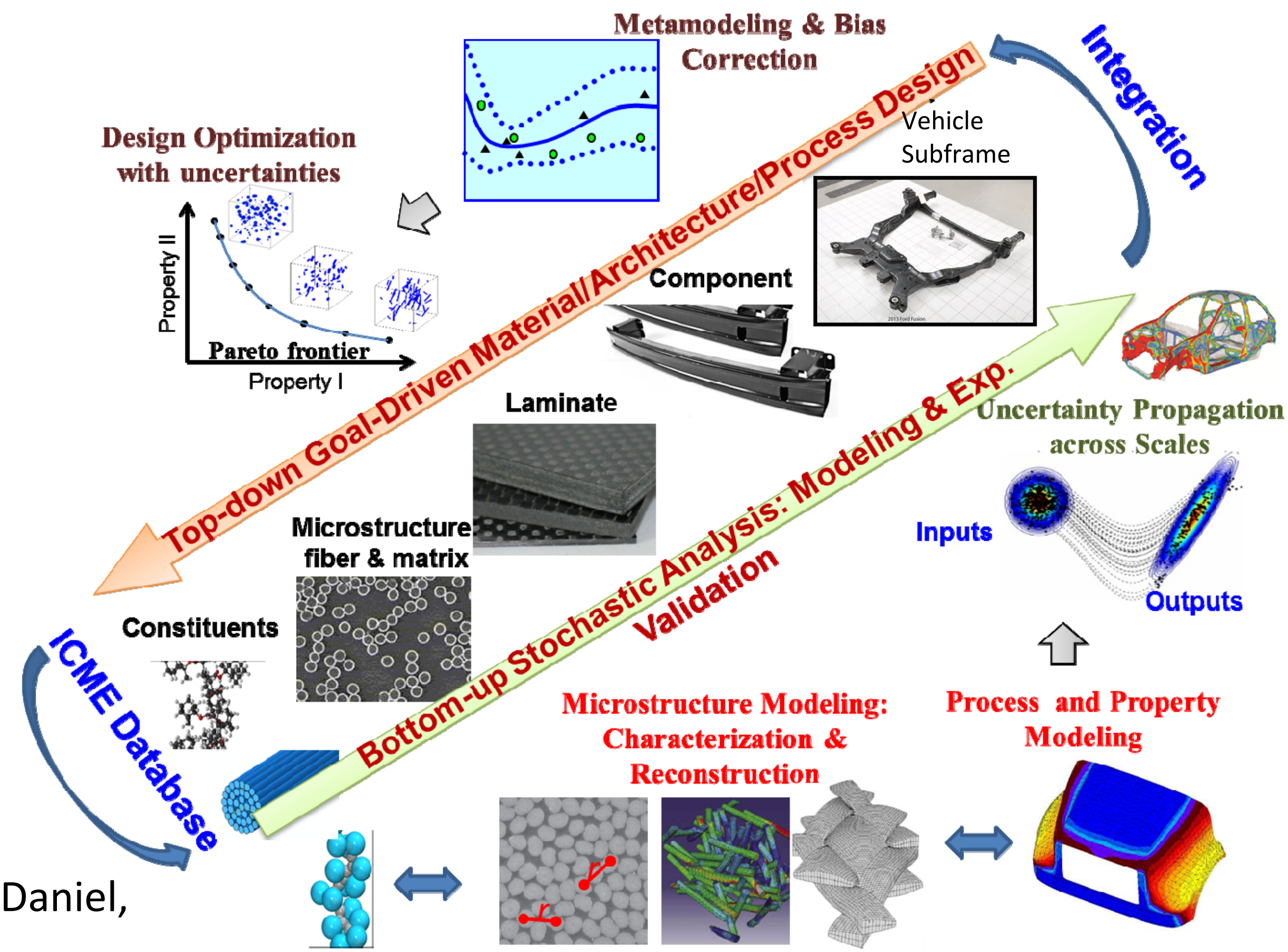
ICME Framework for Carbon Fiber Composite

- Bottom-up multi-physics, multi-scale modeling
- Top-down goal-driven design & optimization
- Integration of uncertainties of materials, processes, and in-service conditions



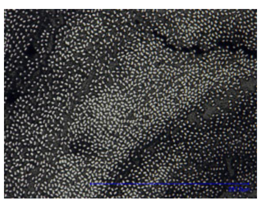
NU PIs:
Cao, Chen, Daniel,
Keten, Liu

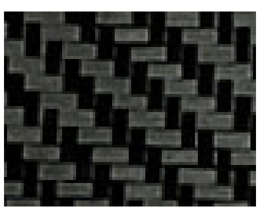
For public release

ICME Development of Carbon Fiber Reinforced Polymer

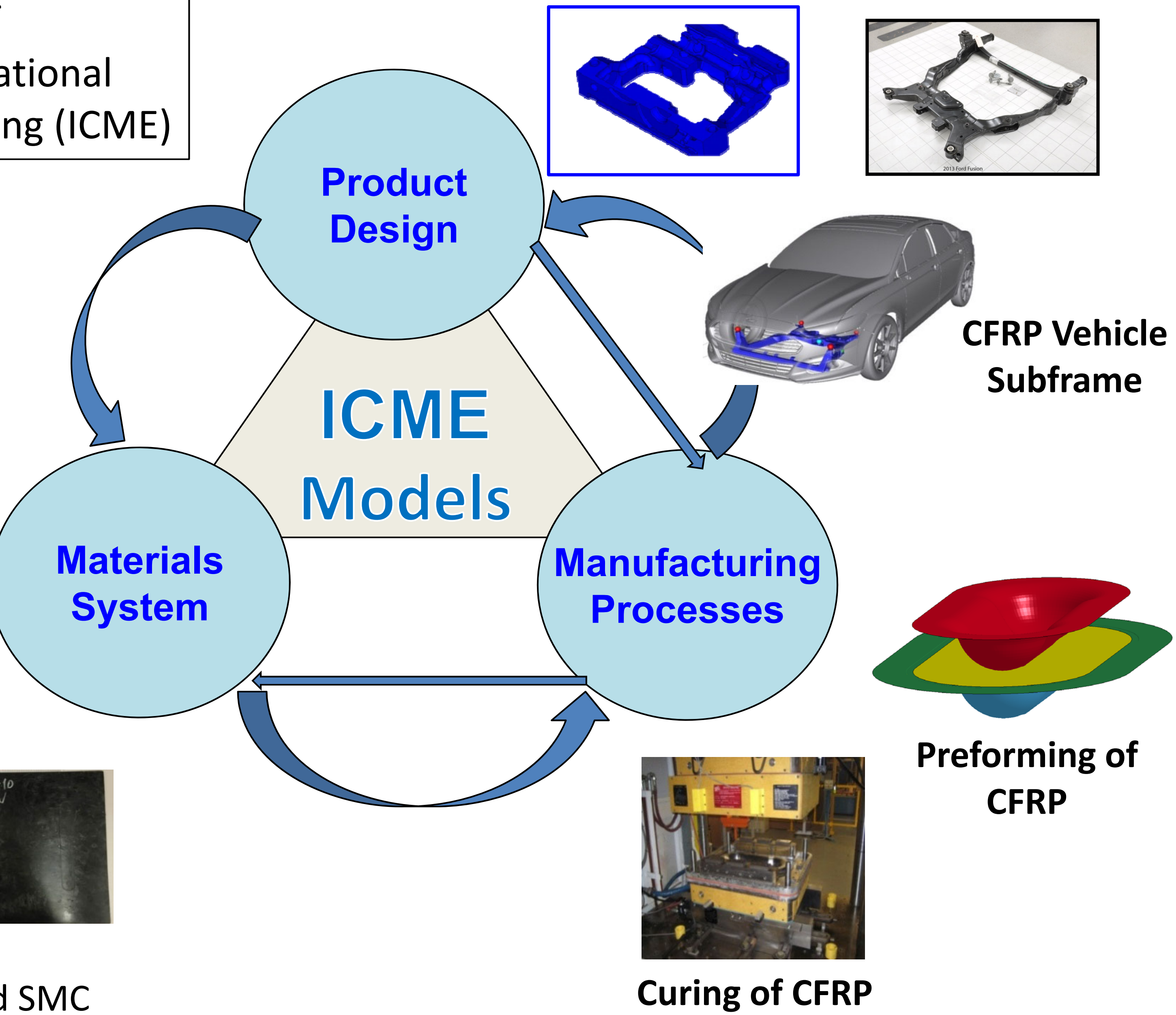
The holy triangle of Integrated Computational Materials Engineering (ICME)

Unidirectional (UD), Woven, and Sheet Molding Compound (SMC) Chopped Fiber





Top: UD
Bottom: Woven and SMC



Project Objective

<u>Overall Objectives</u>

Develop ***<u>predictive</u>*** *<u>Integrated Computational Materials Engineering</u>* (*<u>ICME</u>*) modeling tools for Carbon Fiber Reinforced Polymer (CFRP):

- Precise *<u>materials characterization</u>* for different CFRP systems
- *<u>Materials Constituent</u>* information from *<u>Molecular Dynamic</u>* simulation (Epoxy, Fiber, and Interphase)
- Accurate prediction of *<u>CFRP materials parameters</u>* (≤10% to test data)
- ***<u>Multiscale simulation framework for UD and Woven CFRP</u>***
- Predictive model for *<u>different processes</u>* (preforming, modeling)
  - Material models based on material design and manufacturing processes
  - CAE analysis accounting for local material variations due to process influences
- Integrated CFRP design loop considering all above

<u>Utilize ICME tools to provide design guidance on CFRP material</u>

Project Organization

Department of Energy
Project Manager: *Jerry Parker*
Technology Manager: *Carol Schutte*

Ford Motor Company
Principal Investigator: *Xuming Su, David Wagner*
Business Manager: *Melissa Hendra*

- Northwestern University
- Dow Chemical Company
- University of Maryland / NIST
- LSTC LS-DYNA®
- HBM nCode®
- Autodesk Moldflow®
- ESTECO modeFRONTIER®

