Data-Driven Inverse Characterization for In-situ Microscopic Composite Properties

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Motivations

- Micromechanical or multiscale analysis are developed for modeling complex failure mechanisms in composite material but rely on precise in-situ constituent properties.
- In-situ constituent properties are distinct from bulk material due to difference of manufacture process.
  - In fiber-reinforced composites, in-situ epoxy resin stiffness is different from neat resin and has spatial variation according to nano-indentation tests.

Adapted from, Hardiman 2015

Fiber properties not changed during the curing procedure

Adapted from, Smith 2019
Objectives and background

• Research objectives:
  ➢ Inversely characterize in-situ microscopic resin properties with spatial variability based on image-based measurements (Digital Image Correlation, X-ray tomography, etc.)
  ➢ Propose mathematics framework for robust optimization approach given the noisy measurements.

• Existing characterization approaches:
  ➢ Nano-indentation test:
  ➢ Inverse characterization based on image-based measurements:
    ❖ No existing application for characterizing in-situ composite properties.
    ❖ Easily affected by measurement noise.

Adapted from, Smith 2019

Adapted from, Michopoulos 2011


Inverse characterization approach

➢ Image-based measurement using template matching (TM):

DIC or X-ray microtomography image

Detection of fiber diameter (d)

Distance along x

Displacement $u^e$ from template matching

Displacement $u^s$ from numerical simulations

Adjust constitutive parameter $\theta$

Model Initialization with spatial variation

FEA:

Output

$\theta_{\text{max}}$

$\theta_{\text{min}}$

Minimization?

Yes

No

Assess objective function $\mathcal{L} = f(||u^s - u^e||)$

• Objective function in Normalized Mean Square Error (NMSE) form:

\[ L(\theta) = \frac{\sum_{i=1}^{n} \|u^e_{(i)} - u^s_{(i)}\|^2}{\sum_{i=1}^{n} \|u^e_{(i)}\|^2} \]

- Experimental measurement of displacements \( u^e_{(i)} \)
- Displacements from numerical simulations \( u^s_{(i)} \)
- Unknown constitutive parameters \( \theta \)
- Index of fiber centroid \( i \)

• Asymptotic convergence of objective function with noisy data:

Measurement noise:

\[ u^e_{(i)} = u_{(i)} + \epsilon_{(i)} \]

- True displacement value \( u_{(i)} \)
- Independent random variable with zero mean and standard deviation \( \sigma_\epsilon \)

Asymptotic convergence of objective function by applying law of large number (LLN):

\[ L \to \frac{\sum_{i=1}^{n} \|u_{(i)} - u^s_{(i)}\|^2}{\sum_{i=1}^{n} \|u_{(i)}\|^2} + \frac{2n\sigma_\epsilon^2}{\sum_{i=1}^{n} \|u_{(i)}\|^2} \text{ if } n \to \infty \]

LLN requires continuity of \( u^s \) for each \( \theta \), guaranteed by strict convexity of potential energy with respect to \( u^s \), which is unconditionally satisfied.
Statistical consistency

- Output of optimization:
  \[ \hat{\theta}_n = \arg \min_\theta L \]

- Risk consistency:
  \[ L(\hat{\theta}_n) \rightarrow \frac{\min_\theta \sum_{i=1}^n \| \mathbf{u}_{(i)} - \mathbf{u}_{(i)}^s \|_2 + 2n\sigma^2}{\sum_{i=1}^n \| \mathbf{u}_{(i)} \|_2 + 2n\sigma^2} \quad \text{if } n \rightarrow \infty \]
  If \( \min_\theta \sum_{i=1}^n \| \mathbf{u}_{(i)} - \mathbf{u}_{(i)}^s \|_2 = 0 \), risk consistency is equivalent to: \( \mathbf{u}_{(i)}^s(\hat{\theta}_n) \rightarrow \mathbf{u}_{(i)}(\theta_0) \)

- Estimation consistency:
  \( \hat{\theta}_n \rightarrow \theta_0 \)
  It is satisfied if true parameter is identifiable from the true displacement: \( \mathbf{u}_{(i)}(\theta_0) = \mathbf{u}_{(i)}(\theta_1) \), only if \( \theta_0 = \theta_1 \)

- Discussion about identifiability condition (IC):
  - When the specimen has **uniform resin pocket**, identifiability condition is **not** held regardless of form of spatial variation;
  - If number of resin pockets > 1, the material model determines the minimum number of resin pockets with different sizes.

