Probabilistic Modeling and Computations with Polynomial Chaos for Heterogeneous Multiscale Environments

Roger Ghanem

University of Southern California, Los Angeles, CA, USA

SIAM Conference on Mathematical Geosciences
Houston, TX March 11 2019

Probabilistic Modeling and Computations with

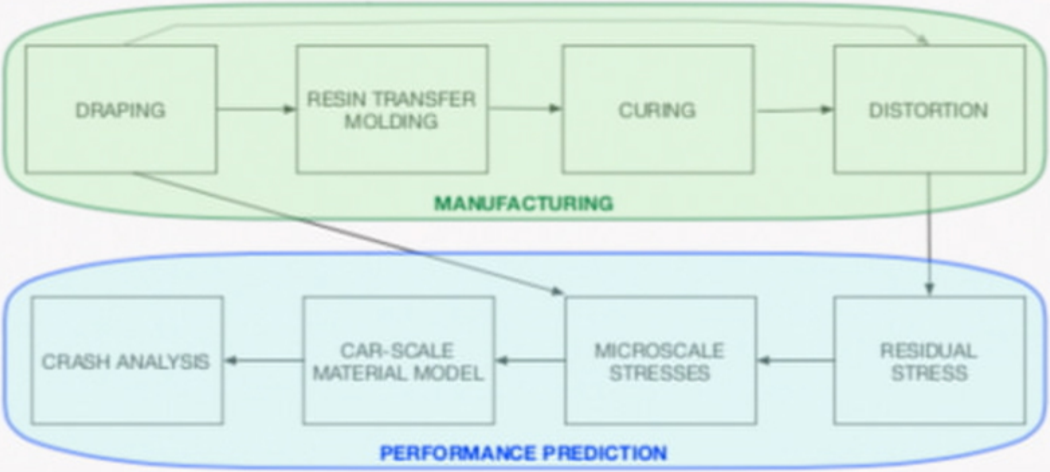
Outline

1. Motivation
2. Review of Polynomial Chaos Constructions
3. Adaptation
4. Stochastic Optimization
5. Stochastic Multiscale Representations

Objective

Design of composite car including material processing.

$$J_{\text{Vehicle}} = f(\text{Fiber, Tow, Lamina, Laminate, Controls})$$



Approach

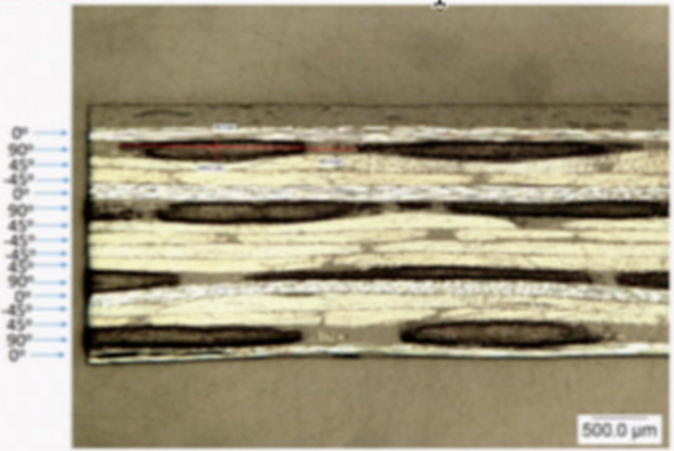
Package information in a suitable manner for impact on purpose.

Information

PHYSICS:

- fabric folding
- resin flow
- resin curing
- residual stresses

DATA:



Approach

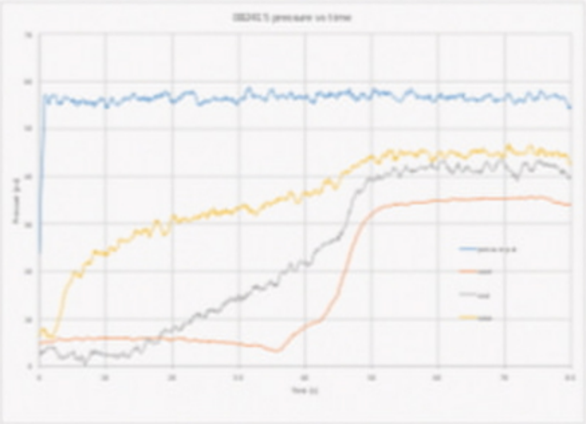
Package information in a suitable manner for impact on purpose.

Information

PHYSICS:

- fabric folding
- resin flow
- resin curing
- residual stresses

DATA:



Approach

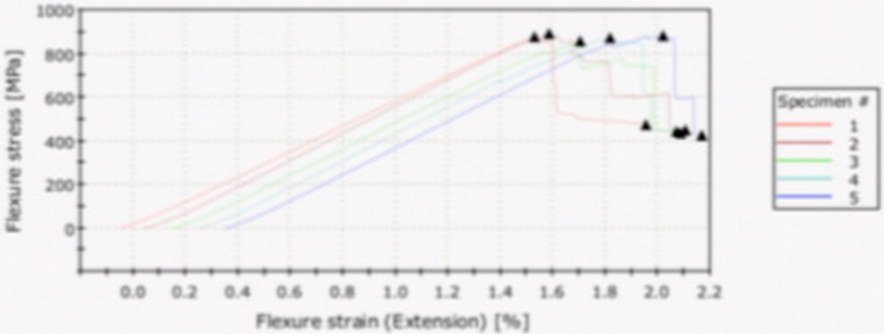
Package information in a suitable manner for impact on purpose.

Information

Physics:

- fabric folding
- resin flow
- resin curing
- residual stresses

Data:



Approach

Package information in a suitable manner for impact on purpose.

Information

PHYSICS:

- fabric folding
- resin flow
- resin curing
- residual stresses

DATA:

Approach

Package information in a suitable manner for impact on purpose.

suitable manner

to leverage big computers and associated highly resolved numerical models.

Approach

Package information in a suitable manner for impact on purpose.

purpose

- Reduce weight of vehicle without adversly affecting occupant safety.
- Optimize the manufacturing process to achieve objective.

Outline

1. Motivation
2. Review of Polynomial Chaos Constructions
3. Adaptation
4. Stochastic Optimization
5. Stochastic Multiscale Representations

Probability Models

standard models:

from observations of K, construct statistics or probability density of K:

$$\text{Data} \mapsto \boxed{f_K(k)}$$

Polynomial Chaos Approach

from observations of K AND understanding of physics:

- postulate dependence of K on subscale features, $\xi : K(\xi) \quad \xi \in \mathbb{R}^d$
- describe this dependence in polynomial form:

$$\text{Data} \oplus \text{Physics} \mapsto \boxed{K(\xi) = \sum_\alpha k_\alpha \, \psi_\alpha(\xi)}$$

- estimate coefficients in that expansion
- observations of K are either experimental or numerical.

Probability Models

standard models:

from observations of K, construct statistics or probability density of K:

$$\text{Data} \mapsto \boxed{f_K(k)}$$

Polynomial Chaos Approach

from observations of K AND understanding of physics:

- postulate dependence of K on subscale features, $\boldsymbol{\xi} : K(\boldsymbol{\xi}) \quad \boldsymbol{\xi} \in \mathbb{R}^d$
- describe this dependence in polynomial form:

$$\text{Data} \bigoplus \text{Physics} \mapsto \boxed{K(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha}} k_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})}$$

- estimate coefficients in that expansion
- observations of K are either experimental or numerical.

A Cameron-Martin Theorem

Let $x(t)$ be a Brownian motion, and let:

- $\{\alpha_i(t)\}$ is a CONS in $L^2[0,1]$
- $\Phi_{m,p}(x) = H_m\left[\int_0^1 \alpha_p(t)dx(t)\right] \quad m = 1, 2, \cdots \ p = 0, 1, \cdots$
- $\Psi_{m_1,\cdots,m_p}(x) = \Phi_{m_1,1}(x)\cdots\Phi_{m_p,p}(x)$

Then

$$\lim_{N\to\infty} \int_C^w \left| F[x] - \sum_{m_1,\cdots,m_N} A_{m_1,\cdots,m_N} \Psi_{m_1,\cdots,m_p}(x) \right|^2 d_w x = 0$$

The polynomial chaos decomposition of any square-integrable functional of the Brownian motion converges in mean-square as N goes to infinity.

For a finite-dimensional representation, the coefficients are functions of the missing dimensions. That is, the coefficients are themselves random variables dependent on the dimensions excluded from the representation.

