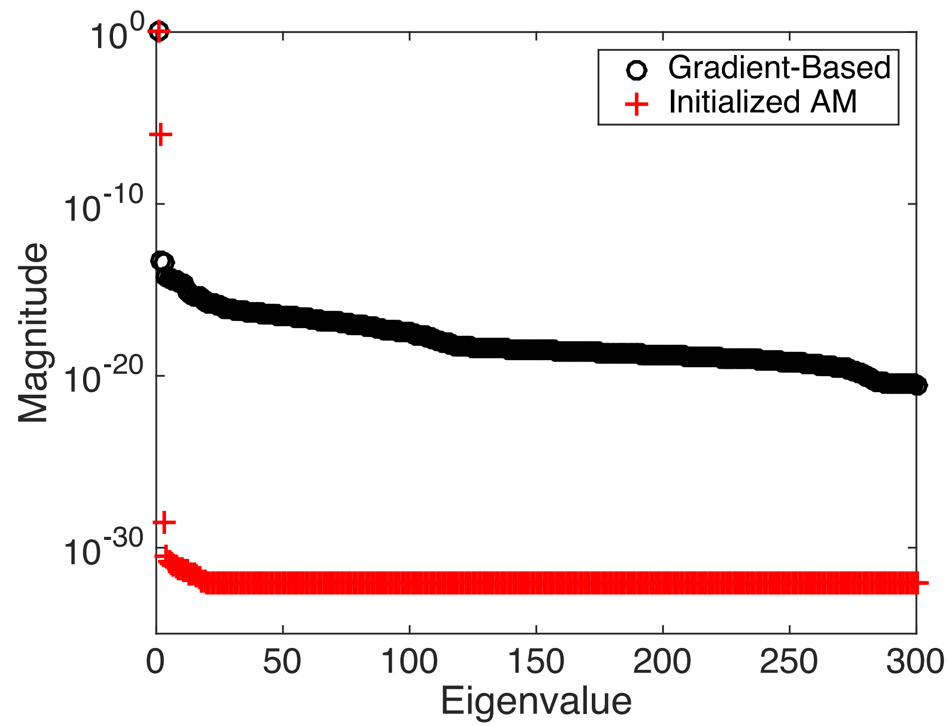
Setup:

- Input Dimension: 7700

SCALE Evaluations:

- Gradient-Based: 1000
- Initialized Adaptive Morris: 18,392
- Projected Finite-Difference: 7,701,000

