NAFEMS

NASMAT

NASA Multiscale Analysis Tool

An Enabling Platform for Achieving Multiscale Multiphysics Analysis of Multiphase Materials

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nafems.org

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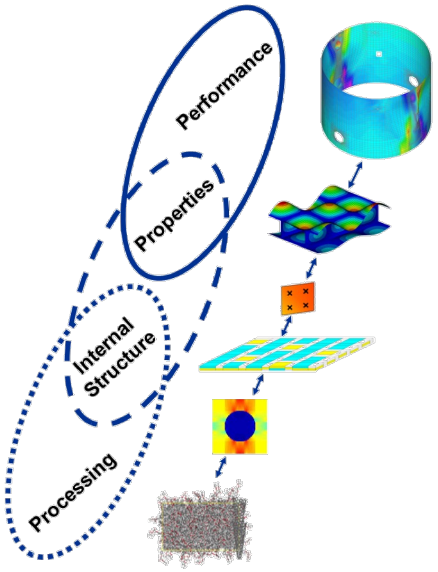
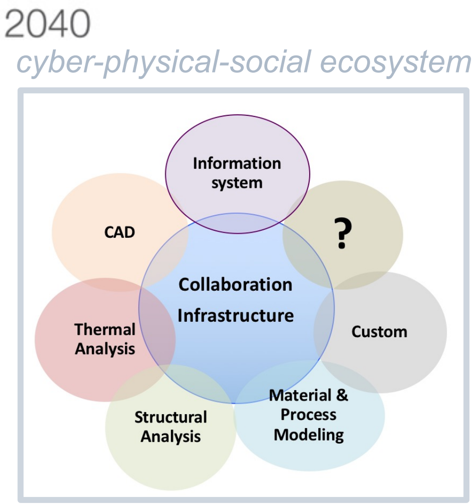
THE INTERNATIONAL ASSOCIATION FOR THE ENGINEERING MODELLING, ANALYSIS, AND SIMULATION COMMUNITY.

Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

Provides a public/private investment strategy for the design of fit-for-purpose materials and structures





NASA CR 2018-219771

https://ntrs.nasa.gov

Nine Identified Key Element Discipline Areas

1. Models and Methodologies
2. Multiscale Measurement & Characterization Tools and Methods
3. Optimization & Optimization Methodologies
4. Decision Making and UQ
5. Verification & Validation
6. Data, Informatics, & Visualization
7. Workflows & Collaboration Frameworks
8. Education & Training
9. Computational Infrastructure

2040 Vision State:

*A cyber-physical-social ecosystem that impacts the supply chain to **accelerate** model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for **affordable**, **producible** aerospace applications*

Identified Critical Gaps & *Possible Subset of Actions Required To Close Each Gap*

Key Element	Critical Gap	Priority Action	Time Frame (2018 2020 2025 2030 2035 2040)	End State Characteristics
1	Underdevelopment of physics-based models that link length and time scales for relevant material systems	Multiscale V&V methods (5.6) Integration of uncertainty across scales (1.13) ICME-based fast process models (1.21) Multiscale models for rare-events/nucleation (1.22) Information framework for 3D/4D model dev. (2.11) Models for key uncertainty sources (1.23)		
2	Inability to conduct real time characterization and measurement of structure and response at appropriate length and time scales	Real-time measurement methods (2.14) Real-time visualization for experiment modeling (6.15) Lifecycle data: automated ingestion and storage (6.23) Protocols: link characterization, test data, models (2.10)		
3	Lack of reliable optimization methods that bridge across scale	New optimization formulation methods (3.13) Education modules: data analytics tools/methods (8.2) Optimization methods with uncertainty incorporated (3.11) Coupled multiphysics and optimization methods (3.5) Surrogate models for large scale optimization (4.15)		
4	Existing models and software codes are not designed to compute input sensitivities and propagate uncertainties to enable UQ	Benchmark characterization methods (2.3) Optimization methods with uncertainty incorporated (3.1) UQ: sensitivity analysis methods (4.19) Holistic test methods (2.16) Models for key uncertainty sources (1.23)		
5	Lack of guidelines and practitioner aids for multiscale/multiphysics (e.g., ICME) V&V	Best practices: data collection (5.7) Multiscale V&V standards and definitions (5.1) Student resources: industry V&V data (8.8) V&V training (5.2) Holistic test methods (2.16)		
6	No widely accepted community standards or schema for materials information storage and communication methods	Workflow data modeling: automation, recognition, tagging (7.1) Training: informatics framework interpretation & integration (6.21) Best practices: data federation (6.1) Best practices: defining multidisciplinary ontologies (6.3)		
7	Lack of open, community/industry standards defining inputs/outputs, needed functionality, data quality, model maturity levels, etc. for smooth operation in the envisioned ecosystem	Access-controlled example workflows (7.9) Best practices: multi-domain workflows (7.16) Data quality and model maturity standards (7.21) Access-controlled adaptive file formats (6.2)		
8	Education/training does not bridge the gap between "essential" or "fundamental" knowledge and industrially relevant skills	Education/Training: decision/UQ approaches (4.7) New computational certifications programs/tracks (8.14) Workforce transition training for students (8.5) V&V training (5.2) Student access to equipment/facilities (8.6)		
9	Lack of support, or adequate business models, for code development and maintenance, particularly for software used in engineering applications	Modernize existing codes (9.6) Best practices: multi-domain workflows (7.16) Web platform for code benchmarking (5.3) Open-source/alternative code writing tools (8.3) Early-stage collaborative code development (9.4) Initiative: support key modeling software tools (9.8)		

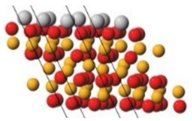
Relevance and Background

Integrated Computational Materials Engineering (ICME) Is The Future

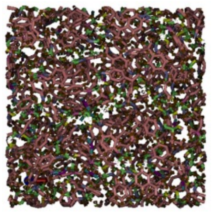
Processing — Internal Structure — Properties — Performance

Design "The" Material ← | → **Design "With" Material**

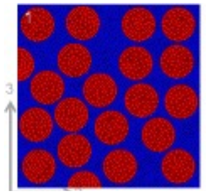
ICME is an approach to the design of products and the materials which comprise them by **linking experimentally validated materials models at multiple length scales**.



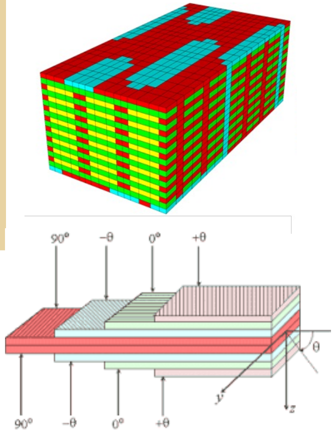
Quantum



Atomistic

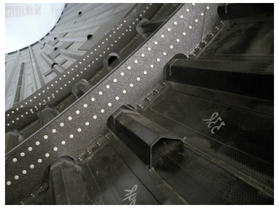


Micro scale



Meso scale

Part



Assembly

System

Handshake via Constitutive Model

Design for Manufacturability, Certifiability and Lowest Cost, with Performance Constraints

Micromechanics / Statistical Mechanics ↔

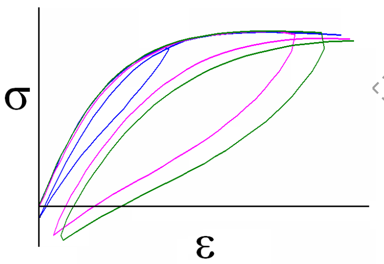
Molecular Dynamics ↔

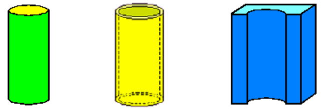
Quantum Mechanics ↔

Continuum Mechanics ↔

Micromechanics: The Link Between Structures and Materials

Constituent Response

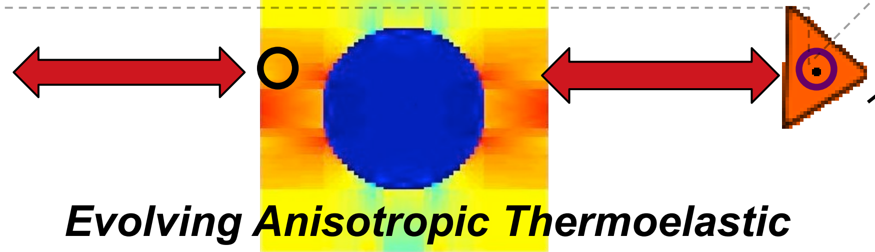




Continuum Deformation and Damage Models

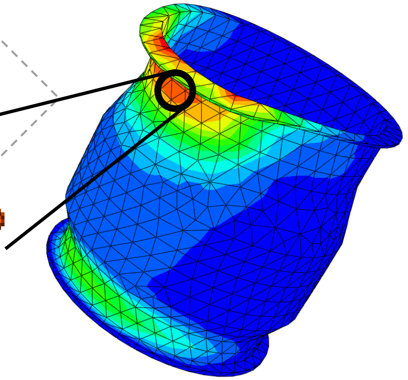
Composite Micromechanics Repeating Unit Cell

Micromechanics Provides the Link Between Structures and Materials



Evolving Anisotropic Thermoelastic Inelastic and Damage Constitutive Model

Structural Model



Micro-level Field Equations (subcell)

$$\varepsilon^{(\alpha\beta\gamma)} = A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}\left(\varepsilon_s^I + \varepsilon_s^T\right)$$

$$\sigma^{(\alpha\beta\gamma)} = C^{(\alpha\beta\gamma)}\left[A^{(\alpha\beta\gamma)}\bar{\varepsilon} + D^{(\alpha\beta\gamma)}\left(\varepsilon_s^I + \varepsilon_s^T\right) - \left(\varepsilon^{I(\alpha\beta\gamma)} + \varepsilon^{T(\alpha\beta\gamma)}\right)\right]$$

Macro-level Constitutive Equations

$$\bar{\sigma} = B^*\left(\bar{\varepsilon} - \bar{\varepsilon}^I - \bar{\varepsilon}^T\right)$$

$$B^* = \frac{1}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)} A^{(\alpha\beta\gamma)}$$

