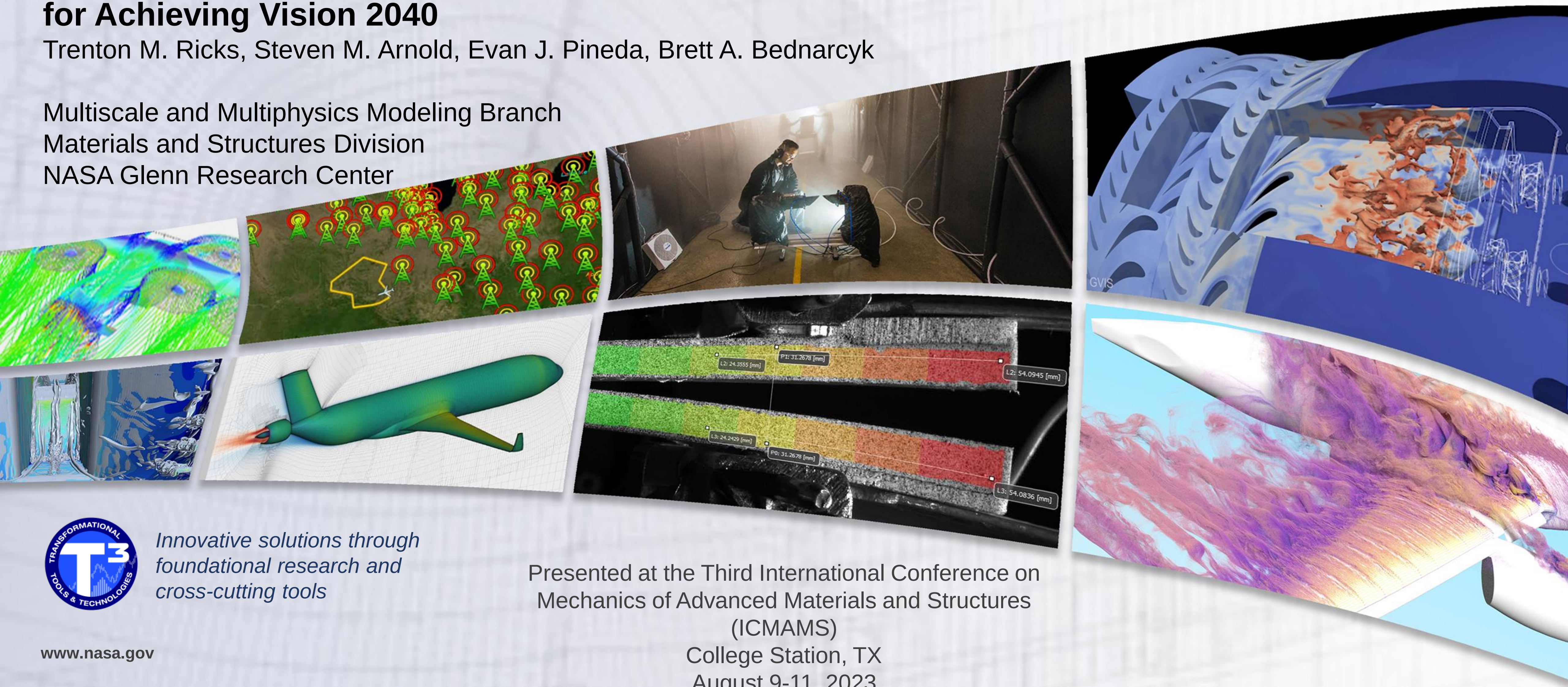
National Aeronautics and Space Administration

Transformational Tools and Technologies (T^3) Project

The NASA Multiscale Analysis Tool: An Enabling Platform for Achieving Vision 2040

Trenton M. Ricks, Steven M. Arnold, Evan J. Pineda, Brett A. Bednarcyk

Multiscale and Multiphysics Modeling Branch
Materials and Structures Division
NASA Glenn Research Center

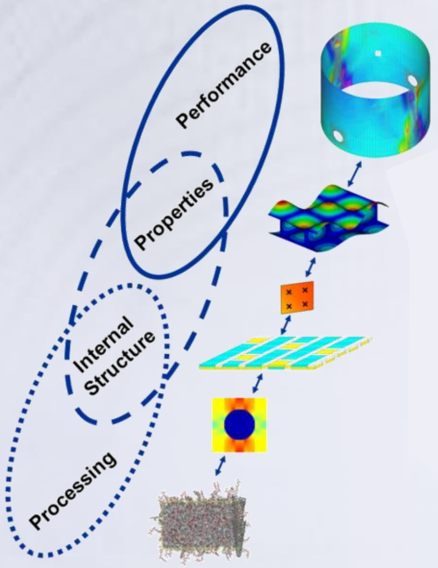


Innovative solutions through foundational research and cross-cutting tools

Presented at the Third International Conference on Mechanics of Advanced Materials and Structures (ICMAMS)
College Station, TX
August 9-11, 2023

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

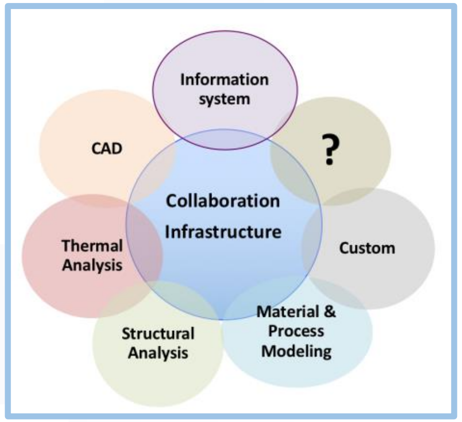
Provides a public/private investment strategy for the design of fit-for-purpose materials and structures



NASA CR 2018-219771

https://ntrs.nasa.gov

cyber-physical-social ecosystem



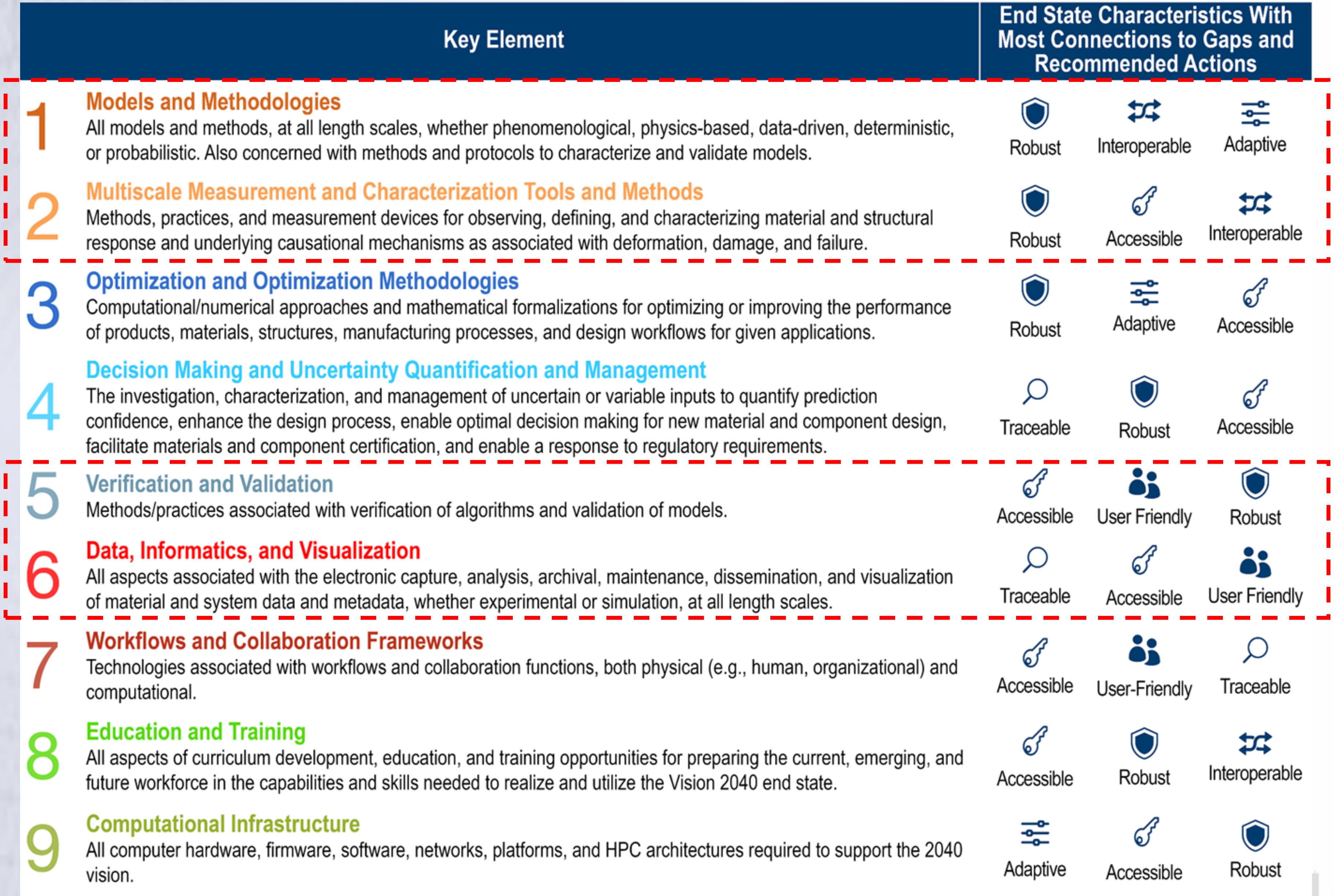
Nine Identified Key Element Discipline Areas

- 🟧 **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:

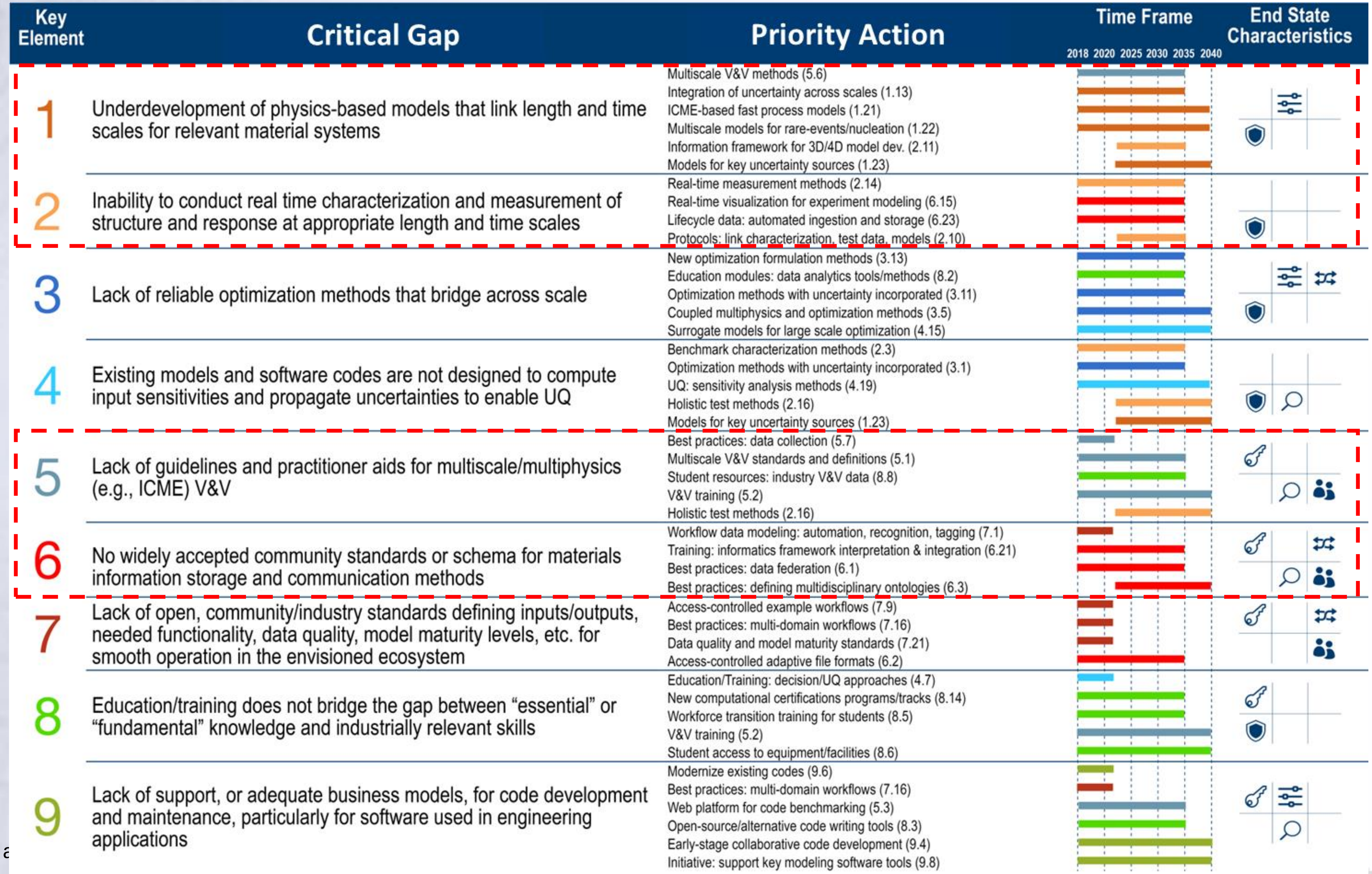
*A cyber-physical-social ecosystem that impacts the supply chain to **accelerate** model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for **affordable**, **producible** aerospace applications*

Study Identified 9 Key Element Domains



	Key Element	End State Characteristics With Most Connections to Gaps and Recommended Actions		
1	**Models and Methodologies** All models and methods, at all length scales, whether phenomenological, physics-based, data-driven, deterministic, or probabilistic. Also concerned with methods and protocols to characterize and validate models.	Robust	Interoperable	Adaptive
2	**Multiscale Measurement and Characterization Tools and Methods** Methods, practices, and measurement devices for observing, defining, and characterizing material and structural response and underlying causational mechanisms as associated with deformation, damage, and failure.	Robust	Accessible	Interoperable
3	**Optimization and Optimization Methodologies** Computational/numerical approaches and mathematical formalizations for optimizing or improving the performance of products, materials, structures, manufacturing processes, and design workflows for given applications.	Robust	Adaptive	Accessible
4	**Decision Making and Uncertainty Quantification and Management** The investigation, characterization, and management of uncertain or variable inputs to quantify prediction confidence, enhance the design process, enable optimal decision making for new material and component design, facilitate materials and component certification, and enable a response to regulatory requirements.	Traceable	Robust	Accessible
5	**Verification and Validation** Methods/practices associated with verification of algorithms and validation of models.	Accessible	User Friendly	Robust
6	**Data, Informatics, and Visualization** All aspects associated with the electronic capture, analysis, archival, maintenance, dissemination, and visualization of material and system data and metadata, whether experimental or simulation, at all length scales.	Traceable	Accessible	User Friendly
7	**Workflows and Collaboration Frameworks** Technologies associated with workflows and collaboration functions, both physical (e.g., human, organizational) and computational.	Accessible	User-Friendly	Traceable
8	**Education and Training** All aspects of curriculum development, education, and training opportunities for preparing the current, emerging, and future workforce in the capabilities and skills needed to realize and utilize the Vision 2040 end state.	Accessible	Robust	Interoperable
9	**Computational Infrastructure** All computer hardware, firmware, software, networks, platforms, and HPC architectures required to support the 2040 vision.	Adaptive	Accessible	Robust

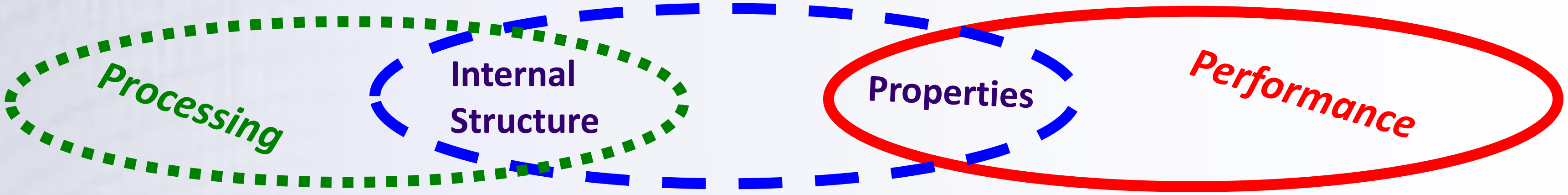
Identified Critical Gaps & *Possible Subset of Actions Required To Close Each Gap*



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

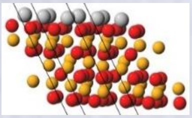
Integrated Computational Materials Engineering (ICME) Is The Future

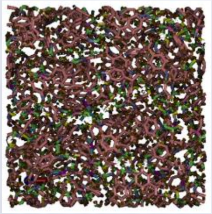


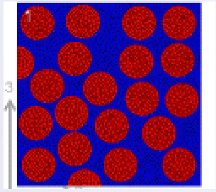
Design "The" Material ←

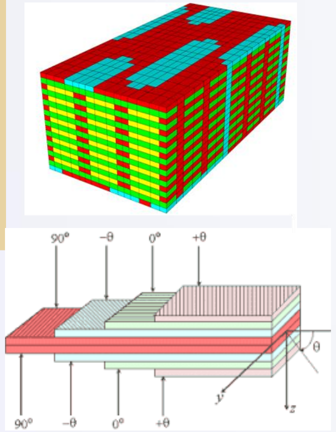
Design "With" Material →

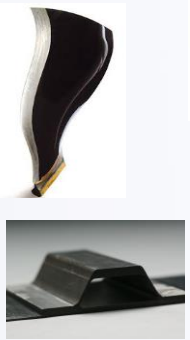
ICME is an approach to the design of products and the materials which comprise them by **linking experimentally validated materials models at multiple length scales**.

