Thermomechanical modeling of woven materials with particle-based, explicit-fiber simulations

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16th Ablation Workshop

ENTRY SYSTEMS MODELING

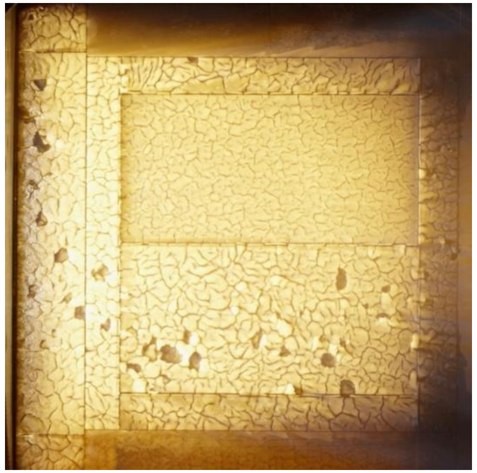
Outline

- Why model TPS thermomechanics and micromechanics?
- The approach and its applicability
- *Focus* on 3mdcp thermal conductivity
  - Yarn
  - Weave
  - Resin
- *An illustrative model:* Weave-driven ablation augmentation

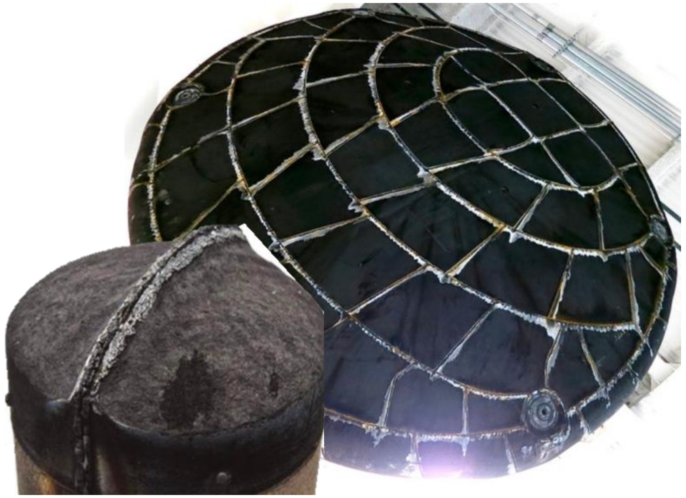
TPS Thermomechanics and fracture during entry

The thermal response of thermal protection systems (TPS) is paramount.

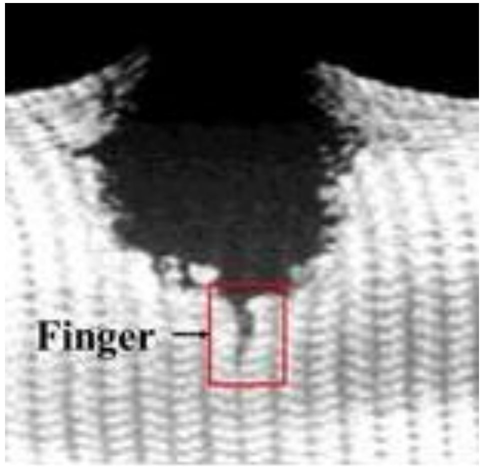
Mechanical behavior of TPS becomes crucial for anomalous cases:
- Manufacturing defects, experimental testing
- Aerothermal loads, CTE mismatch
- Fracture, from entry, MMODs



Avcoat fracture in ArcJet. NASA



Fencing in (left) RTV-PICA and (right) Post-flight Dragon, SpaceX

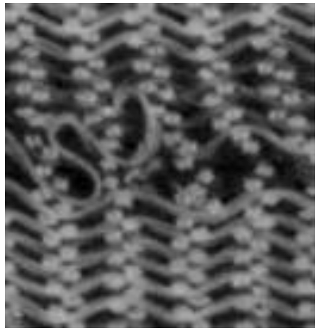


Impact of a woven TPS.