Note: Analytic eigenvalues: 0, 1

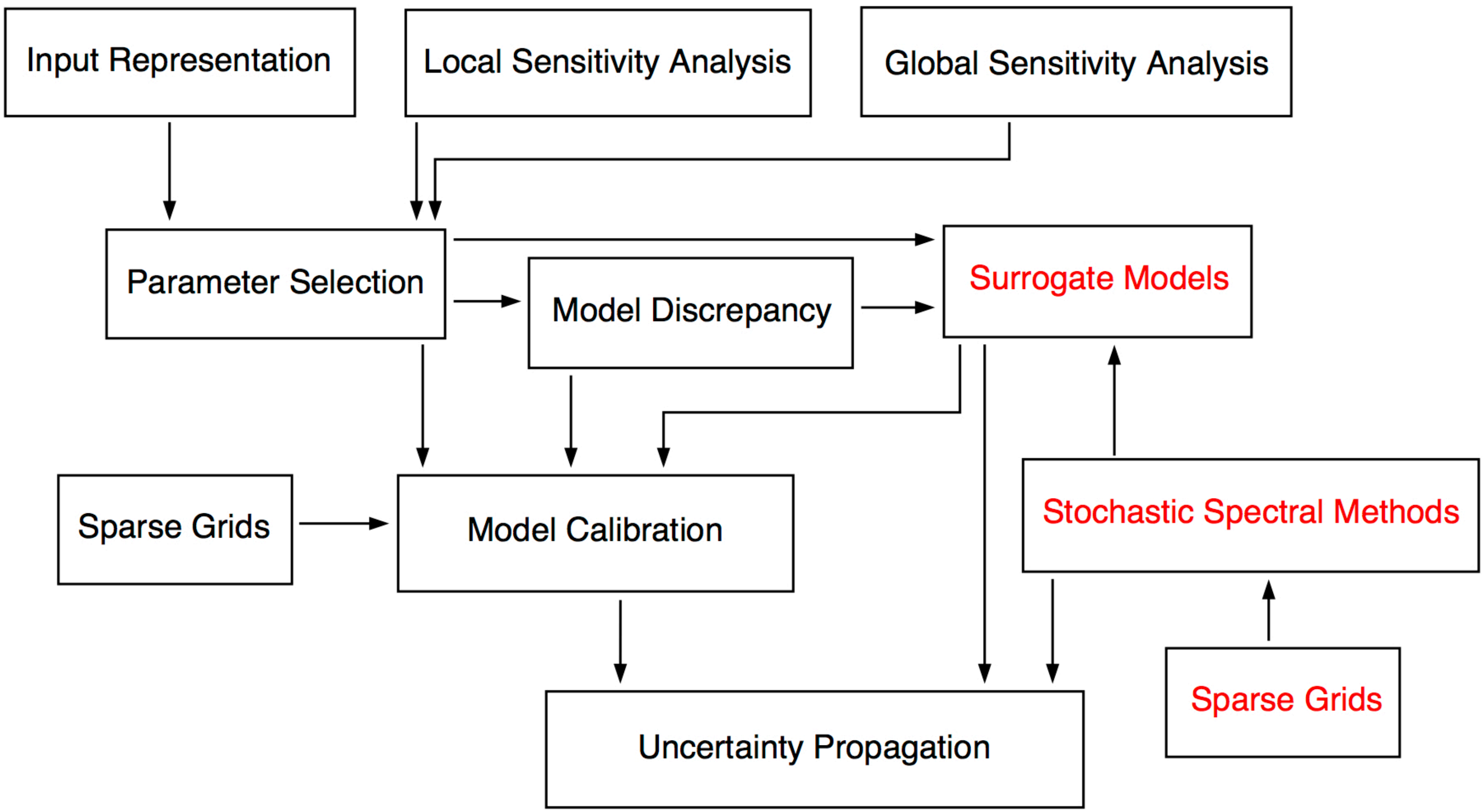


For surrogate sampled off space

Active Subspace Dimensions:

	Gap	PCA				Error Tolerance			
Method		0.75	0.90	0.95	0.99	10^{-3}	10^{-4}	10^{-5}	10^{-6}
Gradient-Based	1	2	6	9	24	1	13	90	233
Initialized AM	1	1	1	1	2	1	2	2	2

Steps in Uncertainty Quantification



Challenge:

- How do we do uncertainty quantification for computationally expensive models?

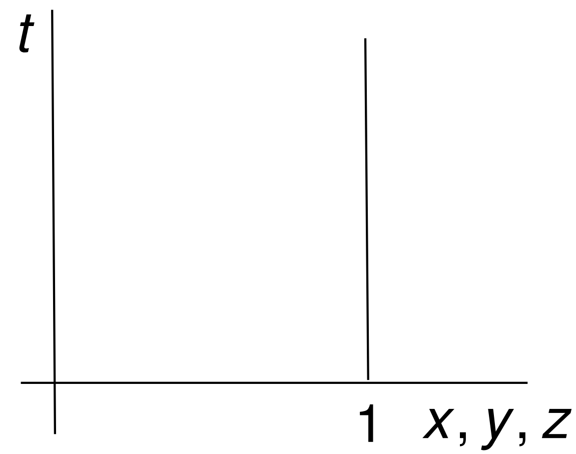
Surrogate Models: Motivation

Example: Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + f(q)$$

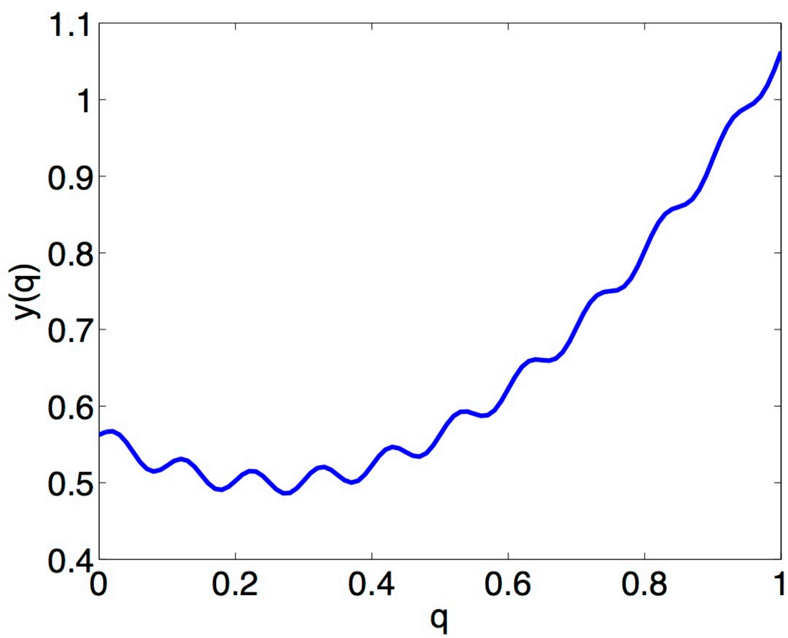
Boundary Conditions

Initial Conditions



with the response

$$y(q) = \int_0^1 \int_0^1 \int_0^1 \int_0^1 u(t,x,y,z)\,dxdydzdt$$



Notes:

- Requires approximation of PDE in 3-D
- What would be a simple surrogate?

