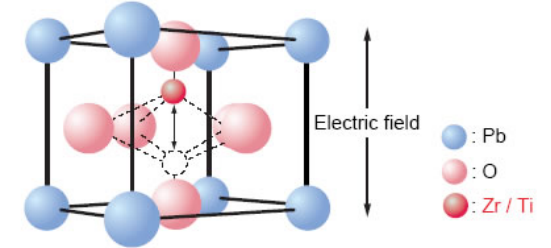
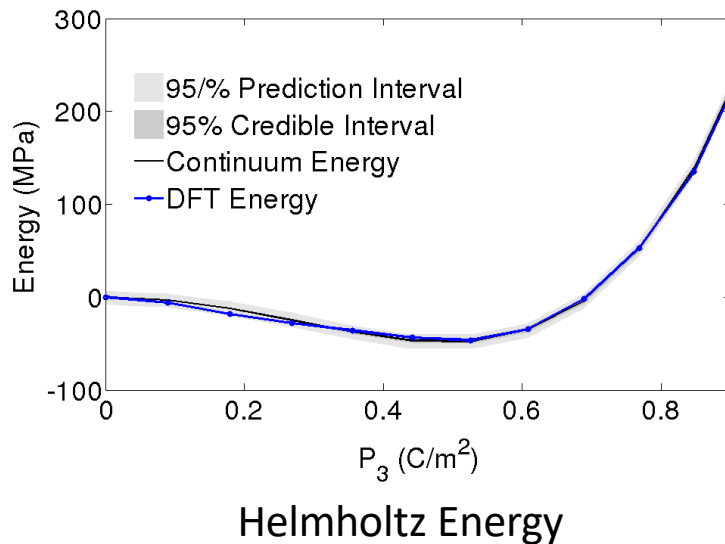


# Statistical Representation of Model Inputs

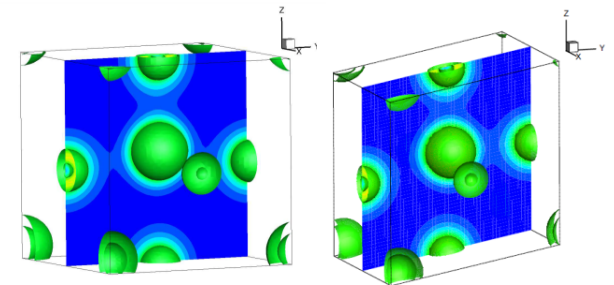
## Example:

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

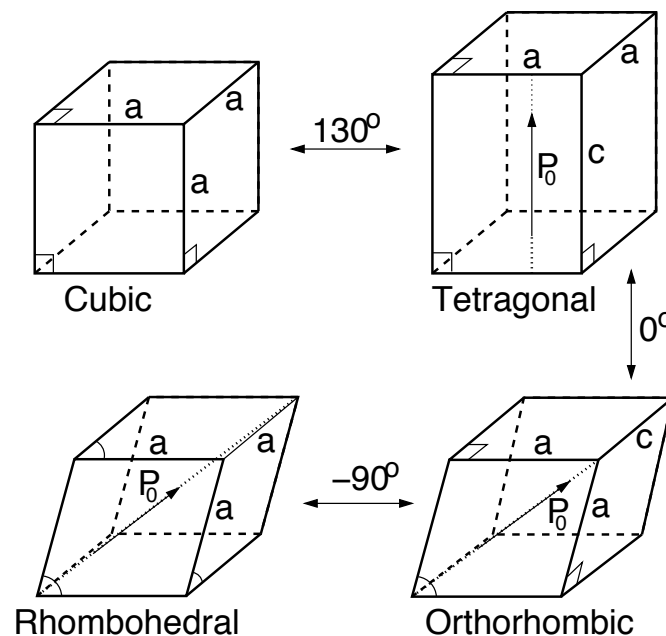
$$\psi(P) = \alpha_1 P^2 + \alpha_{111} P^4 + \alpha_{1111} P^6$$



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation



## UQ and SA Issues:

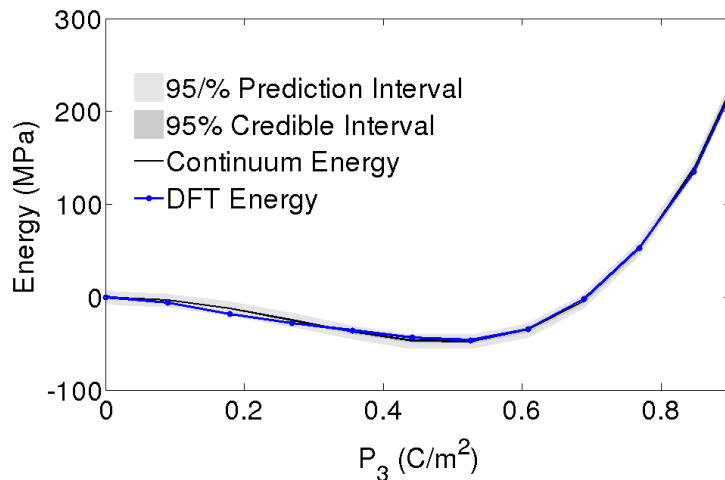
- Is 6<sup>th</sup> order term required to accurately characterize material behavior?
- Note:** Determines molecular structure

# Quantum-Informed Continuum Models

## Objectives:

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

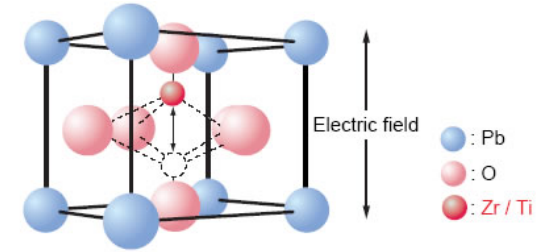
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$



