Multiphysics Multiscale Simulation Platform for Damage, Environmental Degradation and Life Prediction of CMCs in Extreme Environments

PI: Dr. Aditi Chattopadhyay
School for Engineering of Matter, Transport and Energy (SEMTE)
Arizona State University, Tempe, AZ

Major Participants: Dr. Luke Borkowski & Dr. G.V. Srinivasan
Raytheon Technologies Research Center (RTRC)
East Hartford, CT

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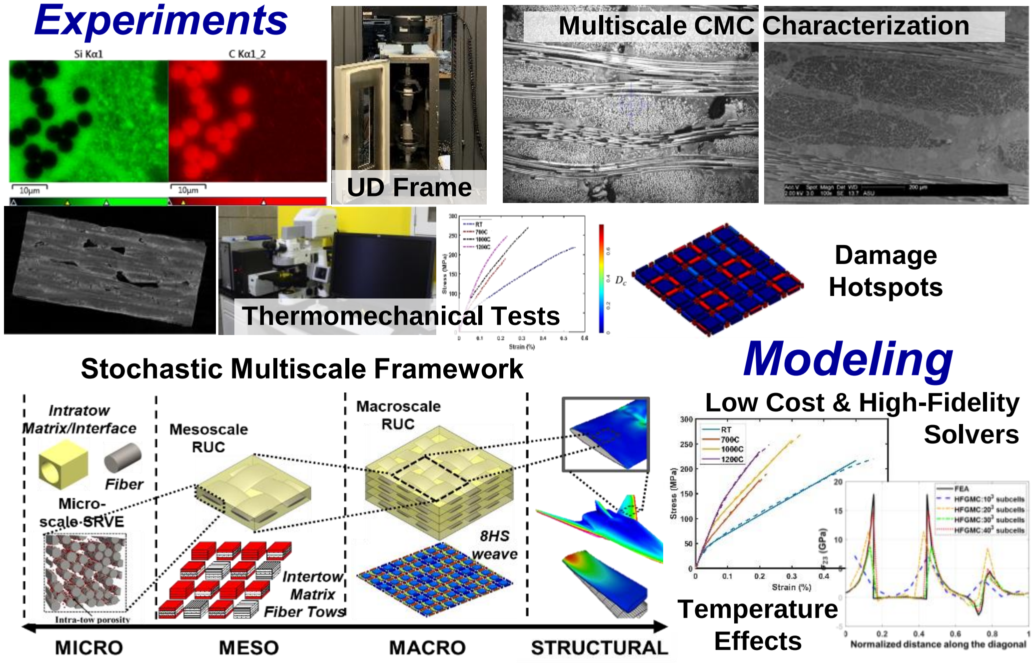
National Energy Technology Laboratory
Program Manager: Matthew F. Adams
Grant Number: DE-FOA-0001993

Project Summary

Methodologies



Objectives

- Develop a stochastic concurrent multiscale framework for accurate analysis of CMC components operating in turbine service environments
- Integrate modeling and experiments
- Incorporate developed models into life prediction methodologies and FEA software for more accurate estimate of service life

Schedule

BP2				BP3				BP1			
10/1/10-9/30/19				10/1/20-9/30/21				10/1/21-8/15/22			
Qtr1	Qtr2	Qtr3	Qtr4	Qtr1	Qtr2	Qtr3	Qtr4	Qtr1	Qtr2	Qtr3	Qtr4
Task 1: Project Management and Planning											
Task 2: Material Characterization and Uncertainty											
Task 3: Multiphysics Constitutive Modeling with Thermomechanical Damage											
Task 4: Integrated Multiscale Framework											
Task 5: Integration into FE Model											
Task 6: Closed Loop Testing and Validation											

Completed: Projected:

Research Team

- Dr. Aditi Chattopadhyay – PI
- Dr. Kranthi Balusu – Postdoc
- Christopher Sorini – PhD Student/Dean's Scholar
- Khaled Khafagy – PhD Student
- Jacob Schichtel – NDSEG fellow, no cost to the grant
- Dr. Luke Borkowski (RTRC)–Major Participant

Overview

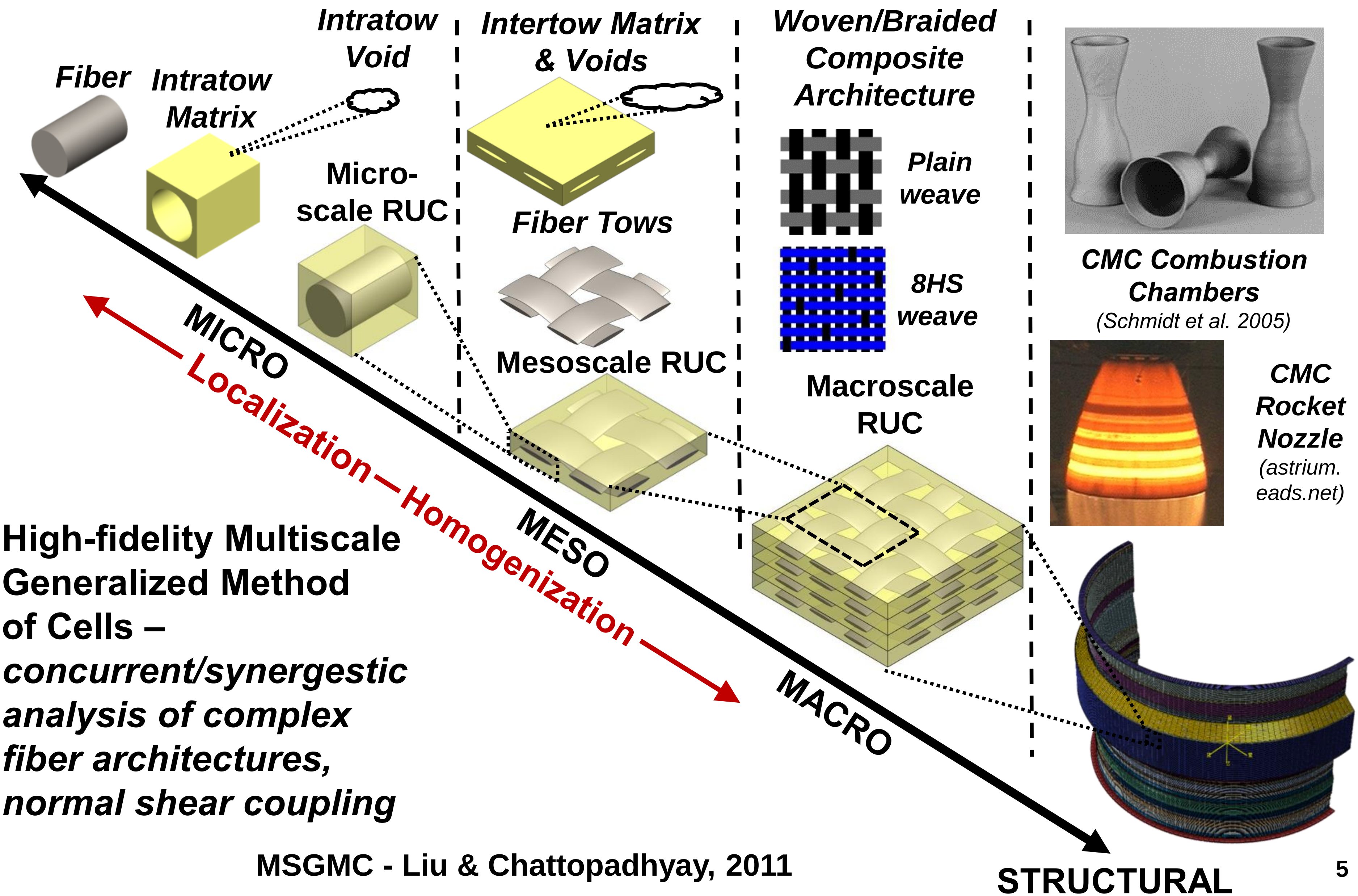
- Key Issues & Objectives
- Tasks & Technical Framework
- Research Progress
  - Material Characterization & Uncertainty Quantification
  - Thermomechanical Progressive Damage Modeling
  - Creep Modeling
  - Damage-diffusion Oxidation Coupling
  - Integrated Multiscale Framework
- Publications
- Concluding Remarks & Future Work
- Acknowledgements

Key Issues & Objectives

- **Next generation CMCs must meet challenges of DOE's advanced turbine concepts, which involve inlet temperatures up to 3100°F, high thermal gradients, multi-regimed oxidation & mechanical loading over long time periods**
- **Limited knowledge of CMC response and damage in operating environment**
- **Significant manufacturing induced flaws and scale-dependent architectural variability**
- **Temperature-dependent damage mechanisms & failure modes**
- **Matrix progressive damage creates pathways for gaseous oxidants to attack CMC interior; distinct effects in intermediate & high temperature**
- **Interface and load sharing between constituents strongly influences material behavior**

Enhance the understanding of CMC degradation & failure in service conditions through more accurate life prediction methodologies - reduce empiricism & enable improved utilization of CMCs in turbine applications

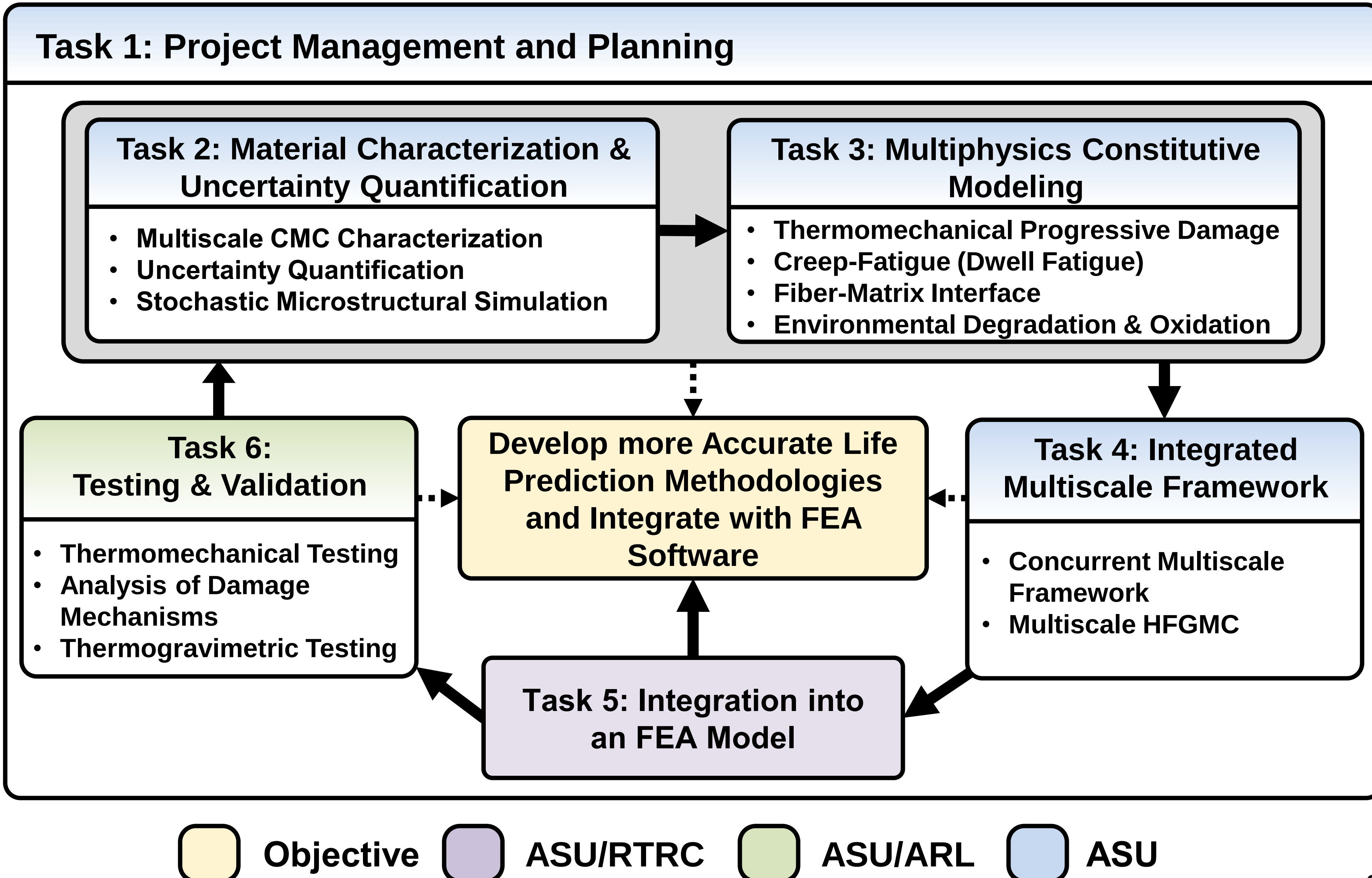
Integrated Multiscale Framework



High-fidelity Multiscale Generalized Method of Cells – ***concurrent/synergestic analysis of complex fiber architectures, normal shear coupling***

MSGMC - Liu & Chattopadhyay, 2011

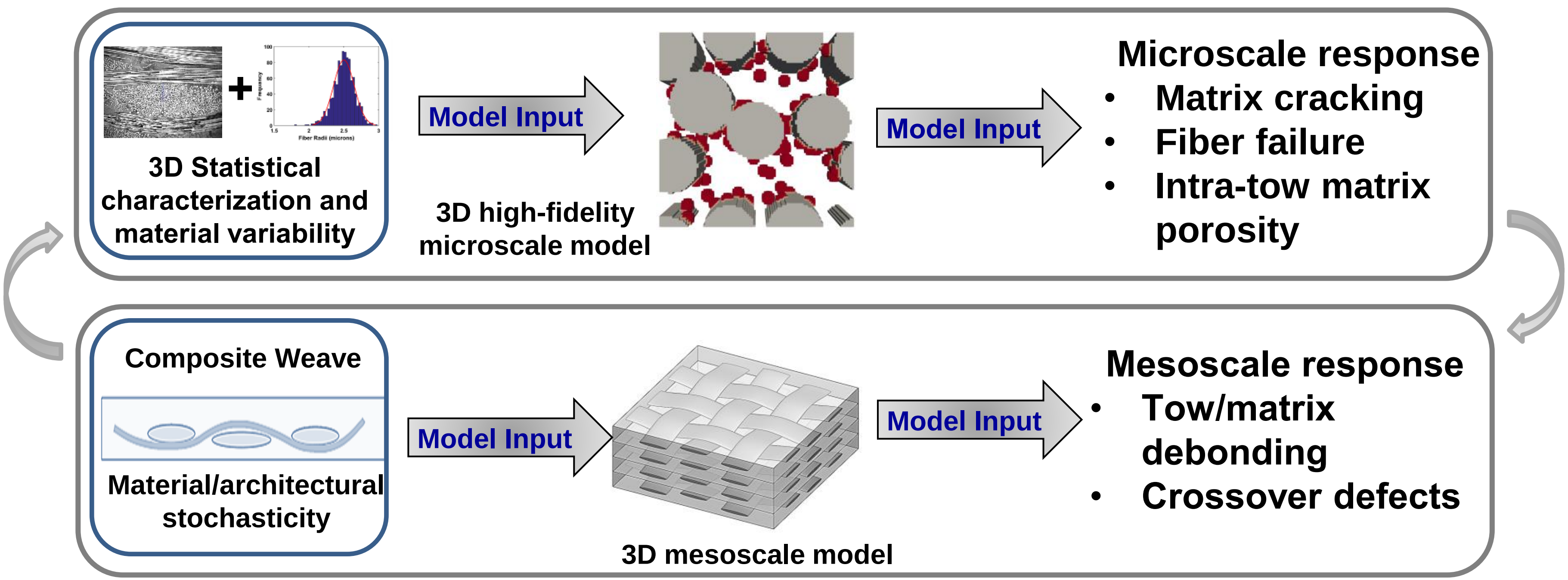
Tasks & Technical Framework



Material Characterization and Uncertainty Quantification

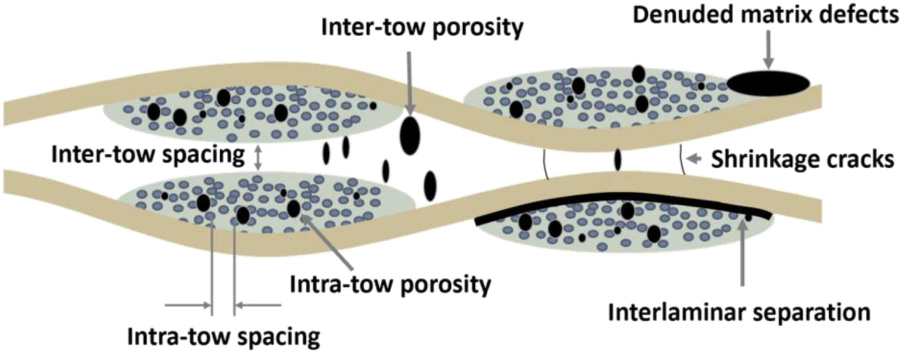
Motivation: Systematically factor uncertainty into the model and capture effects of length-scale dependent variability on CMC response

- Material characterization
- Uncertainty assessment
- Stochastic microstructural simulation & RVEs



Material Characterization

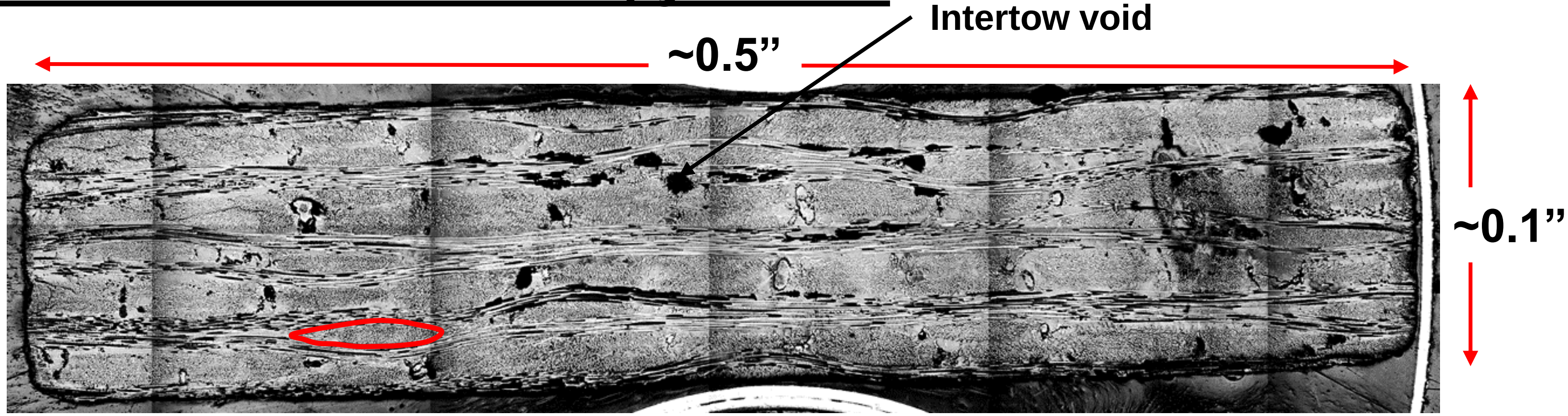
- Characterization, quantification, & representation of multiscale material & architectural variabilities
  - Inter-tow porosity volume fraction
  - Intra-tow porosity volume fraction
  - Fiber volume fraction
  - Fiber radii
  - Inter-tow spacing
  - Intra-tow spacing
  - Tow size & shape



