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Radiation Transport in Random Media With Large Fluctuations

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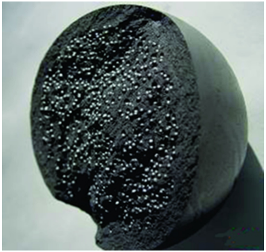
Two Types of Strongly Random Media

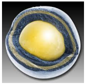
Spatially-continuous mixtures

- Random density/mixing
- Atmospheric radiative transfer
- BWR coolant

Spatially-discontinuous materials

- Random discrete material mixing
- Rayleigh-Taylor instabilities
- Porous materials





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The Random Transport Equation

- Steady-state, one-dimensional, mono-energetic, isotropically-scattering, neutral-particle, stochastic transport equation:

$$\begin{gathered} \mu \frac{\partial \psi(x,\mu,\omega)}{\partial x} + \Sigma_t(x,\omega)\psi(x,\mu,\omega) = \frac{\Sigma_s(x,\omega)}{2}\int_{-1}^{1} d\mu' \psi(x,\mu',\omega), \\ 0 \leq x \leq s; \qquad -1 \leq \mu \leq 1, \\ \psi(0,\mu,\omega) = \delta(1-\mu), \quad \mu > 0; \qquad \psi(s,\mu,\omega) = 0, \quad \mu < 0 \end{gathered} \tag{1}$$

- Quantities of interest (QoI) derived from $\psi(x,\mu,\omega)$
  - e.g., $\langle \phi^m(x) \rangle$, $\langle J^m(x) \rangle$, $P(J^m(x))$

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Random Transport Solution Approach

Spatial Solution Methods:

- MC - Monte Carlo transport
- WMC - MC with Woodcock sampling

Random Geometry Modeling:

- KL - Karhunen-Loève expansion
- lognormal, Nataf transformations

Stochastic Solution Methods:

- RS - Random Sampling
- SC - Stochastic Collocation (isotropic/anisotropic)
- PCE - Polynomial Chaos Expansion

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Spatial Solution Methods

- MC - traditional Monte Carlo particle simulation
- WMC - MC with Woodcock interaction rejection scheme:
  - Choose Σ_t^* equal to or greater than Σ_t for possible particle tracklength
  - Stream based on Σ_t^*
  - Accept or reject interaction based on $\frac{\Sigma_t^*}{\Sigma_t}$

Table: MC and WMC Mechanics

	Stream	Accept?	Scatter?
MC	$\frac{ln(\eta)}{\Sigma_t}$	N/A	$\frac{\Sigma_s}{\Sigma_t}$
WMC	$\frac{ln(\eta)}{\Sigma_t^*}$	$\frac{\Sigma_t^*}{\Sigma_t}$	$\frac{\Sigma_s}{\Sigma_t}$

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Random Geometry Modeling: KL Expansion

Karhunen-Loève (KL) expansion:

$$w(x,\omega) = \langle w \rangle + \sum_{k=1}^{\infty} \sqrt{\gamma_k}\phi_k(x)\xi_k(\omega) \tag{2}$$

- Discrete in random space: countably-infinite number of random variables
- Preserve second order statistics:
  - Mean $\langle w \rangle$
  - Variance v_w
  - Autocovariance $C_w(x, x')$
- Solve transport equation on realizations of KL expansion

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Random Geometry Modeling: Autocovariance

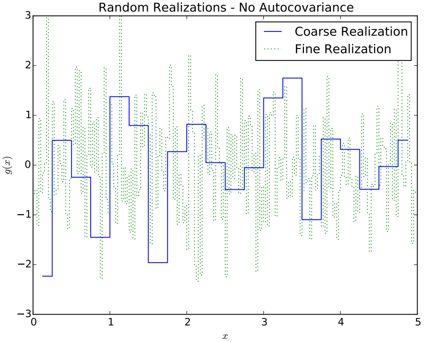

Figure: Two Realizations - Uncorrelated

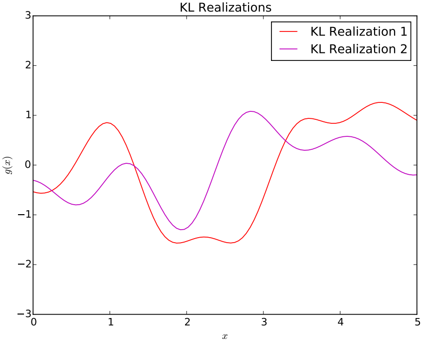

Figure: Two Realizations - Correlated

Numeric KL Eigenvalue and Eigenvector Solution

KL eigenspectrum and eigenvectors from Fredholm integral equation:

$$\int_{\Omega} C_w(x,x')\phi_k(x')dx' = \phi_k(x)\gamma_k \tag{3}$$

Nyström method for numerical solve:

$$\sum_{j=1}^{N} w_j C_w(x_k,x_j)\hat{\phi}_i(x_j) = \hat{\gamma}_i\hat{\phi}_i(x_k), \quad k = 1,\ldots,N \tag{4}$$

or

$$\mathbf{CWy}i = \gamma_i \mathbf{y}_i \quad \rightarrow \quad \mathbf{W}^{\frac{1}{2}}\mathbf{CW}^{\frac{1}{2}}\mathbf{y}_i^* = \hat{\gamma}_i\mathbf{y}_i^*, \quad \mathbf{y}_i = \mathbf{W}^{-\frac{1}{2}}\mathbf{y}_i^* \tag{5}$$

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Motivation for Lognormal Transformation: Positivity

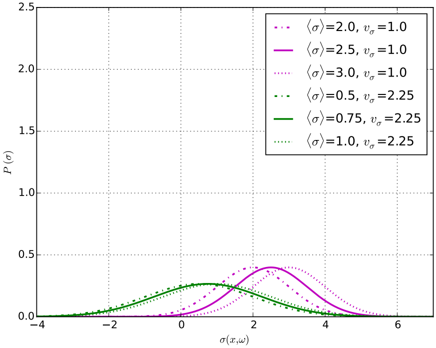

Figure: Gaussian Distributions - "High" and "Low" Variance

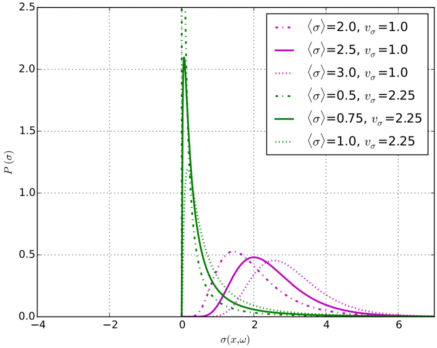

Figure: Lognormal Distributions - "High" and "Low" Variance

Lognormal Transformation

Lognormal Transformation Definition:

$$\Sigma(x,\omega) = exp\left[w(x,\omega)\right], \quad w(x,\omega) = \langle w \rangle + \sum_{k=1}^{K} \sqrt{\gamma_k}\phi_k(x)\xi_k(\omega) \tag{6}$$

Transformation of Second-order Information:

$$\langle w \rangle = \ln\left(\frac{\langle \Sigma \rangle^2}{\sqrt{v_\Sigma + \langle \Sigma \rangle^2}}\right); \quad v_w = \ln\left(\frac{v_\Sigma}{\langle \Sigma \rangle^2} + 1\right) \tag{7}$$

$$\rho_w(x,x') = \frac{\ln\left(\rho_\Sigma(x,x')\frac{v_\Sigma}{\langle \Sigma \rangle} + 1\right)}{\ln\left(\frac{v_\Sigma}{\langle \Sigma \rangle^2} + 1\right)}, \quad \rho_w = \frac{C_w}{v_w}, \rho_\Sigma = \frac{C_\Sigma}{v_\Sigma} \tag{8}$$

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Lognormal and Gaussian Cross Section Realizations