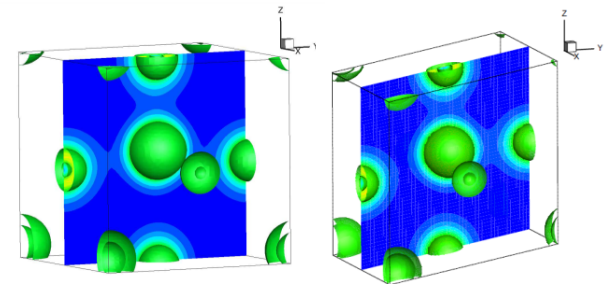
Helmholtz Energy

## UQ and SA Issues:

- Is 6<sup>th</sup> order term required to accurately characterize material behavior?
- **Note:** Determines molecular structure



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation

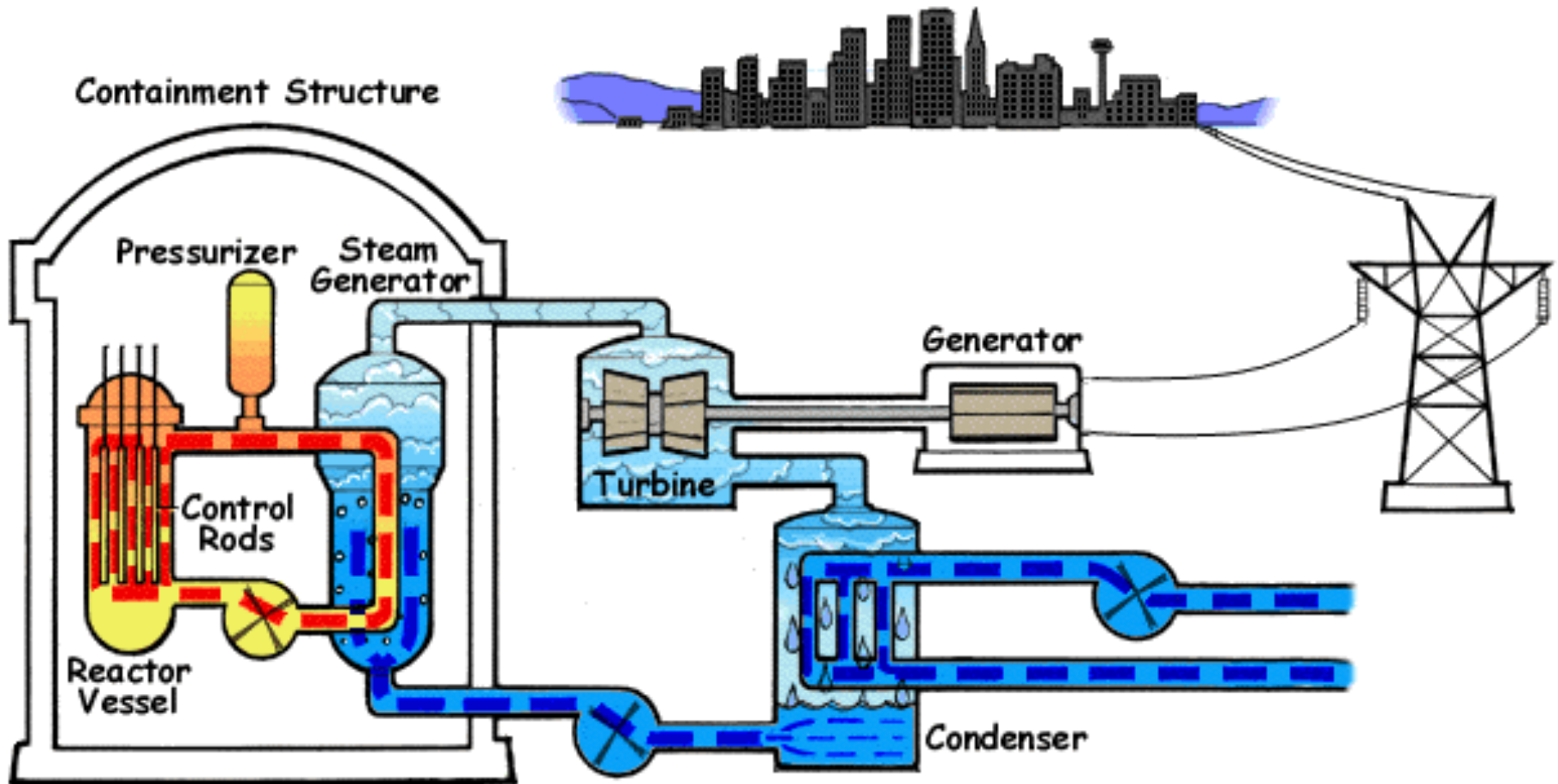
## Broad Objective:

- Use UQ/SA to help bridge scales from quantum to system

## Note:

- Linearly parameterized

## Example 2: Pressurized Water Reactors (PWR)



### Models:

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

**CRUD Measurements:** Consist of low resolution images at limited number of locations.

# Pressurized Water Reactors (PWR)

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

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

$$\begin{aligned} \alpha_f \rho_f \frac{\partial \mathbf{v}_f}{\partial t} + \alpha_f \rho_f \mathbf{v}_f \cdot \nabla \mathbf{v}_f + \nabla \cdot \sigma_f^R + \alpha_f \nabla \cdot \sigma + \alpha_f \nabla p_f \\ = -F^R - F + \Gamma(\mathbf{v}_f - \mathbf{v}_g)/2 + \alpha_f \rho_f \mathbf{g} \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_f \rho_f e_f) + \nabla \cdot (\alpha_f \rho_f \mathbf{e}_f \mathbf{v}_f + T \mathbf{h}) &= (T_g - T_f)H + T_f \Delta_f \\ -T_g(H - \alpha_g \nabla \cdot \mathbf{h}) + \mathbf{h} \cdot \nabla T - \Gamma[\mathbf{e}_f + T_f(\mathbf{s}^* - \mathbf{s}_f)] \\ -\rho_f \left( \frac{\partial \alpha_f}{\partial t} + \nabla \cdot (\alpha_f \mathbf{v}_f) + \frac{\Gamma}{\rho_f} \right) \end{aligned}$$

