



Certification by Analysis of Woven TPS: Fiber- and Weave-Scale Modeling EDL Summer Seminar

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Acknowledgements



Entry Systems Modeling (ESM) Project TPS Certification by Analysis

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Woven Thermal Protection Systems (TPS)



Heat Shield for Extreme Entry Environment Technology (HEEET)

Adaptable Deployable Entry and Placement Technology (ADEPT)







3D Woven Mid-Density Carbon Phenolic (3MDCP)

- Derived from HEEET insulation layer
- Mars Sample Return Earth Entry System (MSR-EES)



Certification by Analysis of Woven TPS



Goal: Develop computational tools and techniques to support certification of woven TPS materials

- > Identify and characterize material features, defects, and damage
- > Determine how these features/defects/damage affect properties, performance, and failure



Weave features or defects

Impact from micrometeoroids and orbital debris (MMOD)



TPS Certification by Analysis Thrusts





Multiscale Materials Modeling

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William Tucker Federico Semeraro Sander Visser



Multiscale Materials Modeling

Glenn Research Center Multiscale & Multiphysics Modeling Branch Trenton Ricks Brett Bednarcyk Subodh Mital

Pappu Murthy Evan Pineda



Machine Learning and Nondestructive Evaluation

Ames Research Center Intelligent Systems Division Kevin Wheeler Vasyl Hafiychuk Michael von Pohle Karan Doss

TPS Cert Activities: Fault Detection



Computational Nondestructive Evaluation (CNDE)





Detection of disbonds by ultrasonic interrogation

POC: Vasyl Hafiychuk (ARC/TI)

Machine Learning



Automated detection of faults in CT scans using deep learning

POC: Michael von Pohle (ARC/TI)

TPS Cert Activities: Damage Simulations

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Progressive Damage Simulations



Stress damage in blended yarns using multiscale recursive micromechanics models

POC: Brett Bednarcyk (GRC)

Impact Simulations



Impact damage using peridynamics simulations with microstructure representation

POC: Justin Haskins (ARC/TSM)

Computational Materials Modeling

Increased Scale and Analysis

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 - Tows' Orientation
- Conclusions & Future Work

Woven TPS Multi-scale Modeling

- In 3D woven composites, some yarns are also weaved through the thickness direction.
- Designing this type of composite for specific applications is not trivial due to the high number of design options.
- This study focuses on multi-scale modeling to obtain the mechanical properties of different 3D woven composites.
 - Modeling steps: Matrix → Yarn → Unit Cell
- Use of PuMA's voxel-based thermal conductivity and stress analysis solver for anisotropic materials.
 - Finite volume
 - Cell-centered discretization

Tools Overview: PuMA

 The PuMA software is able to either generate domains artificially or import them from micro-CT scans and compute material properties such as: porosity, specific surface area, effective thermal conductivity, pore diameter, tortuosity, permeability. It also enables the computation of mechanical properties though its anisotropic elasticity solver.

Tools Overview: PuM

- Lead developers: J.C. Ferguson and F. Semeraro
- Installation: conda install -c conda-forge puma
- Open-source repository: <u>https://github.com/nasa/puma</u>
- Documentation: <u>https://puma-nasa.readthedocs.io</u>
- Community chat: <u>https://gitter.im/puma-nasa/community</u>
- Tutorials: <u>YouTube</u> channel and <u>Colab notebook</u>

PuMA architecture diagram

Tools Overview: TomoSAM

- NASA
- An extension of 3D Slicer using the Segment Anything Model (SAM) from Meta to aid the segmentation of 3D data from tomography or other imaging techniques.
- Lead developers: F. Semeraro
- Open-source repository: <u>https://github.com/fsemerar/SlicerTomoSAM</u>