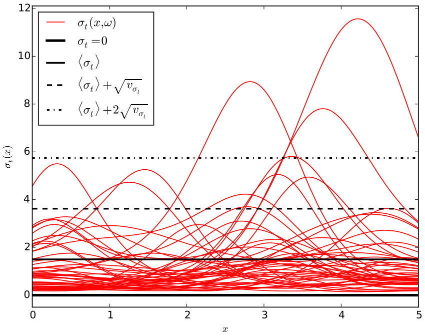

Figure: 50 Lognormal Realizations

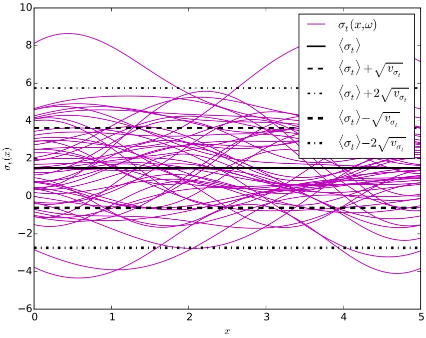

Figure: 50 Gaussian Realizations

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Lognormal Transformation Moment Preservation

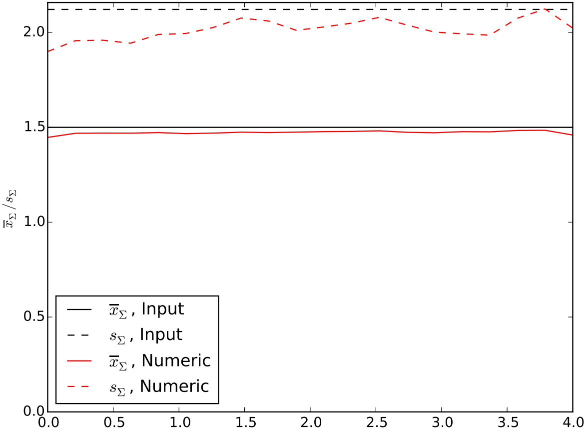

Figure: Observed Cross Section Moments

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Stochastic Solution Methods

Quantity of Interest (QoI) Solution Methods:

- Random Sampling (RS): Monte Carlo
  - QoI moments
  - QoI PDF
- Deterministic Sampling: Stochastic Collocation (SC)
  - QoI moments
- Surrogate Model: Polynomial Chaos Expansion (PCE)
  - QoI moments
  - QoI PDF
  - QoI surface

Solution of Response Moments

Response calculated:

$$\langle \phi^m \rangle = \int_{\xi_N} \cdots \int_{\xi_1} \phi^m(x, \xi_1, \ldots, \xi_N) P(\xi_1, \ldots, \xi_N) d\xi_1 \cdots \xi_N, \quad (9)$$

Probability density $P(\xi_1, \ldots, \xi_N)$ factors into a product of standard normals:

$$P(\xi_1, \ldots, \xi_N) = \prod_{n=1}^{N} P(\xi_n), \; \forall \, \xi_n \in N(0, 1) \quad (10)$$

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Random Sampling (RS) & Stochastic Collocation (SC)

Expectation through RS:

$$\langle \phi^m \rangle \approx \frac{1}{R} \sum_{i=1}^{R} \phi^m(x, \xi_1^i, \ldots, \xi_N^i) \quad (11)$$

Expectation through SC:

$$\langle \phi^m \rangle \approx \sum_{q_N}^{Q_N} \cdots \sum_{q_1}^{Q_1} w_{q_1} \cdots w_{q_N} \, \phi^m(x, \xi_1^{q_1}, \ldots, \xi_N^{q_N}) \quad (12)$$

Table: RS and SC Properties

	RS	SC
Number of samples:	R	$\prod_{n=1}^{N} Q_n$
Convergence rate:	$R^{-0.5}$	variable
Curse of dimensionality:	no	yes, can mitigate with anisotropic SC, e.g., on KL monotonic decrease

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Polynomial Chaos Expansion (PCE)

N-dimensional, K-order model of $\phi(x,\omega)$ as a function of coefficients $u_\kappa(x)$ and Hermite polynomials $H_\kappa(\xi)$:

$$\begin{aligned}\phi(x,\omega) =& u_0(x)H_0 + \sum_{i_1=1}^{N} u_{i_1}(x)H_1(\xi_{i_1}) + \sum_{i_1=1}^{N}\sum_{i_2=1}^{i_1} u_{i_1 i_2}(x)H_2(\xi_{i_1},\xi_{i_2}) + \cdots \\ &+ \sum_{i_1=1}^{N}\cdots\sum_{i_{K-1}=1}^{i_1} u_{i_1\cdots i_{K-1}}(x)H_{K-1}(\xi_{i_1},\cdots,\xi_{i_K})\end{aligned} \quad (13)$$