## Notes:

- Similar relations for gas and bubbly phases
- Surrogate models must conserve mass, energy, and momentum
- Many parameters are spatially varying and represented by random fields

## 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.
- Inference of random fields requires high- (infinite-) dimensional theory.

# Representation of Random Inputs

**Example 1:** Consider the Helmholtz energy

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

with frequency-dependent random parameters

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

**Challenge 1:** Difficult to work with probabilities associated with random events  $\omega \in \Omega$ .

**Solution:** Every realization  $\omega \in \Omega$  yields a value  $q \in Q \subset \Gamma$ . Work in image of probability space  $(\Gamma, \mathcal{B}(\Gamma), \rho(q))$  instead of  $(\Omega, \mathcal{F}, P)$ .

**Challenge 2:** How do we represent random fields; e.g.,  $\alpha_1(f, \omega)$  – that are infinite-dimensional?

**Solution:** Develop a representation and approximation framework

# Example and Motivation

## Example 2: Heat equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \alpha(x, \omega) \frac{\partial T}{\partial x} \right) + f(t, x) \quad , \quad -1 < x < 1, t > 0$$

$$T(t, -1, \omega) = T_\ell(\omega) \quad , \quad T(t, 1, \omega) = T_r(\omega) \quad t > 0$$

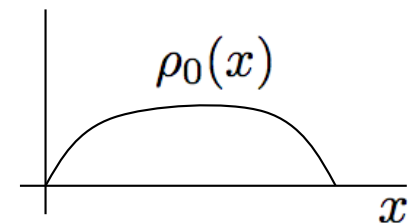
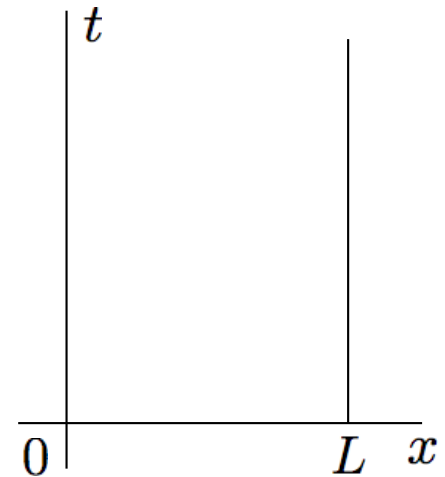
$$T(0, x, \omega) = T_0(\omega) \quad -1 < x < 1$$

## Motivation: Consider

$$\frac{\partial \rho}{\partial t} = \alpha \frac{\partial^2 \rho}{\partial x^2} \quad , \quad 0 < x < L, t > 0$$

$$\rho(t, 0) = \rho(t, L) = 0 \quad t > 0$$

$$T(0, x) = \rho_0(x) \quad 0 < x < L$$



# Example and Motivation

**Motivation:** Consider

$$\frac{\partial \rho}{\partial t} = \alpha \frac{\partial^2 \rho}{\partial x^2} \quad , \quad 0 < x < L, \quad t > 0$$

$$\rho(t, 0) = \rho(t, L) = 0 \quad t > 0$$

$$T(0, x) = \rho_0(x) \quad 0 < x < L$$

**Separation of Variables:** Take

$$\rho(t, x) = T(t)X(x)$$

$$\Rightarrow X(x)\dot{T}(t) = \alpha X''(x)T(t)$$

$$\Rightarrow \frac{X''(x)}{X(x)} = \frac{\dot{T}(t)}{\alpha T(t)} = C$$

Then

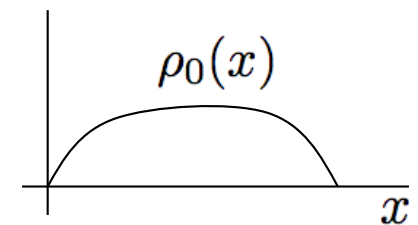
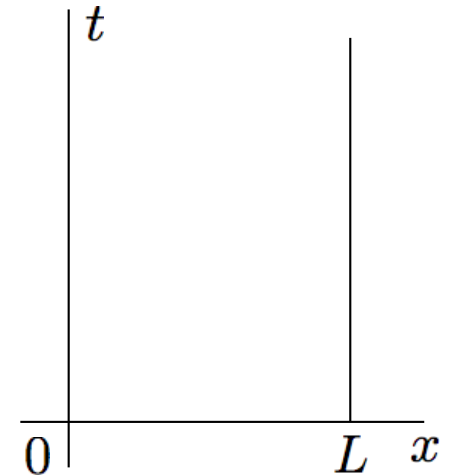
$$X''(x) - cX(x) = 0$$

$$X(0) = X(L) = 0$$

and

$$\dot{T}(t) = c\alpha T(t)$$

$$\Rightarrow T(t) = \beta e^{c\alpha t}$$



**Note:** Heat decays – Mathematical argument

$$\int_0^L [XX'' - cX^2] dx = - \int_0^L [(X')^2 + cX^2] dx = 0$$

If  $c \geq 0$ , this implies that  $X(x) = k = 0$ .