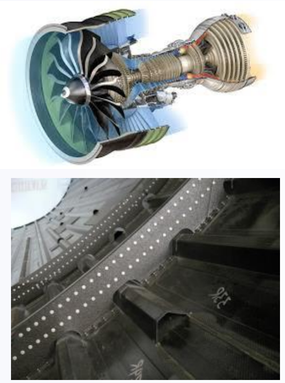

Quantum


Atomistic


Micro scale


Meso scale


Part


Assembly


System

Handshake via Constitutive Model

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

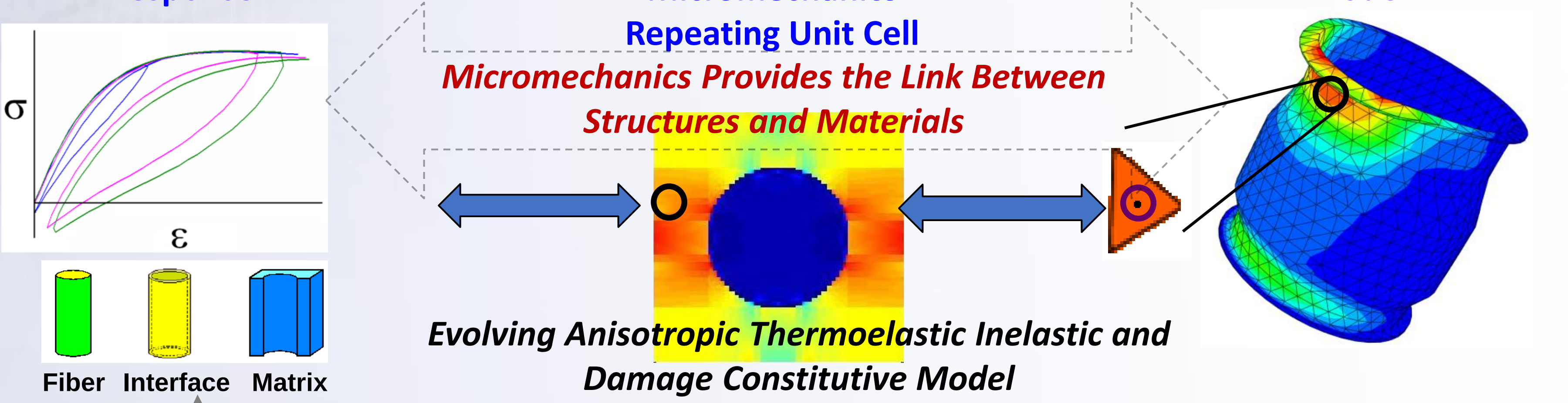
Micromechanics / Statistical Mechanics ↔

Molecular Dynamics ↔

Quantum Mechanics ↔

Continuum Mechanics ↔

Micromechanics: The Link Between Structures and Materials



Constituent Response

Composite Micromechanics Repeating Unit Cell

Structural Model

Micromechanics Provides the Link Between Structures and Materials

Evolving Anisotropic Thermoelastic Inelastic and Damage Constitutive Model

Continuum Deformation and Damage Models

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

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

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

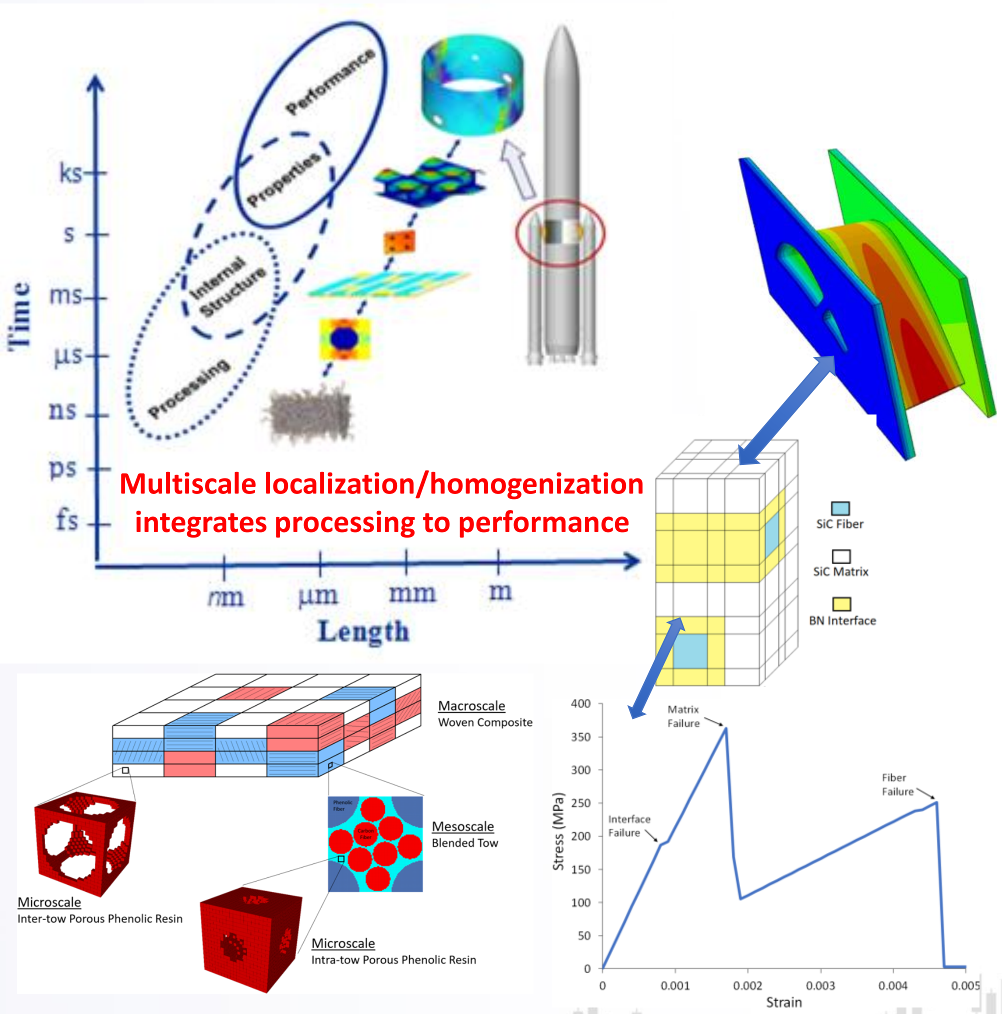
$$\bar{\varepsilon}^I = \frac{-\left[B^*\right]^{-1}}{dhl}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma C^{(\alpha\beta\gamma)}\left(D^{(\alpha\beta\gamma)}\varepsilon_s^I - \varepsilon^{I(\alpha\beta\gamma)}\right)$$

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

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)

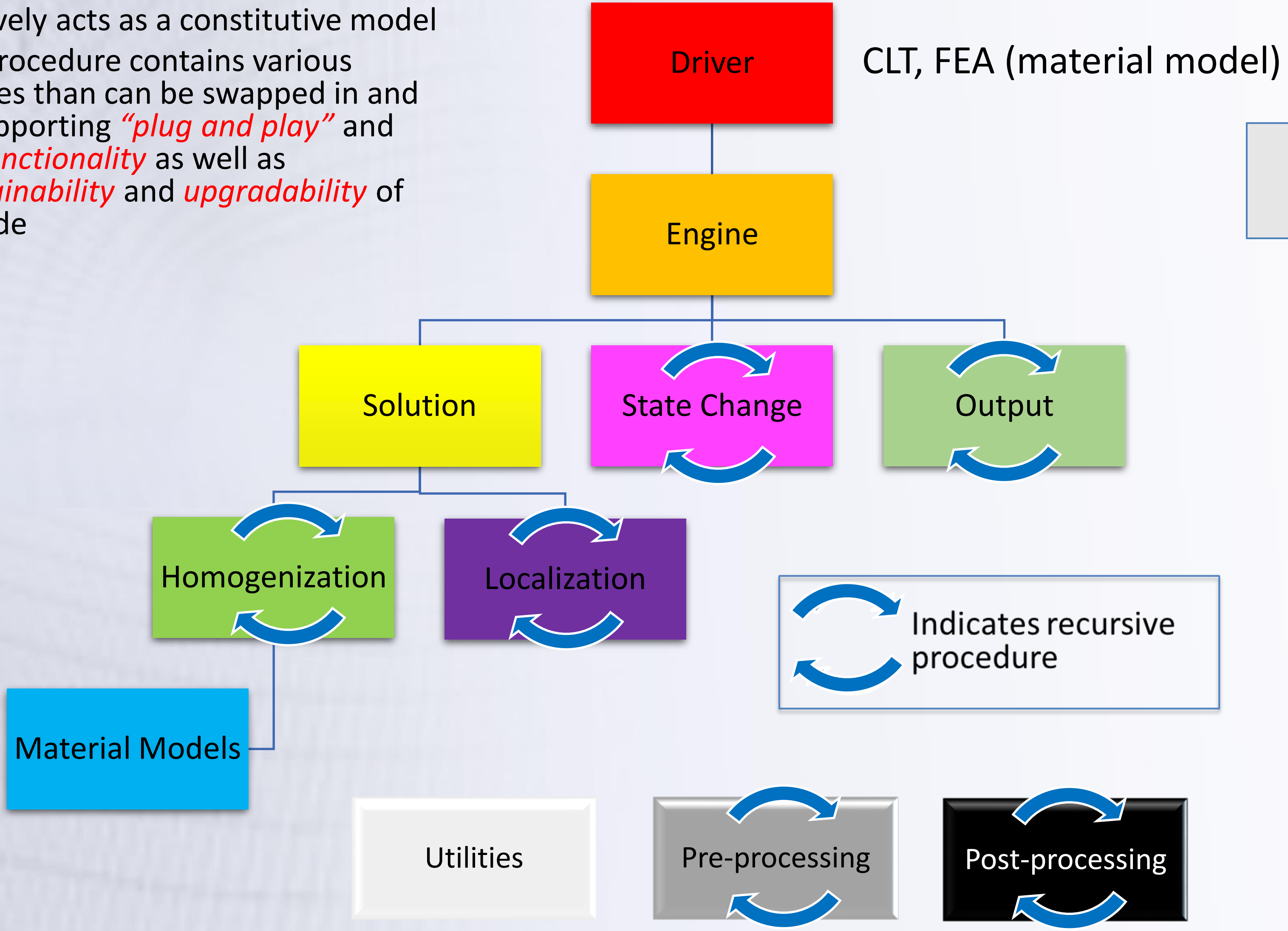
- Clean-sheet development based on legacy MAC/GMC and FEAMAC tools (~30 years of tool development)
- A framework designed to support massively multiscale modeling (M3) on high-performance computing (HPC) systems
  - Solves real, large-scale, non-linear, thermo-mechanical problems
- Modular design to 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 constitutive laws/damage models (including user-defined)
  - Data output in HDF5 file format
- ASCII input, pre/post-processor under development



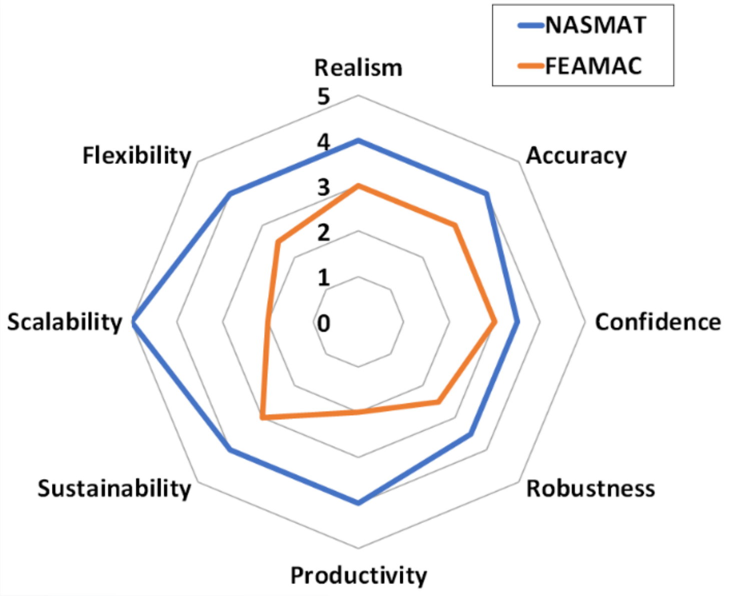
Multiscale localization/homogenization integrates processing to performance

NASMAT Workflow

- Effectively acts as a constitutive model
- Each procedure contains various modules than 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)



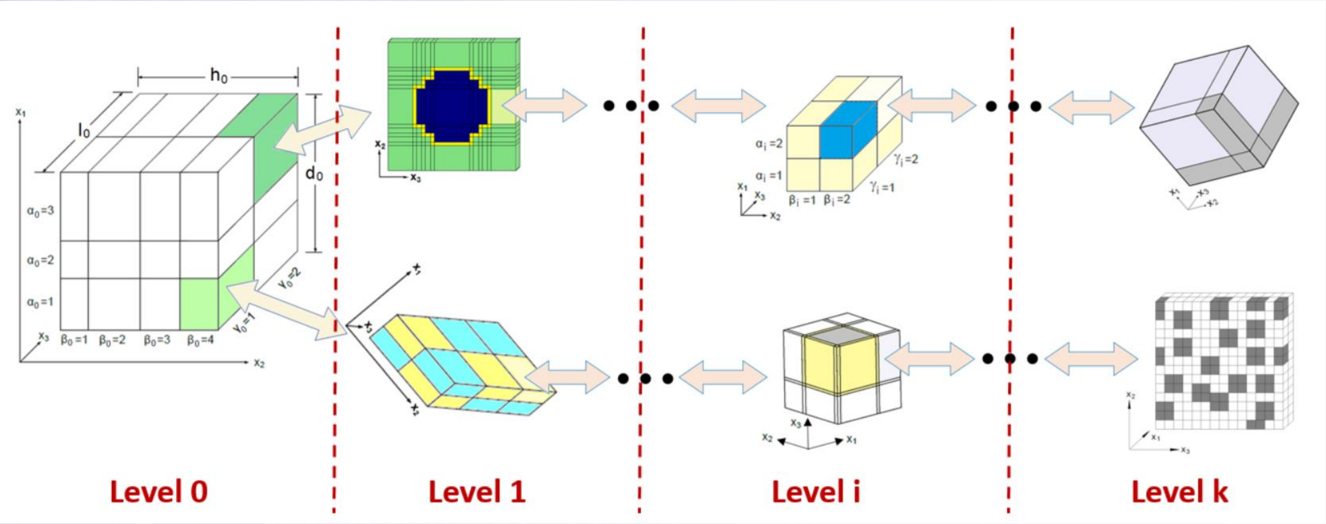
Comparison of Different Modeling Approaches

	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

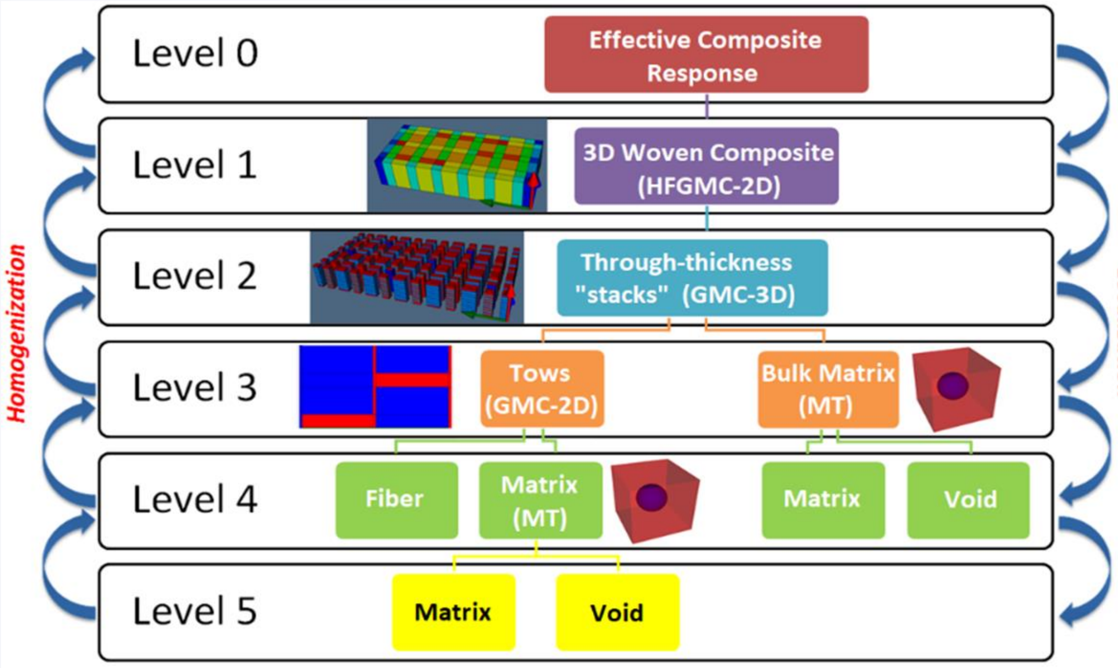
Multiscale Recursive Micromechanics (MsRM)

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



Localization

Homogenization



Homogenization

Localization

Level 0 Effective Composite Response

Level 1 3D Woven Composite (HFGMC-2D)

Level 2 Through-thickness "stacks" (GMC-3D)

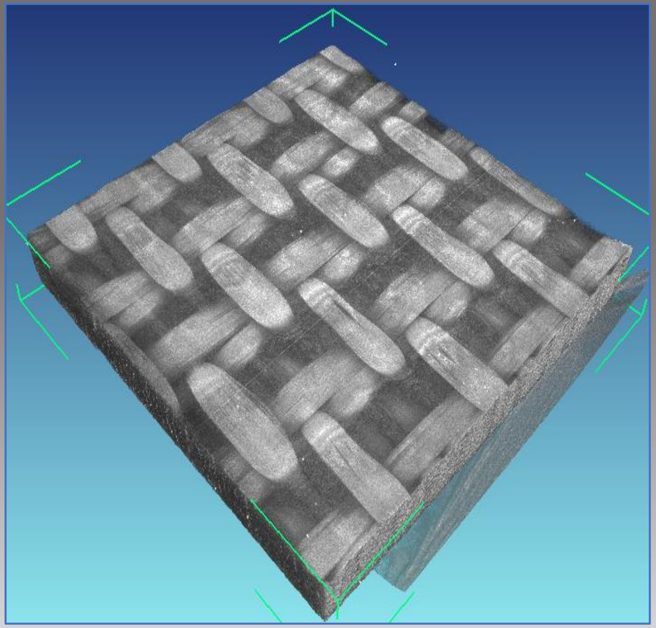
Level 3 Tows (GMC-2D) Bulk Matrix (MT)

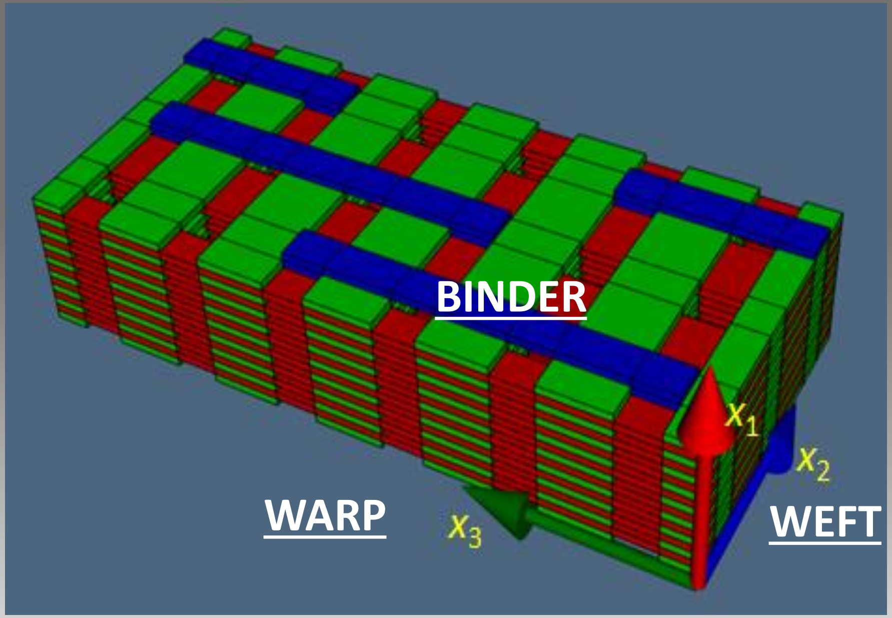
Level 4 Fiber Matrix (MT) Matrix Void

Level 5 Matrix Void

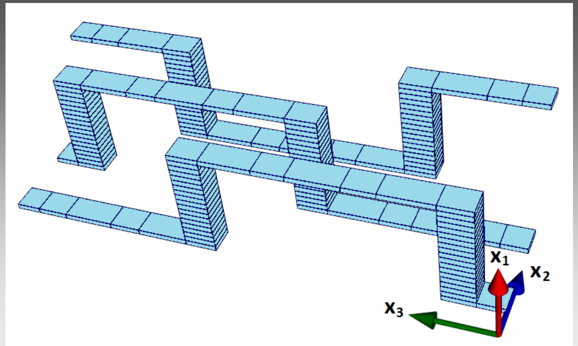
Development of a 3D Woven Repeating Unit Cell (RUC)

