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
Arizona State University, Tempe, AZ

Major Participant: Dr. Luke Borkowski
Raytheon Technologies Research Center
East Hartford, CT

Annual Review Meeting
November 8-10, 2021

U.S. Department of Energy
Program Manager: Matthew F. Adams
Grant Number: DE-FOA-0001993
Overview

- Project Summary
- Motivation
- Research Objectives & Tasks
- Research Progress
  - Material Characterization & Uncertainty Quantification
  - Multiphysics Constitutive Modeling
  - Thermomechanical Testing
  - Integrated Multiscale Framework
  - Machine Learning (ML)-based Surrogate Model
- Concluding Remarks & Future Work
- Publications
- Acknowledgements
Research Objectives

Develop a synergistic multiscale framework, integrating multiphysics constitutive models with scale specific experiments, to understand temporospatial & scale dependent deformation, damage, & degradation mechanisms in CMCs operating in turbine environment.

- Accurate scale-dependent material characterization & uncertainty quantification
- Constitutive modeling of time-dependent damage, inelasticity, and effects of environmental degradation
- Efficient synergistic multiscale analysis
- Incorporation of developed models into commercial finite element (FE) software for CMC component analysis
- Reduced order model (ROM) for computational efficiency
- Closed-loop testing for model calibration & validation
Task 1: Project Management and Planning

Task 2: Material Characterization & Uncertainty Quantification
- Multiscale CMC Characterization
- Uncertainty Quantification
- Stochastic Microstructural Simulation

Task 3: Multiphysics Constitutive Modeling
- Thermomechanical Progressive Damage
- Creep-Fatigue (Dwell Fatigue)
- Fiber-Matrix Interface
- Environmental Degradation & Oxidation

Task 4: Integrated Multiscale Framework
- Synergistic Multiscale Framework
- Multiscale HFGMC

Task 5: Integration into an FEA Model

Task 6: Testing & Validation
- Thermomechanical Testing
- Analysis of Damage Mechanisms
- Thermogravimetric Testing

Develop more Accurate Life Prediction Methodologies and Integrate with FEA Software

Objective

ASU/RTRC

ASU/ARL

ASU
Material Characterization and Uncertainty Quantification

Objective: Systematic quantification of scale-dependent architectural variability & as-produced defects to i) facilitate SRVE development & ii) investigate effects of variability on effective properties & response

- Material characterization
- Uncertainty assessment
- Generation of statistical representative volume elements (SRVEs)

3D Statistical characterization and material variability quantification

Microscale features
- Matrix cracking
- Fiber failure
- Intra-tow matrix porosity

3D high-fidelity microscale model

Mesoscale features
- Tow/matrix debonding
- Crossover defects

3D mesoscale model

Composite Weave

Material/architectural stochasticity
Multiscale graphs allow quantification of architectural & defects variability at respective constituent and weave scales.
Multi Deep NN–based Framework for Multiscale Microstructural Analysis

Feature extraction & variability quantification of microstructures

- Semantic segmentation of microstructural features through Convolutional Neural Network (CNN) layers
- Microstructure variability quantification computed through regression layer

Generation of High-fidelity SRVEs

- Generator produces SRVEs from actual micrograph characteristic features & distribution
- Discriminator enables distinguishing between actual micrograph and generated SRVE for generator optimization

2- Cooper, S. J. et al. npj Computational Materials (2020)
Vanilla Regression Training

Utilized previously-developed SRVE generation algorithm to train DL-based algorithm and further improve variability quantification accuracy.

Prediction from optimized vanilla regression show high coefficient of determination ($R^2$) with respect to ground truth.
- Achieved semantic segmentation for matrix, fiber, fiber/matrix interface and porosity to inform high fidelity micromechanics simulations
- Captured matrix secondary phases and fiber damage regions; critical for accurate damage assessment
Vanilla Regression SiC/SiNC Features Map, Contd.

Confocal microscopy micrograph

Filter A Filter B Filter C

Pixel width

Pixel height

Matrix secondary phases

Intratow defects

Fiber damage

Fiber-Matrix interface

Intratow defects

Modular deep-learning NN: Successfully segmented different microstructure variability: fiber radii, matrix crack shape & distribution and fiber-matrix chemical composition
Microstructure Variability Quantification

- Captured microstructure variability in fiber and porosity volume fractions
- In-progress: fiber radius, intratow spacing, porosity shape and size, & intertow features

**C/ SiNC**
- Fiber VF = 56% ± 6%
- Porosity VF = 3.7% ± 1%

**SiC/ SiNC**
- Fiber VF = 57% ± 3%
- Porosity VF = 4% ± 0.6%
Multiscale Simulation of 5HS Woven C/SiC CMC

Thermomechanical progressive damage model accounting for crack nucleation & growth