Polynomial Chaos

$$K(\boldsymbol{x}, \xi) = \sum_{\alpha \geq 0} k_{\alpha}(\boldsymbol{x})\ \psi_{\alpha}(\xi)$$

- if K is a stochastic process, then k_{α} are function of x.
- ξ reflects uncertainties in model parameters, model form, and data.
- updating the probabilistic model entails updating the coefficients:
- procedure can be recursive:

$$\text{hierarchy of scales: } \xi = \sum_{\beta} z_{\beta}\ \psi_{\beta}(\zeta)$$

$$\text{model/data errors: } k_{\alpha}(\boldsymbol{x}) \rightarrow k_{\alpha}(\boldsymbol{x}, \zeta) = \sum_{\gamma} k_{\alpha,\gamma}(\boldsymbol{x}) \psi_{\gamma}(\zeta)$$

Polynomial Chaos

$$\text{material property model: } k(\boldsymbol{x},\xi) = \sum_{|\boldsymbol{\alpha}|\geq 0} k_{\boldsymbol{\alpha}}(\boldsymbol{x})\ \psi_{\boldsymbol{\alpha}}(\xi)$$

$$\text{physics model:} \quad u = f(k) = f(k(\xi))$$

$$u(\boldsymbol{x},\xi) = \sum_{|\boldsymbol{\alpha}|\geq 0} u_{\boldsymbol{\alpha}}(\boldsymbol{x})\ \psi_{\boldsymbol{\alpha}}(\xi)$$

- if u is a stochastic process, then $u_{\boldsymbol{\alpha}}$ are functions of x.
- ξ reflects uncertainties in model parameters, model form, and data.
- updating the probabilistic model entails updating:

  ξ: models of the fine scale.
  $k_{\boldsymbol{\alpha}}$: how fine scale maps to coarse scale
  $u_{\boldsymbol{\alpha}}$: how prediction depends on fine scale
  k: coarse scale model of property
  u: coarse scale model of prediction

Observations from elementary statistics

Average out the noise (upscaling or CLT)

- $Y \sim \mathcal{N}$

$$Y = \sum_i \xi_i, \qquad \xi_i \sim N(0,1)$$

- $X \sim \chi_d^2$

$$X = \sum_{i=1}^{d} \xi_i^2, \qquad \xi_i \sim N(0,1)$$

- $T \sim t_d$

$$T \propto \frac{\sum_{i=1}^{d} \xi_i}{\sqrt{\sum_{i=n}^{n+d} \xi_i^2}}, \qquad \xi_i \sim N(0,1)$$

Observations from elementary statistics

Average out the noise (upscaling or CLT)

- $Y \sim \mathcal{N}, \quad Y = \sum_i \xi_i, \qquad \xi_i \sim N(0,1)$
- $X \sim \chi^2_d, \quad X = \sum_{i=1}^d \xi_i^2, \qquad \xi_i \sim N(0,1)$
- $T \sim t_d, \quad T \propto \frac{\sum_{i=1}^d \xi_i}{\sqrt{\sum_{i=n}^{n+d} \xi_i^2}}, \qquad \xi_i \sim N(0,1)$

Reverse-engineer CLT:
Features matter: away from mean-field theories

Given coarse observable, construct a functional model from the finer scales:

$$X = f(\xi_1, \cdots, \xi_d) = f(\boldsymbol{\xi})$$

Non-Intrusive Characterization

IF WE KNOW : $\boldsymbol{\xi} \mapsto u(\boldsymbol{\xi})$

We want:

$$u(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}| \geq 0} u_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Orthogonality of $\{\psi_{\boldsymbol{\alpha}}\}$

$$\begin{aligned} u_{\boldsymbol{\alpha}} &= E_{\boldsymbol{\xi}}\{u \, \psi_{\boldsymbol{\alpha}}\} \\ &= \int_{\Gamma_1} \cdots \int_{\Gamma_d} u(\boldsymbol{x}) \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) p_{\boldsymbol{\xi}}(\boldsymbol{x}) \, d\boldsymbol{x} \\ &\approx \sum_{q \in \mathcal{Q}} u(\boldsymbol{x}^{(q)}) \, \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}^{(q)}) \, w_q \end{aligned}$$

Adaptation

We address the challenge of curse of dimensionality

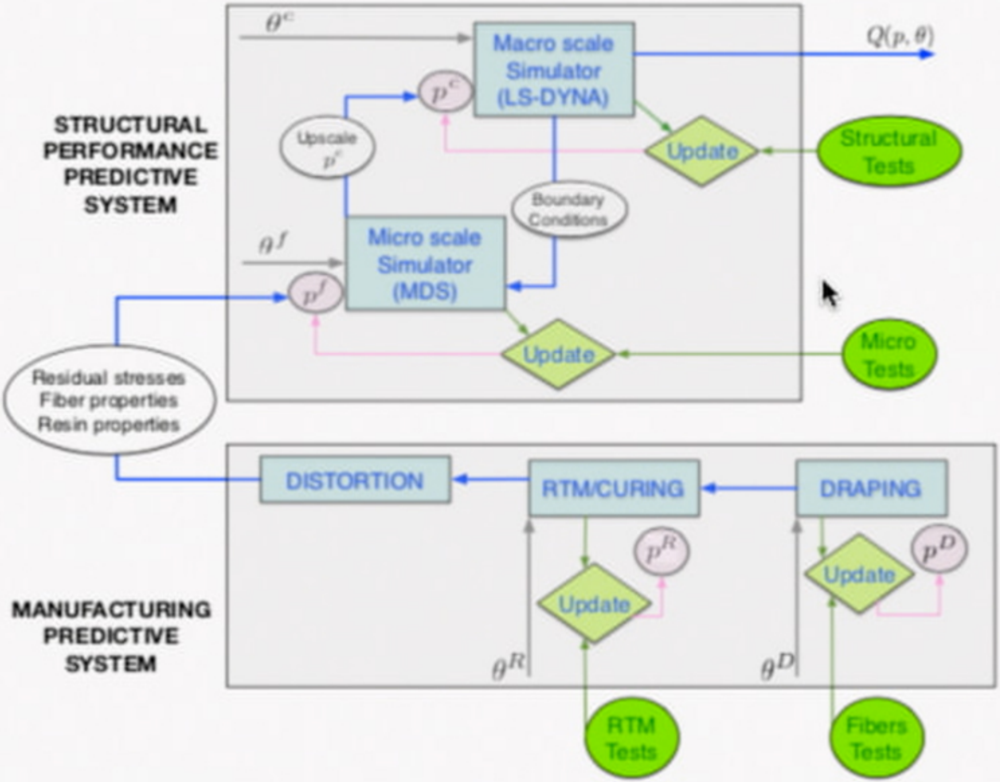
By shifting the complexity of analysis from that of parameter space to that of the Quantity of Interest (QoI).

New challenge: Learn the complexity of the QoI:

We use two different ideas of complexity:

- **Explicit Functional Dependence inherited from Governing Equations:**
  use projections and vector space methods with PCE: Basis adaptation
- **Intrinsic Structure Encoded in Data:**
  use graph analysis and diffusions on manifolds: Manifold sampling

Multiscale Material System: manufacturing to performance



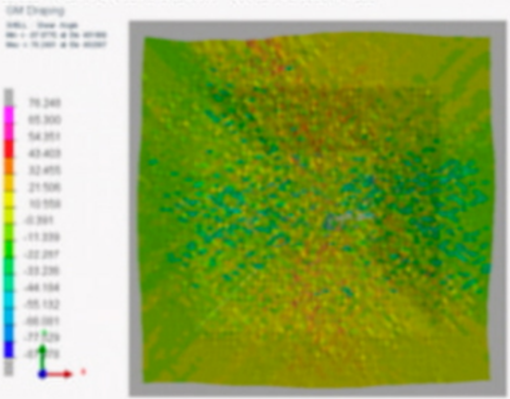
Manufacturing Process

Effect of fluctuations in properties of constituents and manufacturing control variables
on material properties and processing time.