Idealization of Tow Paths from X-Ray CT

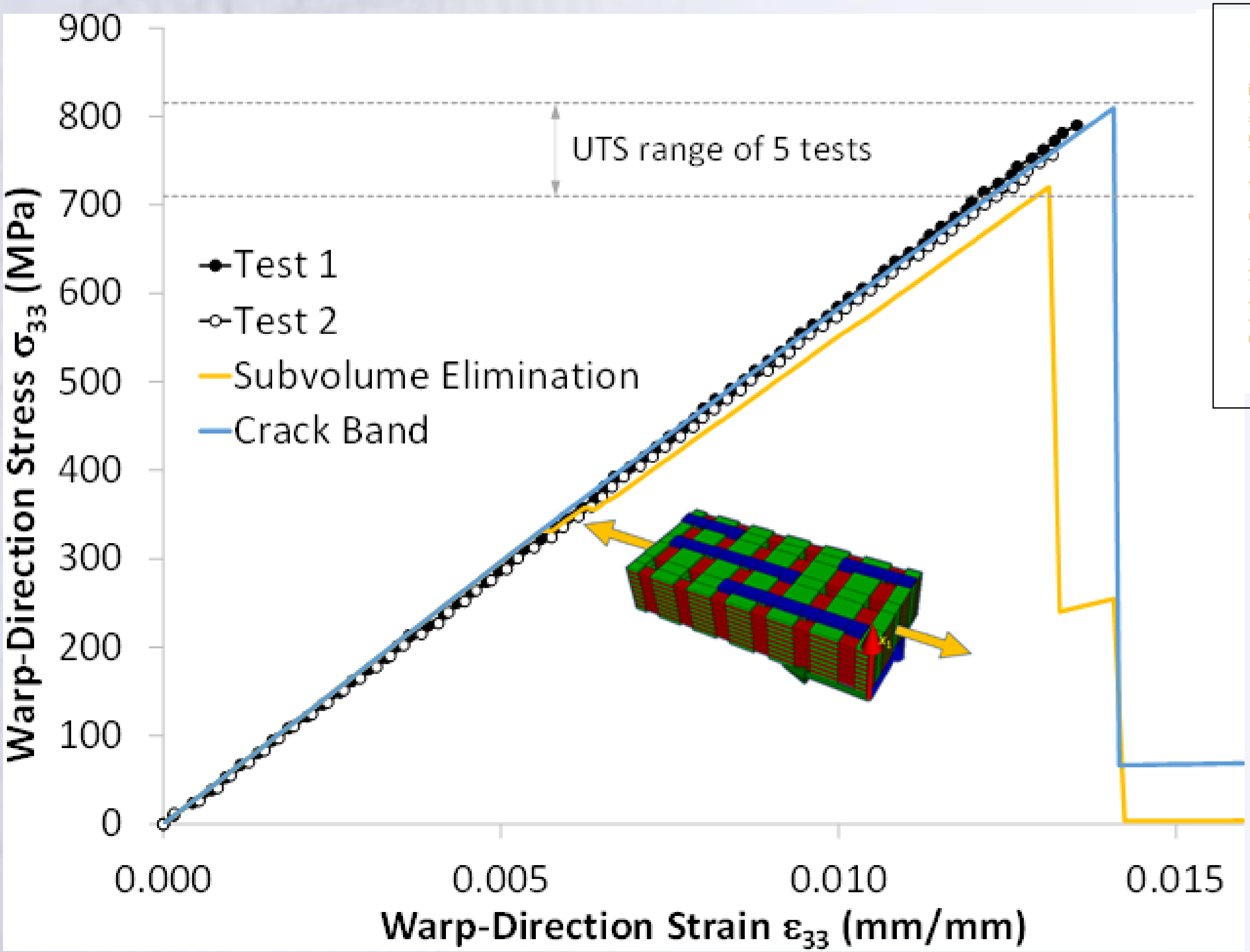


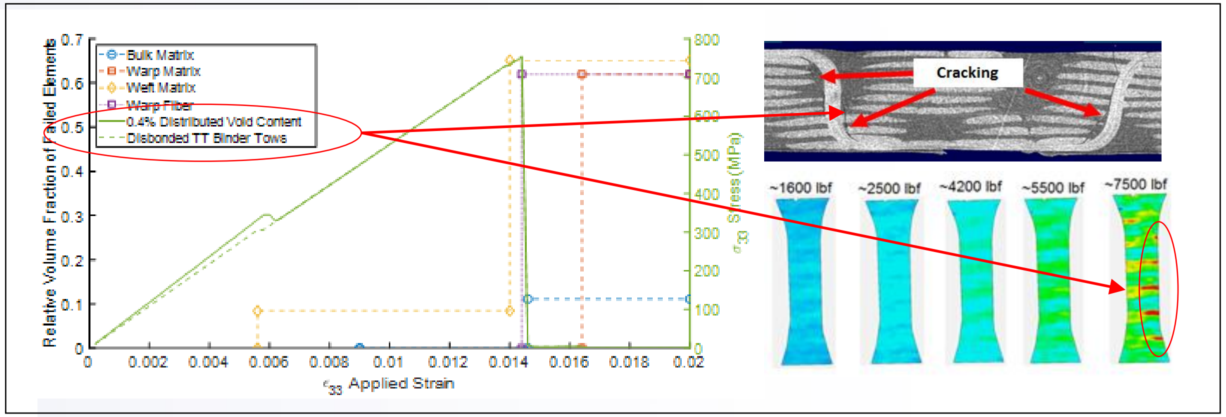


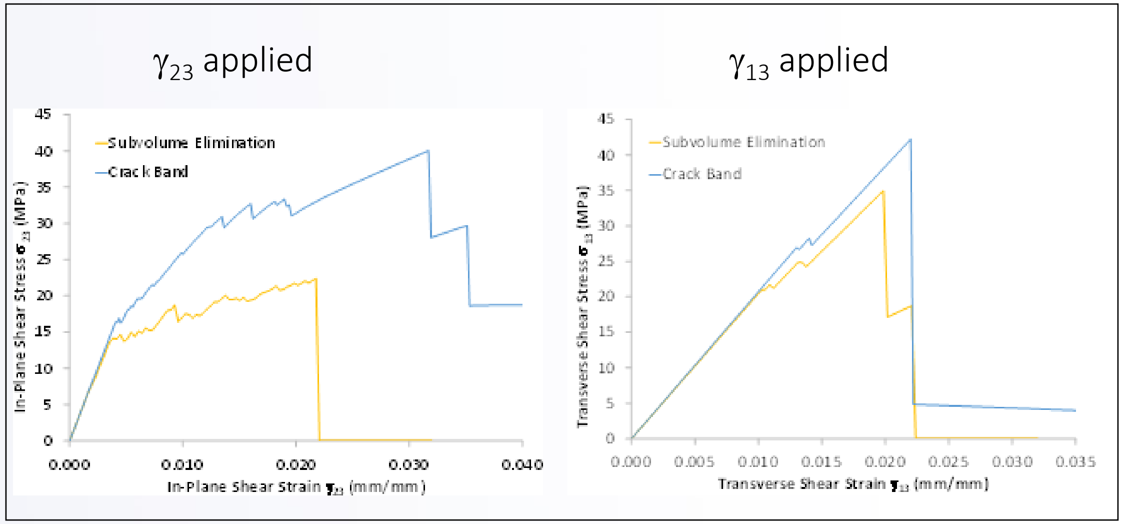
Through-thickness Binder Tow



Failure Prediction of a 3D Woven Composite



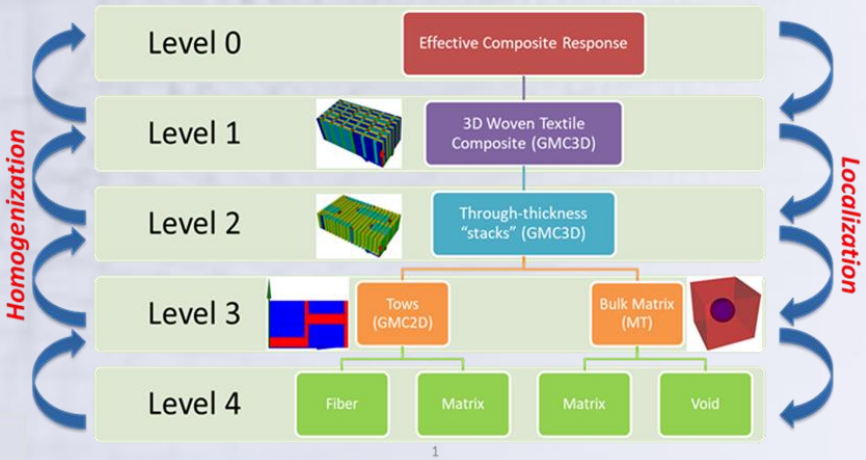


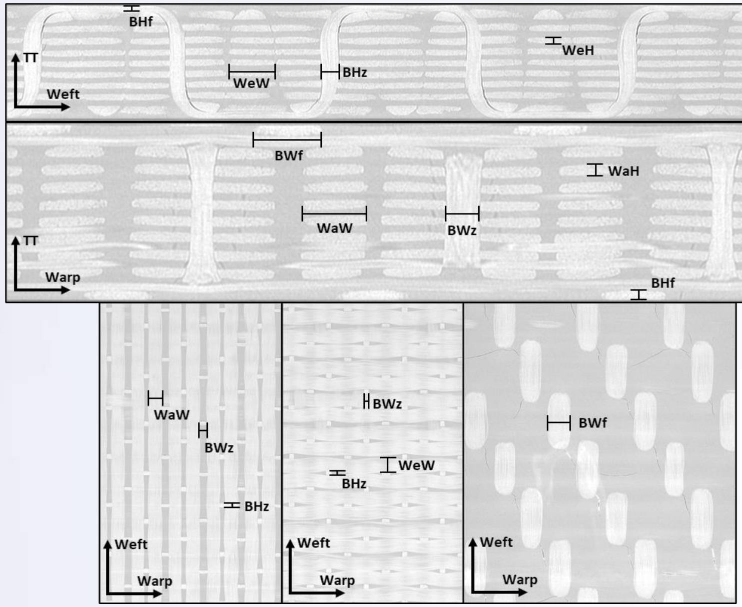


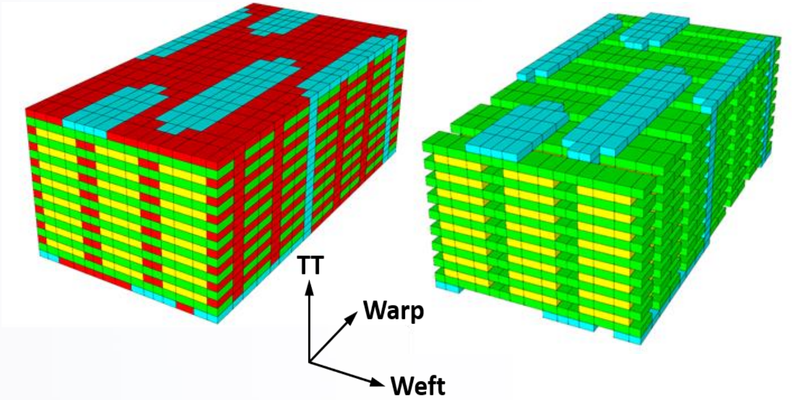
- Warp-direction strength predicted
- Use of quasi-brittle damage model improved overall prediction of stress-strain curve

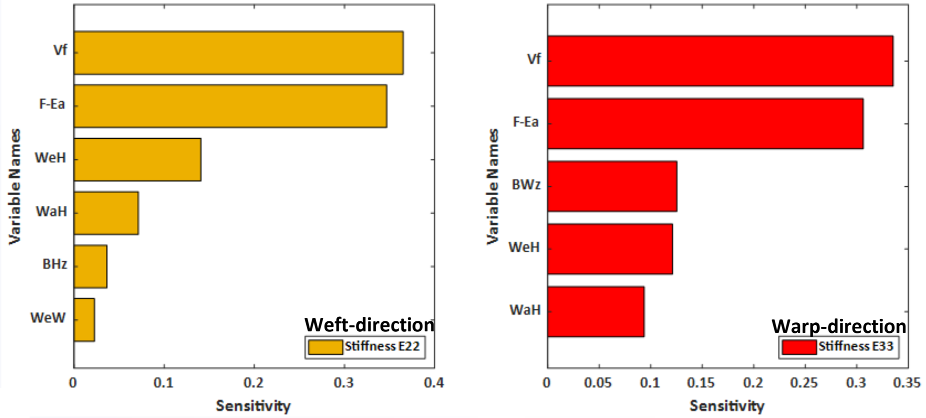
- Failure mode predicted – disbonding of binder tows
- Crack band model results in more shear nonlinearity
- Runtimes: Subvolume elimination ~ 30 sec., crack band ~ 15 min.

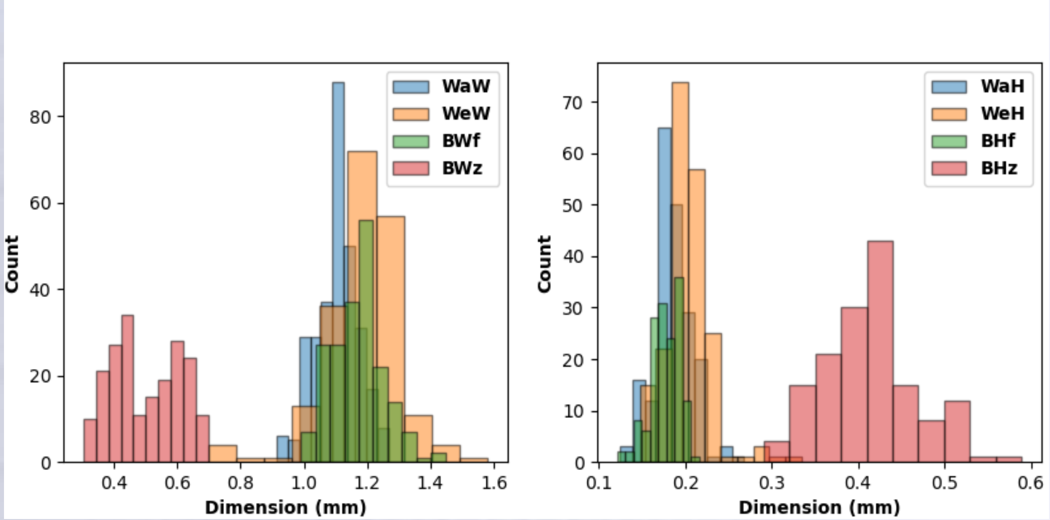
Sensitivity Analysis of 3D Woven Composites







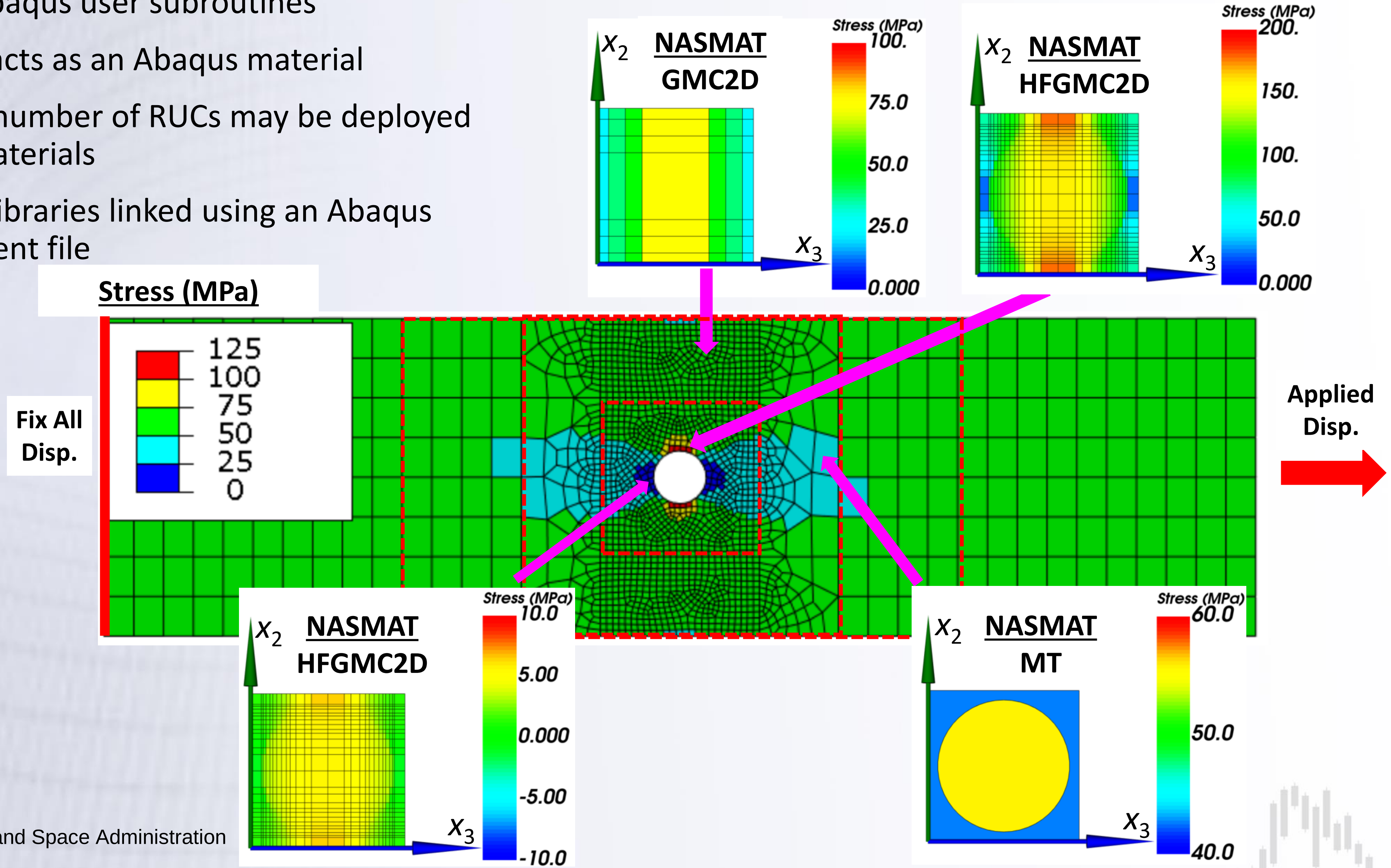




- Ability to capture relevant physics at multiple length scales
- Rapid analysis capability (~sec-min, single CPU) compared to state of the art (~hrs, many CPUs)
- **100k NASMAT simulations in ~6 hours**
- Able to estimate output sensitivities to input variables