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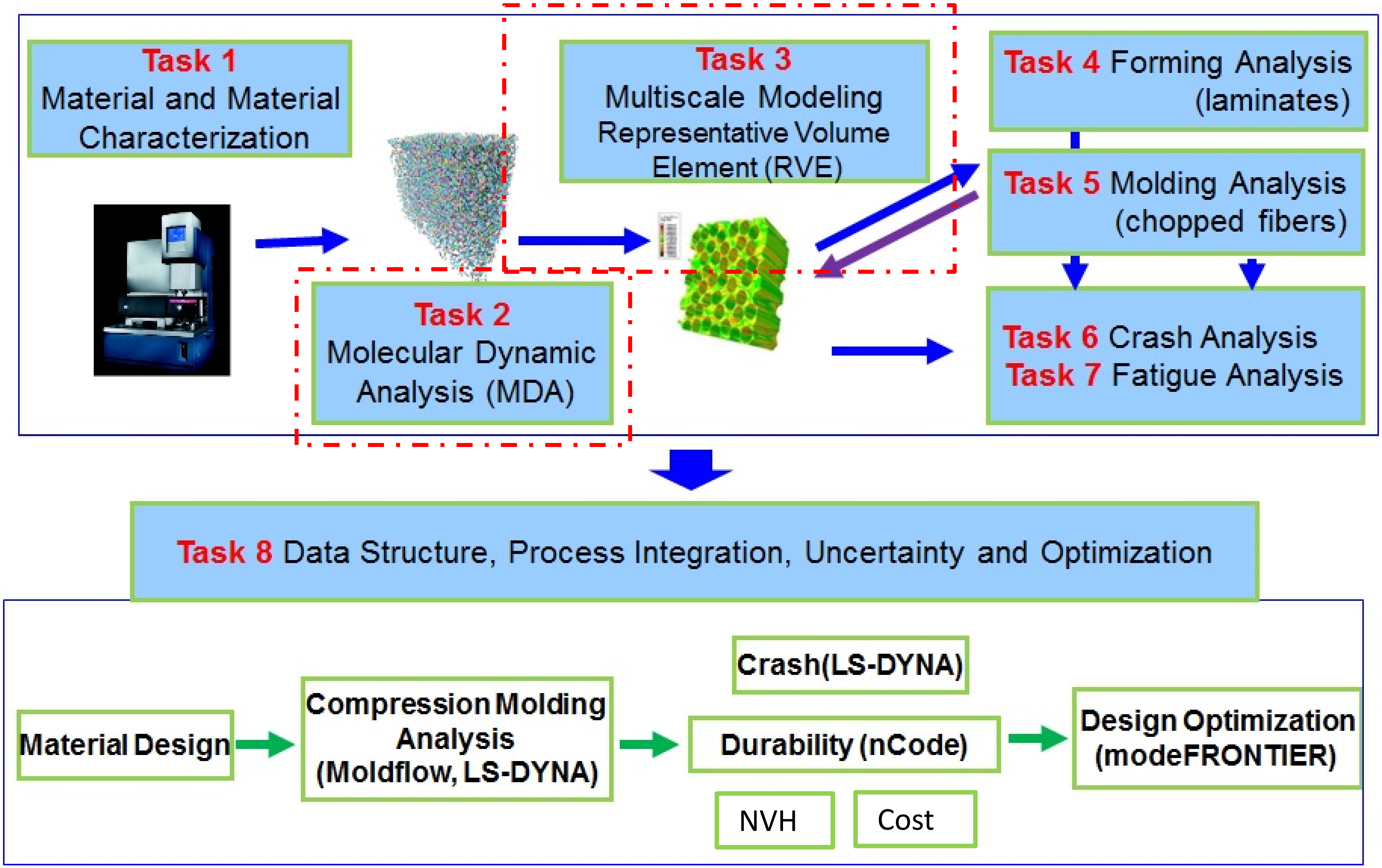
Huaqing Ren
Zeliang Liu

modeFRONTIER
Zhendan Xue

Approach: Task Teams and Task Integration

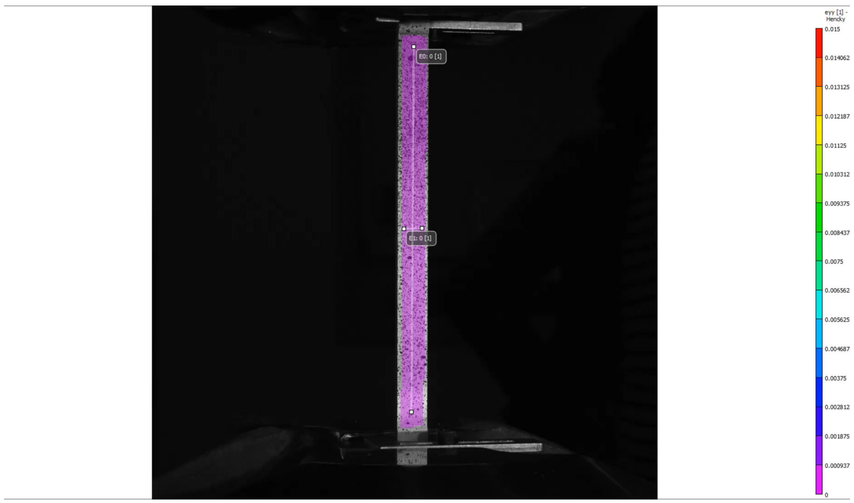


Highlight in Material Characterization (Task 1)

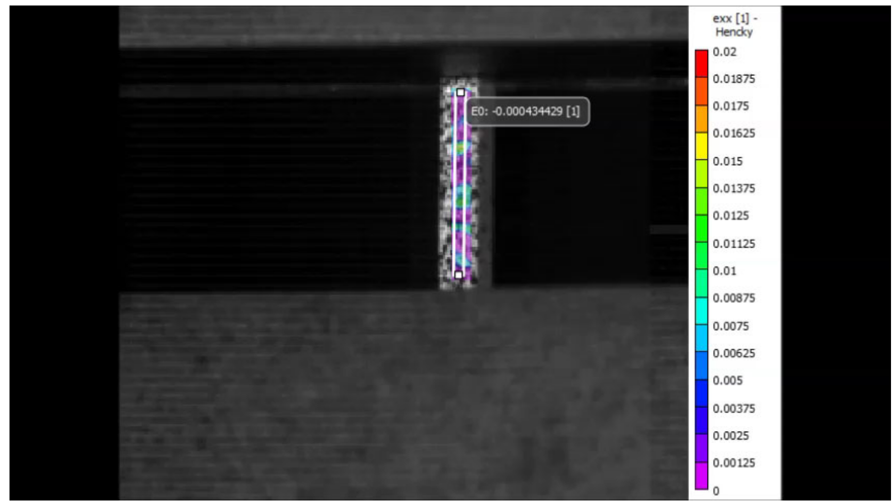
Material Characterization Example: Unidirectional CFRP

Meticulous experiments ensured quality ad quantity of CFRP test data

UD Tension Test (fiber direction)



Quasi-static rate tensile test at 0.0001 per second (nominal strain rate) on regular servohydraulic frame*



*High Rate Tensile Test at ~189 per second (nominal strain rate)**

- UD tests at various strain rate provide data on strain rate dependency.
- Digital Image Correlating (DIC) measurement of surface strain provides data for simulation validation.
- Woven, SMC, and structural level CFRP components are also tested.
- Basic constituents, fiber and matrix, are also tested for simulation input.

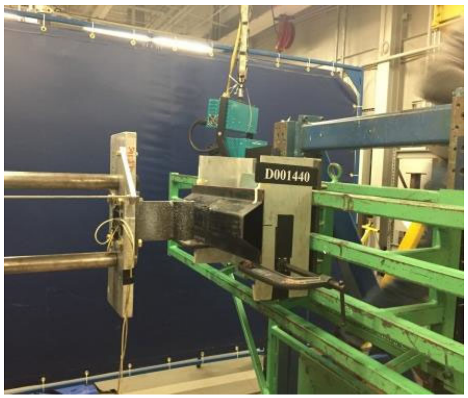
**Courtesy of NIST*

UD Crash Safety Test

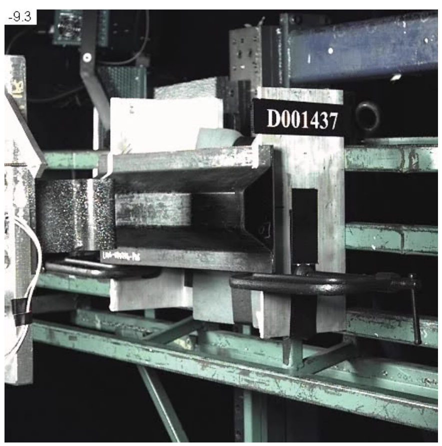
- One UD Hat-section ($[0/90/90/0/0/0]_S$ or $[0/60/-60/0/60/-60]_S$ layup)
- Two different crash test: Dynamic 3-point bending and Axial

Dynamic 3-point bending

Experiment set-up



Impactor
Mass: 25.4kg

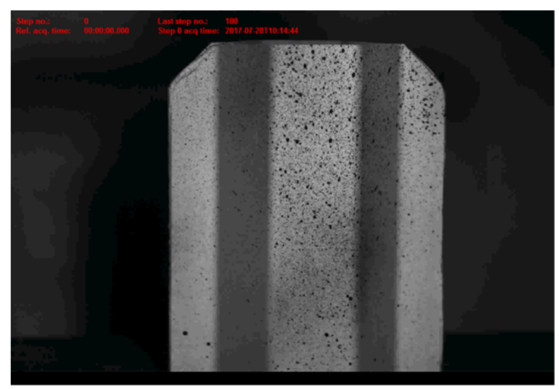


Axial crush

Experiment set-up

Impactor
Mass: 795kg

V=4.4m/s
V=2.2m/s



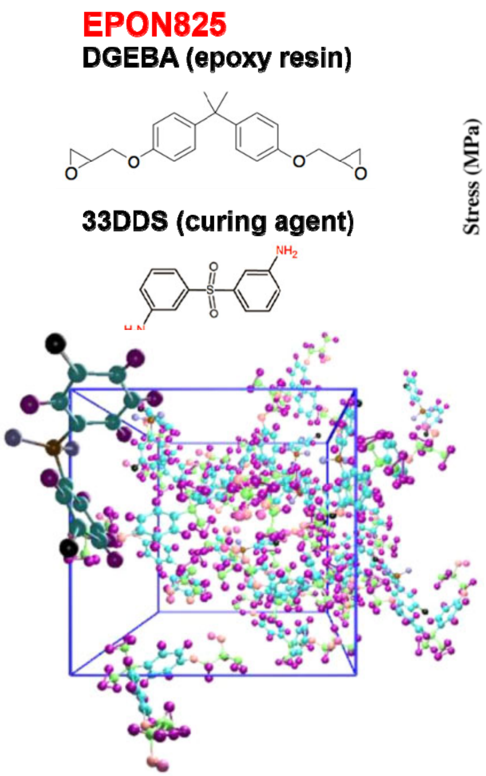
**Courtesy of Ford Motor Company*

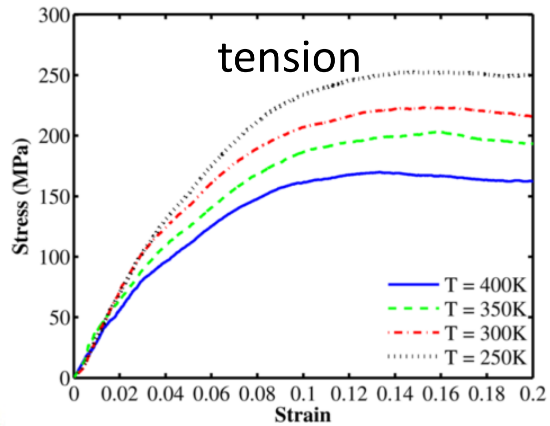
Highlight in Molecular Dynamic Analysis (Task 2)