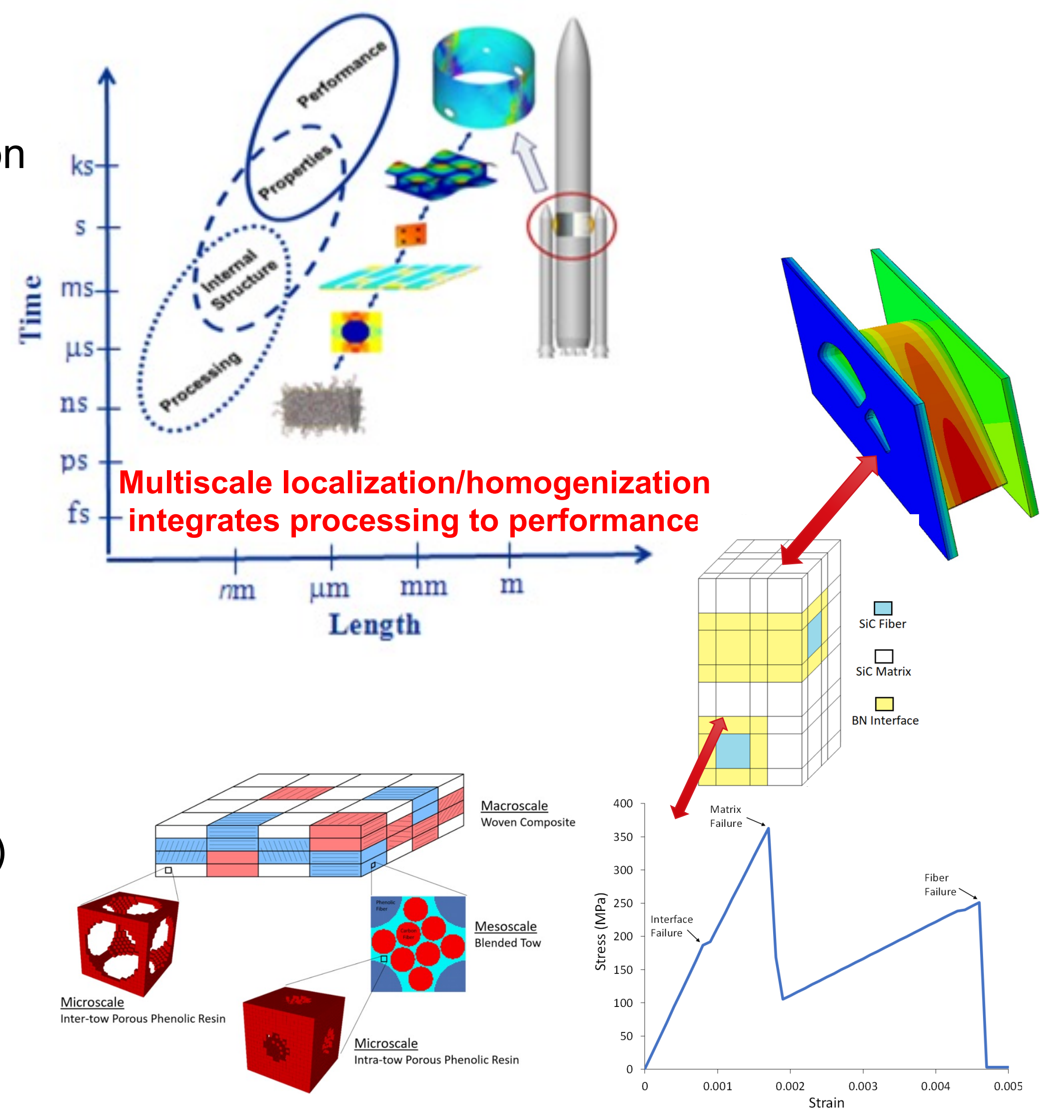
$$\bar{\varepsilon}^I = \frac{-\left[B^*\right]^{-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}\left(D^{(\alpha\beta\gamma)}\varepsilon_s^I - \varepsilon^{I(\alpha\beta\gamma)}\right)$$

$$\bar{\varepsilon}^T = \frac{-\left[B^*\right]^{-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}\left(D^{(\alpha\beta\gamma)}\varepsilon_s^T - \varepsilon^{T(\alpha\beta\gamma)}\right)$$

Aboudi, J., Arnold, S.M., and Bednarcyk, B.A. (2013) *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*, Elsevier, Oxford, UK., pp 1-984.

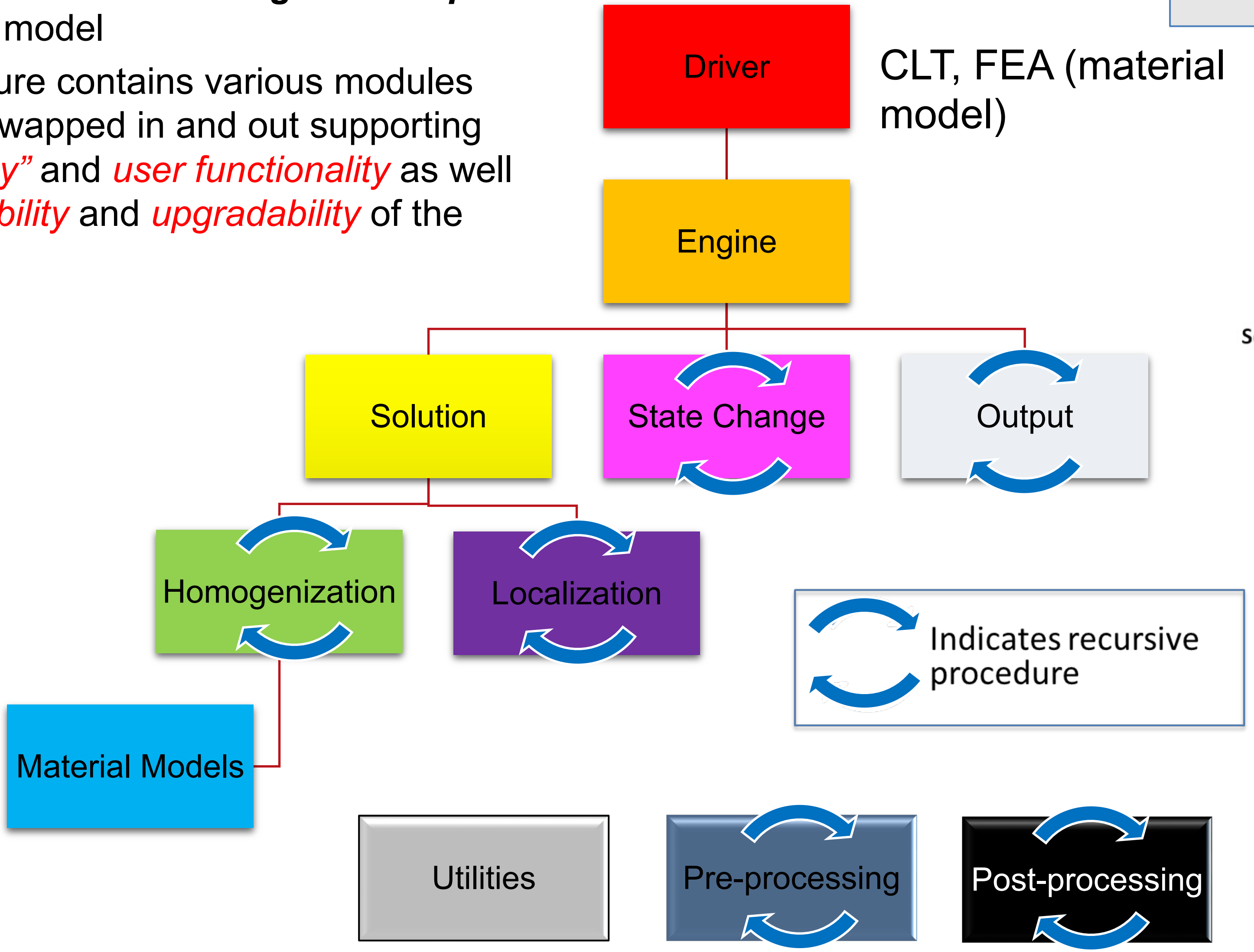
NASA Multiscale Analysis Tool (NASMAT)

- Clean-sheet development based on legacy MAC/GMC and FEAMAC tools (~30 years of tool development)
- A framework designed to support massively multiscale modeling (M^3) on high-performance computing (HPC) systems
  - Solves real, large-scale, non-linear, thermo-mechanical problems
- Modular design to support “plug-and-play” capabilities
  - Operational components categorized into NASMAT procedures
    - Each procedure has access to a library of modules
- Developed for enhanced interoperability
  - Integrates with 3rd party structural analysis codes (e.g., FEA)
  - Arbitrary number of length scales
  - Arbitrary micromechanics theories (including user-defined)
  - Library of constitutive laws/damage models (including user-defined)
  - Data output in HDF5 file format
- ASCII input, pre/post-processor under development

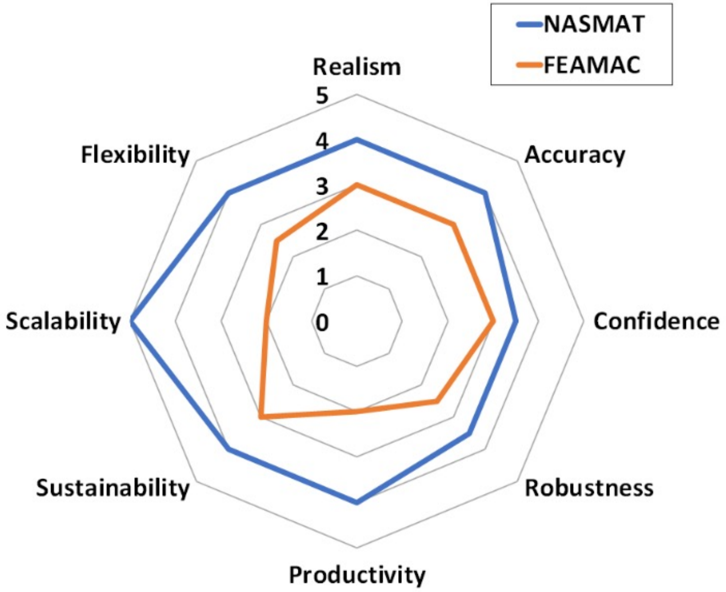


NASMAT Workflow

- Effectively acts as an ***evolving anisotropic constitutive*** model
- Each procedure contains various modules that can be swapped in and out supporting *"plug and play"* and *user functionality* as well as *maintainability* and *upgradability* of the code



Improvements over legacy multiscale software (FEAMAC)



Comparison of Different Modeling Approaches

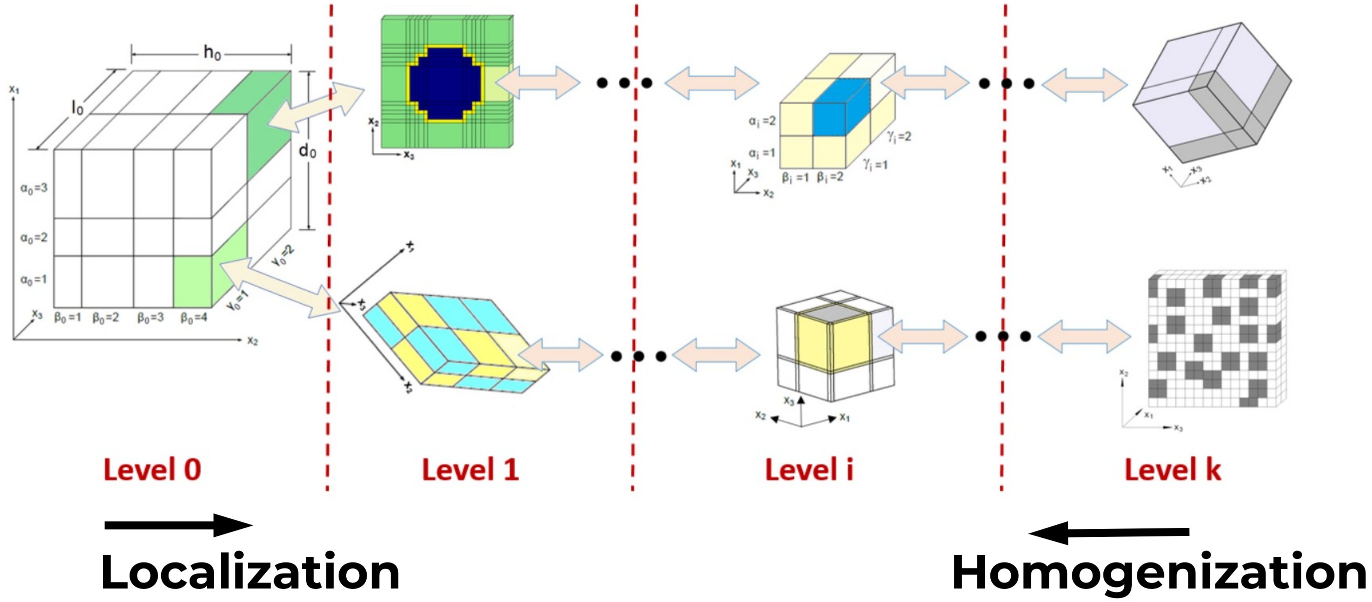
	Mori-Tanaka	GMC	HFGMC	FEA
General Global Accuracy	Good	Very Good	Excellent	Excellent
Computational Efficiency	Superior	Excellent	Fair	Fair
Local Field Accuracy	Poor	Good	Excellent	Excellent
Normal/Shear Coupling	No	No	Yes	Yes
Admits Local Inelasticity	Yes*	Yes	Yes	Yes
Suitable for Inclusion in Structural Models	Excellent	Excellent	Good	Fair
Multi-Axiality	Yes	Yes	Yes	Yes
Ability to Model Debonding	Yes*	Yes	Yes	Yes
Ability to Model Disordered Microstructures	n/a	Fair	Excellent	Excellent
Local Fields Insensitive to Refinements in Mesh	Yes	Yes	No	No