Thus  $c < 0$  so we take  $c = -\lambda^2$  where  $\lambda > 0$ .

# Motivation

## Boundary Value Problem:

$$X''(x) - cX(x) = 0$$

$$X(0) = X(L) = 0$$

$$\text{Solution: } X(x) = A \cos(\lambda x) + B \sin(\lambda x)$$

$$X(0) = 0 \Rightarrow A = 0$$

$$X(L) = 0 \Rightarrow \lambda L = n\pi$$

Thus

$$X_n(x) = B_n \sin(\lambda_n x), \quad \lambda_n = \frac{n\pi}{L}, \quad B_n \neq 0$$

## General Solution:

$$\rho(t, x) = \sum_{n=1}^{\infty} B_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x)$$

$$\text{Initial Condition: } \rho_0(x) = \rho(0, x) = \sum_{n=1}^{\infty} B_n \sin(\lambda_n x)$$

$$\Rightarrow \int_0^L \rho_0(x) \sin(\lambda_m x) dx = \int_0^L \sum_{n=1}^{\infty} B_n \sin(\lambda_n x) \sin(\lambda_m x) dx$$

$$\Rightarrow B_n = \frac{2}{L} \int_0^L \rho_0(x) \sin(\lambda_n x) dx$$



# Motivation

## Boundary Value Problem:

$$X''(x) - cX(x) = 0$$

$$X(0) = X(L) = 0$$

## General Solution:

$$\rho(t, x) = \sum_{n=1}^{\infty} B_n e^{-\alpha \lambda_n^2 t} \sin(\lambda_n x)$$

## Initial Condition:

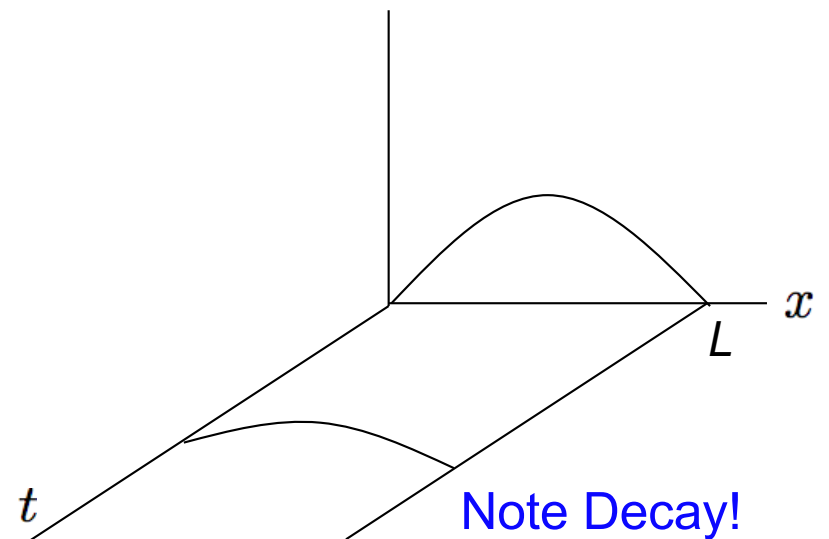
$$B_n = \frac{2}{L} \int_0^L \rho_0(x) \sin(\lambda_n x) dx$$

**Example:**  $\rho_0(x) = \sin\left(\frac{\pi x}{L}\right)$

$$B_n = \frac{2}{L} \int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx$$
$$= \begin{cases} \frac{2}{L} \cdot \frac{L}{2} & , \quad n = 1 \\ 0 & , \quad n \neq 1 \end{cases}$$

## General Solution:

$$\rho(t, x) = e^{-\alpha(\pi/L)^2 t} \sin(\pi x/L)$$



# Random Field Representation

**Random Fields: Strategy** – Represent random field  $\alpha(x, \omega)$  in terms of mean function  $\bar{\alpha}(x)$  and covariance function  $c(x, y)$

**Finite-Dimensional:**  $X \sim MVN(\mu, V)$  ,  $X = [X_1, \dots, X_p]$

$$V = \begin{bmatrix} \text{var}(X_1) & \text{cov}(X_1, X_2) & \cdots & \\ \text{cov}(X_2, X_1) & \text{var}(X_2) & & \\ \vdots & & & \vdots \\ & & & \text{var}(X_p) \end{bmatrix}$$

**Note:** Infinite-dimensional for functions

**Examples:** Short versus long-range interactions

1.  $c(x, y) = \sigma^2 e^{-|x-y|/L}$

**Note:**  $\sigma$  normalizes

$$\mathcal{D} = [-1, 1]$$

Limiting Behavior:

(i)  $L \rightarrow \infty \Rightarrow c(x, y) = 1$  Fully correlated so cannot truncated

(ii)  $L \rightarrow 0 \Rightarrow c(x, y) = \delta(x - y)$  Uncorrelated so easy to truncate

# Random Field Representation

## Examples:

2.  $c(x, y) = \min(x, y)$

1-D Wiener Process

- Used to model Brownian motion
- Can solve eigenvalue problem explicitly

3.  $c(x, y) = \sigma^2 e^{-(x-y)^2/2L^2}$

Gaussian

**MATLAB:** covariance\_exp.m, covariance\_min.m, covariance\_Gaussian.m

## Properties of $c(x, y)$ :

1. Finite-dimensional: e.g.,  $C = V$  symmetric and positive definite

$$C = \Phi \Lambda \Phi^{-1} = \Phi \Lambda \Phi^T$$

$$= \begin{bmatrix} \phi^1 & \dots & \phi^p \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_p \end{bmatrix} \begin{bmatrix} \phi^1 \\ \vdots \\ \phi^p \end{bmatrix}$$

$$= [\lambda_1 \phi^1, \dots, \lambda_p \phi^p] \begin{bmatrix} \phi^1 \\ \vdots \\ \phi^p \end{bmatrix} = \sum_{n=1}^p \lambda_n \phi^n (\phi^n)^T$$