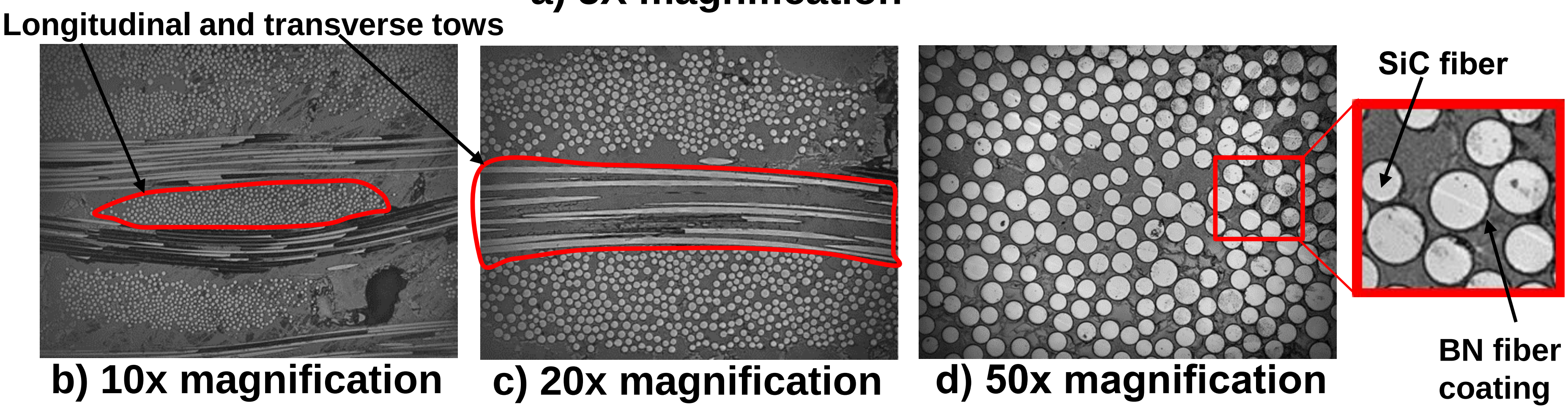
- Image processing algorithms for material feature recognition & image segmentation
- Information used in multiscale analysis

Material Characterization

S200H confocal microscopy results



a) 5X magnification

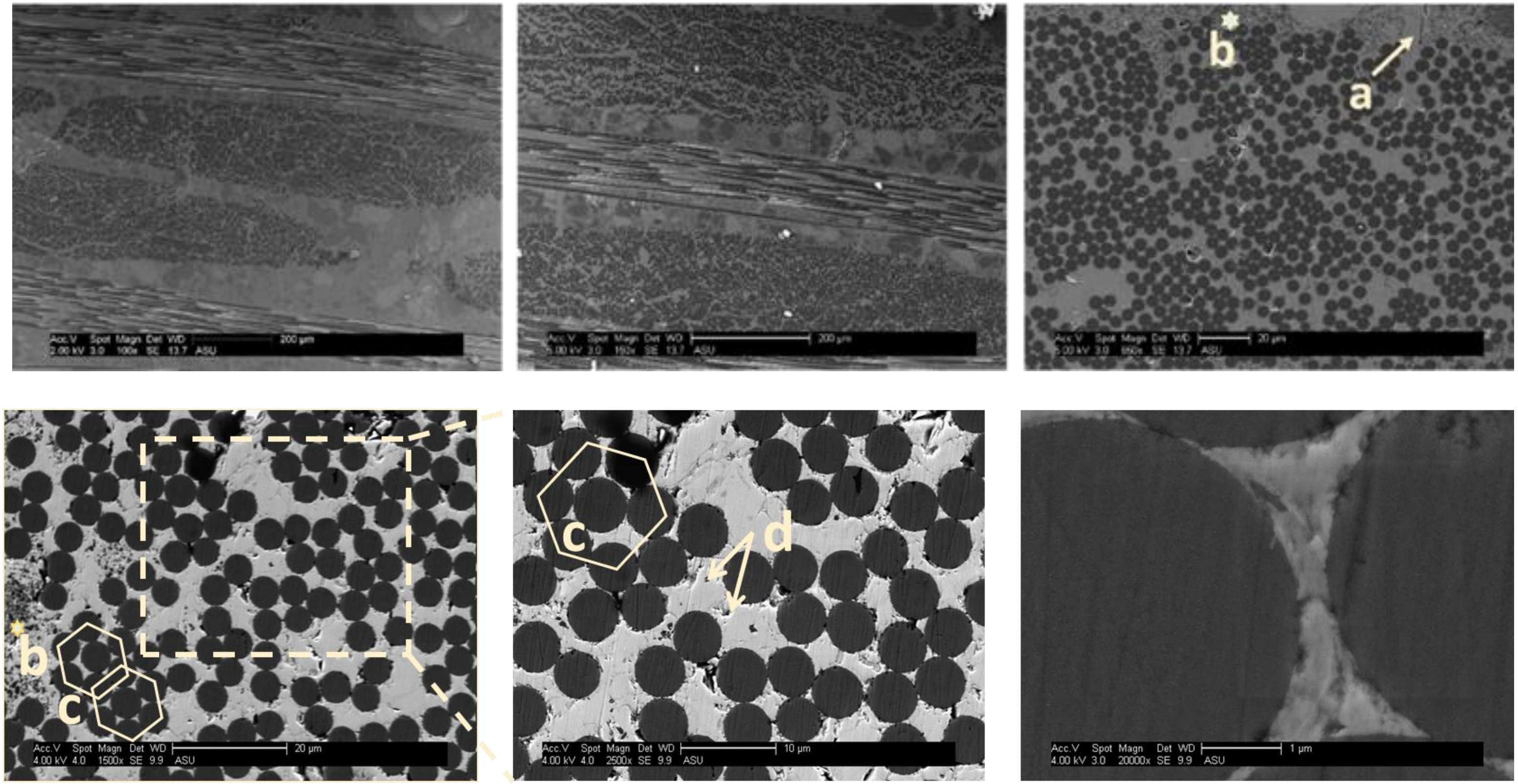


b) 10x magnification c) 20x magnification d) 50x magnification

Confocal microscopy allows more accurate quantification of intratow architectural features over X-ray uCT; micrographs will facilitate construction of microscale S200H SRVEs (Task 2.3)

Material Characterization

Scanning Electron Microscopy (SEM) – S400N C/SiNC CMC



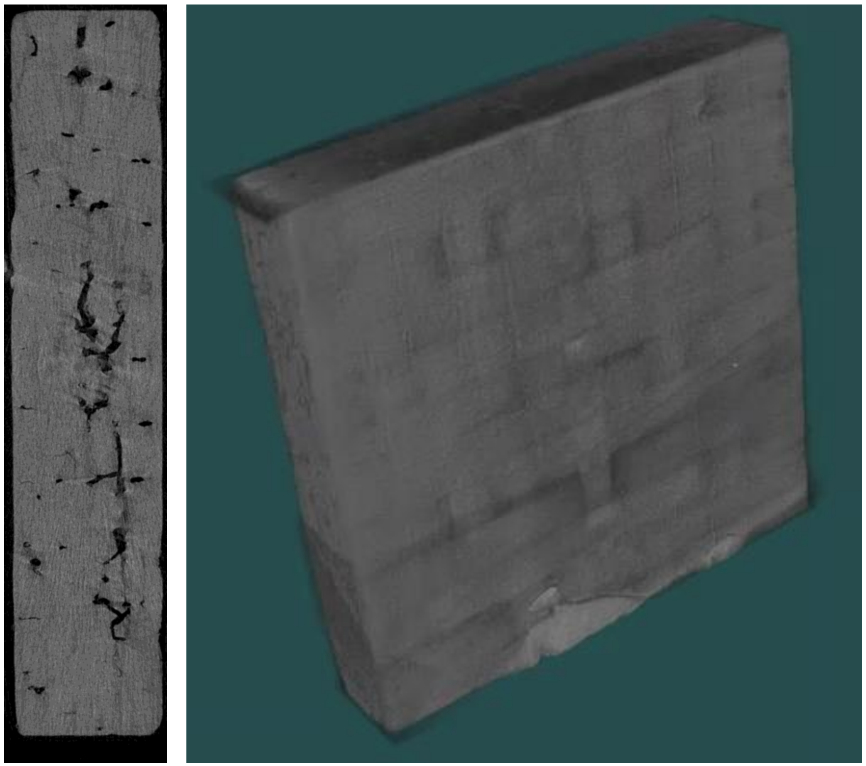
a: shrinkage crack between different ceramic phases (ceramics particles and SiNC matrix)
***b:** different ceramic phases in intratow regions
c: fiber hexagonal close packing
d: intratow porosity

Multiple phases detected in matrix regions; preferable fiber packing structure & intra-tow porosity identified; fiber/matrix interphase layer not visible

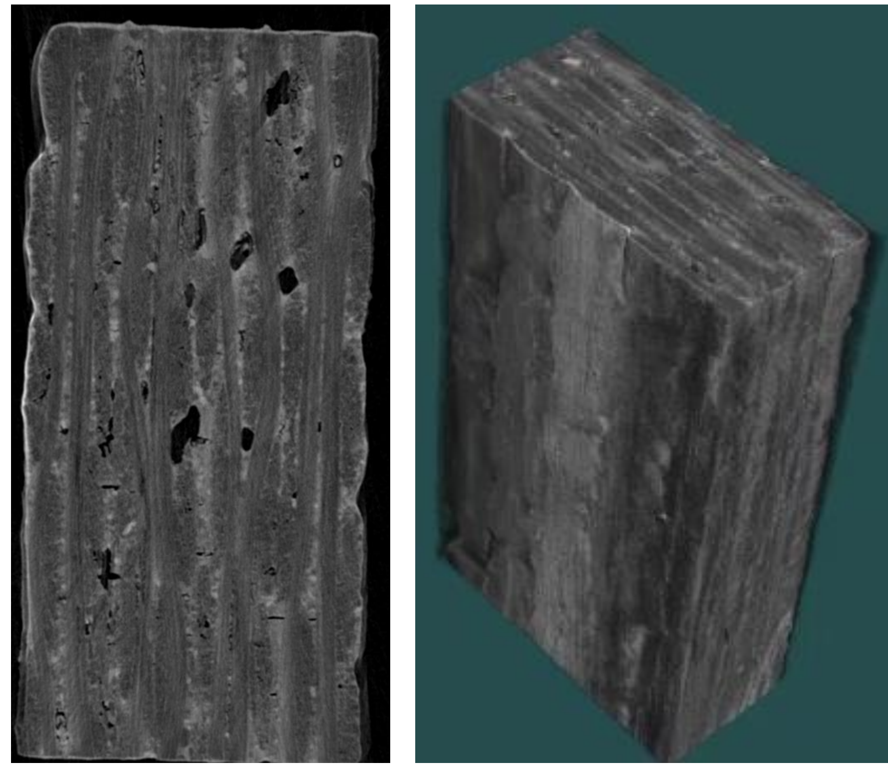
Material Characterization

X-ray Micro-CT

S200H SiC/SiNC CMC



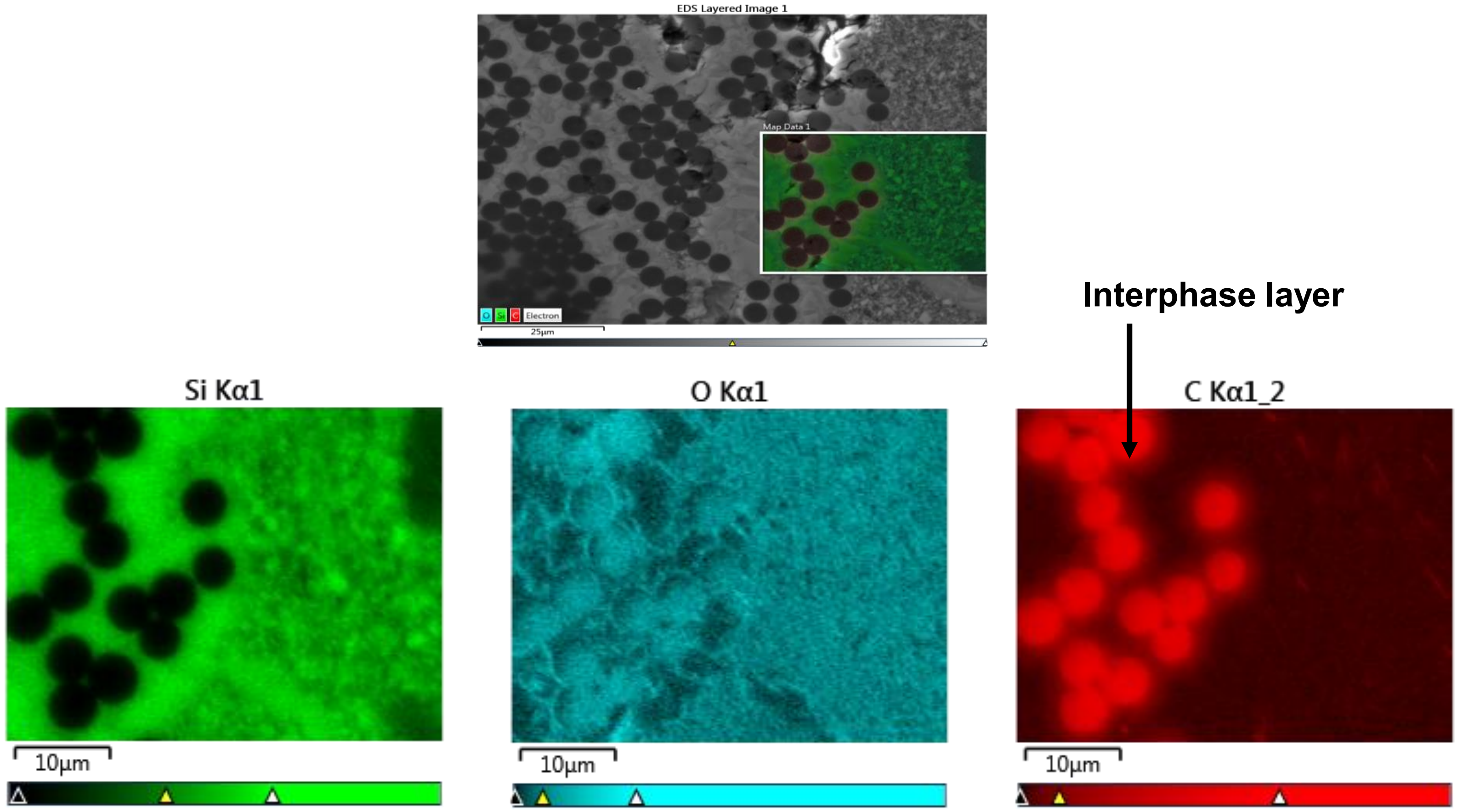
S400N C/SiNC CMC



High-resolution macroscale tomographs show SiC/SiNC versus C/SiNC geometry, internal structure & architectural variability in as-received material

Material Characterization

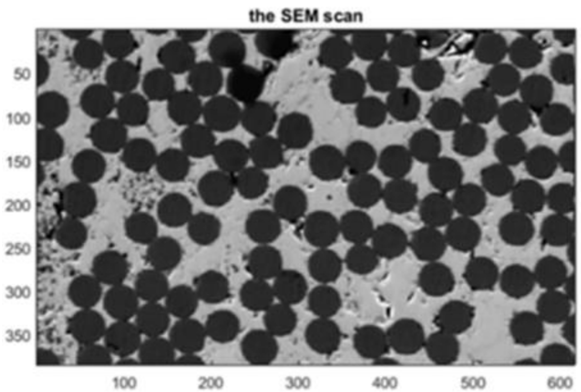
Energy-dispersive spectroscopy (EDS) – S400N C/SiNC CMC



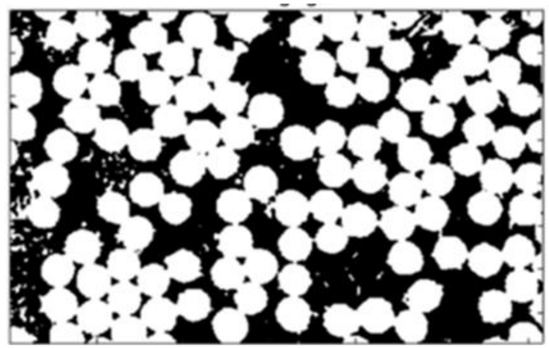
Intertow regions have higher oxidation volume fractions than intratow regions; carbon-rich interphase layer observed around fibers

C/SiNC CMC Variability

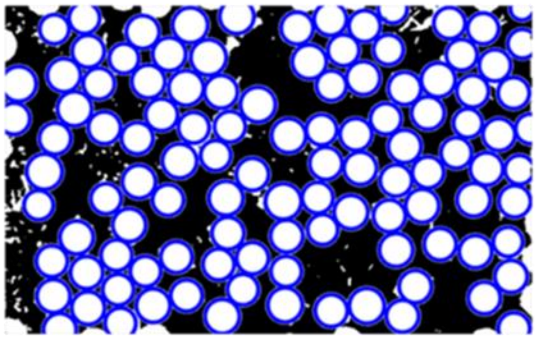
Image processing algorithm developed to detect multiscale structural & defects variability



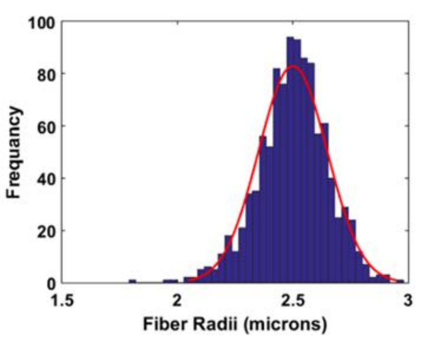
Scanning electron micrograph of intra-tow region

