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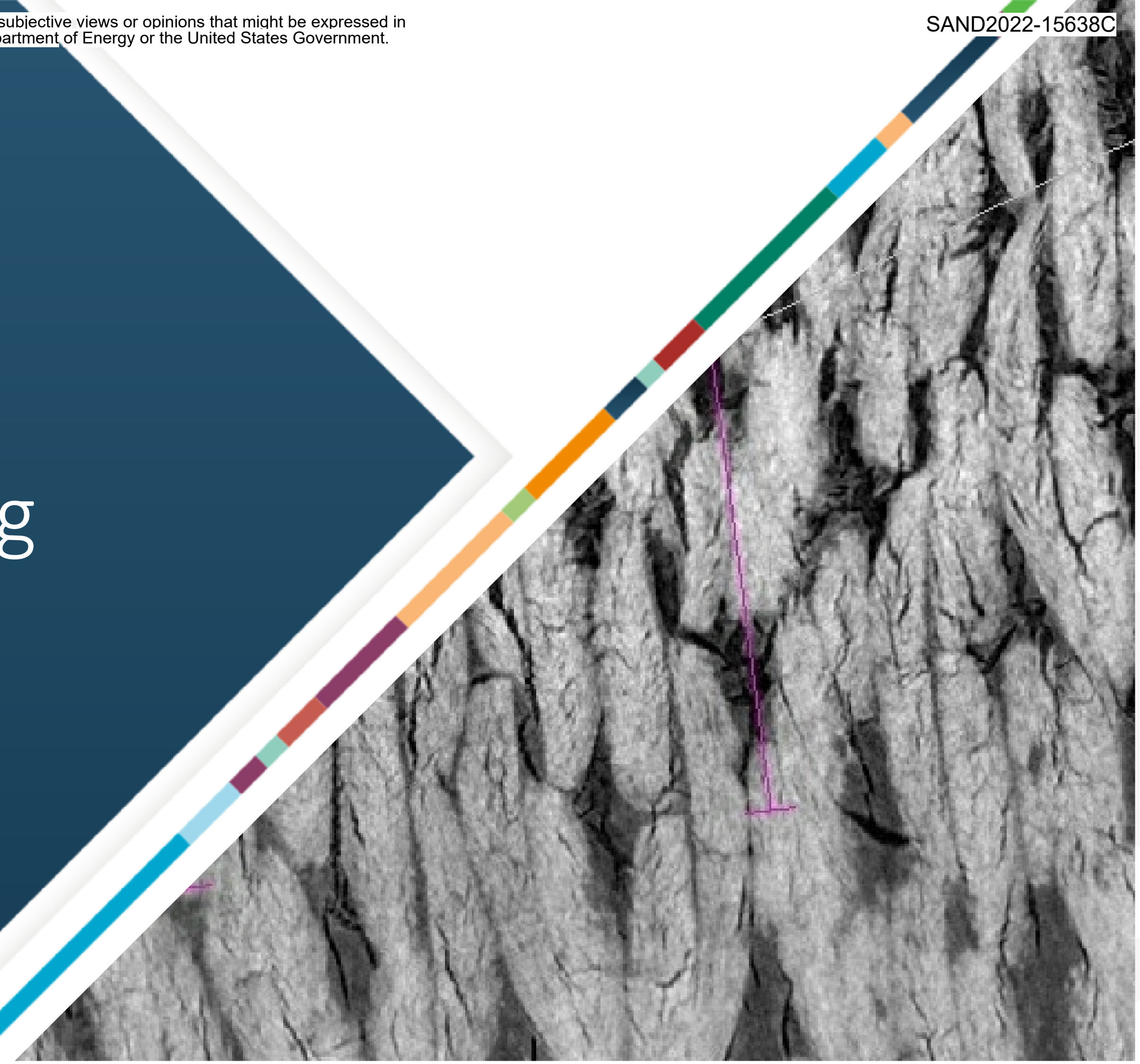

Mesoscale Ablation Modeling

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Engineering Sciences Center

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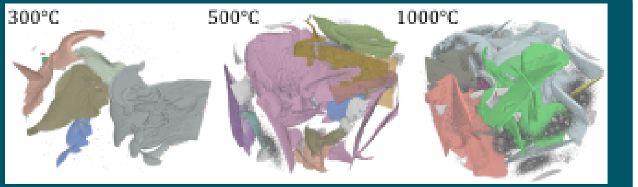
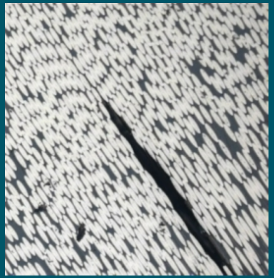
U.S. DEPARTMENT OF ENERGY

NNSA

Material response during atmospheric entry is a multiphysical and multiscale problem

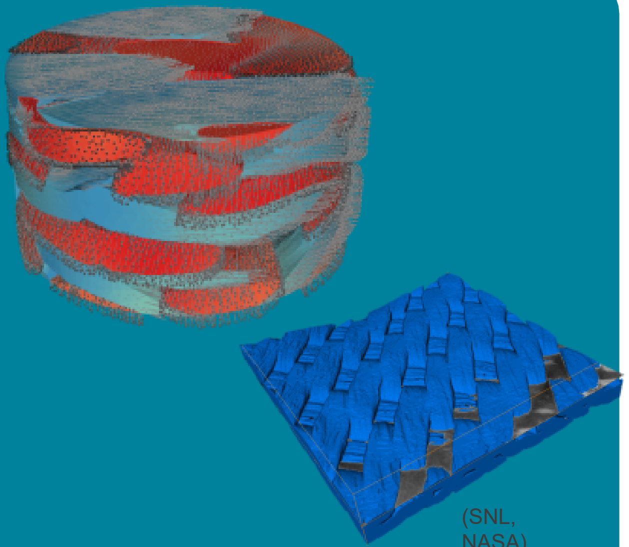
Microscale





- **Constituent materials**
- Pyrolysis chemistry
- Ablation chemistry
- Fiber/resin interface
- Morphology changes

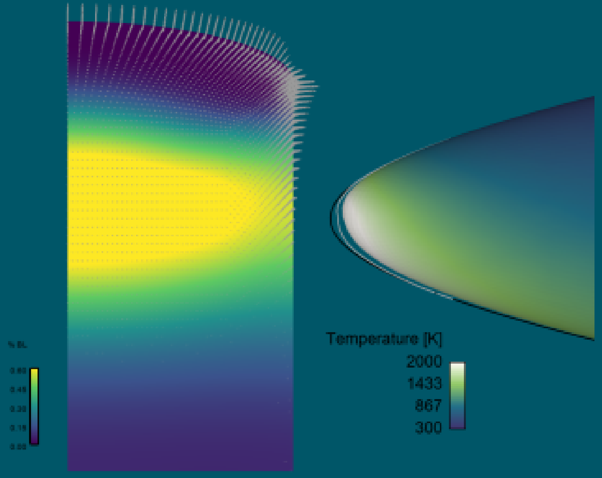
Mesoscale



(SNL, NASA)

- **Structure-property**
- **Local response**
- Property prediction
- Material design
- Stress generation