Surrogate Models: Motivation

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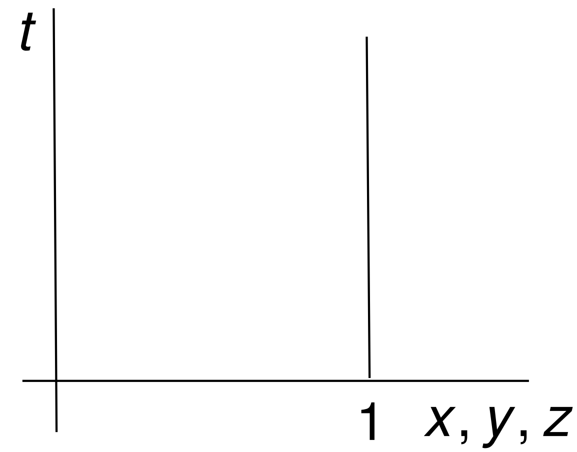
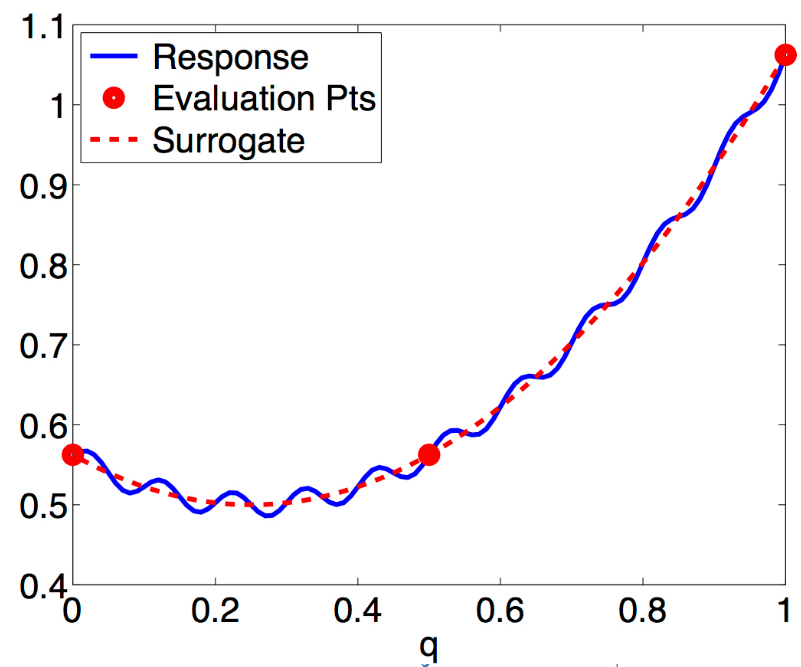


Surrogate: Quadratic

$$y_s(q) = (q - 0.25)^2 + 0.5$$



Question: How do you construct a polynomial surrogate?

- Regression
- Interpolation

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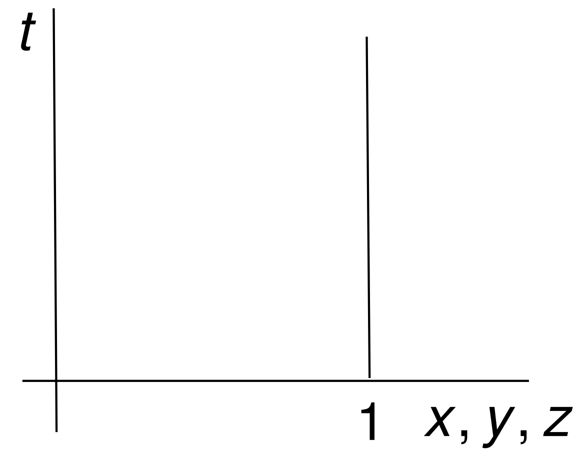

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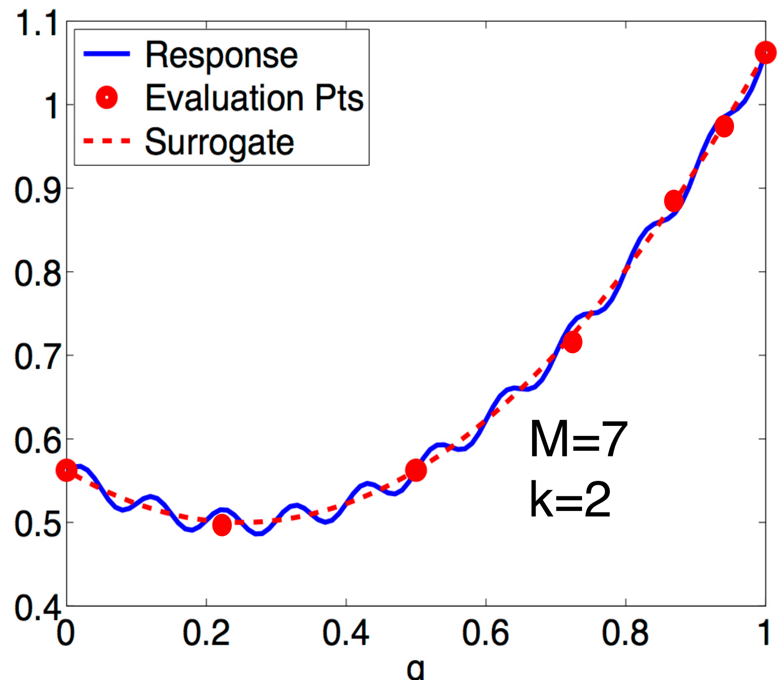