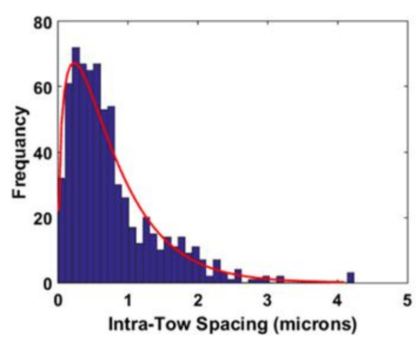


Segmented grayscale image



Fiber cross sections & intra-tow defects



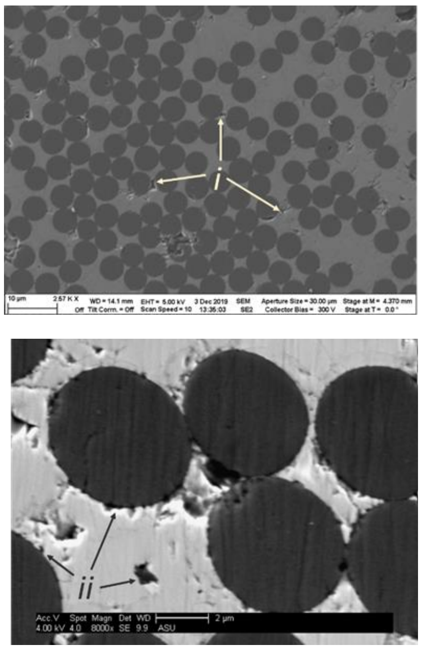


- **Porosity volume fractions: Intra-tow ~3%; Inter-tow: ~5%**
- **Tow cross section: 1498.221μm x 172.673μm**
- **Fiber radius: 2.4846 μm (mean); standard deviation 0.1489 μm**
- **Fiber volume fraction: 49.59%**

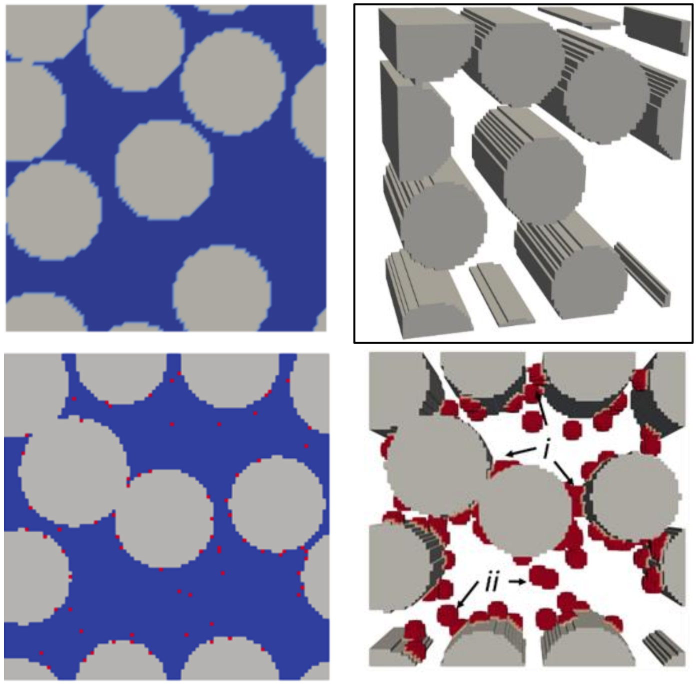
Khafagy, K., Datta S. & Chattopadhyay, A., “Multiscale Characterization and Representation of Variability in Ceramic Matrix Composites", *Journal of Composite Materials (in press).*

Microstructural Simulation & SRVE

Image processing algorithms under development to generate detailed 3D stochastic representative volume elements (SRVEs)



Micrographs illustrating intra-tow matrix porosity

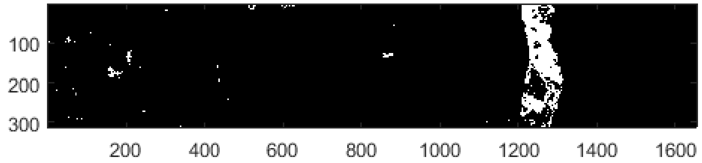


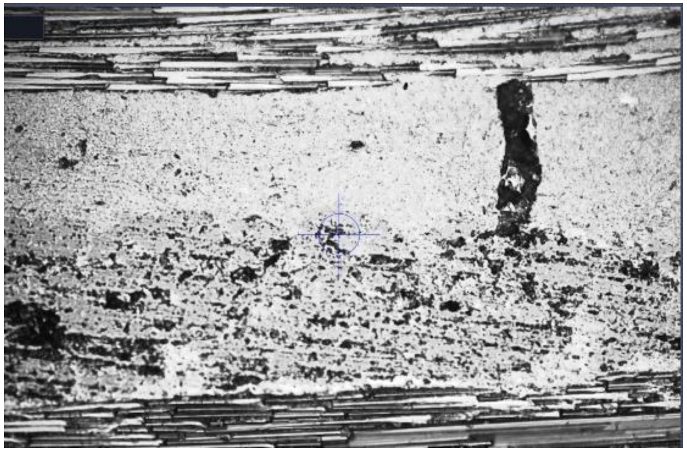
Microscale SRVEs containing intra-tow matrix porosity

Accurate in-situ microstructural representation will facilitate accurate modeling of damage initiation, progression, & subsequent failure

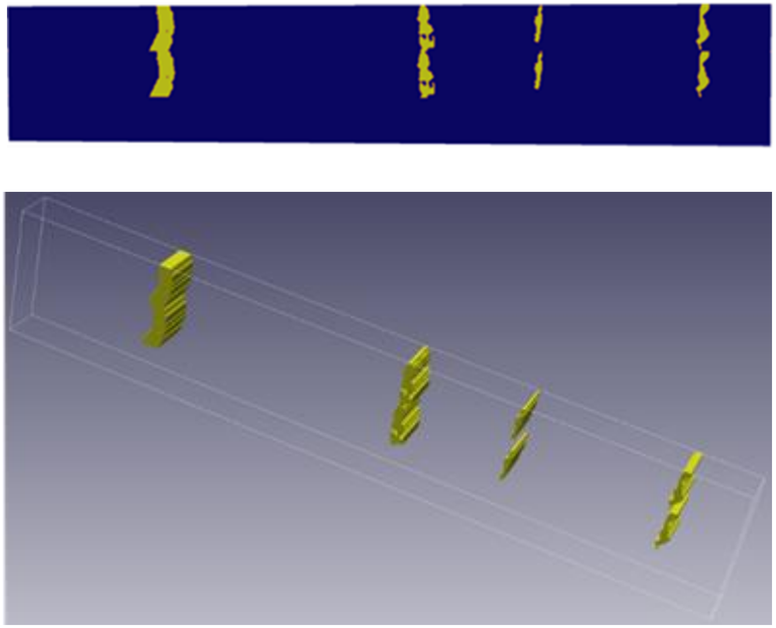
Microstructural Simulation & SRVE

Image processing algorithms currently under development to generate detailed 3D stochastic representative volume elements (SRVEs)





Micrographs illustrating inter-tow matrix porosity



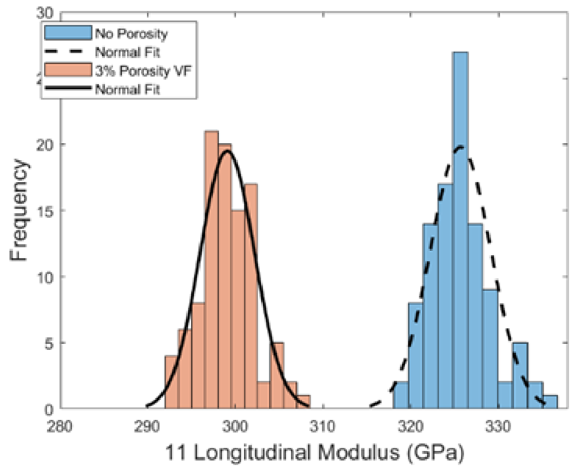
Microscale SRVEs containing inter-tow matrix porosity

Accurate in-situ microstructural representation will facilitate accurate modeling of damage initiation, progression, & subsequent failure

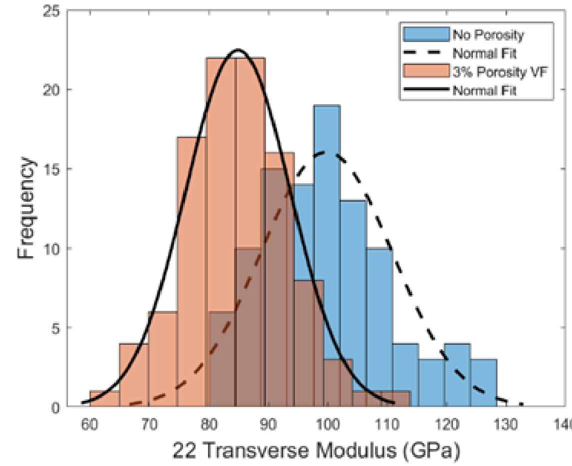
Microstructural Simulation & SRVE

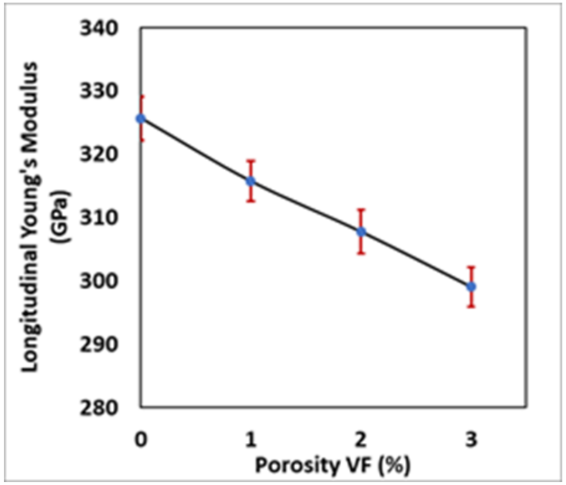
- 400 SRVEs generated with 1-3% intra-tow porosity VF
- Elastic properties obtained using high fidelity micromechanics theory

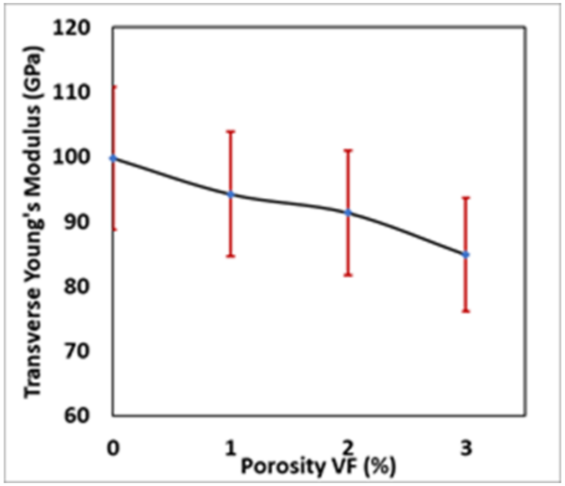
Longitudinal modulus

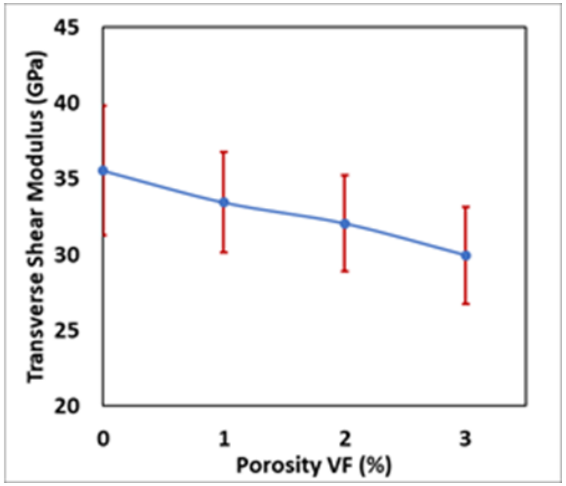


Transverse modulus









Presence of intra-tow matrix porosity deteriorates elastic properties of UD C/SiNC CMC. Larger standard deviation in transverse & shear

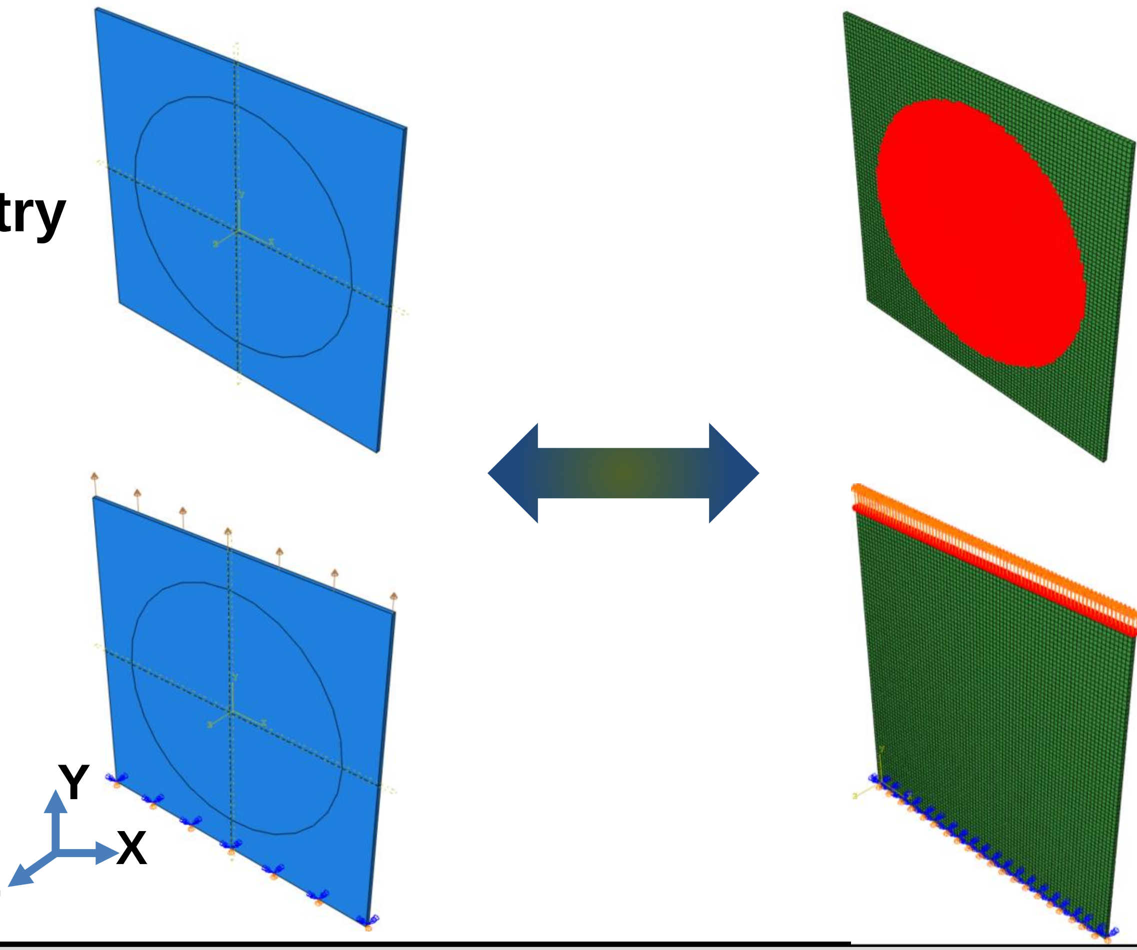
Converted high-fidelity SRVEs to finite element (FE) based grids

FE geometry

Developed SRVE generator

BCs and loading (along y)

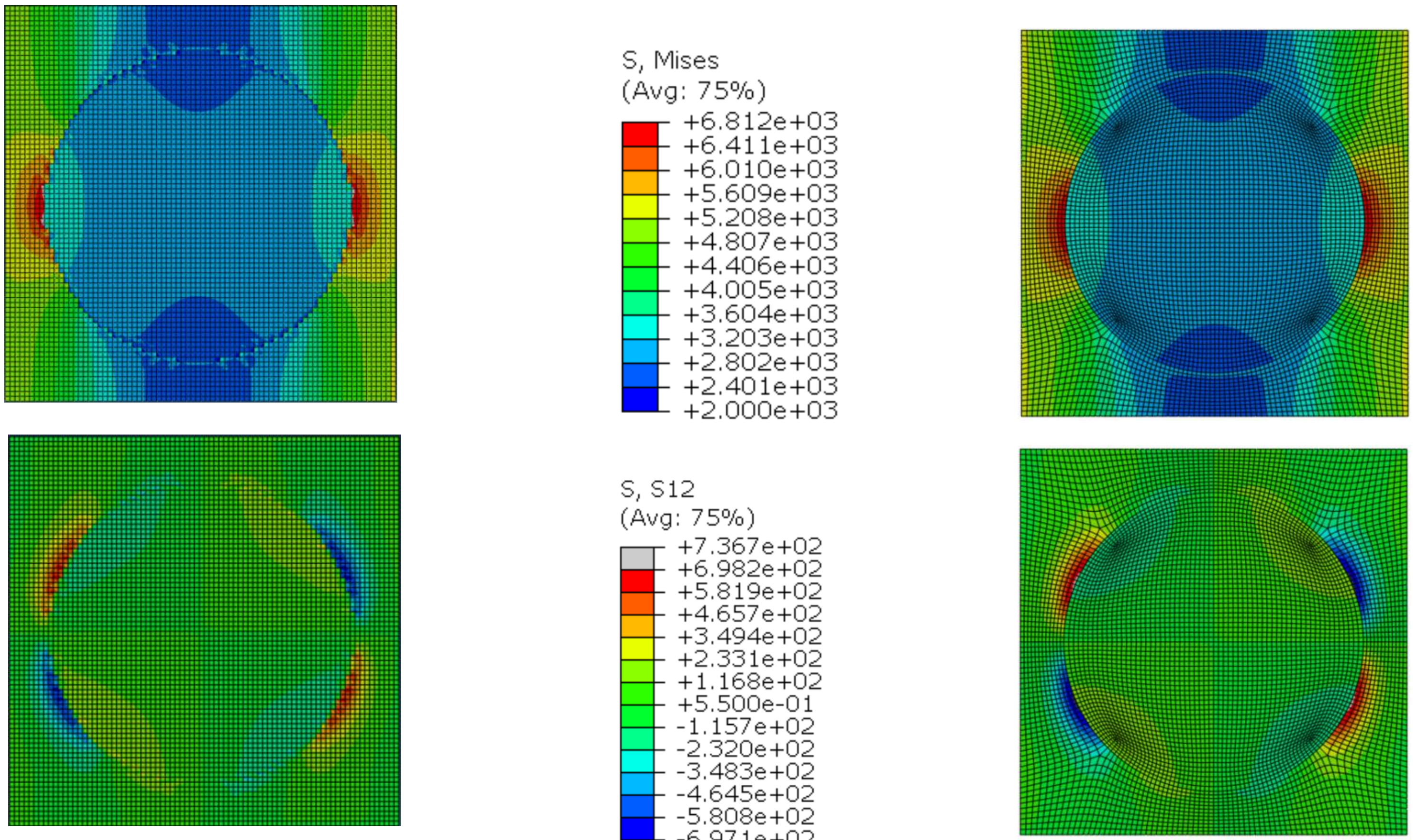
BCs and loading conditions



Geometry for single fiber from the developed generator & FE-based geometry

Microstructural Simulation & SRVE

von-Mises & shear stress comparison



Structured grid (SRVE generator)