- IC is not satisfied
- IC is satisfied depending on material modeling.
Increasing sampling number of displacement

- Statistical consistency indicates that increasing sampling points can mitigate the noise effect.
- Ways of increasing sampling points for mitigating noise:
  - Increasing fiber number by enlarging specimen size with fixing fiber volume fraction.
    - Increasing fiber volume fraction will be later shown to be more sensitive to noise.
  - Combining measurements from multiple of experiments ($p$ times) regardless of loading conditions and specimen, while each experiment contains different noise.

\[
\min_{\theta} \frac{\sum_{i=1}^{n} \| u^e_{(i)} - u^s_{(i)} \|_2}{\sum_{i=1}^{n} \| u^e_{(i)} \|_2}
\]
Characterization tests using synthetic measurement

- Consider a two-dimensional (2-D) numerical specimen subjected to 1% strain-controlled compressive loading with \( p \) times.
- The synthetic measurements are generated from fiber centroid displacements, added with Gaussian noise \( N(0,0.1) \).
- The optimization problem is solved for characterizing spatial variance parameter \( E_{\text{int}} \) and \( \alpha \).

\[ E_{\text{int}} \]

- Assess objective function \( L \) at grid points in parameter space

\[ \min L \]

\[ \alpha \]

\[ u_{(i)}^c \] from \( p \) times loading

**Enumeration algorithm**

\[ E_{\text{int}} \]

Resin stiffness variation evidenced by nanoindentation test:

\[ E_m(y) = \left( E_{\text{int}} - \bar{E}_m \right) \exp(-\alpha l) + \bar{E}_m \]

- \( E_{\text{int}} \) – stiffness at fiber/matrix interface
- \( \alpha \) – variation of stiffness distribution
- \( \bar{E}_m \) – bulk stiffness
- \( l \) – distance from nearest fiber/matrix interface

Adapted from, Hardiman 2015

Convergence of prediction error

- 200 microns, 500 microns, 1 mm specimens with 55% volume fraction are respectively loaded different times ($p=1,2,5,10,20$).
- 100 optimizations are solved for the measurement assemblies with the sampling number of $n$.
- The variance (whisker) of prediction error due to randomness of noise reduces with increasing times of experiment.
Convergence of estimation error

- The estimation error is calibrated by maximum relative error of resin stiffness within the distribution:

\[ \epsilon_{\text{max}} = \max_{y} \left[ \frac{\hat{E}_m(y) - E_m(y)}{E_m(y)} \right] \]

- The error plot for 200 microns, 500 microns, 1 mm specimens loaded different times (p=1,2,5,10,20) are combined as a function of total sampling numbers \( n \).
- Bias and variance of maximum relative error of resin stiffness reduces from 40% to < 2% with more sampling number \( n \).
Effect of fiber volume fraction

- 500 microns specimens with 55%, 42%, 30%, 15% volume fraction are loaded different times (p=1,2,5,10,20).
- 100 optimizations are solved for the measurement assemblies with sampling number of $n$.
- Lower volume fraction enhance the precision of variation term $\alpha$, because more stiffness variance is revealed in larger resin pocket size.
- Characterization of spatial variation in resin-rich region is more precise with the presence of noise, although the number of measurement points is decreased.

$$e_{\text{max}} = \max_y \left[ \frac{\bar{E}_m(y) - E_m(y)}{E_m(y)} \right]$$
Sequential quadratic programming (SQP) is more applicable for parameter characterization with higher dimensions.

Finite difference method is employed for evaluating gradient of objective function with respect to parameters.

Multi-start method is employed. Each initialization is selected in the stratified region within the parameter space.

Characterization test of $E_{int}$, $\alpha$ and $\nu_m$ for 1 mm specimen loaded 10 times ($p=10$) with noise of $N(0,0.1)$.

The maximum stiffness error within the distribution ($e_{max}$) and the error of $\nu_m$ are respectively 1.28% and 0.05%.
Conclusions

• This study aims to inversely characterize \textit{in-situ spatially heterogeneous resin properties} in composite based on image-based measurement (e.g., fiber template matching).

• In the presence of noise, the displacement prediction and estimation of constitutive parameters converge to optimal value with incorporating more measurement points, by:
  ➢ increasing fiber samplings (enlarging specimen size with fixing fiber volume fraction)
  ➢ increasing experiment times or more loading frames.

• Resin-rich region can enable more accurate prediction of spatial variation with the presence of noise.

• SQP approach is applicable for characterization of more than two constitutive parameters, the estimation error is about 1%.
Thank you!