Manufacturing process

Draping/Fabric Forming

11 uncertain variables



Manufacturing process

Draping/Fabric Forming

11 uncertain variables

Resin Transfer Molding + Curing

30 uncertain variables

Distortion

34 uncertain variables

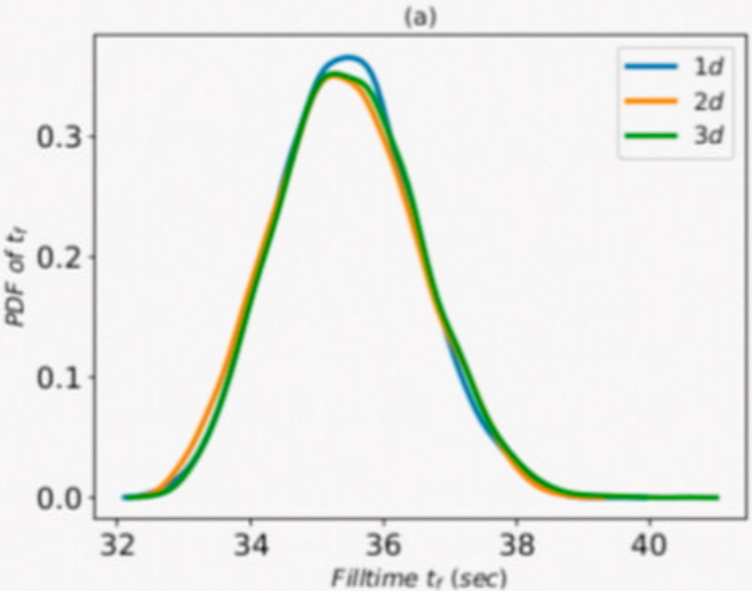
Total dimension of parameter space

75 uncertain variables

Manufacturing process

75-dimensional parameter space for material processing

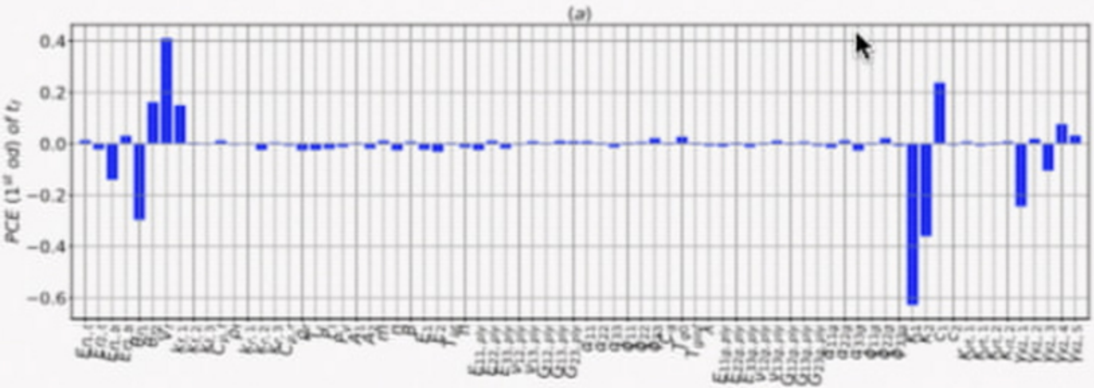
QoI: Fill Time (75d)



Manufacturing process

75-dimensional parameter space for material processing

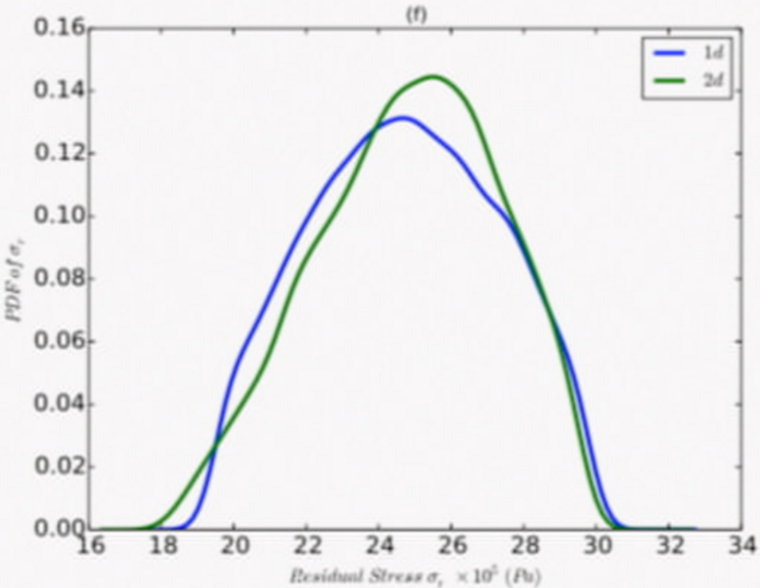
QoI: Fill Time (75d): First order coefficients



Manufacturing process

75-dimensional parameter space for material processing

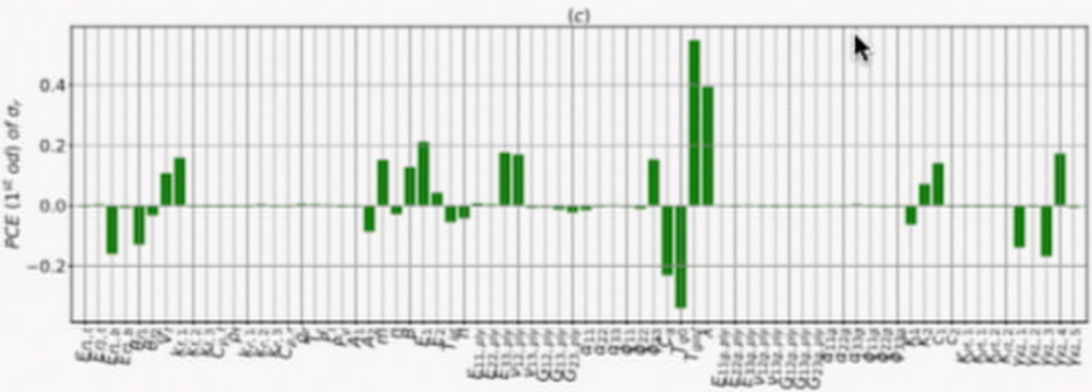
QoI: Maximum residual stress (75d)



Manufacturing process

75-dimensional parameter space for material processing

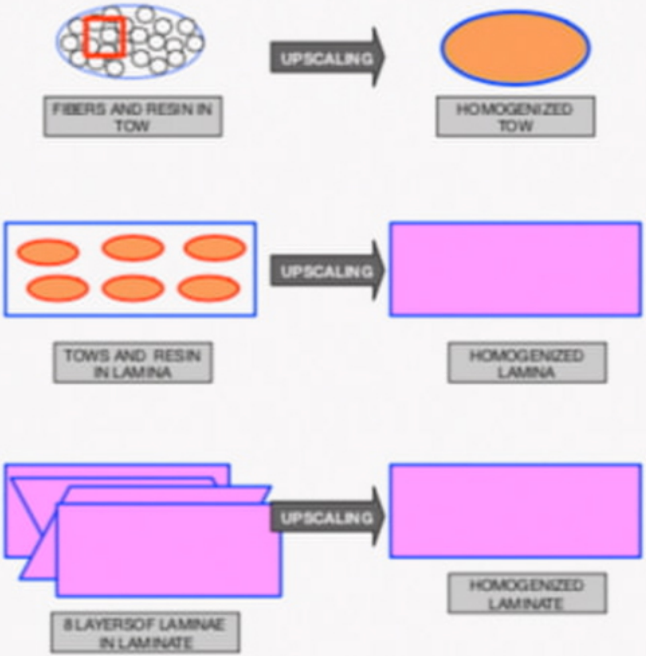
QoI: Maximum Residual Stress (75d): First order Coefficients

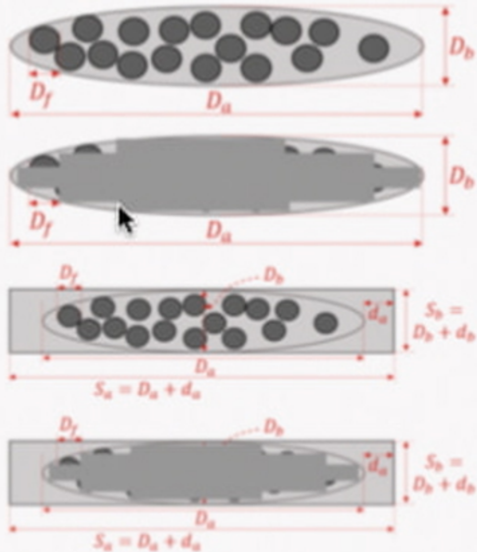


Structural Performance

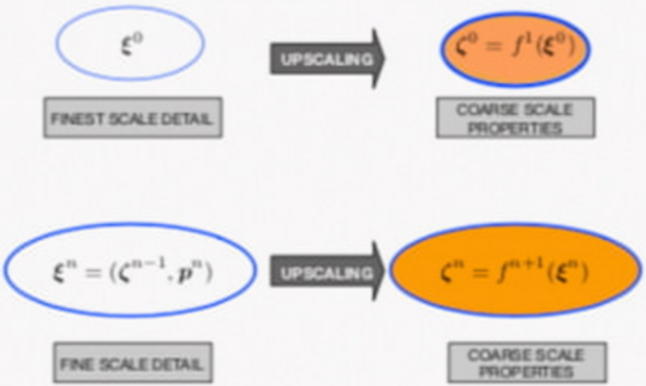
Effect of fluctuations in microstructure of manufactured material on the performance of the structure.

