Transformational Tools and Technologies (T³) 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

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

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

Nine Identified Key Element Discipline Areas

- 1. Models and Methodologies
- 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

NASA CR 2018-219771
https://ntrs.nasa.gov
**Study Identified 9 Key Element Domains**

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

<table>
<thead>
<tr>
<th>Key Element</th>
<th>Critical Gap</th>
<th>Priority Action</th>
<th>Time Frame</th>
<th>End State Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Underdevelopment of physics-based models that link length and time scales for relevant material systems</td>
<td>Multiscale V&amp;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) Informatics framework for 3D4O model dev. (2.11) Models for key uncertainty sources (1.23)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>2</td>
<td>Inability to conduct real-time characterization and measurement of structure and response at appropriate length and time scales</td>
<td>Real-time measurement methods (2.14) Real-time visualization for experiment modeling (6.15) Lifecycle data: automated ingestion and storage (6.23) Propagation path characterization, test data models (8.19)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>3</td>
<td>Lack of reliable optimization methods that bridge across scale</td>
<td>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)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>4</td>
<td>Existing models and software codes are not designed to compute input sensitivities and propagate uncertainties to enable UQ</td>
<td>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)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>5</td>
<td>Lack of guidelines and practitioner aids for multiscale/multiphysics (e.g., ICME) V&amp;V</td>
<td>Best practices: data collection (5.7) Multiscale V&amp;V standards and definitions (5.1) Student resources: industry V&amp;V data (8.8) V&amp;V training (5.2) Holistic test methods (2.16)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>6</td>
<td>No widely accepted community standards or schema for materials information storage and communication methods</td>
<td>Workflow data modeling: automation, recognition, tagging (7.1) Training: informatics framework interpretation &amp; integration (6.21)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>7</td>
<td>Lack of open, community/industry standards defining inputs/outputs, needed functionality, data quality, model maturity levels, etc. for smooth operation in the envisioned ecosystem</td>
<td>Access-controlled example workflows (7.5) Best practices: multi-domain workflows (7.16) Data quality and model maturity standards (7.21) Access-controlled adaptive file formats (6.2)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>8</td>
<td>Education/Training does not bridge the gap between “essential” or “fundamental” knowledge and industrially relevant skills</td>
<td>Education/Training: decision UQ approaches (4.7) New computational certifications programs/tracks (8.14) Workforce transition training for students (8.5) V&amp;V training (5.2) Student access to equipment/facilities (8.6)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
<tr>
<td>9</td>
<td>Lack of support, or adequate business models, for code development and maintenance, particularly for software used in engineering applications</td>
<td>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)</td>
<td>2016 2018 2020</td>
<td>+ + + + +</td>
</tr>
</tbody>
</table>
Relevance and Background

**Integrated Computational Materials Engineering (ICME) Is The Future**

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.

- **Processing**
  - Internal Structure
  - Properties
  - Performance

**Design “The” Material**
**Design “With” Material**

- **Internal Structure**
  - Meso scale
  - Micro scale

- **Atomistic**
  - Quantum

- **Micromechanics / Statistical Mechanics**
  - Molecular Dynamics

- **Continuum Mechanics**
  - Design for Manufacturability, Certifiability and Lowest Cost, with Performance Constraints

- **Handshake via Constitutive Model**

**Relevance and Background**

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  - Quantum

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- **Handshake via Constitutive Model**

- **Design for Manufacturability, Certifiability and Lowest Cost, with Performance Constraints**
Micromechanics: The Link Between Structures and Materials

Continuum Deformation and Damage Models

Micro-level Field Equations (subcell)

\[
\epsilon^{(app)} = A^{(app)} \bar{e} + D^{(app)} (\epsilon_i^T + \epsilon_j^T)
\]

\[
\sigma^{(app)} = C^{(app)} \left[ A^{(app)} \bar{e} + D^{(app)} (\epsilon_i^T + \epsilon_j^T) - \left( \epsilon^{(app)} + \epsilon^{(app)}^T \right) \right]
\]

Composite Micromechanics Repeating Unit Cell

Micromechanics Provides the Link Between Structures and Materials

Structural Model

Evolution Anisotropic Thermoelastic Inelastic and Damage Constitutive Model

Macro-level Constitutive Equations

\[
\bar{\sigma} = B' (\bar{\epsilon} - \bar{\epsilon}' - \bar{\epsilon}^T)
\]

\[
B' = \frac{1}{d\tilde{h}} \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_y} \sum_{\gamma=1}^{N_z} \int_d \sum_{\mu=1}^{N_d} \sum_{\nu=1}^{N_n} d\tilde{h} \tilde{h}' C^{(app)} A^{(app)}
\]

\[
\bar{\epsilon}' = -\left[ B'^{-1} \right] \frac{1}{d\tilde{h}} \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_y} \sum_{\gamma=1}^{N_z} \int_d \sum_{\mu=1}^{N_d} \sum_{\nu=1}^{N_n} d\tilde{h} \tilde{h}' C^{(app)} D^{(app)} \epsilon_i^T - \epsilon_j^T
\]

\[
\bar{\epsilon}'' = -\left[ B'^{-1} \right] \frac{1}{d\tilde{h}} \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_y} \sum_{\gamma=1}^{N_z} \int_d \sum_{\mu=1}^{N_d} \sum_{\nu=1}^{N_n} d\tilde{h} \tilde{h}' C^{(app)} D^{(app)} \epsilon_i^T - \epsilon_j^T
\]