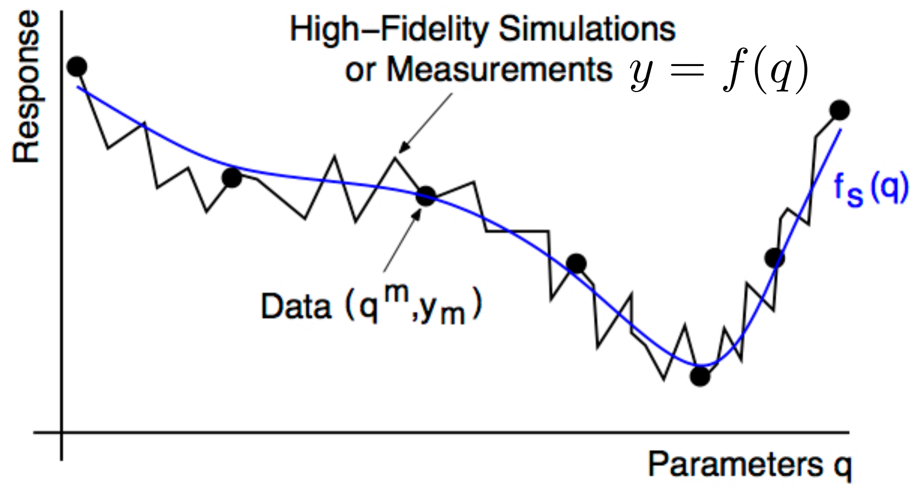
Question: How do you construct a polynomial surrogate?

- Interpolation
- Regression

Data-Fit Models

Notes:

- Often termed response surface models, surrogates, emulators, meta-models.
- Rely on interpolation or regression.
- Data can consist of high-fidelity simulations or experiments.



Strategy: Consider high fidelity model

$$y = f(q)$$

with M model evaluations

$$y_m = f(q^m)\ ,\ \ m = 1, \ldots, M$$

Statistical Model: $f_s(q)$: Surrogate for $f(q)$

$$y_m = f_s(q^m) + \varepsilon_m\ ,\ \ m = 1, \ldots, M$$

Surrogate:

$$y^K(Q) = f_s(Q) = \sum_{k=0}^{K} \alpha_k \Psi_k(Q)$$

Note: $\Psi_k(Q)$ orthogonal with respect to inner product associated with pdf

e.g., $Q \sim N(0,1)$: Hermite polynomials

$Q \sim U(-1,1)$: Legendre polynomials

Orthogonal Polynomial Representations

Representation:

$$y^K(Q) = \sum_{k=0}^{K} \alpha_k \Psi_k(Q)$$

Note: $\Psi_0(Q) = 1$ implies that

$$\mathbb{E}[\Psi_0(Q)] = 1$$

$$\begin{aligned}\mathbb{E}[\Psi_i(Q)\Psi_j(Q)] &= \int_\Gamma \Psi_i(q)\Psi_j(q)\rho(q)dq \\ &= \delta_{ij}\gamma_i\end{aligned}$$

where $\gamma_i = \mathbb{E}[\Psi_i^2(Q)]$

Properties:

(i) $\mathbb{E}[y^K(Q)] = \alpha_0$

(ii) $\text{var}[y^K(Q)] = \sum_{k=1}^{K} \alpha_k^2 \gamma_k$

Note: Can be used for:

- Uncertainty propagation
- Sobol-based global sensitivity analysis

Issue: How does one compute α_k , $k = 0, \ldots, K$?

- Stochastic Galerkin techniques (Polynomial Chaos Expansion – PCE)
- Nonintrusive PCE (Discrete projection)
- Stochastic collocation
- Regression-based methods with sparsity control (Lasso)

Note: Methods nonintrusive and treat code as blackbox.

Orthogonal Polynomial Representations

Nonintrusive PCE: Take weighted inner product of $y(q) = \sum_{k=0}^{\infty} \alpha_k \Psi_k(q)$ to obtain

$$\alpha_k = \frac{1}{\gamma_k} \int_\Gamma y(q) \Psi_k(q) \rho(q) dq$$

Quadrature:

$$\alpha_k \approx \frac{1}{\gamma_k} \sum_{r=1}^{R} y(q^r) \Psi_k(q^r) w^r$$

Note:

(i) Low-dimensional: Tensored 1-D quadrature rules – e.g., Gaussian

(ii) Moderate-dimensional: Sparse grid (Smolyak) techniques

(iii) High-dimensional: Monte Carlo or quasi-Monte Carlo (QMC) techniques

Regression-Based Methods with Sparsity Control (Lasso): Solve

$$\min_{\alpha \in \mathbb{R}^{K+1}} \|\Lambda \alpha - d\|^2 \quad \text{subject to} \quad \sum_{k=0}^{K} |\alpha_k| \leqslant \tau$$

Note: Sample points $\{q^m\}_{m=1}^{M}$

$$\Lambda \in \mathbb{R}^{M \times (K+1)} \quad \text{where} \quad \Lambda_{jk} = \Psi_k(q^j)$$

