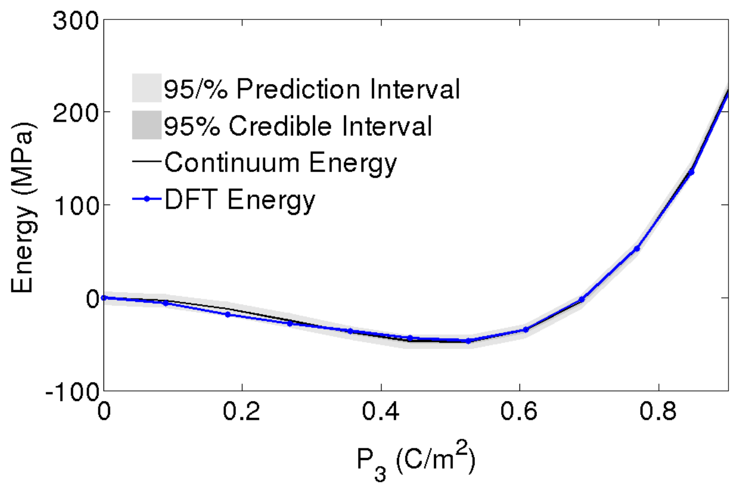
Lecture 5: Statistical Representation of Model Inputs

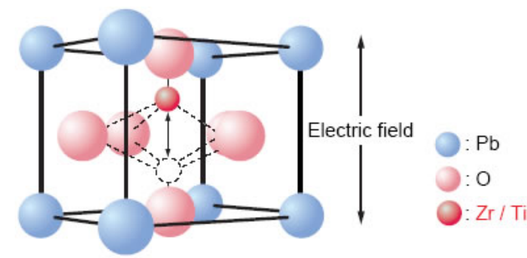
Example:

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

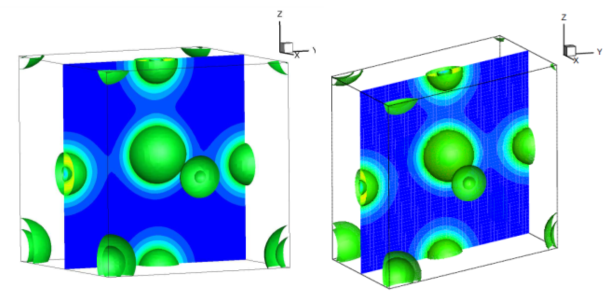
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$



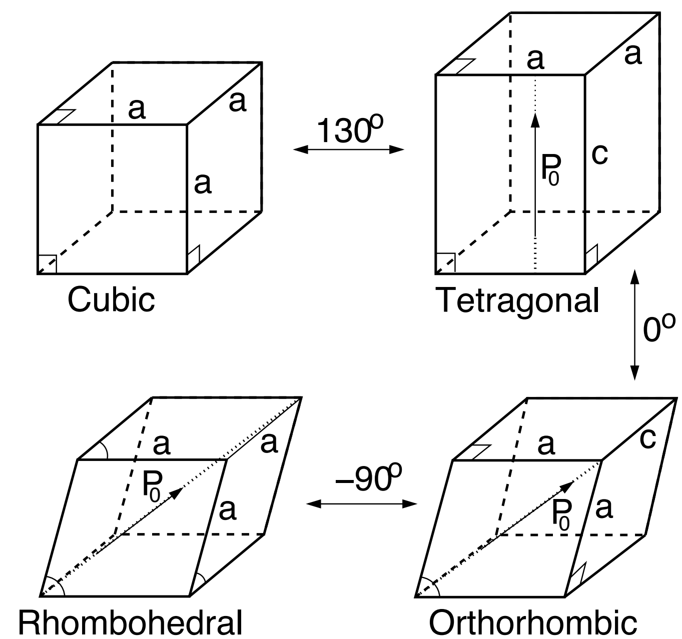
Helmholtz Energy



Lead Titanate Zirconate (PZT)



DFT Electronic Structure Simulation



UQ and SA Issues:

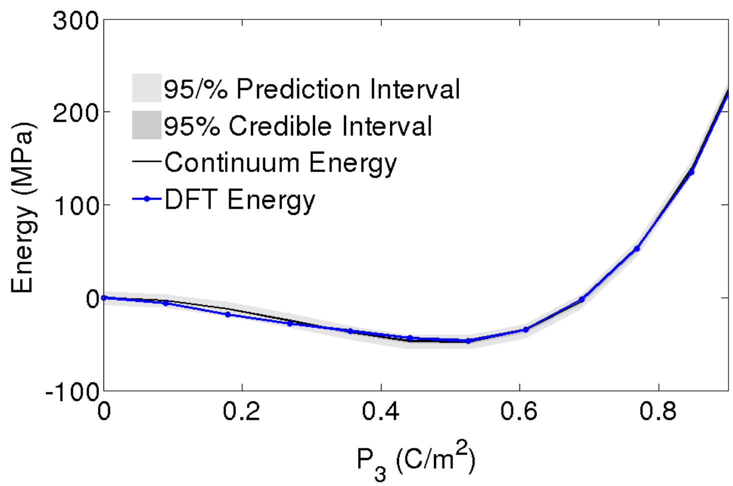
- Is 6th order term required to accurately characterize material behavior?
- **Note:** Determines molecular structure

Quantum-Informed Continuum Models

Objectives:

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

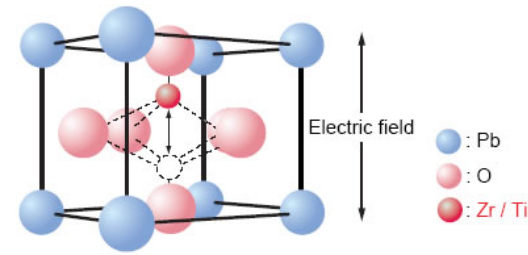
$$\psi(P) = \alpha_1 P^2 + \alpha_{11} P^4 + \alpha_{111} P^6$$



Helmholtz Energy

UQ and SA Issues:

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



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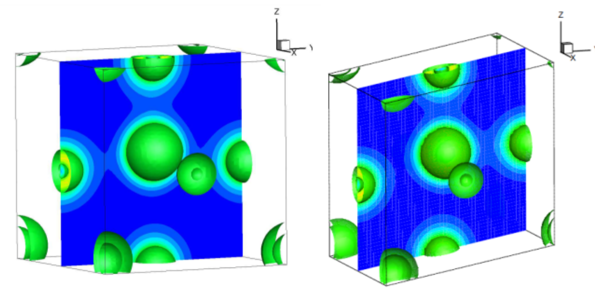