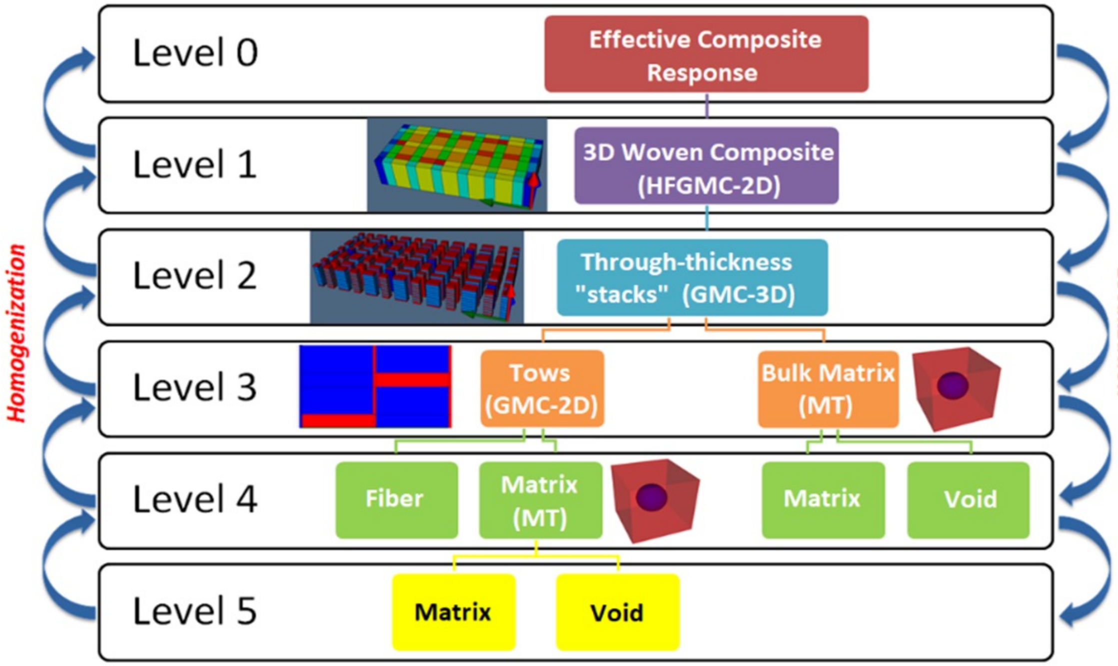
*Features not in NASMAT

Multiscale Recursive Micromechanics (MsRM)

- Efficient, semi-analytical micromechanics theories
- Call each other (or themselves, recursively)
- Captures microstructure on **arbitrary** number of scales
  - ➢ No limit on depth of scales

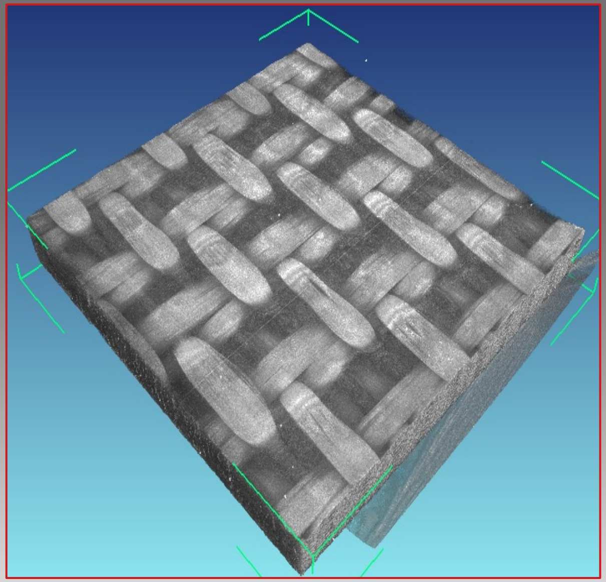
Any micromechanics theory can be used at any level!

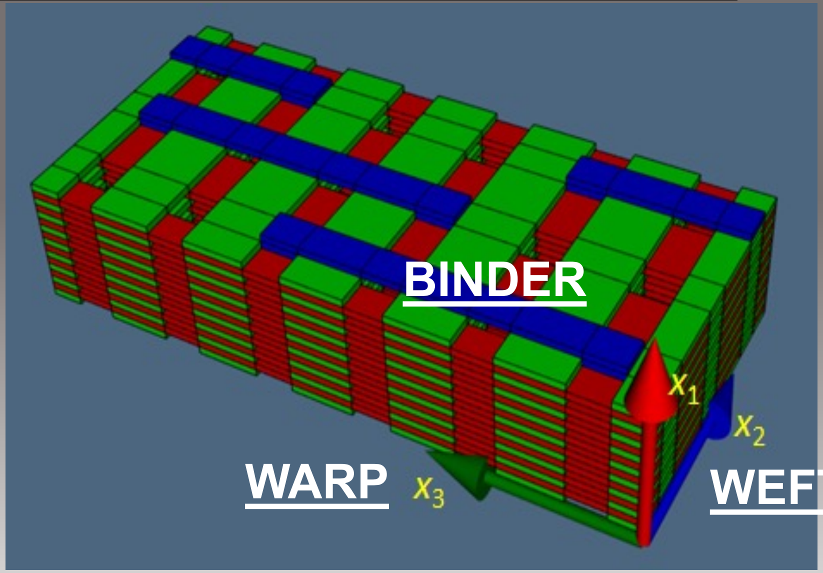




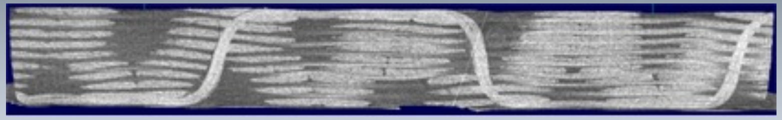
Development of a 3D Woven Repeating Unit Cell (RUC)