# Random Field Representation

**Mercer's Theorem:** (Infinite Dimensional) – If  $c(x,y)$  is symmetric and positive definite, it can be expressed as

$$c(x, y) = \sum_{n=1}^{\infty} \lambda_n \phi_n(x) \phi_n(y)$$

where

$$\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}$$

and

$$\int_{\mathcal{D}} \phi_n(x) \phi_m(x) dx = \delta_{mn} \quad \textbf{Note:} \text{ Eigenfunctions are orthonormal}$$

**Karhunen-Loeve Expansion:**

$$\alpha(x, \omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)$$

# Random Field Representation

## Karhunen-Loeve Expansion:

$$\alpha(x, \omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)$$

## Statistical Properties: Take

$$\alpha(x, \omega) = \bar{\alpha}(x) + \beta(x, \omega)$$

where  $\beta(x, \omega)$  has zero mean and covariance function  $c(x, y)$ . Take

$$\beta(x, \omega) = \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)$$

$$\Rightarrow \beta(x, \omega) \beta(y, \omega) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} Q_n(\omega) Q_m(\omega) \sqrt{\lambda_n \lambda_m} \phi_n(x) \phi_m(y)$$

**Recall:** For random variables  $X, Y$

$$\text{cov}(X, Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$$

**Notation:**  $\mathbb{E}[Y] = \langle Y \rangle = \int y \rho(y) dy$

# Random Field Representation

**Statistical Properties:** Because  $\beta(x, \omega)$  has zero mean,

$$\begin{aligned}c(x, y) &= \mathbb{E}[\beta(x, \omega)\beta(y, \omega)] \\ &= \langle \beta(x, \omega)\beta(y, \omega) \rangle \\ &= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \langle Q_n(\omega)Q_m(\omega) \rangle \sqrt{\lambda_n\lambda_m}\phi_n(x)\phi_m(y)\end{aligned}$$

Since eigenfunctions are orthogonal,

$$\begin{aligned}\lambda_k\phi_k(x) &= \int_{\mathcal{D}} c(x, y)\phi_k(y)dy \\ &= \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega) \rangle \sqrt{\lambda_n\lambda_k}\phi_n(x)\end{aligned}$$

Multiplication by  $\phi_\ell(x)$  and integration yields

$$\begin{aligned}\lambda_k \int_{\mathcal{D}} \phi_k(x)\phi_\ell(x)dx &= \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega) \rangle \sqrt{\lambda_n\lambda_k}\delta_{n\ell} \\ \Rightarrow \lambda_k\delta_{k\ell} &= \sqrt{\lambda_k\lambda_\ell} \langle Q_k(\omega)Q_\ell(\omega) \rangle\end{aligned}$$

**Note:**

$$\begin{aligned}k = \ell &\Rightarrow \langle Q_k(\omega)Q_\ell(\omega) \rangle = 1 \\ k \neq \ell &\Rightarrow \langle Q_k(\omega)Q_\ell(\omega) \rangle = 0 \\ \Rightarrow \langle Q_k(\omega)Q_\ell(\omega) \rangle &= \delta_{k\ell}\end{aligned}$$

# Random Field Representation

## Karhunen-Loeve Expansion:

$$\alpha(x, \omega) = \bar{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)$$

where

$$\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}$$

**Result:** The random variables satisfy

- (i)  $\mathbb{E}[Q_n] = 0$                       Zero mean
- (ii)  $\mathbb{E}[Q_n Q_m] = \delta_{mn}$         Mutually orthogonal and uncorrelated

**Question:** How do we choose  $c(x,y)$  and compute solutions to

$$\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D}$$

# Common Choices for $c(x,y)$

## 1. Radial Basis Function:

$$c(x, y) = e^{-|x-y|/L} \quad , \quad \mathcal{D} = [-1, 1]$$

**Note:**  $L$  is correlation length, which quantifies smoothness or relation between values of  $x$  and  $y$ .

so

$$\int_{-1}^1 e^{-|x-y|/L} \phi_n(y) dy = \lambda_n \phi_n(x)$$

Analytic Solution:

$$\lambda_n = \begin{cases} \frac{2L}{1+L^2 w_n^2} & , \quad \text{if } n \text{ is even,} \\ \frac{2L}{1+L^2 v_n^2} & , \quad \text{if } n \text{ is odd,} \end{cases}$$

$$\phi_n(x) = \begin{cases} \frac{\sin(w_n x)}{\sqrt{1 - \frac{\sin(2w_n)}{2w_n}}} & , \quad \text{if } n \text{ is even,} \\ \frac{\cos(v_n x)}{\sqrt{1 + \frac{\sin(2v_n)}{2v_n}}} & , \quad \text{if } n \text{ is odd} \end{cases}$$

**Note:**  $w_n$  and  $v_n$  are the solutions of the transcendental equations

$$Lw + \tan(w) = 0 \quad , \quad \text{for even } n,$$

$$1 - Lv \tan(v) = 0 \quad , \quad \text{for odd } n$$



# Common Choices for $c(x,y)$

## 1. Radial Basis Function:

$$c(x, y) = e^{-|x-y|/L}, \quad \mathcal{D} = [-1, 1]$$

**Note:**  $L$  is correlation length

so

$$\int_{-1}^1 e^{-|x-y|/L} \phi_n(y) dy = \lambda_n \phi_n(x)$$

Limiting Cases:

(i)  $c(x, y) = 1$  Fully correlated ( $L \rightarrow \infty$ )

(ii)  $c(x, y) = \delta(x - y)$  Uncorrelated ( $L \rightarrow 0$ )

$$\int_{\mathcal{D}} \phi_n(y) dy = \lambda_n \phi_n(x) = k_n$$

Then

$$\phi_n(x) = \lambda_n \phi_n(x)$$

$$\Rightarrow \lambda_n = 1 \quad \text{for all } n$$

Recall:  $c(x, y) = 1 = \sum_{n=1}^{\infty} \lambda_n \phi_n(x) \phi_n(y)$

Take

$$\phi_1(x) = \phi_1(y) = \frac{\sqrt{2}}{2}$$

$$\lambda_1 = 2$$

$$\lambda_n = 0 \text{ for } n = 2, 3, \dots$$

**Note:** Because uncorrelated, we cannot truncate series!

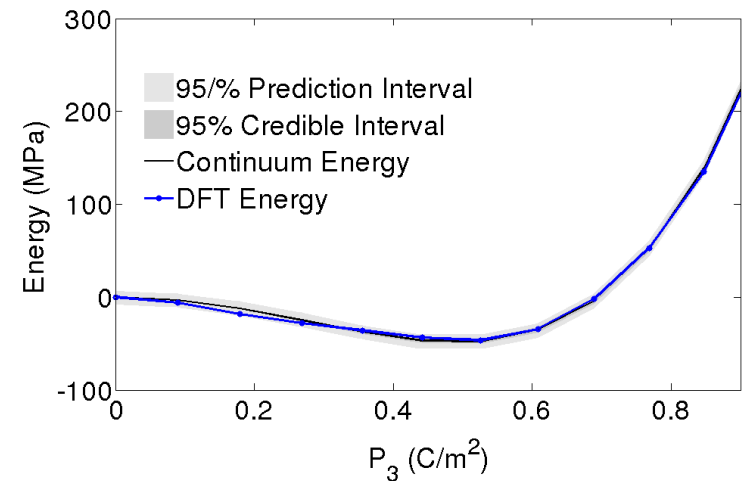
# Construction of $c(x,y)$

**Question:** If we know underlying distribution  $\omega \in \Omega$ , can we approximate the covariance function  $c(x,y)$ ? Yes ... via sampling!

**Example:** Consider the Helmholtz energy

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

and take  $x = P$  for  $x = P \in [0, 1]$



**Note:** Assume we can evaluate  $\alpha(x_j, \omega^k)$  for various polarizations  $x_j = P_j$  and values  $\omega^k$  from the underlying distribution

**Required Steps:**

- Approximation of the covariance function  $c(x,y)$
- Approximation of the eigenvalue problem

$$\int_{\mathcal{D}} c(x, y) \phi_n(y) dy = \lambda_n \phi_n(x) \text{ for } x \in \mathcal{D} \quad \text{with} \quad \int_{\mathcal{D}} \phi_n(x) \phi_m(x) dx = \delta_{mn}$$

# Construction of $c(x,y)$

## Step 1: Approximation of covariance function $c(x,y)$

For  $N_{MC}$  Monte Carlo samples  $\omega^k$ , covariance function approximated by

$$c(x, y) \approx c^{N_{MC}}(x, y) = \frac{1}{N_{MC} - 1} \sum_{k=1}^{N_{MC}} \alpha_c(x, \omega^k) \alpha_c(y, \omega^k)$$

where the centered field is

$$\alpha_c(x, \omega^k) = \alpha(x, \omega^k) - \bar{\alpha}(x)$$

and the mean is

$$\bar{\alpha}(x) \approx \frac{1}{N_{MC}} \sum_{j=1}^{N_{MC}} \alpha(x, \omega^j)$$

# Construction of $c(x,y)$

**Step 2 (Nystrom's Method):** Approximate eigenvalue problem

$$\int_{\mathcal{D}} c(x,y)\phi_n(y)dy = \lambda_n\phi_n(x) \text{ for } x \in \mathcal{D} \text{ with } \int_{\mathcal{D}} \phi_n(x)\phi_m(x)dx = \delta_{mn}$$

Consider composite quadrature rule with  $N_{quad}$  points and weights  $\{(x_j, w_j)\}$ .

Discretized Eigenvalue Problem:

$$\sum_{j=1}^{N_{quad}} c(x_i, x_j)\phi_n(x_j)w_j = \lambda_n\phi_n(x_i), \quad i = 1, \dots, N_{quad}$$

Matrix Eigenvalue Problem:

$$CW\phi_n = \lambda_n\phi_n$$

where

$$\phi_n^i = \phi_n(x_i)$$

$$C_{ij} = c(x_i, x_j)$$

$$W = \text{diag}(w_1, \dots, w_{N_{quad}})$$

Symmetric Matrix Eigenvalue Problem:

$$W^{1/2}CW^{1/2}\tilde{\phi}_n = \lambda_n\tilde{\phi}_n$$

where

$$\tilde{\phi}_n = W^{1/2}\phi_n \Rightarrow \phi_n = W^{-1/2}\tilde{\phi}_n$$

$$\tilde{\phi}_n^T\tilde{\phi}_n = 1 \Rightarrow \phi_n^T W\phi_n = 1$$

$$W^{1/2} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_{N_{quad}}})$$

# Algorithm to Approximate $c(x,y)$

## Inputs:

- (i) Quadrature formula with nodes and weights  $\{(x_j, w_j)\}$
- (ii) Functions evaluations  $\{\alpha(x_j, \omega^k)\}$ ,  $j = 1, \dots, N_{quad}$ ,  $k = 1, \dots, N_{MC}$

## Output: Eigenvalues, eigenvectors and KL modes

(1) Center the process

$$\alpha_c(x_i, \omega^k) = \alpha(x_i, \omega^k) - \frac{1}{N_{MC}} \sum_{j=1}^{N_{MC}} \alpha(x_i, \omega^j)$$

for  $i = 1, \dots, N_{quad}$  and  $k = 1, \dots, N_{MC}$ .