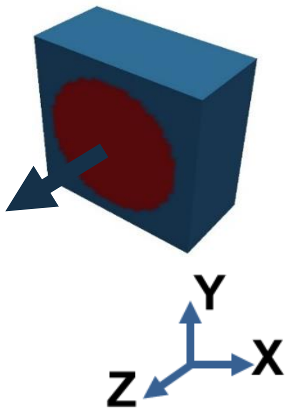
Structured mesh (ABAQUS geometry)

Good agreement with results from FE geometry and ABAQUS

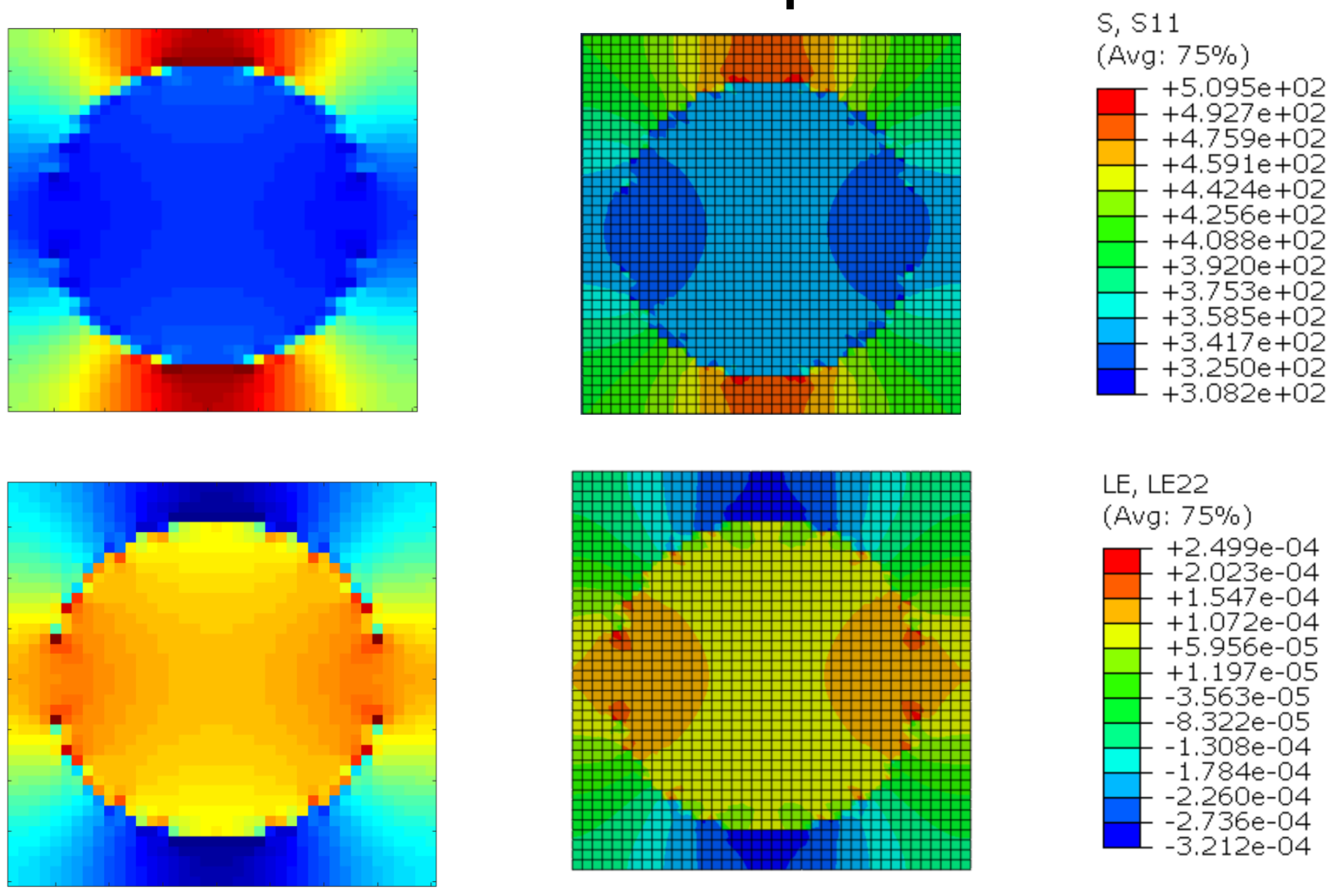
Microstructural Simulation & SRVE

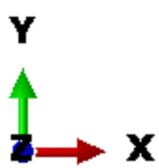
Incorporated SRVEs in parallelized HFGMC (pHFGMC)

Transverse stresses & strains comparison



RUC domain size:
40x40x20
Loading:
along fiber



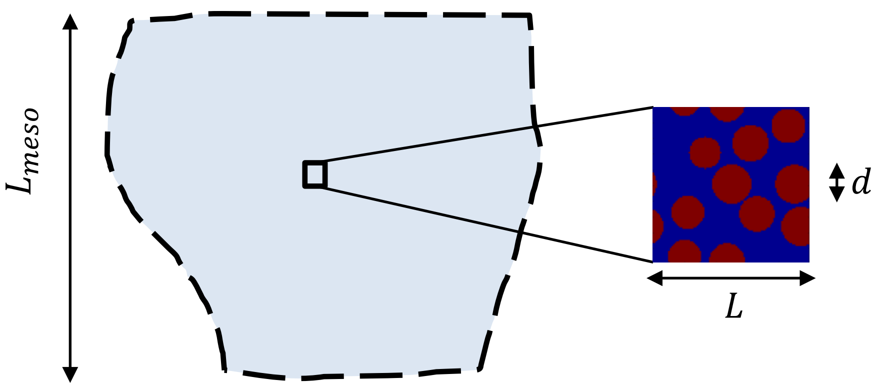


pHFGMC solver **ABAQUS solver**

Good agreement between FE and pHFGMC solvers

Size Effect in Stochastic Representative Volume Elements (SRVE)

- Multiscale analysis uses localization & homogenization schemes to bridge the length scales - key issue is the size of the RVE over which homogenization is conducted
- Stochastic RVE (SRVE): RVE in the presence of disorder/stochasticity in the microstructure
- A minimum SRVE size is required to approximate the mesoscale material behavior
- Minimum SRVE size increases
  - As stochasticity increases*
  - Critical for simulating nonlinear mechanical behaviors (plasticity, damage, failure)**



Characteristic lengths

d: Microscale (e.g., fiber diameter)
L: SRVE
L_{meso}: Mesoscale

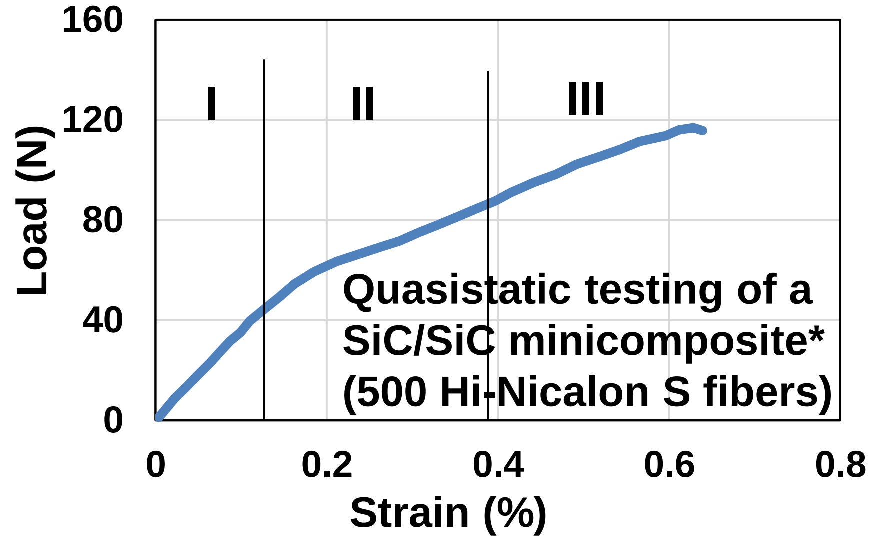
Weak stochasticity $d <$
Large stochasticity $d \ll$
$\} L \ll L_{meso}$

*Ostoja-Starzewski (2006) **Trias (2006)

Size Effect in Stochastic Representative Volume Elements (SRVE)

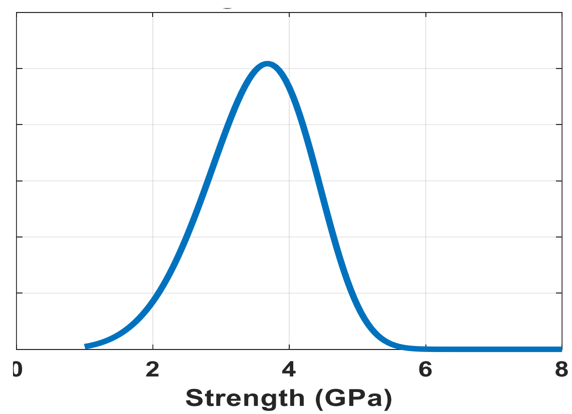
Example: SRVE for Tow Failure

- Unknown SRVE size for tow failure



Experimentally observed tow behavior:

- I: Linear elastic behavior
- II: Nonlinear behavior with matrix cracking until saturation
- III: Nonlinear behavior with sequential fiber failure



Experimental distribution of strength for Hi-Nicalon fiber**

Model assumptions:

- No fiber failure occurs in region II
- Matrix has no load sharing role in region III
- Stochasticity arises from varying fiber strengths

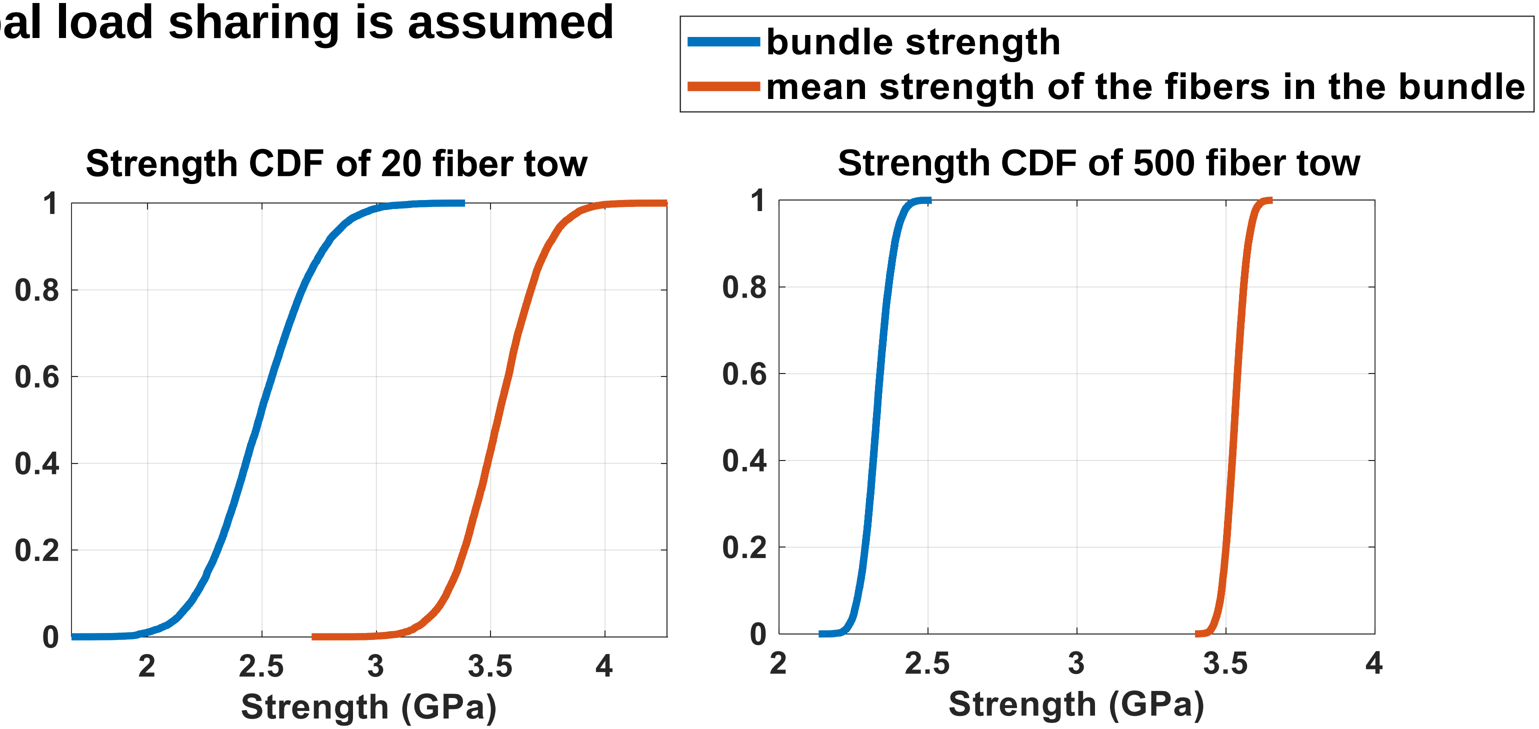
Stochasticity in tow failure behavior due to varying fiber strengths

*Chateau (2014); **Calard, V., & Lamon, J. (2004)

Size Effect in Stochastic Representative Volume Elements (SRVE)

SRVE for Tow Failure

- Force controlled loading until failure
- Fiber strengths randomly sampled from experimental Weibull distribution
- Global load sharing is assumed



Increase in number of fibers decreases stochasticity

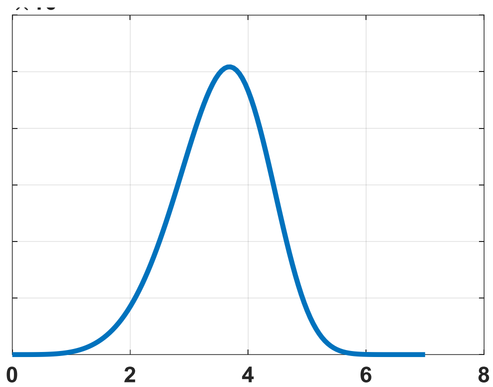
Tow strength prediction strongly depends on number of fibers - illustrates importance of minimum SRVE size

Size Effect in Stochastic Representative Volume Elements (SRVE)

<u>SRVE for Tow Failure: Modified Fiber Damage Model</u>

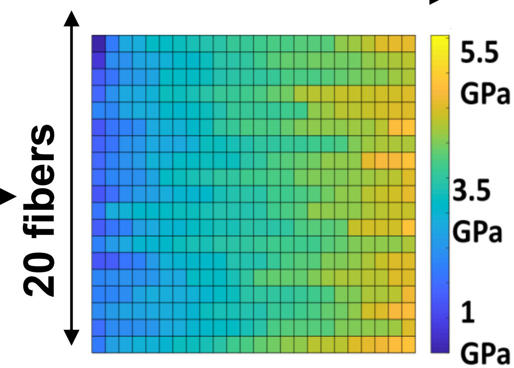
- **Objective: Simulate strength of tows with 500 fibers using an equivalent <u>20-fiber SRVE</u>**
- **Each fiber consist of 25 pseudo fibers with same cross-sectional area & initial elastic stiffness**

Experimental Weibull distribution of strength for Hi-Nicalon fiber*



Random sampling

25 pseudo fibers each (ascending order of strengths)



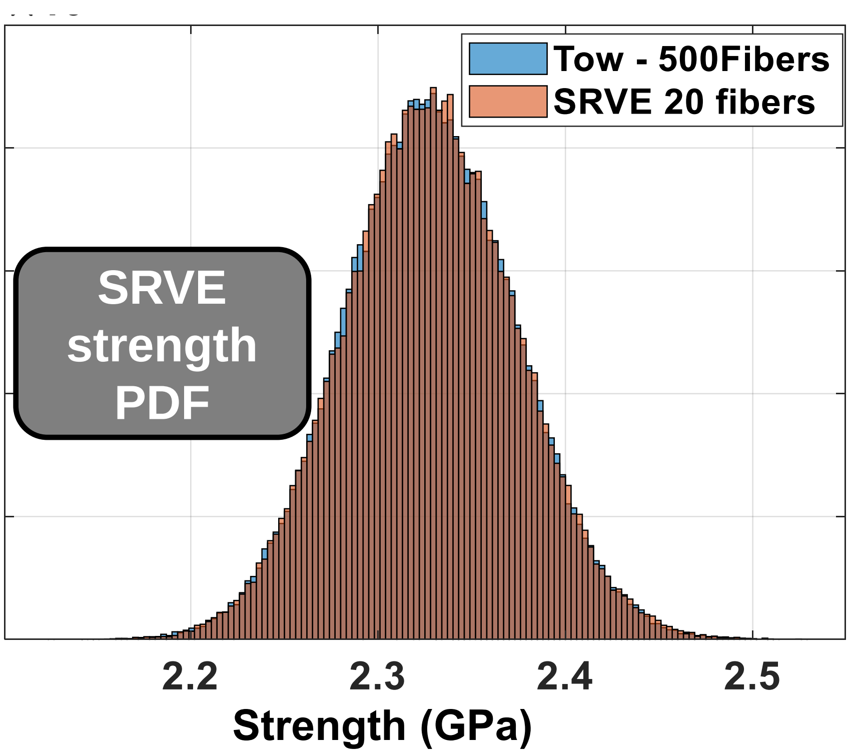
Each pixel denotes a different fiber strength