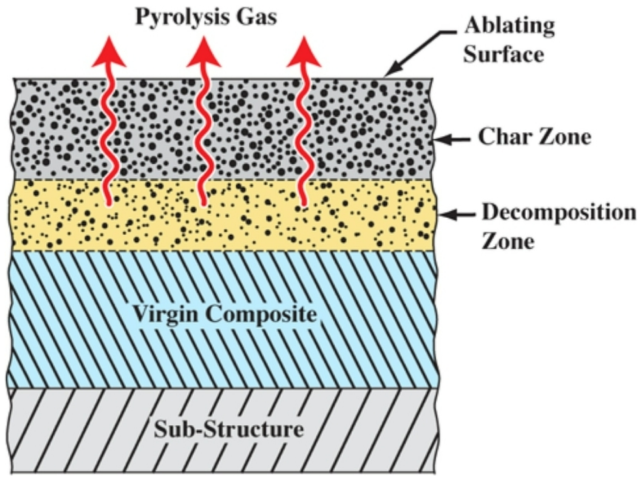
Macroscale



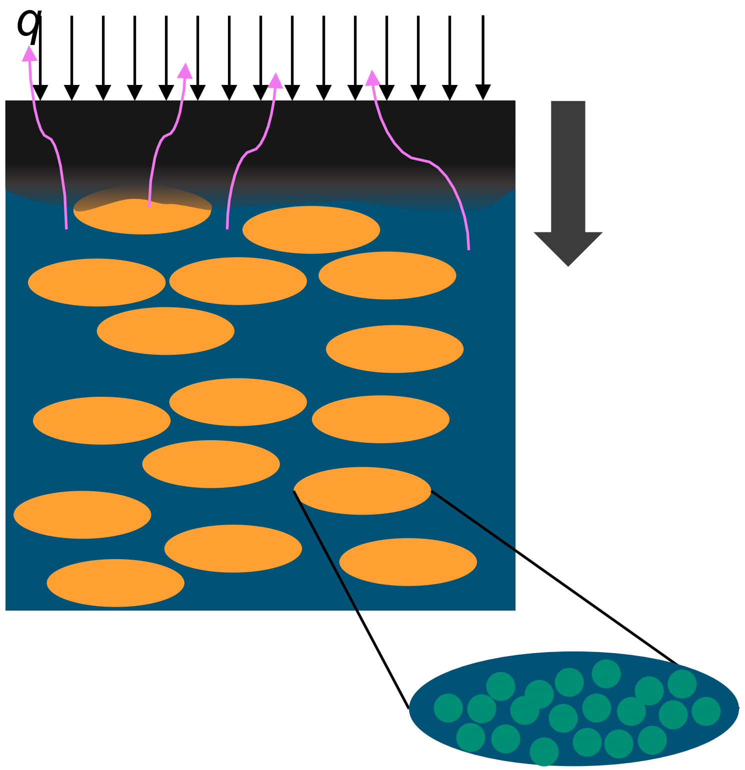
- **Engineering + analysis**
- Bulk properties
- Thermal protection
- Shape change
- GSI/FSI

Mesoscale mod/sim offers a connection between research efforts

Mesoscale model development



(Amar)



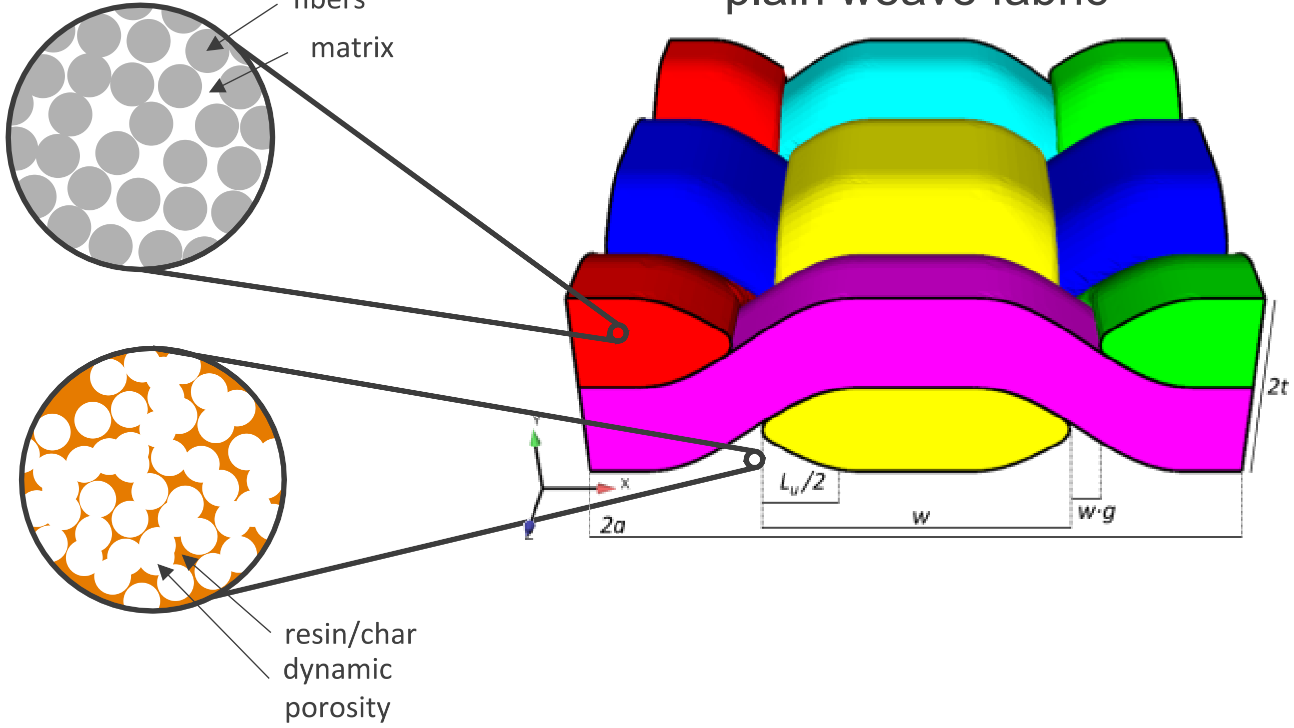
- Differing decomposition characteristics in composite regions
- Improved characterization of pyrolysis gases as function of heating rate/composition etc.
- Ideal proving ground for high-fidelity in-depth chemistry models
- Non-equilibrium pyrolysis gas composition, coking, in-depth oxidation and interaction with boundary layer
- Role and importance of species tracking and/or ROM for chemistry
- Mechanical response

Mesoscale ablation model

- Mesoscale **porous** media
  - Two-phase
  - Matrix and yarn domains
- Porous **enthalpy** transport
  - Localized transport
  - Anisotropy
  - Uptake from gas phase
- **Arrhenius** decomposition
  - Inert fibers
  - Volumetric
- **Dynamic** material properties
  - Temperature and decomposition
- Pyrolysis **gas transport**
  - Darcy flow
  - **Pressure development**
  - Generalized species transport
  - Gas-phase reactions (secondary pyrolysis)
  - Surface reaction with char
- Locally varying **ablation rates**
  - **Development of surface roughness**