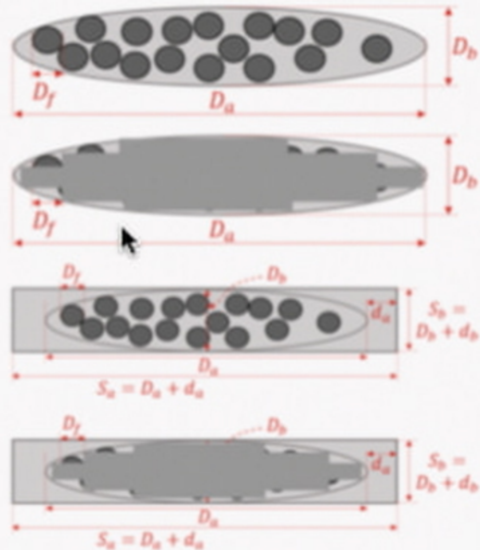
Multiple Scales



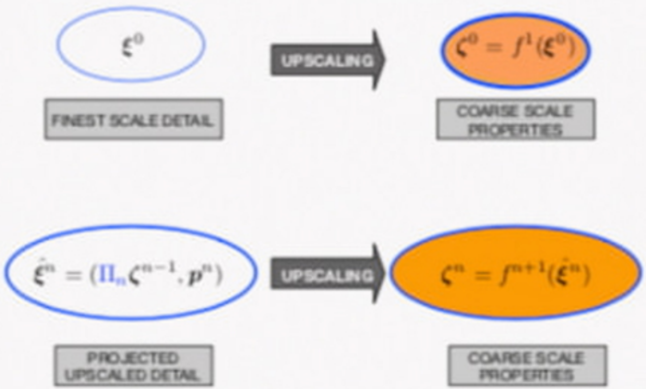


Multiple Scales





Multiple Scales

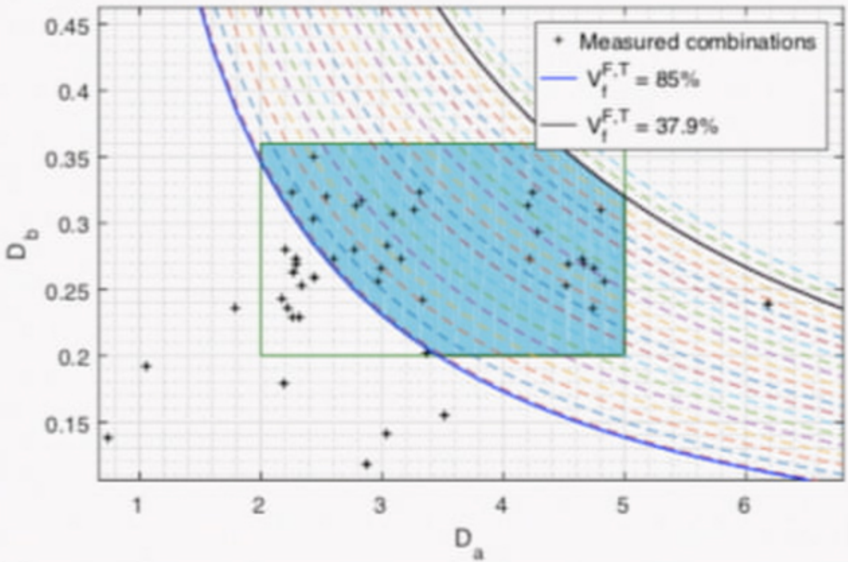


Random variable	Mean value	Lower limit	Upper limit	C.O.V.
V_f %	83.4	76.4	90.4	4 %
E_{fA}	230.0e9	200e9	240e9	2.51 %
E_{fT}	20.0e9	14.8e9	25.2e9	15 %
G_{fA}	25.0e9	20.7e9	29.3e9	10 %
ν_{fA}	0.016	0.013	0.019	10 %
ν_{fT}	0.400	0.331	0.469	10 %
E_m	3.40e9	2.81e9	3.99e9	10 %
ν_m	0.335	0.294	0.376	7 %
D_a	3.47	0.74	6.2	45.4 %
d_a	0.505	0.01	1.0	56.6 %
D_b	0.27	0.12	0.42	32.1 %

Macro-scale structural behavior

16-dimensional parameter space

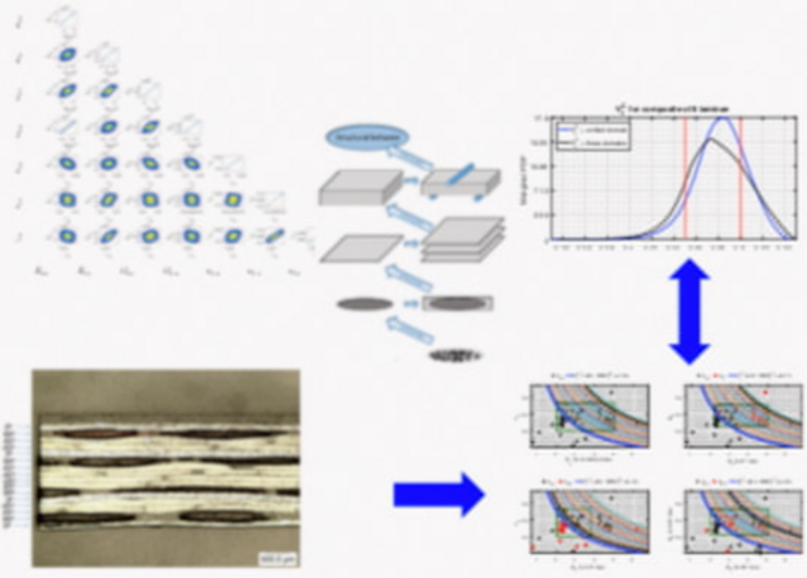
Tow geometry model:
statistical dependence at microscale with coarse scale constraints



Macro-scale structural behavior

16-dimensional parameter space: resin/fiber/towGeometry

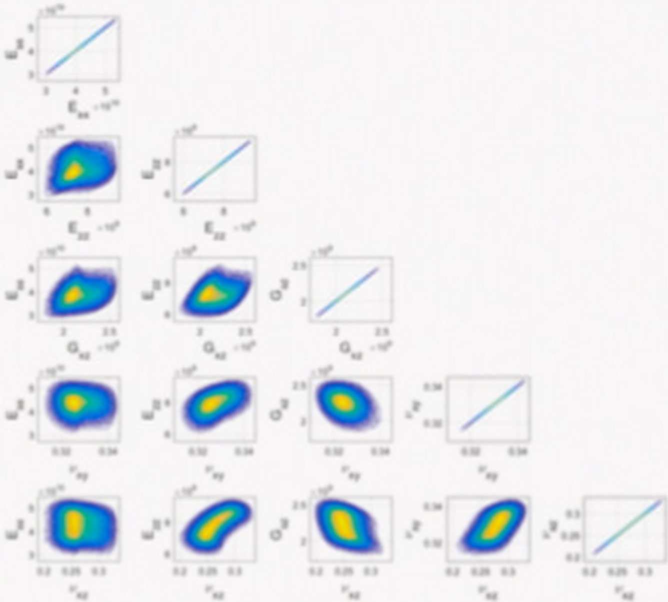
Stochastic Structural System Performance



Macro-scale structural behavior

16-dimensional parameter space

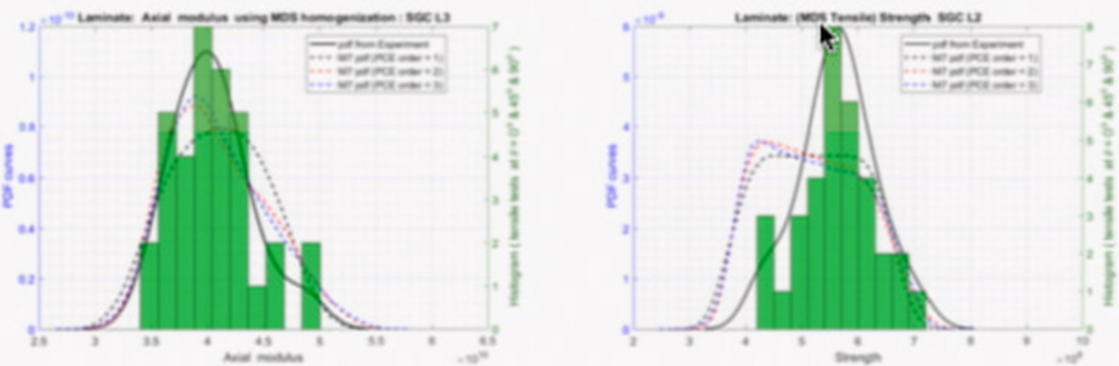
Predicted Joint PDF for coarse scale properties