- Includes flaw statistics, temperature dependent material properties
- Crack growth kinetics governed by fracture mechanics

Simulated 5HS weave architecture

Need to account for material initial damage state & residual stress effects due to cooldown during manufacturing process

Skinner, T., & Chattopadhyay, A., Composite Structures (2021)
Areas with high residual tensile stress have shrinkage cracks; high stress areas in cooldown framework accumulate damage & exhibit degraded initial properties in damage direction.
High-fidelity FE Creep Modeling

3D coupled viscoplasticity-damage model:
- Norton-Bailey creep power law
- Hill orthotropic plastic potential
- Arrhenius temperature dependence
- Associative flow rule
- Time- and strain-hardening formulations
- Fracture mechanics-informed matrix damage model
- Curtin progressive fiber damage model

Captured transient creep stage due to large constituent creep mismatch, followed by steady-state stage
Excellent agreement with CMC total longitudinal strain & constituent longitudinal stress time-history
Effects of intratow porosity on creep behavior

Prescribed loading: 100 MPa (constant), 1300 °C

Presence of intratow voids affects load transfer mechanism between constituents & results in complex stress “hot spots” in vicinity of voids - potential damage initiation sites
Matrix cracks create passages for oxygen to diffuse into material

- Oxidation of fiber interphase or fusion of SiC fiber to SiNC matrix impairs load transfer
- Oxidation reaction of oxygen-exposed SiNC matrix activates at extreme temperatures, resulting in a multi-regime response

Physics-based modeling

- Model oxidation coupling through the chemical reaction source terms for concentrations of oxygen and material
- Model damage-driven diffusion through approximations of the partial differential equations

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

Oxidation of fiber interface


Oxygen diffusing through cracks

Damage-diffusion Oxidation Coupling, Contd.

Five degrees of freedom (DOFs) per node: displacement (x, y, z), concentration (O$_2$, BN)

For $c_{(O_2)}$ DOF:  
$$ \dot{c}_{(O_2)} - \nabla \cdot (D \nabla c_{(O_2)}) + R c_{(BN)} c_{(O_2)} = 0 $$

For $c_{(BN)}$ DOF:  
$$ \dot{c}_{(BN)} + R c_{(BN)} c_{(O_2)} = 0 $$

For displacement DOFs:  
$$ \nabla \cdot \sigma = 0 $$

Oxidation reaction 1:  
$$ 2BN(s) + \frac{3}{2} O_2(g) \rightarrow B_2O_3(l) + N_2(g) $$

Diffusion crack path matrix:  
$$ P = \begin{bmatrix} \frac{d_{22}h_{22}+d_{33}h_{33}}{2} & 0 & 0 \\ 0 & \frac{d_{11}h_{11}+d_{33}h_{33}}{2} & 0 \\ 0 & 0 & \frac{d_{22}h_{22}+d_{11}h_{11}}{2} \end{bmatrix} $$

For SiC:  
$$ \sigma = MC \varepsilon $$

For Interphase:  
$$ \sigma = \left(1 - \frac{c_{(BN)}}{c_{(max)}}\right) C \varepsilon $$

Stress:

Effective oxygen diffusivity:  
$$ D = P \cdot D_{air(O_2)} $$

$$ D = \left(1 - \frac{c_{(BN)}}{c_{(max)}}\right) D_{air(O_2)} I $$
In-situ Tensile Testing

Experimental set-up

1. DIC speckle pattern
2. Amteco Furnace (>1400 °C)
3. 30kN MTS load frame
4. Hydraulic grip system
5. Digital image correlation

- Two independent heating zones for better temperature uniformity control
- View port access for in-situ (DIC) experiments

High & room temperature quasi-static (QS) & creep testing for SiC/SiNC using MTS load frame and in-situ digital image correlation (DIC) technique
SiC/SiNC CMC stress-strain response and strength

- Loading conditions: QS strain rate = 1e-5/sec
- Temperature conditions: Room temperature = 24 °C
- Gauge region dimensions: 99.0 x 10.2 x 2.5 (mm)

Average tensile strength = 409.34 MPa (0/90°) & 193.24 MPa (+/-45°)

Average failure strain = 0.4731% (0/90°) & 0.52 % (+/-45°)

Results show good agreement with data from literature

Integrated Multiscale Framework

Challenge & Goal:

Raytheon’s role includes evaluating multiscale models for industrial applications (i.e., relevant materials, geometries, loads)

Outcomes:

▪ Assessment of accuracy and efficiency of lifing model for material systems, geometries, and loads relevant to RTX
▪ Technology readiness level (TRL) evaluation of modeling framework
▪ Validate simulation results against in-house lifing tools
Machine Learning Surrogate Model

**Approach:**

Surrogate models will help bridge gap between high-fidelity multiscale models and industrial application