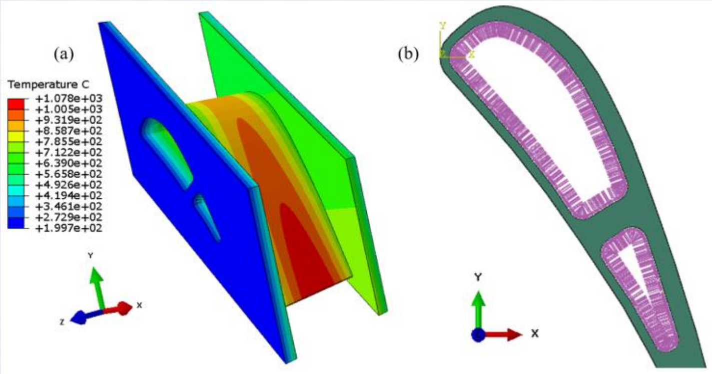
Multifidelity Integration with Abaqus

- 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

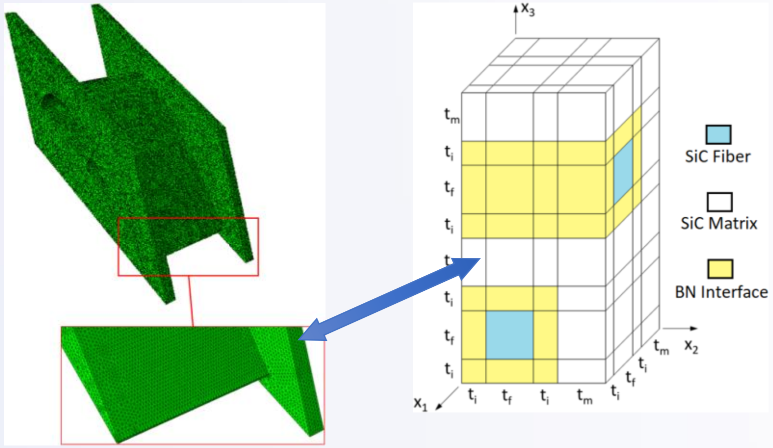


Application to a Realistic, Industrial Sized Problems

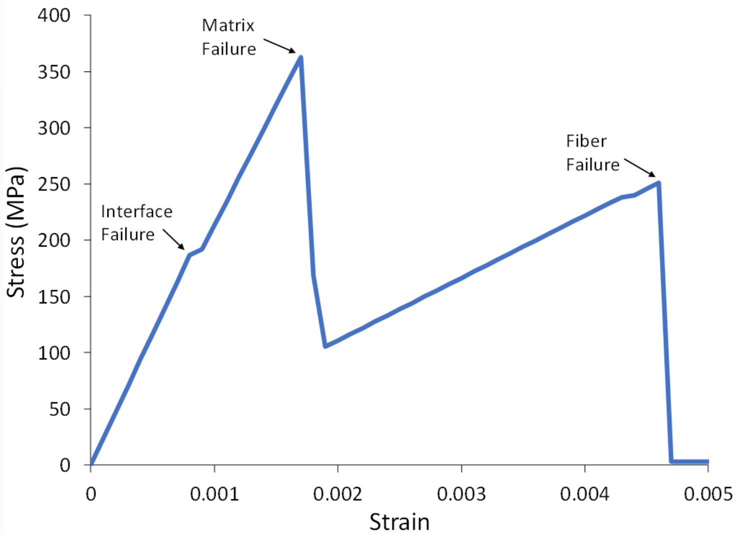
- Multiscale simulation of realistic SiC/SiC CMC turbine vane subjected to thermal and internal pressure loading
  - Fully integrated nonlinear analysis
    - 5.5 hrs, 102 CPUs



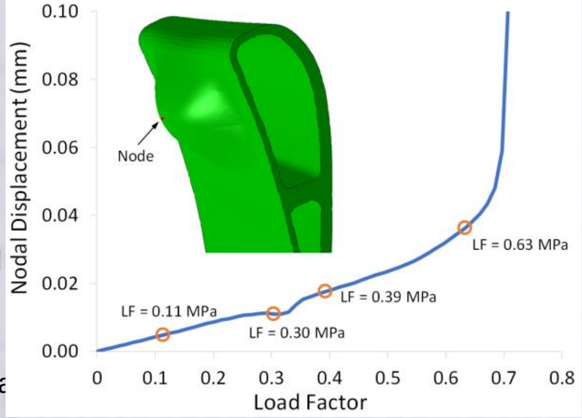
- FE Mesh ~0.5M C3D10 quadratic tets
- GMC3D SiC/SiC CMC RUC
  - 128 subcells



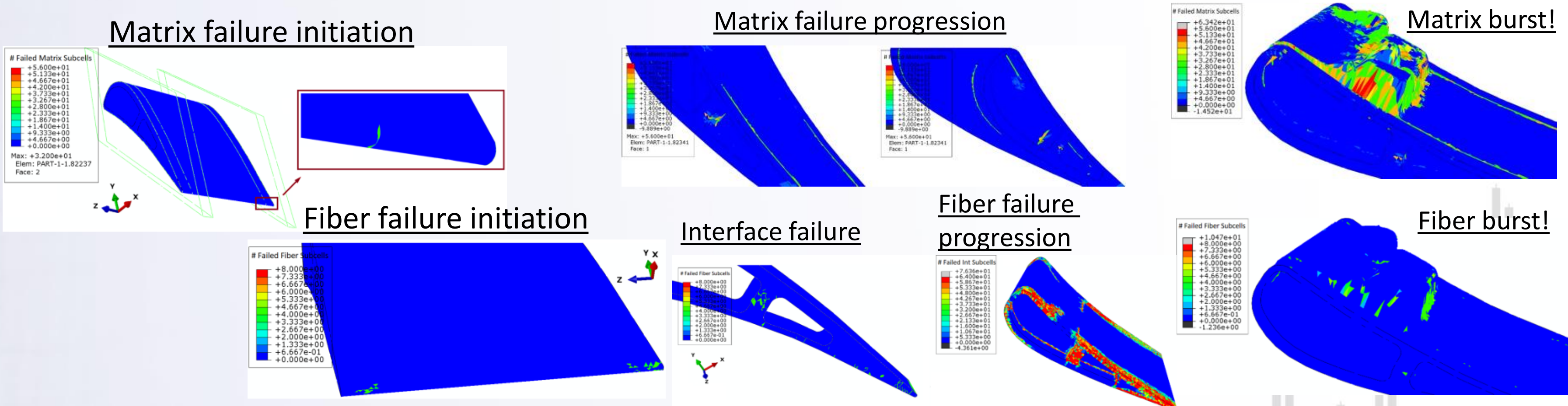
- Failure invoked at the microscale in the constituents



- Nodal displacement monitored as cavity bursts



- Failure progression monitored in constituent



Matrix failure initiation

Matrix failure progression

Matrix burst!

Fiber failure initiation

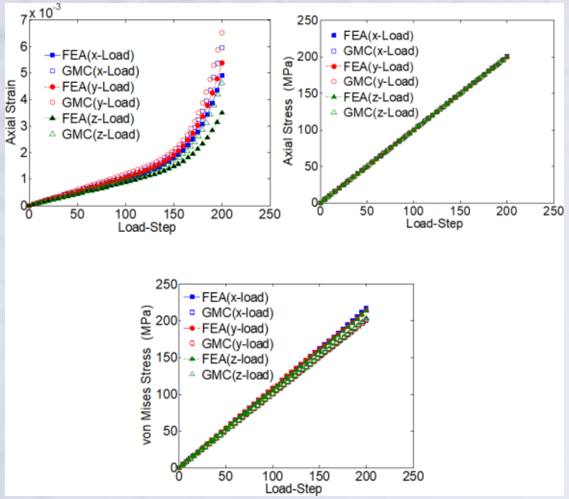
Interface failure

Fiber failure progression

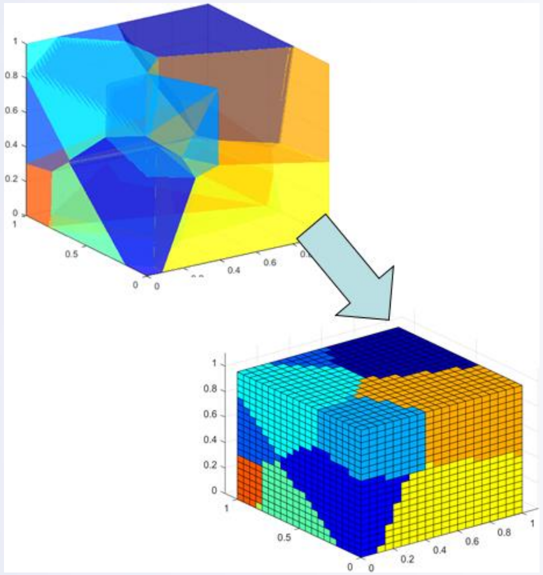
Fiber burst!

Microscale Tailoring of a Multiphase Metallic Alloy Disk

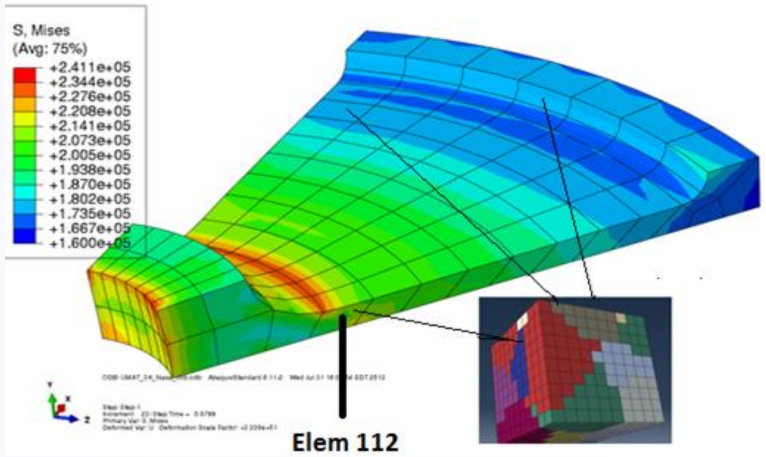
Single-crystal plasticity – collab. with **Achuthan (Clarkson University)**



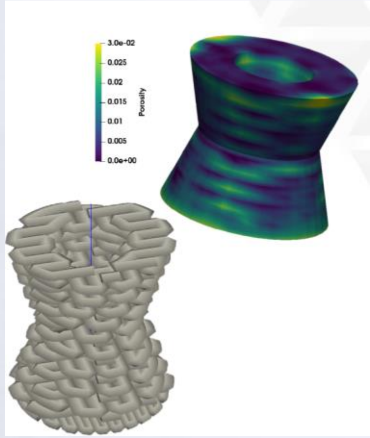
Voxelization of polycrystalline RUC for HFGMC analysis

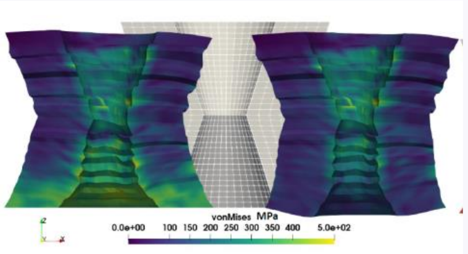


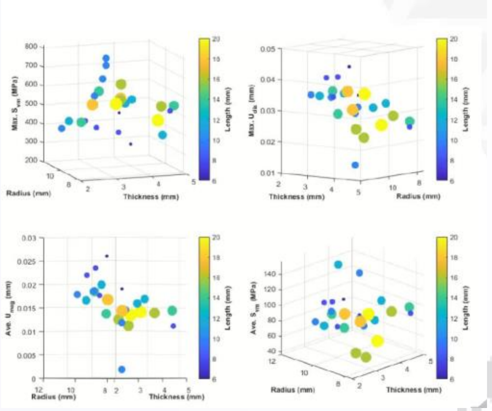
Multiscale Modeling: Supported through NASA SBIR – **ADDITIVE MANUFACTURING INNOVATIONS, LLC; PI: Ajit Achuthan**



Additive Manufacturing: collab. with **Gustafson** (**Western Michigan University)**





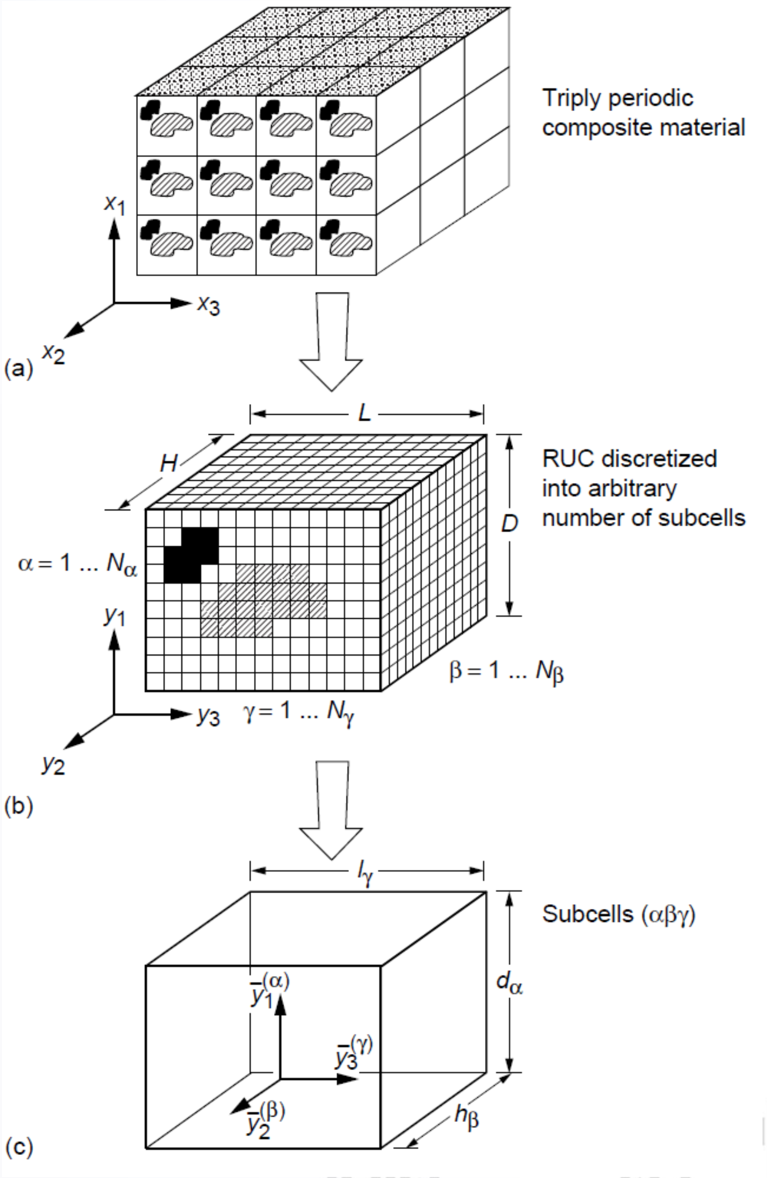


Multiphysics Governed by Vector Constitutive Laws

- 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:

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

- System of $3N_\alpha N_\beta N_\gamma$ algebraic equations: $\mathbf{K}\,\mathbf{\Omega} = \mathbf{f}$
- Concentration equation: $\boxed{\mathbf{X}^{(\alpha\beta\gamma)} = \mathbf{A}^{(\alpha\beta\gamma)}\,\bar{\mathbf{X}}}$
- Global (effective) constitutive equation: $\bar{\mathbf{Y}} = \mathbf{Z}^*\,\bar{\mathbf{X}}$
- Where, effective property tensor is: $\boxed{\mathbf{Z}^* = \frac{1}{DHL}\sum_{\alpha=1}^{N_\alpha}\sum_{\beta=1}^{N_\beta}\sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma\, \mathbf{Z}^{(\alpha\beta\gamma)}\,\mathbf{A}^{(\alpha\beta\gamma)}}$

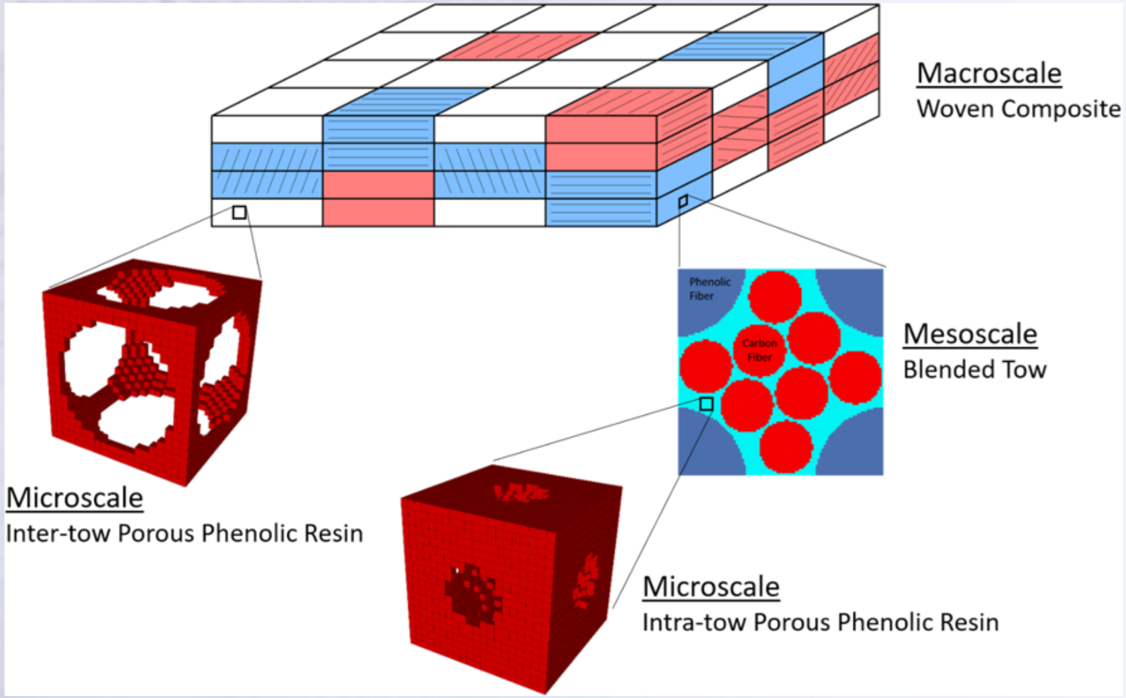


Physics Governed by Vector Constitutive Laws

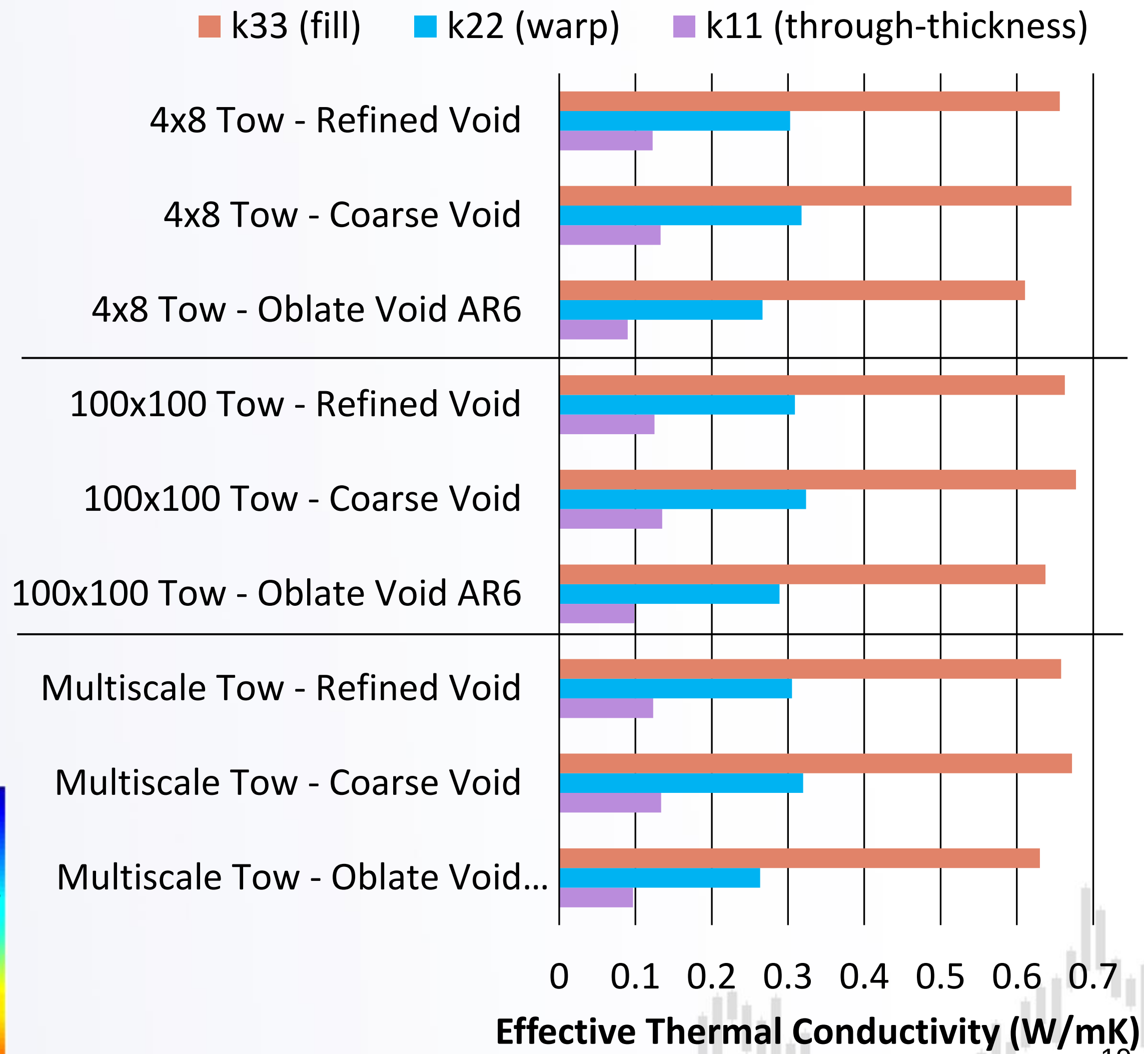
Heat conduction (Fourier's Law)	$\mathbf{q} = -\boldsymbol{\kappa}\nabla T$	$\mathbf{q} = heat\ flux\ vector$ $\boldsymbol{\kappa} = 2nd\ order\ thermal\ conductivity\ tensor$ $T = temperature$	
Electrical conduction	$\mathbf{J} = -\boldsymbol{\sigma}\nabla\phi$	$\mathbf{J} = electic\ current\ density\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

