

A Bayesian Framework for Assessing the Strength Distribution of Composite Structures with Random Defects

SIAM CSE

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Overview

Goal: Model deformations of composite materials used in aerospace engineering

Outline:

- 1. Problem formulation
- **2.** MCMC
- 3. Preconditioning
- 4. Surrogate Models
- 5. Outlook





Problem formulation: Composite Materials







Modelling Challenges for Composite Materials

Classical Finite Elements (FE) on grid T_h , find $\mathbf{u}_h \in V$ such that

$$\int_{\Omega} \boldsymbol{C}(\mathbf{x})\varepsilon(\mathbf{u}_h):\varepsilon(\mathbf{v}_h)\ d\mathbf{x} = \int_{\Omega} \mathbf{f}\cdot\mathbf{v}_h\ d\mathbf{x} + \int_{\Gamma} (\sigma\cdot\mathbf{n})\cdot\mathbf{v}_h\ d\mathbf{x} \quad \forall \mathbf{v}_h \in V_h$$

leads to system of matrix equations: Au = b, $u \in \mathbb{R}^M$

- C(x) Elasticity Tensor varies over small length scales (<mm) application/component on > 10m scale → massive systems of equations!
- High Contrast Fibre to Resin (~ 10 : 1) → very ill-conditioned equations!
- Strongly Anisotropic (often non-grid aligned) → non-local coupling in A!



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Defects in Composites

- **Defects** can form when manufacturing complex aerospace components.
- Reduce testing by using numerical simulations
 - Requires good mathematical / mechanical models for composite failure
 - Efficient stochastic algorithms to calculate the probability distribution of failure
- Inverse problems might avoid expensive/infeasible scans.





FE modeling

 Requires high number of degrees of freedom to resolve, plies, interfaces, wrinkles



 Very coarse FE modelnot possible as at least one element per layer is needed

Characterising Wrinkles

Let $\{\psi_i(\mathbf{x})\}$ define the orthonormal basis over which wrinkles are defined

- The deformation induced by W(x, ξ) should not self-intersect. At this stage it is sufficient to choose ψ_i not self-intersecting, and impose the constraint det J(x, ξ) > 0 during the posterior sampling
- The misalignment is computed as follows

$$an \phi_j(\mathbf{x}, \boldsymbol{\xi}) = \sum_{i=1}^{N_w} a_i \frac{d\psi_i(\mathbf{x}, \mathbf{b})}{dx_j} ext{ for } j = 1 ext{ and } 2.$$
 (1)

 the choice of basis ψ_i is important as it constrains the representation of wrinkles, it should be left as general as possible

Characterising Wrinkles



Estimating alignment at a point by minimizing the integral of the gray scale over the trial fibre using the MFIA algorithm.



Characterising Wrinkles



Randomly sampled points are used to reconstruct an alignment over the domain. Samples are concentrated in areas of high misalignment in a multilevel scheme.



Wrinkle parameterisation



Represent a wrinkle using a Karhunen-Loéve expansion:

$$W(\mathbf{x}) = \sum_{i=1}^{N_{KL}} a_i \underbrace{\Psi_i(\lambda, x_1)}_{ ext{KL modes}} \underbrace{\mathcal{F}(\mathbf{x})}_{ ext{Decay fct}},$$

where the decay functions

$$F(\mathbf{x}) = \prod_{j=1}^{3} \exp\left[-\frac{(x_j - X_j)^n}{\lambda_D}\right]$$

account for the localized nature of the wrinkles.

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Defect Modeling

A Markov chain is a sequence of samples $\{\xi^{(0)}, \xi^{(1)}, \dots, \xi^{(m)}\}$. The first set of coefficients is generated randomly from $\mathcal{N}(0, 1)$. Subsequent samples are generated by preconditioned Crank-Nicolson proposal with tuning parameter $\beta \in \mathbb{R}$:

$$\boldsymbol{\xi'} = \sqrt{(1-eta^2)} \, \boldsymbol{\xi}^{k-1} + eta \underline{\omega}; \quad 1 \leqslant k \leqslant m$$

For the proposal we calculate its fit to the data $\mathbf{A} = \{\mathbf{a}^{(0)}, \dots, \mathbf{a}^{(n)}\}$

$$\mathcal{L}(\boldsymbol{\xi'}) = \exp\left[-\frac{1}{2}\sqrt{n} \min_{i=1,\dots,n} ||\mathbf{a}^{(i)} - \boldsymbol{\xi}'_j||_2\right]$$

The proposal ξ' is accepted as the next sample $\xi^{(k)}$ with probability

$$\alpha(\boldsymbol{\xi}', \boldsymbol{\xi}^{k-1}) = \min\left\{1, \frac{\mathcal{L}(\boldsymbol{\xi}')}{\mathcal{L}(\boldsymbol{\xi}^{k-1})}\right\}$$

otherwise $\boldsymbol{\xi}^{k} = \boldsymbol{\xi}^{k-1}$.

Markov Chain Monte-Carlo

- We initialize five independent Markov chains
- By computing the autocorrelation length Λ we approximate the subsampling interval for which the samples are independent, i.e. $\Xi = \{\xi^{(\Lambda)}, \xi^{(2\Lambda)}, \dots, \xi^{S\Lambda}\}$ and $S\Lambda = m$.
- Subsampling only occurs after a burn-in period to remove influence of the start of the chain on the distribution.