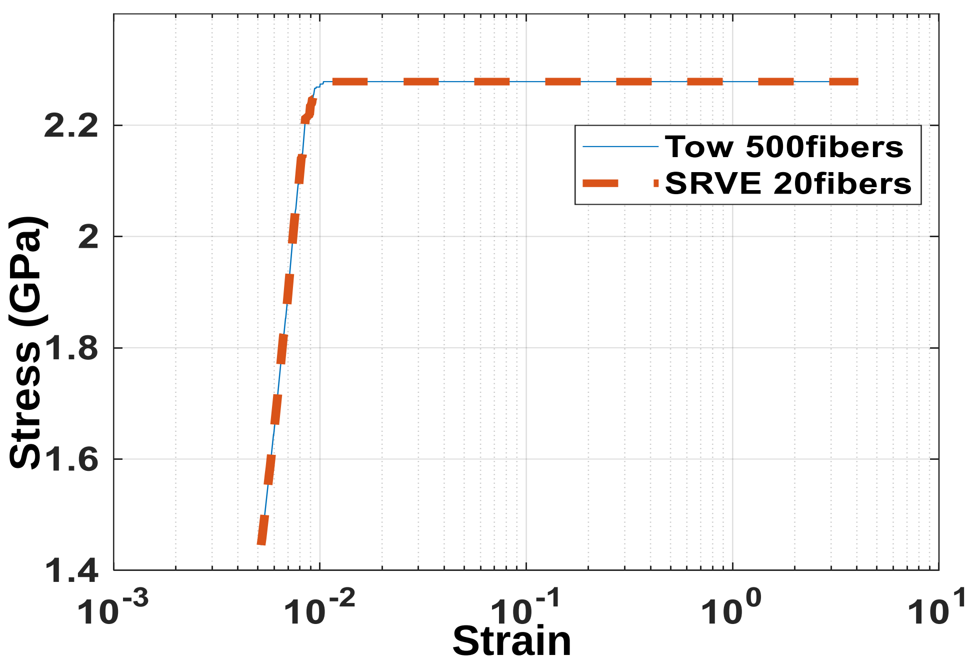
- **Fiber failure model modified to a discrete-progressive damage model**
- **If the stress on a fiber exceeds the strength of one of its pseudo fibers, then that pseudo fiber fails**
  - **Fiber stiffness degraded accordingly**
  - **Strengths of remaining pseudo fibers degraded by same fraction**

*Calard, V., & Lamon, J. (2004)

Size Effect in Stochastic Representative Volume Elements (SRVE)

SRVE for Tow Failure: Modified Fiber Damage Model





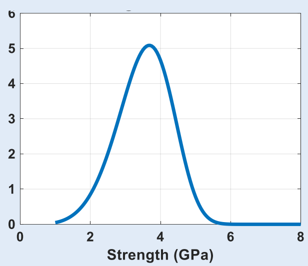
- Tow strength distributions with the 20-fiber SRVE compare well with 500-fiber tows
- Stress-strain responses show excellent agreement

The modified fiber damage model enables the SRVE to capture stochasticity in tow fiber failure strength with significantly reduced number of fibers

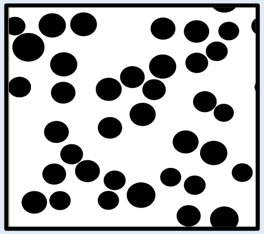
Bayesian framework for uncertainty assessment

Model input parameters: θ

Prior estimates of the parameters: $P(\theta)$

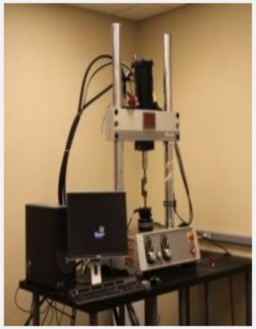


The probability of observations X_{obs} given the parameters (θ) and uncertainty: $P(X_{obs}|\theta)$



Multiscale model (Task 3)

Observations: X_{obs}



Experimental testing (Task 6)

Bayesian inference

$$P(\theta|X_{obs}) \propto P(\theta)P(X_{obs}|\theta)$$

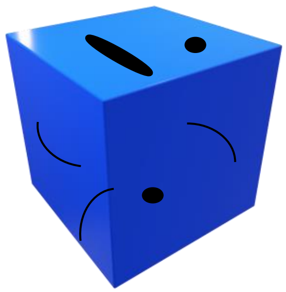
Updated probability distributions of the parameters: $P(\theta|X_{obs})$

Bayesian inference for estimating parameters of material behavior models based on sparse characterization data & experimental observations

Thermomechanical Progressive Matrix Damage Model

Thermomechanical progressive damage model accounting for crack growth & nucleation and micropore formation

- **Incorporation of flaw statistics, temperature dependent material properties**
- **Crack & void growth governed by fracture mechanics, crack growth kinetics**
- **Matrix cracks activate when stress intensity factor exceeds critical value; crack growth rate affected by temperature, environment**



Matrix RUC with flaws

$$\sigma_{ij} = (1 - D)C_{ijkl}(\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{p} - \varepsilon_{kl}^{D} - \varepsilon_{kl}^{T})$$

$$\dot{D} = \begin{cases} \dot{D}_p & K_I \leq K_{IC} \\ \dot{D}_c & K_I > K_{IC} \end{cases}$$

C: Elastic stiffness tensor
ε^{tot}: Total strain
ε^{p}: Porosity-based strain
ε^{D}: Flaw growth-based strain
ε^{T}: Thermal strain

D: Damage ISV
D_p: Porosity ISV
D_c: Matrix cracking ISV
K_I: Stress intensity factor (SIF)
K_{IC}: Critical SIF

Skinner and Chattopadhyay (2020) Composite Structures

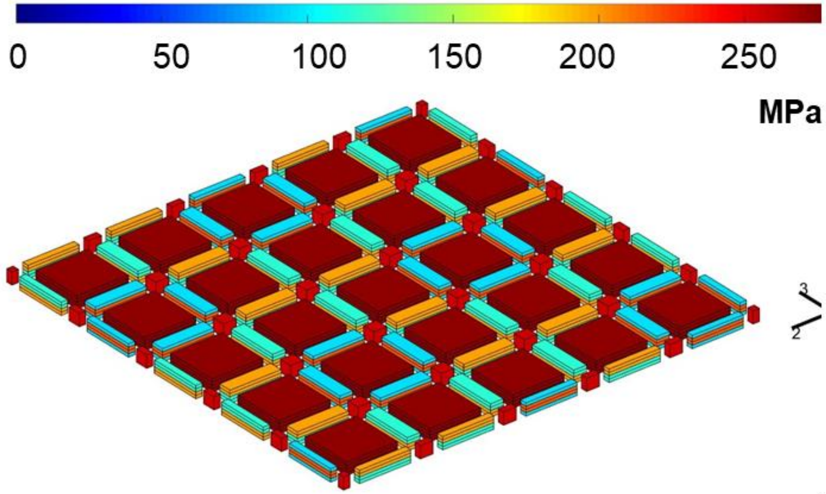
Thermomechanical Progressive Matrix Damage Model

Cooldown Framework

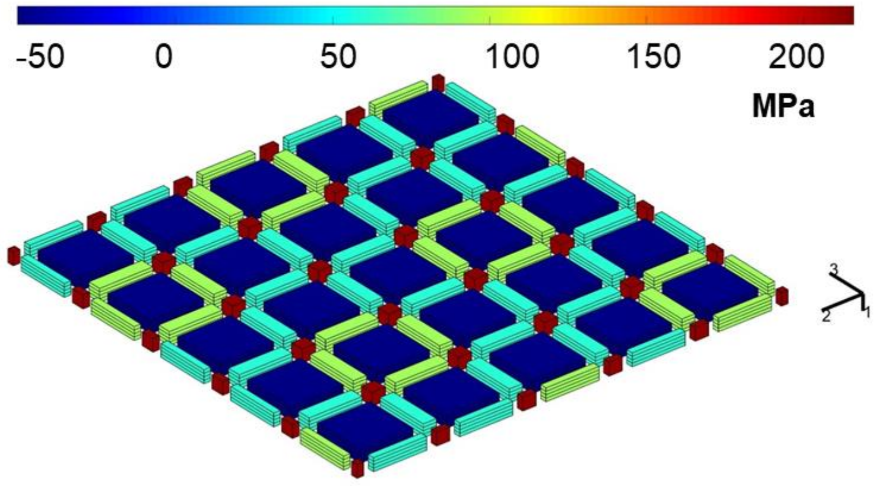
- CMC response highly dependent on as-produced thermal residual stress and damage state
- Developed multiscale cooldown simulation framework to determine thermal residual stress at micro-, meso-, and macroscales in CMC weave
- Applied temperature-dependent damage model with cooldown framework to capture manufacturing-induced damage and residual stresses

Thermal Residual Stresses

2D Woven C/SiC (5HS weave architecture)



Residual effective stress



Residual through-thickness stress

Cooldown framework captures realistic initial state with thermal residual stress profiles, initial damage distribution

Thermomechanical Progressive Matrix Damage Model

Cooldown Framework

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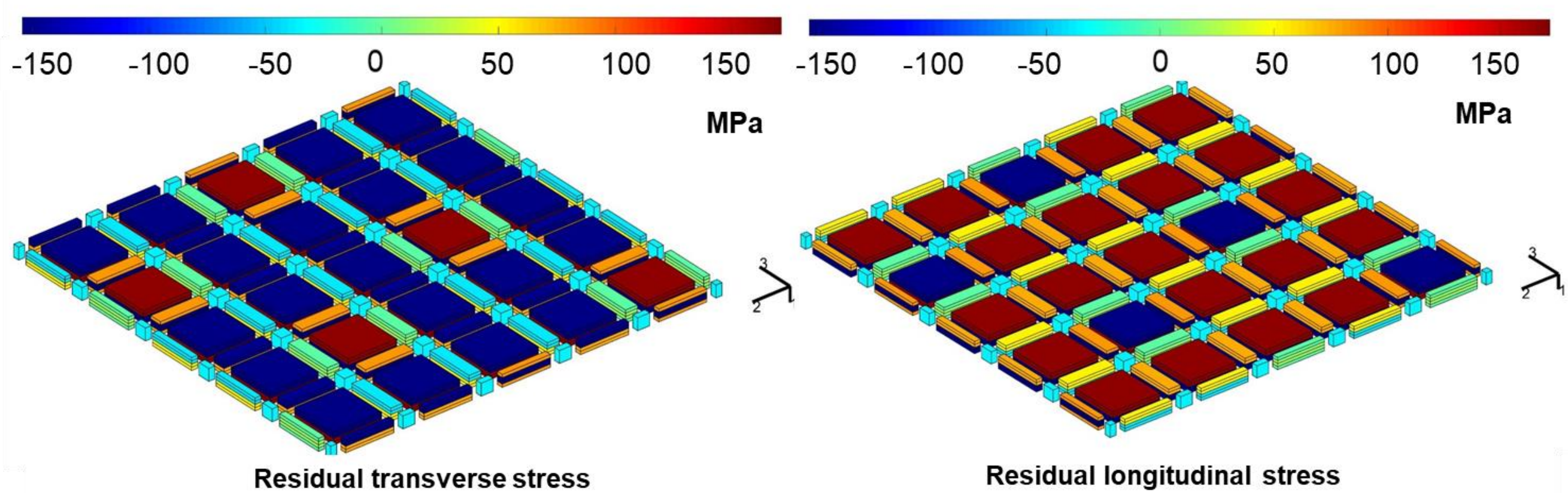
- Applied temperature-dependent damage model with cooldown framework to capture manufacturing-induced damage and residual stresses

Thermal Residual Stresses



Cooldown framework captures realistic initial state with thermal residual stress profiles, initial damage distribution. Damage initiates in undulating tows and propagates to the intertow matrix subcells.

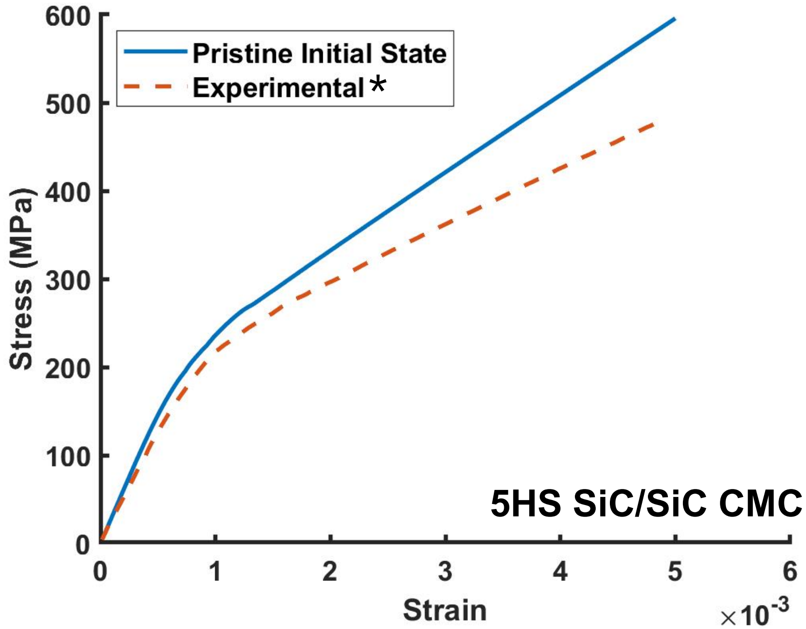
Thermomechanical Progressive Matrix Damage Model

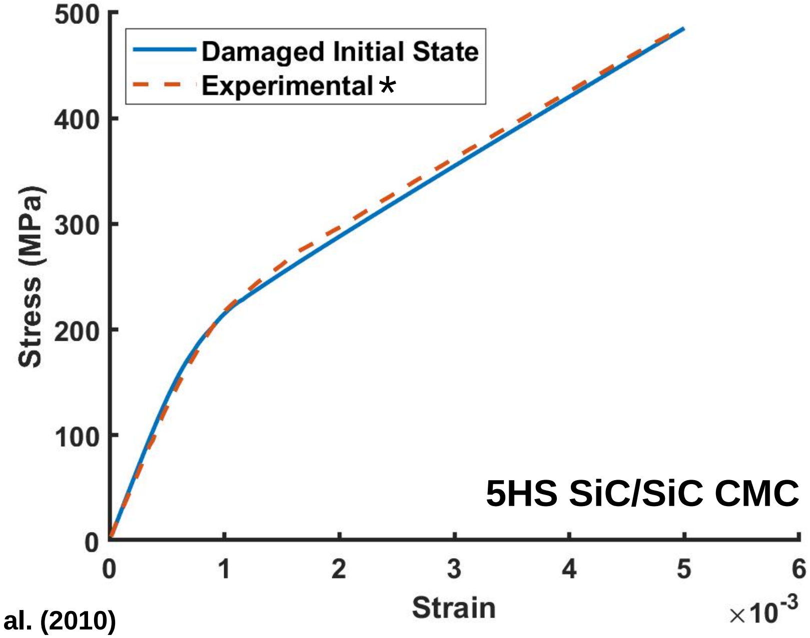
Results

- Cooldown framework captures realistic initial state, accounts for manufacturing-induced damage, thermal residual stresses
- Mechanical loading simulation captures nonlinear elastic material behavior, first matrix cracking

Comparison with Experiment

Loading direction: Longitudinal





* Gowayed et al. (2010)

Cooldown simulation followed by mechanical loading simulation makes framework applicable to entire range of CMC operating temperatures

Creep Modeling

Complex creep behavior in CMC components, under sustained loading & elevated service temperatures, occurs across multiple length scales and interacts with the inherent brittle damage behavior of the individual constituents.

Accurate CMC component life prediction requires in-depth understanding of creep, creep-fatigue, and damage interactions across the length scales

Key Issues

- **Time-dependent constituent load transfer due to differing creep rates; CMC creep consists of creep & relaxation in constituents**
- **Damage mechanisms & failure modes depend on constituent creep susceptibility**
- **Thermal residual stresses in as-produced CMC parts affect subsequent creep behavior**

Develop a 3D viscoplasticity model; integrate into a micromechanics framework to simulate constituent creep & subsequent time-dependent load transfer

Khafagy, K., Sorini, C., Skinner, T. & Chattopadhyay, A., "Modeling Creep Behavior in Ceramic Matrix Composites", *Ceramics International,* (submitted 2020).