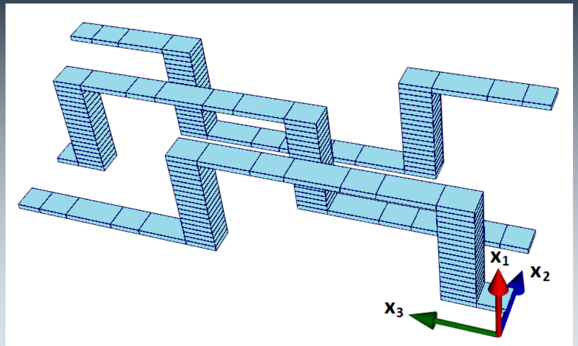
Idealization of Tow Paths from X-Ray CT



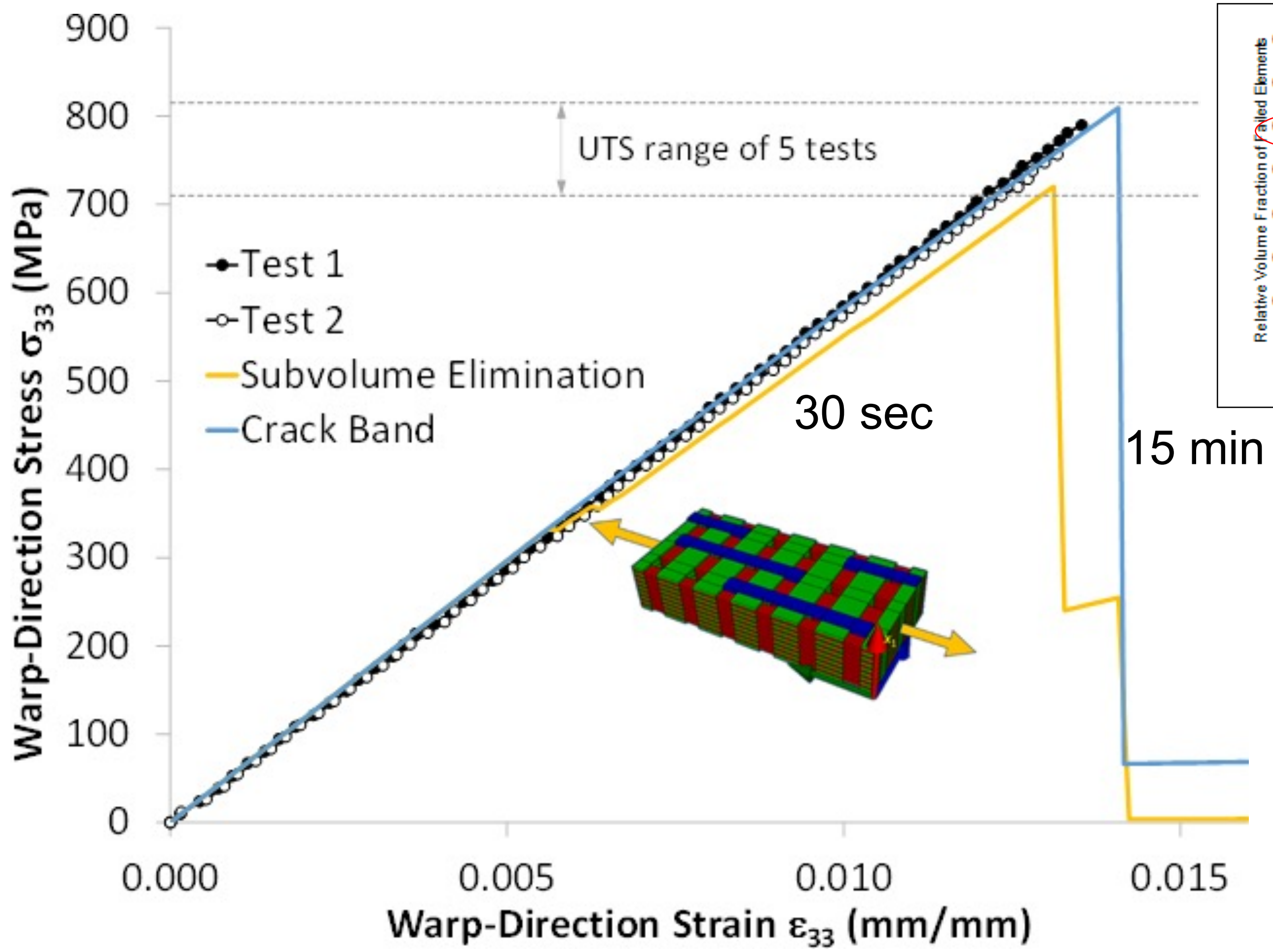


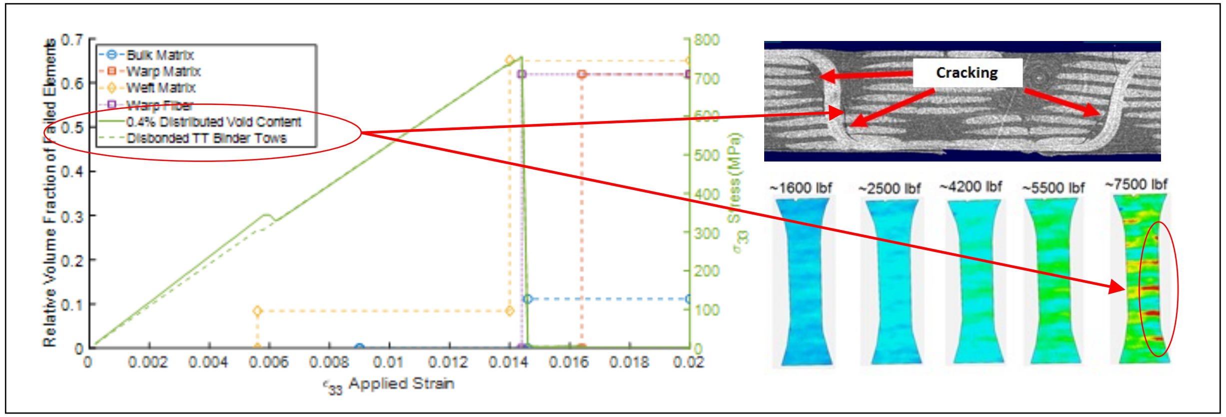
Through-thickness Binder Tow

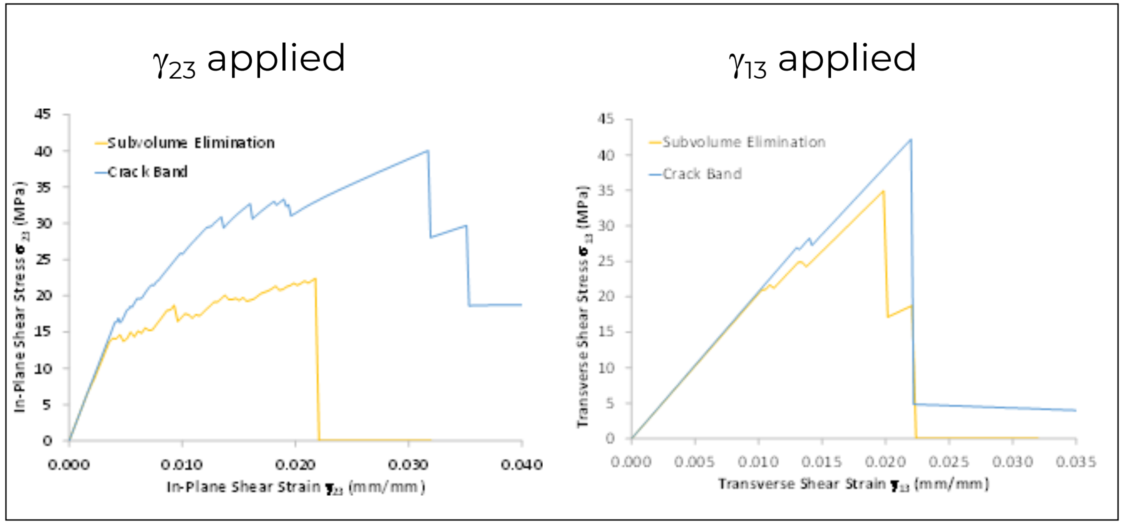




Failure Prediction of a 3D Woven Composite



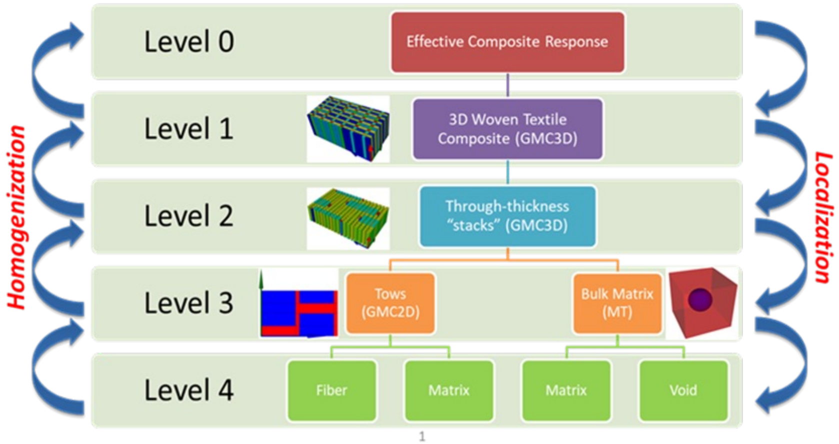


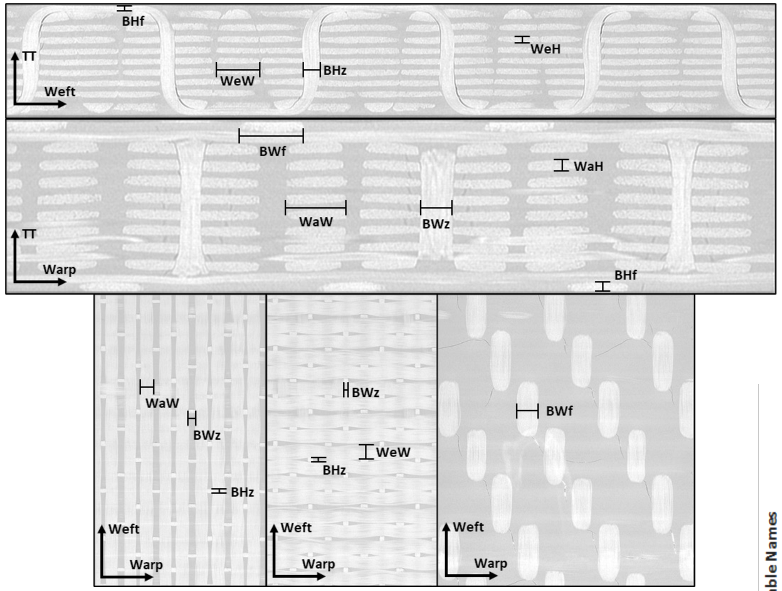


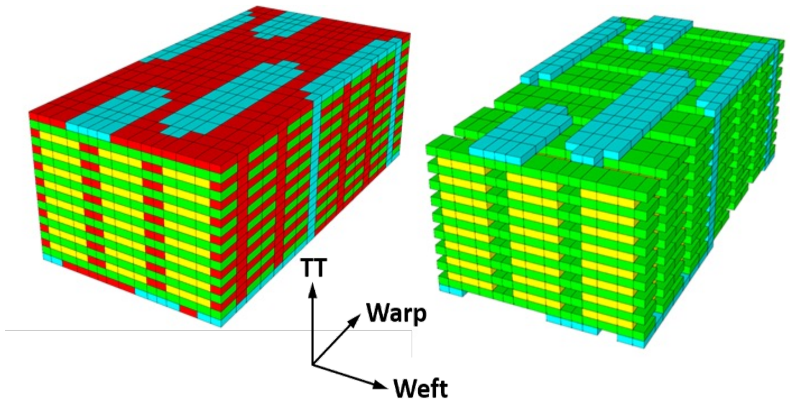
- Warp-direction strength predicted
- Use of quasi-brittle damage model improved overall prediction of stress-strain curve

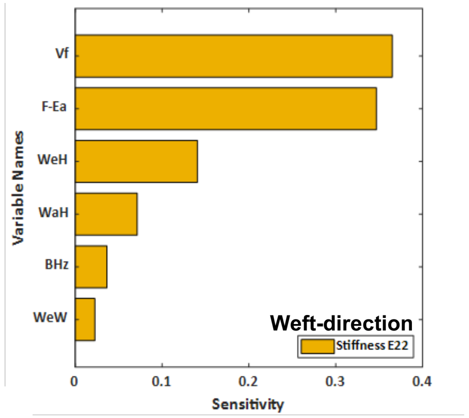
- Failure mode predicted – disbonding of binder tows
- Crack band model results in more shear nonlinearity

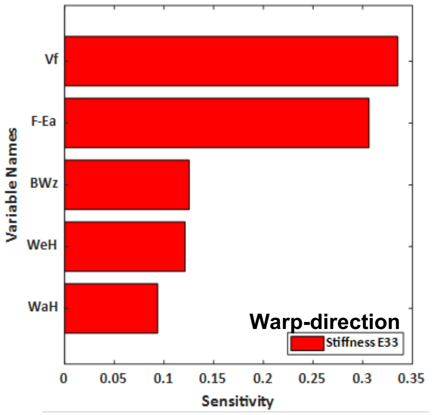
Sensitivity Analysis of 3D Woven Composites