Material models

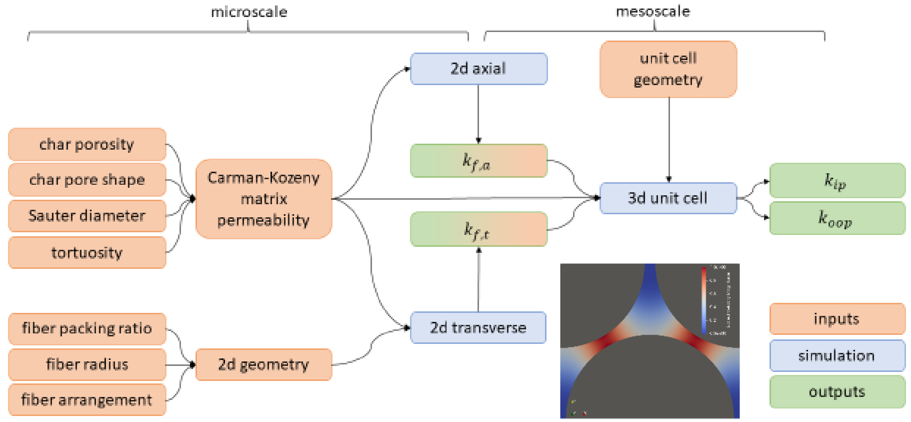
plain weave fabric



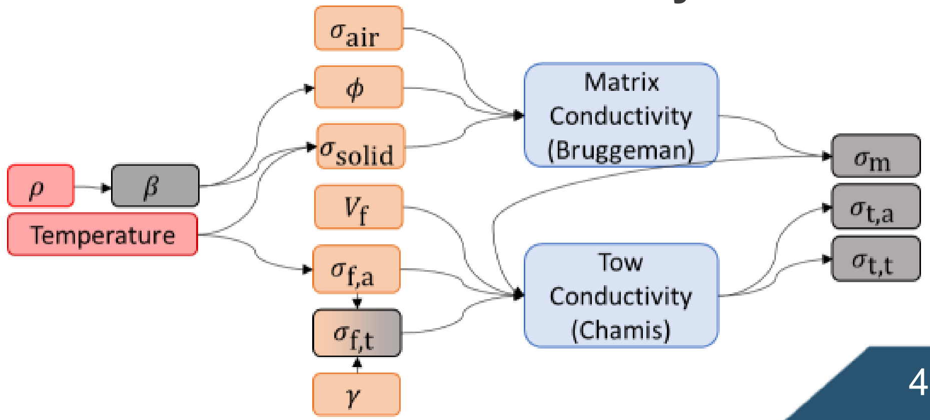
geometric properties

t	w	g	u
thickness	width	gap	undulation

permeability



thermal conductivity



Material geometry

- Analytical forms, TexGen, image-based reconstruction

Refined constituent material characterization

Dynamic material properties

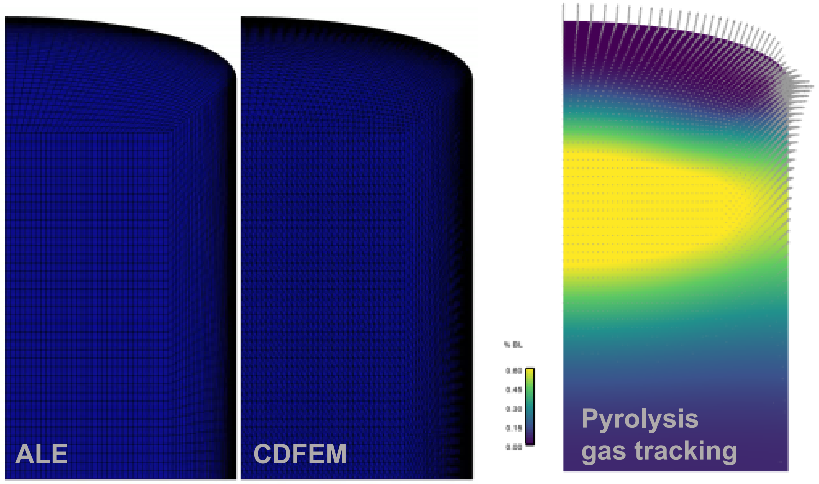
- Nonlinear dependence of $k(\beta, T)$
- Multi-scale calculation of permeability
- Consistent porosity evolution w.r.t. decomposition

Material response modeling with SIERRA/Aria

COMPSIM
THERMAL FLUIDS

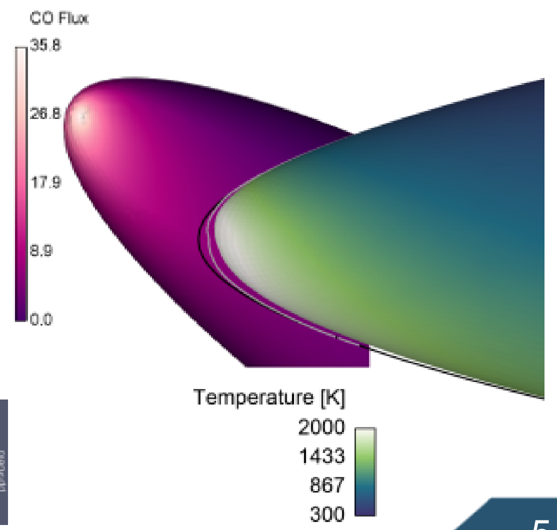
SIERRA/Aria

- Generalized thermal/fluids finite element code
  - Multi-physics native and through coupling (mechanics, dynamics, high-Mach CFD)
  - Multi-phase capabilities with stabilization (CVFEM)
- Ablator material response modeling
  - Implementation and modernization of legacy models and methods
  - B’ tables for ablation for non-decomposing, decomposing
  - Heat of ablation models
  - Effective property calculations
  - Coupling to system models and aero CFD
- Advanced mesh motion
  - Coupled to transport equations
  - ALE/TALE/CDFEM
- General Chemistry module
  - Multiple species reactive transport
  - Pyrolysis decomposition (volumetric)
  - Interface/surface chemistry with dynamic/nonlinear surface quantiti
  - Easily scripted for automatic input generation and parametric studi

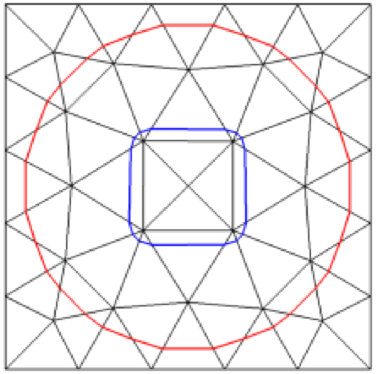


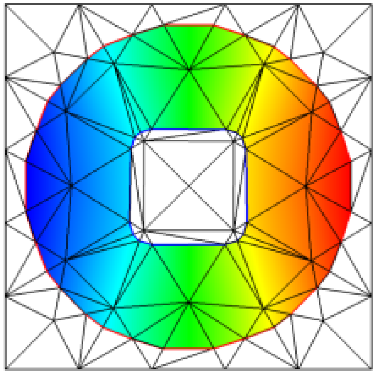
TACOT Type III

Park model with SPARC test vehicle



Conformal decomposition (CDFEM)





Concept

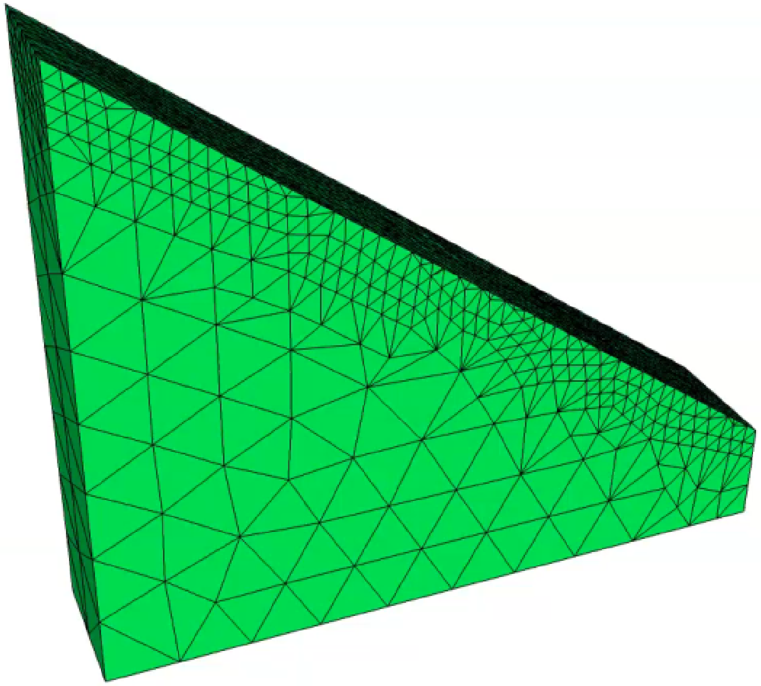
- Use level set fields to define phases
  - Solve for signed distance from interface

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0 \qquad \vec{n} = \nabla \phi, \kappa = \nabla \cdot \nabla \phi$$

- Propagate level-set with **velocity from B' tables**
- Decompose non-conformal elements into conformal ones