Written more succinctly:

$$\phi(x,\omega) = \sum_{\kappa=0}^{K_t} \widehat{u}_{\mathbf{k}(\kappa)}(x) H_{\mathbf{k}(\kappa)}(\boldsymbol{\xi}) \quad (14)$$

Where the number of terms is:

$$K_t + 1 = \frac{(N+K)!}{N!K!} \quad (15)$$

Solution of PCE Coefficients Using SC (SC-PCE)

- Begin with the expansion and note i.i.d. bases for factoring joint polynomials into univariate polynomials:

$$\phi(x,\omega) = \sum_{\kappa=0}^{K_t} \widehat{u}_{\mathbf{k}(\kappa)}(x) H_{\mathbf{k}(\kappa)}(\boldsymbol{\xi}); \qquad H(\xi_1,\ldots,\xi_N) = \prod_{n=1}^{N} H(\xi_n) \tag{16}$$

- Take multi-dimensional inner-product:

$$\left\langle \phi(x,\boldsymbol{\xi}), H_{\mathbf{j}}(\boldsymbol{\xi}) \right\rangle = \widehat{u}_{\mathbf{k}}(x) \left\langle \sum_{\kappa=0}^{K_t} H_{\mathbf{k}}(\boldsymbol{\xi}), H_{\mathbf{j}}(\boldsymbol{\xi}) \right\rangle = \frac{\widehat{u}_{\mathbf{j}}(x)}{a_{\mathbf{j}}}, \quad a_{\mathbf{j}} = \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi} j_n! \delta_{k_n j_n}} \tag{17}$$

- Solve flux coefficients:

$$\widehat{u}_{\mathbf{k}}(x) = a_{\mathbf{k}} \left\langle \phi(x,\boldsymbol{\xi}), H_{\mathbf{k}}(\boldsymbol{\xi}) \right\rangle \tag{18}$$

- Integrate using stochastic collocation

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Lognormal KL Flux Averages

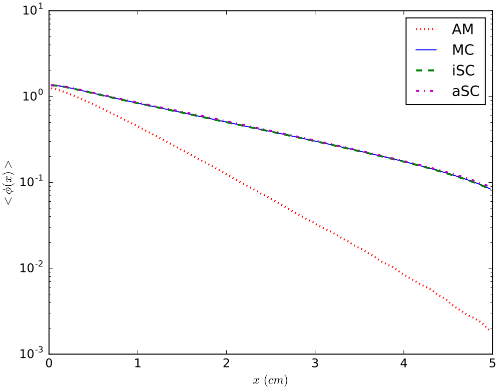

Figure: Flux Averages

AM: Atomic Mix

RS (MC): 10,000 realizations

iSC: $K_s = K_a = 4$, $Q_n = 3$
(6561 realizations)

aSC: $K_s = 4$, $Q_{k_s} = \{4, 3, 3, 2\}$
$K_a = 3$, $Q_{k_a} = \{4, 3, 2\}$
(1728 realizations)

Lognormal KL Flux Standard Deviations

AM: Atomic Mix

RS (MC): 10,000 realizations

iSC: $K_s = K_a = 4$, $Q_n = 3$
(6561 realizations)

aSC: $K_s = 4$, $Q_{k_s} = \{4, 3, 3, 2\}$
$K_a = 3$, $Q_{k_a} = \{4, 3, 2\}$
(1728 realizations)

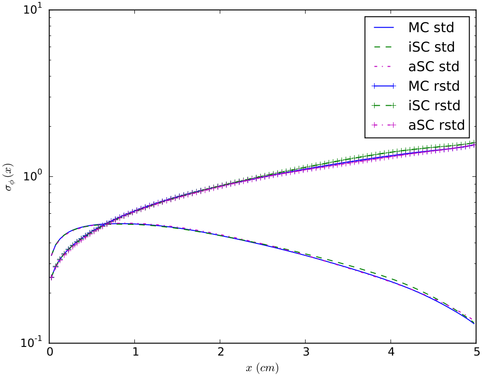

Figure: Flux Standard Deviations

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Lognormal KL Transmission Moments