DFT Electronic Structure Simulation

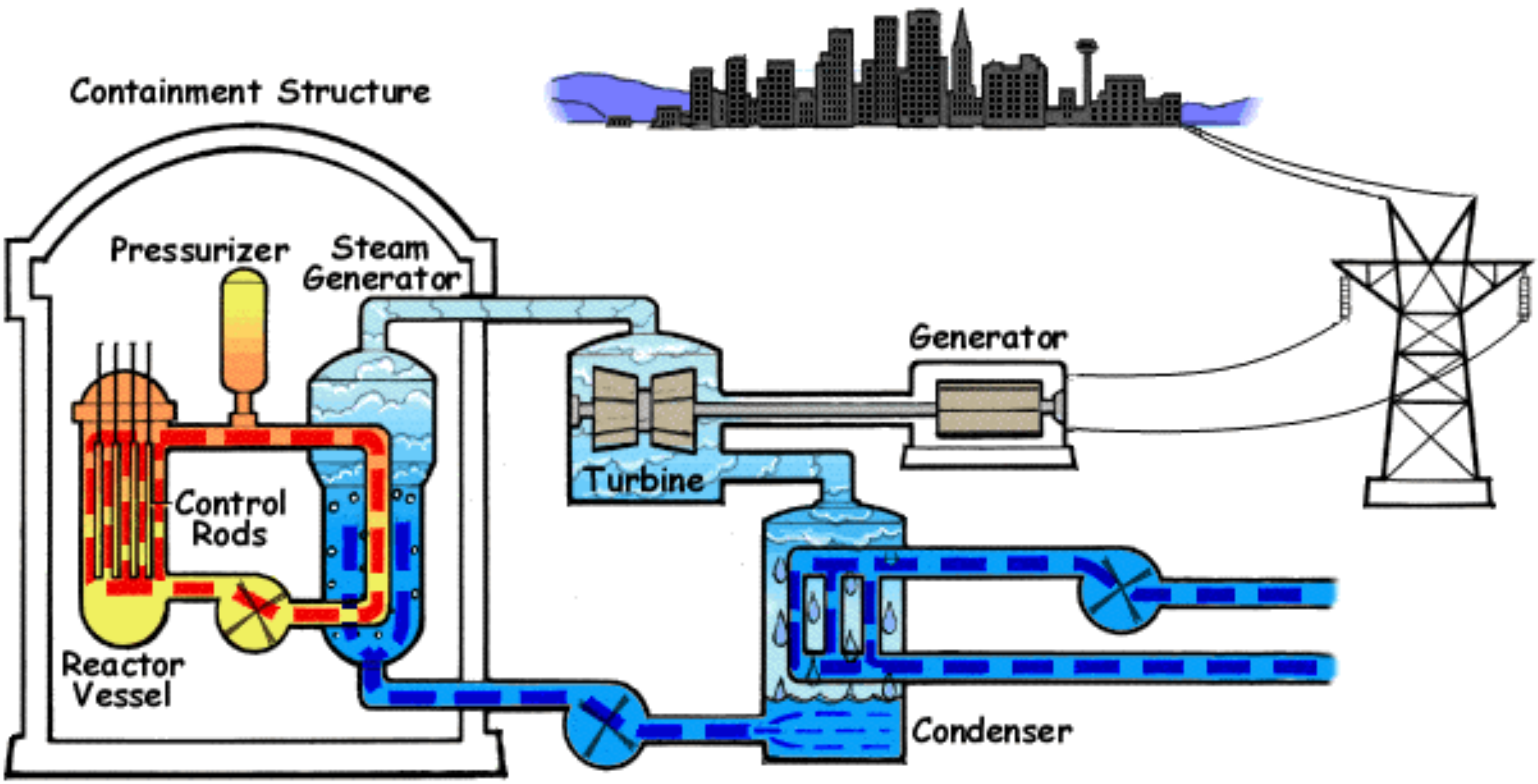
Broad Objective:

- 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

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

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

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

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

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

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

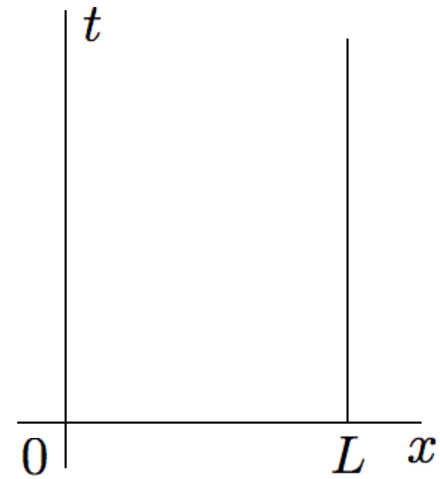
$$T(0,x,\omega) = T_0(\omega) \quad -1 < x < 1$$