$$d = [y(q^1), \ldots, y(q^m)]$$

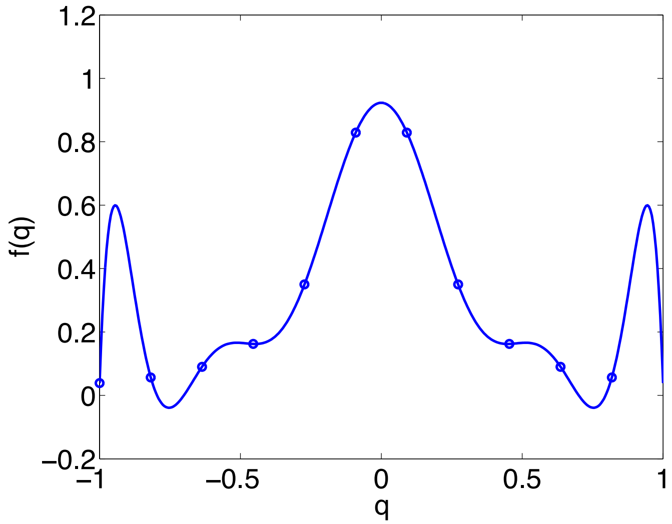
e.g., SPGL1

- MATLAB Solver for large-scale sparse reconstruction

Surrogate Models: Grid Choices

Example: Consider the Runge function $f(q) = \frac{1}{1+25q^2}$ with points

$$q^j = -1 + (j-1)\frac{2}{M} \; , \; j = 1, \ldots, M$$



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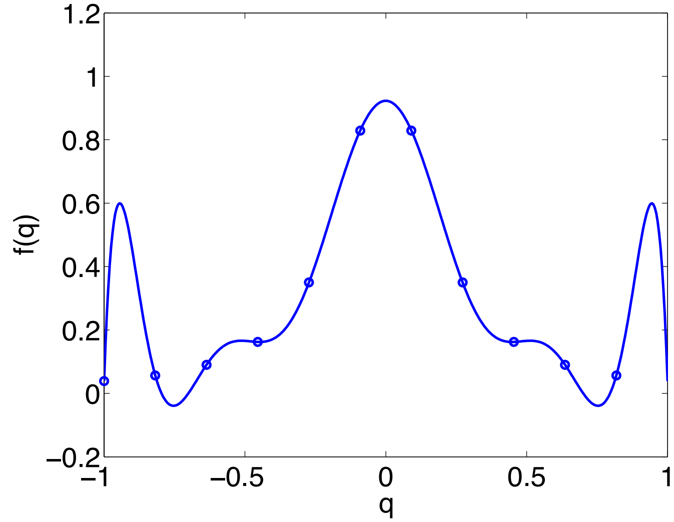
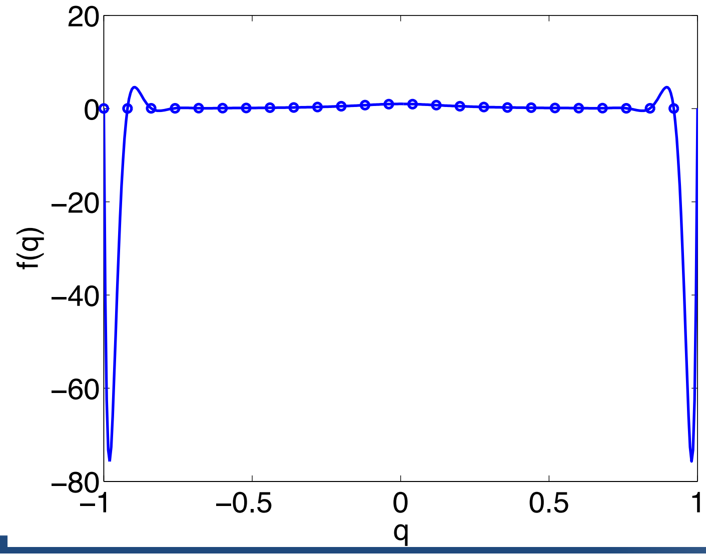
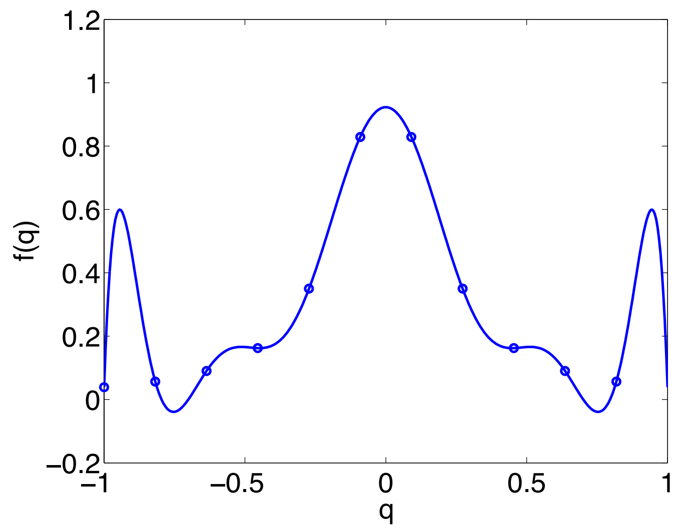