Creep Modeling

Development of 3D thermomechanical orthotropic viscoplasticity model

- Norton-Bailey creep power law
- Hill orthotropic plastic potential
- Arrhenius temperature dependence
- Associative flow rule
- Time-hardening and strain-hardening formulations

- Matrix damage modeled with previously developed thermomechanical progressive damage model (Task 3.1)
- Curtin progressive damage model applied to simulate stiffness reduction due to successive fiber failure

Constitutive law: $\sigma_{ij} = (1 - D)C_{ijkl}\left(\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{I} - \varepsilon_{kl}^{th}\right)$

where $\varepsilon_{ij}^{I} = \int_0^t \dot{\varepsilon}_{ij}^{I}\, dt$ **and** $\mathrm{D} = \int_0^t \dot{D}\, dt$

Constituent model parameters will be determined from in-house creep-fatigue tests

Creep Modeling

3D orthotropic viscoplasticity formulation incorporated into generalized method of cells (GMC) micromechanics framework

- **Effective stiffness matrix**

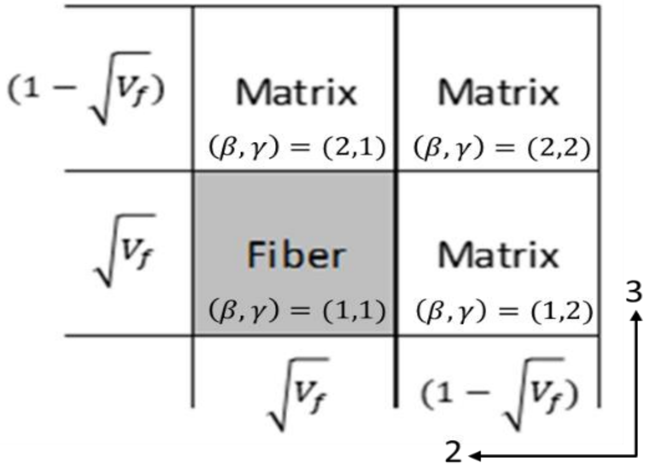
$$\bar{\boldsymbol{C}} = \frac{1}{h_{tot} l_{tot}} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} \boldsymbol{C}^{(\beta,\gamma)} \boldsymbol{A}^{(\beta,\gamma)} h_\beta \, l_\gamma$$

- **Global RUC stresses**

$$\bar{\boldsymbol{\sigma}} = \frac{1}{h_{tot} l_{tot}} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} \boldsymbol{\sigma}^{(\beta,\gamma)} h_\beta \, l_\gamma$$

$\boldsymbol{A}$: Strain concentration tensor
h_β, l_γ: Subcell dimensions
h_{tot}, l_{tot}: RUC dimensions
$\boldsymbol{N_\beta}, \boldsymbol{N_\gamma}$: Number of subcells in each dimension

Unidirectional GMC RUC

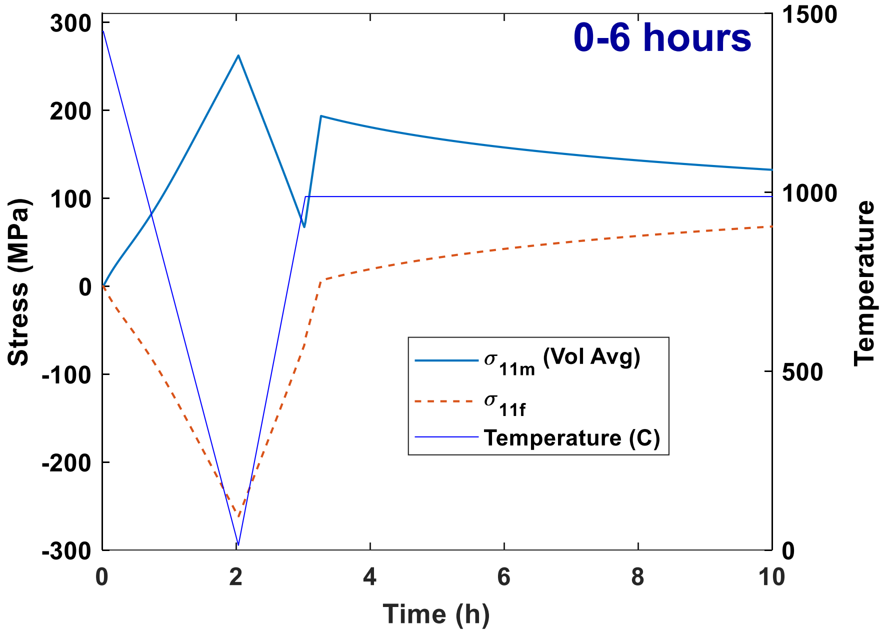


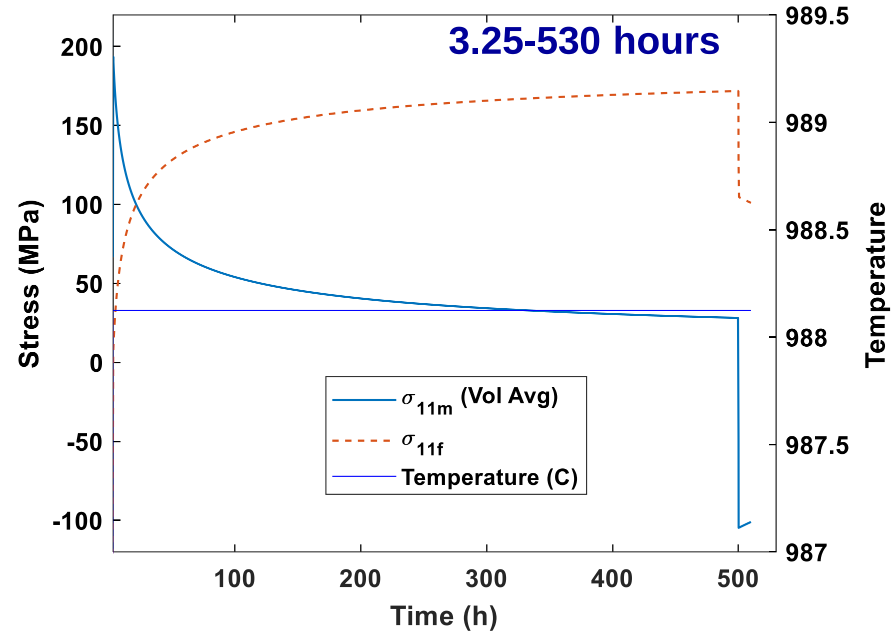
GMC integration facilitates simulation of CMCs with arbitrary microstructures & ply/weave architectures; enables simulation of creep in individual constituents & associated constituent load transfer

Creep Modeling

Thermal residual stress effects, Contd.

- Simulated response – Hi Nicalon SiC/CVD-SiC microcomposite* subjected to thermal cooldown from 1450 °C to RT followed by 100 MPa creep at 1000 °C





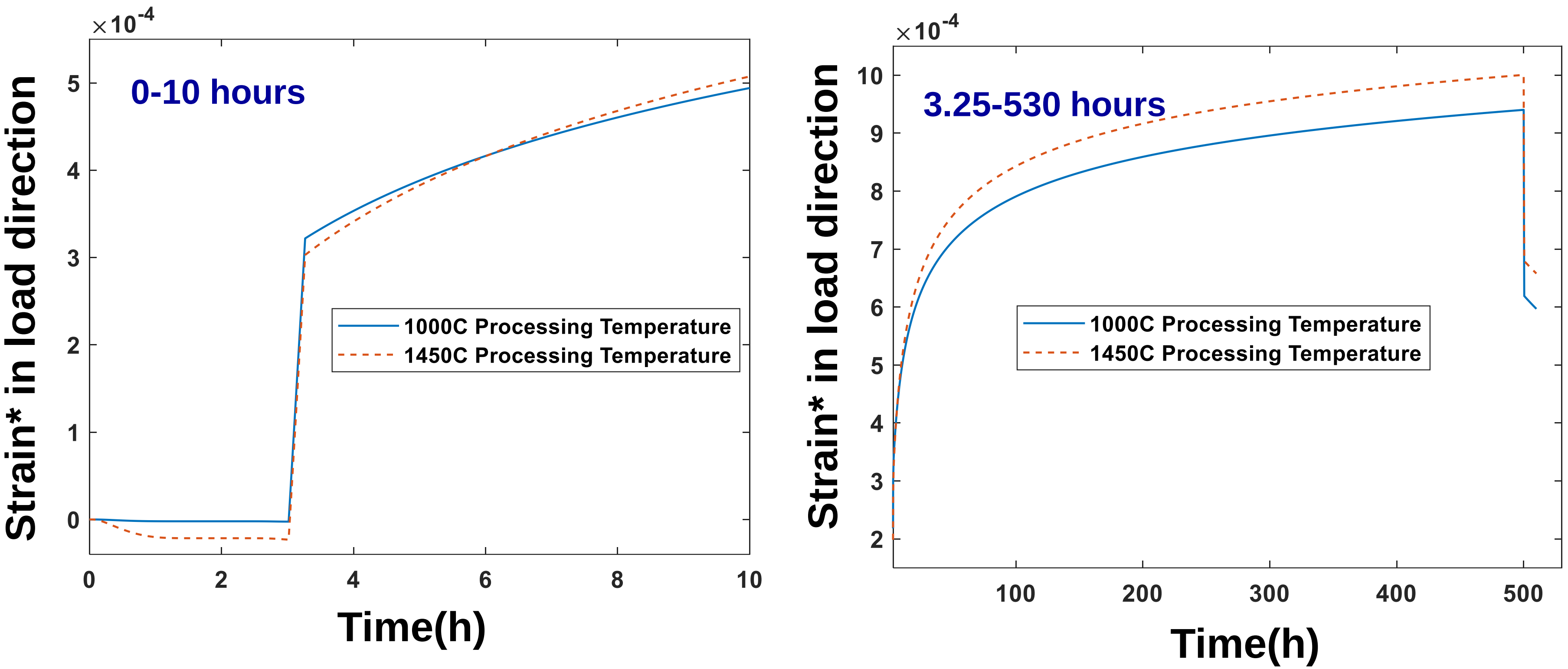
Constituent stresses in load direction vs. time

- Post-manufacturing cooldown causes as-produced tensile stress in matrix & compressive stress in fiber (matrix CTE > fiber CTE)
- Creep causes redistribution of constituent residual stresses; matrix creeps first and sheds load to fiber; matrix is in compression and fibers are in tension upon unloading

* Model calibrated using microcomposite creep test results presented in Rugg et al. (1999)

Creep Modeling

Effect of processing temperature: 1000ºC vs. 1450ºC



Microcomposite strain* vs. time

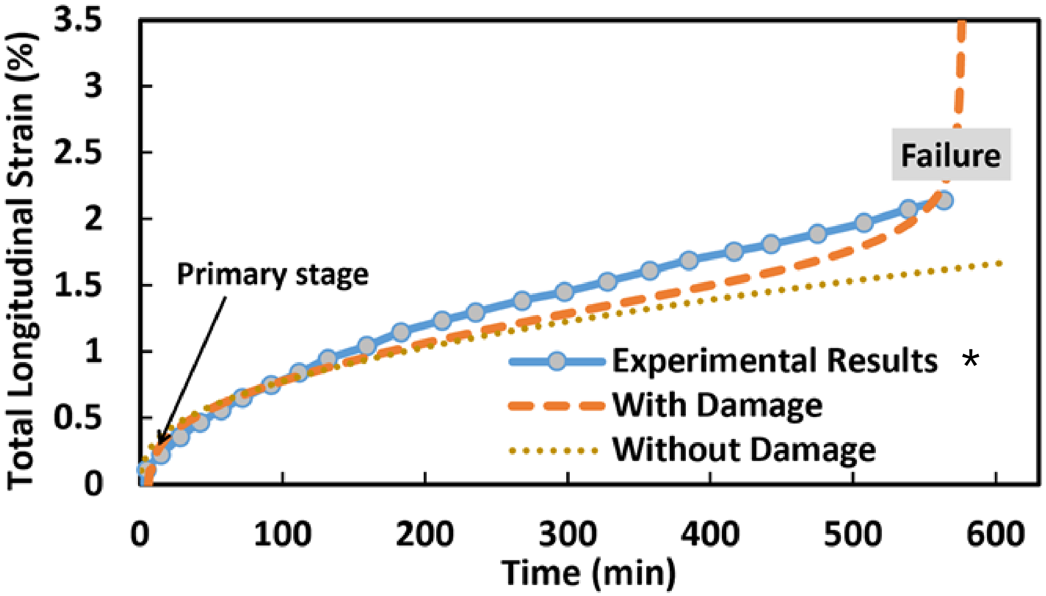
Higher predicted inelastic (creep) strain for higher processing temperature due to process-induced compressive stress in matrix, <u>which is less creep-resistant</u> than fiber for the SiC/SiC microcomposite

*** Plotted strain is $\varepsilon_{11}^{total} - \varepsilon_{11}^{thermal}$**

Creep-damage Modeling

Simulated total longitudinal strain time history for Hi-Nicalon/CVD-SiC CMC single fiber microcomposite

- **Prescribed loading: 381 MPa (constant), 1300 °C**
- **Matrix damage simulated with developed thermomechanical progressive damage model**
- **Fiber damage & failure simulated with Curtin progressive damage model**



Total longitudinal strain vs. time

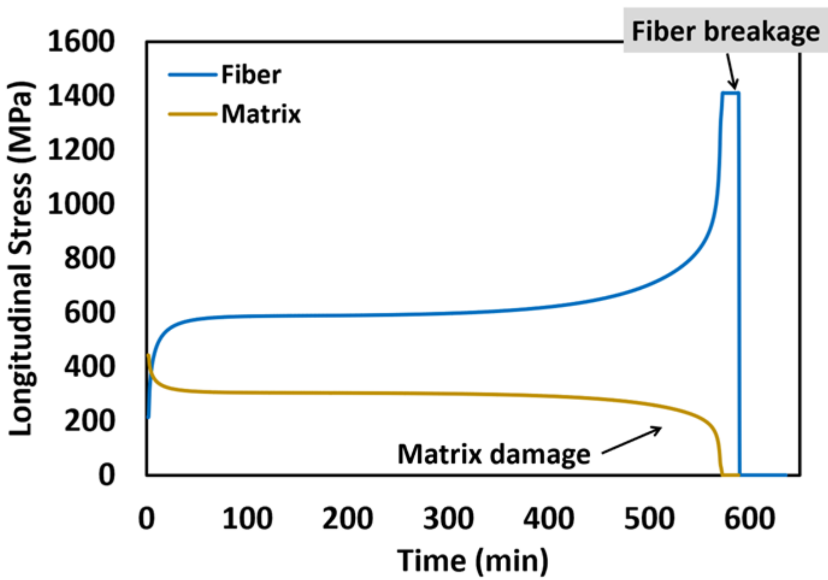
Incorporation of matrix and fiber progressive damage models permit simulation of i) tertiary creep; ii) microcomposite progressive damage; iii) microcomposite failure

* Rugg et al. (1999).

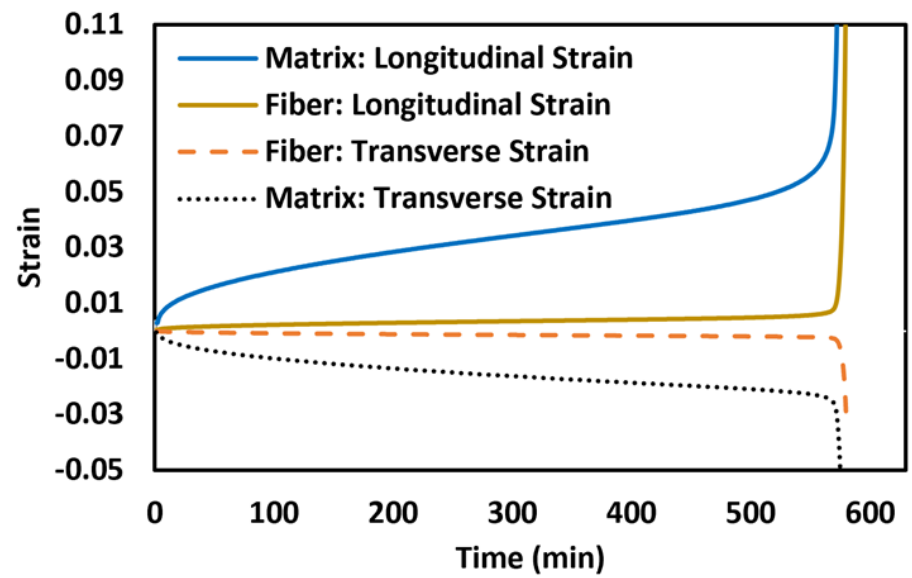
Creep-damage Modeling

Simulated constituent stress and strain time history for Hi-Nicalon/CVD-SiC CMC single fiber microcomposite

- **Prescribed loading: 381 MPa (constant), 1300 °C**



Constituent longitudinal stress vs. time



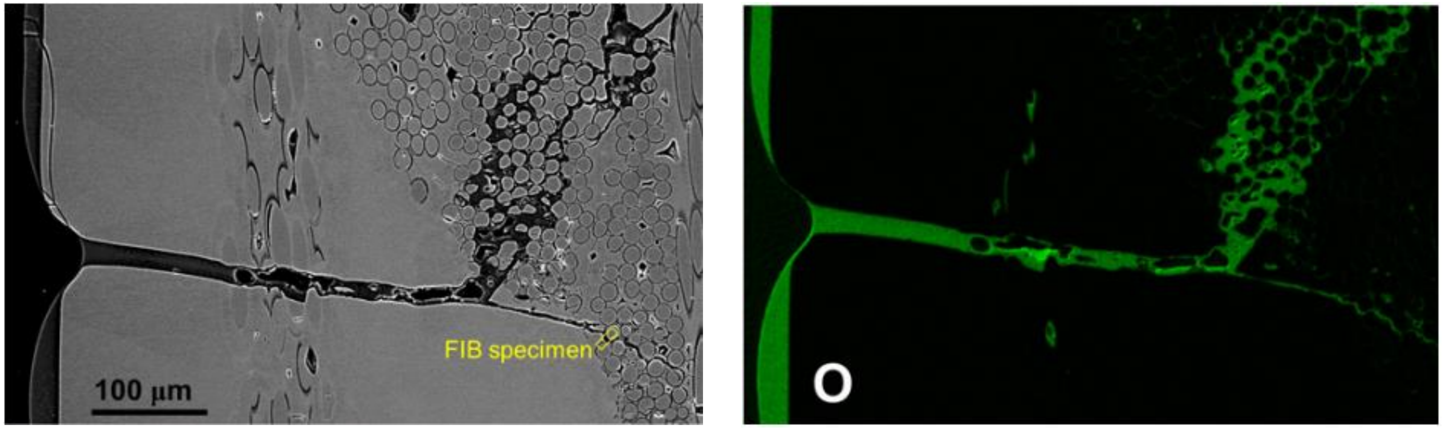
Constituent longitudinal and transverse strains vs. time

Incorporation of matrix and fiber progressive damage models permit simulation of i) tertiary creep; ii) microcomposite progressive damage; iii) microcomposite failure

Damage-diffusion Oxidation Coupling

Oxidation plays a major role in the response of CMCs at elevated temperatures

- **Matrix cracks create passages for oxygen to diffuse into the material**
- **Oxidation of the fiber interphase or the fusion of the SiC fiber to the SiNC matrix impairs load transfer capabilities**
- **Oxidation reaction of oxygen-exposed SiNC matrix activates at extreme temperatures, resulting in a multi-regimed response**



Terrani (2014) “Silicon carbide oxidation in steam up to 2 MPa”. Journal of the American Ceramic Society.

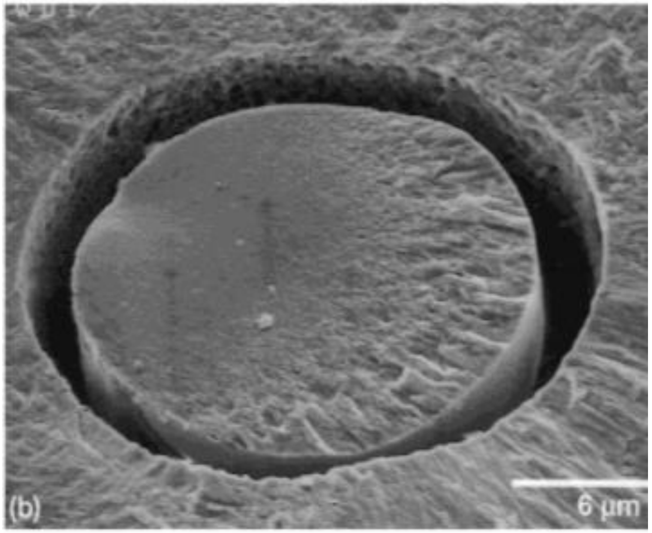
Model under development to address complex coupling between anisotropic damage, diffusion, crack closure, & oxidation of the fiber-matrix interphase at the microscale

Damage-diffusion Oxidation Coupling

Model under development

- Anisotropic damage model with crack closure
- Nonlinear damage-diffusion coupling
- Oxidation model - couple concentrations of gaseous oxygen to interface material
- User defined elements (UELs) with additional concentration degrees of freedom developed & integrated into Abaqus FE software

Oxidation of Fiber Interface



Jacobson (1999) "High-Temperature Oxidation of Boron Nitride: II, Boron Nitride Layers in Composites".