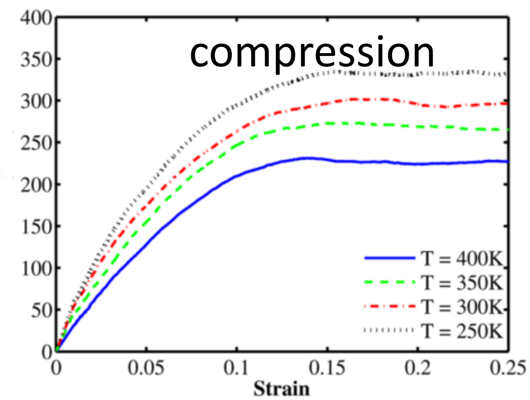
The ***paraboloidal yield surface constants*** can be computed by Molecular dynamics (MD) simulations

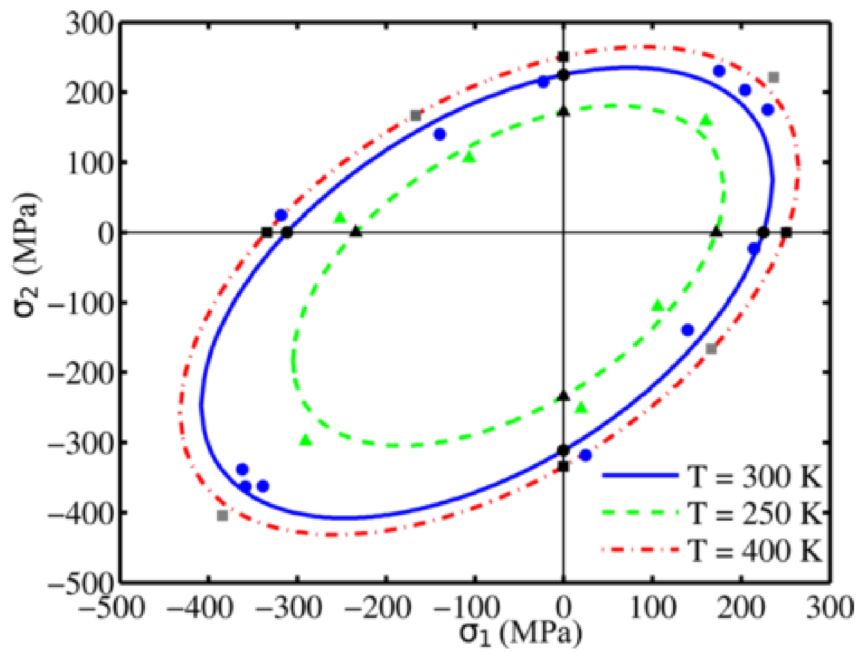
$$f(\boldsymbol{\sigma}, \boldsymbol{\sigma_c}, \boldsymbol{\sigma_T}) = 6J_2 + 2(\boldsymbol{\sigma_c} - \boldsymbol{\sigma_T})I_1 - 2\boldsymbol{\sigma_c}\boldsymbol{\sigma_T}$$

where $\boldsymbol{\sigma_T}$ and $\boldsymbol{\sigma_c}$ are tensile and compressive yield stresses, I_1 is the first stress invariant, and J_2 is the second invariant of deviatoric stress tensor.









The yield criterion is determined uniquely by compressive and tensile yield stresses

[1] N. Vu-Bac et al., Macromolecules, 2015 [2] Argon, AS. Philos. Mag. 1973, 28, 839−865. [3] Heinz, SR.; Wiggins, JS. Polym. Test. 2010, 29, 925−932. ; [4] Ma, J.; Mo, M.-S.; Du, X.-S.; Rosso, P.; Friedrich, K.; Kuan, H.-C. Polymer 2008, 49, 3510−3523

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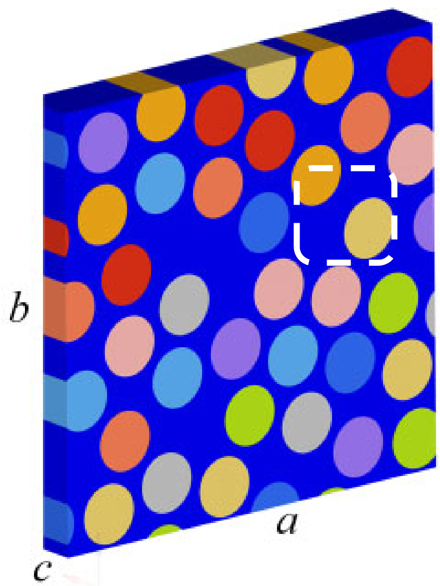
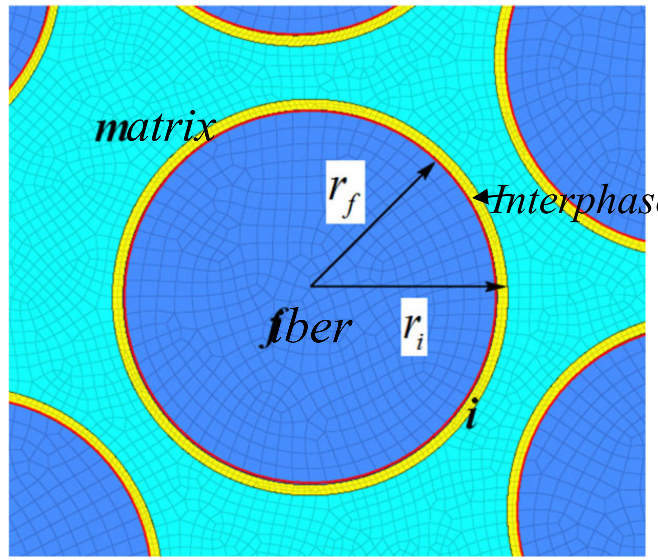
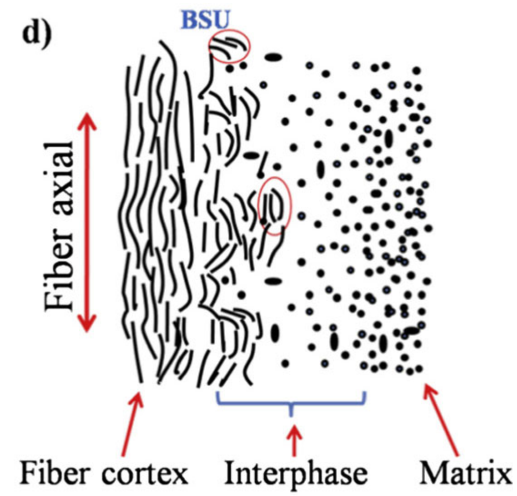
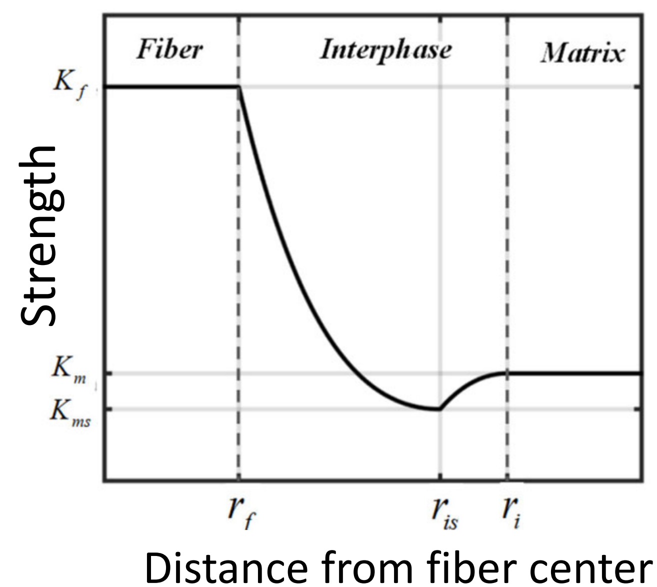
Interphase Region Between Fiber And Matrix







- **Interphase properties predicted by MD results.**
- Trend assumed to be a exponential variation model.
- Interphase average properties are found to be stronger and stiffer than the matrix, providing extra load bearing capability of the composites.



Meng, Zhaoxu, Miguel A. Bessa, Wenjie Xia, Wing Kam Liu, and Sinan Keten. "Predicting the macroscopic fracture energy of epoxy resins from atomistic molecular simulations." *Macromolecules* 49, no. 24 (2016): 9474-9483.