Multiscale Thermal Conductivity – C/Phenolic TPS Material

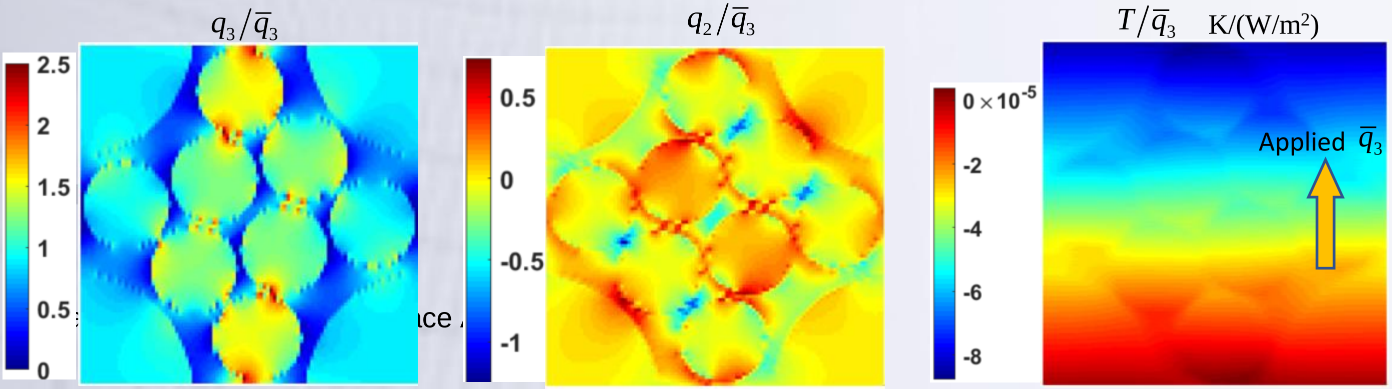
- Three scales (woven composite/tows/voids)



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

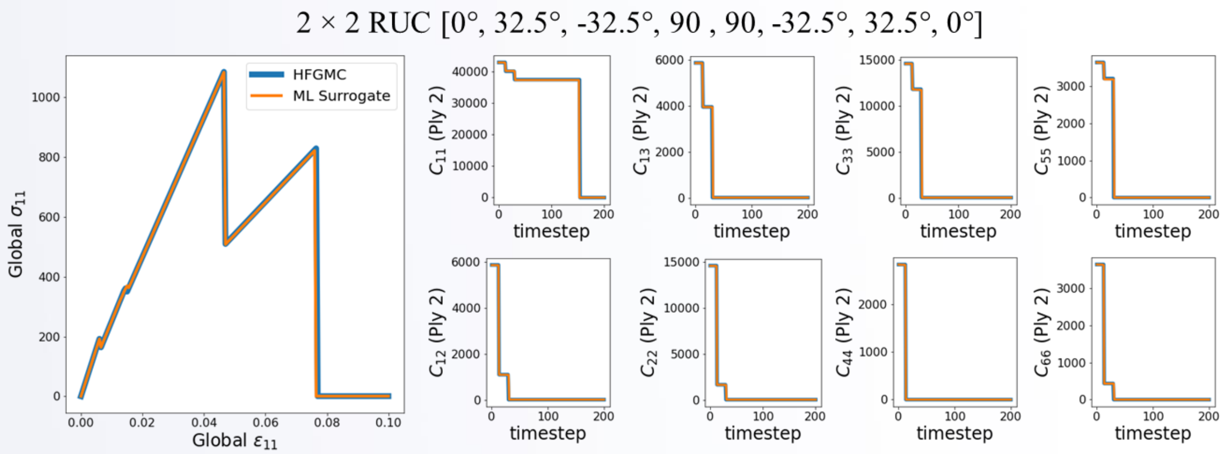


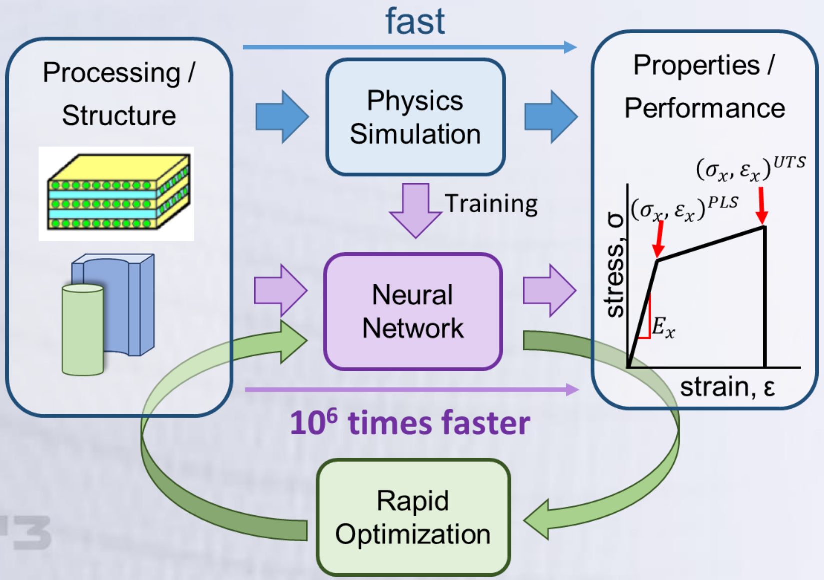
Sample local flux and temperature fields in tow (normalized)

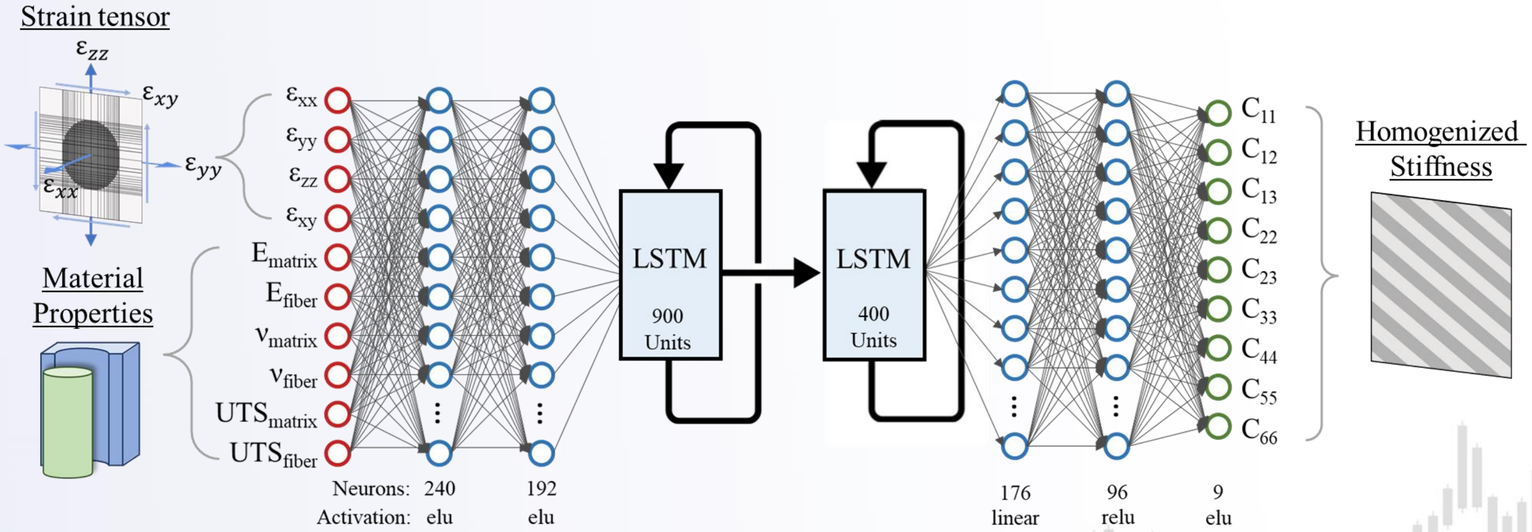


Coupling NASMAT with Machine Learning Tools

- 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







POC: J. Stuckner

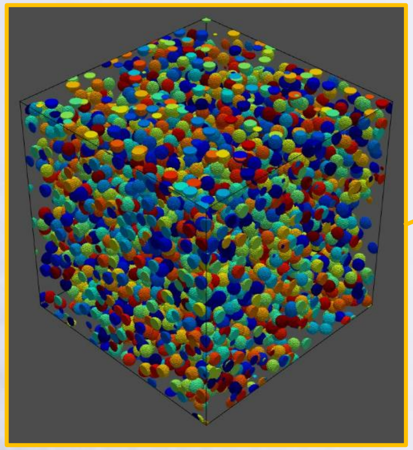
Framework for Multiscale Process Modeling

Hierarchical process modeling approach (FEA)

- Analysis outputs at lower length scales become inputs to analysis at higher length scales
- Allows characterization of in-situ residual stresses
  - Proposed key driver of initial damage

Abaqus Fortran Python

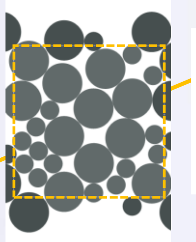
Porous Microstructure Analysis (PuMA)



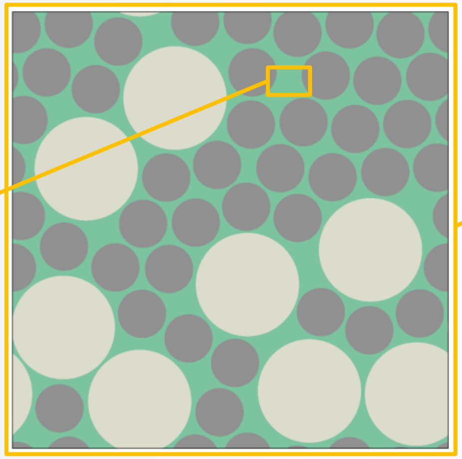
Highly porous phenolic matrix

Microscale Level I

Random RVE generator



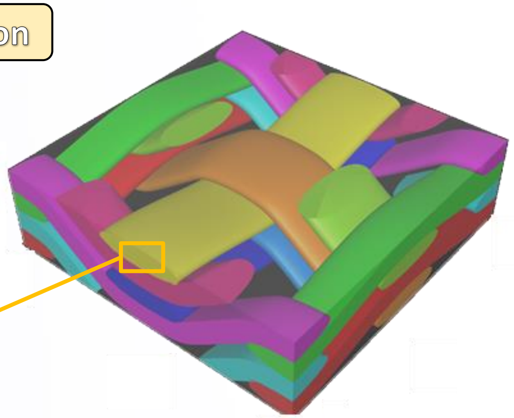
UMASS LOWELL



Blended carbon/phenolic tow microstructure

Microscale Level II

TexGen



3D medium density carbon phenolic (3MDCP) textile

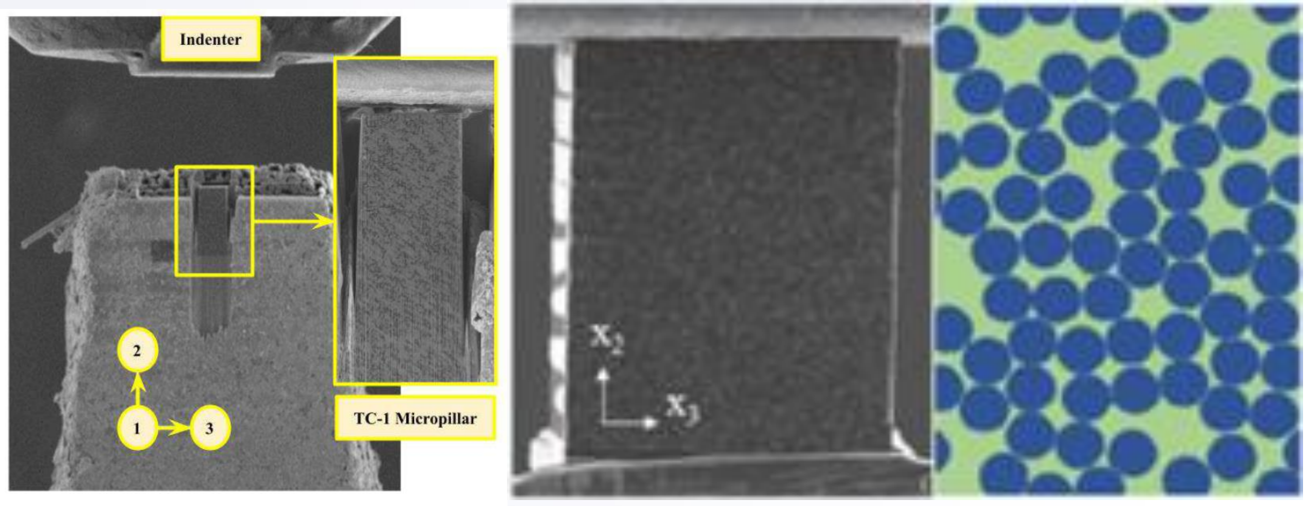
Mesoscale

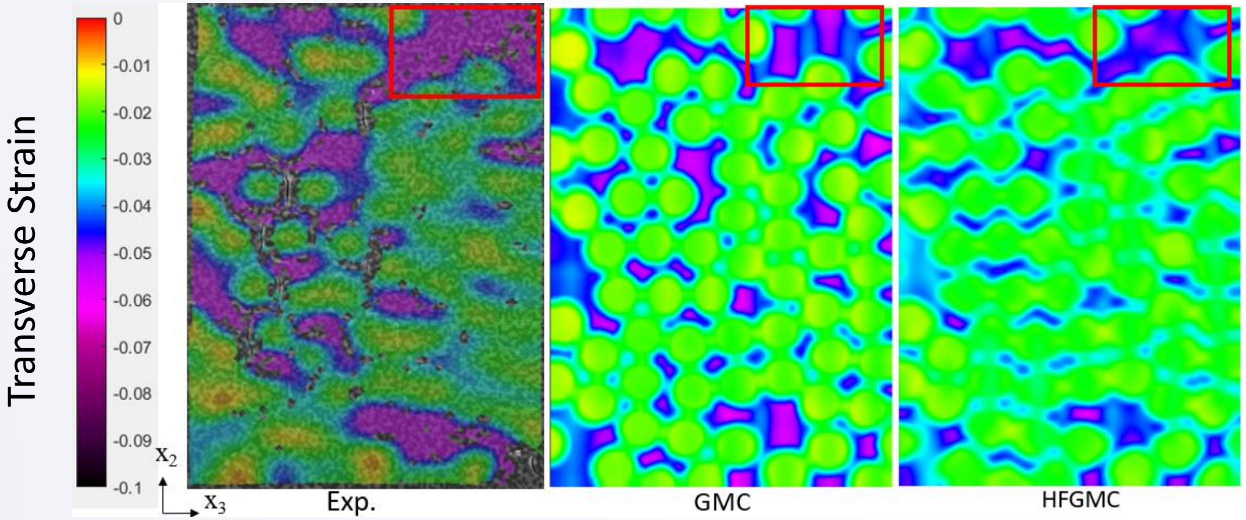
Plans to incorporate into NASMAT

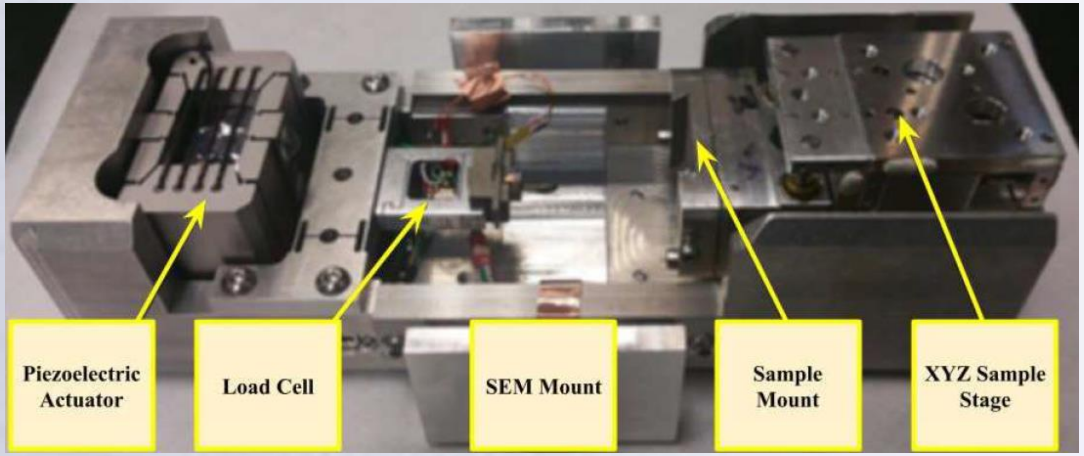
***collaboration with T^3-funded NRA (M. Maiaru – U. Mass. Lowell)**

Micropillar Composite Testing to Validate Microscale Modeling

- Novel compression testing of micropillar composites (AFRL – M. Flores)
- Test useful for validating microscale modeling approaches
- Modeling performed with NASMAT/Abaqus
- Stiffness prediction close to experiments
- Exploring methods for comparing local DIC/ model fields
- Planning to model compressive failure