Results



Domain Decomposition Methods



- Additive Schwarz methods solve on each small subdomain Ω and use these local approximations of K^{-1} as a preconditioner
- Performance reduces with increasing number of domains/processors \rightarrow does not scale to large problem sizes
- Strong connectivity between subdomains (fibre direction) may not be captured in large problems

GenEO Preconditioner

Idea: Add a global coarse space to add information from neighboring subdomains [GenEO]

$$M_{AS,2}^{-1} = \underbrace{R_H^T K_H^{-1} R_H}_{\text{coarse space}} + \underbrace{\sum_{j=1}^N R_j^T K_j^{-1} R_j}_{\text{AS 1}}$$

- Robust for Composite Applications
- Condition of preconditioned system stays constant with increasing number of domains/processors
- Fine scale behaviour of the fibres is captured

[GENEO] Spillane et al, Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps, 2014.

GenEO Coarse Space

Definition (Generalized eigenproblems in the overlaps)

For each subdomain j = 1, ..., N, we define the generalized eigenproblem

$$a_{\Omega_j}(oldsymbol{
ho},oldsymbol{v}) = \lambda a_{\Omega_j^o}(\Xi_j(oldsymbol{
ho}), \Xi_j(oldsymbol{v})) orall oldsymbol{v} \in V_h(\Omega_j),$$

where Ξ_j is the partition of unity and a_{Ω_j} , $a_{\Omega_j^o}$ is the bilinear form restricted to the subdomain Ω_i and the overlap respectively.

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Definition (GenEO coarse space)

For each subdomain j = 1, ..., N, let $(p_k^j)_{k=1}^{m_j}$ be the eigenfunctions from the eigenproblem in definition corresponding to the m_j smallest eigenvalues. Then the GenEO coarse space is defined as

$$V_H := \text{span} \{ R_j^T \Xi_j(p_k^j) : k = 1, \dots, m_j; j = 1, \dots, N \}.$$

GenEO Coarse Space

Definition (Generalized eigenproblems in the overlaps)

For each subdomain j = 1, ..., N, we define the generalized eigenproblem

$$a_{\Omega_j}(\boldsymbol{\rho}, \boldsymbol{v}) = \lambda a_{\Omega_j^o}(\Xi_j(\boldsymbol{\rho}), \Xi_j(\boldsymbol{v})) \forall \boldsymbol{v} \in V_h(\Omega_j),$$

where Ξ_j is the partition of unity and a_{Ω_j} , $a_{\Omega_j^o}$ is the bilinear form restricted to the subdomain Ω_j and the overlap respectively.

Sample eigenfunctions:



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Performance



GenEO as a surrogate model

• Find $u \in V := H_0^1(\Omega)$, such that

$$-
abla \cdot oldsymbol{c}(\mathbf{x})
abla u(\mathbf{x}) = 1 \quad orall \mathbf{x} \in \Omega := [0, 1]^d$$

 $u(\mathbf{x}) = \mathbf{0} \ \forall \mathbf{x} \in \partial \Omega$

- c(x) Log-normal random field
- Variations over small length scales and high contrast



- Subdivide into 16 subdomains
- Overlap subdomain by O layers
- dim $V_h = 4.0 \times 10^4$
- Babuska I & Lipton R, Optimal Local Approximation Spaces for Generalized Finite Element Methods with Application to Multiscale Problems, *Multiscale Model Simul*, 2011.





Motivating Example: Incompressible Darcy Flow

First 5 eigenfunctions on Ω_6 . Lowest $\lambda_6^{(1)} = 0$ as Ω_6 has no Dirichlet boundary

$$\lambda_6^{(1)} = 0.0 \qquad \lambda_6^{(2)} = 0.0193 \quad \lambda_6^{(3)} = 0.0511 \quad \lambda_6^{(4)} = 0.0937 \quad \lambda_6^{(5)} = 0.2056$$



Fine model dim $V_h = 4 \times 10^4$



Coarse Model dim $V_H = 320$ m = 20, O = 5



Conclusions



- Often in composite structures there is little data, since large composite parts are expensive to make. → not possible to infer much about the strength distribution of a component from such limited data without the use of statistical tools
- The GenEO preconditioner is robust and scales well up to thousands of cores
- Alternatively, a good multiscale method can capture finescale behaviour with fewer degrees of freedom
- Avoid expensive scans/invasive testing

Citations

- **[GENEO]** Spillane N, Dolean V, Hauret P, Nataf F, Pechstein C & Scheichl R, Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps. Numerische Mathematik,126(4), pp. 741-770, 2014.
- **[MCMC]** A. Sandhu, A. Reinarz, T. Dodwell, A bayesian framework for assessing the strength distribution of composite structures with random defects, Composite Structures, 2018.
- [composites] R. Butler et al, dune-composites an open source, high performance package for solving large-scale anisotropic elasticity problems, submitted.
- [DUNE] M. Blatt, A. Burchardt, A. Dedner, C. Engwer, J. Fahlke, B. Flemisch, C. Gersbacher, C. Gräser, F. Gruber, C. Grüninger, D. Kempf, R. Klöfkorn, T. Malkmus, S. Müthing, M. Nolte, M. Piatkowski, O. Sander., *The Distributed and Unified Numerics Environment, Version 2.4.* Archive of Numerical Software, 2016.