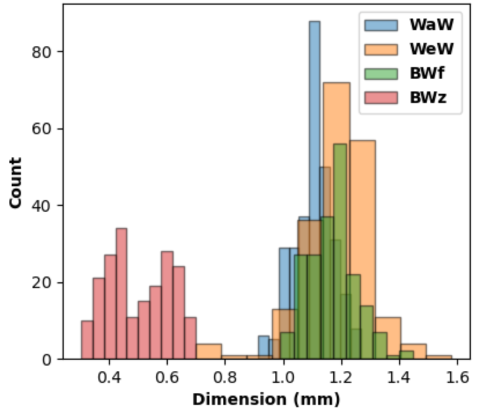


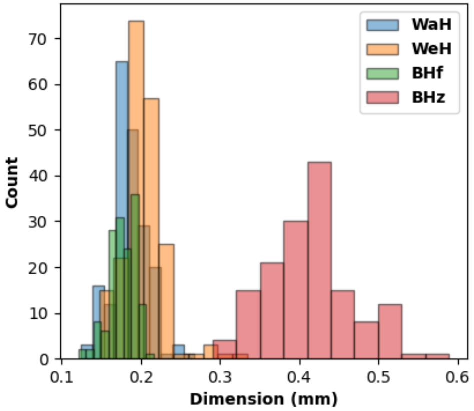








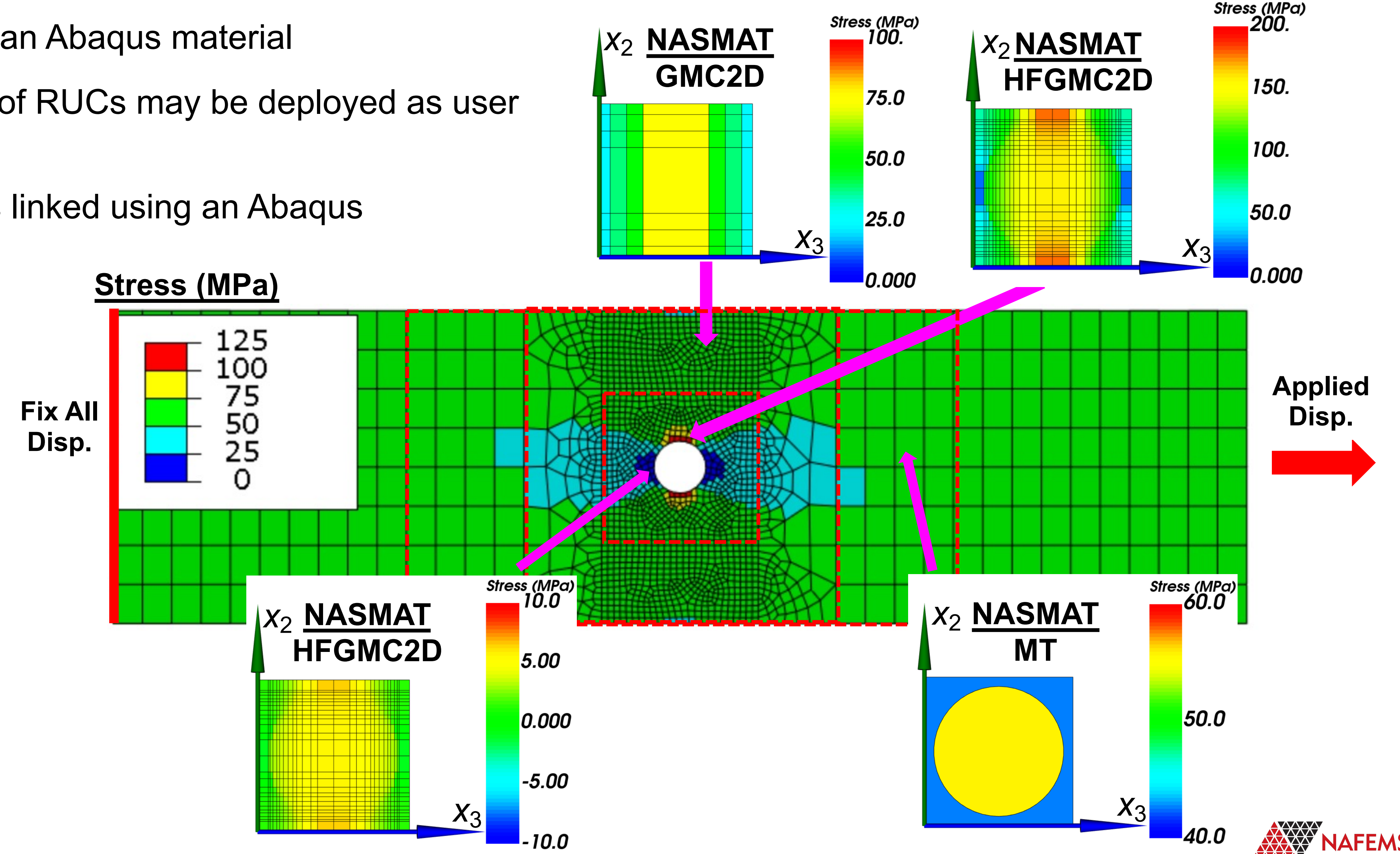




- Ability to capture relevant physics at multiple length scales
- Rapid analysis capability (~sec-min, single CPU) compared to state of the art (~hrs, many CPUs)
- **100k NASMAT simulations in ~6 hours**
- Able to estimate output sensitivities to input variables

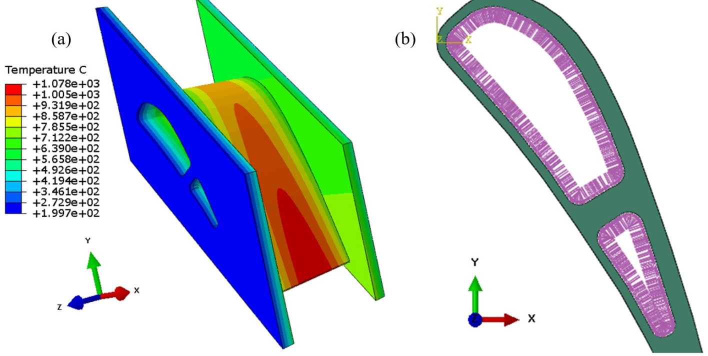
Multifidelity Integration with Abaqus

- Utilizes Abaqus user subroutines
- NASMAT acts as an Abaqus material
- Arbitrary number of RUCs may be deployed as user materials
- NASMAT libraries linked using an Abaqus environment file

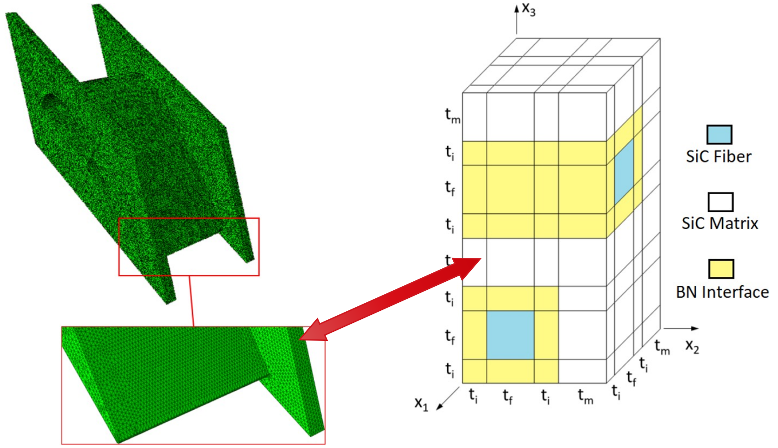


Application to a Realistic Industrial Sized Problem

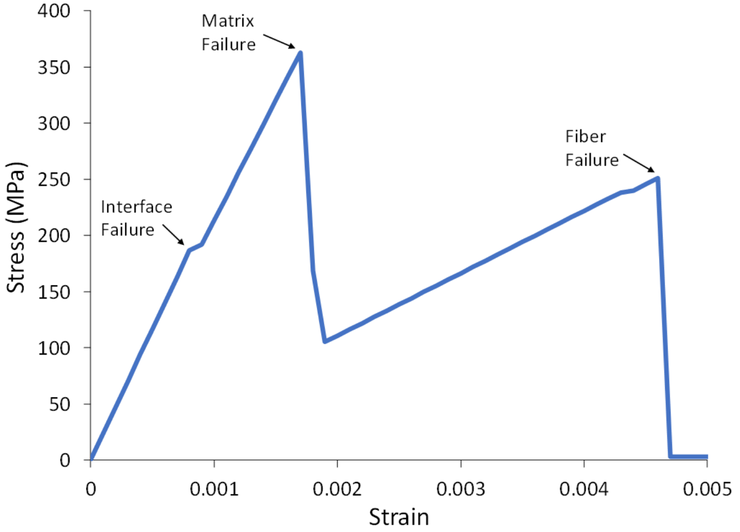
- Multiscale simulation of a realistic SiC/SiC CMC turbine vane subjected to thermal and internal pressure loading
  - Fully integrated nonlinear analysis
    - **5.5 hrs, 102 CPUs**



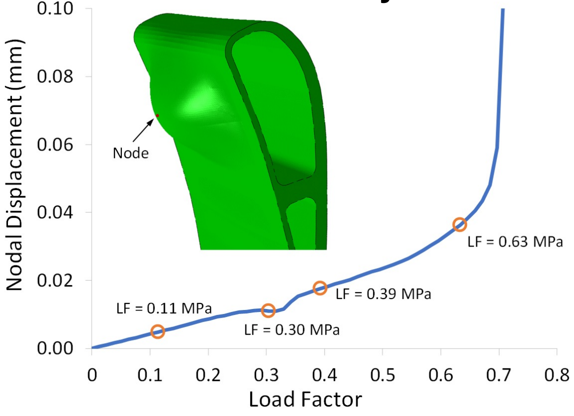
- FE Mesh ~0.5M C3D10 quadratic tets
- GMC3D SiC/SiC CMC RUC
  - – 128 subcells/ int. pt.



- Failure invoked at the microscale in the constituents

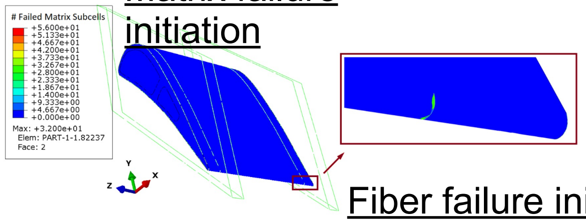


- Nodal displacement monitored as cavity bursts

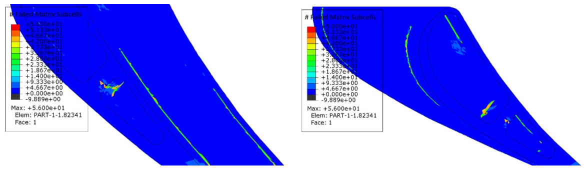


- Failure progression monitored in constituent

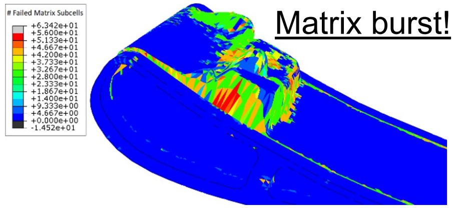
Matrix failure initiation



Matrix failure progression

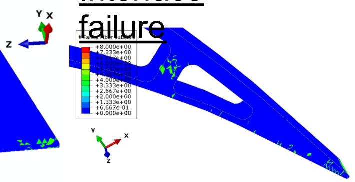


Matrix burst!

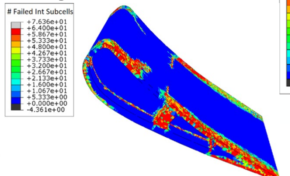


Fiber failure initiation

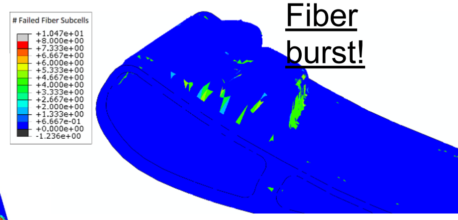
Interface failure



Fiber failure progression



Fiber burst!