Oruganti, et al. ICTMS (2024)
Libben, et al. FIODC (2019)

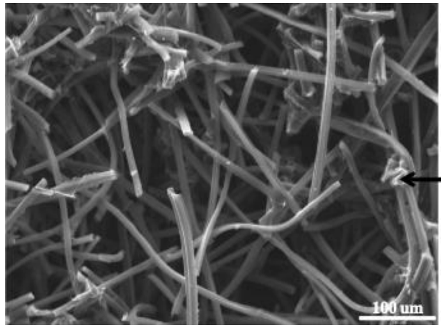
Micromechanics are important to TPS entry

TPS fracture and manufacturing-based variability are strongly influenced by the **fiber microstructure** and interactions.



Weaving defects

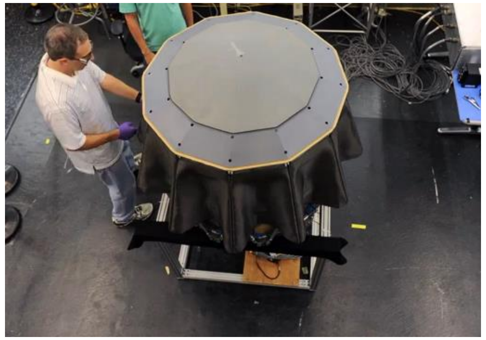
Felting, compaction, MERINO/NASA



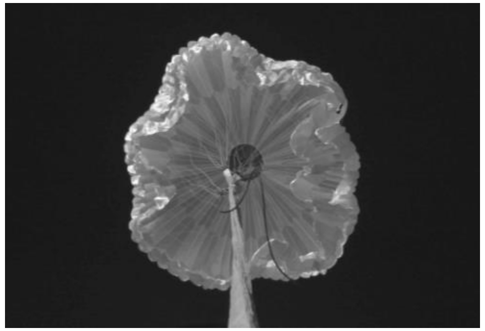
Fiber type: Rayon/lyocell/PAN

Deployable TPS undergoes large-scale deformation

LOFTID deployment before entry. NASA



Adept deploying. NASA



Perseverance parachute opening. NASA

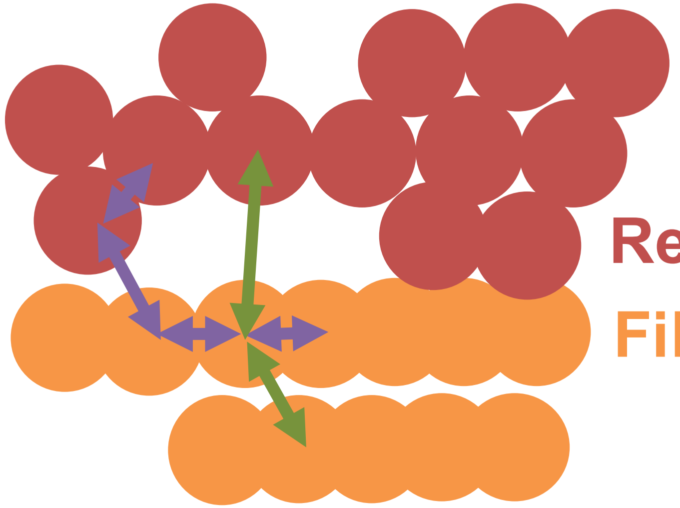
Discrete elements with bonded particle models can capture these features.

Bonded Particle Model Parameters

Inherently captures fiber anisotropy

Micromechanics-informed model:

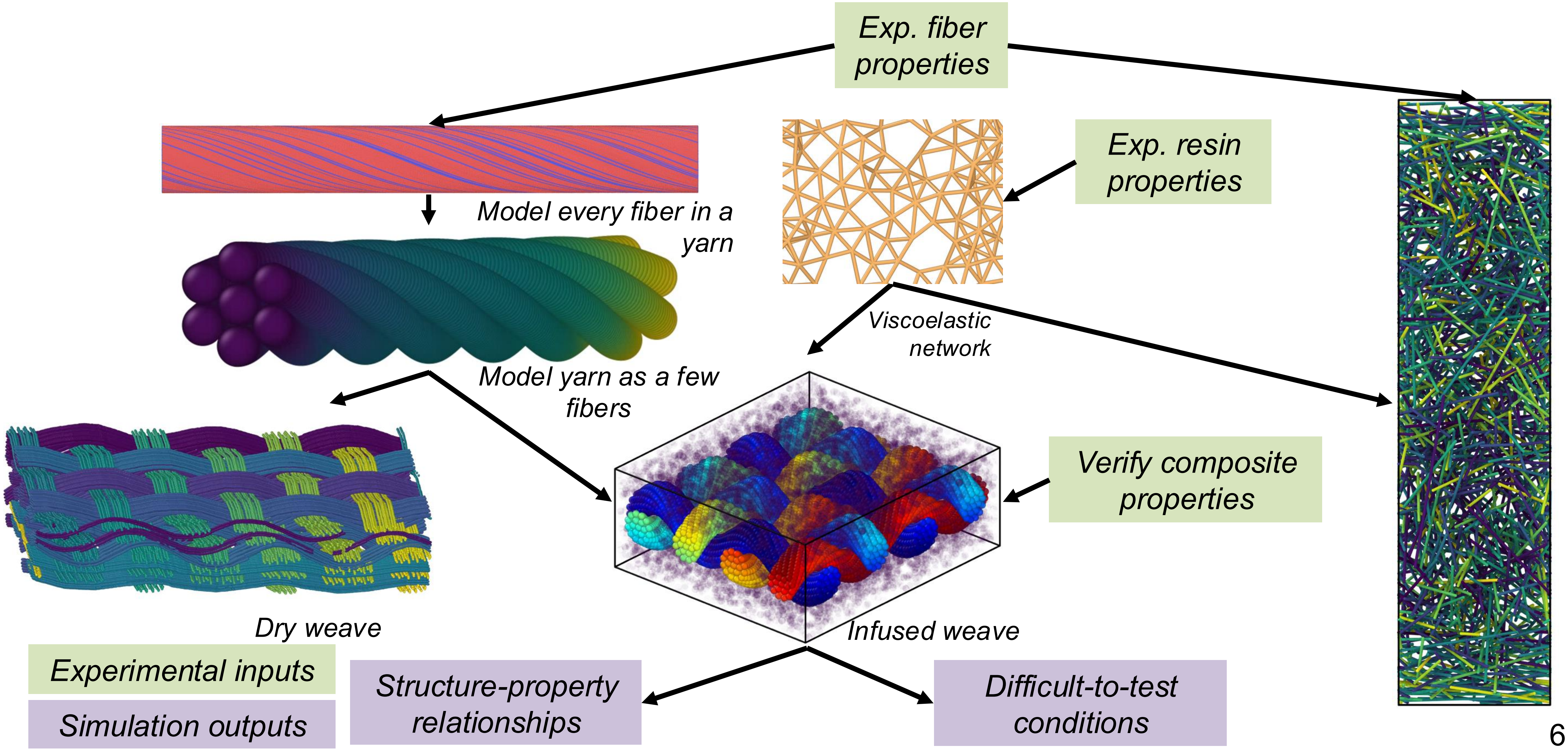
- Intra-fiber, fiber-resin, resin-resin[1,2], bonded forces
  - Elastic stretch, bend, shear, twist
  - Viscous damping
  - Rupture
- Inter[3]-fiber and fiber-(void)-resin, contact forces (DEM)
  - Friction
  - Viscoelastic repulsion
  - Cohesion



Component	Input Property
Resin	porosity, tanδ
Fibers	density, diameter, friction, contact modulus
Resin, fibers, resin-fiber bonds	conductivity, heat capacity tensile, shear, flexural moduli & strength,

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

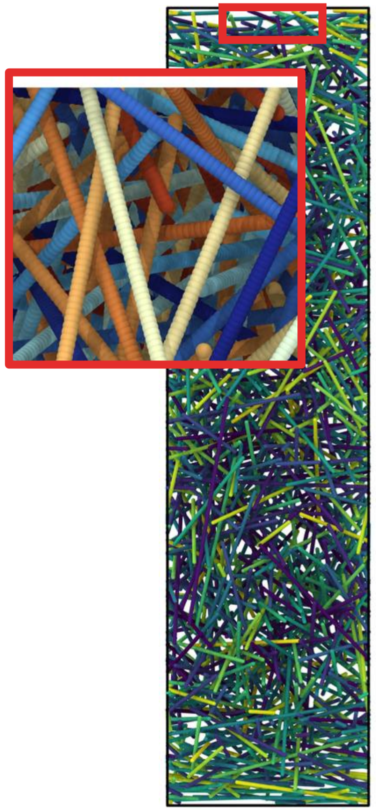
Bonded Particle Models for TPS Composites