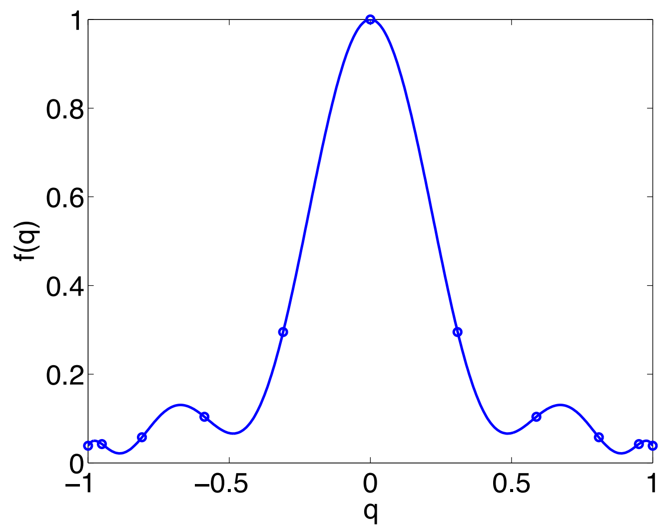


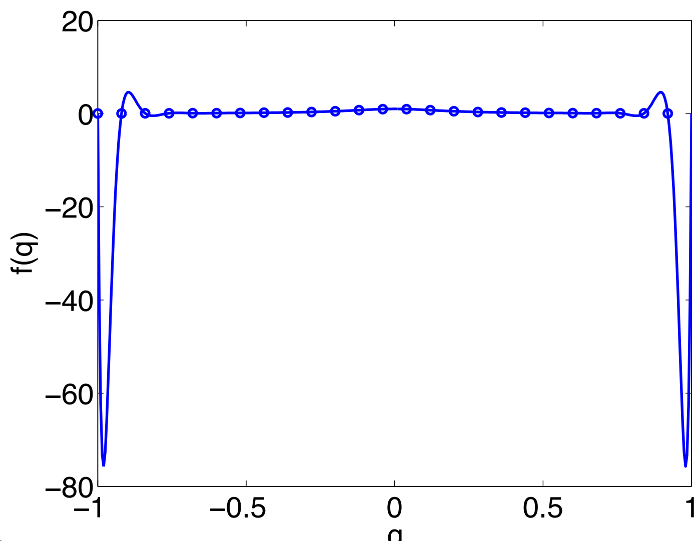
Surrogate Models: Grid Choices

Example: Consider the Runge function $f(q) = \frac{1}{1+25q^2}$ with points

$$q^j = -1 + (j-1)\frac{2}{M}\ ,\ j = 1, \ldots, M \qquad q^j = -\cos\frac{\pi(j-1)}{M-1}\ ,\ j = 1, \ldots, M$$







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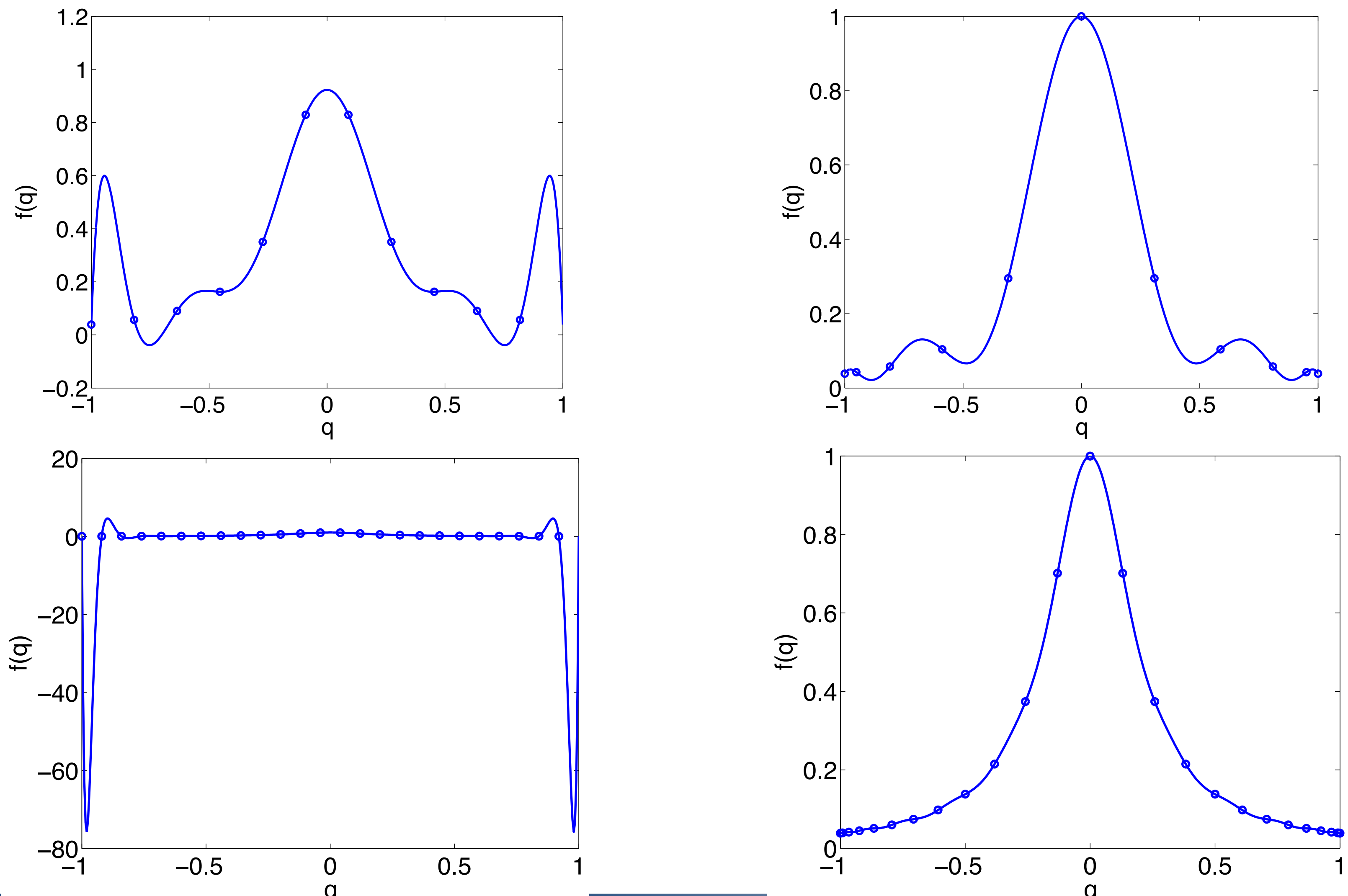
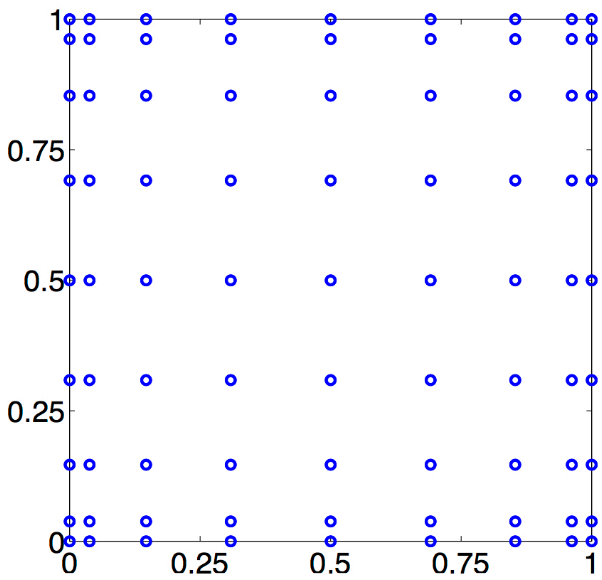
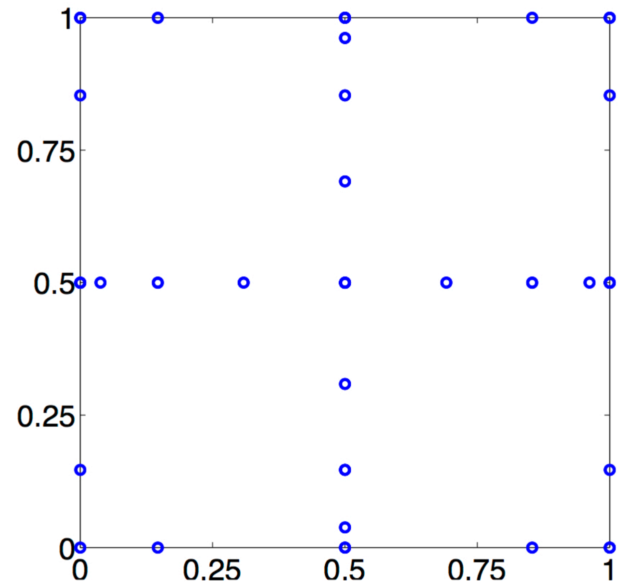