Physics Governed by Vector Constitutive Laws

Heat conduction (Fourier's Law)	$\mathbf{q} = -\boldsymbol{\kappa}\nabla T$	$\mathbf{q} = \textit{heat flux vector}$ $\boldsymbol{\kappa} = \textit{2nd order thermal conductivity tensor}$ $T = \textit{temperature}$	
Electrical conduction	$\mathbf{J} = -\boldsymbol{\sigma}\nabla\phi$	$\mathbf{J} = \textit{electic current density vector}$ $\boldsymbol{\sigma} = \textit{2nd order electric conductivity tensor}$ $\phi = \textit{electical potential}$	*Electric field*: $\mathbf{E} = -\nabla\phi$
Diffusion (Fick's Law)	$\mathbf{j} = -\mathbf{d}\nabla C$	$\mathbf{j} = \textit{permeant flux vector}$ $\mathbf{d} = \textit{2nd order diffusivity tensor}$ $C = \textit{concentration}$	
Magnetic permeability	$\mathbf{B} = -\boldsymbol{\mu}\nabla\xi$	$\mathbf{J} = \textit{magnetic flux density vector}$ $\boldsymbol{\sigma} = \textit{2nd order magnetic permeability tensor}$ $\xi = \textit{magnetic potential}$	*Magnetic field*: $\mathbf{H} = -\nabla\xi$
Electrical permittivity	$\mathbf{D} = -\boldsymbol{\varepsilon}\nabla\phi$	$\mathbf{D} = \textit{electric displacement vector}$ $\boldsymbol{\varepsilon} = \textit{2nd order electric permittivity tensor}$ $\phi = \textit{electric potential}$	*Electric field*: $\mathbf{E} = -\nabla\phi$
In General	$\mathbf{Y} = -\mathbf{Z}\nabla\psi = \mathbf{Z}\mathbf{X}$	Governing Equation: $\nabla \cdot \mathbf{Y} = 0$	

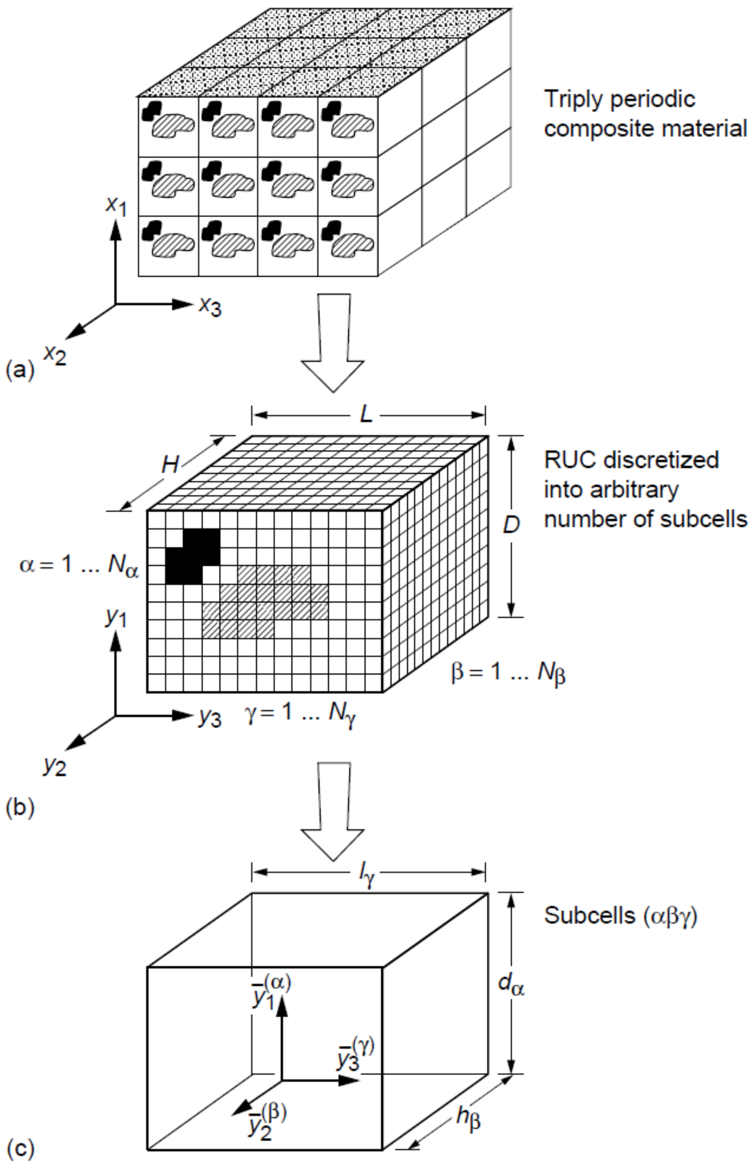
Multiphysics Governed by Vector Constitutive Laws

- New HFGMC formulation can solve any physics governed by vector constitutive law
- Predicts:
    - Effective properties (given constituent properties and arrangement)
    - Local fields (given global field loading)
- Second order potential or (temperature, etc.) expansion:

$$\psi^{(\alpha\beta\gamma)} = \bar{X}_j x_j + \theta_{(000)}^{(\alpha\beta\gamma)} + \bar{y}_1^{(\alpha)}\theta_{(100)}^{(\alpha\beta\gamma)} + \bar{y}_2^{(\beta)}\theta_{(010)}^{(\alpha\beta\gamma)} + \bar{y}_3^{(\gamma)}\theta_{(001)}^{(\alpha\beta\gamma)}$$
$$+ \frac{1}{2}\left(3\bar{y}_1^{(\alpha)2} - \frac{d_\alpha^2}{4}\right)\theta_{(200)}^{(\alpha\beta\gamma)} + \frac{1}{2}\left(3\bar{y}_2^{(\beta)2} - \frac{h_\beta^2}{4}\right)\theta_{(020)}^{(\alpha\beta\gamma)} + \frac{1}{2}\left(3\bar{y}_3^{(\gamma)2} - \frac{l_\gamma^2}{4}\right)\theta_{(002)}^{(\alpha\beta\gamma)}$$

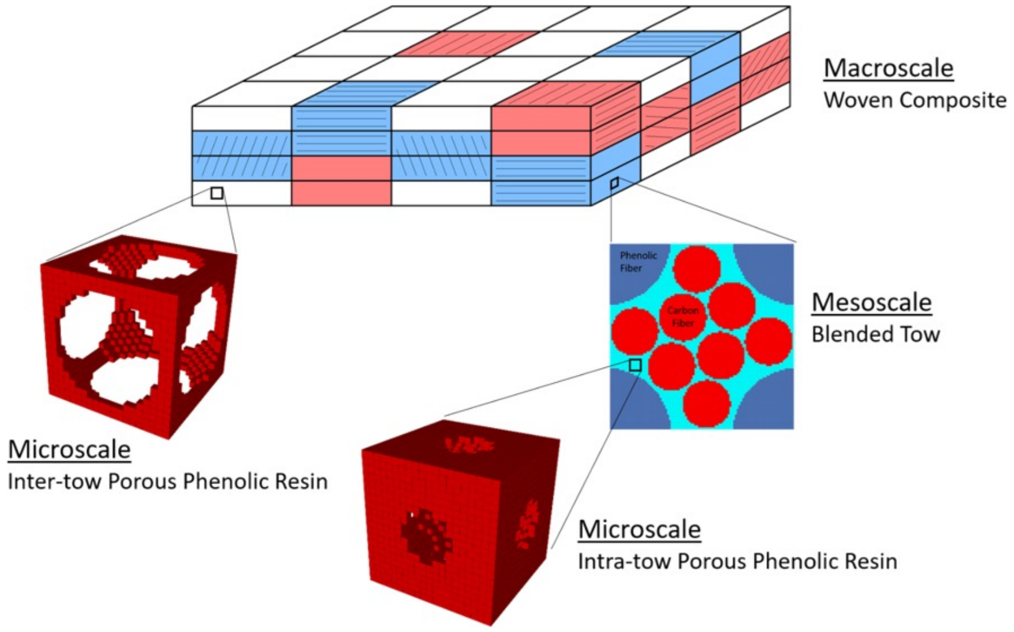
- System of $3N_\alpha N_\beta N_\gamma$ algebraic equations: $\mathbf{K}\,\mathbf{\Omega} = \mathbf{f}$
- Concentration equation: $\mathbf{X}^{(\alpha\beta\gamma)} = \mathbf{A}^{(\alpha\beta\gamma)}\bar{\mathbf{X}}$
- Global (effective) constitutive equation: $\bar{\mathbf{Y}} = \mathbf{Z}^*\bar{\mathbf{X}}$
- Where, effective property tensor is:

$$\mathbf{Z}^* = \frac{1}{DHL}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma\, \mathbf{Z}^{(\alpha\beta\gamma)}\mathbf{A}^{(\alpha\beta\gamma)}$$

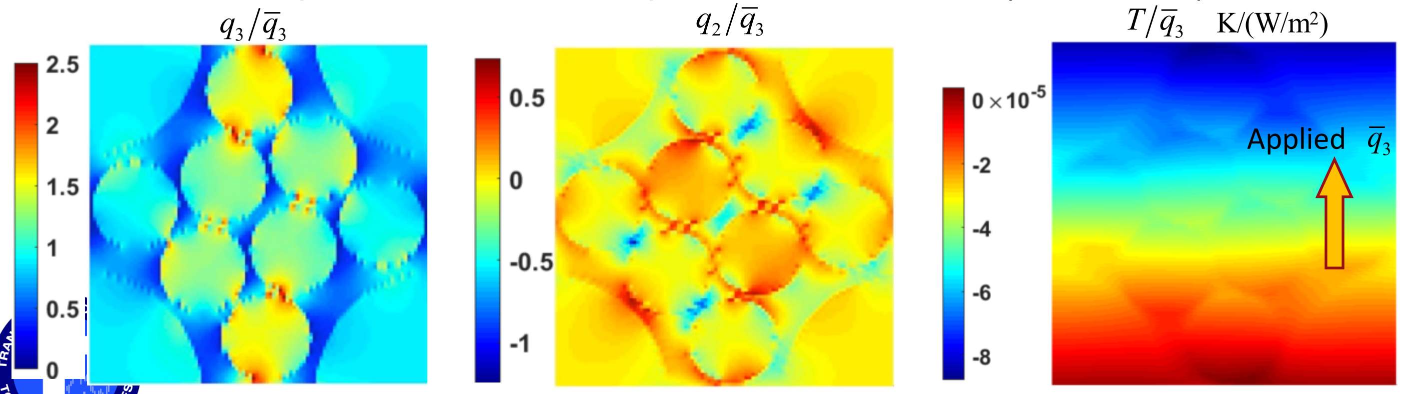


Multiscale Thermal Conductivity – C/Phenolic TPS Material

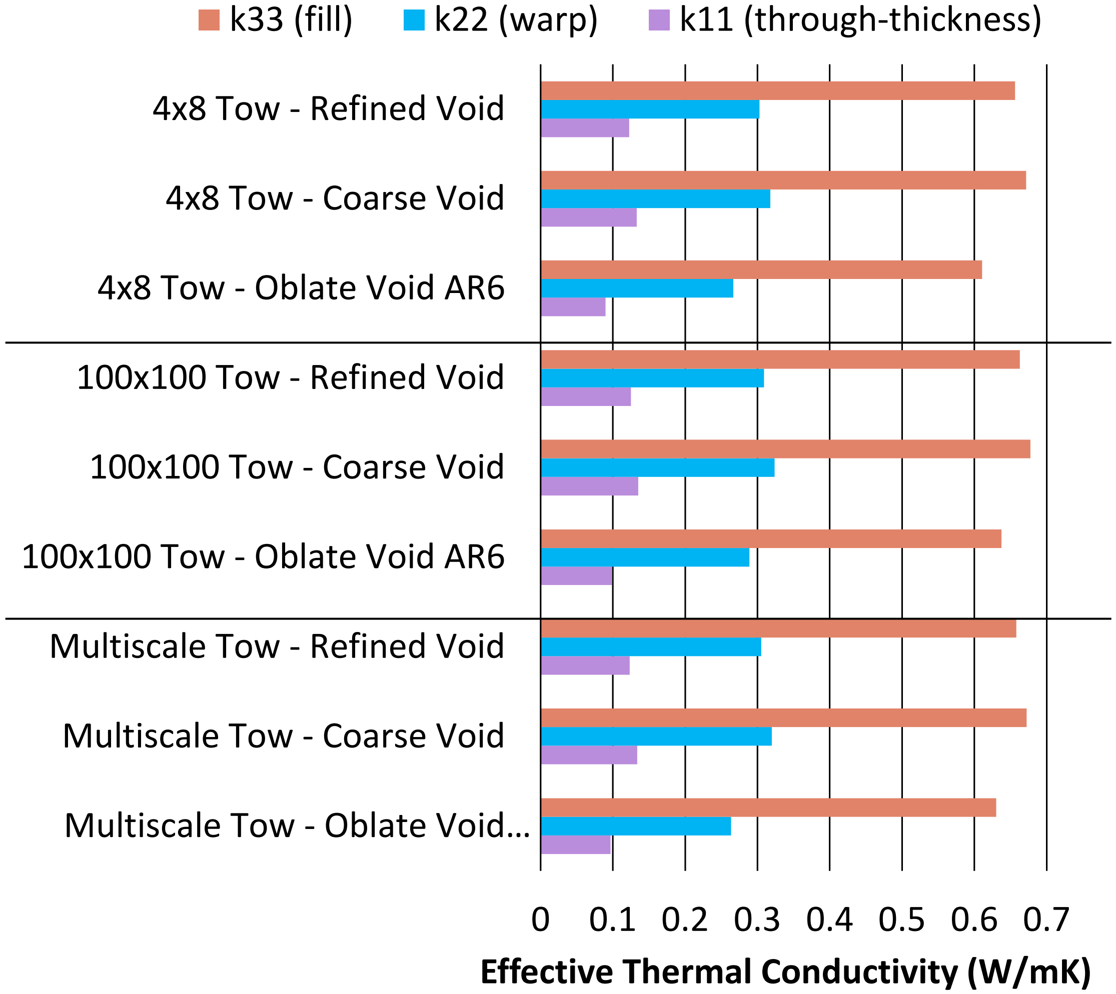
- Three scales (woven composite/tows/voids)