2) Form covariance matrix  $C = [C_{ij}]$  that discretizes covariance function  $c(x, y)$

$$C_{ij} = \frac{1}{N_{MC} - 1} \sum_{k=1}^{N_{MC}} \alpha_c(x_i, \omega^k) \alpha_c(x_j, \omega^k)$$

for  $i, j = 1, \dots, N_{quad}$ .

# Algorithm to Approximate $c(x,y)$

**Output:** Eigenvalues, eigenvectors and KL modes

(3) Let  $W = \text{diag}(w_1, \dots, w_{N_{quad}})$  and solve

$$W^{1/2} C W^{1/2} \tilde{\phi}_n = \lambda_n \tilde{\phi}_n$$

for  $n = 1, \dots, N_{quad}$ .

(4) Compute the eigenvectors  $\phi_n = W^{-1/2} \tilde{\phi}_n$ .

(5) Exploit the decay in the eigenvalues  $\lambda_n$  to choose a KL truncation level  $N_{KL}$  and compute discretized KL modes  $Q_n(\omega)$ . Consider

$$\begin{aligned} \alpha(x, \omega) &\approx \bar{\alpha}(x) + \sum_{n=1}^{N_{KL}} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega) \\ \Rightarrow \alpha_c(x, \omega) &\approx \sum_{n=1}^{N_{KL}} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega) \\ \Rightarrow Q_n(\omega) &= \frac{1}{\sqrt{\lambda_n}} \int_{\mathcal{D}} \alpha_c(x, \omega) \phi_n(x) dx \\ &\approx \frac{1}{\sqrt{\lambda_n}} \sum_{j=1}^{N_{quad}} w_j \alpha_c(x_j, \omega) \phi_n^j. \end{aligned} \tag{1}$$

# Algorithm to Approximate $c(x,y)$

**Output:** Eigenvalues, eigenvectors and KL modes

(6) Sample  $\omega^k$  and construct surrogate  $\tilde{Q}_n(\omega^k)$ ; e.g., polynomial, spectral polynomial, Gaussian process.

**Example:** Consider the Helmholtz energy

$$\alpha(x, \omega) = \alpha_1(\omega)x^2 + \alpha_{11}x^4 + \alpha_{111}x^6$$

for  $x \in [0, 1]$

Mean Values: Based on DFT

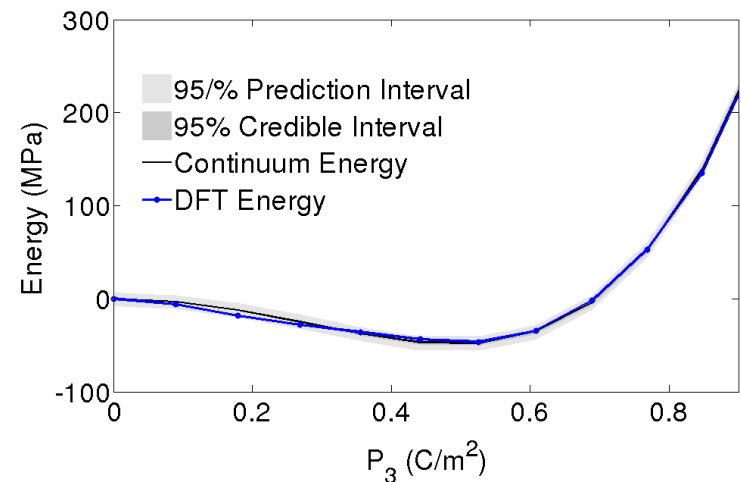
$$\bar{\alpha}_1 = -389.4, \quad \bar{\alpha}_{11} = 761.3, \quad \bar{\alpha}_{111} = 61.5.$$

Distribution:

$$\alpha = [\alpha_1, \alpha_{11}, \alpha_{111}] \sim \mathcal{U}([\alpha_{1l}, \alpha_{1r}] \times [\alpha_{2l}, \alpha_{2r}] \times [\alpha_{3l}, \alpha_{3r}])$$

where  $\alpha_{1l} = \bar{\alpha}_1 - 0.2\bar{\alpha}_1$ ,  $\alpha_{1r} = \bar{\alpha}_1 + 0.2\bar{\alpha}_1$  with similar intervals for  $\alpha_{11}$  and  $\alpha_{111}$

Eigenvalues:  $\lambda_1 = 417.88$ ,  $\lambda_2 = 1.2$  and  $\lambda_3 = 0.009$  so truncate series at  $N_{KL} = 3$



**MATLAB:** covariance\_construct.m

# Example and Motivation

## Example 2: Heat equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \alpha(x, \omega) \frac{\partial T}{\partial x} \right) + f(t, x) \quad , \quad -1 < x < 1, t > 0$$

$$T(t, -1, \omega) = T_\ell(\omega) \quad , \quad T(t, 1, \omega) = T_r(\omega) \quad t > 0$$

$$T(0, x, \omega) = T_0(\omega) \quad -1 < x < 1$$

## Note: Well-posedness requires

$$0 < \alpha_{\min} \leq \alpha(x, \omega) \leq \alpha_{\max}$$

Take

$$\alpha(x, \omega) = \alpha_{\min} + e^{\tilde{\alpha}(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} \phi_n(x) Q_n(\omega)}$$

