Atomistically Informed Nano to Macroscale Modeling of Advanced Composites

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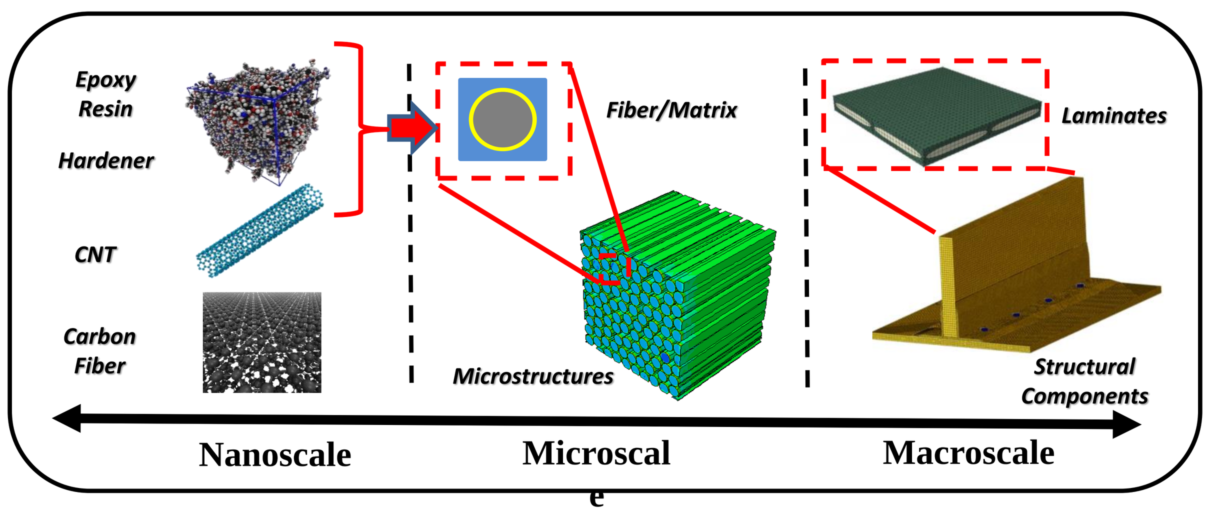
Objectives:

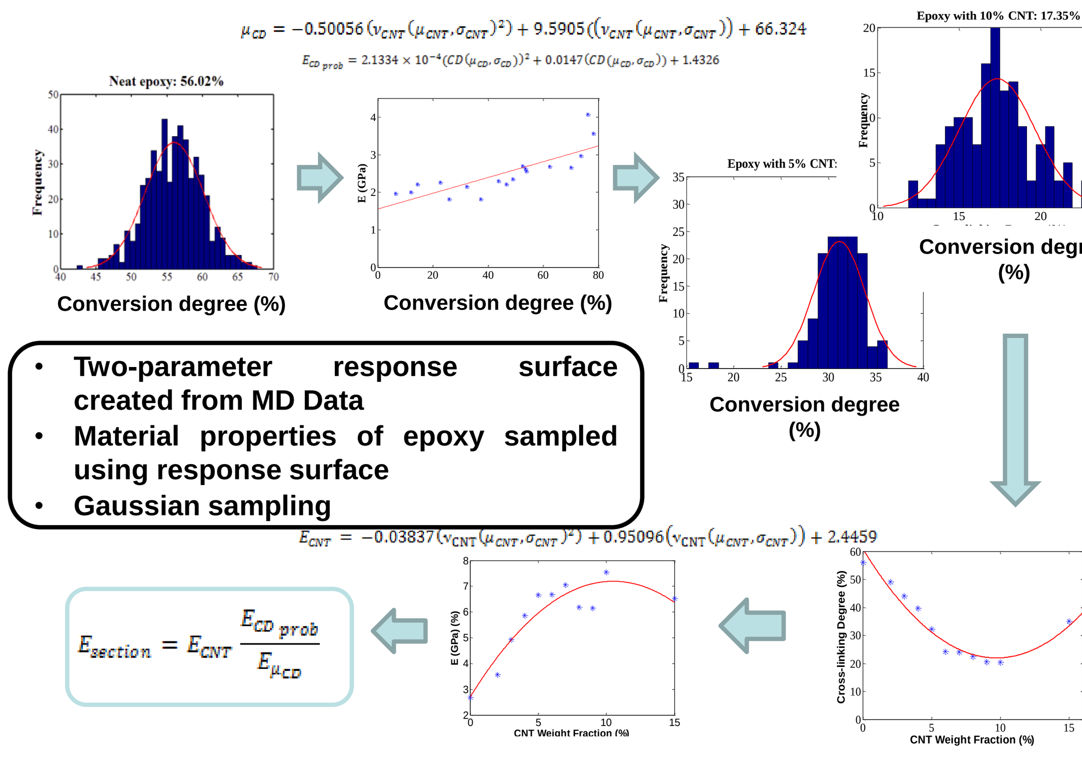
- Develop stochastic multiscale model for CFRPs and CNT/CFRP structures which utilize nanoscale information
- Investigate nonlinear, multifunctional, and causal effects of damage initiation and propagation in advanced composites
- Utilize low fidelity damage models for macroscale integration and analysis of composite structures