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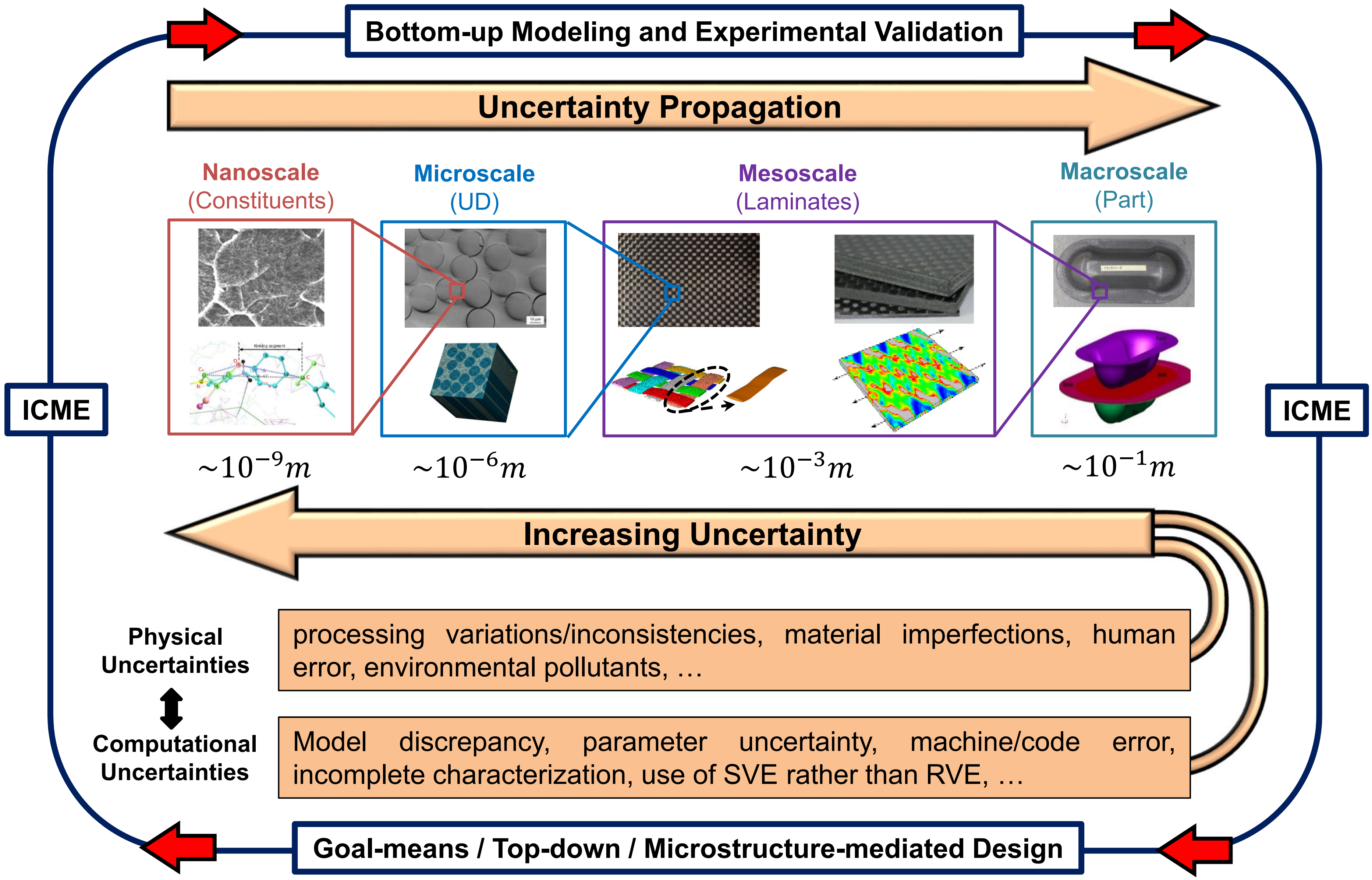
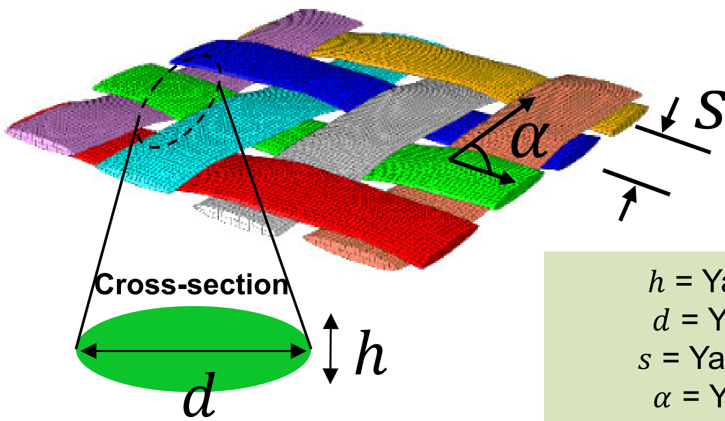
Highlight in Multiscale Modeling (Task 3)



Uncertainties in Multiscale Model

Most *prior works* on fiber composites have focused on mesoscale:

- Sensitivity of orthogonal woven fabrics to the yarn geometry via two-level factorial design [1]:
  - Material properties, s, d, and h were found to be important.
- Sensitivity of dry orthogonal woven composites to friction coefficient and yarn height has been illustrated in [2] via Sobol indices.
- The stiffness of orthogonal woven composites significantly decreases as the fiber misalignment increases [3].



h = Yarn Height
d = Yarn Width
s = Yarn Spacing
α = Yarn Angle

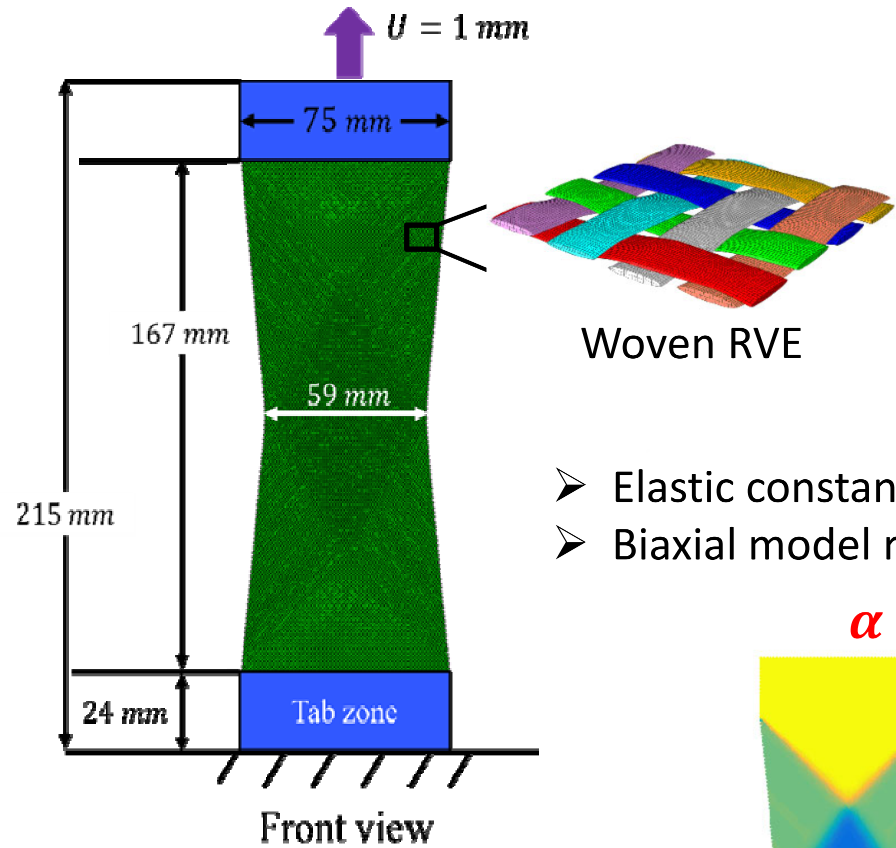
Limitations of prior work:

- **Spatial variations** are not considered.
- Uncertainties are modeled with random variables rather than **random fields**.
- **Multiscale** simulations have not been considered.

[1] Komeili, M. and A. Milani. Computers & Structures, 2012. **90**: p. 163-171.
[2] Akmar, A.I., et al.Composite Structures, 2014. 116: p. 1-17.
[3] Vanaerschot, A., et al. Applied Mechanics and Materials. 2015. Trans Tech Publ.

Hierarchical* Multiscale Modeling with Uncertainties

Cured Woven Biaxial Tension Simulation (elastic only)

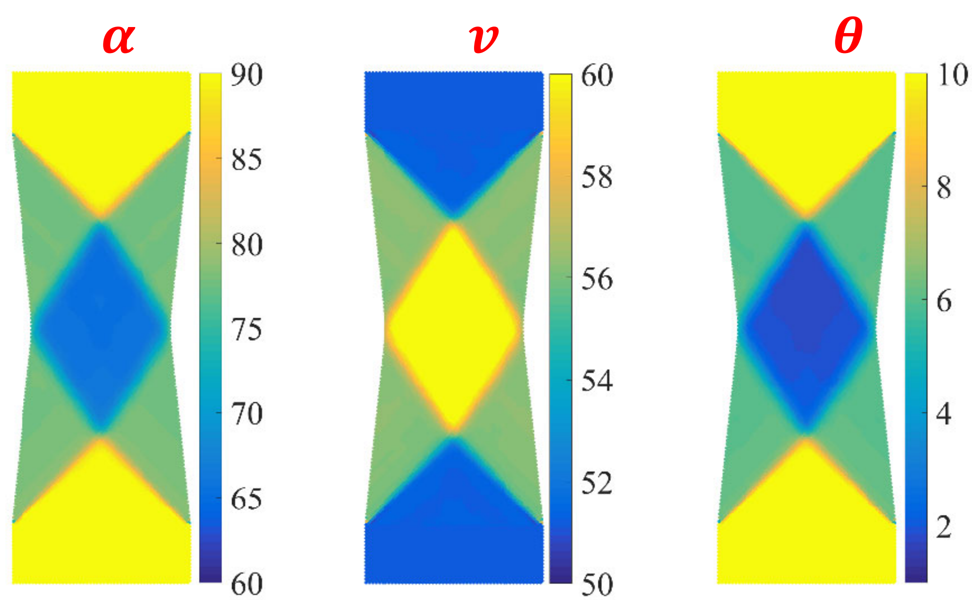


With consideration of:

- ***Spatial variation of α (yarn angle)***
- ***Spatial variation of ν (fiber volume fraction)***
- ***Spatial variation of θ (fiber misalignment)***

Different woven RVEs required

- Elastic constants of woven RVEs stored as $\mathbf{C}(\alpha, \nu, \theta)$
- Biaxial model reads **C** at each integration point



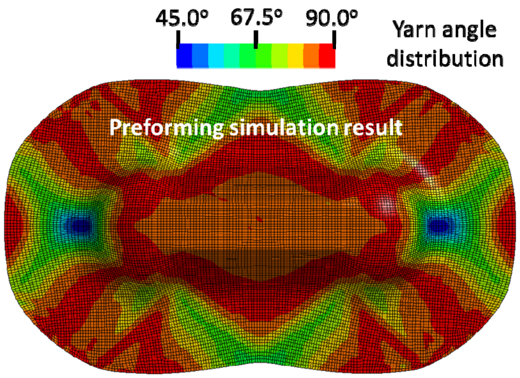
*Concurrent Simulation approach will be introduced in later sections

Manuscript in Preparation

Highlight in Twill Woven Forming Analysis (Task 4)

Information Flow from *Preforming* to *Performance Analysis*

Preforming simulation:



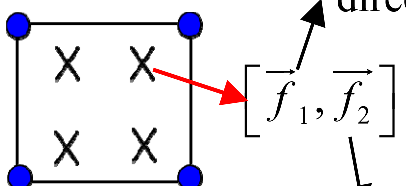
Geometry →

- Stress or strain field within the composite structure;
- Failure or damage prediction.