Properties

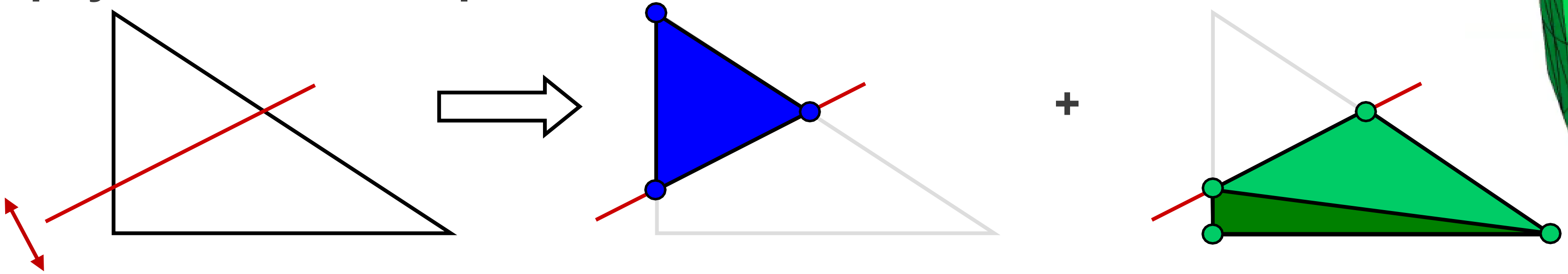
- Supports wide variety of dynamic interfacial conditions
- Avoids manual generation of boundary fitted mesh
- Supports general topological evolution



What about bad elements?

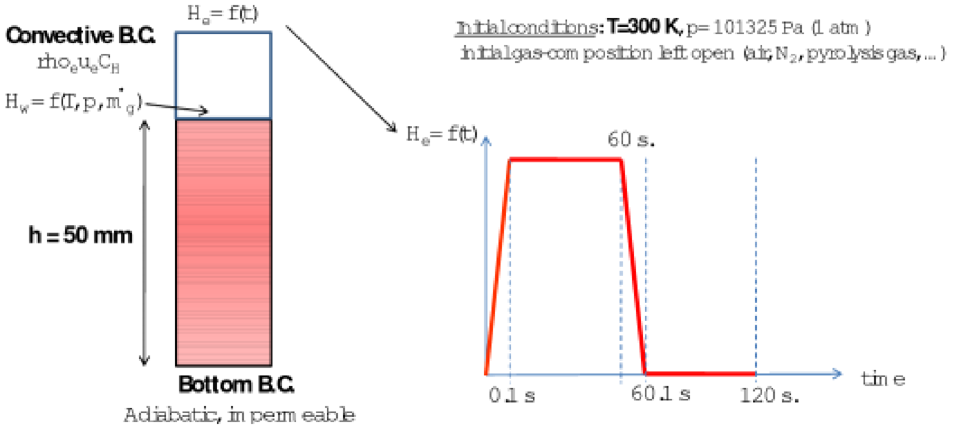
- snapping: movement of background nodes prior to cutting
- edge collapses, face swaps, and edge swaps

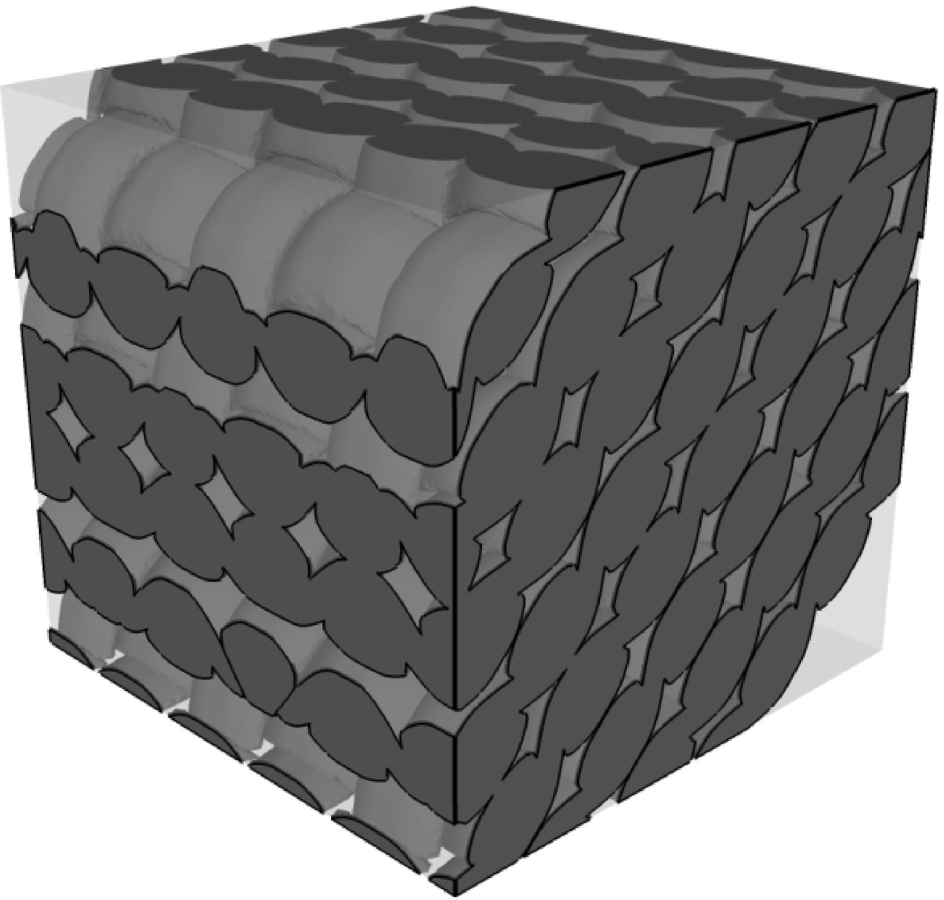
Interface CFL condition couples mesh motion and physics to time step selection



(Noble, 2010; Kramer, 2014; Roberts, 2018)