Motivation



- Advanced composite structures present many mechanical/multifunctional benefits
- Nanocomposites with CNTs: Stiff and strong, ideal filler material
- Lack of accurate predictive models for material engineering or structural analysis
- Experimental trial and error is too expensive and time consuming
- *Large divide between theory and experiments*

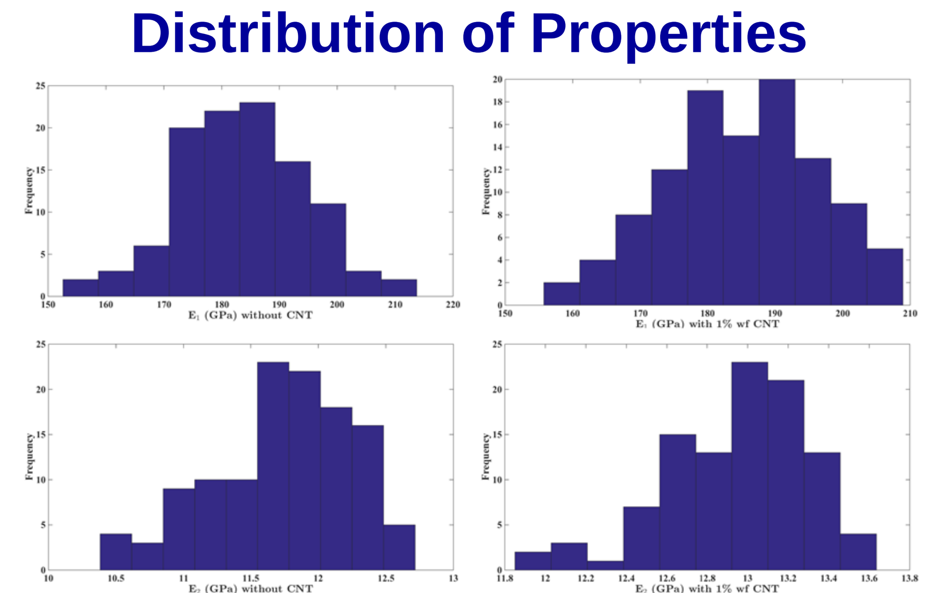
Bridging Elastic information



- Two-parameter response surface created from MD Data
- Material properties of epoxy sampled using response surface
- Gaussian sampling