Macro-scale structural behavior

16-dimensional parameter space

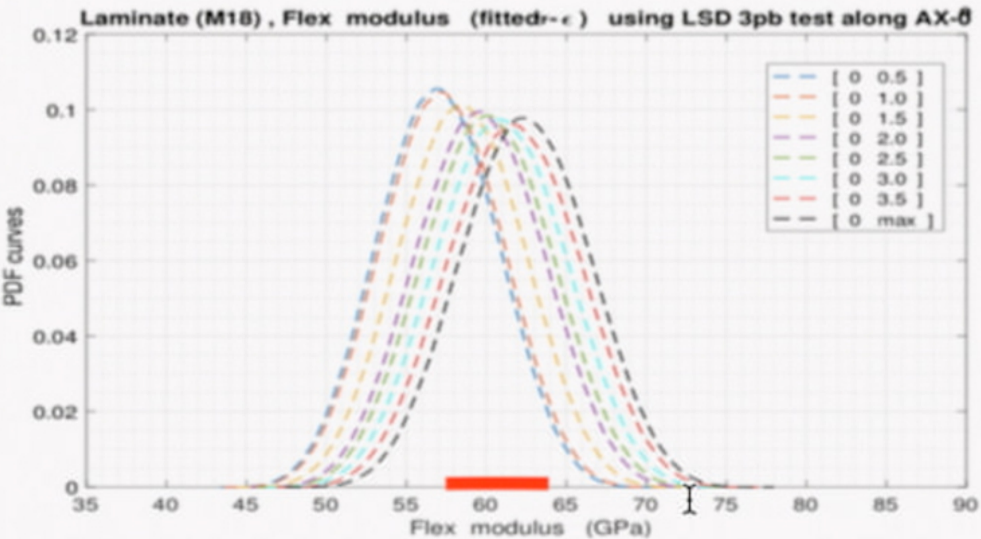
Modulus and strength comparison with experiments in tension test



Validation Results

Validation with 3PB tests

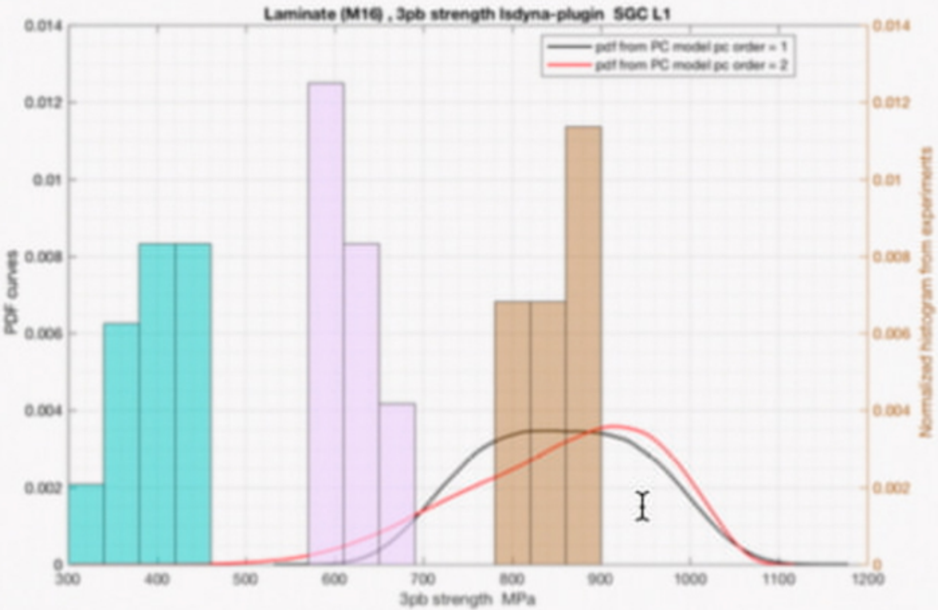
Elasticity Modulus



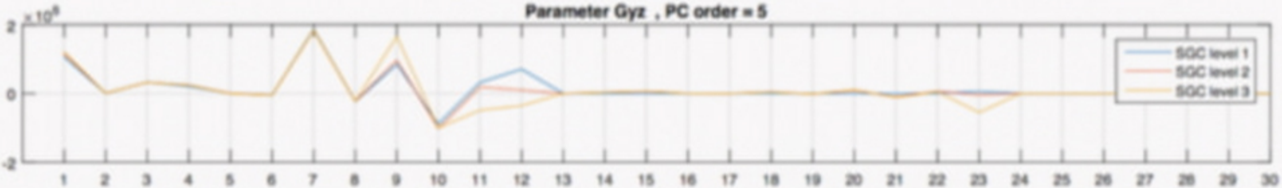
Validation Results

Validation with 3PB tests

Strength Modulus



Polynomial Chaos representation



This is our prior model that encodes physics knowledge and simulation codes.

Required innovation

Mathematical/Statistical

Compute likelihood and statistical dependence of various quantities across scales and across physics/models.

Algorithms

Curse of dimensionality: address large parametric dimension through stochastic basis adapation.

Software

Multi-models exchange distinct stochastic representations, spatial discretizations, and homogenized variables.

Outline

Basis Adaptation: Context

Numerical model is parameterized with random parameters $\boldsymbol{k}$:

These are mapped to d independent random variables.

$$\boldsymbol{k} = \boldsymbol{f}(\boldsymbol{\xi}), \qquad \boldsymbol{\xi} \in \mathbb{R}^d$$

QoI is expressed as function of $\boldsymbol{\xi}$

$$Q(\boldsymbol{\xi}) \triangleq h[u(\boldsymbol{\xi})] = \sum_{|\boldsymbol{\alpha}| \leq p} q_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Basis Adaptation: Basic Idea

Idea:

Compute sensitivity with respect to all possible
linear combinations of the variables.

Challenge:

Linear combinations of the variables become statistically dependent with complicated probability density functions that depend on the weights. unless they are gaussian.

We use nonlinear maps to transport nonGaussian densities to Gaussians.

Basis Adaptation: Basic Idea/ Gaussian germ

Rotate ξ

$$\boldsymbol{\eta} = \boldsymbol{A}\boldsymbol{\xi}$$

Since $\boldsymbol{\xi}$ is Gaussian, $\boldsymbol{\eta}$ is also Gaussian and

$$Q(\boldsymbol{\eta}) \equiv Q(\boldsymbol{\xi})$$

PCE for rotated variables:

$$\sum_{|\boldsymbol{\alpha}|\geq 0} q_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}|\geq 0} q_{\boldsymbol{\alpha}}^{\boldsymbol{A}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{A}\boldsymbol{\xi})$$

- the sparsities of truncated expansions are different and depend on $\boldsymbol{A}$
- choose $\boldsymbol{A}$ to concentrate the expansion of Q in the first few $\eta_i, i = 1, \cdots, n$
- best $\boldsymbol{A}$ depends on the specific Q

Basis Adaptation: Constructing the rotation

Gaussian adaptation

Align η_1 with the Gaussian components of Q: $\eta_1 = \sum_{i=1}^{d} q_i \xi_i$
Other η_i obtain through Gram-Schmidt.

Compresisve sensing

Find $\boldsymbol{A}$ to minimize least squares distance between adapted-basis prediction and available full-dimension samples.

Various optimality criteria

- closest 1d match to CDF of available samples
- diagnolize a full second order fit
- Maximum likelihood estimator for $\boldsymbol{A}$
- Bayesian posterior for $\boldsymbol{A}$ over manifold of rotation matrices.

Isometry on Gaussian Space

Let $\boldsymbol{A}$ be an Isometry
Let $\boldsymbol{\eta} = \boldsymbol{A}\boldsymbol{\xi}$
Then

$$\forall n \geq 1 \quad span\{\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), |\boldsymbol{\alpha}| = n\} = span\{\psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}), |\boldsymbol{\alpha}| = n\}$$

Let $\psi^{\boldsymbol{A}}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta})$
and

$$q(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathcal{I}_p} q_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \qquad q^{\boldsymbol{A}}(\boldsymbol{\eta}) = \sum_{\boldsymbol{\alpha} \in \mathcal{I}_p} q^{\boldsymbol{A}}_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}) \ ,$$

Projection on Transformed Space

Consider a subspace $V_{\mathcal{I}}$ of $L^2(\Omega)$ spanned by $\{\psi^{\mathbf{A}}_{\beta}; \beta \in \mathcal{I} \subset \mathcal{I}_p\}$.