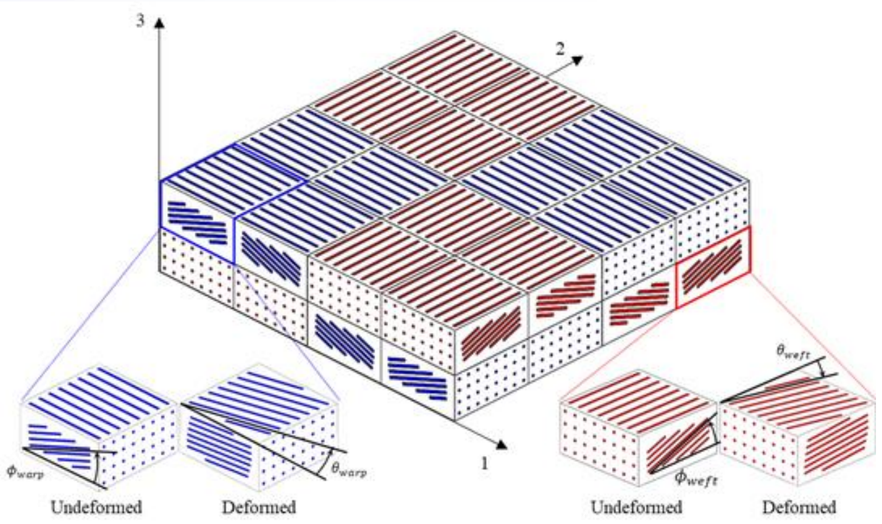


	Experiment	GMC	HFGMC	FEA
Transverse Stiffness (GPA)	10.79	9.37	10.05	10.06

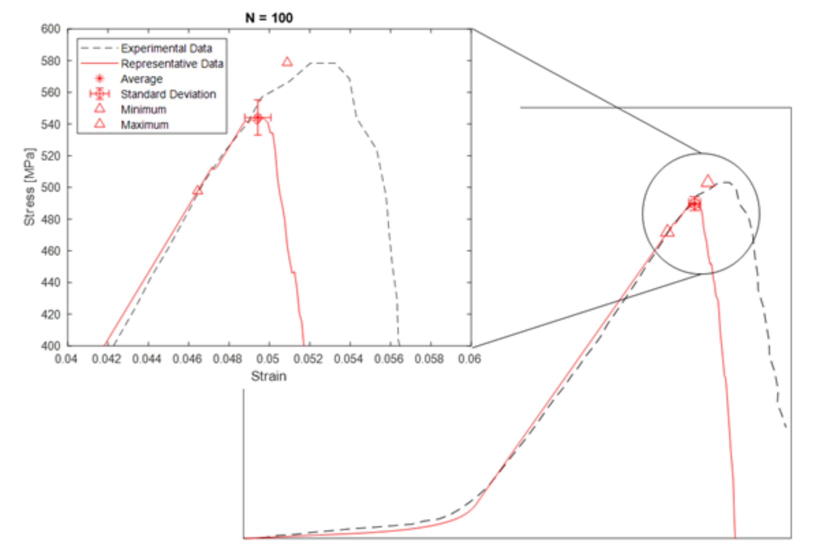
***Partnership with AFRL**

Dry Fabrics for Entry Parachute Applications

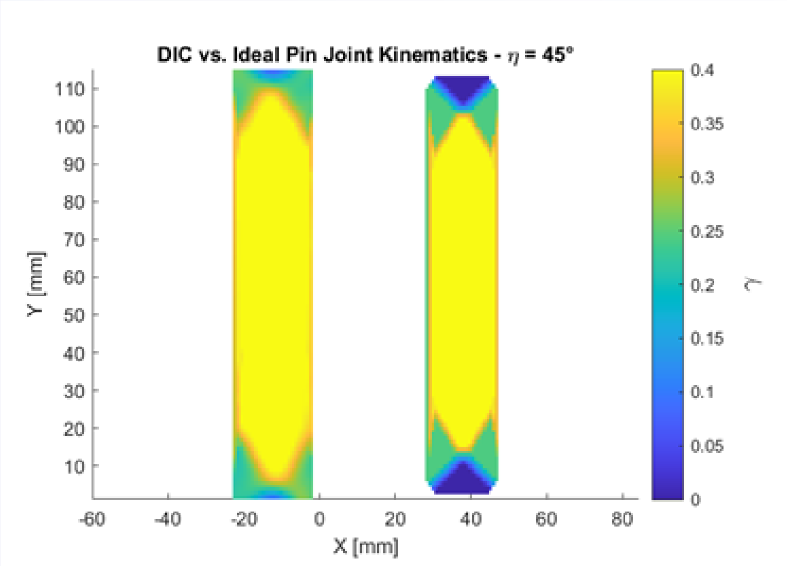
- Simulate dry fabric behavior by allowing the tow orientation in each subcell to change with applied loading
  - ϕ – Crimp or tow undulation angle
  - ϑ – Relative tow rotation angle
- Failure predicted for both fiber breakage and yarn pullout
  - Fiber breakage accounts for statistical variation observed experimentally
  - Yarn pullout failure criteria developed for macroscale (coupon)
    - Able to capture full field strain development



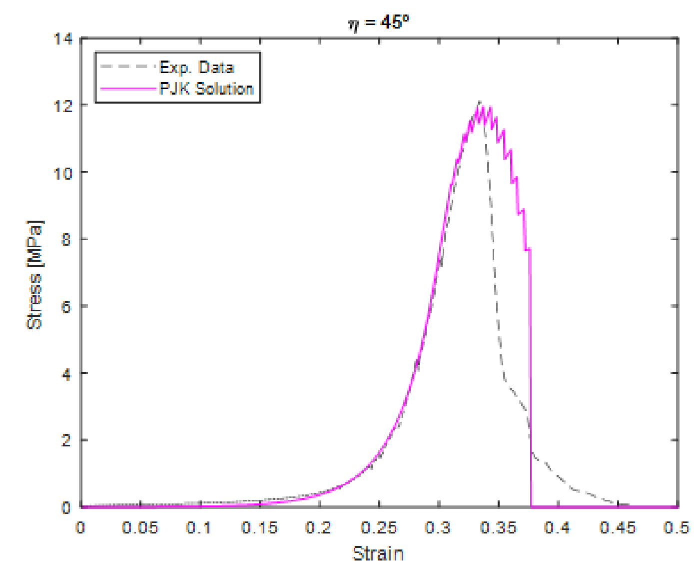
Fabric RUC with defining angles



Warp-Aligned Uniaxial Tension (100 simulations)



Bias Extension Shear Strain Development

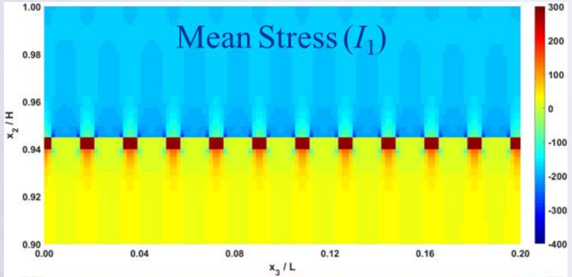


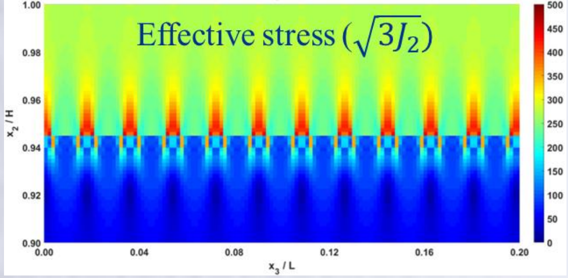
Bias Extension Simulation

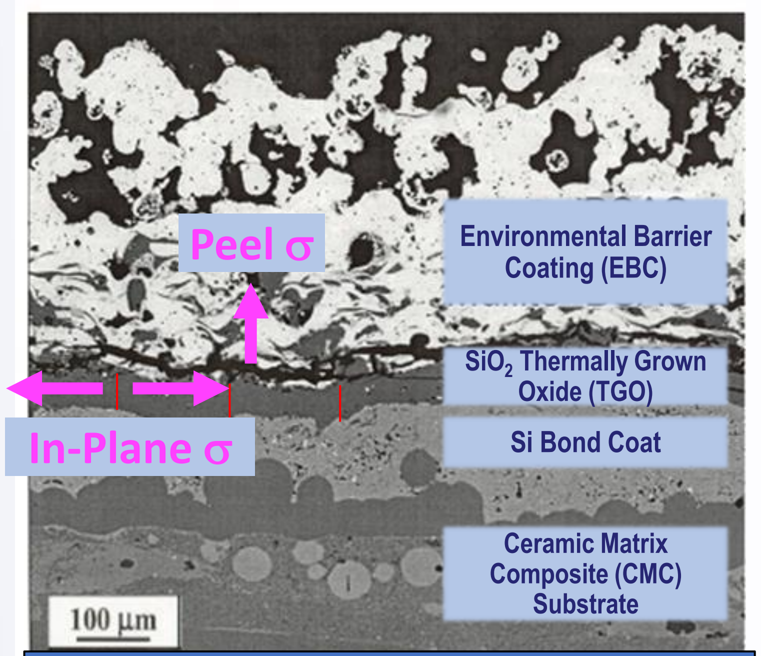
POC: B. Hearley

Modeling of Ceramic Matrix Composite (CMC) / Environmental Barrier Coating (EBC) Systems

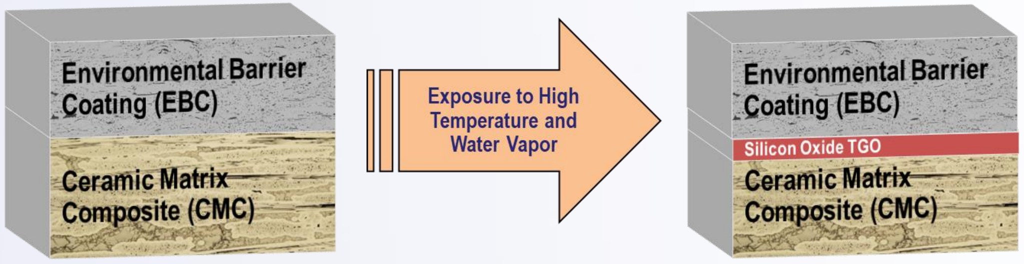
- Coupled thermal-mechanical analysis performed using legacy tools and FEA
- Porting legacy capability over to NASMAT to analyze
- Focused on understanding driving forces
- Modeling captures temperature dependence, creep, volumetric changes
- Generating more realistic models by incorporating measured data (roughness, thickness, crack spacing)
- Developing lifing methodology for CMC/EBC systems

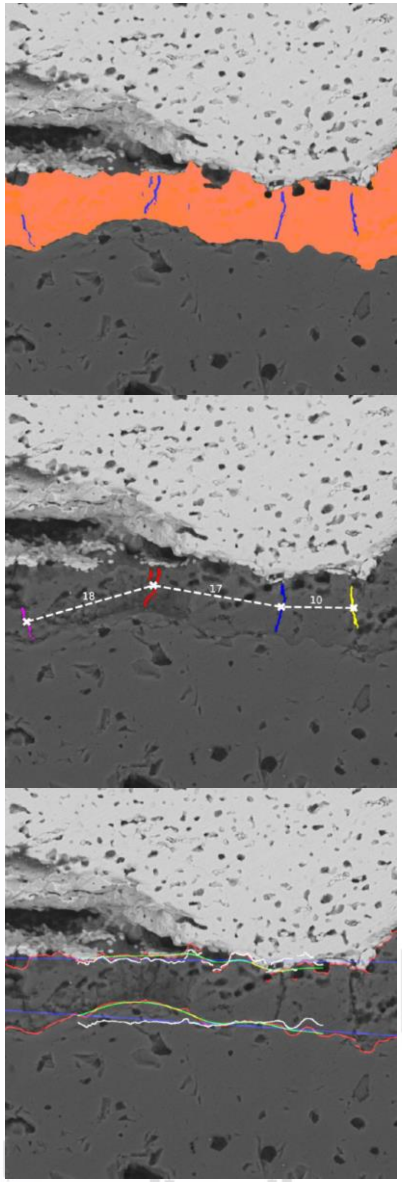






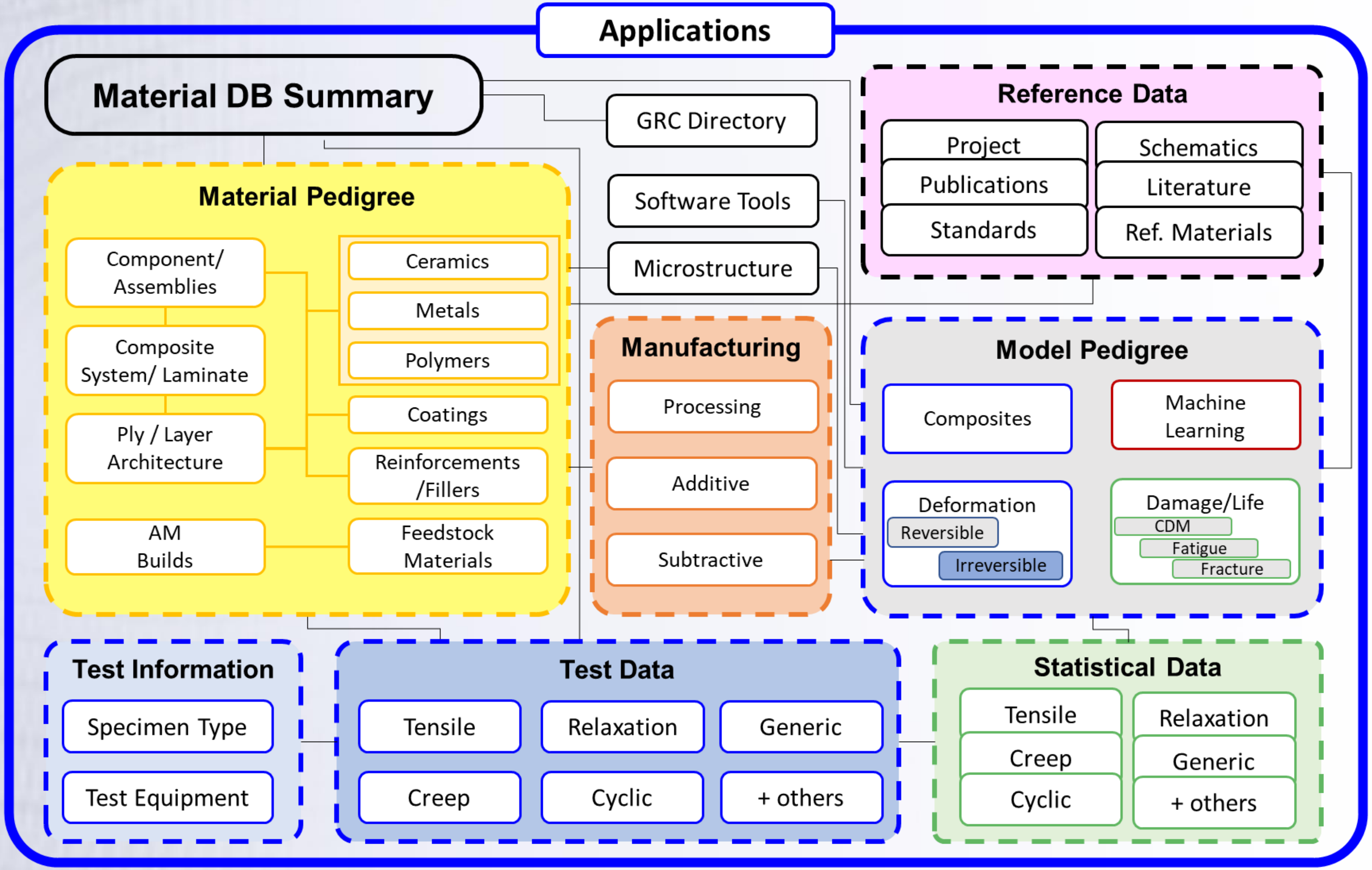
Environmental Barrier Coating system after 15,144h test





POCs: S. Mital/J. Stuckner

NASA GRC Database Schema for ICME



Applications

Material DB Summary

- GRC Directory
- Software Tools
- Microstructure

Reference Data

- Project
- Publications
- Standards
- Schematics
- Literature
- Ref. Materials

Material Pedigree

- Component/ Assemblies
- Composite System/ Laminate
- Ply / Layer Architecture
- AM Builds
- Ceramics
- Metals
- Polymers
- Coatings
- Reinforcements /Fillers
- Feedstock Materials

Manufacturing

- Processing
- Additive
- Subtractive

Model Pedigree

- Composites
- Machine Learning
- Deformation
  - Reversible
  - Irreversible
- Damage/Life
  - CDM
  - Fatigue
  - Fracture