↑ Output

Discretization ↓

Shell/solid elements:



Warp yarn direction

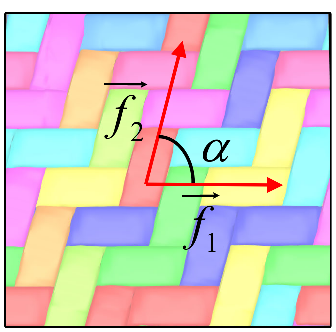
Weft yarn direction

- At macro-integration point, stress update with user-define material model:

$$[\boldsymbol{\sigma}] = \left[\mathbf{C}\left(\vec{f}_1, \vec{f}_2\right)\right][\boldsymbol{\varepsilon}]$$

↑ Input to FEM Software

Composite cured RVE:



Homogenization →

- Effective constitutive law:

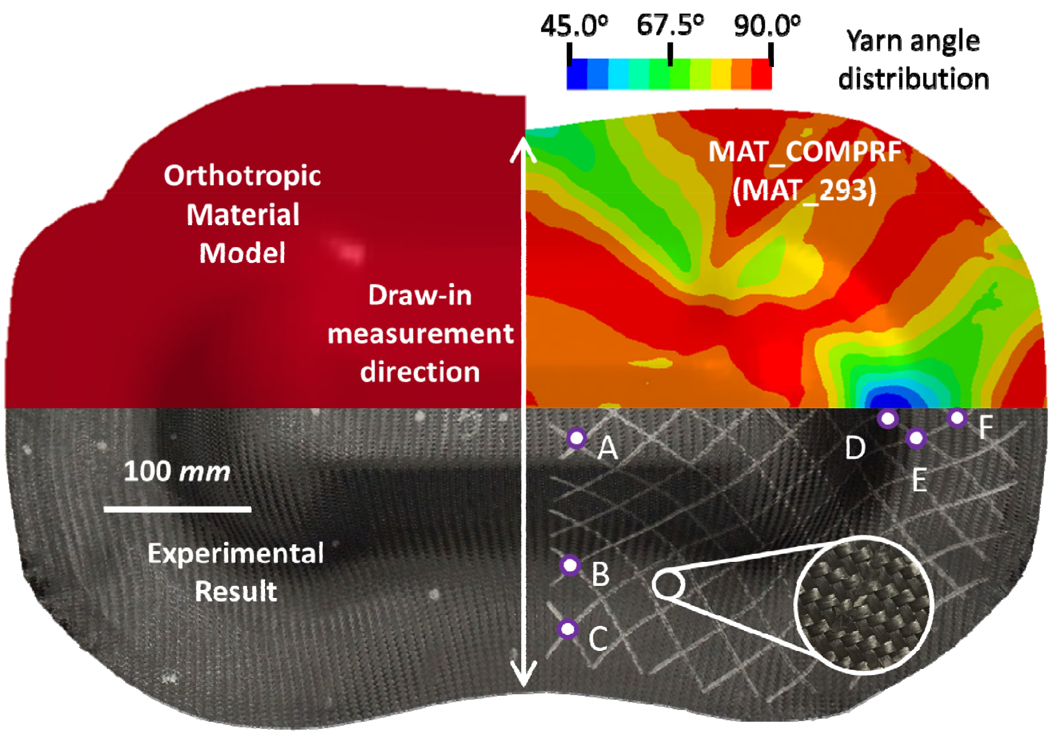
$$\mathbf{C}\left(\vec{f}_1, \vec{f}_2\right)$$

A non-orthogonal material model is needed

Zhang, Weizhao, Huaqing Ren, Biao Liang, Danielle Zeng, Xuming Su, Jeffrey Dahl, Mansour Mirdamadi, Qiangsheng Zhao, and Jian Cao. "A non-orthogonal material model of woven composites in the preforming process." *CIRP Annals-Manufacturing Technology* (2017).

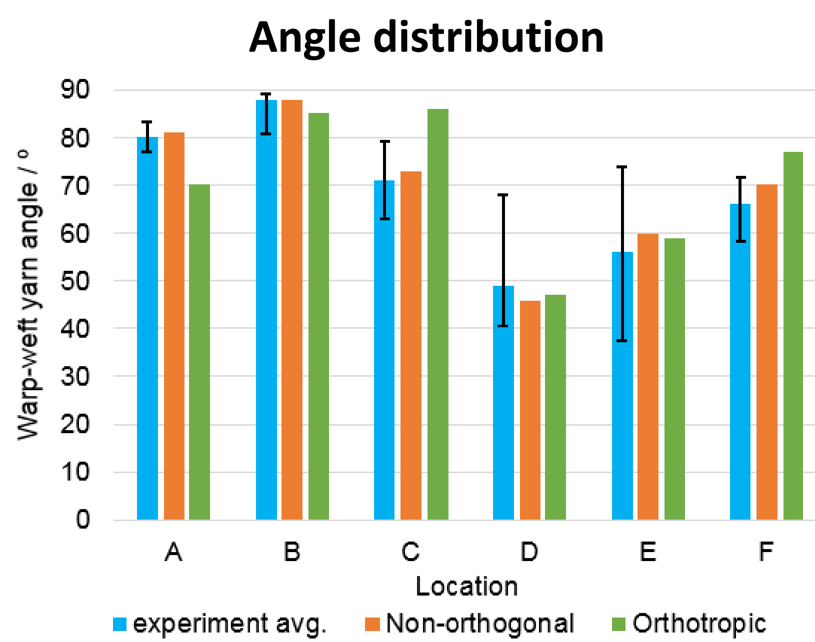
- Preforming validation: non-orthotropic v.s. orthotropic

➢ Simulation with non-orthogonal model is able to achieve less than 15% error of yarn angle and draw-in prediction at various sampling points.



Y-direction draw-in distance

	experiment	Non-ortho	Ortho
Draw-in / mm	49±4	42 (85.7%)	73 (149.0%)

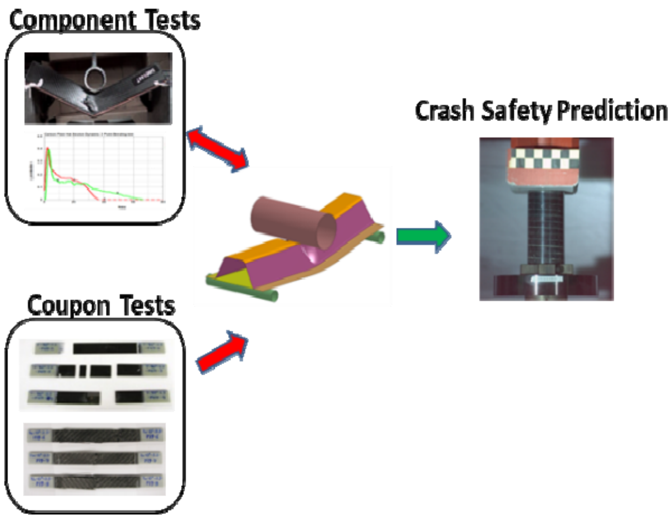


➢ Non-orthogonal model makes a great prediction improvement of fiber angle and draw-in over orthotropic material model.

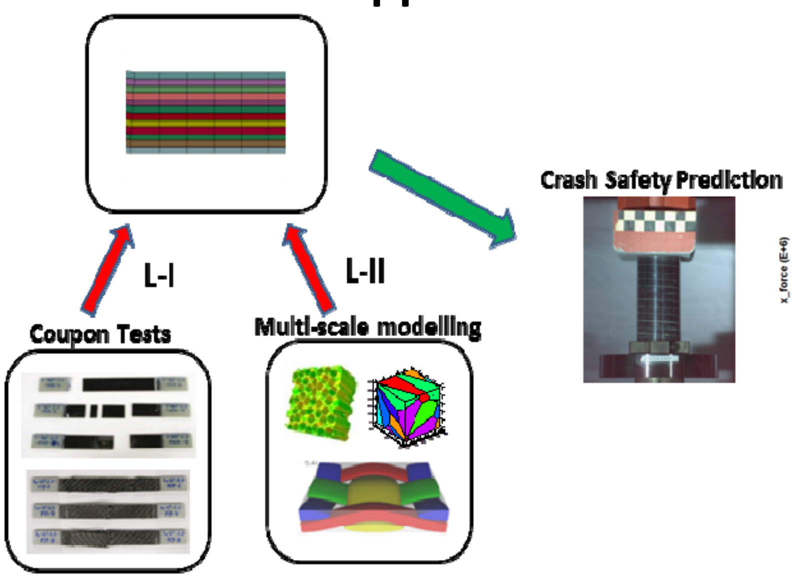
Highlight in Crash Analysis (Task 6)