TomoSAM graphical user interface

Micro-CT workflow diagram

Porous Matrix Modeling: Elasticity

Fully dense isotropic phenolic resin: E = 4.5 GPa, v = 0.30Random intersecting spherical pores: $\Phi = 0.0 / 0.2 / 0.4 / 0.6$ Pore diameter sensitivity study: 4 – 20 voxels Domain: 100 x 100 x 100 voxels

Fig.5 - Voxelized models of porous resin matrix (top) and different pore sizes (bottom)

Fig.6 - Micrograph of cured porous phenolic resin [3]

Results compared with semi-empirical equations found in the literature:

- Bert: solid with spherical pores following a hexagonal distribution, $\phi_{max} = 0.7405$ and c = 2 ϕ_{max} [4]
- Roberts: solid with random overlapping spherical pores, $\phi_{max} = 0.818$ and c = 1.65 [5]

$$E_{\phi} = E_0 \left(1 - \frac{\phi}{\phi_{max}} \right)^{\alpha}$$

Porous Matrix Modeling: Elasticity

- Pore diameter of the simulations shown: D = 16 voxels
- Assumed isotropic material
- RVE homogenization method:
 - Model's face in XY plane fixed
 - Displacement of 1 voxel in +X
 - Symmetry BC in the other 4 faces
- Top: Displacement field (X)
- Bottom: Direct stress field (X)

Displacement field (top) and direct stress field (bottom) in the X direction

Porous Matrix Modeling: Elasticity

- 9 pore diameters analyzed, up to 30 simulations each to minimize the random generation uncertainty.
- Pore diameter selected for this study: d = 20 voxels.
- Great agreement with Robert's equation.

Porous Matrix Modeling: Thermal Conductivity

- Porous phenolic model generated via random intersecting spherical voids.
- Fully dense isotropic phenolic resin (SC-1008): k = 0.25 W/mK
- Pores filled with air: k = 0.0257 W/mK
- Pore diameter = 20 voxels
- Domain = 300 x 300 x 300 voxels
- Multiple simulations $\Phi = [0 1]$

Phenolic resin thermal conductivity as function of porosity (PuMA)

Temperature and heat flux fields for different porosity values

Yarns made of carbon and porous phenolic resin (hex distribution). Porous phenolic: mechanical properties from this study, $\Phi = 0.0 - 0.6$ Carbon fibers: $E_L = 230$ GPa, $E_T = 15$ GPa, $v_{LT} = 0.20$, $v_{TT} = 0.20$ Fiber volume fraction in tow: $V_f = 0.5 / 0.6 / 0.7 / 0.8$ Domain: 25 x 100 x 173 voxels

Voxelized tow models, $V_f = 0.6, 0.8$

Results compared with theoretical and semi-empirical equations found in the literature:

- Rule of Mixtures (ROM): good approximation for E_L and v_{LT}
- Halpin-Tsai: better approximation of E_T than ROM with empirical parameter for hex distribution ξ = 1 (η = 1) [7]
- Nielsen: modified Halpin-Tsai equation with maximum fiber packing parameter η = 0.907 [8]
- Chamis: widely used due its simplicity and greater accuracy compared to ROM [9]

Yarns made of carbon and porous phenolic resin (hex distribution). Porous phenolic: mechanical properties from this study, $\Phi = 0.0 - 0.6$ Carbon fibers: $E_L = 230$ GPa, $E_T = 15$ GPa, $v_{LT} = 0.20$, $v_{TT} = 0.20$ Fiber volume fraction in tow: $V_f = 0.5 / 0.6 / 0.7 / 0.8$ Domain: 25 x 100 x 173 voxels

Voxelized tow models, V_f = 0.6, 0.8

ROM
$$E_L = E_{f_L}V_f + E_mV_m$$
 $v_{LT} = v_{f_{LT}}V_f + v_mV_m$
Halpin-Tsai $E_T = E_m \frac{1 + \xi \eta V_f}{1 - \psi \eta V_f}$ where, $\eta = \frac{r - 1}{r + \xi}$ $r = \frac{E_{f_T}}{E_m}$
Chamis $E_T = \frac{E_m}{1 - \sqrt{V_f} \left(1 - \frac{E_m}{E_{f_T}}\right)}$

