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

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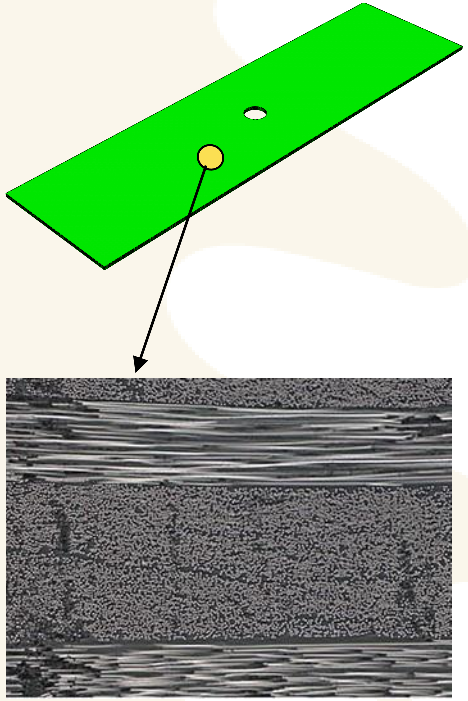
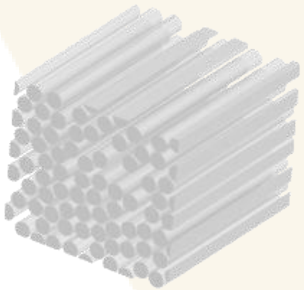
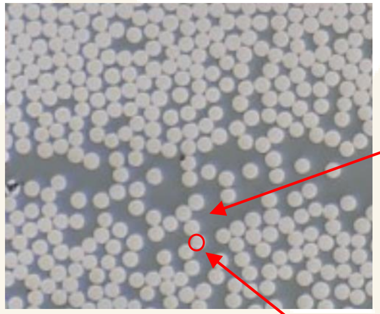
Motivations

- 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.