Bonded particle models for TPS

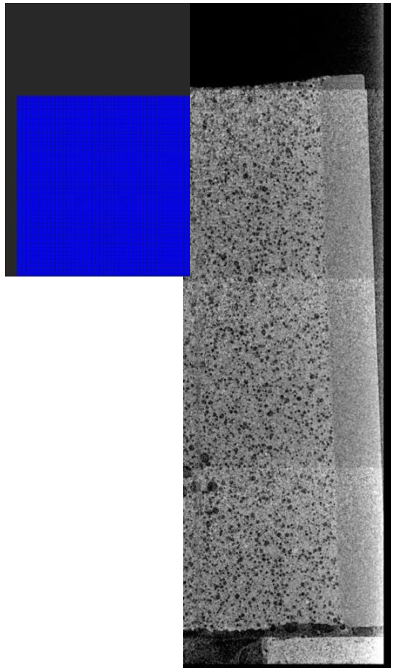
These methods are being applied to understand phenomena and properties in other TPS and entry/descent materials

FiberForm/PICA



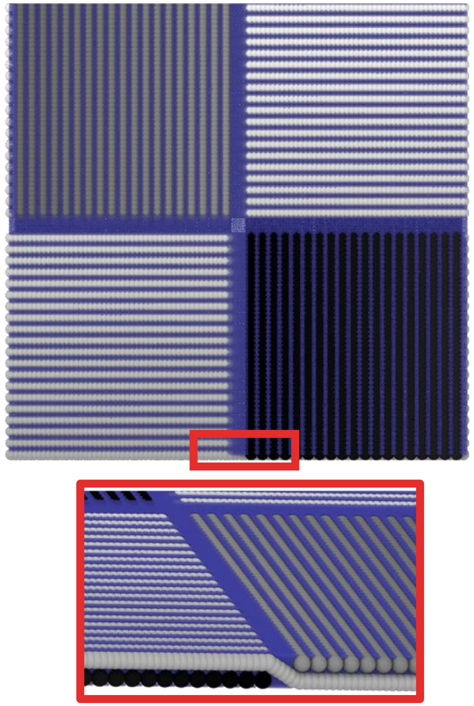
Network of rigid fibers using a BPM

RTV



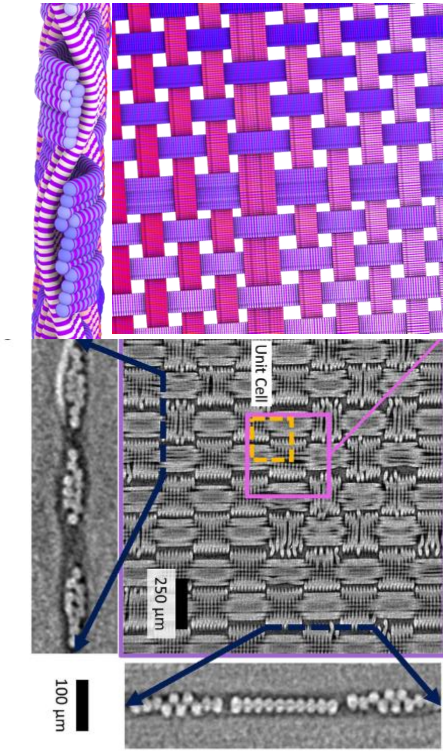
(left) peridynamics modeling [Kyle Watson] (right) in-situ heating at the ALS by Bessire, Hiss, Pokharel et al.

Carbon-epoxy (face sheet)



Part of effort comparing BPM, FEM and FVM.