- Efficiently approximate output of physics-based models
- Neural-network based surrogate model – trained on experimental and simulation data
- Physics-based regularization to enforce physical laws

\[ l_T = \lambda_{MSE} l_{MSE} + \lambda_P l_P \]
\[ l_{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - y_i^p)^2 \]
\[ l_P = \text{ReLU}(w^P) \]

Surrogate model will run much faster than numerical solution - making large-scale multiscale simulations more feasible

This page contains no technical data subject to the EAR or the ITAR.
Results:

As proof-of-concept, surrogate model trained and evaluated using nonlinear plasticity numerical model

Validation results – Piecewise linear reverse loading

Validation results – Cyclic random amplitude, random frequency loading

Excellent agreement between ML surrogate and training data

*Borkowski, Sorini and Chattopadhyay (2021)*

This page contains no technical data subject to the EAR or the ITAR.
Surrogate model developed, trained, and tested for woven CMC under cyclic loading conditions

- RNN-based surrogate model prediction includes homogenized constitutive response of multiple constituents (fiber, matrix, interphase)

- Physics-based regularization to enforce physical laws (e.g., tangent stiffness matrix positive semi-definiteness) and maintain linear elastic unloading

- Nonlinear tensile cyclic loading response of plain weave CMC governed by progressive matrix damage model

Mathematical expressions:

\[ l_T = \lambda_{MSE} l_{MSE} + \lambda_{TM} l_{TM} + \lambda_{PSD} l_{PSD} \]

\[ l_{MSE} = \frac{1}{n} \sum_{i=1}^{n} (\sigma_i - \sigma_i^p)^2 \]

\[ l_{TM} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\partial \sigma_i}{\partial \varepsilon_i} - \frac{\partial \sigma_i^p}{\partial \varepsilon_i} \right)^2 \]

\[ l_{PSD} = \text{ReLU} \left( - \frac{\partial \sigma_i^p}{\partial \varepsilon_i} \right) \]
Surrogate model shown to perform well in predicting CMC cyclic behavior, including unloading

- Training data generated using Multiscale Generalized Method of Cells (MSGMC) micromechanics model

- Uniaxial load / unload cycles applied (up to four) at random points during loading and of varying unload magnitudes

Sample loading histories

Surrogate model validation

Test case 45

Test case 3
Concluding Remarks

- Developed concurrent & efficient high-fidelity multiscale simulation methodology
- Characterized scale-dependent architectural variability & defects in C/SiNC and SiC/SiNC CMCs material systems using SEM, EDS, X-ray Micro-CT, and confocal microscopy
- Developed microstructure generation algorithm accounting for material variability and defects, captured from detailed characterization study
- Developed ML-based techniques to facilitate image segmentation, scale-dependent variability quantification, and SRVE generation
- Developed multiscale cooldown framework and temperature-dependent damage model - i) simulates manufacturing-induced damage & thermal residual stresses; ii) captures nonlinear thermomechanical response
- Developed 3D orthotropic viscoplastic creep constitutive model & implementation in i) GMC micromechanics framework; ii) ABAQUS commercial FEA via UMAT
- Formulated oxidation model with complex coupling between anisotropic damage, diffusion, crack closure, & hygrothermal effects
- Developed NN-based surrogate model to facilitate computationally efficient information transfer across multiple analysis length scales
- Conducted *in-situ* quasi-static tensile testing using digital image correlation
Future Work

- Development of conditional generative adversarial network for experimentally-inspired SRVEs
- Hybrid μCT-microscopy segmentation approach for mesoscale 8HS SiC/SiNC CMC SRVE
- High-fidelity SRVE simulations including damage and creep
- Integration of oxidative-damage model into multiscale framework
- Extension of ML-surrogate model to account for viscoplasticity and damage anisotropy
- Dwell-fatigue testing & modeling
Publications

Journals


Conferences


Acknowledgements

Program Manager: Matthew F. Adams

- Dr. Patcharin Burke – National Energy Technology Laboratory
- Dr. Edgar Lara-Curzio – Oak Ridge National Laboratory
- Dr. Anindya Ghoshal – Army Research Lab (ARL)
- Dr. Ojard, Dr. Kumar & Dr. G.V. Srinivasan – RTRC
- Dr. Amjad Almansour & Dr. Robert Goldberg – NASA Glenn Research Center
- Dr. Luis Bravo – ARL, DoD HPC hours, Uncertainty-based compressible multiphase flow and material models for rotorcraft FVL propulsion

Research Team

- Dr. Luke Borkowski (RTRC) – Major Participant
- Christopher Sorini – PhD Student
- Khaled Khafagy – PhD Student
- Mohamed Hamza – PhD Student
- Jacob Schichtel – NDSEG Fellow