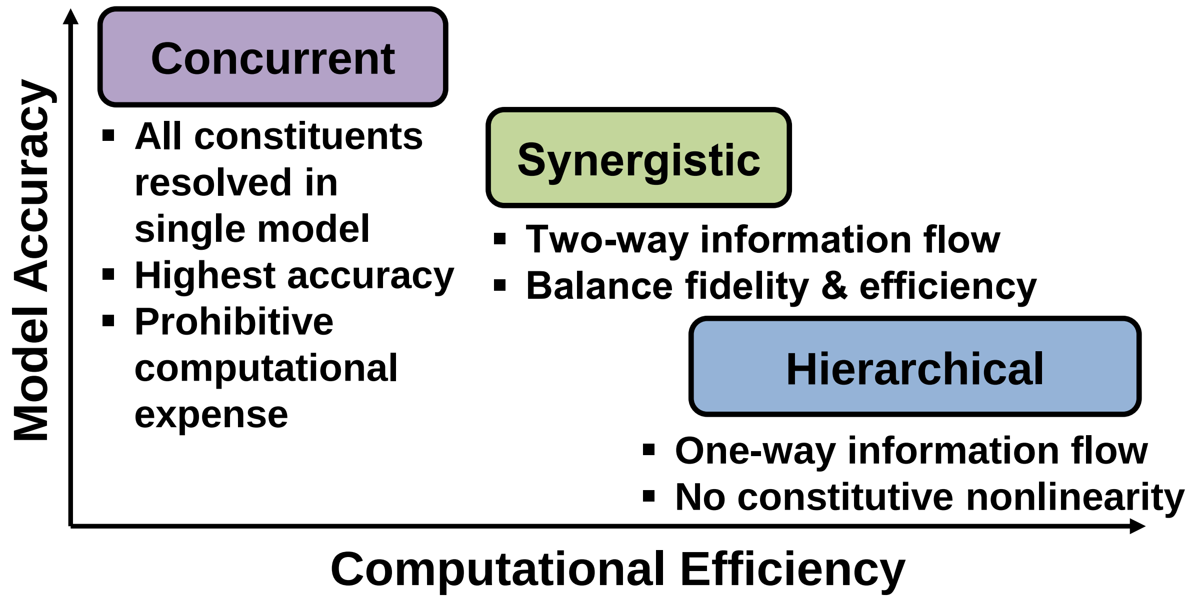
Need for Computational Efficiency

Necessary to balance fidelity & efficiency to enable model scalability

- Multiscale handshaking methods: Hierarchical, concurrent, synergistic
- Hierarchical models unable to admit constitutive nonlinearity; precludes simulation of creep & progressive damage
- Concurrent models prohibitively computationally expensive
- Part & component simulation require parallelization & model order reduction

Additional efficiency required in presence of:

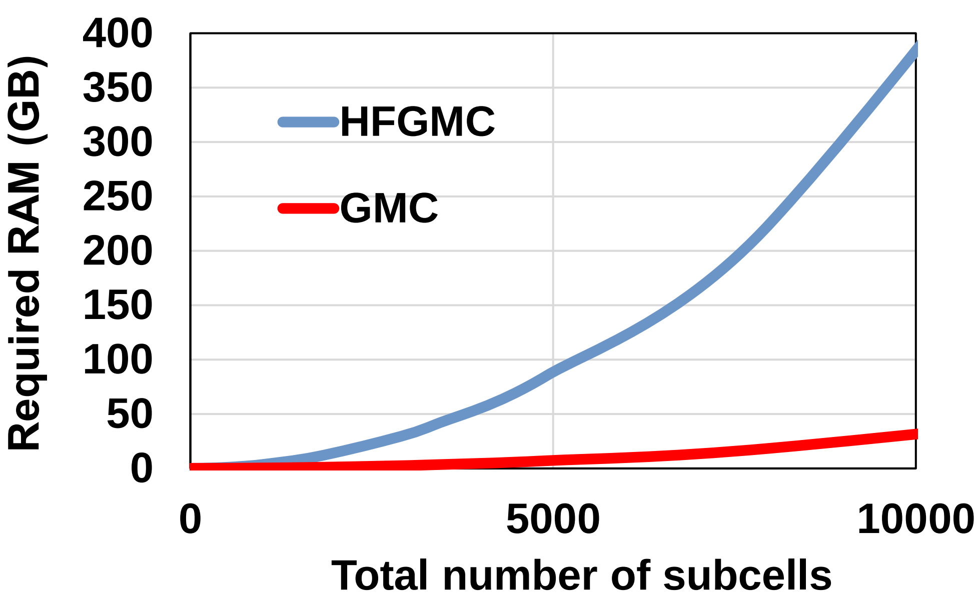
- Complex geometry
- Multiple analysis scales
- Material & geometric uncertainty
- Time-dependent nonlinear material behavior



Approach: Increase computational efficiency & model scalability via parallelization & model order reduction techniques

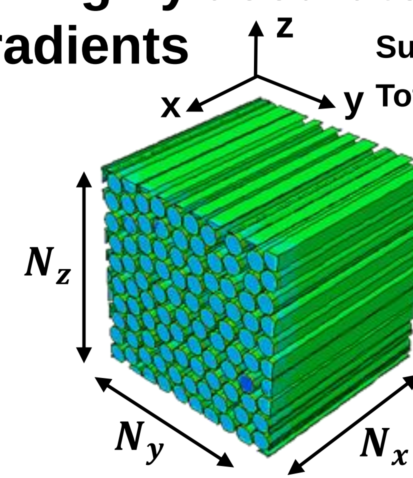
Need for Computational Efficiency

- GMC*: First-order local fields – highly efficient; lack of normal-shear coupling & local field gradients*
- Higher order local fields necessary to accurately model nonlinear response and failure
- HFGMC***: Second-order local fields – highly accurate; admits normal-shear coupling & local field gradients

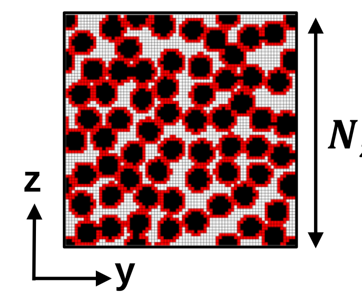


Subcells in direction i: N_i

Total subcells in RVE: $N_x N_y N_z$



Microscale RVE



Microscale RVE mesh

Number of equations to be solved:

GMC: $6N_xN_yN_z$ HFGMC: $21N_xN_yN_z$

- Improved fidelity of HFGMC comes at significant computational cost
- Efficient HFGMC implementation necessary for model scalability

*GMC: Generalized Method of Cells; **Aboudi et al., (2012) ***HFGMC: High Fidelity Generalized Method of Cells

Efficiency Improvement

Methodology to achieve computational efficiency

- Most memory & time-consuming operation in HFGMC is inversion of global stiffness matrix
- Global stiffness matrix must be computed every time local subvolume experiences damage
- Multiscale simulations require solution of multiple expensive micromechanics simulations at every time increment

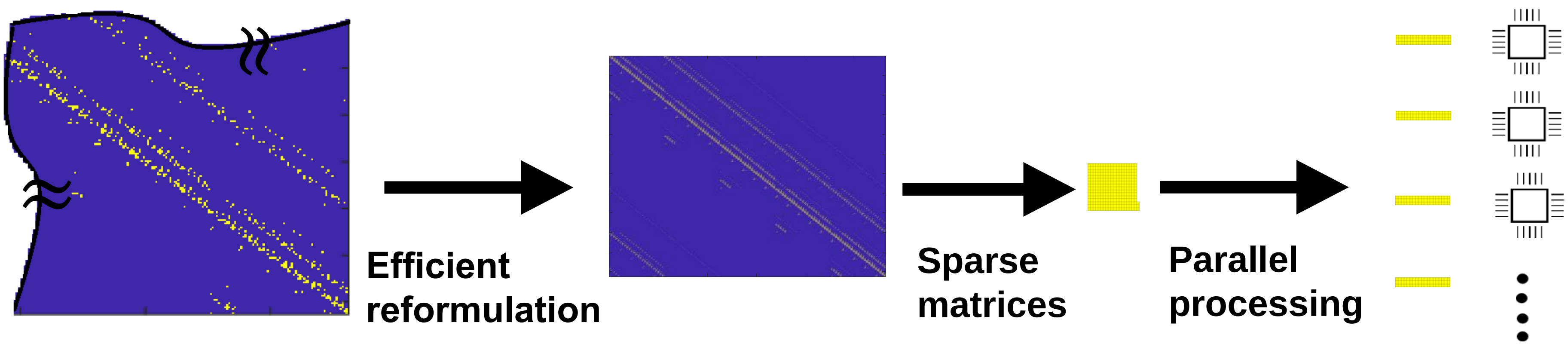


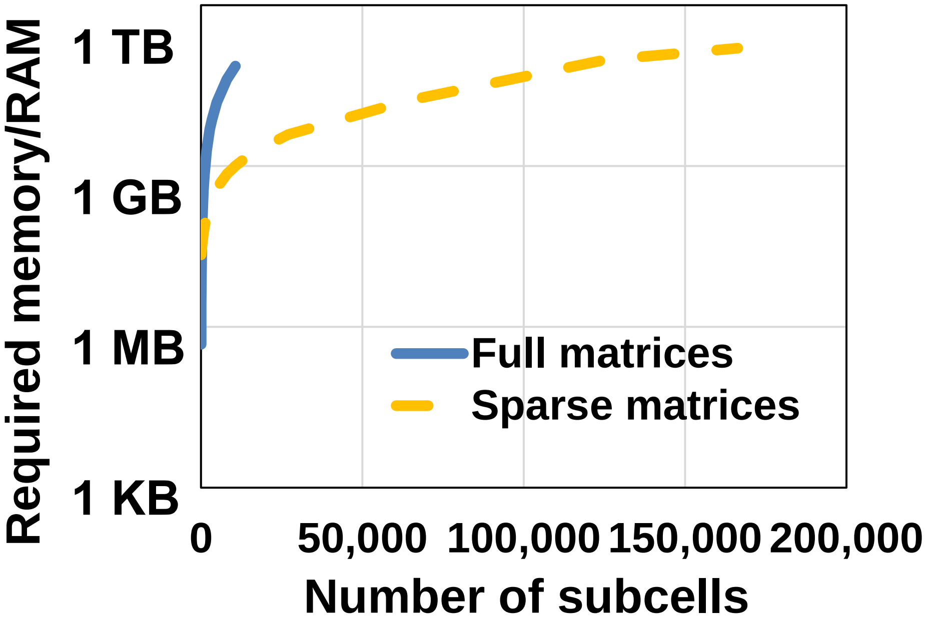
Illustration of sparsity in global stiffness matrix & methodology used to achieve computational efficiency

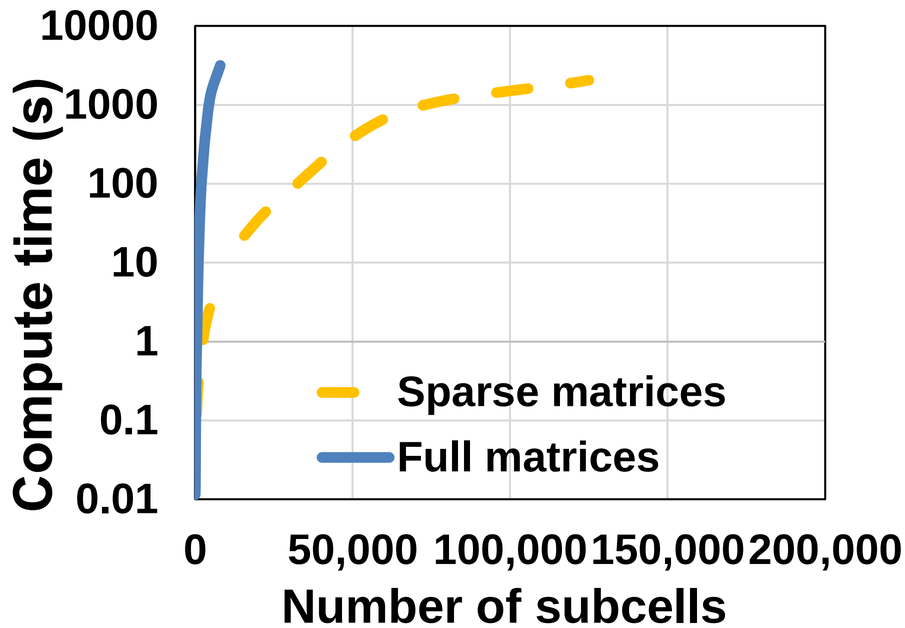
Combination of efficient reformulation, sparse matrix representation & parallel processing used to achieve improved computational efficiency

Balusu & Chattopadhyay, *Comput. Mat. Sci.* (2021)

Efficiency Improvement

HFGMC computational performance results





- Computation time and memory savings increase when larger subcell configurations are simulated
- Additional time savings achieved using parallel processing

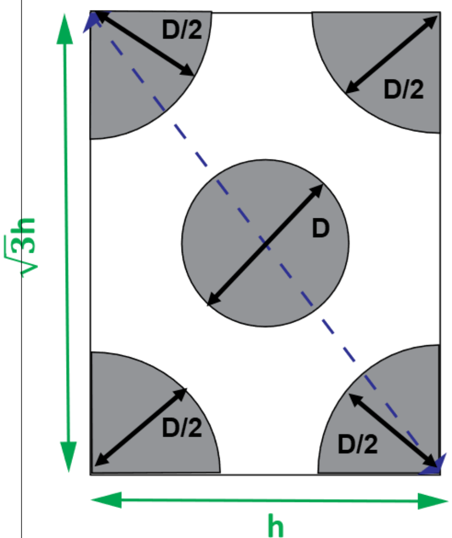
- Improved HFGMC efficiency through use of sparse matrices & parallelization techniques
- Memory required and computation time reduced by two orders of magnitude

Balusu & Chattopadhyay, *Comput. Mat. Sci.* (2021)

Integrated Multiscale Framework

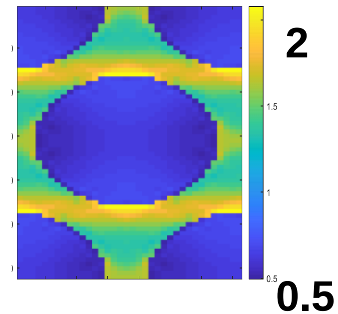
Efficient HFGMC Implementation – Verification

Benchmark problem*

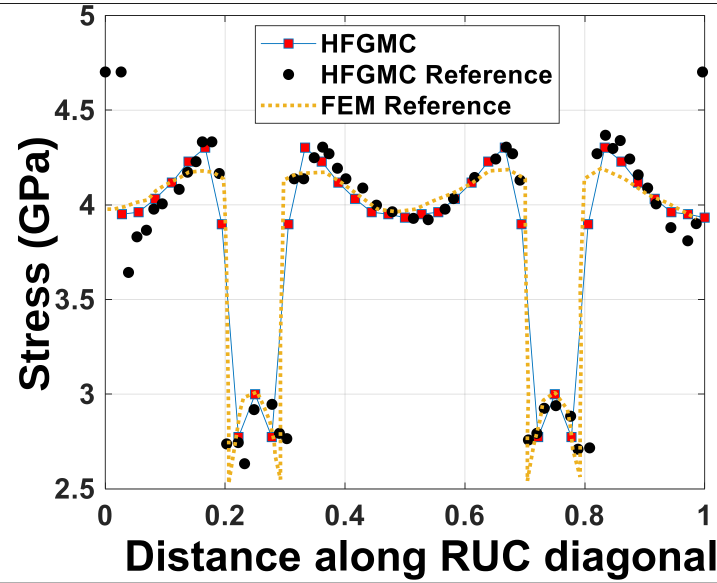


Unidirectional composite RUC

In-plane shear strain



- **HFGMC second order displacement field captures normal-shear coupling**



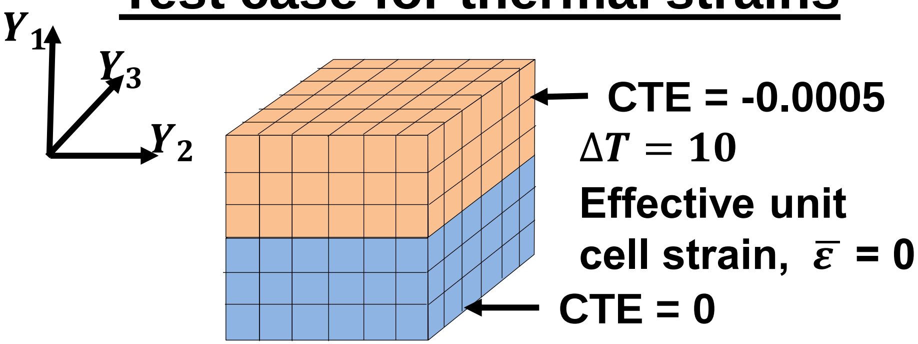
- **Local stress fields in agreement with reference values**
- **Current HFGMC implementation performs better, i.e. closer to FEM, than reference HFGMC* at boundaries**

Results compare well with benchmark problem; verifies efficient HFGMC implementation

*Sertse et al. (2018); Balusu & Chattopadhyay, *Comput. Mat. Sci.* (2021)

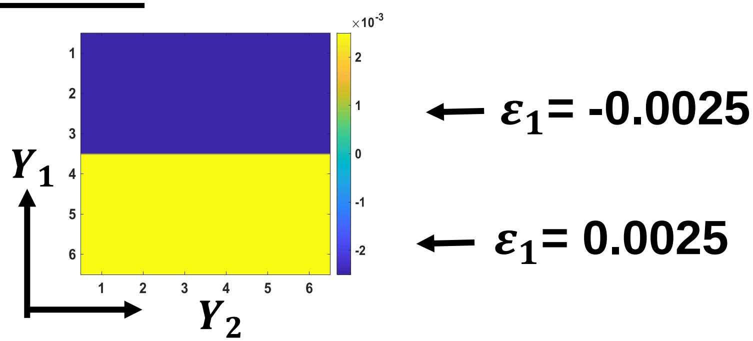
Incorporation of Plasticity and Thermal Effects in HFGMC