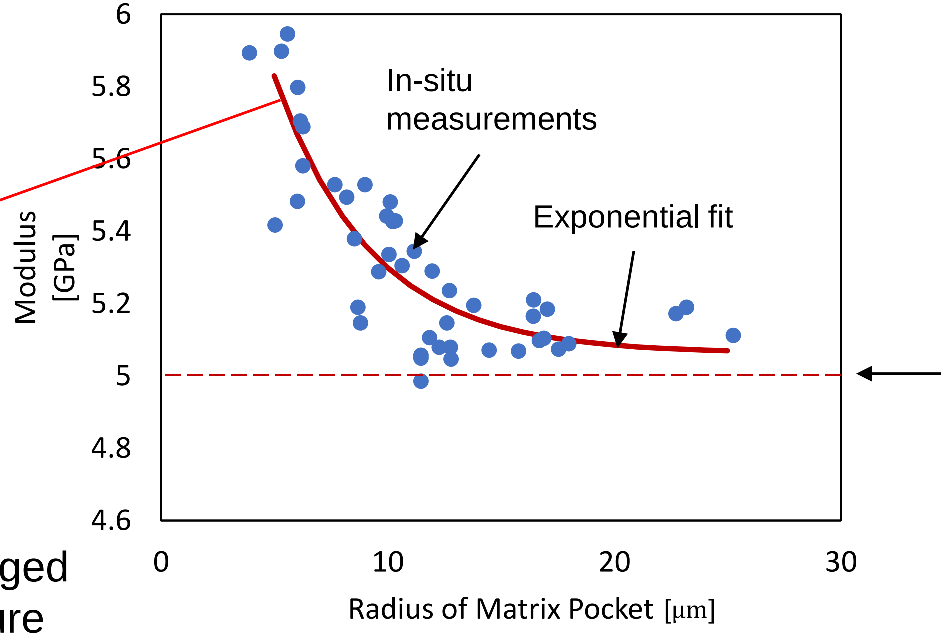


Adapted from, Smith 2019

Epoxy resin properties

Fiber properties not changed during the curing procedure

Adapted from, Hardiman 2015

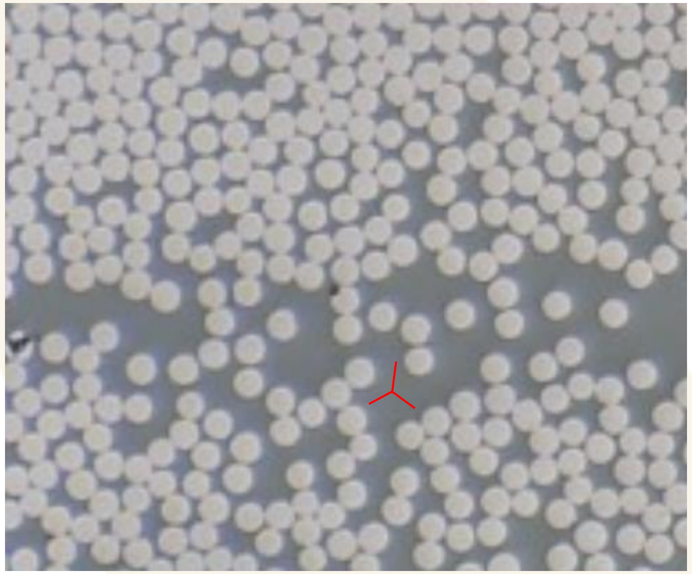


Austin J. Smith, "Microscale characterization and ply level modeling of transverse fracture in polymer-matrix composites", Master Thesis, University of Utah, 2019.

Hardiman, M., T. J. Vaughan, and C. T. McCarthy. "Fibrous composite matrix characterisation using nanoindentation: The effect of fibre constraint and the evolution from bulk to in-situ matrix properties." Composites Part A: Applied Science and Manufacturing 68 (2015): 296-303.

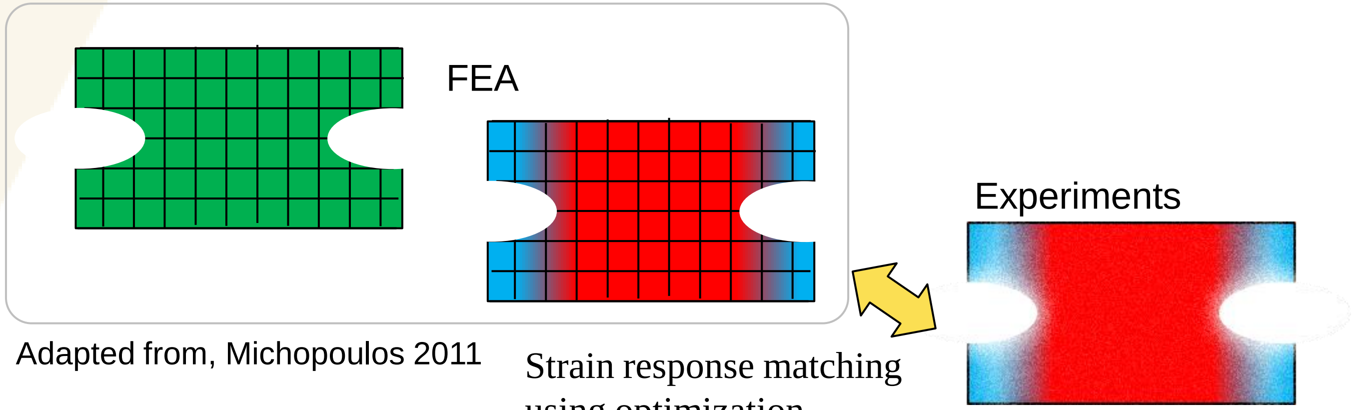
Objectives and background

- 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:



Adapted from, Smith 2019

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



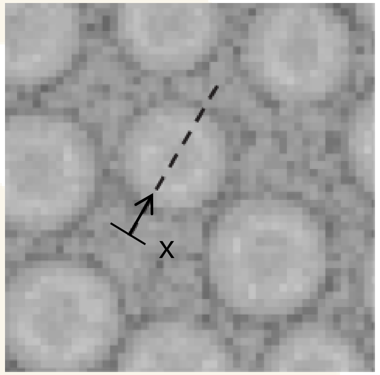
Adapted from, Michopoulos 2011

Strain response matching using optimization

Michopoulos, John G., et al. "On the constitutive response characterization for composite materials via data-driven design optimization." International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. Vol. 547
Austin J. Smith, “Microscale characterization and ply level modeling of transverse fracture in polymer-matrix composites“, Master Thesis, University of Utah, 2019.