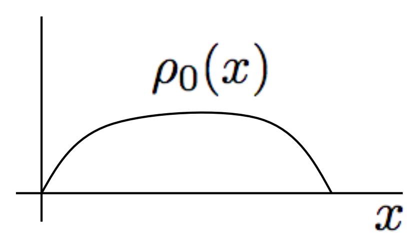
Motivation: Consider

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

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

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





Example and Motivation

Motivation: Consider

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

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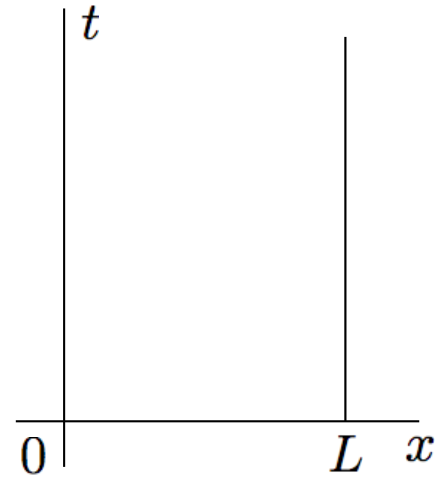
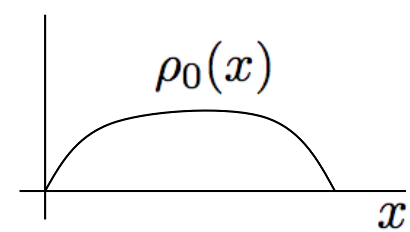


Separation of Variables: Take

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

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

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



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

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

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

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

Motivation

Boundary Value Problem:

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

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

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

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

General Solution:

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

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:

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

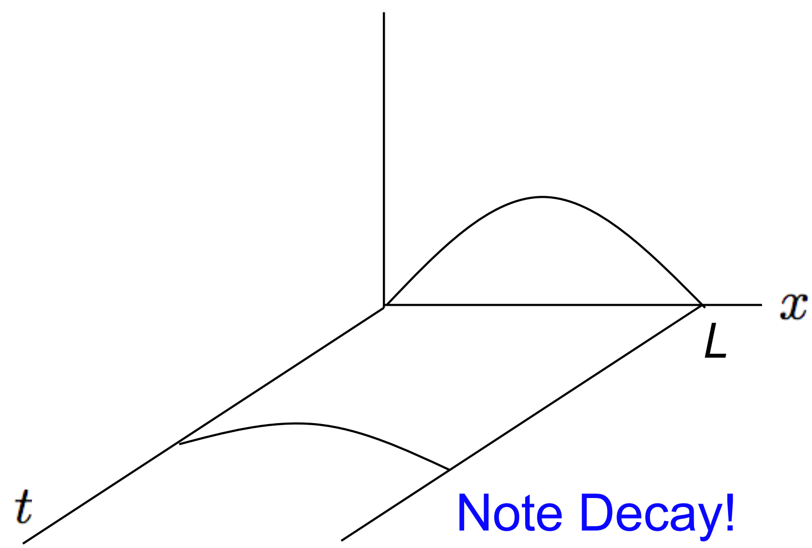
Example: $\rho_0(x) = \sin\left(\frac{\pi x}{L}\right)$

$$B_n = \frac{2}{L}\int_0^L \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx$$

$$= \begin{cases} \frac{2}{L}\cdot\frac{L}{2} & , \quad n = 1 \\ 0 & , \quad n \neq 1 \end{cases}$$

General Solution:

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



Note Decay!

Random Field Representation

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

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

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

Note: Infinite-dimensional for functions

Examples: Short versus long-range interactions

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

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

   Limiting Behavior:

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

   (ii) $L \to 0 \Rightarrow c(x,y) = \delta(x-y)$ 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

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

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

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

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

$$\int_{\mathcal{D}} \phi_n(x)\phi_m(x)dx = \delta_{mn}$$

Note: 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

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

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

$$\lambda_k \int_{\mathcal{D}} \phi_k(x)\phi_\ell(x)dx = \sum_{n=1}^{\infty} \langle Q_n(\omega)Q_k(\omega)\rangle \sqrt{\lambda_n\lambda_k}\delta_{n\ell}$$

$$\Rightarrow \lambda_k\delta_{k\ell} = \sqrt{\lambda_k\lambda_\ell}\,\langle Q_k(\omega)Q_\ell(\omega)\rangle$$

Note:

$$k=\ell \quad\Rightarrow\quad \langle Q_k(\omega)Q_\ell(\omega)\rangle = 1$$

$$k\neq\ell \quad\Rightarrow\quad \langle Q_k(\omega)Q_\ell(\omega)\rangle = 0$$

$$\Rightarrow \langle Q_k(\omega)Q_\ell(\omega)\rangle = \delta_{k\ell}$$

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:

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

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

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:

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

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 $(L \to \infty)$

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

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

Take

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

$$\lambda_1 = 2$$

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

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

Then

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

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

Note: Because uncorrelated,
we cannot truncate series!