The projection of $q^{\mathbf{A}}$ on $V_{\mathcal{I}}$ is:

$$\begin{aligned} q^{\mathbf{A},\mathcal{I}}(\boldsymbol{\eta}) &= \sum_{\beta \in \mathcal{I}} q^{\mathbf{A}}_{\beta} \psi_{\beta}(\boldsymbol{\eta}) = \sum_{\beta \in \mathcal{I}} \sum_{\alpha \in \mathcal{I}_p} q_{\alpha} (\psi_{\alpha}, \psi^{\mathbf{A}}_{\beta}) \psi_{\beta}(\boldsymbol{\eta}) \\ &= \sum_{\gamma \in \mathcal{I}_p} q^{\mathcal{I}}_{\gamma} \psi_{\gamma}(\boldsymbol{\xi}) \, . \end{aligned}$$

This yields,

$$q^{\mathcal{I}}_{\gamma} = \sum_{\beta \in \mathcal{I}} \sum_{\alpha \in \mathcal{I}_p} q_{\alpha} (\psi_{\alpha}, \psi^{\mathbf{A}}_{\beta})(\psi^{\mathbf{A}}_{\beta}, \psi_{\gamma})$$

Case 1: Adaptation to Gaussian Components

$$\text{Take} \qquad \eta_1 = \sum_{\boldsymbol{\alpha}\in\mathcal{I}_1} q_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \sum_{i=1}^{d} q_{\mathbf{e}_i}\xi_i$$

$$\mathcal{I} = \mathcal{I}_p \cap \mathcal{E}_1 \ .$$

Then:

$$q^{\mathbf{A}}(\boldsymbol{\eta}) = q_0^{\mathbf{A}} + q_{\mathbf{e}_1}^{\mathbf{A}}\eta_1 + \sum_{\substack{1<|\boldsymbol{\beta}|\le p \\ \boldsymbol{\beta}\in\mathcal{E}_1}} q_{\boldsymbol{\beta}}^{\mathbf{A}}\psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) + \sum_{\substack{1<|\boldsymbol{\beta}|\le p \\ \boldsymbol{\beta}\notin\mathcal{E}_1}} q_{\boldsymbol{\beta}}^{\mathbf{A}}\psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) \ .$$

and

$$q^{\mathbf{A},\mathcal{I}}(\boldsymbol{\eta}) = q_0^{\mathbf{A}} + \sum_{\boldsymbol{\beta}\in\mathcal{E}_1} q_{\boldsymbol{\beta}}^{\mathbf{A}}\psi_{\boldsymbol{\beta}}(\boldsymbol{\eta})$$

Error

$$q^{\mathbf{A}}(\boldsymbol{\eta}) - q^{\mathbf{A},\mathcal{I}}(\boldsymbol{\eta}) = \sum_{\substack{1<|\boldsymbol{\beta}|\leq p \\ \boldsymbol{\beta}\notin\mathcal{E}_1}} q^{\mathbf{A}}_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta})$$

Case 2: Adaptation to Quadratic Components

$$\text{Take } \boldsymbol{A} \text{ to diagonalize } q_0 + \sum_{i=1}^{d} \hat{q}_i \xi_i + \sum_{i=1}^{d} \sum_{j=1}^{d} \hat{q}_{ij}(\xi_i \xi_j - \delta_{ij})$$

$$\boldsymbol{A}\hat{\boldsymbol{S}}\boldsymbol{A} = \boldsymbol{D}$$

Then:

$$q^{\boldsymbol{A}}(\boldsymbol{\eta}) = q_0 + \sum_{i=1}^{d} b_i \eta_i + \sum_{i=1}^{d} d_i(\eta_i^2 - 1) + \sum_{|\boldsymbol{\beta}|>2} q_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) \ ,$$

$$q^{\boldsymbol{A},\mathcal{I}} = q_0 + \sum_{i=1}^{d} \sum_{\boldsymbol{\beta} \in \mathcal{E}_i} q_{\boldsymbol{\beta}}^{\boldsymbol{A}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) \ ,$$

Error

$$q^{\mathbf{A}}(\boldsymbol{\eta}) - q^{\mathbf{A},\mathcal{I}}(\boldsymbol{\eta}) = \sum_{\substack{2<|\boldsymbol{\beta}|\leq p \\ \boldsymbol{\beta}\notin\mathcal{E}}} q^{\mathbf{A}}_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) \ .$$

Case 3: Adaptation to CDF of QoI

$$\text{Take } A \text{ such that:} \quad \boldsymbol{A} = \arg\min \sum_{i=0}^{p} \|q_i(\boldsymbol{A}) - \hat{q}_i\| w_i$$

$$\mathcal{I} = \mathcal{E}_1 \qquad \text{where} \quad \hat{q} \equiv F^{-1}\Phi(\xi) = \sum_i \hat{q}_i \psi_i(\xi)$$

Then:

$$q^{\boldsymbol{A}}(\boldsymbol{\eta}) = q_0^{\boldsymbol{A}} + q_{\boldsymbol{e}_1}^{\boldsymbol{A}} \eta_1 + \sum_{\substack{1<|\boldsymbol{\beta}|\le p \\ \boldsymbol{\beta}\in\mathcal{E}_1}} q_{\boldsymbol{\beta}}^{\boldsymbol{A}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) + \sum_{\substack{1<|\boldsymbol{\beta}|\le p \\ \boldsymbol{\beta}\notin\mathcal{E}_1}} q_{\boldsymbol{\beta}}^{\boldsymbol{A}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta}) \,.$$

and

$$q^{\boldsymbol{A},\mathcal{I}}(\boldsymbol{\eta}) = q_0^{\boldsymbol{A}} + \sum_{\boldsymbol{\beta}\in\mathcal{E}_1} q_{\boldsymbol{\beta}}^{\boldsymbol{A}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta})$$

Error

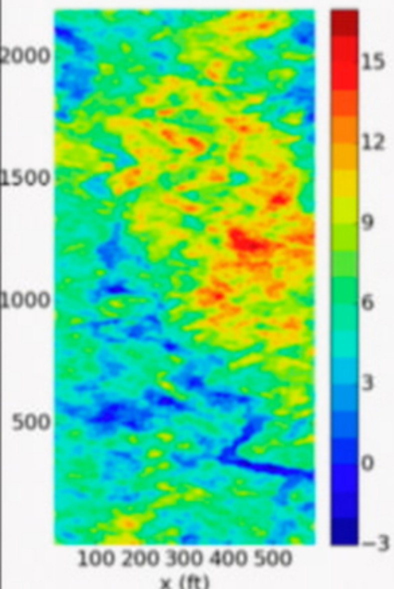
$$q^{\boldsymbol{A}}(\boldsymbol{\eta}) - q^{\boldsymbol{A},\mathcal{I}}(\boldsymbol{\eta}) = \sum_{\substack{1<|\boldsymbol{\beta}|\le p \\ \boldsymbol{\beta}\notin\mathcal{E}_1}} q_{\boldsymbol{\beta}}^{\boldsymbol{A}} \psi_{\boldsymbol{\beta}}(\boldsymbol{\eta})$$

Outline

1. Motivation
2. Review of Polynomial Chaos Constructions
3. Adaptation
4. **Stochastic Optimization**
5. Stochastic Multiscale Representations

Basis Adaptation for Optimization: $\boldsymbol{A}(\boldsymbol{d})$

Focus on QoI in Design Optimization:
$\boldsymbol{d}^*$= Locations of Injection/Production wells



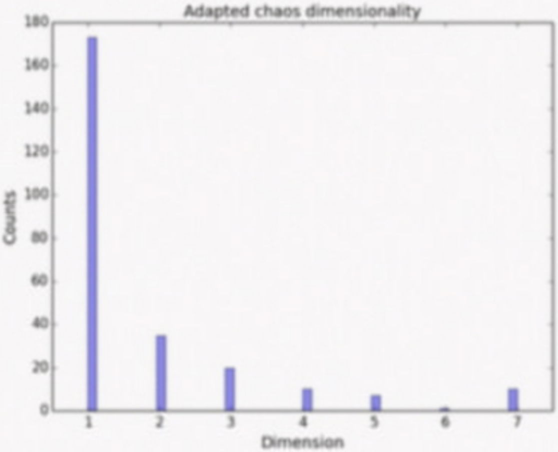
Find: $\boldsymbol{d}^* = \arg\max J(\boldsymbol{d})$
$J(\boldsymbol{d}) = Q(\alpha)$