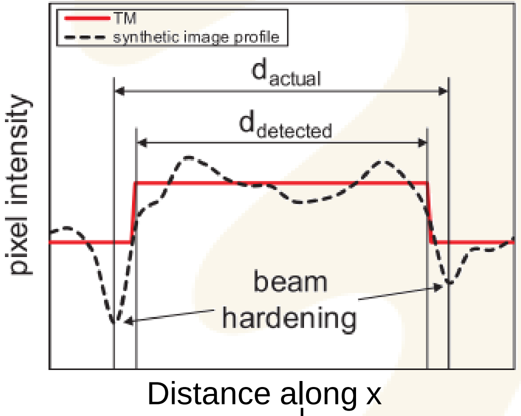
➢ Image-based measurement using template matching (TM):

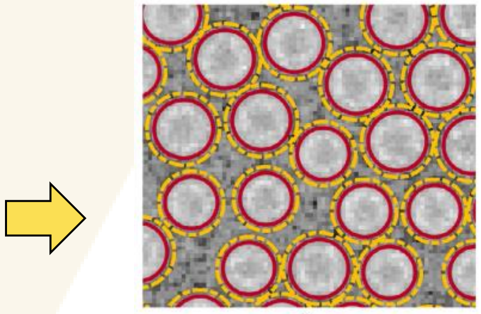
DIC or X-ray microtomography image

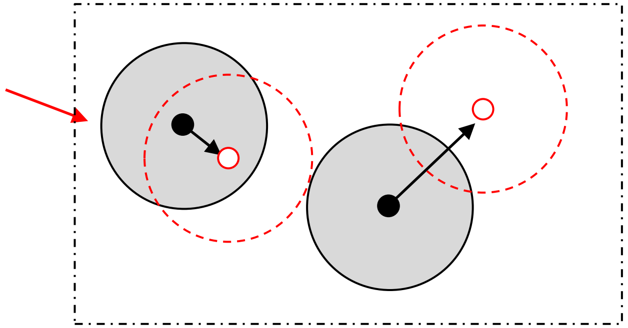


Creveling 2019

Detection of fiber diameter (d)

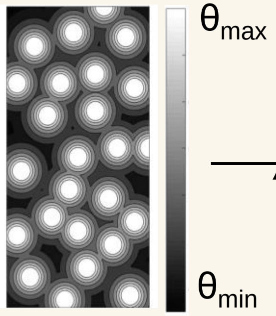




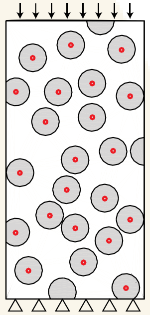


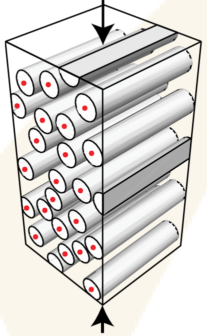
➢ Inverse characterization procedure:

Model Initialization with spatial variation



FEA:





Displacement $\mathbf{u}^e$ from template matching

Displacement $\mathbf{u}^s$ from numerical simulations

Assess objective function

$\mathscr{L} = f\left(\|\mathbf{u}^s - \mathbf{u}^e\|\right)$

Minimization?

Yes → Output

No → Adjust constitutive parameter θ

Creveling, Peter J., William W. Whitacre, and Michael W. Czabaj. "A fiber-segmentation algorithm for composites imaged using X-ray microtomography: Development and validation." Composites Part A: Applied Science and Manufacturing 126 (2019): 105606.