Sparse Grid Techniques

Tensored Grids: Exponential growth



Sparse Grids: Same accuracy



p	R_ℓ	Sparse Grid $\mathcal{R}$	Tensored Grid $R = (R_\ell)^p$
2	9	29	81
5	9	241	59,049
10	9	1581	$> 3 \times 10^9$
50	9	171,901	$> 5 \times 10^{47}$
100	9	1,353,801	$> 2 \times 10^{95}$

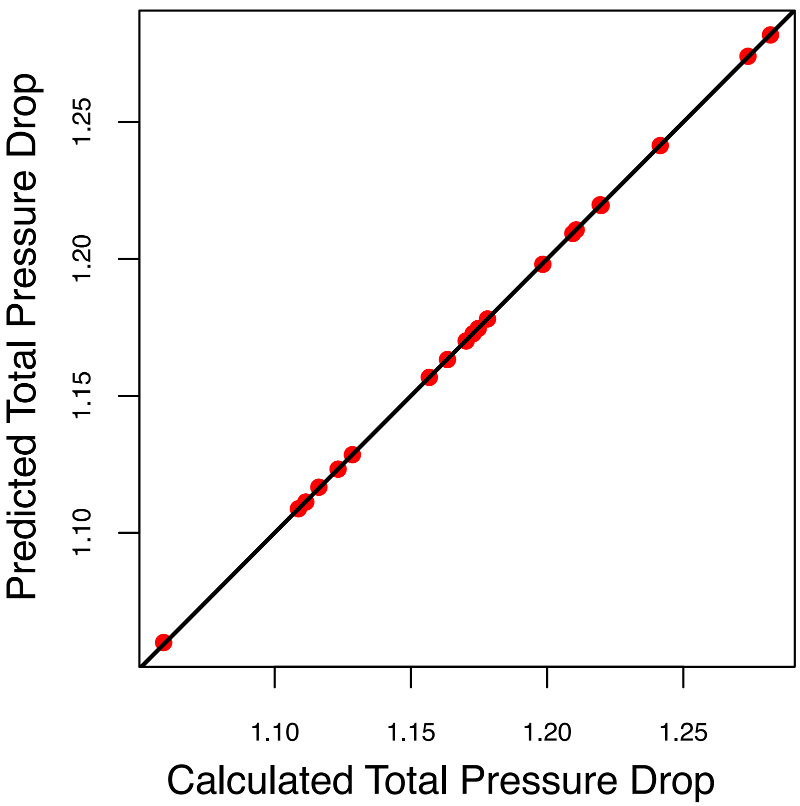
Surrogate Construction: CASL

Subchannel Code (COBRA-TF): 33 VUQ parameters reduced to 5 using SA

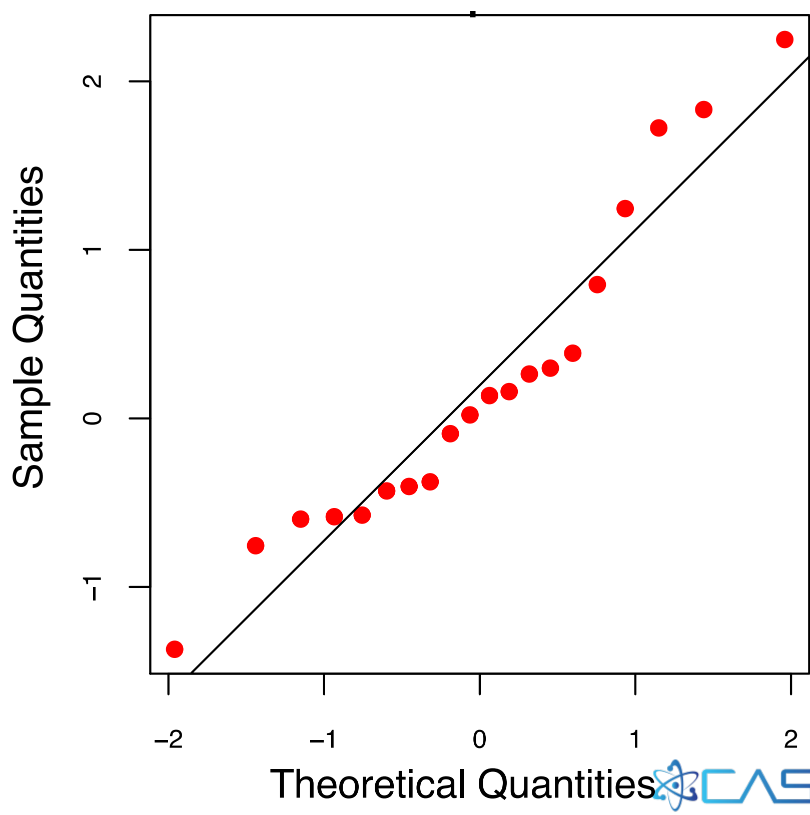
Surrogate: Total pressure drop

• Kriging (GP) emulator constructed using 50 COBRA-TF runs perturbing 5 active inputs.

• Use remaining computational budget to evaluate quality of surrogate using post-processed Dakota outputs.



Out-of-Sample Validation



Concluding Remarks

Notes:

• UQ requires a synergy between engineering, statistics, and applied mathematics.

• Model calibration, model selection, uncertainty propagation and experimental design are natural in a Bayesian framework.

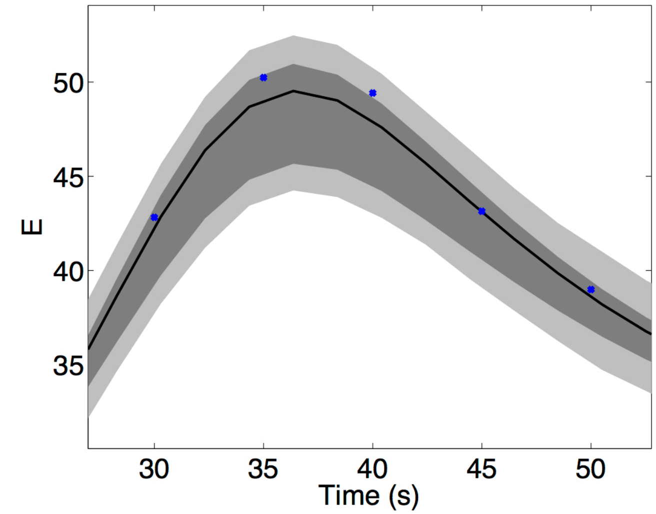
• Goal is to predict model responses with quantified and reduced uncertainties.

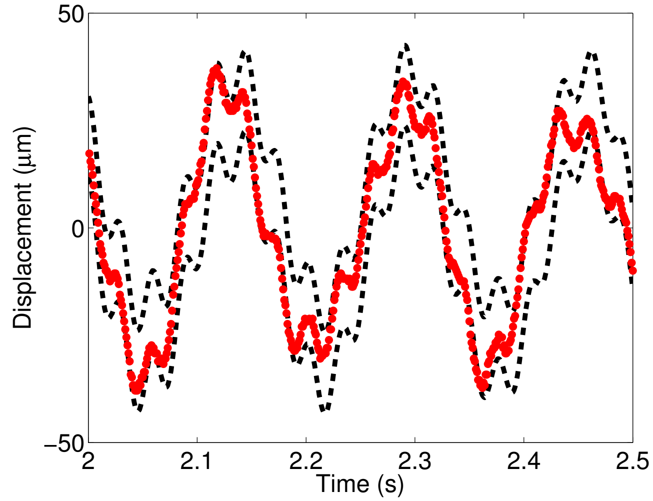
• Parameter selection is critical to isolate identifiable and influential parameters.

• Surrogate models critical for computationally intensive simulation codes.

• Codes and packages: Sandia Dakota, R, MATLAB, Python, nanoHUB.

• *Prediction is very difficult, especially if it's about the future*, Niels Bohr.





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