Exemplar formulation



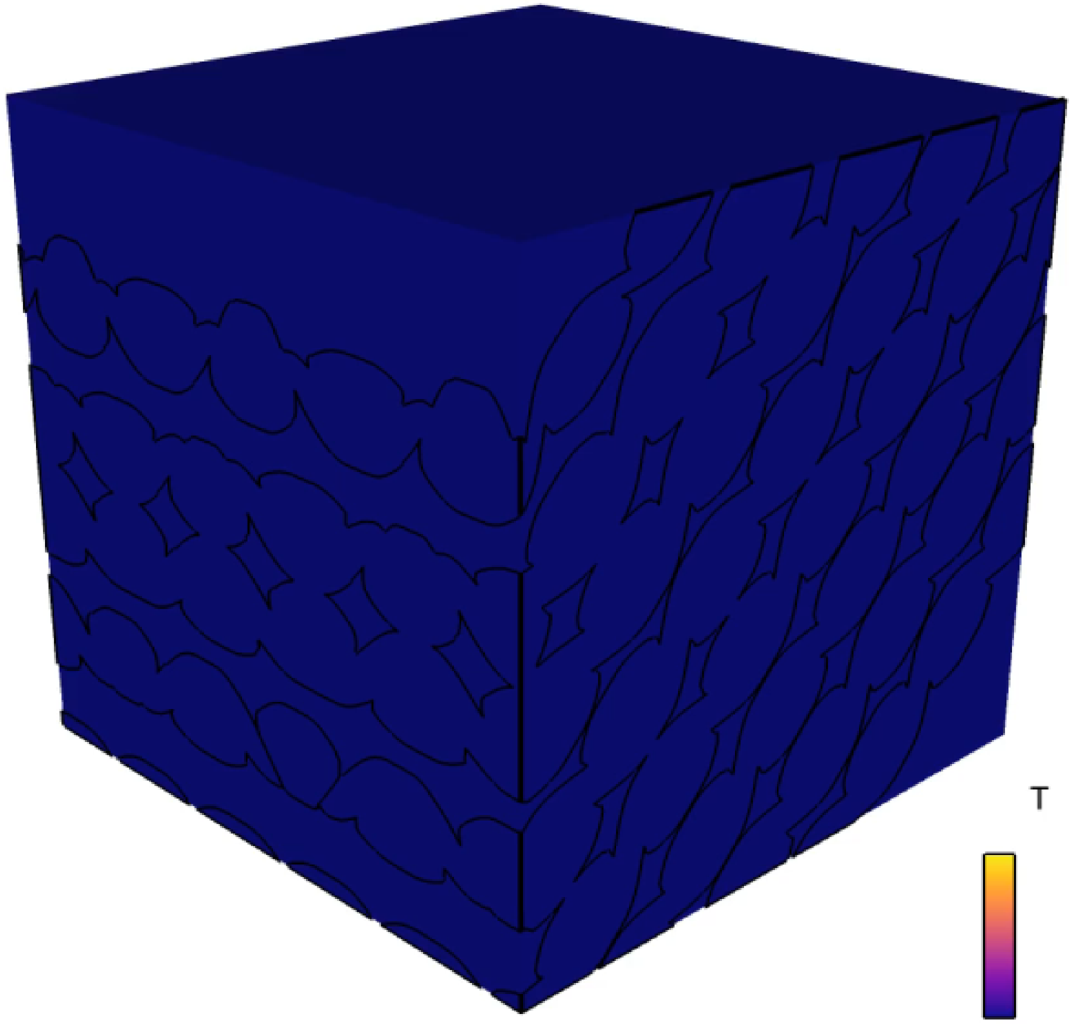


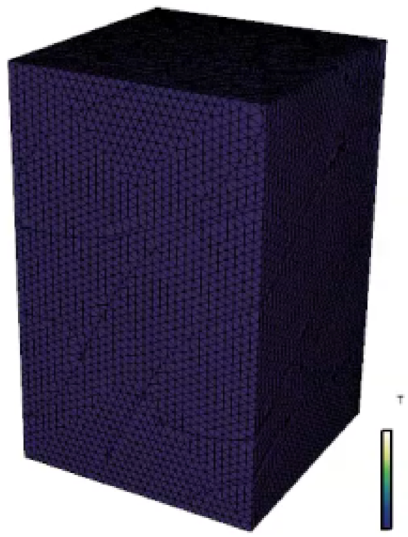
Materials

- Fictitious woven composite
  - TACOT decomposition kinetics for dense resin
  - AWS Test Case II heating, BCs, thermochemistry table
    - Ablating fabric reinforcement
  - Anisotropic material properties
    - *k*(fabric) >> *k*(resin)

- Track interface motion using CDFEM

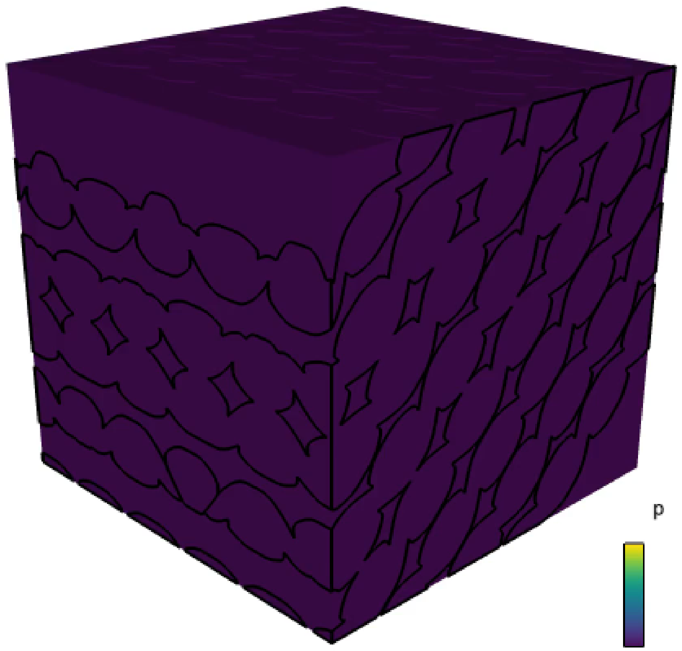
Thermal response

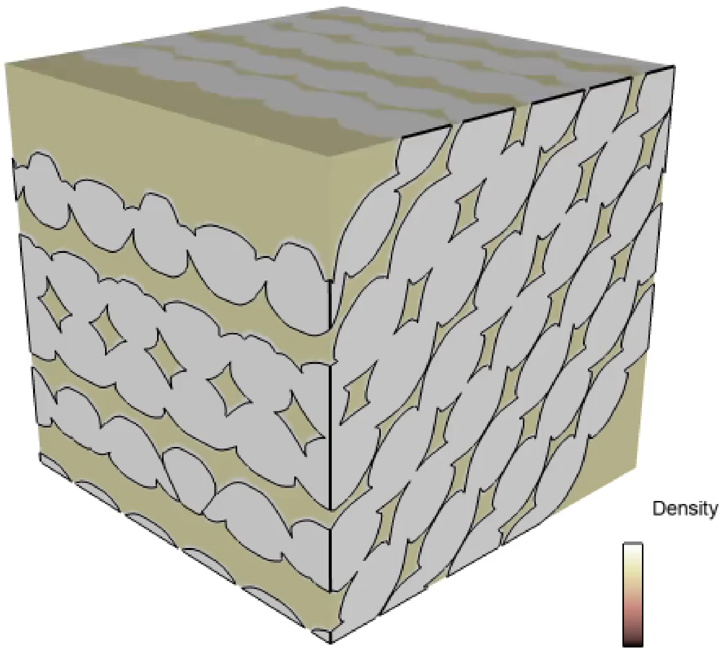


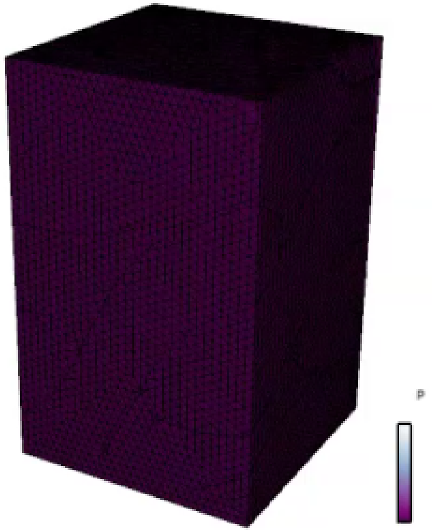


- Local thermal response creates uneven surface temperature and recession early
- Material anisotropy is essential
- Matrix between layers act as strong insulator
  - Arrangement dependent
- Largely isothermal
- **How to handle small domain size?**
  - Periodic BCs, remove adiabatic condition, coupling?