Optimization with noise

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

$$L(\boldsymbol{\theta}) = \frac{\sum_{i=1}^{n} \|\mathbf{u}_{(i)}^{e} - \mathbf{u}_{(i)}^{s}\|_2}{\sum_{i=1}^{n} \|\mathbf{u}_{(i)}^{e}\|_2}$$

$\mathbf{u}_{(i)}^{e}$ - Experimental measurement of displacements $\mathbf{u}_{(i)}^{s}$ - Displacements from numerical simulations

θ - Unknown constitutive parameters i - index of fiber centroid

- Asymptotic convergence of objective function with noisy data:

Measurement noise: $\mathbf{u}_{(i)}^{e} = \mathbf{u}_{(i)} + \boldsymbol{\epsilon}_{(i)}$

$\mathbf{u}_{(i)}$ - True displacement value $\boldsymbol{\epsilon}_{(i)}$ - independent random variable with zero mean and standard deviation of σ_{ε}

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

$$L \rightarrow \frac{\sum_{i=1}^{n} \|\mathbf{u}_{(i)} - \mathbf{u}_{(i)}^{s}\|_2 + 2n\sigma_{\epsilon}^2}{\sum_{i=1}^{n} \|\mathbf{u}_{(i)}\|_2 + 2n\sigma_{\epsilon}^2} \quad \text{if} \quad n \rightarrow \infty$$

LLN requires continuity of u^s for each θ, guaranteed by *strict convexity* of potential energy with respect to u^s, which is unconditionally satisfied.

- Output of optimization: $$\hat{\boldsymbol{\theta}}_n = \arg\min_{\boldsymbol{\theta}} L$$

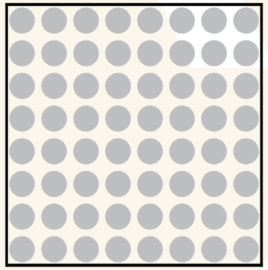
- Risk consistency: $$L(\hat{\boldsymbol{\theta}}_n) \rightarrow \frac{\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \|\mathbf{u}_{(i)} - \mathbf{u}^s_{(i)}\|_2 + 2n\sigma_\epsilon^2}{\sum_{i=1}^{n} \|\mathbf{u}_{(i)}\|_2 + 2n\sigma_\epsilon^2} \quad \text{if} \quad n \rightarrow \infty$$

If $\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \|\mathbf{u}_{(i)} - \mathbf{u}^s_{(i)}\|_2 = 0$, risk consistency is equivalent to: $\mathbf{u}^s_{(i)}(\hat{\boldsymbol{\theta}}_n) \rightarrow \mathbf{u}_{(i)}(\boldsymbol{\theta}_0)$

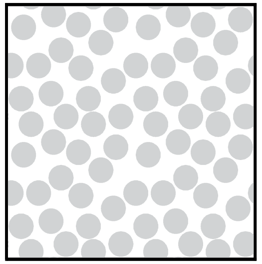
- Estimation consistency: $$\hat{\boldsymbol{\theta}}_n \rightarrow \boldsymbol{\theta}_0$$

It is satisfied if *true parameter is identifiable* from the true displacement: $\mathbf{u}_{(i)}(\boldsymbol{\theta}_0) = \mathbf{u}_{(i)}(\boldsymbol{\theta}_1)$, only if $\boldsymbol{\theta}_0 = \boldsymbol{\theta}_1$

- 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.



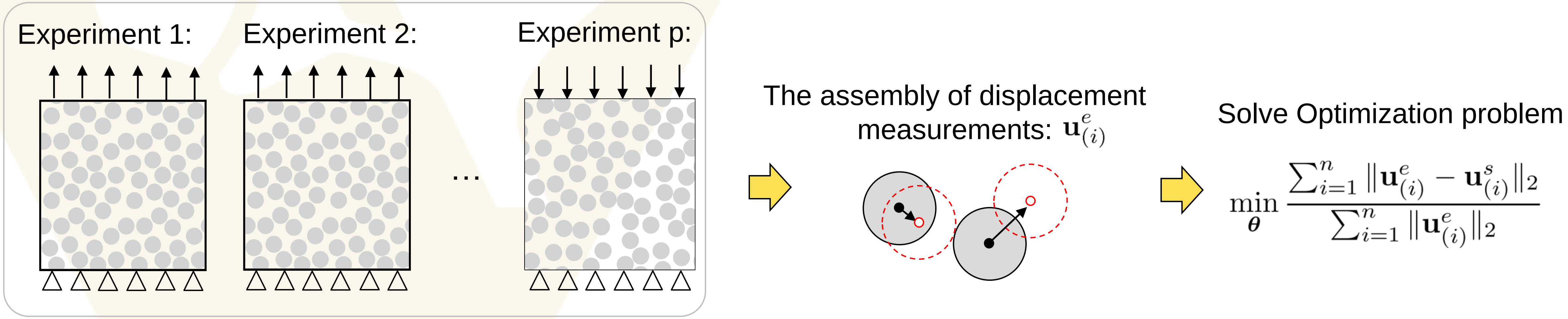
IC is not satisfied



IC is satisfied depending on material modeling.