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 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

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

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

Idealization of Tow Paths from X-Ray CT

Through-thickness Binder Tow

WARP

WEFT

BINDER
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

Fiber failure initiation

Interface failure

Fiber failure progression

Matrix burst!

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

Additive Manufacturing; collab. with Gustafson (Western Michigan University)

Multiscale Modeling: Supported through NASA SBIR – ADDITIVE MANUFACTURING INNOVATIONS, LLC; PI: Ajit Achuthan
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:
  \[
  \psi^{(a\beta\gamma)} = \bar{X}_1 x_1 + \theta^{(a\beta\gamma)}_{(000)} + \bar{Y}_{(a)} \theta^{(a\beta\gamma)}_{(100)} + \bar{Y}_{(\beta)} \theta^{(a\beta\gamma)}_{(010)} + \bar{Y}_{(\gamma)} \theta^{(a\beta\gamma)}_{(001)} \\
  + \frac{1}{2} \left( 3\bar{Y}_{(a)}^2 - \frac{d_{a}^2}{4} \right) \theta^{(a\beta\gamma)}_{(200)} + \frac{1}{2} \left( 3\bar{Y}_{(\beta)}^2 - \frac{h_{\beta}^2}{4} \right) \theta^{(a\beta\gamma)}_{(020)} + \frac{1}{2} \left( 3\bar{Y}_{(\gamma)}^2 - \frac{l_{\gamma}^2}{4} \right) \theta^{(a\beta\gamma)}_{(002)}
  \]
- System of \(3N_\alpha N_\beta N_\gamma\) algebraic equations:
  \[\mathbf{K} \mathbf{\Omega} = \mathbf{f}\]
- Concentration equation:
  \[\mathbf{X}^{(a\beta\gamma)} = \mathbf{A}^{(a\beta\gamma)} \mathbf{\bar{X}}\]
- Global (effective) constitutive equation:
  \[\mathbf{\bar{Y}} = \mathbf{Z}^* \mathbf{\bar{X}}\]
- Where, effective property tensor is:
  \[\mathbf{Z}^* = \frac{1}{DHL} \sum_{a=1}^{N_a} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} d_{a} h_{\beta} l_{\gamma} \mathbf{Z}^{(a\beta\gamma)} \mathbf{A}^{(a\beta\gamma)}\]
### Physics Governed by Vector Constitutive Laws

<table>
<thead>
<tr>
<th>Phenomenon</th>
<th>Equation</th>
<th>Variables</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat conduction (Fourier’s Law)</td>
<td>$\mathbf{q} = -\mathbf{k} \nabla T$</td>
<td>$\mathbf{q}$ = heat flux vector, $\mathbf{k}$ = 2nd order thermal conductivity tensor, $T$ = temperature</td>
<td></td>
</tr>
<tr>
<td>Electrical conduction</td>
<td>$\mathbf{J} = -\mathbf{\sigma} \nabla \phi$</td>
<td>$\mathbf{J}$ = electric current density vector, $\mathbf{\sigma}$ = 2nd order electric conductivity tensor, $\phi$ = electrical potential</td>
<td>$\mathbf{E} = -\nabla \phi$</td>
</tr>
<tr>
<td>Diffusion (Fick’s Law)</td>
<td>$\mathbf{j} = -\mathbf{d} \nabla C$</td>
<td>$\mathbf{j}$ = permeant flux vector, $\mathbf{d}$ = 2nd order diffusivity tensor, $C$ = concentration</td>
<td></td>
</tr>
<tr>
<td>Magnetic permeability</td>
<td>$\mathbf{B} = -\mu \nabla \zeta$</td>
<td>$\mathbf{B}$ = magnetic flux density vector, $\mu$ = 2nd order magnetic permeability tensor, $\zeta$ = magnetic potential</td>
<td>$\mathbf{H} = -\nabla \zeta$</td>
</tr>
<tr>
<td>Electrical permittivity</td>
<td>$\mathbf{D} = -\varepsilon \nabla \phi$</td>
<td>$\mathbf{D}$ = electric displacement vector, $\varepsilon$ = 2nd order electric permittivity tensor, $\phi$ = electric potential</td>
<td>$\mathbf{E} = -\nabla \phi$</td>
</tr>
<tr>
<td>In General</td>
<td>$\mathbf{Y} = -\mathbf{Z} \nabla \psi = \mathbf{Z} \mathbf{X}$</td>
<td>Governing Equation: $\nabla \cdot \mathbf{Y} = 0$</td>
<td></td>
</tr>
</tbody>
</table>
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