Subject to:

$$1 - F_{\boldsymbol{d}}(Q_\alpha) = P(q(\boldsymbol{d}, \boldsymbol{\theta}) > Q_\alpha) = 1 - \alpha$$

Basis Adaptation for Optimization: $\boldsymbol{A}(\boldsymbol{d})$

Focus on QoI in Design Optimization:
$\boldsymbol{d}^*$= Locations of Injection/Production wells



Find: $\boldsymbol{d}^* = \arg\max J(\boldsymbol{d})$

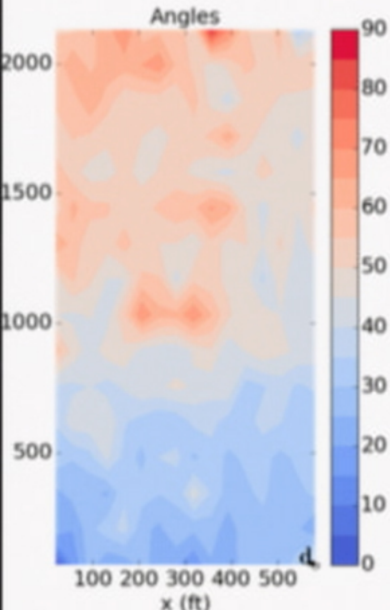
$$J(\boldsymbol{d}) = Q(\alpha)$$

Subject to:

$$1 - F_{\boldsymbol{d}}(Q_\alpha) = P(q(\boldsymbol{d}, \boldsymbol{\theta}) > Q_\alpha) = 1 - \alpha$$

Basis Adaptation for Optimization: $A(\boldsymbol{d})$

Focus on QoI in Design Optimization:
$\boldsymbol{d}^*$= Locations of Injection/Production wells



Find: $\boldsymbol{d}^* = \arg\max J(\boldsymbol{d})$

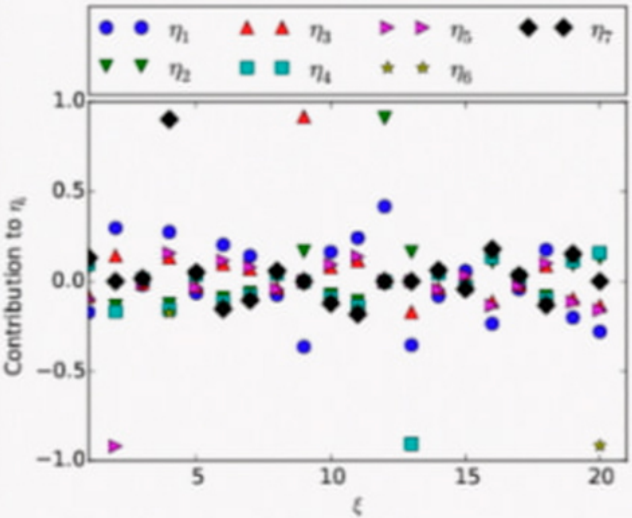
$$J(\boldsymbol{d}) = Q(\alpha)$$

Subject to:

$$1 - F_{\boldsymbol{d}}(Q_\alpha) = P(q(\boldsymbol{d}, \boldsymbol{\theta}) > Q_\alpha)$$
$$= 1 - \alpha$$

Basis Adaptation for Optimization: $\boldsymbol{A}(\boldsymbol{d})$

Focus on QoI in Design Optimization:
$\boldsymbol{d}^*$= Locations of Injection/Production wells



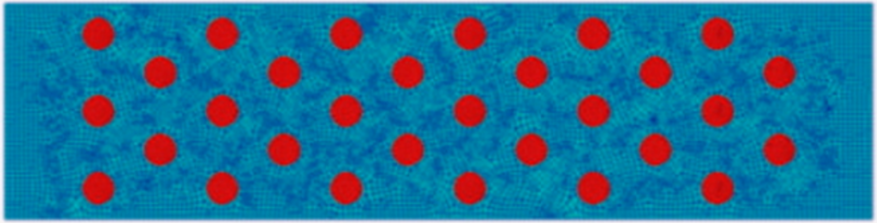
Find: $\boldsymbol{d}^* = \arg\max J(\boldsymbol{d})$

$$J(\boldsymbol{d}) = Q(\alpha)$$

Subject to:

$$1 - F_{\boldsymbol{d}}(Q_\alpha) = P(q(\boldsymbol{d}, \boldsymbol{\theta}) > Q_\alpha) = 1 - \alpha$$

Adapted Stochastic Upscaling

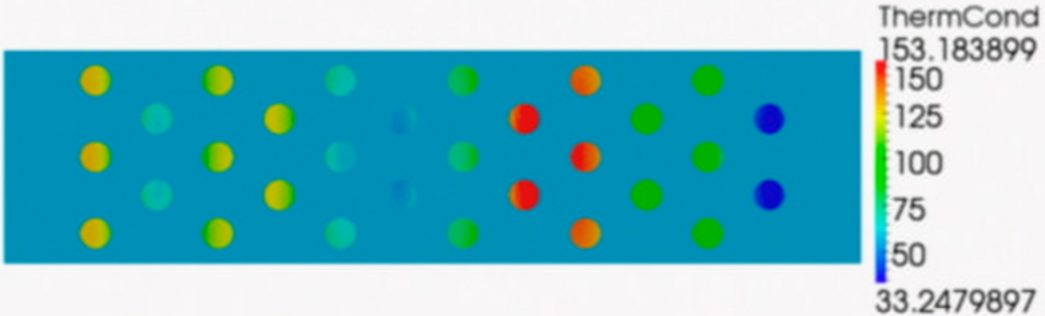


Fluid passing through heated inclusions

Random Thermal Conductivity of Inclusions

$c_{p,s}(x) = \sum_i c_i(x)\psi_i(\xi) \qquad \xi \in \mathbb{R}^d$

Stochastic Process with d Dimensions



One realization of thermal conductivity process.

Governing Equations

Steady-state laminar flow

- continuity $\rho_f(\nabla \cdot \boldsymbol{u}) = 0$
- conservation of momentum $\rho_f (\nabla \cdot \boldsymbol{u})\, \boldsymbol{u} = -\nabla P + \mu_f \nabla^2 \boldsymbol{u} + \rho_f \boldsymbol{f}$
- conservation of energy $\rho_f c_{p,f} [\nabla \cdot (\boldsymbol{u} T)] = k_f \nabla^2 T$

B.C.: Constant material flux and constant temperature on left side.

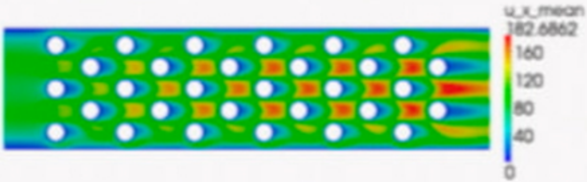
- ρ_f is the density of the fluid,
- μ_f is the viscosity of the fluid,
- k_f is the thermal conductivity of the fluid,
- $c_{p,f}$ is specific heat of the fluid.

Steady-state heat conduction in solid

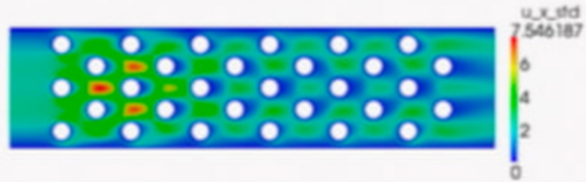
$$\rho_s c_{p,s} [\nabla \cdot (\boldsymbol{u} T)] = k_s \nabla^2 T$$

B.C.: Constant flux at center of each inclusion.