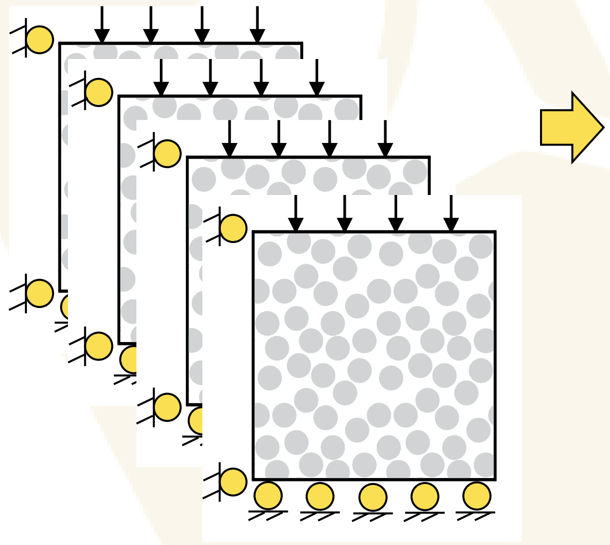
Increasing sampling number of displacement

- 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.

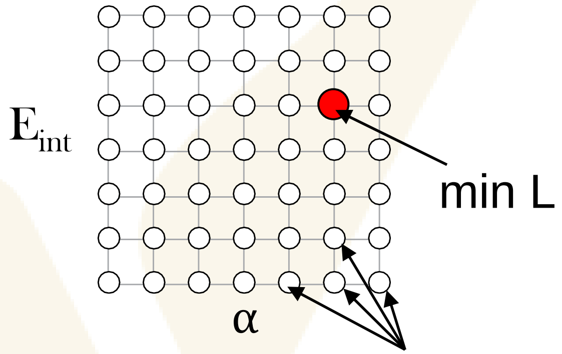


- Consider a two-dimensional (2-D) numerical specimen subjected to 1% strain-controlled compressive loading with p times.
- The synthetic measurements are generated from fiber centroid displacements, added with Gaussian noise N(0,0.1).
- The optimization problem is solved for characterizing spatial variance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