Results compared with theoretical and semi-empirical equations found in the literature:

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- Nielsen: modified Halpin-Tsai equation with maximum fiber packing parameter η = 0.907 [8]
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- Fully dense phenolic matrix for the simulations shown.
- RVE homogenization method:
 - Model's face in XY plane fixed
 - Displacement of 1 voxel in +Z
 - Periodic BC in the other 4 faces
- Top: Displacement field (Z)
- Bottom: Direct stress field (Z)

Displacement field (top) and direct stress field (bottom) in the Z direction

 Halptin-Tsai shows the best agreement with the results from PuMA for E_T

Fig.16 - Yarns Transverse Young's modulus

 ROM shows great agreement with results from PuMA for E_L and v_{LT}

Fig.17 - Longitudinal Young's modulus and Poisson's ratio

- Segmentation of HEEET-IL microscopy images is important to obtain more accurate material properties and composition data of the TPS constituents.
- A UNet CNN was trained to automate the segmentation process leveraging Dragonfly's Deep Learning capabilities.
- Approach followed for the segmentation:
 - Mask out the in-plane tows to clean up the images and train the UNet CNN only with the through-thickness tows.
 - Segment manually a few regions to start training the UNet CNN and use the initial model's predictions to help with the segmentation of additional regions.
 - Correct the segmentation of the predicted labels and continue training the UNet model with the new data.
 - Continue the process with different microscopy images to generate additional training data.

HEEET-IL microscopy image (NASA-GRC) though the steps of masking out the in-plane tows

Selection of regions segmented of the HEEET-IL microscopy image (NASA-GRC) to train the UNet CNN

Segmented microscopy image using the trained UNet model

- Once the microscopy data is fully segmented, PuMA can calculate the average thermal conductivity of a tow.
- Selected 75 regions or "frames" of sizes between 500² and 1600² pixels for thermal conductivity evaluation.

Frames selected for thermal conductivity calculation, 2023-1-10-HEEET_IL_Warp_L2 (left) and 2023-1-10-HEEET_IL_Tow-Area-2-4-7 (right)

- AS4 carbon fiber: k_{axial} = 6.9 W/mK, k_{transverse} = 2.52 W/mK
- Phenolic fiber assumed fully dense phenolic resin: k = 0.25 W/mK
- Porosity of infiltrated phenolic resin considered.
- Final conductivity value computed by volume averaging the results for all frames.

Tow Properties	Value
VF Cracks	
VF Phenolic Resin	
VF Carbon Fibers	
VF Phenolic Fibers	
k _{transverse}	
k _{axial}	

Ji, X. et al. Carbon **2022**, 197, 1–9.

HEEET_IL_Tow-Area-2-4-7 frame #36, temperature_x (left), heat flux_x (center) and heat flux_z (right) fields.

Unit Cell: Micro-CT Data

- Micro-CT data provided by Kyle Hendrickson, infused sample "HEEET-24-016-001-12"
- Sample object of this study taken from the middle section of the reconstructed image.
- Tows made of four twisted sub-tows, and visible matrix cracks.
- Sample resolution:
 - X (R) 472px (Fill)
 - Y (A) 497px (Warp)
 - Z (S) 330px (Thickness)

Raw and cropped micro-CT data

HEEET-24-016-001-12 sample (credits: Kyle Hendrickson)

Unit Cell: Micro-CT Segmentation

Segmented 3MDCP visualizations

Unit Cell: Micro-CT Orientation

- Orientation of the tows computed for the full resolution micro-CT data.
- Orientation fields are important to apply different mechanical properties or thermal conductivity values along and across the sub-tows.
- Tow's orientation computed using PuMA's Structure Tensor method for each tow individually.
- Final orientation values obtained by averaging the results for each crosssection of each tow to reduce errors.