Parachutes

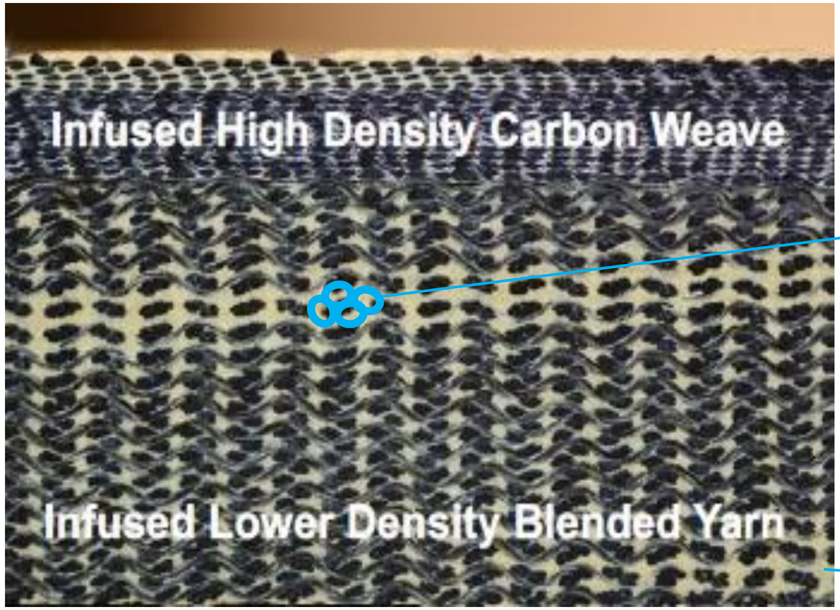


(top) BPM snapshot (bottom) Phillippe, et al., AIAA J.,62 (4691–4700), 2024.

Focus on 3MDCP

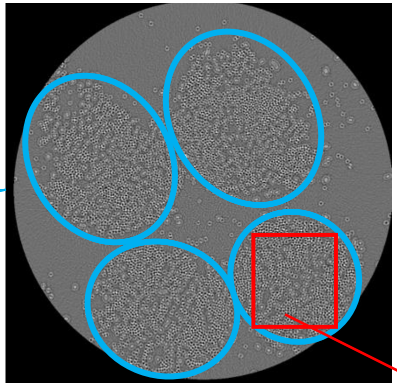
- Mid density 3D woven TPS (3MDCP), fills a density and structural robustness TPS gap
  - Capturing multiscale features of the composite requires unique models

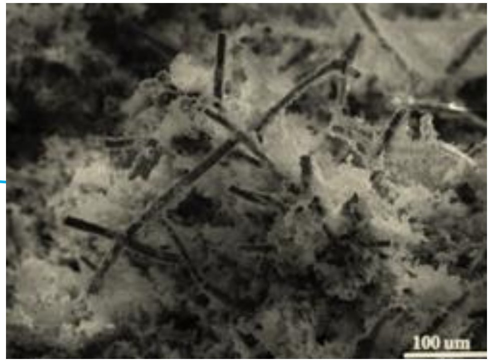
HEEET Weave



3D woven carbon-phenolic blended yarns infused with phenolic resin

4-Ply Twisted Tow Stretch Broken



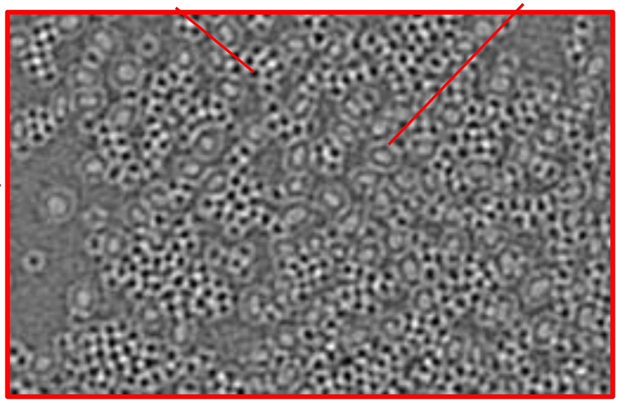


Phenolic

Blended Yarn

Carbon fiber

Phenolic fiber



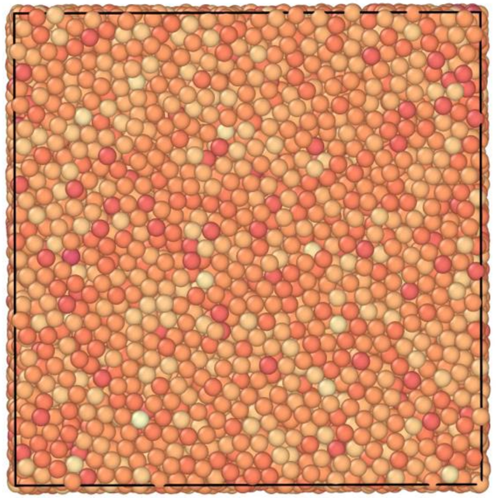
D Ellerby et al, MS&T, 2019
Agrawal, Chavez-Garcia, *J. Spacecraft Rockets*, (4) 50, 2013
CT Scans by Kyle Hendrickson

Porosity and crosslinking to resin model

Phenolic resin provides excellent ablative properties.
Varying crosslinking and density are used in TPS.