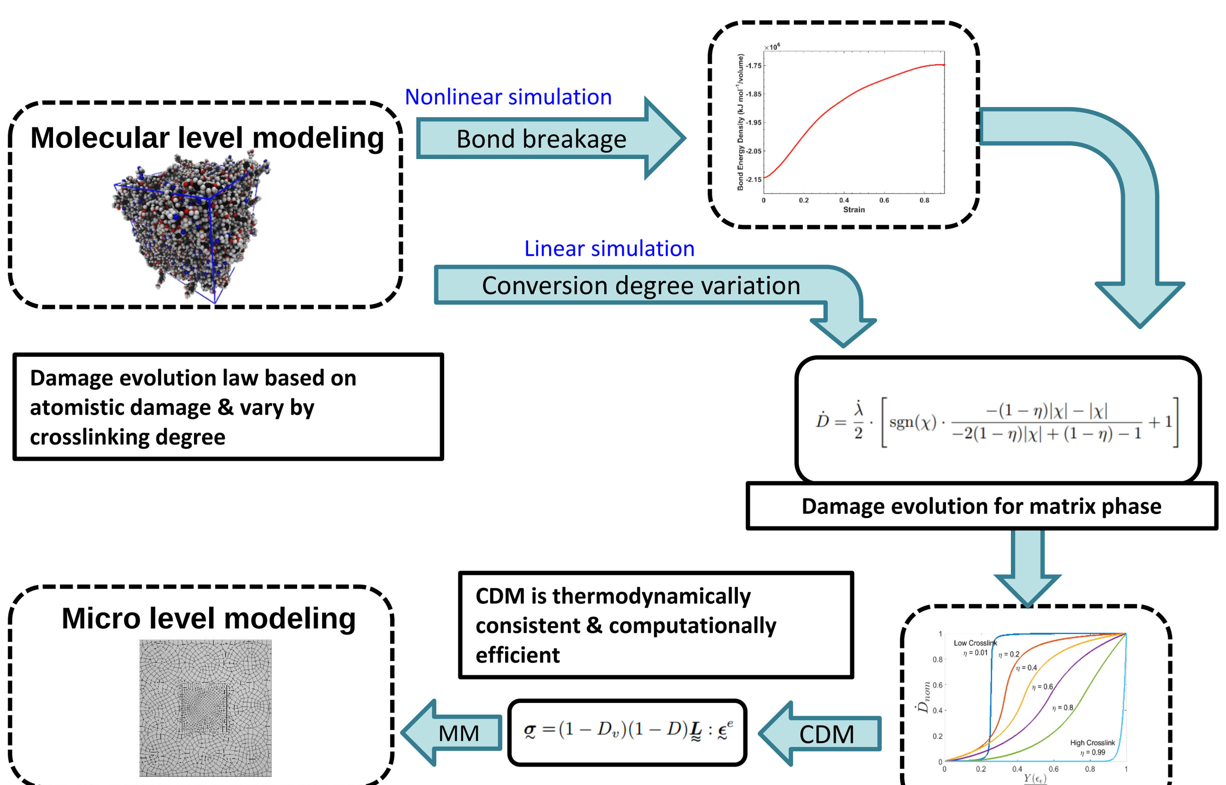
$$E_{section} = E_{CNT}\frac{E_{CD\,prob}}{E_{\mu_{CD}}}$$

Distribution of Properties



- Obtained a PDF of elastic constants
- Comparisons with experiments:
  - 0.3% error in mean of E1
  - 3.1% error in standard deviation of E1
  - 2.3% error in mean of E2
  - 10.6% error in standard deviation of E2

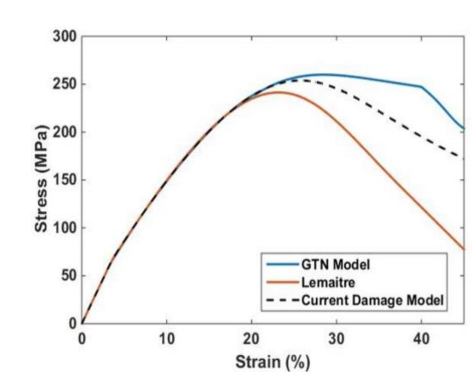
Information Transfer

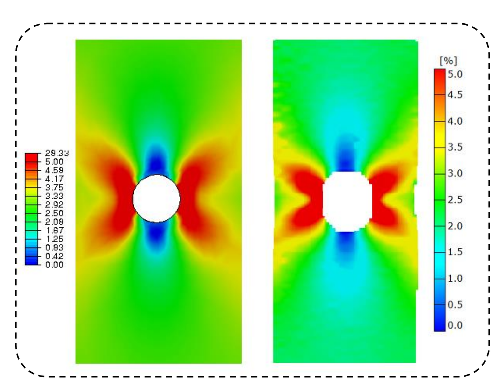


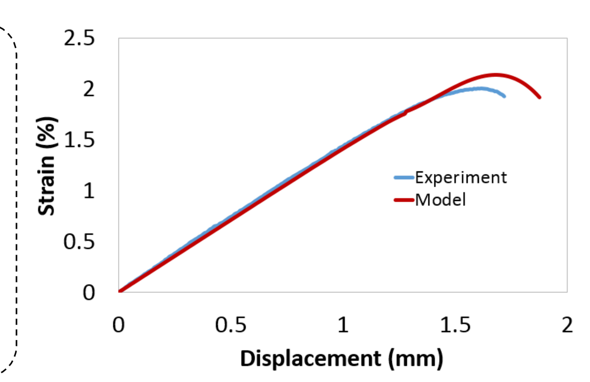
Rai et al., J of Comp (2016)

Polymer Damage Model Validation

- Various validation strategies used:
  - *Benchmarking with established models*
  - *Experimental approaches*
  - *Comparing local stress fields*