RS (MC): 10,000 realizations

iSC: $K_s = K_a = 4$, $Q_n = 3$
(6561 realizations)

iSC-PCE: $K = 3$

aSC: $K_s = 4$, $Q_{k_s} = \{4, 3, 3, 2\}$
$K_a = 3$, $Q_{k_a} = \{4, 3, 2\}$
(1728 realizations)

aSC-PCE: $K = 3$

Table: Transmission Moments

	$\bar{x}_T$	s_T	$s_{\bar{x}_T}$
RS	0.06629	0.10529	0.00105
iSC	0.06422	0.10484	N/A
iSC-PCE	0.06422	0.10436	N/A
aSC	0.06866	0.10585	N/A
aSC-PCE	0.06866	0.10557	N/A

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Nataf Transformation

Transform Gaussian field $Y(x)$ to discrete field $Z^*(x)$ and normalize to zero mean and unit variance ($E[Z]=0,\ V[Z]=1$) :

$$Z^*(x) = \begin{cases} 1 & \text{if} \quad \text{in mat 1} \\ 0 & \text{if} \quad \text{in mat 0} \end{cases} \Rightarrow \quad Z(x) = \begin{cases} \frac{p_0-1}{\sqrt{p_0(1-p_0)}} & \text{if} \quad \text{in mat 1} \\ \frac{p_0}{\sqrt{p_0(1-p_0)}} & \text{if} \quad \text{in mat 0} \end{cases} \qquad (19)$$

Solve Gaussian value w_t for which $F_Y(w_t) = p_0$:

$$F_Y(w_t) = \int_{-\infty}^{w_t} \frac{1}{\sqrt{2\pi}} exp\left[-\frac{(x)^2}{2}\right] dx' = p_0 \quad \Rightarrow \quad w_t = \sqrt{2} erf^{-1}(2p_0 - 1) \quad (20)$$

Utilize w_t in definition of Nataf transformation:

$$z = c(w) = \begin{cases} \frac{p_0-1}{\sqrt{p_0(1-p_0)}} & \text{if} \quad w < w_t \\ \frac{p_0}{\sqrt{p_0(1-p_0)}} & \text{if} \quad w > w_t \end{cases} \qquad (21)$$

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Nataf Transformation: Gaussian Covariance Function

Relate Gaussian (R_{YY}) and field (R_{ZZ}) covariance:

$$\begin{aligned} R_{ZZ}(x_1, x_2) &= E[Z(x_1), Z(x_2)] = E[c(Y(x_1)), c(Y(x_2))] \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c(w_1)c(w_2)p_{yy}(w_1, w_2, R_{YY})dw_1 dw_2 \end{aligned} \tag{22}$$

Expand bivariate Gaussian pdf (p_{yy}) with Hermite polynomials (H_m) and simplify:

$$R_{ZZ} = \sum_{m=0}^{\infty} K_m^2 R_{YY}^m, \qquad K_m = \frac{1}{\sqrt{m!}}\int_{-\infty}^{\infty} c(y)H_m(y)\phi(y)dy \tag{23}$$

Solve $R_{YY}(r)$, $r = |x_1 - x_2|$, numerically.

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Discrete KL Realization Visualization