Sample local flux and temperature fields in tow (normalized)

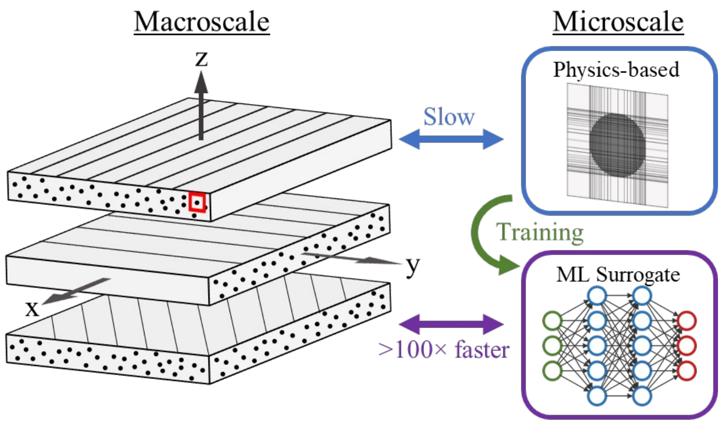


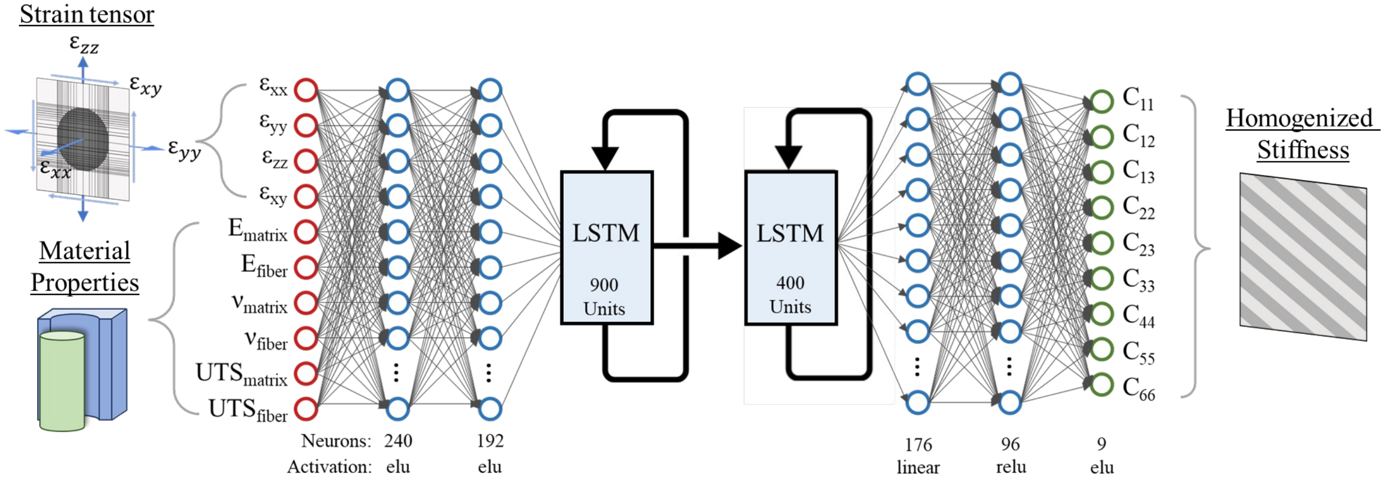
Anisotropic effective thermal conductivity as a function of tow and void representation



Coupling NASMAT with Machine Learning Tools

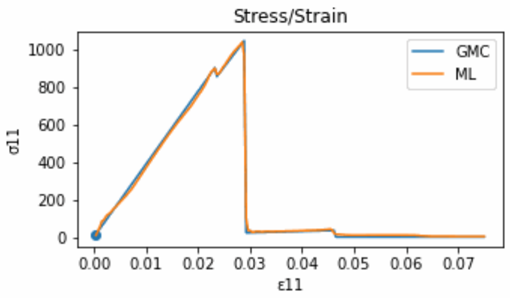
- Surrogate model interface to NASMAT developed
  - Couples Tensorflow to NASMAT
- Machine learning models developed to accurately replace physics-based models
- Currently validating approach for large-scale problems

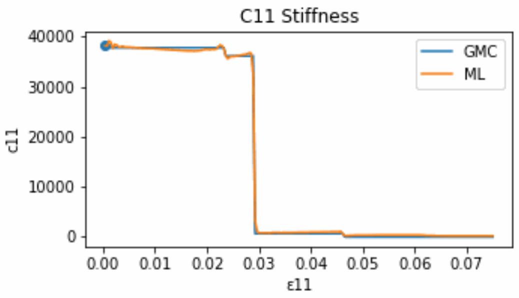


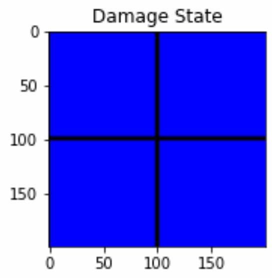


ACCOMPLISHMENT

- Laminate model with embedded ML surrogate was able to calculate the composite laminate response 145 times faster while maintaining an accuracy of 98% compared to the original physics-based model
- Industrial required speed with research level of accuracy



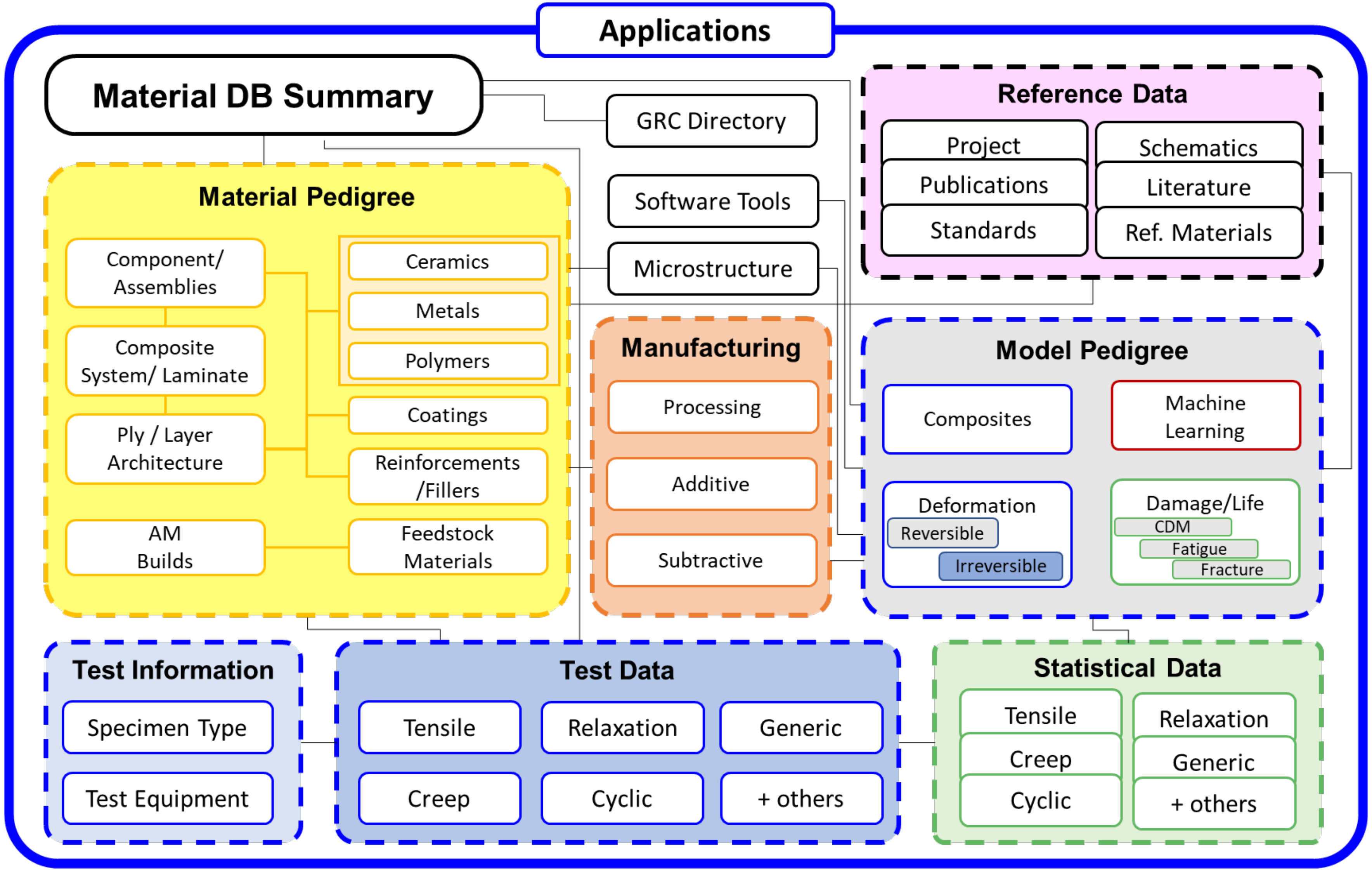




Stuckner, J., Graeber, S., Weborg, B., Ricks, T. M., & Arnold, S. M. (2021). Tractable Multiscale Modeling with An Embedded Microscale Surrogate. In AIAA Scitech 2021 Forum (p. 1963).
Sorini, A., Pineda, E. J., Stuckner, J., & Gustafson, P. A. (2021). A Convolutional Neural Network for Multiscale Modeling of Composite Materials. In AIAA Scitech 2021 Forum (p. 0310).