- NASA
- RVE homogenization method: displacement of 1 voxel in +X, +Y and +Z respectively with periodic BCs.

Fig.18 - Displacement field with matrix visible (top) and matrix hidden (bottom) in the X, Y and Z directions

- NASA
- RVE homogenization method: displacement of 1 voxel in +X, +Y and +Z respectively with periodic BCs.

Fig.19 – Direct stress field with matrix visible (top) and matrix hidden (bottom) in the X, Y and Z directions

The same methodology used at the micro-scale for the constituents was applied to obtain the
effective mechanical properties of the unit cell.

- X = 1
- Y = 2
- Z = 3

0.8

Conclusions

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- This work described a methodology to carry out multi-scale analyses of porous 3D woven materials using artificially generated models, and models segmented from microscopy / micro-CT data.
- This methodology can be applied to any type of composite material to obtain its homogenized orthotropic mechanical properties, and anisotropic thermal conductivity.
- The PuMA software allowed us to analyze the constituents at the micro-scale and then use those results to accurately model the unit cell at the macro-scale.
- Results were validated for the elasticity results of the porous matrix and the yarns by comparing them to analytical expressions listed in the literature.
- Future work investigate as-manufactured weaves.

Computational Materials Modeling

Increased Scale and Analysis

Particle-based/Meshless/Lagrangian Woven TPS Modeling

Goal of the bottom-up approach

- if the fiber model is correct, the weave will be correct
- extract fiber-level behavior and contribution in weaves and yarns during damage, impact or ablation

Molecular dynamics

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microscale

Phenomena Captured by Explicit-Fiber Modeling

Explicit-fiber modeling captures certain experimental observations where continuum is unable

Impact with friction^ Explicit-fiber applications

a) Po

Yarn evolution during Braiding [#]

Physics incorporated with explicit-fiber models

- Role of geometry and directionality
- Fiber-fiber friction
- Rupture
- Dynamic collective motion

Friction controlled deformation with localized failure ⁺

*Liu, D. et al. J. App. Mech. **2019**, 86 (11). <u>doi.org/10.1115/1.4044014</u>

*Ghaedsharaf, M. et al. Composites Part B 2021, 218, 108938. doi.org/10.1016/j.compositesb.2021.108938
*Wang, Y. et al. Int. J. Impact Eng. 2016, 97, 66–78. doi.org/10.1016/j.ijimpeng.2016.06.007
*Wang, Y.; et al. Int. J. Impact Eng 2016, 97, 66–78. doi.org/10.1016/j.ijimpeng.2016.06.007

Configuration Generation with Relevant Features

- Idealized and realistic yarn and weave configurations are required to calibrate and verify fiber models and test hypotheses on weaves
- Python package, yarn_generator, developed to generate fiber-level models of yarns and weaves

Two ways to generate a weave

Yarn Features

processing conditions

optimal circle-in-circle or random 2d blended packing

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The yarn generator builds configurations with the relevant features

• Woven heat shields use yarns composed of different fibers and

Explicit-fiber simulations model the yarn microstructure

Yarn-Weave Manipulation

- Yarn manipulation can control the weave density or yarn packing
- Enables wrinkle and other behaviors
- Satisfies contact mechanics

Explicit-Fiber Simulation Methodology

Explicit-fiber simulations allow for the fibers to evolve independently during yarn-weave manipulation, parameterization and entry phenomena

Plimpton, S. J. et al., LAMMPS Comp. Phys. Comm. 2022, 271, 108171

Fiber Model Details

- Explicit-fiber simulation forces model each contact and internal mode independently
- Analysis of trajectories and forces can highlight the magnitude and directionality of each mode's contribution

Micromechanics-informed model:

- Intra^{1,2}-fiber, bonded forces
 - Stretch
 - Bend
 - Shear
 - Twist
 - Rupture
- Inter³-fiber, contact forces
 - Friction
 - Viscoelastic repulsion
 - Cohesion