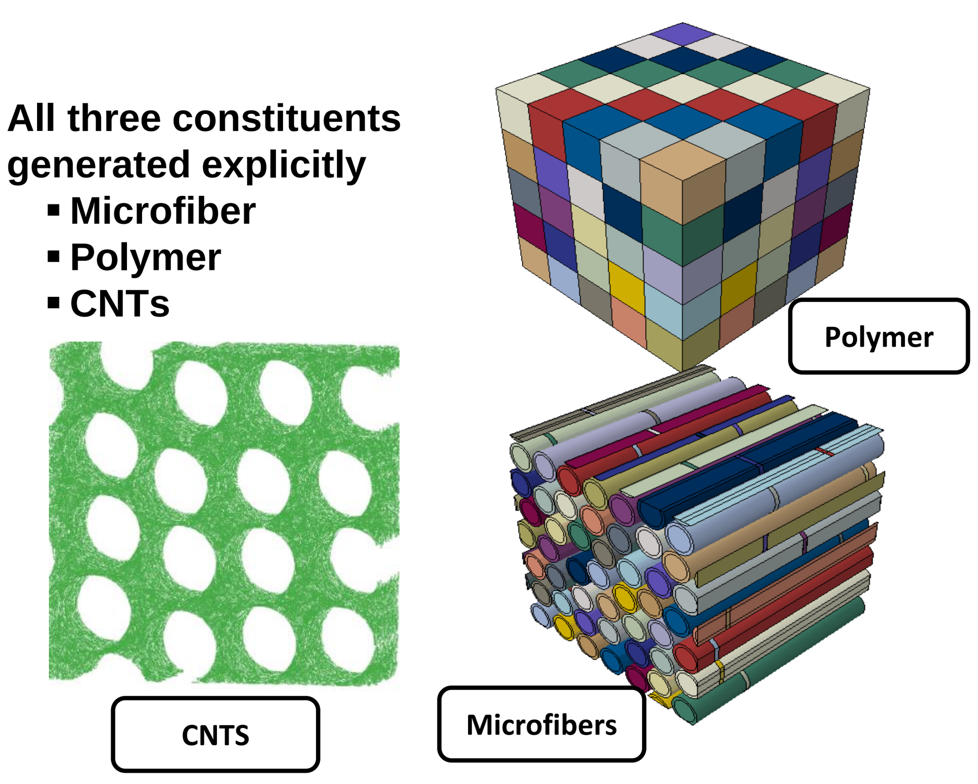




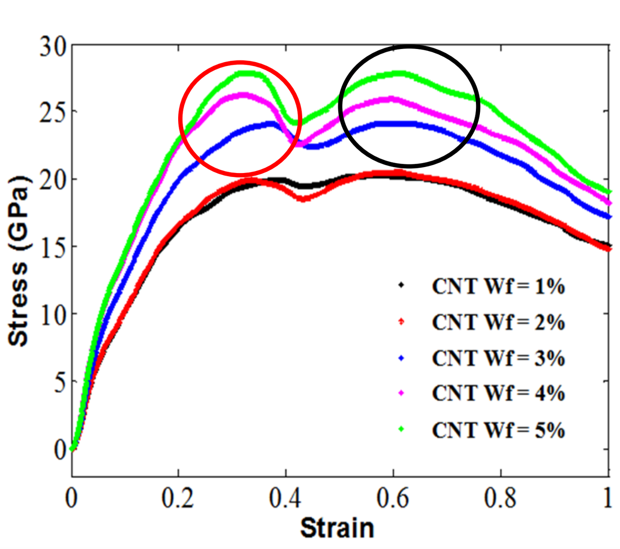


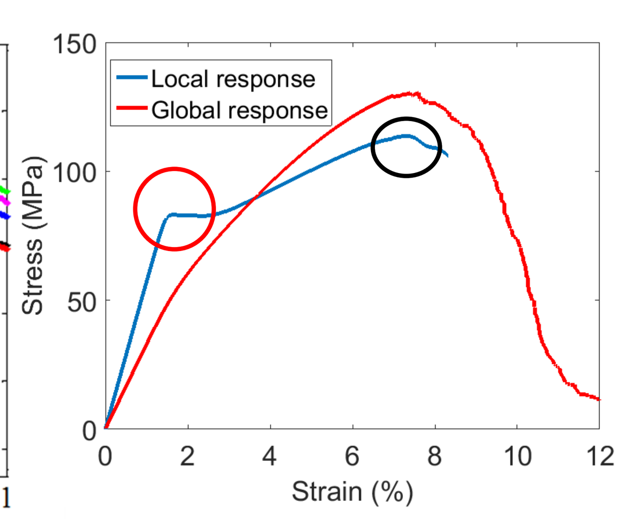
Microstructure Generation

- All three constituents generated explicitly
  - Microfiber
  - Polymer
  - CNTs