Crash safety simulation

Mesoscale Approach



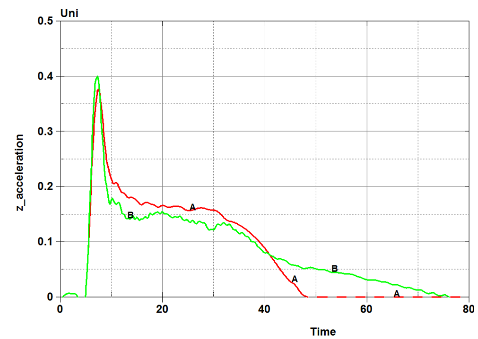
ICME Approach



Experimental Work on CFRP Crash Analysis

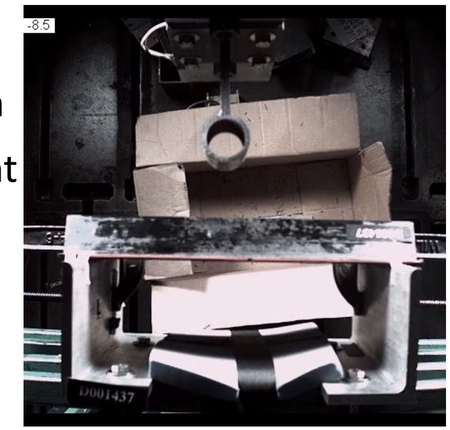
Dynamic 3-point bending

Acceleration history



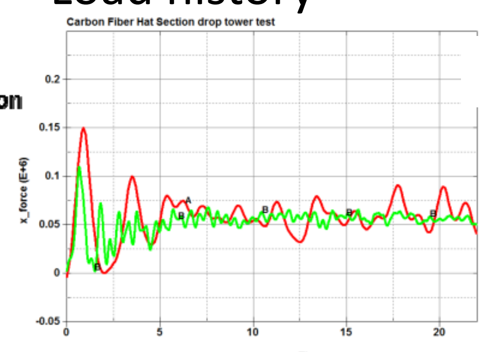
Simulation

Experiment



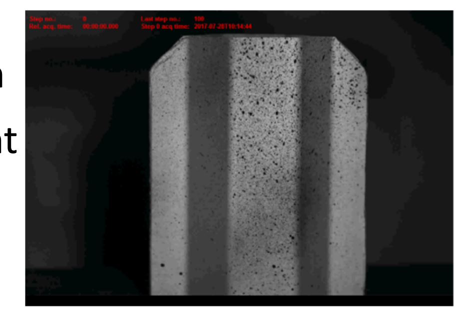
Axial crush

Load history



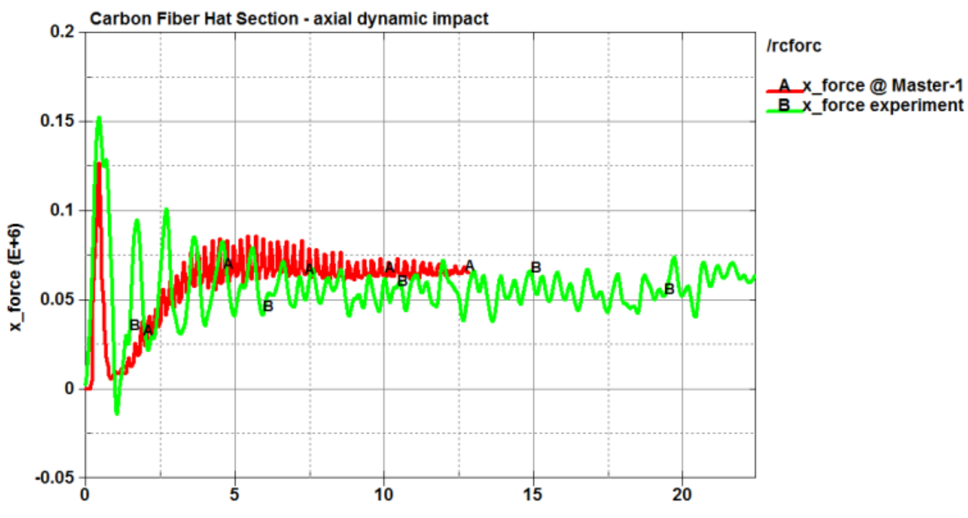
Simulation

Experiment

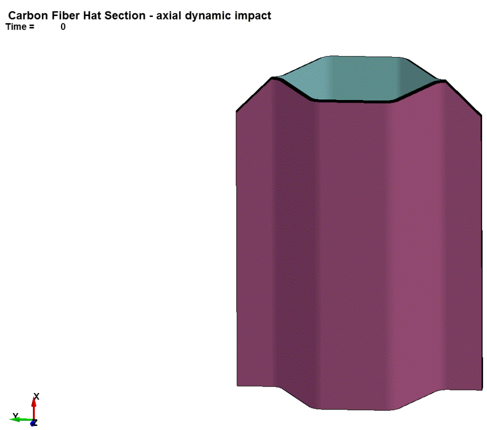


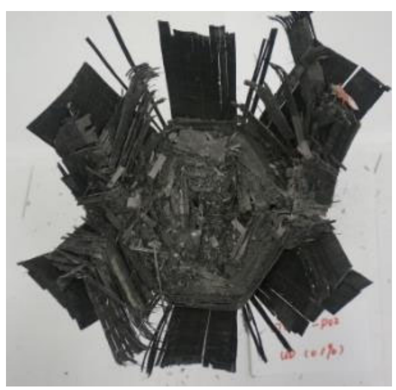
Axial crush – UD Laminate Model

[0/90/90/0/0/0]$_S$

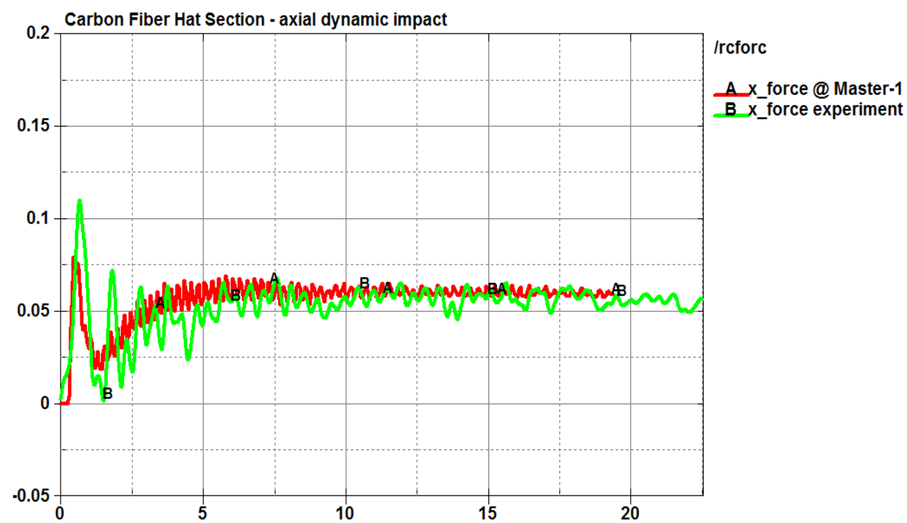


Impact Velocity = 4.4 m/s

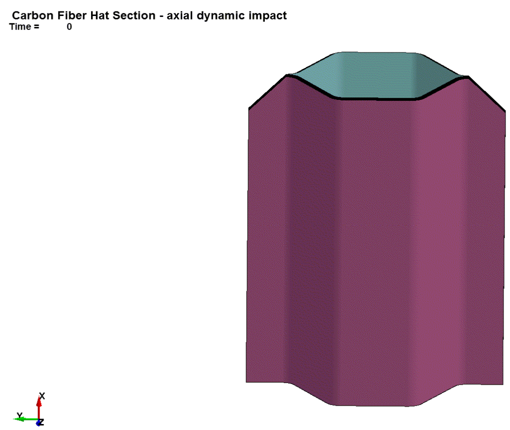


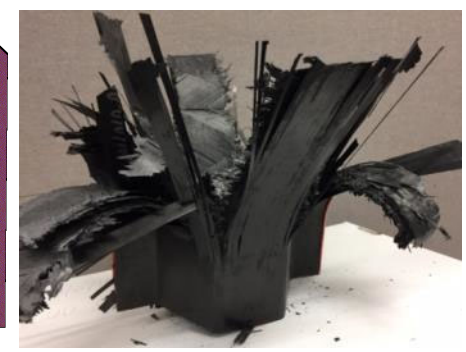


[0/60/-60/0/60/-60]$_S$



Impact Velocity = 4.4 m/s



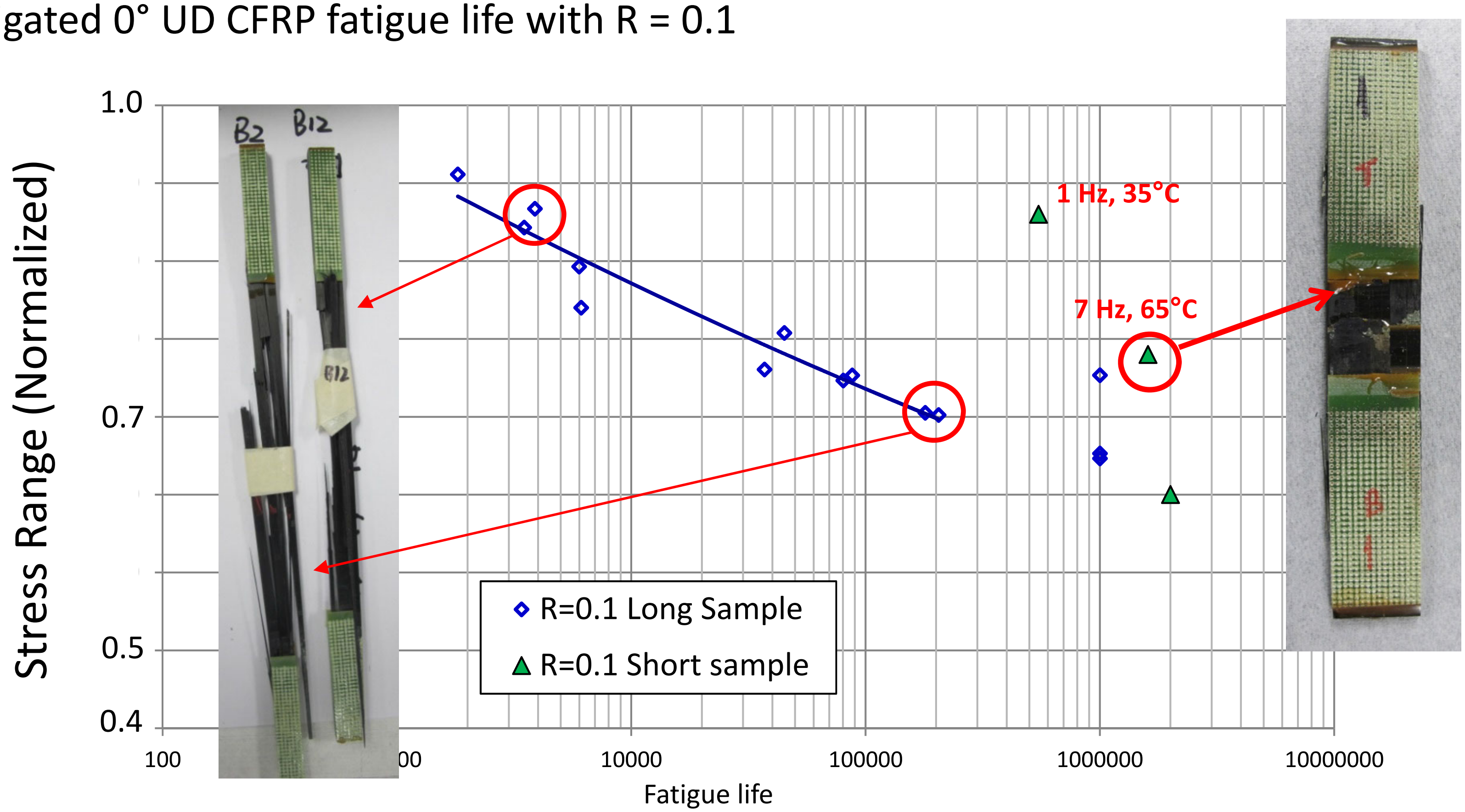


- Thick shell element with calibrated UD constitutive law
- No microstructure information

Northwestern University

Highlight in Fatigue Analysis (Task 7)

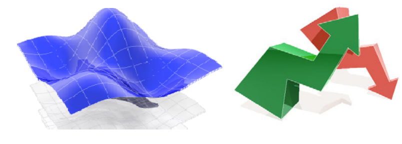
Investigated 0° UD CFRP fatigue life with R = 0.1



- Large stress amplitude reduces fatigue life significantly
- Similar damage pattern on UD coupon
- Short coupon exhibits longer fatigue life, but coupon tab fails before UD specimen