Pressure development

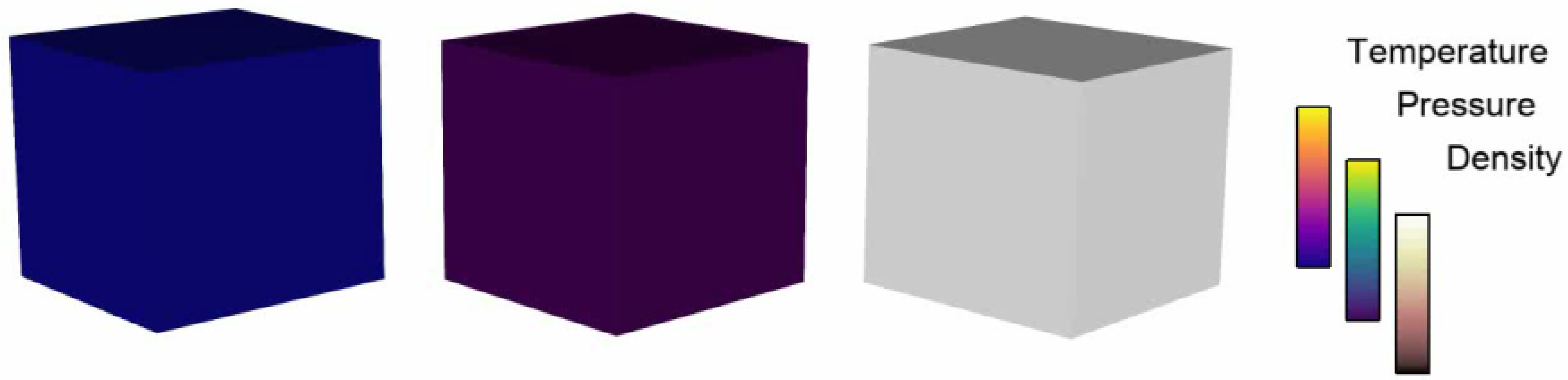


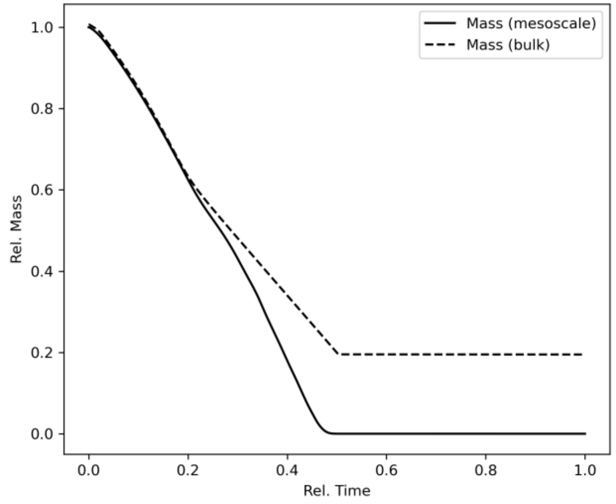


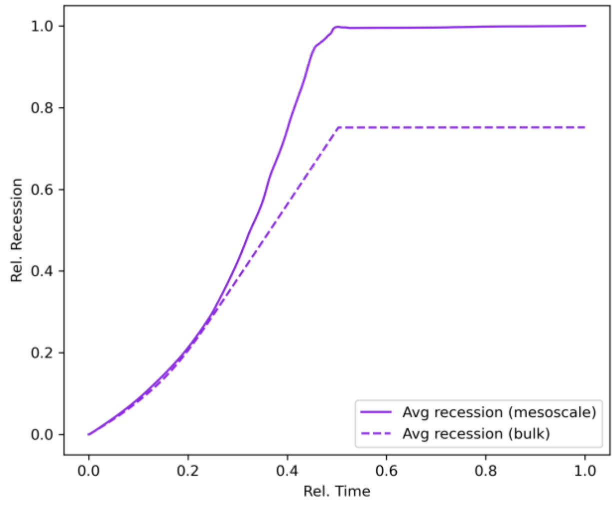


- Pyrolysis gas flow strongly follows connected charred matrix phase
- Anisotropic permeability likely less significant
- Significant pressure generation between layers and upon initial degradation

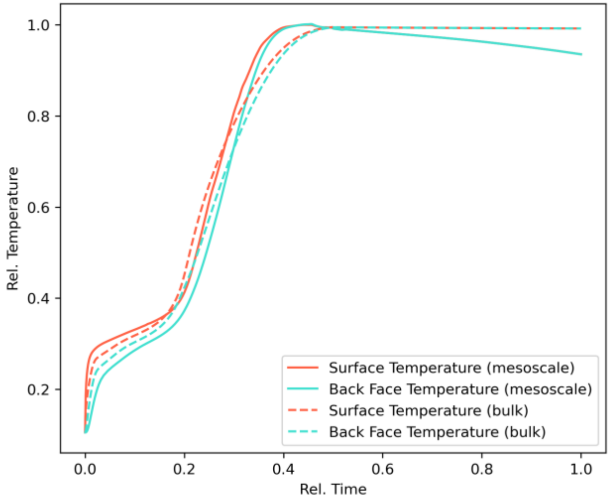
Comparison with bulk

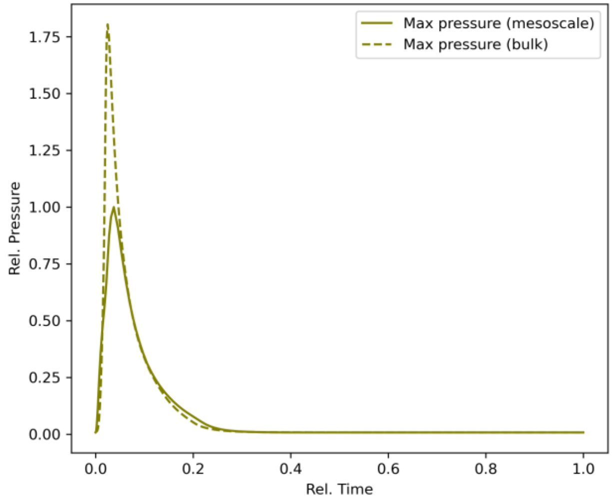






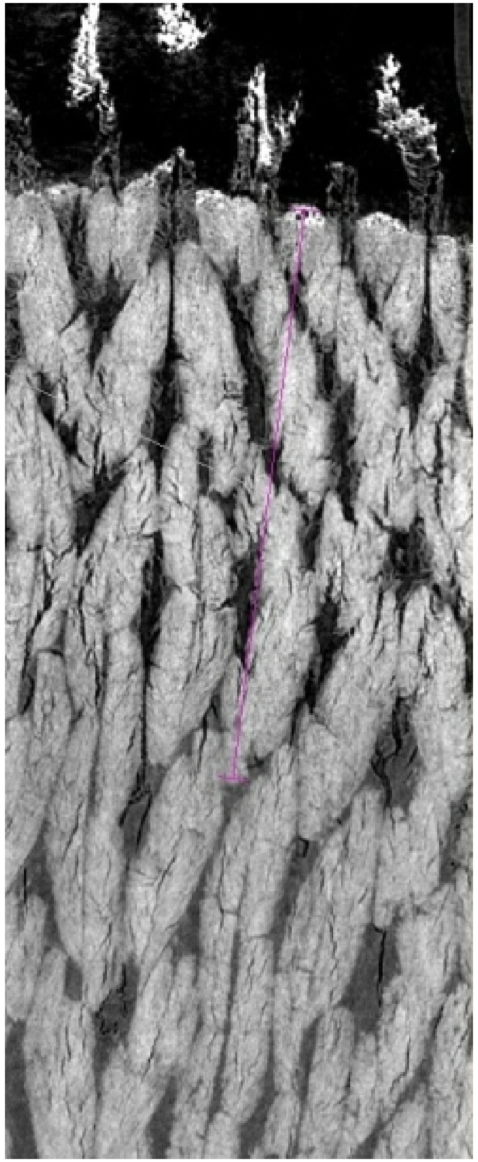
Approximate volume averaging of composite properties *





*** Work in progress**

Outlook



- **Material anisotropy is essential.**
- **How to use these simulations?**
  - Explore structure/property relation and material design
  - How to use developed surface roughness?
  - What about upscaling?
- **How to handle small domain size?**
  - How to push upper limits of simulation cost?
  - Sustained blowing through char?
- **What features are missing?**
  - Explore stress generation, deformation, and failure.
  - What about the aerodynamic heating boundary conditions?
  - Integration of high-fidelity chemistry (pyrolysis and ablation).
  - Resolving the created pore space.
  - Explore as-manufactured materials.

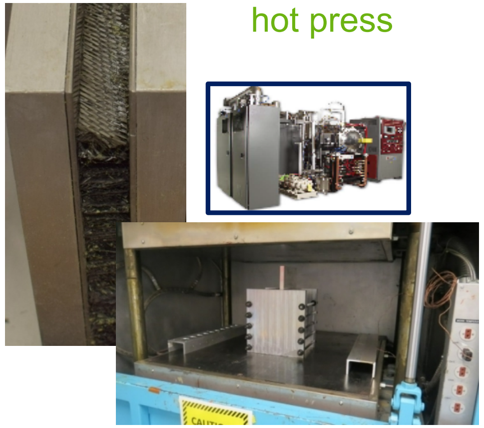
Thank you!