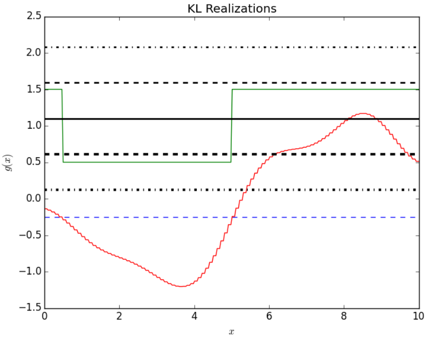

Figure: Discrete KL Realization

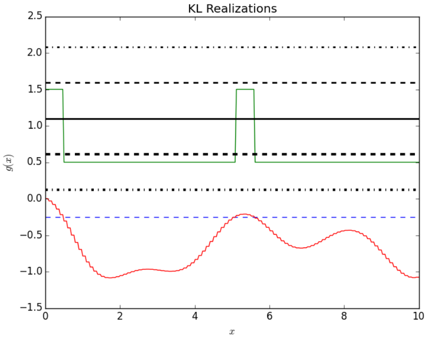

Figure: Discrete KL Realization

Example Markov Realizations

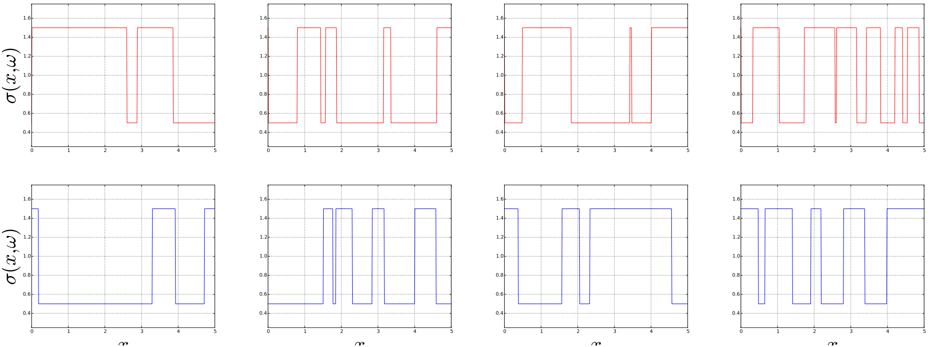

Figure: Chord Length Sampling (Top), Discrete KL (Bottom)

Discrete KL Moment Preservation

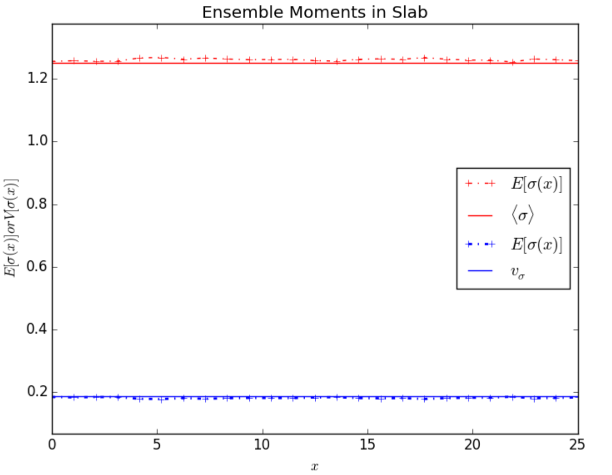

Figure: Observed Cross Section Moments

Numerical Sampling of Discrete KL Covariance

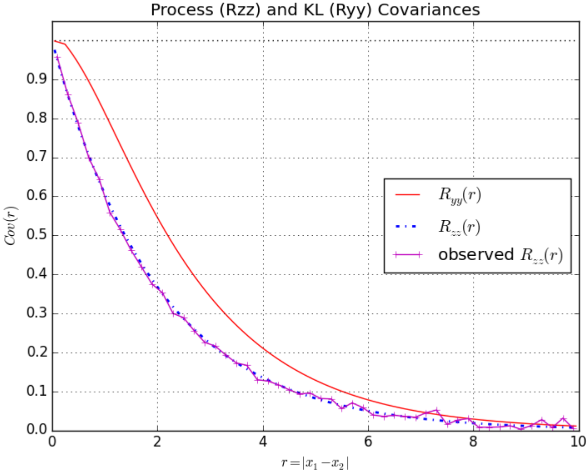

Figure: Process, Gaussian, and Sampled Covariances

Conclusions

- Lognormal transform of Gaussian process maintains positivity in reconstructions
- Karhunen-Loève models which require a relatively-low truncation order can be computed on efficiently using stochastic collocation, especially anisotropic stochastic collocation
- Polynomial Chaos Expansion models allow PDF generation using SC scheme
- Discontinuous media can be modeled with Gaussian input distributions using the Nataf transformation

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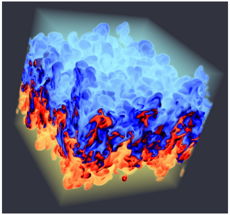
Future Work

Planned:

- Complete full-transport implementations
- Perform convergence studies to investigate stochastic smoothness

Possible:

- Examine non-exponential covariance functions for discontinuous media
- Extend discontinuous media modeling to multi-D



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Questions?