Highlight in Design Optimization Loop for CFRP (Task 8)

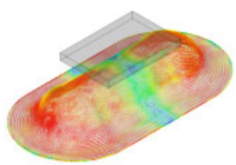
Design Optimization under Uncertainty



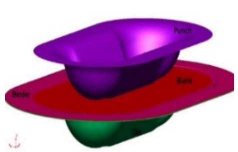
Manufacturing Process Simulation → **Multiscale Material Modeling** → **Performance Analysis considering Process Information**

Manufacturing Process Simulation

- **Chopped Fiber SMC Compression Molding Analysis** - *Moldflow*

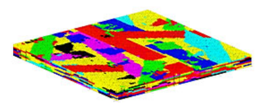


- **Preforming & Compression Molding Analysis** - *LSDYNA*

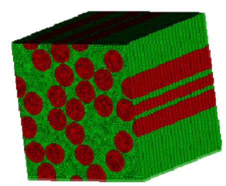


Multiscale Material Modeling

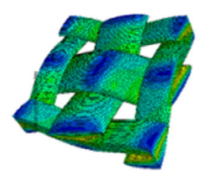
- **SMC** RVE



- **UD** RVE

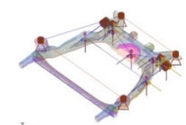


- **Woven** RVE

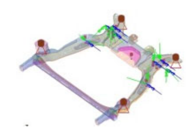


Performance Analysis considering Process Information

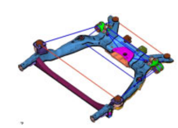
- **NVH** - *NASTRAN* (fiber orientation)



- **Durability** - *nCode* (fiber orientation)



- **Crash** - *LSDYNA* (fiber orientation, delamination, etc.)



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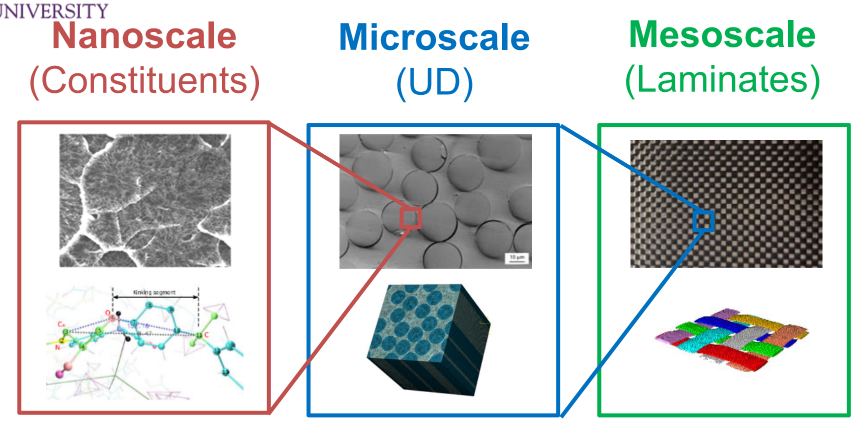
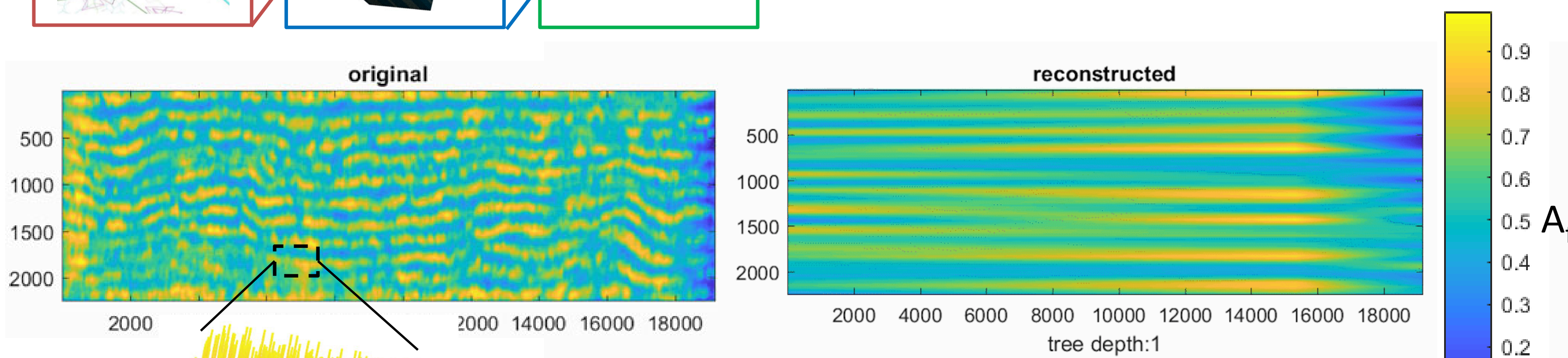
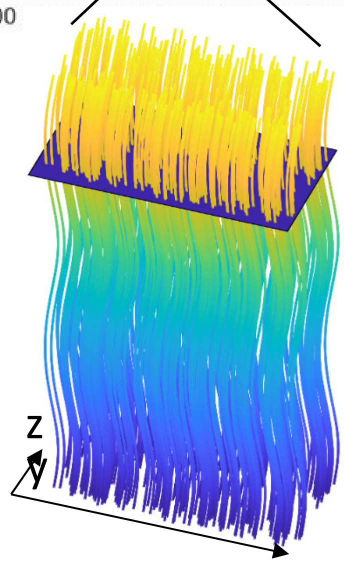
Microscale Uncertainties



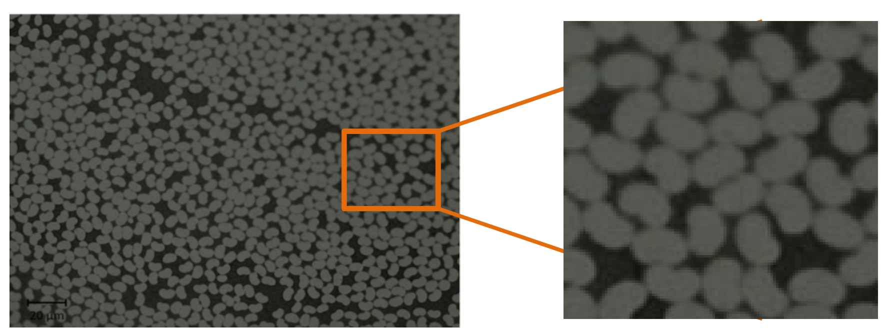
Uncertainties include:

- Local fiber area fraction (A_f)
- Geometry of the fiber cross-section (circular, bean-shape, …)
- Spatial distribution of the fibers





Non-uniform fiber A_f in UD cross-section
(Reconstructed using random tree)



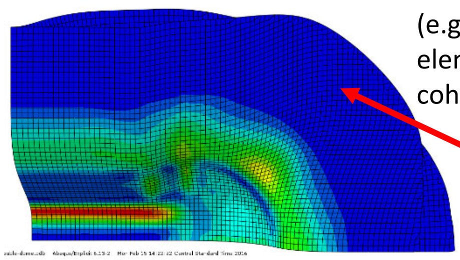
UD microscopy

Irregular fiber shape

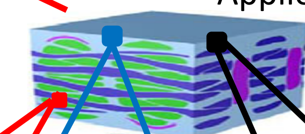
Multiscale Modeling for CFRP

*Liu et al; Microstructural Material Database for Self-consistent Clustering Analysis of Elastoplastic Strain Softening Materials, Computer Methods in Applied Mechanics and Engineering, accepted.
*Liu et al., *Self-consistent clustering analysis: An effcient multi-scale scheme for inelastic heterogeneous materials*, Computer Methods in Applied Mechanics and Engineering, (2016).

Macroscale Model



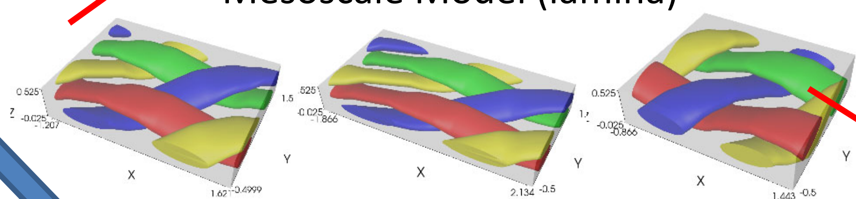
Laminates
(e.g. n layers of shell elements with cohesive elements)



Dimension: 775 mm x 490 mm x n mm
Number of elements: 3980

Macro to Meso sampling
Random field & correlation functions:
1) Tow size
2) Tow spacing within the woven composite
3) Woven angles in different layers

Mesoscale Model (lamina)

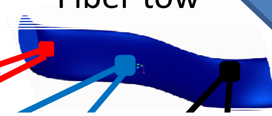


Dimension: 9 mm x 9mm x 1 mm
Number of elements: 683000

Meso to Macro homogenization:
Material law at each integration point in the Macroscale model.

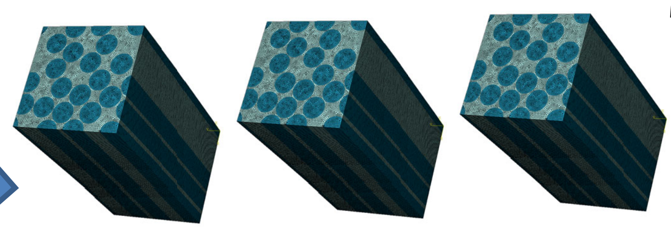
Meso to Micro sampling
Random field & correlation functions:
1) Fiber misalignment
2) Volume fraction
3) Interfacial strength

Fiber tow



Dimension: 9mm x 2mm x 0.5mm

Microscale Model (UD)



Micro to Meso homogenization:
Material law at each integration point in the Mesoscale model.