**Parameters:**  $Q = [T_\ell, T_R, T_0, Q_1, \dots, Q_N]$



# Example

**Example 3:** Pressure distribution for single-phase flow

$$-\nabla \cdot (\kappa \nabla p) = b \quad , \quad \text{in } \mathcal{D} \quad \mathcal{D} = (-1, 1) \times (0, 1)$$

$$p = 0 \quad , \quad \text{on } \Gamma_D$$

$$\kappa \nabla p \cdot \hat{n} = 0 \quad , \quad \text{on } \Gamma_T,$$

**Note:** Random permeability fields

$$\log \kappa(x, \omega) = \alpha(x, \omega) = \bar{\alpha} + \sigma^2 z(x, \omega)$$

Take

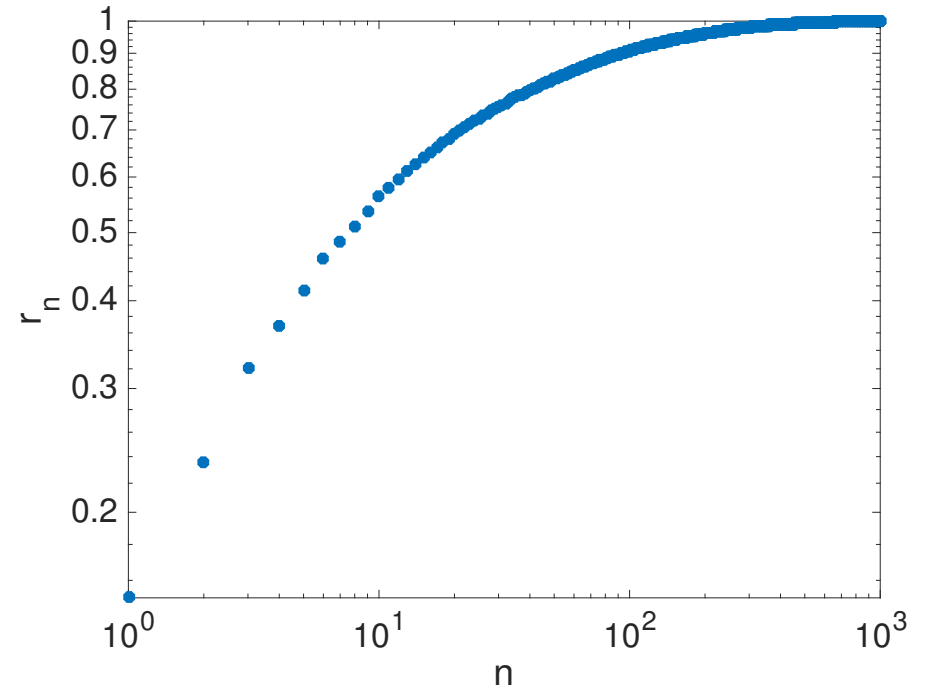
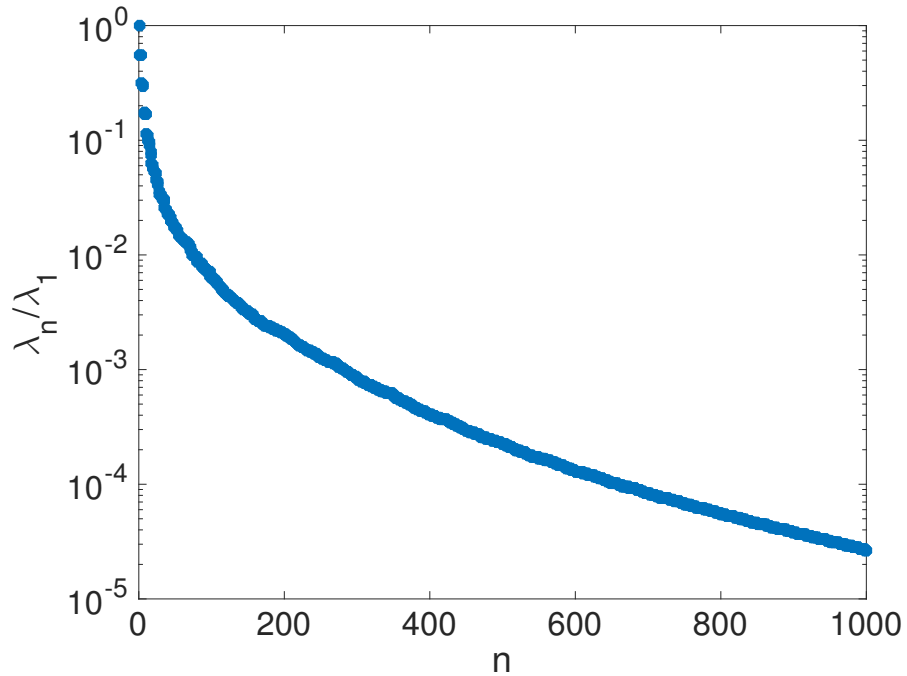
$$c_z(x, \omega) = \exp \left( -\frac{|x_1 - y_1|}{L_x} - \frac{|x_2 - y_2|}{L_y} \right) , \quad x, y \in \mathcal{D}$$

with

$$L_x = \frac{1}{2} , \quad L_y = \frac{1}{4}$$

# Example

**Results:** Normalized eigenvalues and ratios  $r_N = \frac{\sum_{n=1}^N \lambda_n}{\sum_{n=1}^{\infty} \lambda_n}$



**Note:**  $r_N > 0.9$  for  $N = 129$

# Example

**Results:** Two realizations of the permeability field