Test case for thermal strains



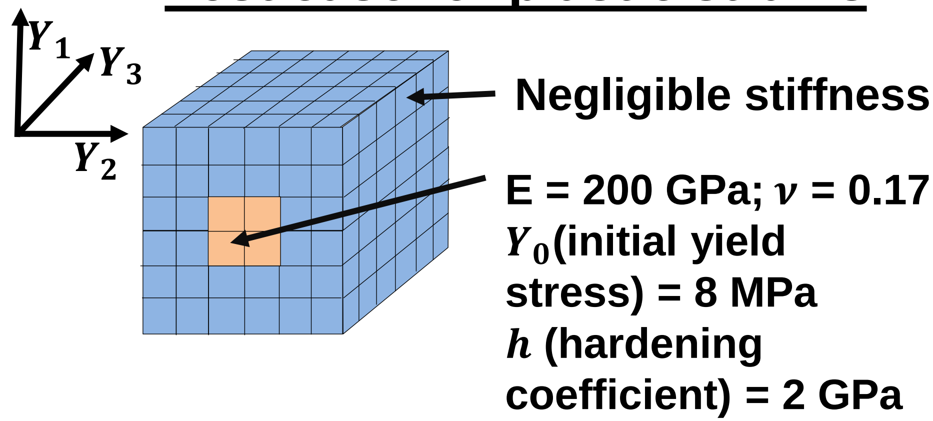
- Negligible stiffness in directions 2 & 3

Results

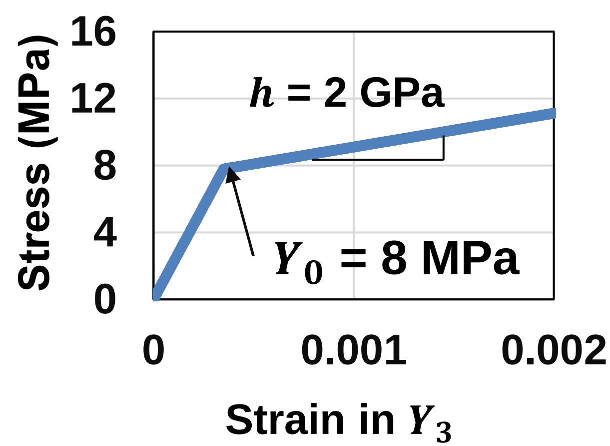


Matches analytical solution

Test case for plastic strains



Results



Expected linear strain hardening behavior recovered

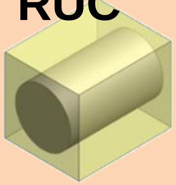
The methodology will allow accurate analysis of processing-induced thermal residual stresses, creep & damage

Integration into an FEA Model – Assessment and Feedback

HFGMC (elastic case) has been implemented into Abaqus as a user-defined material subroutine for implicit (UMAT) and explicit (VUMAT) FEA in Abaqus

- **VUMAT/UMAT will be extended to include <u>inelastic</u> and <u>thermal</u> effects**

Microscale



Using HFGMC

Inputs
- Material constituent properties
- Fiber/Void/Interphase volume fractions and arrangement
- Fiber orientation

Jacobian $\left(\frac{\partial\Delta\sigma}{\partial\Delta\varepsilon}\right)$ and $\Delta\sigma$ →

UMAT

← $\Delta\varepsilon$

$\Delta\sigma$ →

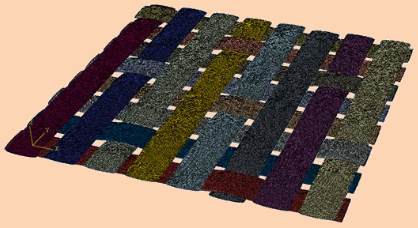
VUMAT

← $\Delta\varepsilon$

Finite elements in Abaqus

At every integration point in every element

Mesoscale

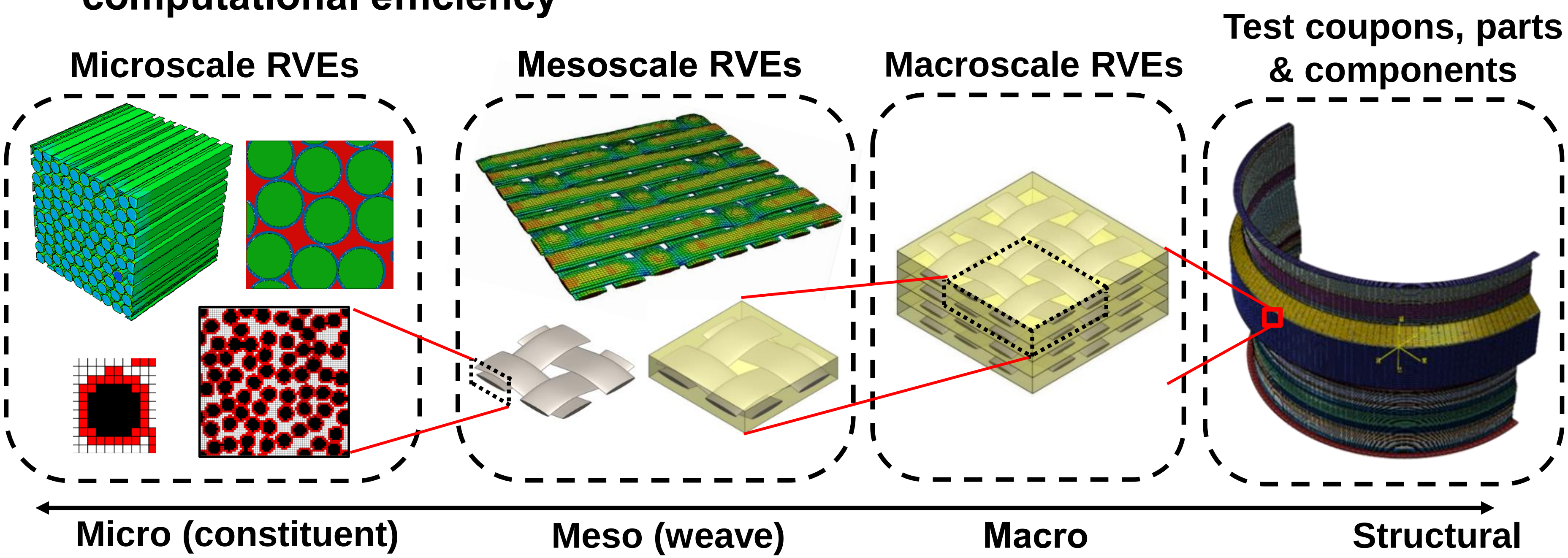


HFGMC UMAT will facilitate simulation of realistic coupon/part geometries & boundary conditions while accounting for microstructural architectural features

Machine Learning-based Reduced Order Model (ROM)

Background and Motivation

- *High-fidelity multiscale* simulation of CMCs requires solution of *multiple* scale-dependent SRVEs
- Woven CMC architecture requires at least two analysis scales
- Efficient handshaking & structural scale integration requires additional computational efficiency



Model order reduction necessary to enable i) efficient handshaking across multiple scales; ii) integration of developed tools into continuum-scale life prediction tools

Machine Learning-based Reduced Order Model (ROM)

Approach

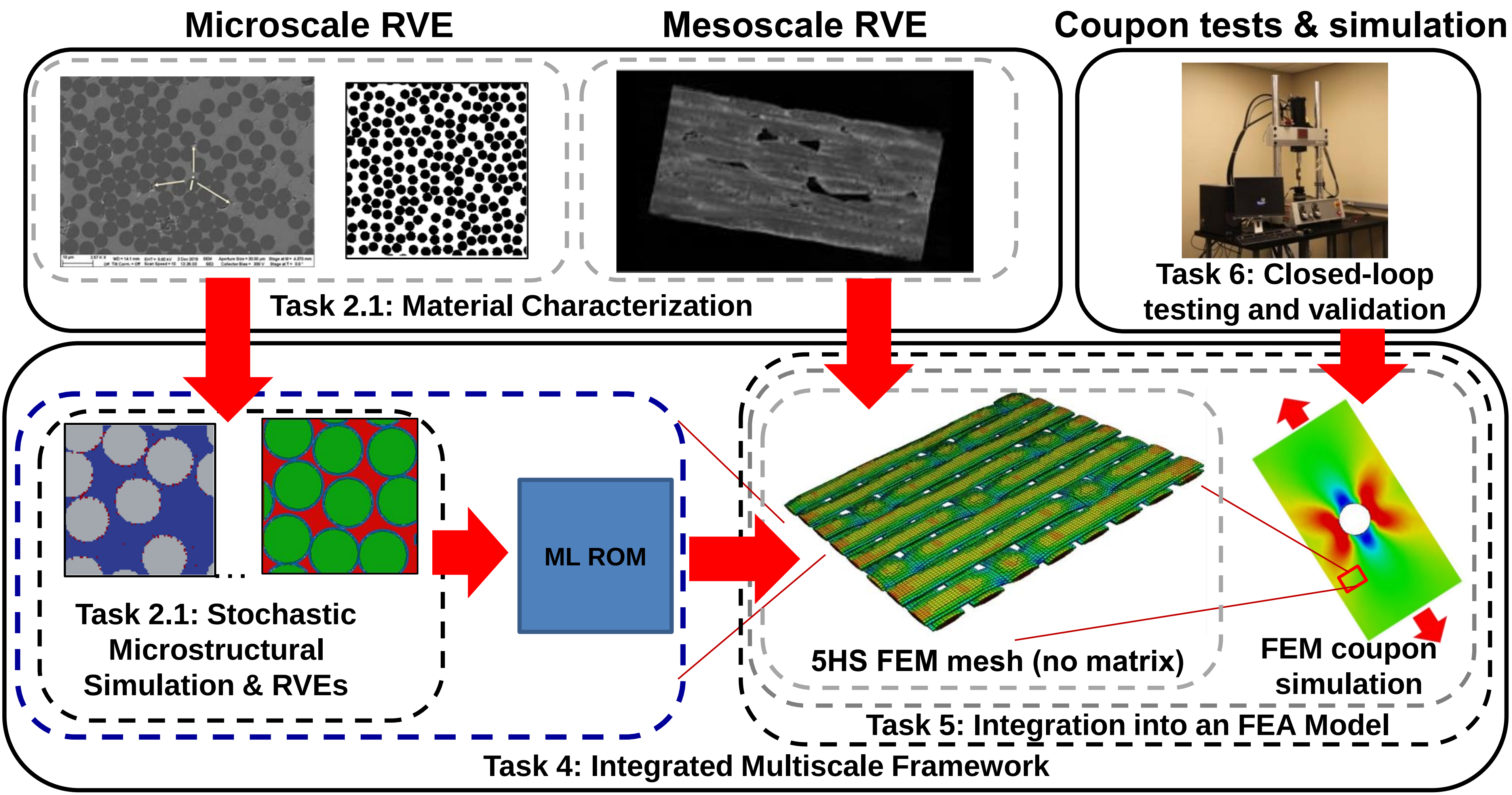
Machine learning (ML)-based reduced order model (ROM) to improve computational efficiency & facilitate structural scale integration; enforcement of governing physical laws & constraints will guide inference & ensure physical consistency & model stability

- **Replace effective nonlinear constitutive law of microscale SRVEs with ML-based reduced order model (ROM)**
- **Use of custom layers to endow NN architecture with domain-specific knowledge to i) guide model inference; ii) satisfy physical laws & constraints**
- **Custom layers will solve constrained convex optimization problems to enforce physical consistency; optimization problem solved within layer <u>need not have closed form solution</u>**

Challenge – learned constitutive law must be thermodynamically consistent; numerical integration requires symmetric positive definite tangent stiffness matrix

Machine Learning-based Reduced Order Model (ROM)

Schematic of ROM implementation in multiscale framework



Initial development of ML-based ROM focused on replacing microscale SRVEs; model architecture amenable to other scales in integrated multiscale framework

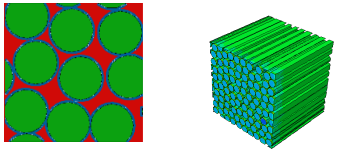
Closed Loop Testing and Validation

Experiments

- Multiscale material characterization
- Low, intermediate & high test temperatures
- Quasi-static tensile testing
- Creep-fatigue testing in air and inert atmosphere
- Thermal properties of interest: specific heat, thermal diffusivity, CTEs

Project Tasks

- Material Characterization and Uncertainty Quantification
- Multiphysics Constitutive Modeling
- Integrated Multiscale Framework
- Integration into FE Model
- Testing & Validation



- Calibrate creep model parameters
- Inform/update damage model
- Identify key micro mechanisms that govern creep-fatigue
- Identify PEL change

Publications

Journals

1. **Khafagy, K., Datta S. & Chattopadhyay, A., "Multiscale Characterization and Representation of Variability in Ceramic Matrix Composites",** ***Journal of Composite Materials,*** **2020 (in press).**
2. **Khafagy, K., Sorini, C., Skinner, T. & Chattopadhyay, A., "Modeling Creep Behavior in Ceramic Matrix Composites",** ***Ceramics International,*** **2020 (submitted).**
3. **Skinner, T. & Chattopadhyay, A., "Multiscale temperature-dependent ceramic matrix composite damage model with thermal residual stresses and manufacturing-induced damage". Composite Structures (in preparation).**
4. **Khafagy, K., Venkatesan, K. & Chattopadhyay, A., "Micromechanics modeling of damage propagation and failure in ceramic matrix composites". Composite Structures (in preparation).**

Conferences

1. **Khafagy, K., Sorini, C., Skinner, T. & Chattopadhyay, A., "A Three-Dimensional Orthotropic Viscoplasticity Formulation for Creep in Ceramic Matrix Composites",** ***AIAA Science and Technology Forum and Exposition, January 11-15,*** **(2021), Nashville, TN, USA.**
2. **Khafagy, K., Venkatesan, K., Balusu, K., Datta, S. & Chattopadhyay, A., "Stochastic microstructural analysis of failure mechanisms in ceramic matrix composites using a high-fidelity multiscale framework",** ***AIAA Science and Technology Forum and Exposition, January 11-15*****, (2021), Nashville, TN, USA.**

Concluding Remarks

Development of integrated multiscale multiphysics framework to model CMC material response under service conditions

- **Characterized SiC-SiNC and C-SiNC CMCs using SEM, EDS, Micro-CT, and confocal microscopy**
- **Quantified uncertainty and generated detailed 3D SRVEs**
- **Incorporated 3D SRVE in structural scale FE simulation**
- **Developed cooldown framework and temperature-dependent damage model - i) simulates manufacturing-induced damage & thermal residual stresses; ii) captures nonlinear thermomechanical response**
- **Developed a novel 3D orthotropic creep model**
- **Formulated a model for the microscale oxidation of fiber interface with complex coupling between anisotropic damage, diffusion, crack closure, & oxidation**
- **Developed parallelized efficient pHFGMC framework; accounted for plasticity & thermal effects**
- **Initiated NN-based ROM development to improve computational efficiency**

Future Work

- **Thermomechanical testing**
- **Bayesian framework for UQ**
- **Model refinement & validation**
- **Oxidation model and integration with multiscale analysis**

Acknowledgements

Program Manager: Matthew F. Adams

- **Dr. Patcharin Burke – *National Energy Technology Laboratory***
- **Dr. Edgar Lara-Curzio – *Oak Ridge National Laboratory***
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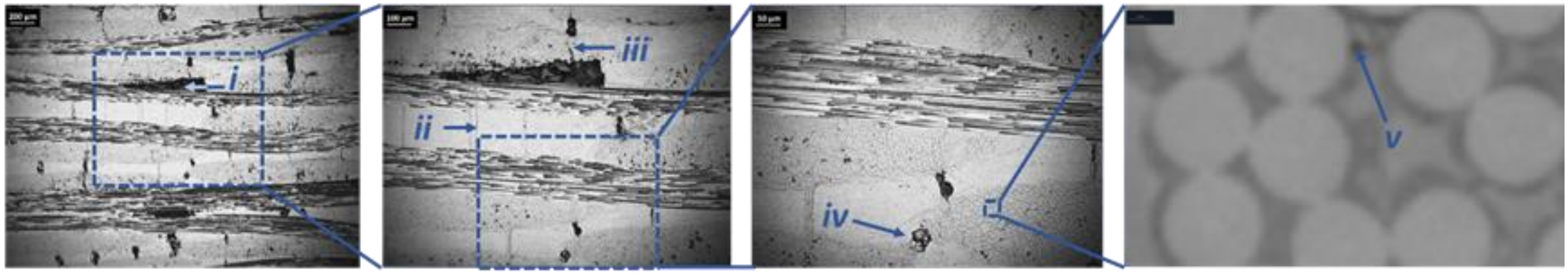
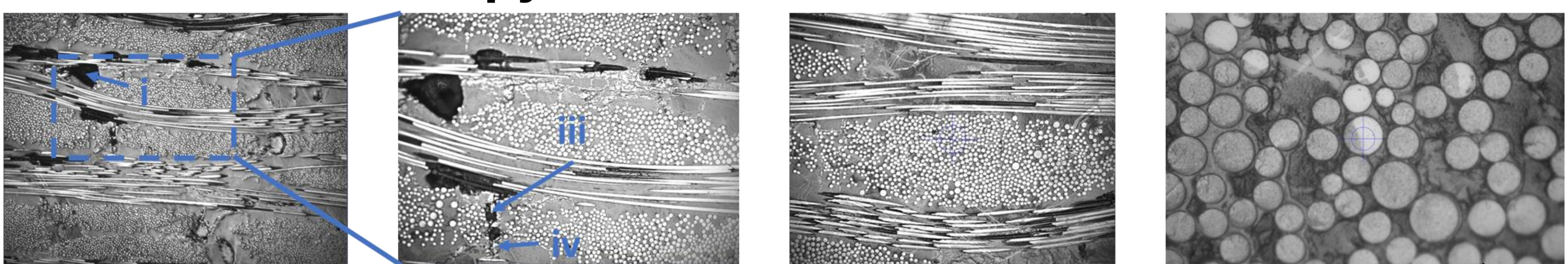
- **Dr. Ojard, Dr. Kumar, and Dr. G.V. Srinivasan – *RTRC***
- **Dr. Luis Bravo – ARL, DoD HPC hours*, Uncertainty-based compressible multiphase flow and material models for rotorcraft FVL propulsion***

Material Characterization

Confocal Microscopy – S400N C/SiNC CMC



Confocal Microscopy – S200H SiC/SiNC CMC



Increasing magnification

Micrographs illustrating SiC/SiNC and C/SiNC CMC weave structure and defect types such as (i) denuded matrix, (ii) shrinkage cracks, (iii) inter- and intra-tow defects interactions, (iv) open porosity, and (v) intra-tow porosity