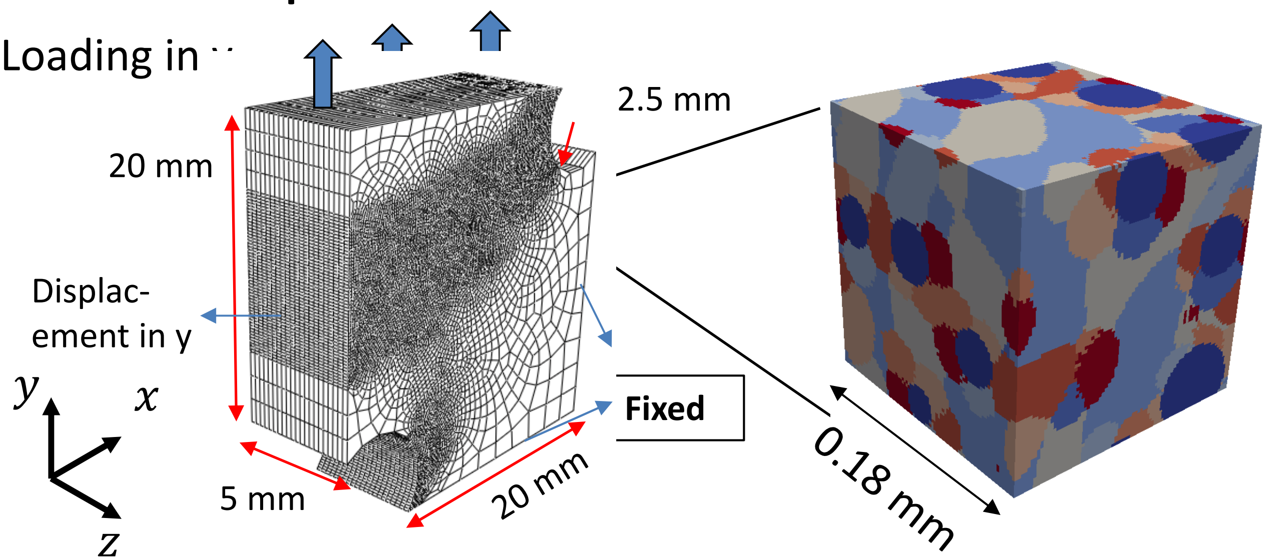
Number of DOFs in the full-field system:
$3980 \times 683000 \times 68700 = 1.9 \times 10^{15}$

Number of DOFs in the reduced order system*:
$3980 \times 20 \times 20 = 1.6 \times 10^{6}$

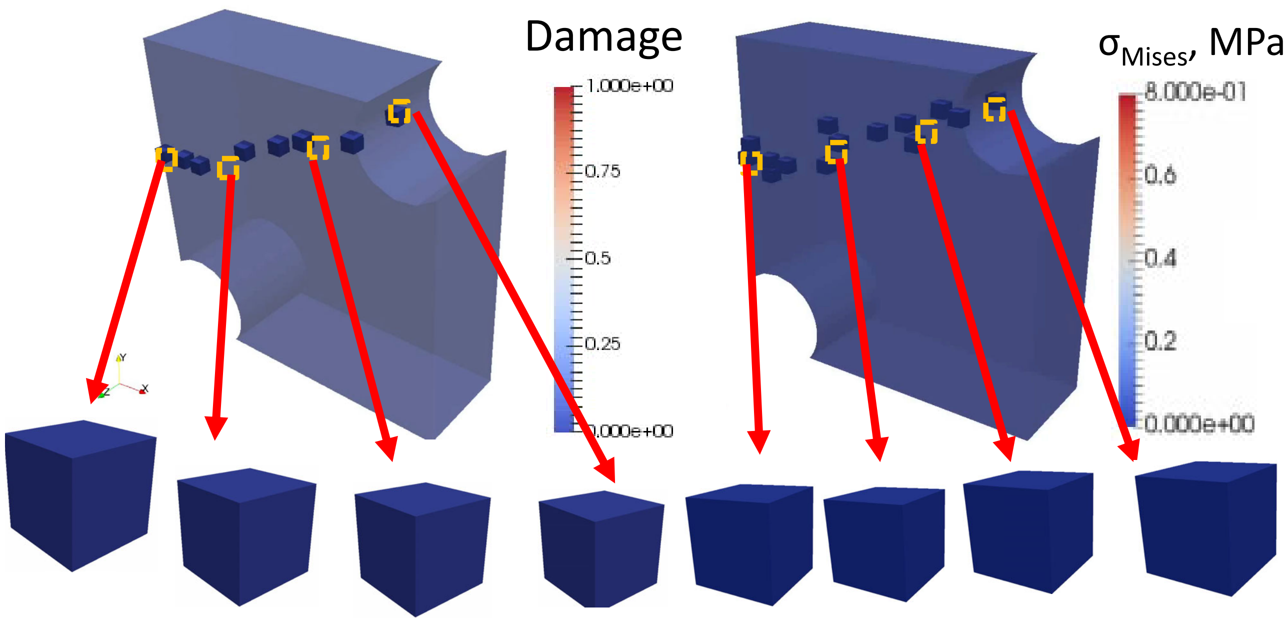
***By Self Consistent Clustering Analysis (SCA)**

Concurrent Simulation of 3D Double-Notched Coupon

Macroscale coupon | **Microscale SCA model**



Damage field | von Mises Stress field



<u>Macroscale</u>
Gauss Points: *154371*
Volume fraction: 20%

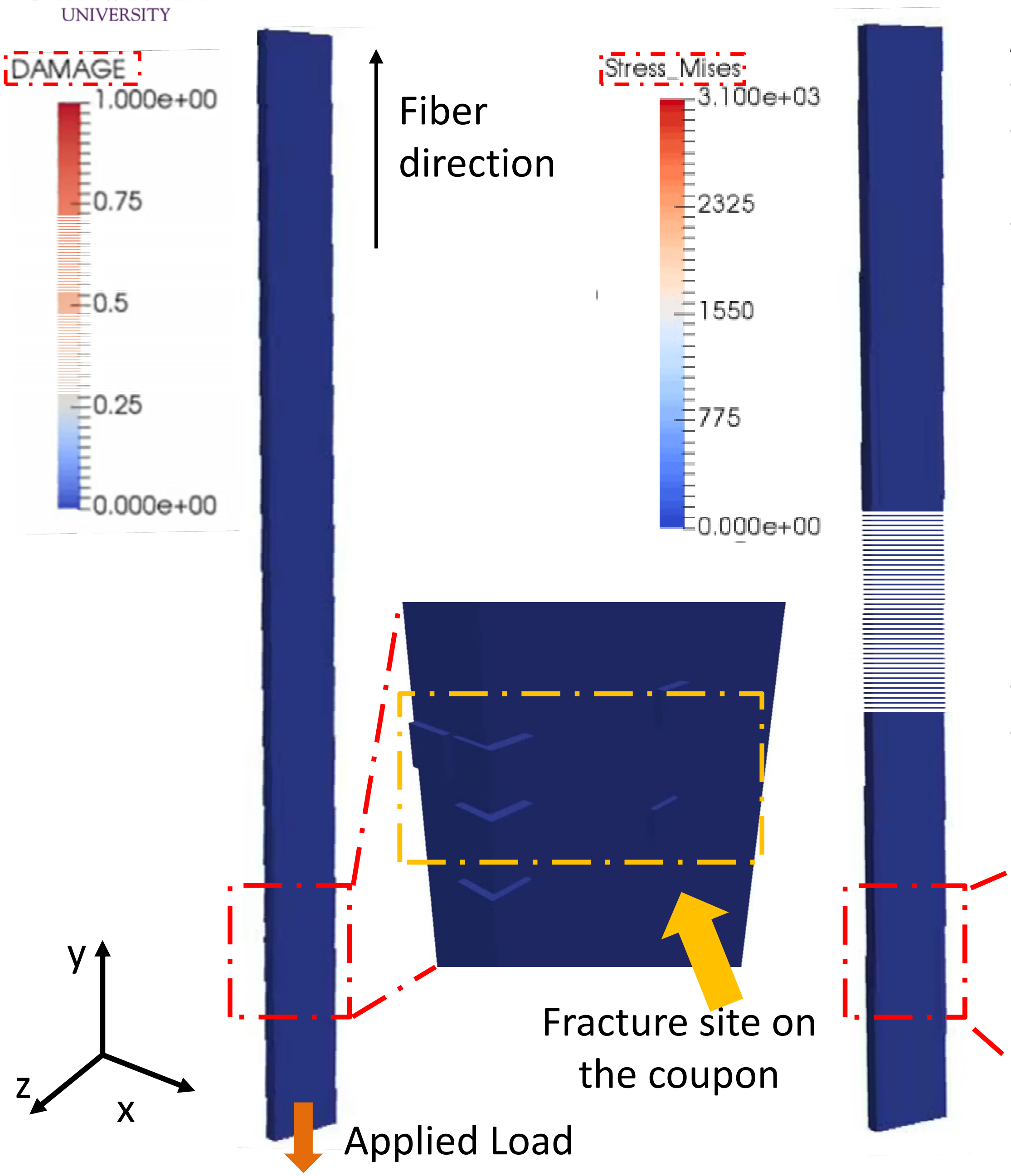
<u>Microscale</u>
RVE DNS Mesh: *512,000*
Computational Effort:
154,371*512,000* =**
<u>79,037,952,000</u>

SCA Model: *10* Clusters
Matrix: <u>8</u> clusters
Inclusion: <u>2</u> clusters
Computational Effort:
154,371*10* =**
<u>1,543,710</u>

<u>The concurrent simulation with SCA (10 clusters) takes 56 hours on 72 cpus.</u>
<u>Speed-Up: 43,000</u>

<u>Based on RVE record, it is estimated that the DNS will take more than 1×10^5 days ...</u>

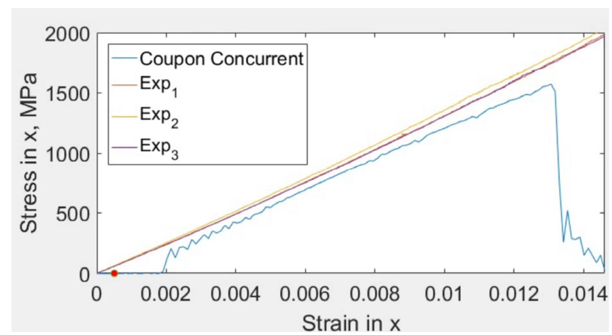
0° Coupon Concurrent Simulation



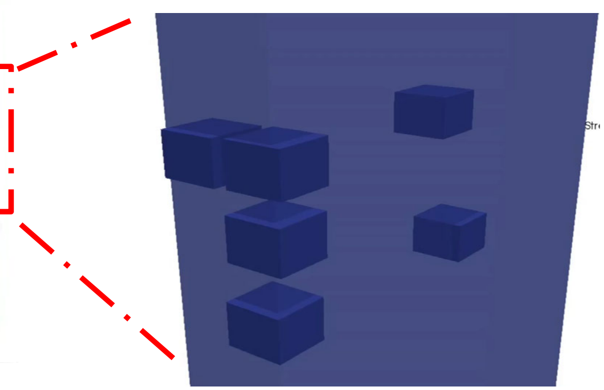
Key Observation:

- Concurrent simulation of 0° CFRP coupon
- Macroscale damage field and microscale RVE damage field observed simultaneously
- Cause of macroscale structure damage can be tracked down to microstructure

Stress vs. Strain Curve



- Oscillation due to mass-scaling
- Fiber stiffening effect not captured by elastic fiber properties



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