- 4x8 Tow - Refined Void
- 4x8 Tow - Coarse Void
- 4x8 Tow - Oblate Void AR6
- 100x100 Tow - Refined Void
- 100x100 Tow - Coarse Void
- 100x100 Tow - Oblate Void AR6
- Multiscale Tow - Refined Void
- Multiscale Tow - Coarse Void
- Multiscale Tow - Oblate Void...
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

Porous Microstructure Analysis (PuMA)

- Highly porous phenolic matrix
  - Microscale Level I

Random RVE generator

Blended carbon/phenolic tow microstructure
  - Microscale Level II

3D medium density carbon phenolic (3MDCP) textile
  - Mesoscale

Plans to incorporate into NASMAT

*collaboration with T³-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

<table>
<thead>
<tr>
<th>Transverse Stiffness (GPA)</th>
<th>Experiment</th>
<th>GMC</th>
<th>HFGMC</th>
<th>FEA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10.79</td>
<td>9.37</td>
<td>10.05</td>
<td>10.06</td>
</tr>
</tbody>
</table>
Dry Fabrics for Entry Parachute Applications

- Simulate dry fabric behavior by allowing the tow orientation in each subcell to change with applied loading
  - $\phi$ – Crimp or tow undulation angle
  - $\theta$ – 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

Warp-Aligned Uniaxial Tension (100 simulations)
Bias Extension Shear Strain Development

Fabric RUC with defining angles

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

POCs: S. Mital/J. Stuckner
NASA GRC Database Schema for ICME

Material DB Summary

Material Pedigree
- Component/Assemblies
- Composite System/Laminate
- Ply/Layer Architecture
- AM Builds

Manufacturing
- Processing
- Additive
- Subtractive

Reference Data
- Project
- Publications
- Standards

Model Pedigree

Deformation
- Reversible
- Irreversible

Machine Learning

Statistical Data
- Tensile
- Creep
- Cyclic
- + others

Test Information
- Specimen Type
- Test Equipment

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

POC: B. Hearley
Material Pedigree
- Reinforcements/Fillers
- Composite System/Laminate

Architecture

Software Tools

Model Pedigree
- Composite Models
- Deformation Models
- Damage Models

NASMAT

Automation of read/write and tool execution in background

Nanoscale
- Change the fiber material in a composite → update lamina properties

Microscale

Mesoscale

Macroscale

Application
- Optimizer

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
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)
Questions

Contact: Trenton.M.Ricks@nasa.gov
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.

<table>
<thead>
<tr>
<th>Today’s Design Paradigm</th>
<th>2040 Design Paradigm</th>
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<tbody>
<tr>
<td>Stages Of The Product Development Lifecycle Are <em>Segmented</em></td>
<td>Stages Of The Product Development Lifecycle Are <em>Seamlessly Joined</em></td>
</tr>
<tr>
<td>Tools, Ontologies, And Methodologies Are <em>Domain-specific</em></td>
<td>Tools, Ontologies, And Methodologies Are <em>Usable Across The Community</em></td>
</tr>
<tr>
<td>Materials Properties Are Based On <em>Empiricism</em></td>
<td>Materials Properties Are <em>Virtually Determined</em></td>
</tr>
<tr>
<td>Product Certification Relies Heavily On <em>Physical Testing.</em></td>
<td>Product Certification Relies Heavily On <em>Simulation</em></td>
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</table>
Virtual Testing Can Enable Significant Cost Savings in Certification Process

Experimental Test Pyramid

Numerical Simulation Pyramid

Model Building Block Approach

A robust validated computational platform is essential for sustainable, cost-effective technology development program ➢ reduced testing and time to certify!

$$\textit{Savings!}$$

Experimental Building Block Approach
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

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**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
Transverse Loading
50% Glass/Epoxy

~11,000 GPS Elements
676 Subcells
1024 Subcells

von Mises stress ($J_2$)
Pressure
($= -\sigma_{\text{mean}}$)
(MPa)

Fidelity vs. Efficiency in Composite Micromechanics

Simpler Methods
Mean Field

FEA
GMC
HFGMC
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

Local Heat Flux Fields

Above “percolation threshold”
Multiscale Process Modeling of Thermoplastics

- 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
- 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)

<table>
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<tr>
<td>91,125</td>
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<td>10</td>
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</tbody>
</table>

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