$\mathbf{u}^e_{(i)}$ from p times loading

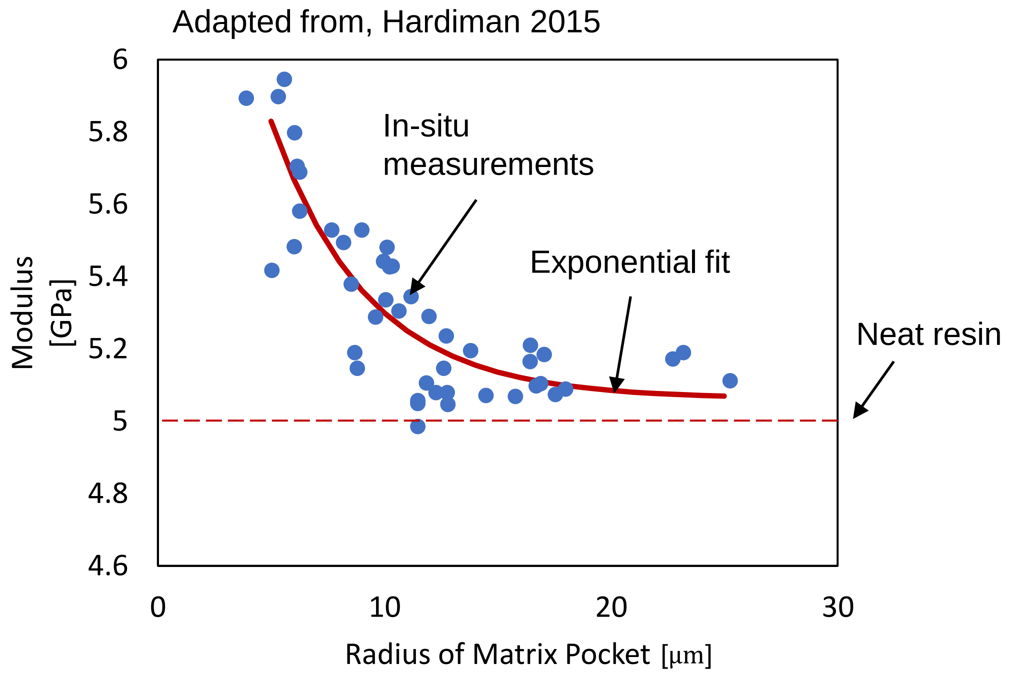


Enumeration algorithm



Assess objective function L at grid points in parameter space

Resin stiffness variation evidenced by nano-indentation test :



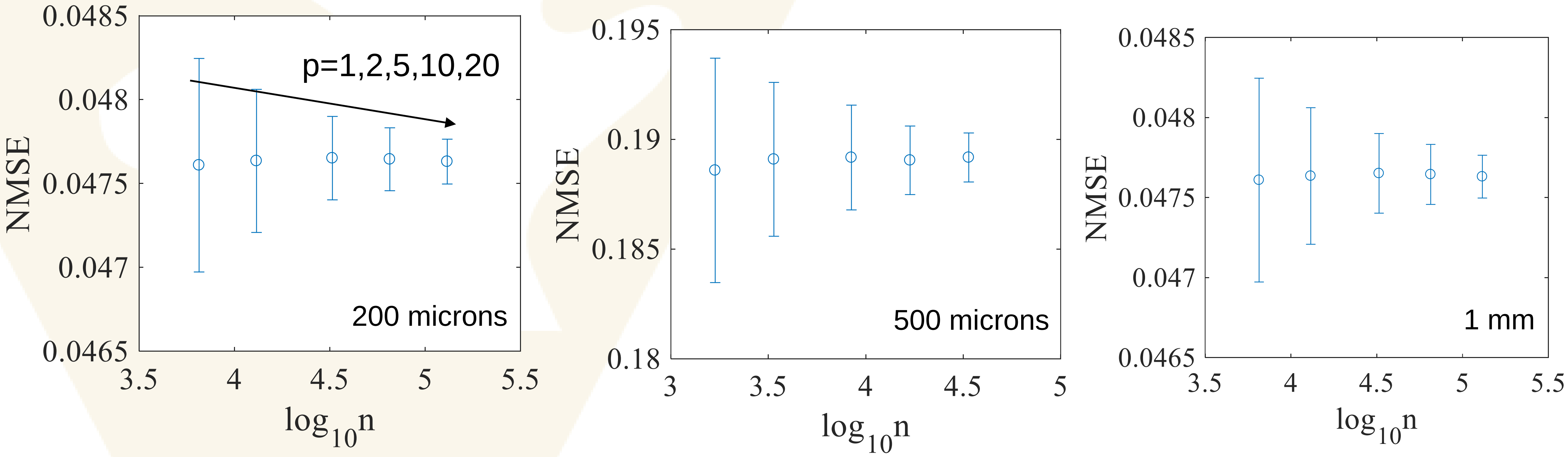
$$E_{\mathrm{m}}(\mathbf{y}) = \left(E_{\mathrm{int}} - \bar{E}_{\mathrm{m}}\right) \exp\left(-\alpha l\right) + \bar{E}_{\mathrm{m}}$$

E_{int} – stiffness at fiber/matrix interface
α – variation of stiffness distribution
$\bar{E}_{\mathrm{m}}$ –bulk stiffness
l – distance from nearest fiber/matrix interface

Hardiman, M., T. J. Vaughan, and C. T. McCarthy. "Fibrous composite matrix characterisation using nanoindentation: The effect of fibre constraint and the evolution from bulk to in-situ matrix properties." Composites Part A: Applied Science and Manufacturing 68 (2015): 296-303.