Test Information

- Specimen Type
- Test Equipment

Test Data

- Tensile
- Relaxation
- Generic
- Creep
- Cyclic
- + others

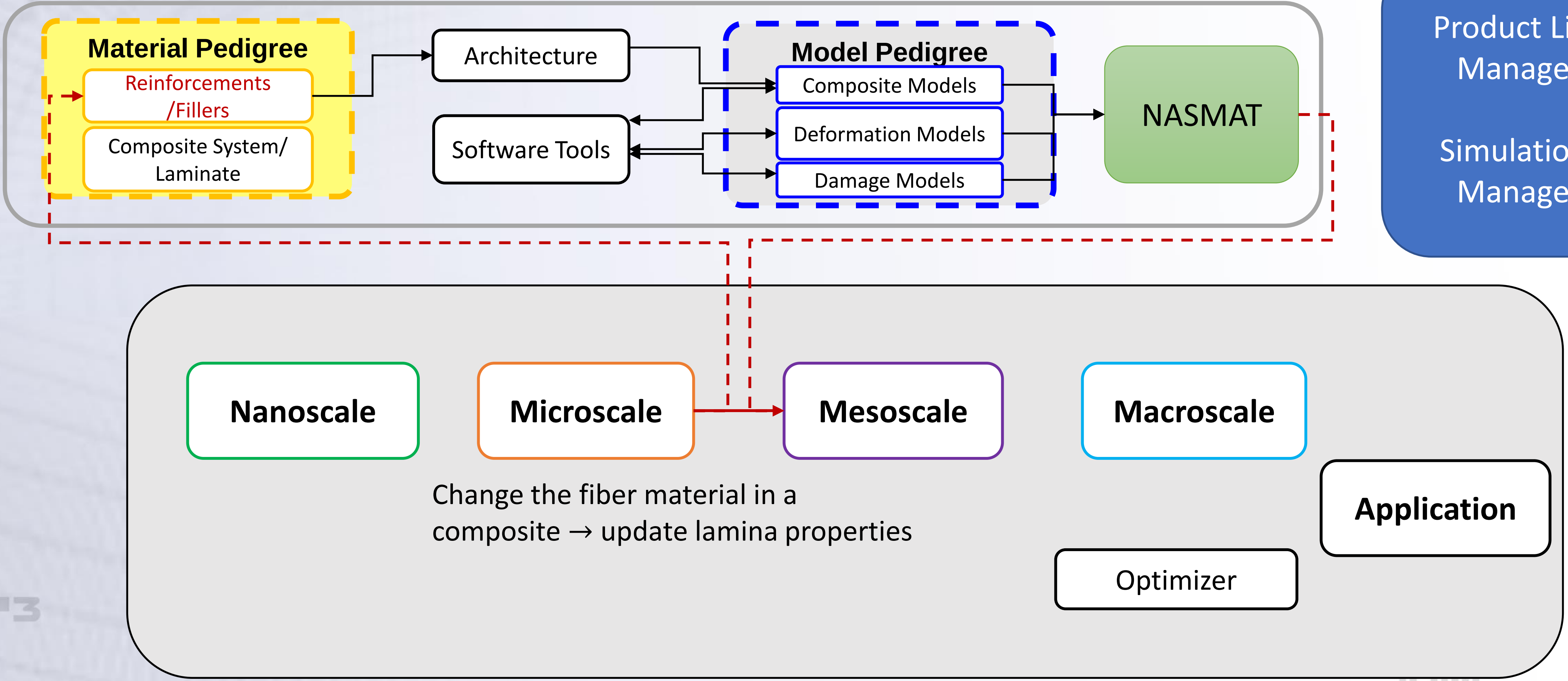
Statistical Data

- Tensile
- Creep
- Cyclic
- Relaxation
- Generic
- + others

POC: B. Hearley

Database/Simulation Management in ICME

Automation of read/write and tool execution in background



Material Pedigree

Reinforcements /Fillers

Composite System/ Laminate

Architecture

Software Tools

Model Pedigree

Composite Models

Deformation Models

Damage Models

NASMAT

Nanoscale

Microscale

Mesoscale

Macroscale

Application

Optimizer

Change the fiber material in a composite → update lamina properties

Product Lifecycle Management

Simulation Data Management

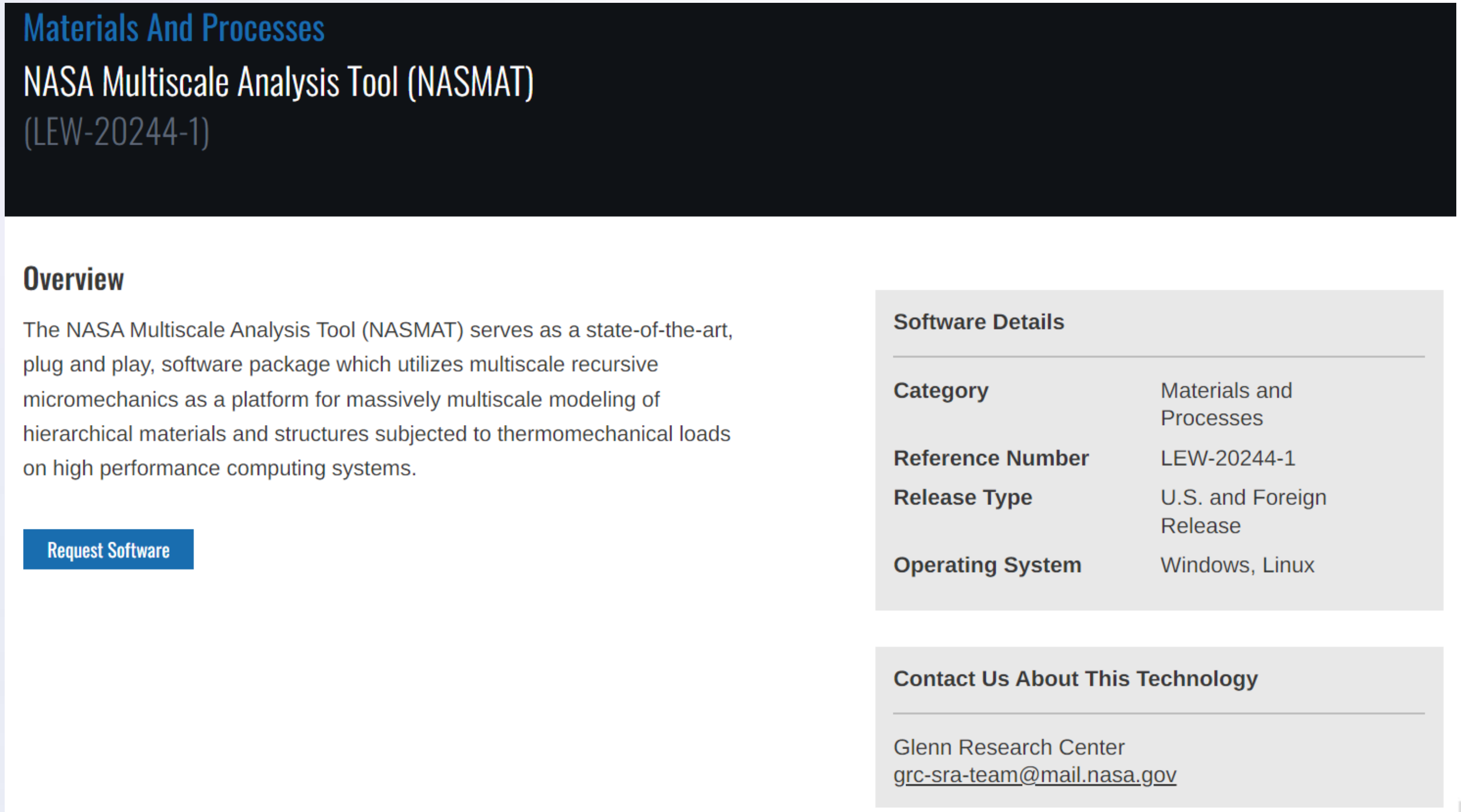
POC: B. Hearley

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

How to Get

- NASA Software Catalog
- https://software.nasa.gov/software/LEW-20244-1
- 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.

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

Acknowledgements

- NASA GRC co-workers (P. Gustafson, B. Hearley, I. Kaleel, S. Mital, P. Murthy, P. Naghipour, J. Stuckner)
- NASMAT primarily developed with support from the NASA ARMD Transformational Tools & Technologies Project
- Support also obtained from multiple other sources:
  - 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
  - Many university partners (especially interns and fellows)

Thanks for Your Attention

Questions

Contact: Trenton.M.Ricks@nasa.gov

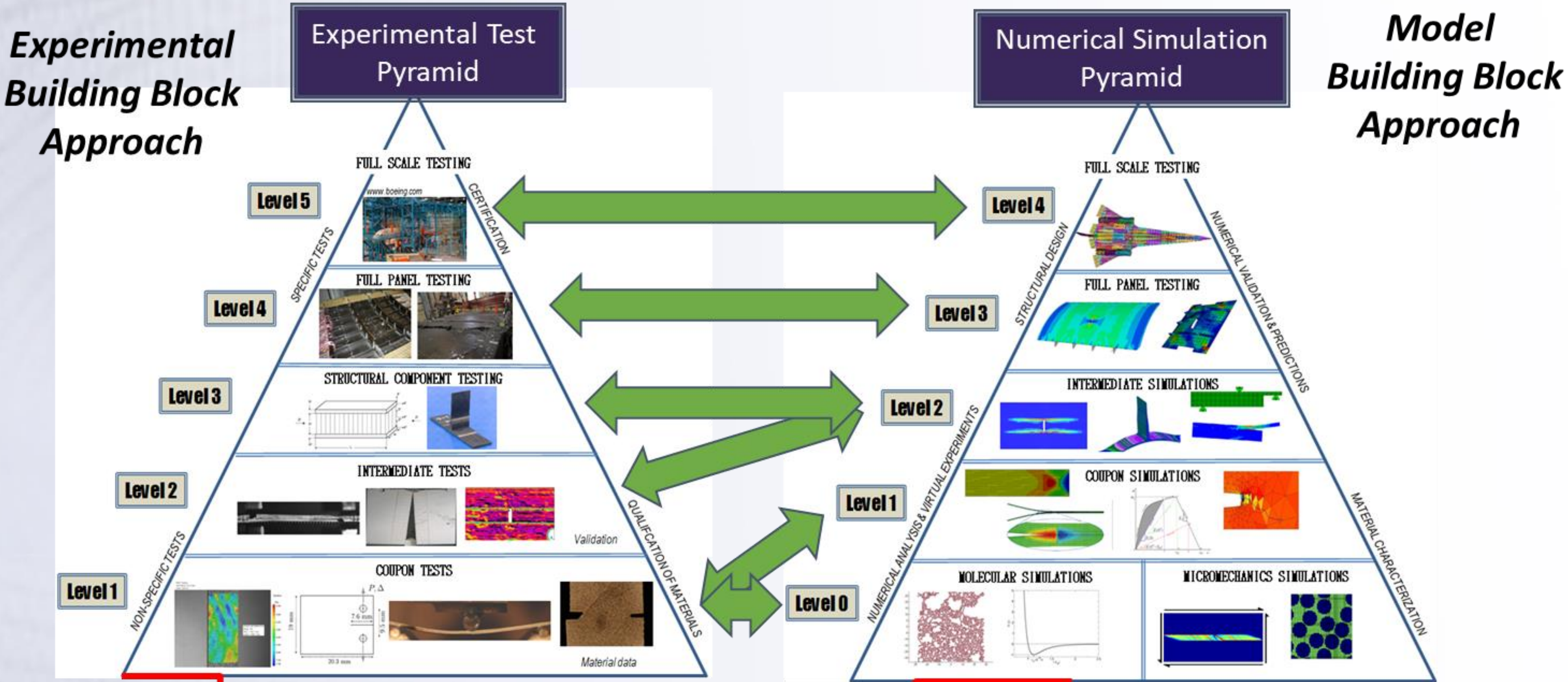
BACKUP

2040 Ecosystem Revolutionizes Design Paradigm

The cyber-physical-social ecosystem that marries "the design of materials" (material scientist viewpoint) with "the design with materials" (structural analyst viewpoint) approaches into one concurrent transformational digital paradigm.

Today' s Design Paradigm	2040 Design Paradigm
Design Of Materials And Systems Is ***Disconnected***	Design Of Materials And Systems Is ***Integrated***
Stages Of The Product Development Lifecycle Are ***Segmented***	Stages Of The Product Development Lifecycle Are ***Seamlessly Joined***
Tools, Ontologies, And Methodologies Are ***Domain-specific***	Tools, Ontologies, And Methodologies Are ***Usable Across The Community***
Materials Properties Are Based On ***Empiricism***	Materials Properties Are ***Virtually Determined***
Product Certification Relies Heavily On ***Physical Testing***.	Product Certification Relies Heavily On ***Simulation***

Virtual Testing Can Enable Significant Cost Savings in Certification Process

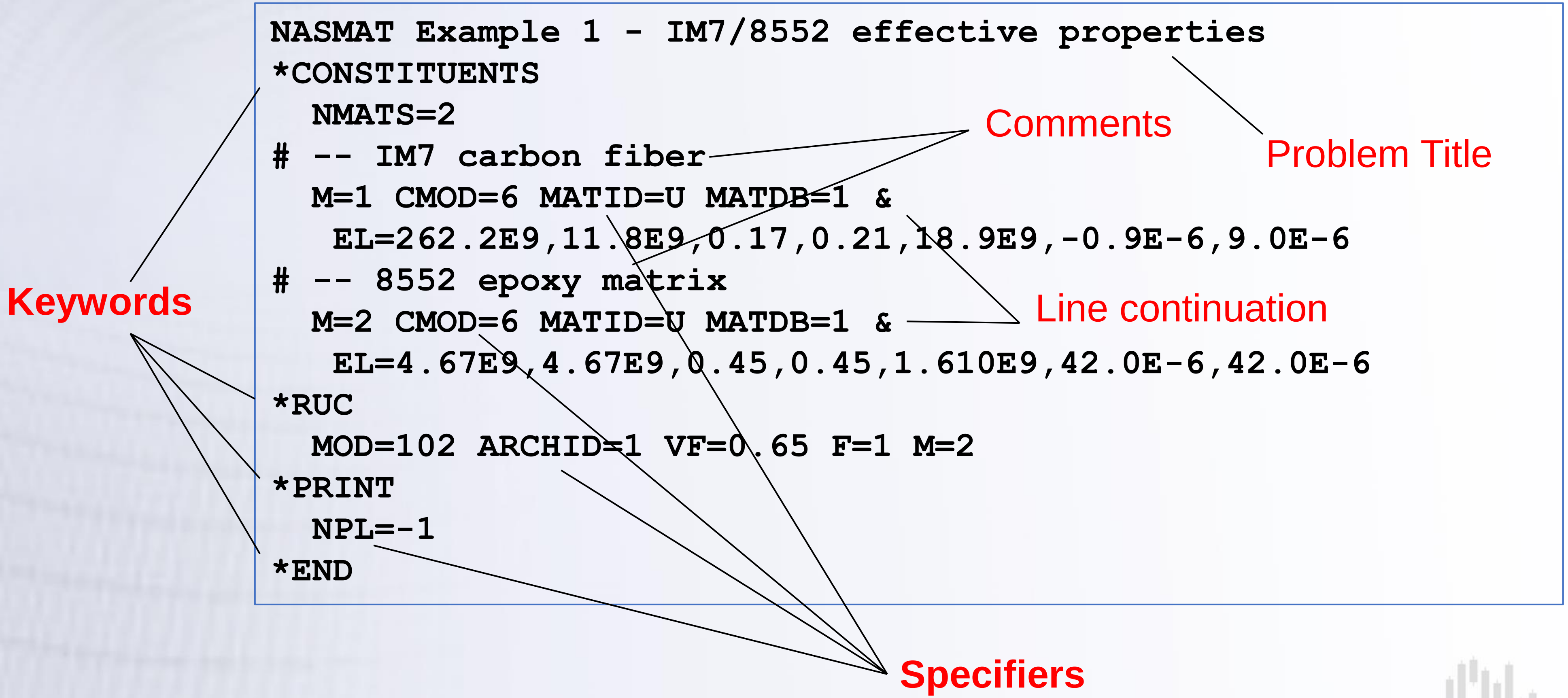


A robust **validated computational** platform is **essential** for *sustainable, cost-effective technology development program*

- ➢ *reduced testing and time to certify!*

NASMAT Input File

- Input file is an ASCII text file – use any text editor
- **Keywords** and **Specifiers** described in user manual (distributed with code)
- Pre/Post-processor under development to aid users

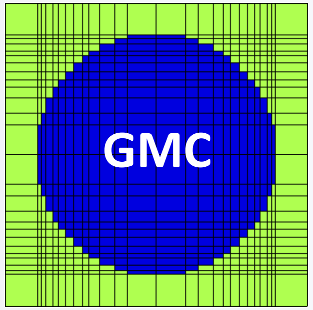


```
NASMAT Example 1 - IM7/8552 effective properties
*CONSTITUENTS
  NMATS=2
# -- IM7 carbon fiber
  M=1 CMOD=6 MATID=U MATDB=1 &
   EL=262.2E9,11.8E9,0.17,0.21,18.9E9,-0.9E-6,9.0E-6
# -- 8552 epoxy matrix
  M=2 CMOD=6 MATID=U MATDB=1 &
   EL=4.67E9,4.67E9,0.45,0.45,1.610E9,42.0E-6,42.0E-6
*RUC
  MOD=102 ARCHID=1 VF=0.65 F=1 M=2
*PRINT
  NPL=-1
*END
```

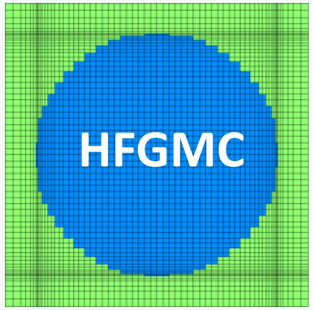
Fidelity vs. Efficiency in Composite Micromechanics

Transverse Loading
50% Glass/Epoxy

~11,000 GPS Elements



676 Subcells

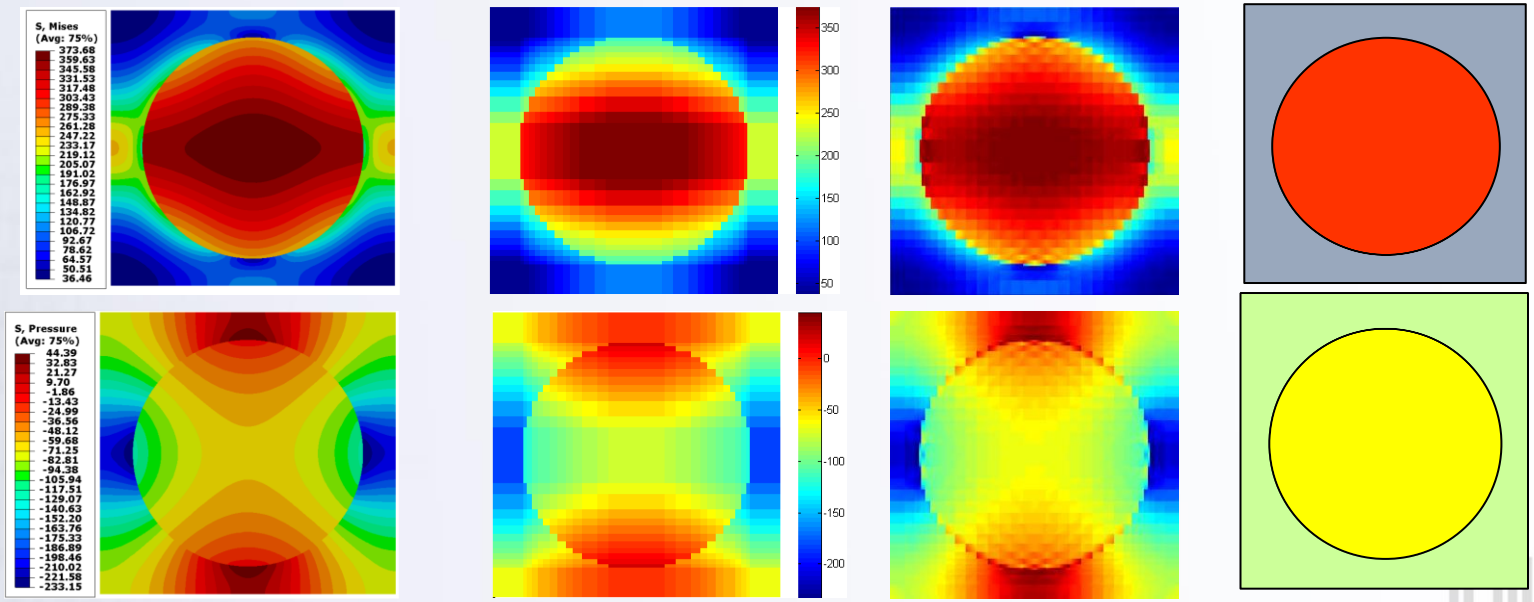


1024 Subcells

Simpler Methods
Mean Field

von Mises stress (J_2)

Pressure (= $-\sigma_{mean}$) (MPa)