Stress Field in Vicinity of Nanofillers





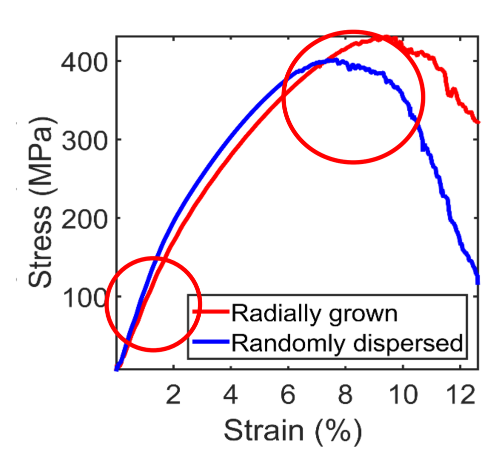
Two softening phases observed in MD
Two softening phases observed in local FE

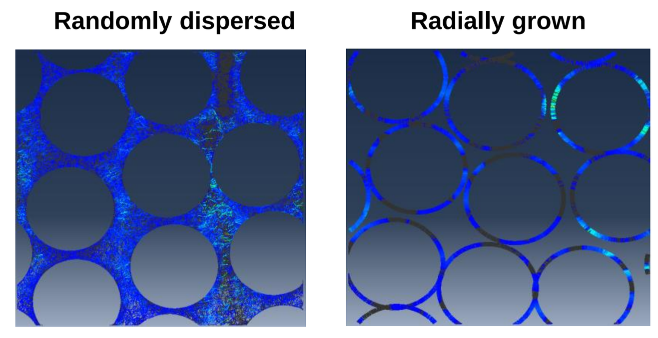
Microstructure Investigations

- Microstructures with 0.1% wf CNT generated
- Tested in transverse direction
- Elastic and damage response was studied

Randomly dispersed configuration shows slightly higher elastic behavior

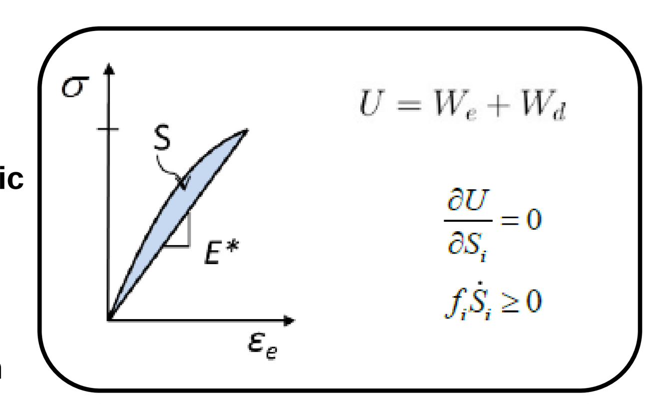
Radially grown configuration shows better damage behavior





Low-fidelity Damage Model for Matrix

- Represent matrix response using Schapery potential theory
- Straight forward for isotropic damage since single ISV required
- Orthotropic response requires modified definition of the ISVs
- One ISV for strain in each direction
- ISV as a function of binary parameters activated on existence of strain
- Elastic constants are a function of ISVs



$$U = W_e + W_d \qquad \frac{\partial U}{\partial S_i} = 0 \qquad f_i\dot{S}_i \geq 0$$

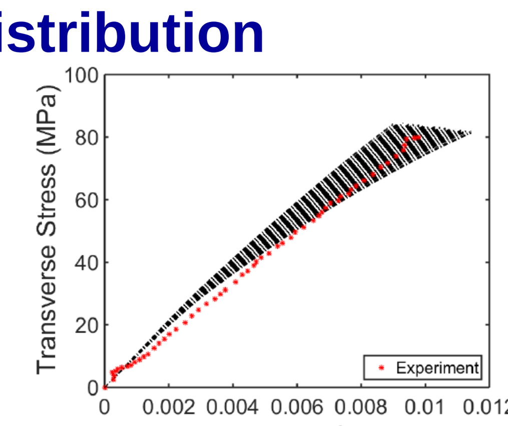
$$W_d = \sum_{i=1}^{i=6} S_i \qquad S_i = \delta_i s_i$$