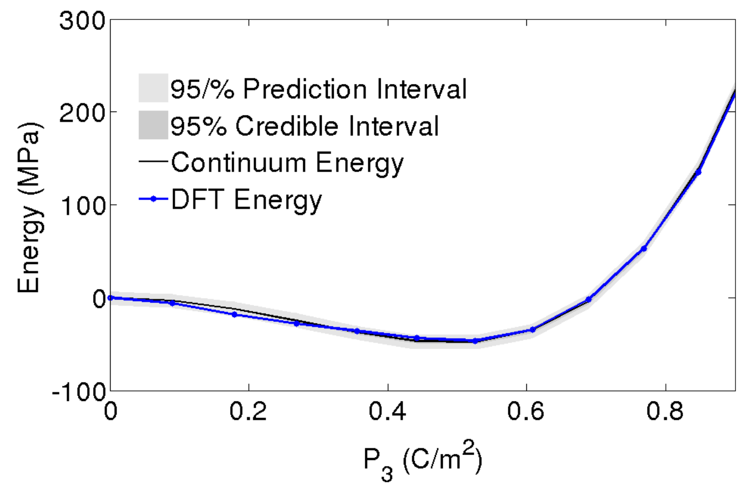
Construction of c(x,y)

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 ω^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 ω^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

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

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

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

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

Discretized Eigenvalue Problem:

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

Matrix Eigenvalue Problem:

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

where

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

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

$$W = \mathrm{diag}(w_1, \ldots, w_{N_{quad}})$$

Symmetric Matrix Eigenvalue Problem:

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

where

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

$$\widetilde{\phi}_n^T \widetilde{\phi}_n = 1 \Rightarrow \phi_n^T W \phi_1 = 1$$

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

Algorithm to Approximate c(x,y)

Inputs:

(i) Quadrature formula with nodes and weights $\{(x_j, w_j)\}$

(ii) Functions evaluations $\{\alpha(x_j, \omega^k)\}$, $j = 1, \ldots, N_{quad}$, $k = 1, \ldots, N_{Mc}$

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

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

Algorithm to Approximate c(x,y)

Output: Eigenvalues, eigenvectors and KL modes

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

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

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

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

(5) Exploit the decay in the eigenvalues λ_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)

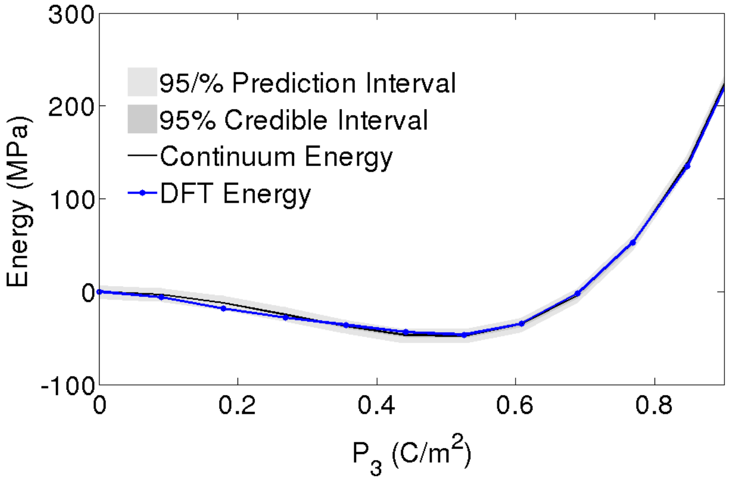
Output: Eigenvalues, eigenvectors and KL modes

(6) Sample ω^k and construct surrogate $\widetilde{Q}_n(\omega^k)$; 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

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

Distribution:

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

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

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

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

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

Note: Well-posedness requires

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

Take

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

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