Contact: Lincoln N. Collins, lcolli@sandia.gov

Team Members: Scott A. Roberts, Martin DiStefano, Peter Creveling, Collin Foster

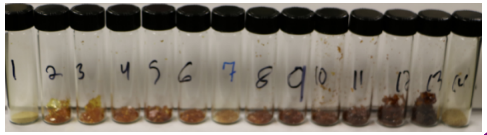
Sandia's multi-scale, multi-disciplinary approach to ablation

Processing: prepreg, hot press



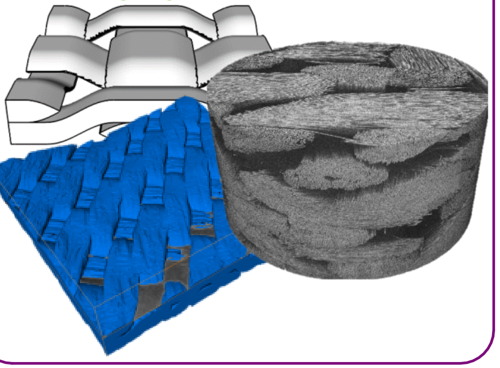
Nanoscale + Microscale

Composition: Property measurement, performance prediction, interface characterization, chemistry (MD)



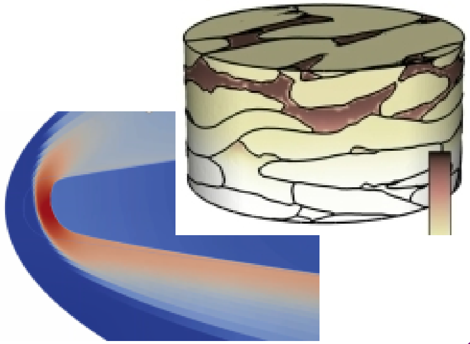
Mesoscale

Structure: Parametric studies, thermal, mechanical, 3D imaging



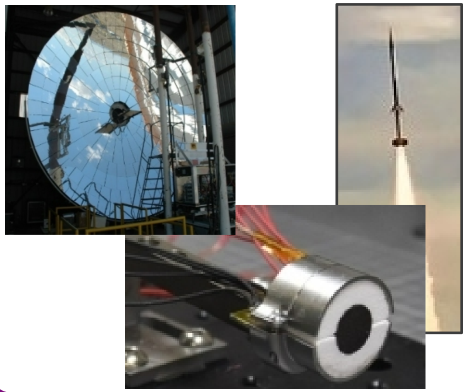
Macroscale

Behavior: mesoscale simulation, measurement, full system ablation



Coupon/vehicle scale

Performance: Thermal, recession, mechanical



Simulation