Convergence of prediction error

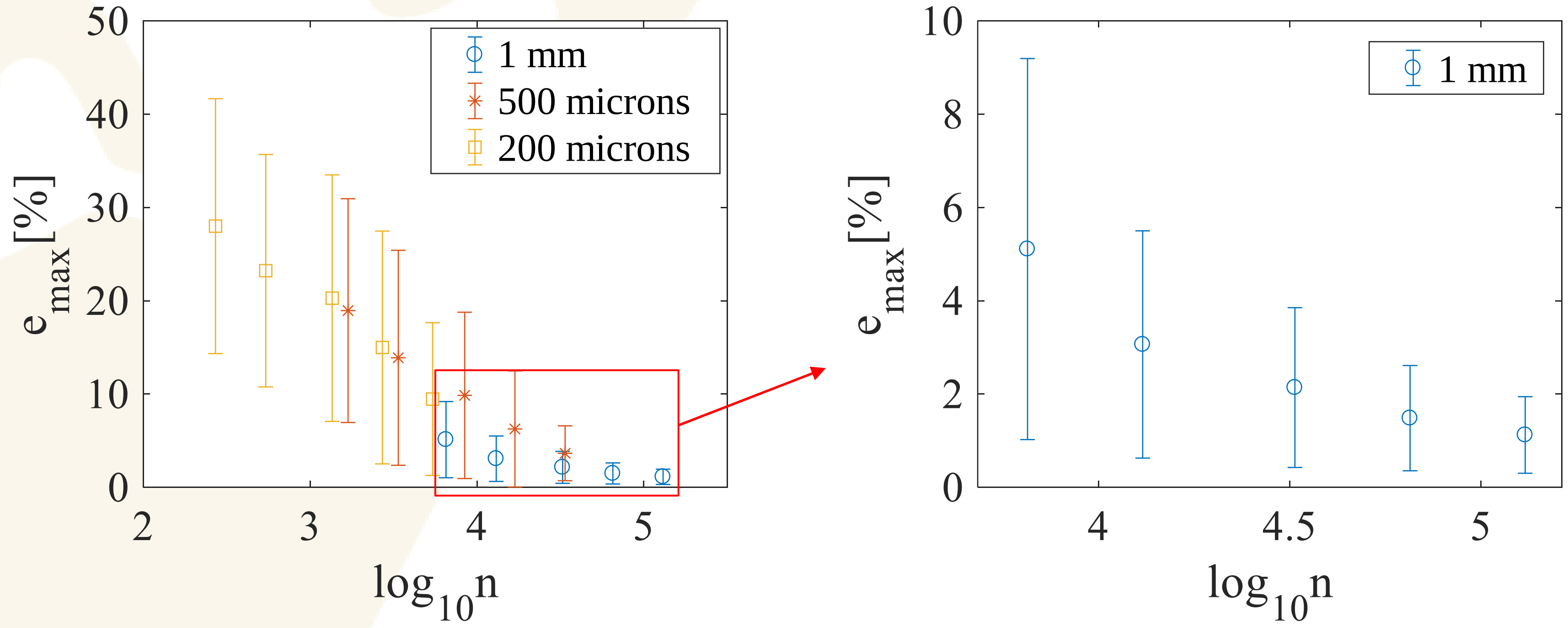
- 200 microns, 500 microns, 1 mm specimens with 55% volume fraction are respectively loaded different times (p=1,2,5,10,20).
- 100 optimizations are solved for the measurement assemblies with the sampling number of *n.*
- The variance (whisker) of prediction error due to randomness of noise reduces with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