POC: J. Stuckner

NASA GRC Database Schema for ICME

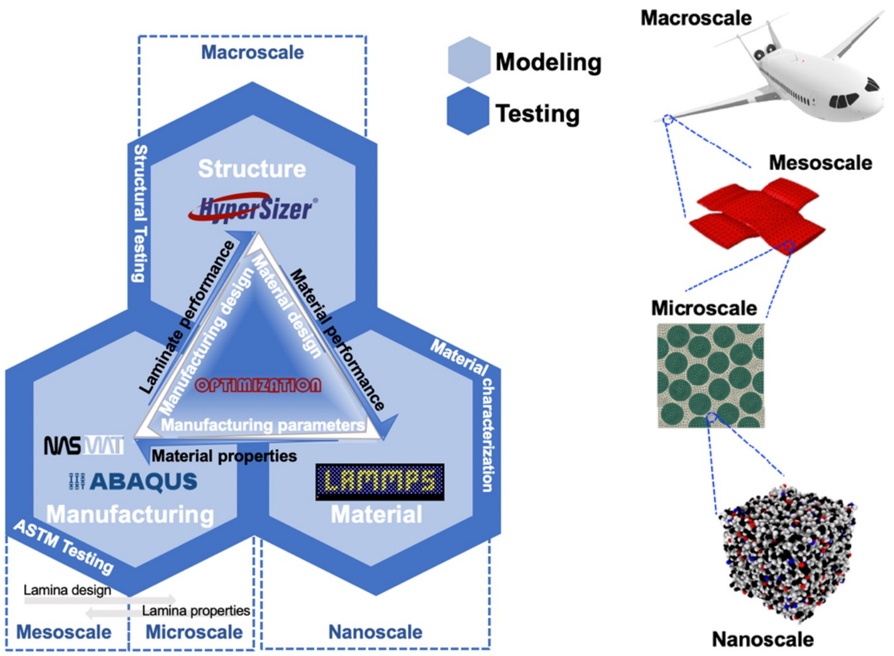


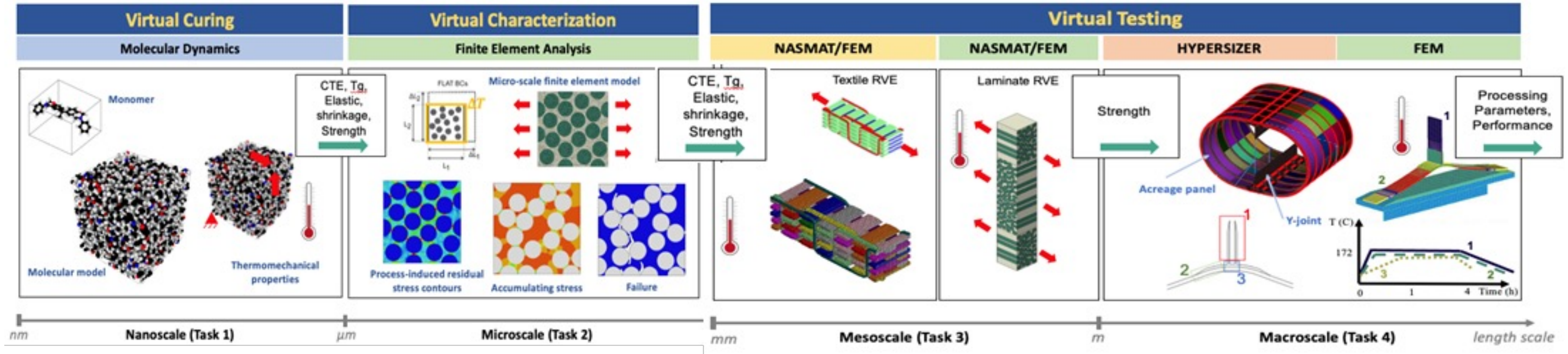
POC: B. Hearley

ICME Optimization of Advanced Composite Components of the Aurora D8 Aircraft: Digital Twin/Digital Thread

Multi Org. Collaboration: Univ Mass Lowell, Univ Michigan Tech, NASA, Aurora, Collier

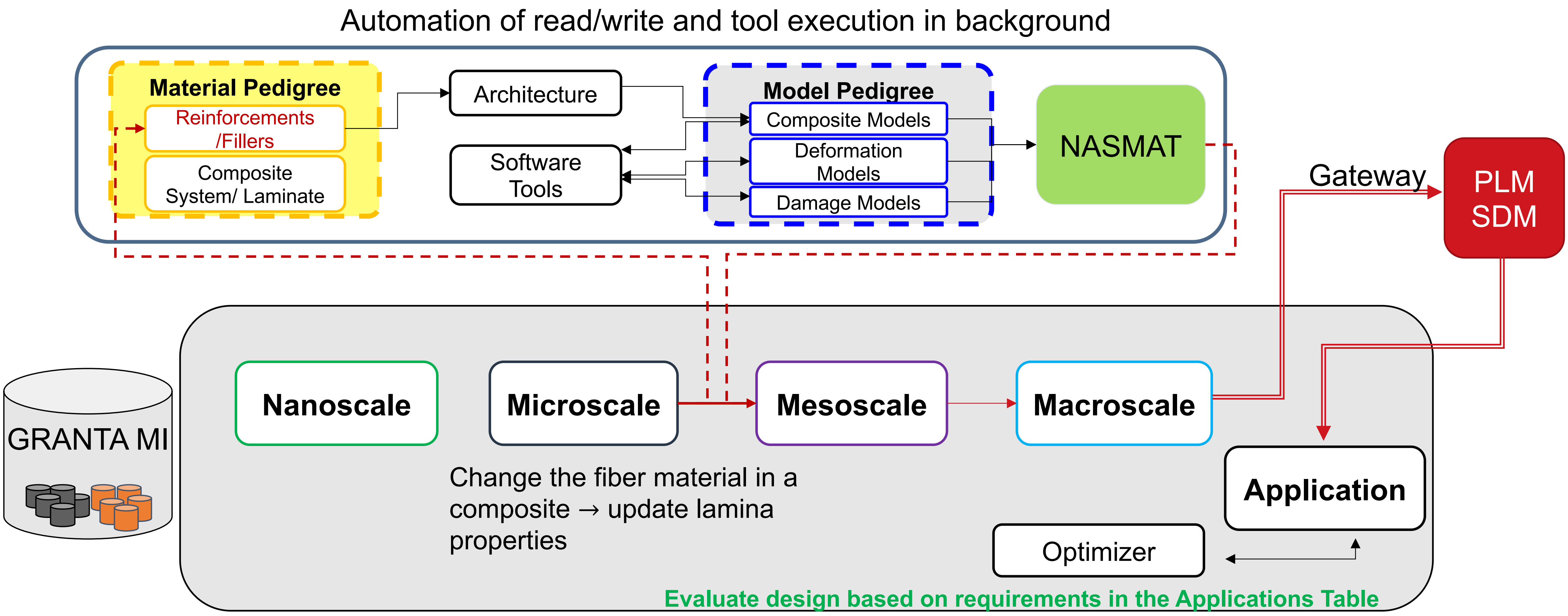
- NRA Objective is to develop an **integrated approach** to design and optimize the composite Y-joints and composite acreage panels used in the Aurora D8 aircraft
- Approach link material models, structural models, and experiments at multiple length scales
- Benchmark problem will serve to demonstrate the benefits of the ICME (compared to traditional approach)
  - **Digital Twins** at each scale
  - Input/output from each scale will constitute the **digital thread** of this ICME framework
- Use case within AIAA Digital Twin Implementation paper (Multiscale – ICME Schema)





AIMAOS Orchestrates ICME Process

Fit-for-Purpose Material Design



- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Summary

- NASMAT is an efficient and accurate nonlinear deformation and damage framework for the design and analysis of composite materials and structures (laminated and woven)
- NASMAT is an enabling tool to realize Vision 2040
- Suitable for modeling various materials (composite, fabrics, metallics)
- Able to capture relevant mechanisms at multiple scales
- Variable fidelity models available to balance computational efficiency and accuracy
- Has multi-physics modeling capability (including sequentially coupled)
- Can be coupled to external third-party software (e.g., FEA)
- Ongoing work focused on parallelizing multiscale recursive models within NASMAT

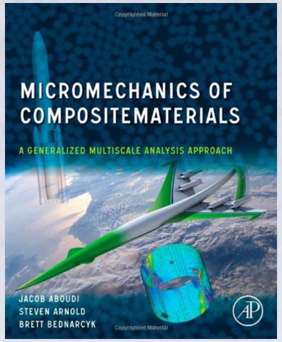
Thanks for Your Attention

Questions

Contact: Steven.M.Arnold@nasa.gov

Key References

Aboudi, J., Arnold, S.M., and Bednarcyk, B.A. (2013) *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*, Elsevier, Oxford, UK., pp 1-984.



Outline

1) Introduction
2) Constituent Material Modeling
3) Fundamentals of the Mechanics of Multiphase Materials
4) The Method of Cells Micromechanics
5) The Generalized Method of Cells Micromechanics
6) The High Fidelity Generalized Method of Cells Micromechanics
7) Multiscale Modeling of Composites
8) Fully Coupled Thermomechanical Analysis of Multiphase Composites
9) Finite Strain Micromechanical Modeling of Multiphase Composites
10) Micromechanical Analysis of Smart Composite Materials
11) Higher-Order Theory for Functionally Graded Materials
12) Wave Propagation in Multiphase and Porous Materials
13) Micromechanics Software

Published July 2021

"Written with both ***students and practitioners*** in mind and is coupled with a fully functional MATLAB code to enable solution of technologically relevant micromechanics problems. The many illustrative example problems and exercises highlight key concepts and rely heavily on the MATLAB code"

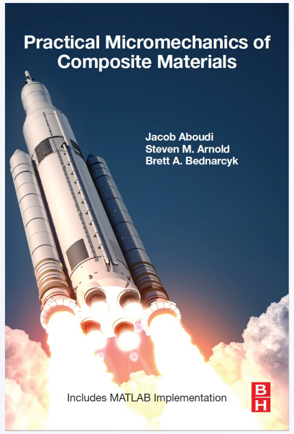


Table of Contents

1. Introduction
2. Lamination Theory Using Macromechanics
3. Closed Form Micromechanics
4. Failure Criteria and Margins of Safety
5. The Generalized Method of Cells (GMC) Micromechanics Theory
6. The High-Fidelity Generalized Method of Cells (HFGMC) Micromechanics Theory
7. Progressive Damage and Failure

Features:

- Thermoelastic Material Behavior
- Emphasis on Local fields via Strain and Stress Concentration Tensors;
- General MATLAB open-source code provided
  - four micromechanics theories MT, MOC, GMC, HFGMC
  - four failure criteria, along with consistent treatment of Margins of Safety (MoS)
  - Emphasis on PMC & CMC, order and disorder microstructures
  - https://github.com/nasa/Practical-Micromechanics
- Extensive Practical Examples; ~ 15 Exercises /Chapter (Solution Manual available to professors)

How to Get

- NASA Software Catalog
- Format: Windows/Linux standalone executable and Abaqus compiled libraries
- Prerequisites: Intel OneAPI Base and HPC toolkits, HDF5 (1.10.6)
- Contact: nasmat@lists.nasa.gov

Materials And Processes

NASA Multiscale Analysis Tool (NASMAT)

(LEW-20244-1)

Overview

The NASA Multiscale Analysis Tool (NASMAT) serves as a state-of-the-art, plug and play, software package which utilizes multiscale recursive micromechanics as a platform for massively multiscale modeling of hierarchical materials and structures subjected to thermomechanical loads on high performance computing systems.

Request Software

Software Details

Category	Materials and Processes
Reference Number	LEW-20244-1
Release Type	U.S. and Foreign Release
Operating System	Windows, Linux

Contact Us About This Technology

Glenn Research Center
grc-sra-team@mail.nasa.gov

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  - NASA STMD Composite Technologies for Exploration
  - NASA STMD Entry Systems Modeling
  - NASA STMD Thermoplastics Development for Exploration Activities
  - Office of Naval Research
- Special thanks to collaborators:
  - NASA Langley Research Center, Ames Research Center
  - NASA OSTEM and NASA Postdoctoral Program
  - Air Force Research Laboratory
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