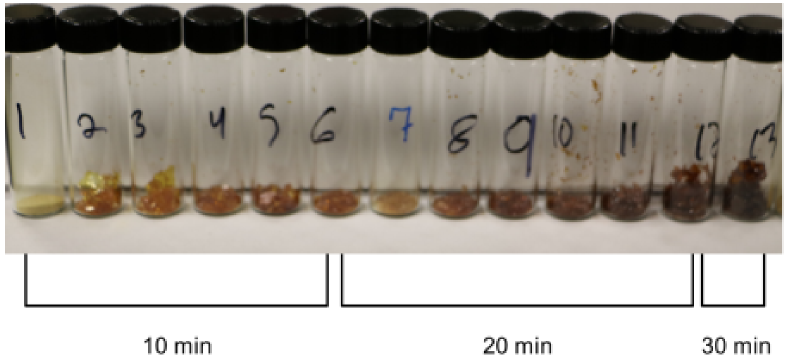
Experiment

Combined

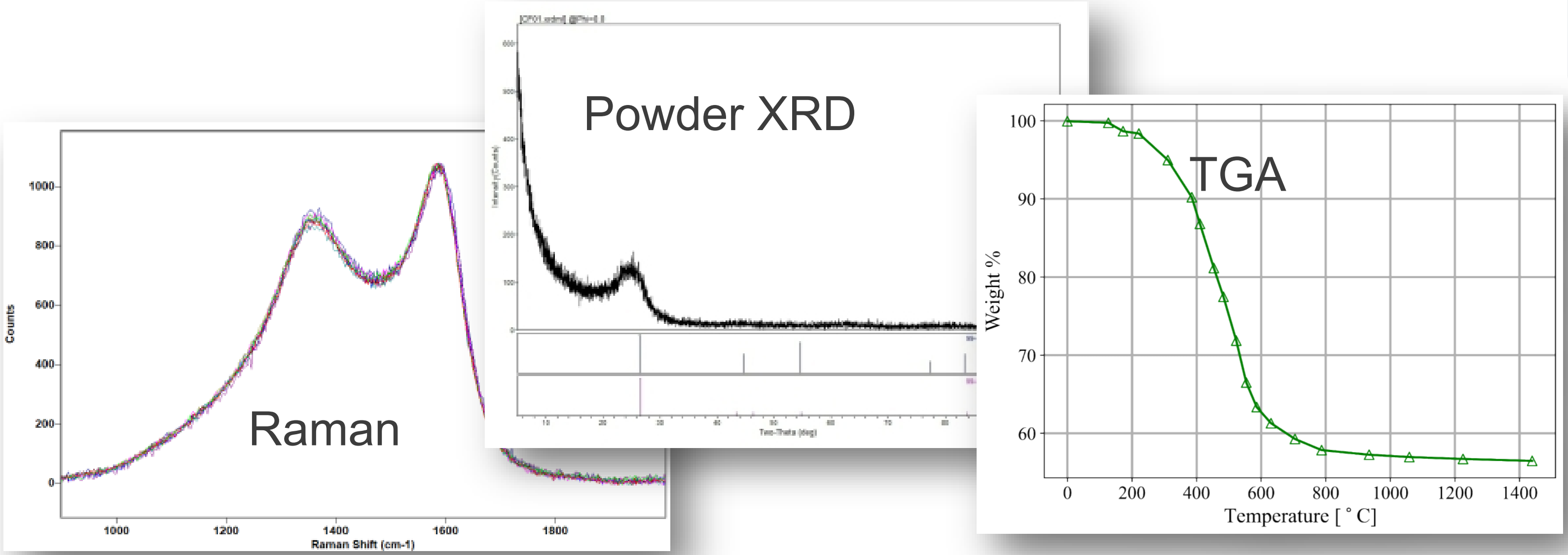
Length Scale

Complexity of Understanding

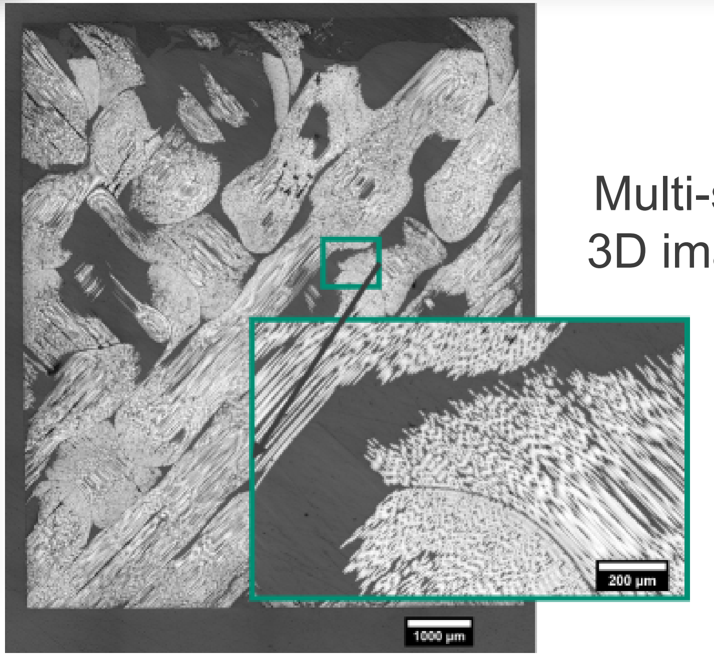
Materials and manufacturing research



Constituent material characterization

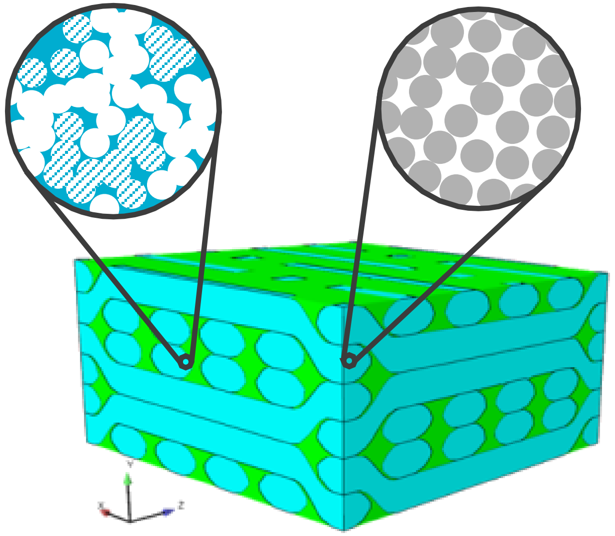


Composite manufacturing

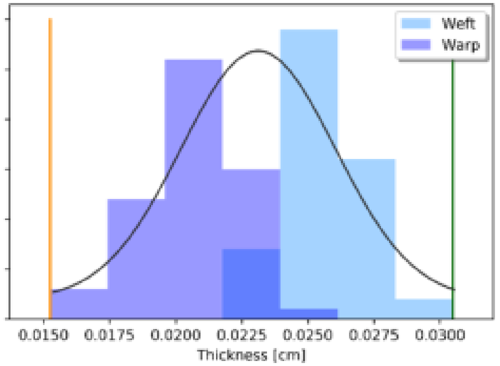


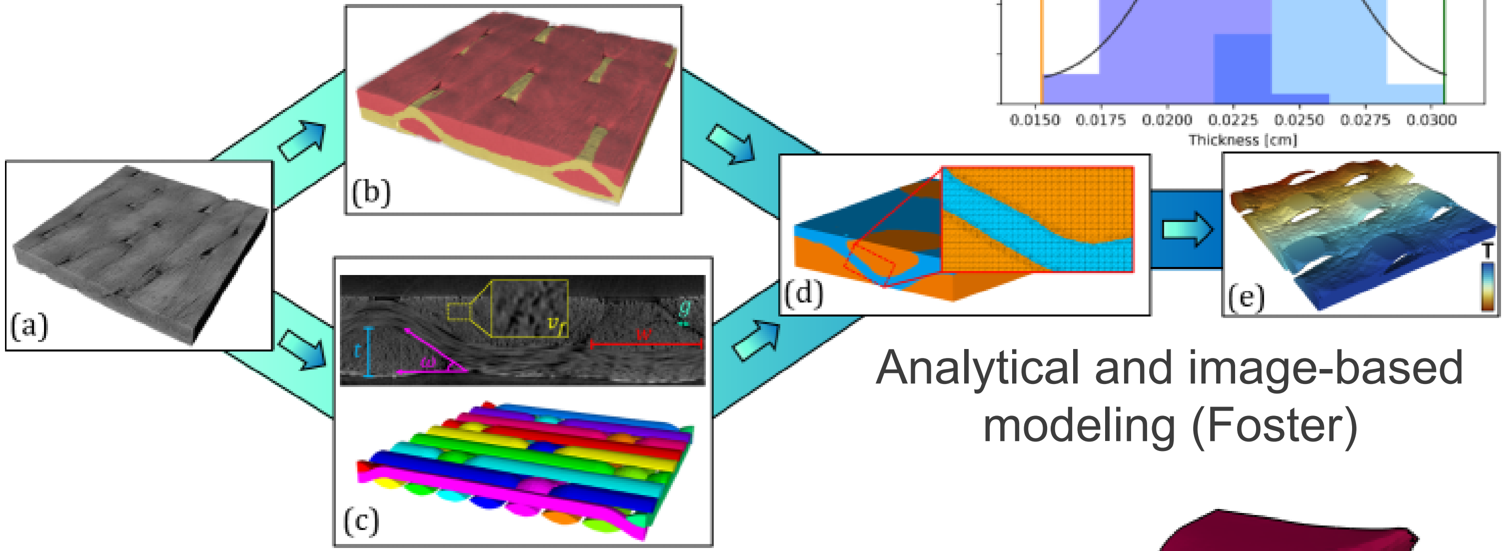
Multi-scale 3D imaging

Microscale and mesoscale modeling

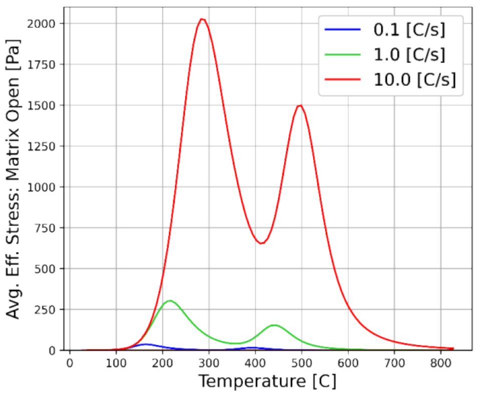


Micro- and meso-scale modeling

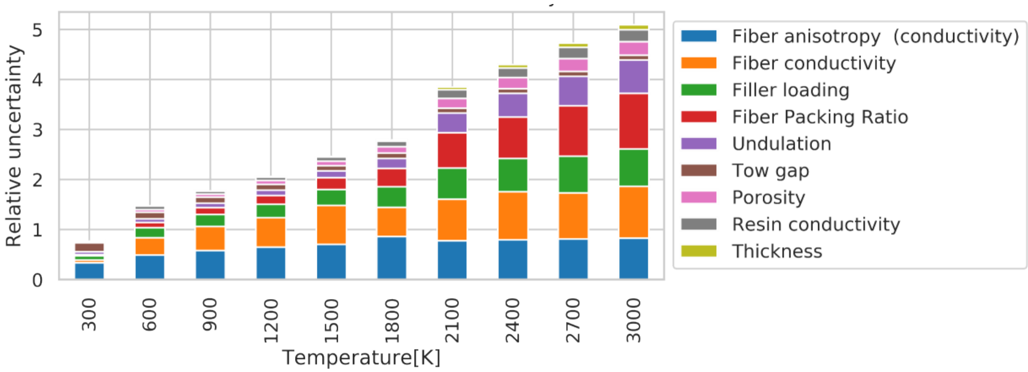




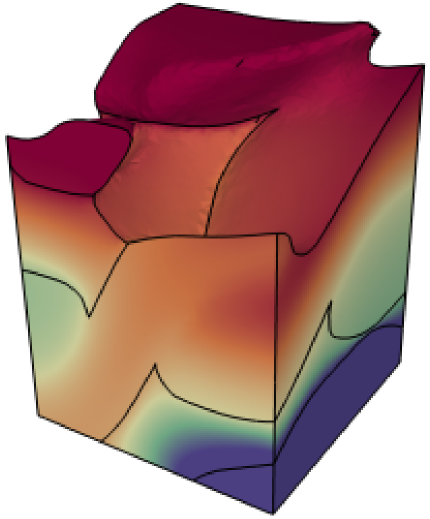
Analytical and image-based modeling (Foster)



Manufacturing of C-C



Property prediction, interpolation, and UQ



Ablation predictions (Collins)