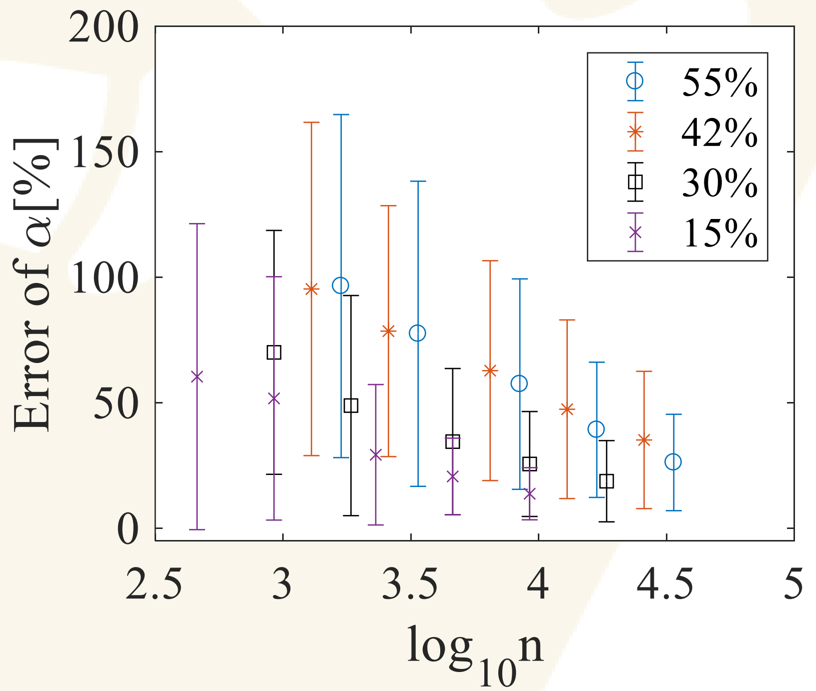
- The estimation error is calibrated by maximum relative error of resin stiffness within the distribution:

$$e_{\max} = \max_{\mathbf{y}} \left[\hat{E}_m(\mathbf{y}) - E_m(\mathbf{y}) \right] / E_m(\mathbf{y})$$

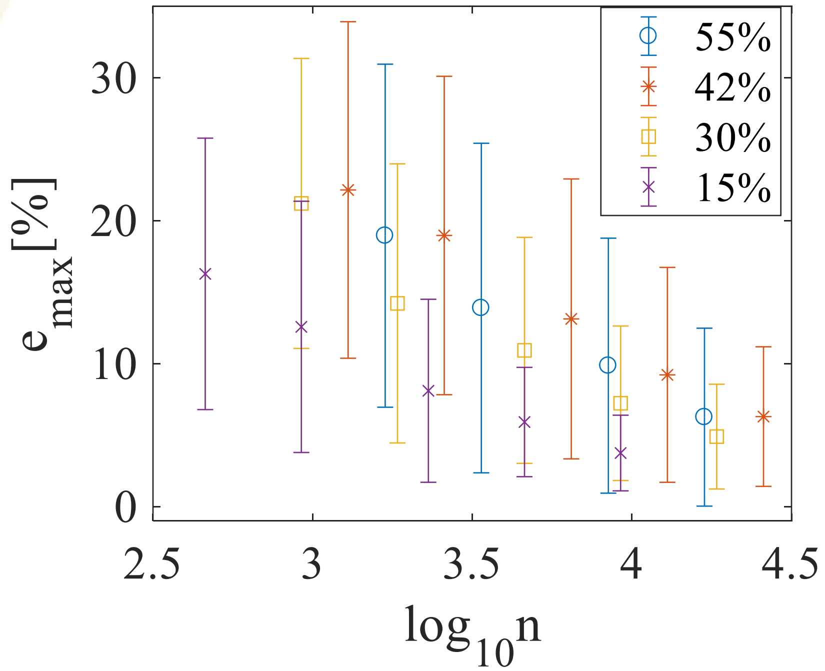
- The error plot for 200 microns, 500 microns, 1 mm specimens loaded different times (p=1,2,5,10,20) are combined as a function of total sampling numbers *n*.
- Bias and variance of maximum relative error of resin stiffness reduces from 40% to < 2% with more sampling number *n*.



- 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 α, 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.



$$e_{\max} = \max_{\mathbf{y}} \left[\hat{E}_m(\mathbf{y}) - E_m(\mathbf{y}) \right] / E_m(\mathbf{y})$$



Characterization using SQP approach

- 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} , α and ν_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 ν_m are respectively 1.28% and 0.05%.

Conclusions

- This study aims to inversely characterize *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!