Most model forces are modeled as a Hookean spring + damping

Method

- Meshless
- dynamic
- apply heat and deformation
- microstructure can change during simulation
- implemented in an open-source parallelized code⁴

$$f_r = k_r(r-r_0)$$

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¹Chen, X. et al. Comparative Assessment and Unification of Bond Models in DEM Simulations. *Granular Matter* 2021, 24 (1), 29.
 ²Wang, Y. and Sun, X. Digital-Element Simulation of Textile Processes. *Composites Sci. Tech.* 2001, 61 (2), 311–319.
 ³Silbert, L. E. et al., Granular Flow down an Inclined Plane: Bagnold Scaling and Rheology. *Phys. Rev. E* 2001, 64 (5), 051302.
 ⁴Plimpton, S. J. et al., LAMMPS *Comp. Phys. Comm.* 2022, 271, 108171

Tensile, Bending and Shear Moduli

Tuning model spring parameters can capture the rupture behavior due to different modes for carbon fibers, *e.g.*, enabling experimental comparison

Rod Thermal Conduction Model

- Explicit-fiber models can characterize conduction along and across fibers
- New model enables thermo-mechanical processes
- Yarn feature-property relationships can be tested

7 twisted Kynol phenolic fibers

- Yarn coarse-graining changes the conduction timescale to steady-state due to
 - Number of fibers changes the contact area
 - Exterior fibers are longer than interior fibers in twisted yarns

Weave Simulations of Heat Shield Ablation

The multi-fiber yarn representation can be incorporated into a full weave

We can apply weave simulations to test hypotheses, such as heat shield ablation

State of Ablation Modeling

Available ablation model (FIAT) shows that the standard approach to ablation (chemical only) underpredicts experimental recession values

• Ablation augmentation factor (AF) was proposed to scale chemical ablation rate to fit experiments:

$$\frac{\partial m}{\partial t} = (1 + AF) \frac{\partial m_c}{\partial t}$$

- The AF is not well posed but does appear to correlate to available surface shear stresses in some cases
- What are the contributing factors to non-chemical ablation augmentation?

ADEPT Weave

Ablative Disconnection of Yarns

• Erosion of the weave such that regions of tows become disconnected and "fall off" from having no structural connection to the remaining weave

47

Model of Weave Ablation and Connectivity

- Ablation front moves into the material and removes particles
- Forces applied such that disconnected portions of fibers are ejected from the surface into the ablation zone

ablation zone

Fiber tension: harmonic bonds *Fiber-fiber repulsion*: viscoelasticity

Augmentation from Loss of Weave Connectivity

- Large portions of weft yarns ablate faster due to the 3D geometry
- Weave disconnection enhances erosion by ~47%
- Other phenomena, such as pitting, are likely present
- With more development, the method could predict this behavior

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Explicit-Fiber Simulation Conclusions

- Yarn processing, like twist, changes material properties, requiring explicit-fiber simulations
- Enabled modeling of thermo-mechanical behavior
- 3D woven heat shields have enhanced ablation, ~47%, due to the weave geometry

Future work

- Incorporate material-specific, coarse-grained yarn-models into full weaves
- Identify defect deformation mechanisms

Fiber and Weave Modeling Conclusions

- Entry System Modeling Certification by Analysis task is ٠
 - Multi-center (ARC-TSM, ARC-TI and GRC) and ٠
 - **Multi-method** (non-destructive evaluation, machine learning, • material characterization, finite element, peridynamics, explicit-fiber)
- The PuMA software •
 - Measured the orthotropic mechanical properties, and ulletanisotropic thermal conductivity
 - Modeled a composite woven system, and it's constituents, ٠ including the porous matrix and yarns
- Explicit-fiber simulations ٠
 - Demonstrated a $\sim 47\%$ ablation enhancement due to the • weave geometry

Porous Microstructure Analysis (PuMA)

Particle-based, discrete-element methods (LAMMPS, HYDRA)