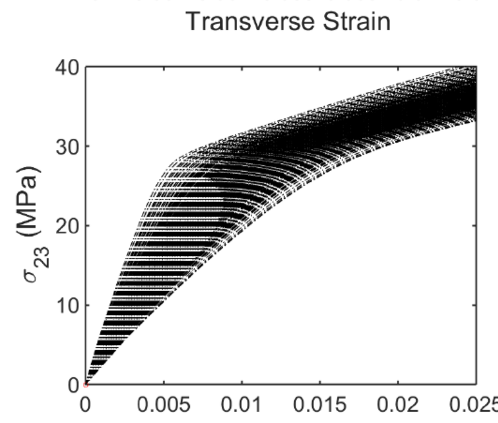
$$\delta_i = \begin{cases} 1 & \text{when } |\epsilon_{11}| > 0 \text{ and} \\ 0 & \text{when } |\epsilon_{11}| = 0 \end{cases}$$

$$\frac{\partial W_e}{\partial s_i} = -\delta_i$$

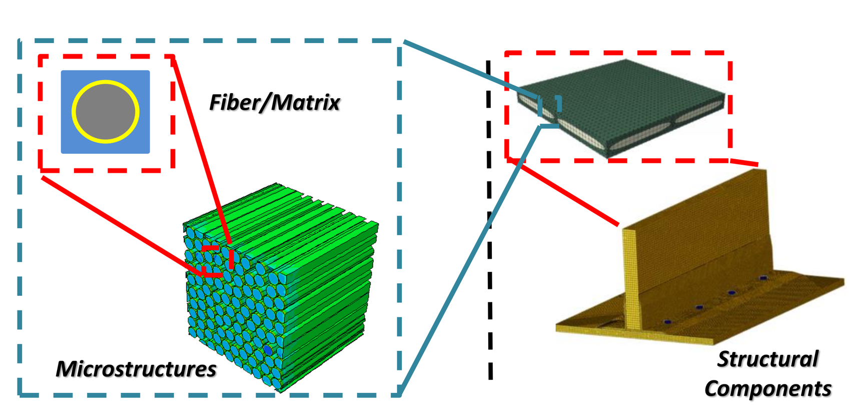
Response Distribution

- Two sources of variability:
  - Volume fraction
  - Matrix properties
- 1000 simulations, randomly sampled
- Processing time: 30-45 minutes
- Transverse loading – tight response, failure strain change
- Shear loading – large spread; higher non-linearity for stiff response
- Average response discouraged for design



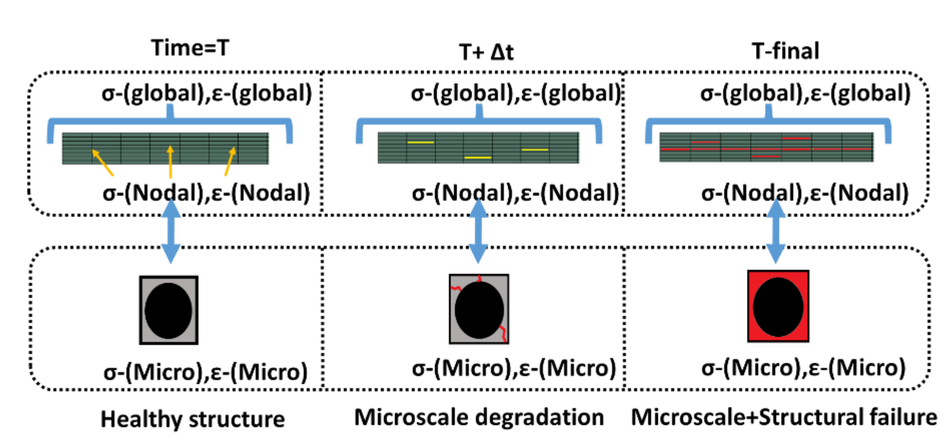


Integration to the Macroscale



- Macroscale model integration for structural analysis
- Structural composite bonded joints as case study
  - Limited use due to lack of appropriate analysis methods and damage initiation, progression and failure criteria
  - Introduction of bolts leading to overdesign
  - Unoptimized designs
- Can be used more effectively with comprehensive models to predict damage and failure

Methodology



- Structural Analysis -> FE
- FE integration point - > Microstructure representation
- Microstructure Analysis -> MoC Micromechanics
- Matrix -> Low fidelity damage models
- Matrix analysis -> atomistically informed damage model

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