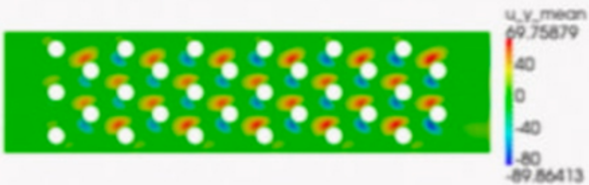
Fine scale results using Albany- u_x and u_y



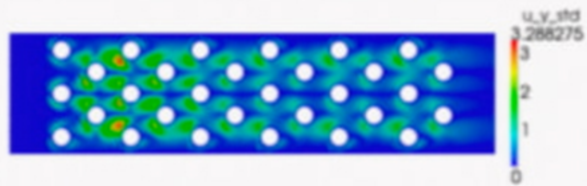
(a) Mean of u_x



(b) std. dev. of u_x



(c) Mean of u_y

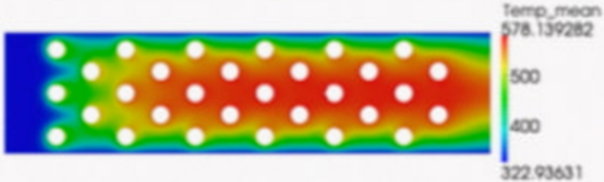


(d) std. dev. of u_y

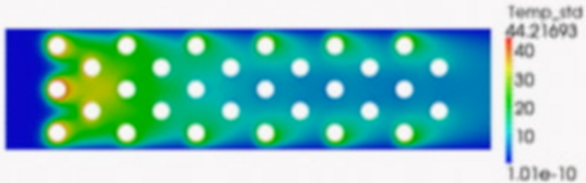
Fine scale results using Albany - pressure and temperature

(e) Mean of pressure

(f) std. dev. of presure



(g) Mean of temperature



(h) std. dev. of temperature

Coarse scale model: Brinkman-Darcy equations

Fluid flow continuity equation

$$\rho_f(\nabla \cdot \tilde{\boldsymbol{u}}) = 0$$

Darcy-Brinkmann Momentum Equation:

$$\rho_f \frac{\rho_f}{\phi}(\nabla \cdot \tilde{\boldsymbol{u}})\tilde{\boldsymbol{u}} = -\phi \nabla \tilde{P} + \mu_f \nabla^2 \tilde{\boldsymbol{u}} - \frac{\phi \mu_f}{K}\tilde{\boldsymbol{u}} + \phi \rho_f \tilde{\boldsymbol{f}}$$

Fluid and solid phase equations collapse to one

$$\nabla \cdot \left(\bar{\rho}\bar{C}\tilde{\boldsymbol{u}}\bar{T}\right) = \bar{k}_{eff}\nabla^2 \bar{T} + \dot{\bar{Q}}$$

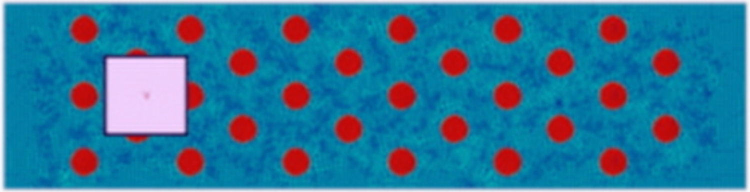
- $\tilde{\boldsymbol{u}}$ is the volume averaged Darcy seepage velocity
- $\tilde{P}$ is the volume averaged fluid pressure in the porous media,
- ϕ is the porosity of the medium,
- K is the permeability,
- $\bar{C}_{eff}$ is effective heat conductivity of porous media.
- Brinkman term $\mu_f \nabla^2 \tilde{\boldsymbol{u}}$ accounts for transitional flow between the solid boundaries

Stochastic upscaling

Spatial Average over RVE

Permeability

$$-\frac{\partial \langle P \rangle}{\partial x_i} = \mu k_{ij}^{-1} \langle u_j \rangle$$



Obtain: For each RVE, $k_{ij}(x)$ as function of $\boldsymbol{\xi} \in \mathbb{R}^d$.

Stochastic upscaling

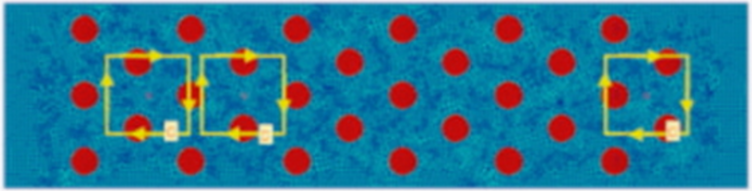
Spatial Average over RVE

Thermal Conductivity

$$\bar{\rho}\bar{C}\nabla\cdot(\tilde{\boldsymbol{u}}\bar{T}) = \bar{C}_{\text{eff}}\nabla\cdot(\nabla\bar{T})$$

By Gauss-divergence theorem

$$\bar{\rho}\bar{C}\int_C \vec{n}\cdot(\boldsymbol{u}T)\,ds = \bar{C}_{\text{eff}}\int_C \vec{n}\cdot(\nabla T)ds,$$



Obtain: for each RVE, $C_{\text{eff}}(x)$ as function of $\boldsymbol{\xi}\in\mathbb{R}^d$.

Parameter of Upscaled Model

We want a random field model for coarse scale permeability K and C_{eff}:

$$k(x,\xi) = \sum_{i=0}^{P} k_i(x)\psi_i(\boldsymbol{\xi}),$$

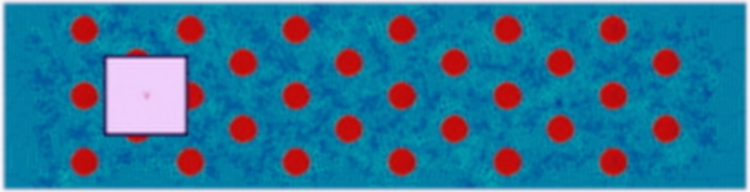
This is a model in d dimensional space. Still too expensive.

Stochastic upscaling

Spatial Average over RVE

QoI is Permeability

$$-\frac{\partial \langle P \rangle}{\partial x_i} = \mu k_{ij}^{-1} \langle u_j \rangle$$



Obtain: For each RVE, $k_{ij}(x)$ as function of one η.

Stochastic upscaling

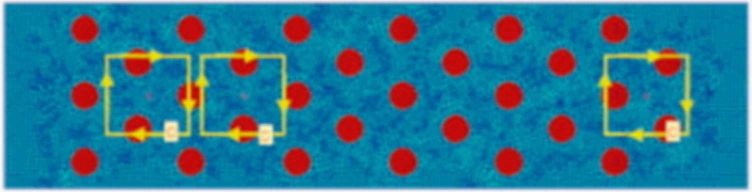
Spatial Average over RVE

QoI is Thermal Conductivity

$$\bar{\rho}\bar{C}\nabla\cdot(\tilde{\boldsymbol{u}}\bar{T}) = \bar{C}_{\text{eff}}\nabla\cdot(\nabla\bar{T})$$

By Gauss-divergence theorem

$$\bar{\rho}\bar{C}\int_C \vec{n}\cdot(\boldsymbol{u}T)\,ds = \bar{C}_{\text{eff}}\int_C \vec{n}\cdot(\nabla T)ds,$$



Obtain: for each RVE, $C_{\text{eff}}(x)$ as function of one η.

QoI is RVE-upscaled variable:

We want a coarse scale random field for permeability K and C_{eff}:

$$k(x,\xi) = \sum_{i=0}^{P} k_i(x)\psi(\boldsymbol{\xi}),$$

Linear basis adaptation for each RVE

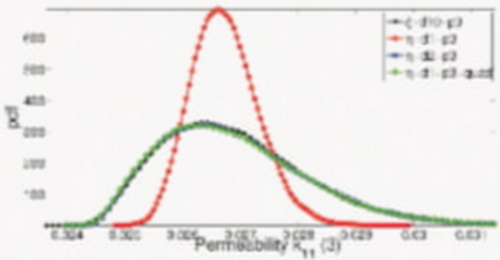
$$\eta(x) = \sum_{i=1}^{d} w_i(x)\xi_i$$

$$k(x,\xi) = \sum_{i} k_i(x)\psi_i(\eta(x))$$

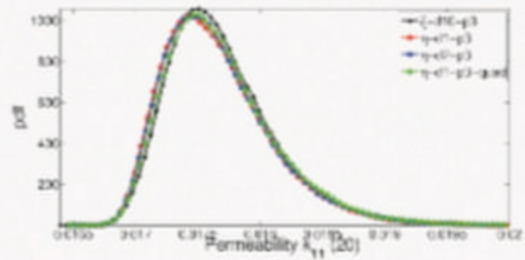
Challenge:

Considered over the whole spatial domain, it is likely that all ξ_i are activated: no reduction in complexity.

Upscaled Permeability: Is not one-dimensional



(i) Permeability at point 3



(j) Permeability at point 20

Figure: Permeability computed at points 3 is 3-dimensional and at point 20 is 1-dimensional.

Upscaled variables are statistically dependent

Depend on same fine scale fluctuations

$$k(x) = \sum_{\boldsymbol{\alpha}} k_{\boldsymbol{\alpha}}(x)\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

$$C_{\text{eff}}(x) = \sum_{\boldsymbol{\alpha}} C_{\text{eff},\boldsymbol{\alpha}}(x)\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Concluding Remarks

- PCE is fundamentally a representation of stochastic variables and processes.
- The coefficients can be constrained by physics from across scales.
- Adaptation and other projections can be leveraged to yield massive computational reductions.