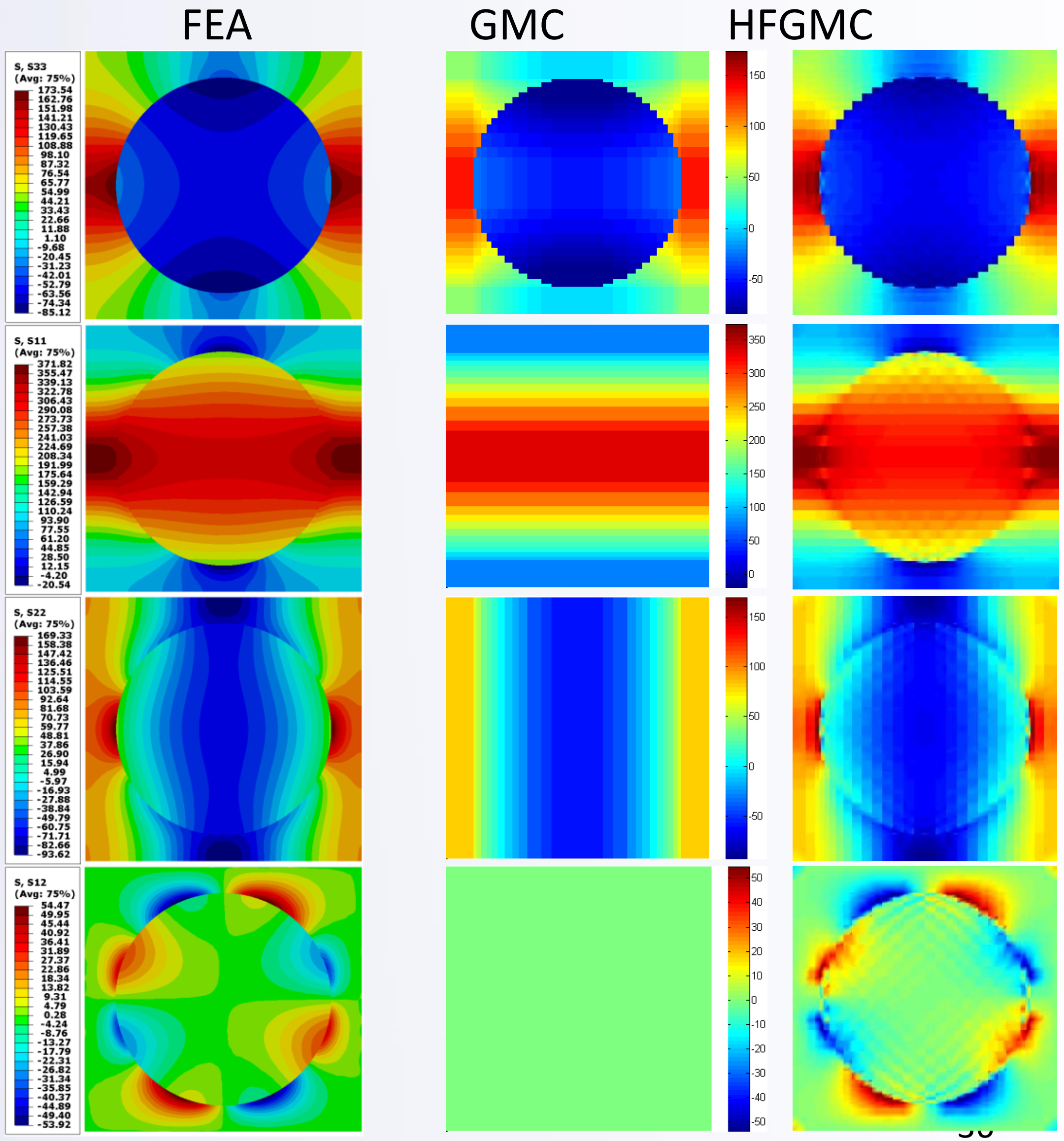
Individual Stress Components

Axial stress (MPa)

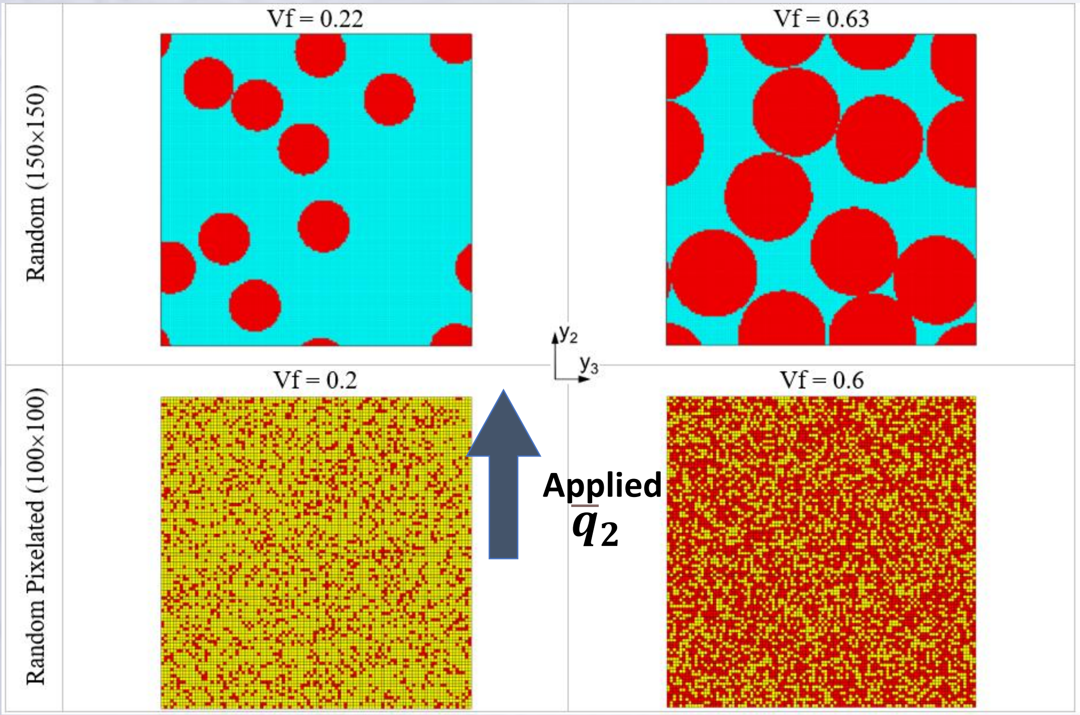
Transverse stress in loading direction (MPa)

Transverse stress (MPa) normal to loading direction

Transverse shear stress (MPa)

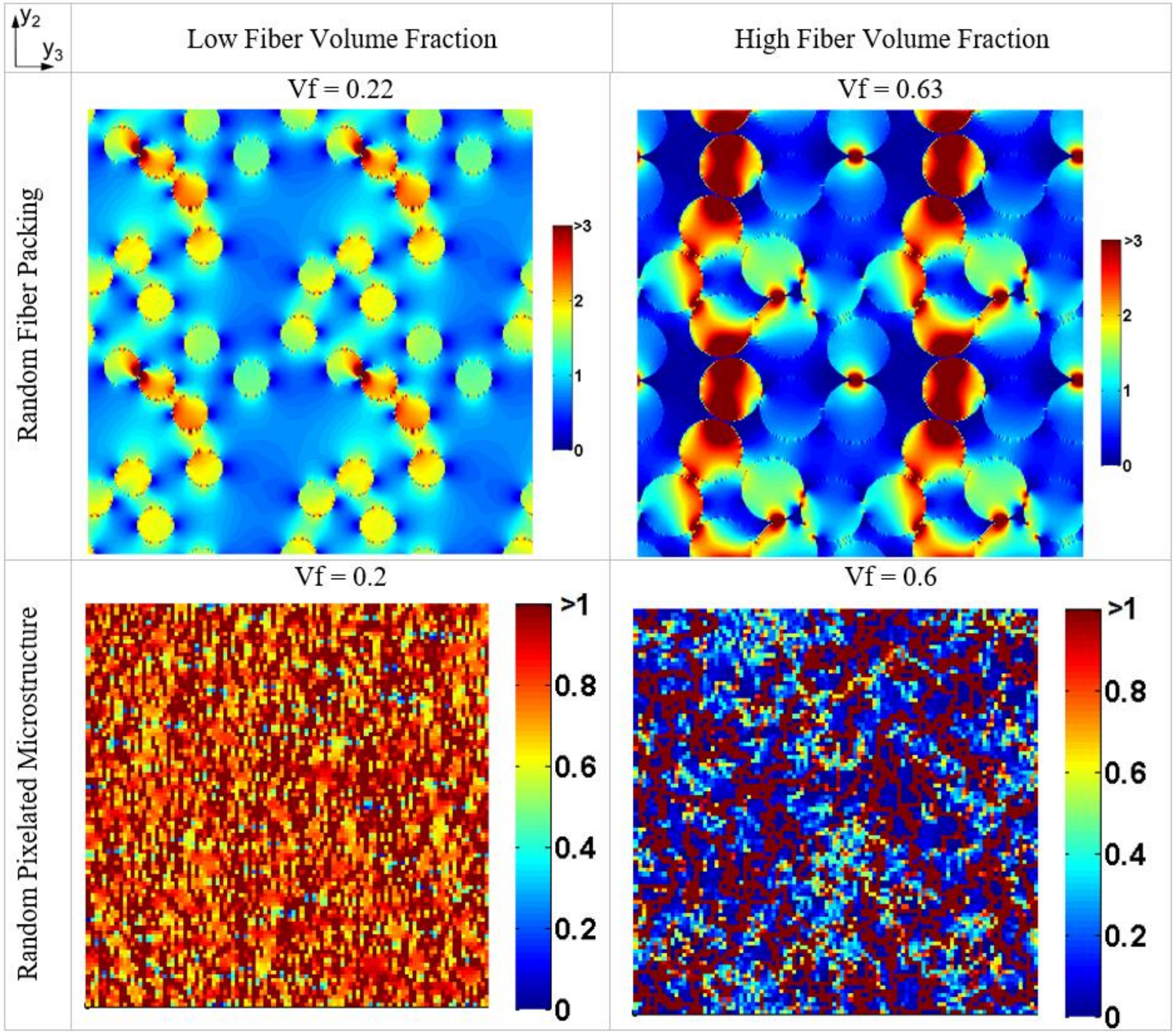


Application to Random Microstructures



Applied $\bar{q}_2$

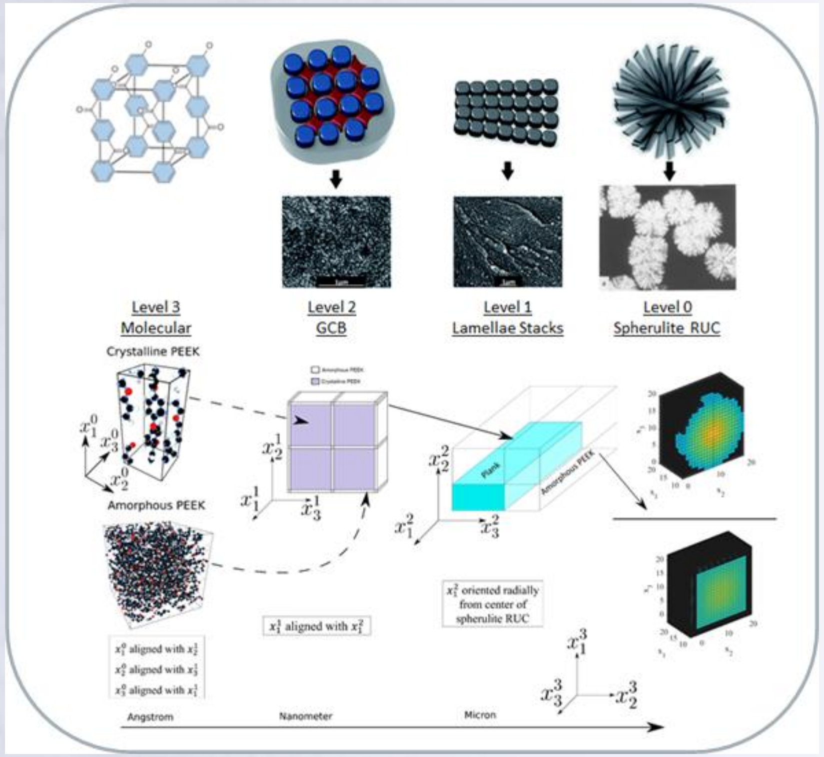
Local Heat Flux Fields

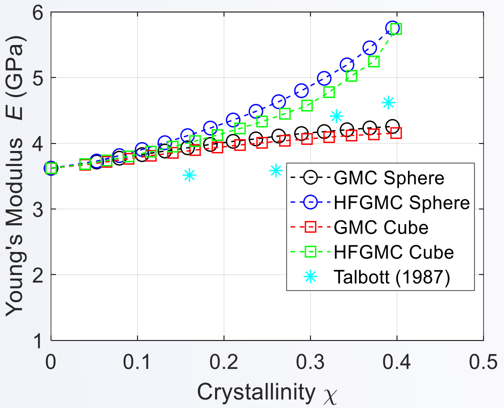


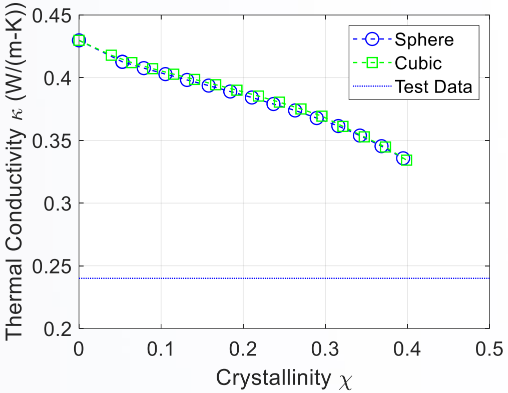
Above “percolation threshold”

Multiscale Process Modeling of Thermoplastics

Bulk Thermoplastic

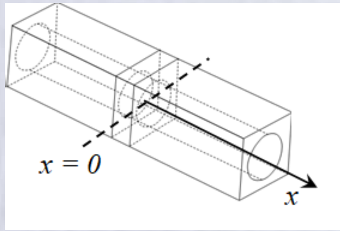


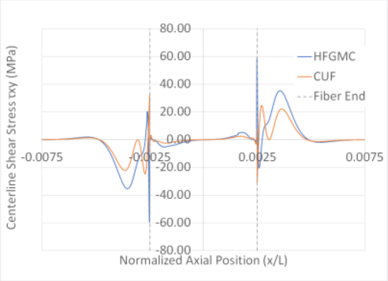




- Semi-crystalline thermoplastic involves 4 separate scales
  - Nano -> micro
- Can ***predict*** stiffness, CTE, thermal conductivity as ***function of crystallinity***
  - ***Purely computational*** prediction
    - MD at lowest scale, integrated micromechanics at other scales

Discrete Long Fiber Composite



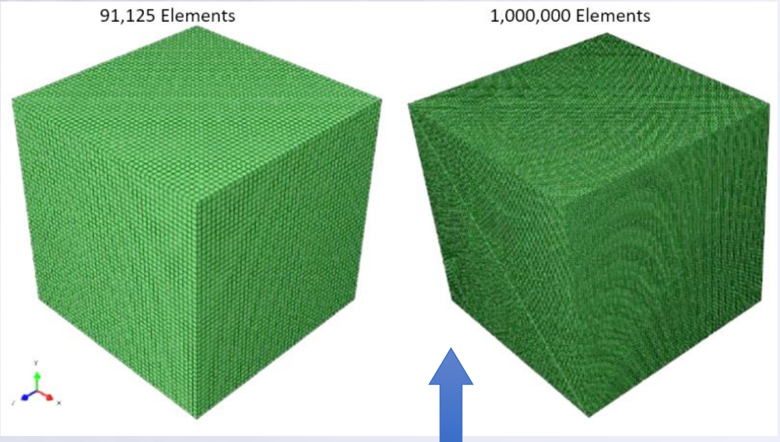


- Repeating unit cell (RUC) model of discrete long fiber composites
- ***Can capture*** complex local stress state due to ***shear lag effect***
  - Critical for nonlinear predictions
- Next phase will link thermoplastic and discrete fiber models together

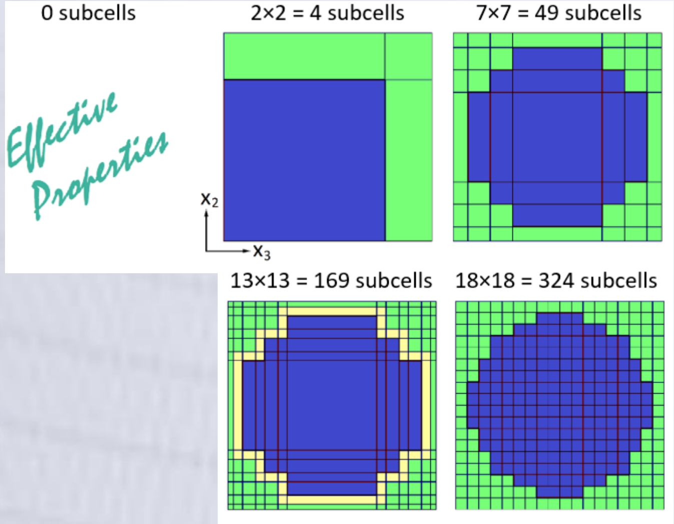
Multiscale HPC Performance, NASMAT with Abaqus

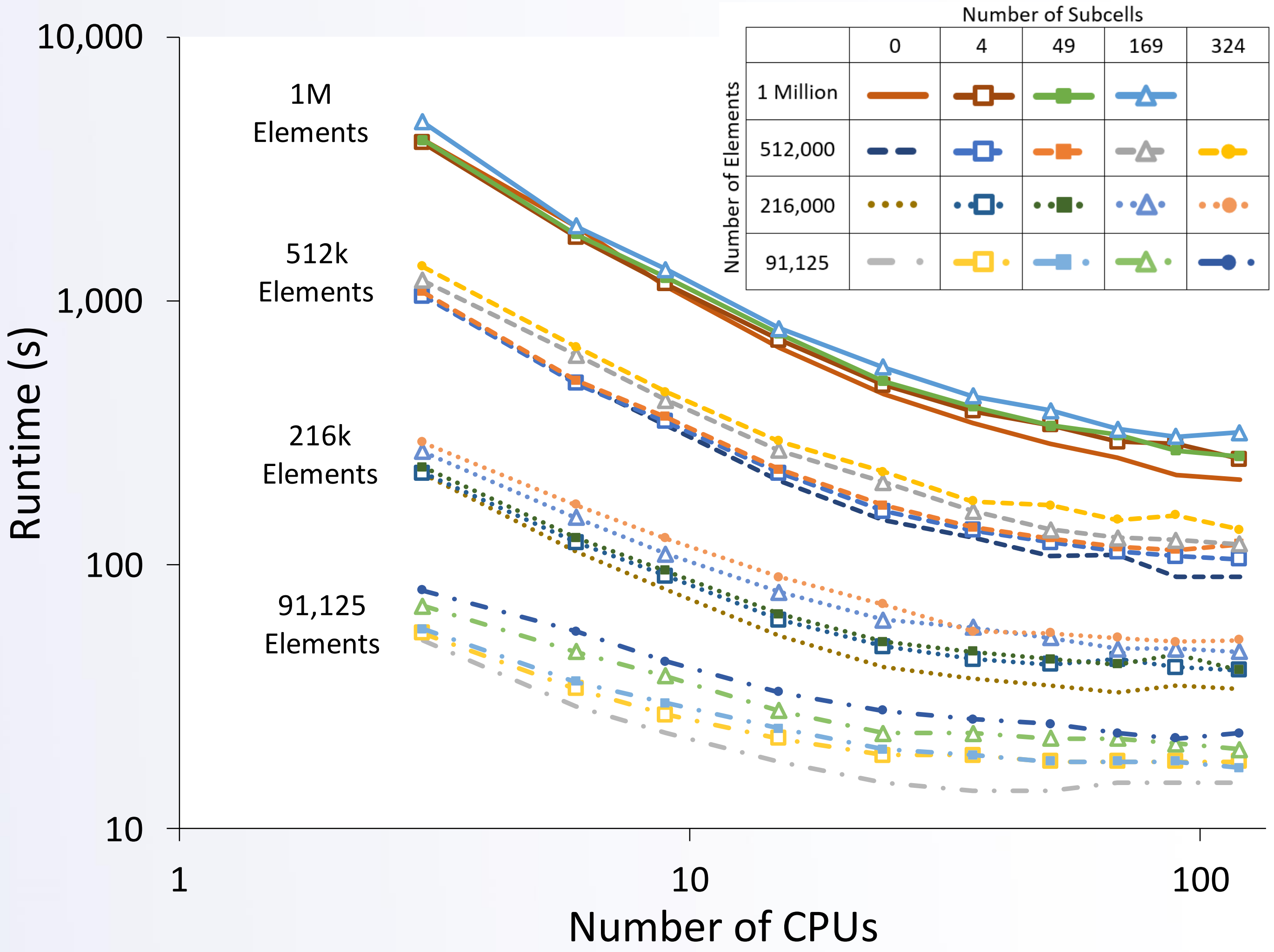
- Profiling of 4 mesh densities, each element int. pt. calling micro model (5 microscale refinements)

Structural Abaqus Model



Micromechanics Model





- Strong performance dependence on FEM density
- Weak dependence on micromechanics model refinement