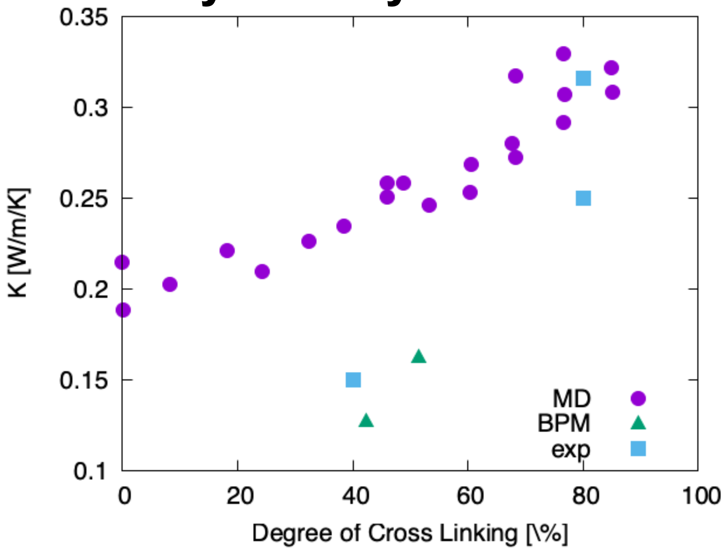
- The bonded particle model properties are set to match dense Young's modulus and thermal conductivity
- Experimental trends are matched by decreasing bonds/particle (crosslinking) and adding pores

Resin model resolves complex fracture paths



Phenolic resin bonded particle model tensile simulation, particles are colored by number of bonds (black:0 to orange:17)

Explicit porosity and crosslinking, captures conductivity-density and -crosslinking trends



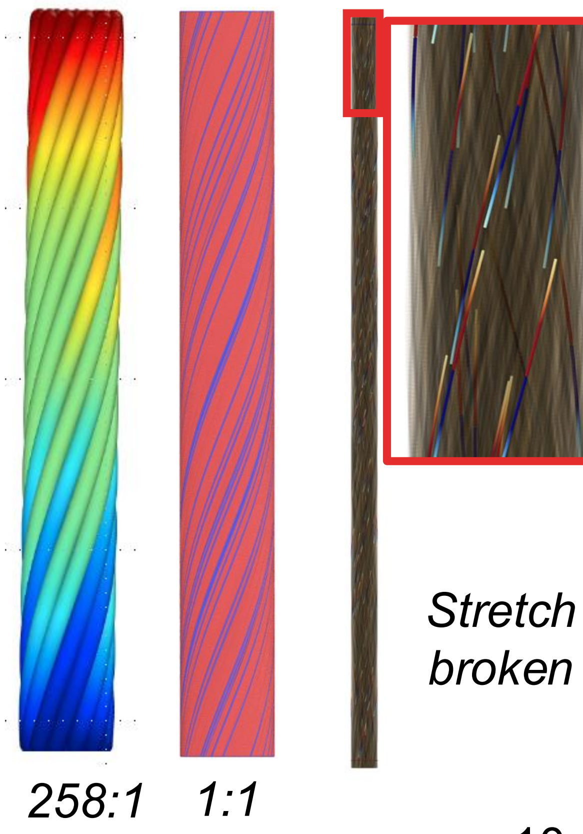
Conductivity as a function of cross linking in MD, BPM and experiments.

Monk, J. D. et al. *Macromol.* **2015**, *48* (20), 7670–7680

Coarse-grained 1-ply Dry 3MDCP Yarn

- **Coarse-grained explicit-fiber method agrees with PuMA and NASMAT**
  - **full yarn model conductivity is much lower and being investigated**

	Material	Conductivity [W/m-K]
components	*carbon fiber (exp)*	6.83
	kynol fiber (exp)	0.000190
	phenolic resin	~0.1
Explicit yarn	Area averaging	1x
	twisted/continuous/dry	0.063x
	twisted/stretch-broken/dry	0.013x
	twisted/stretch-broken/infused	0.1x



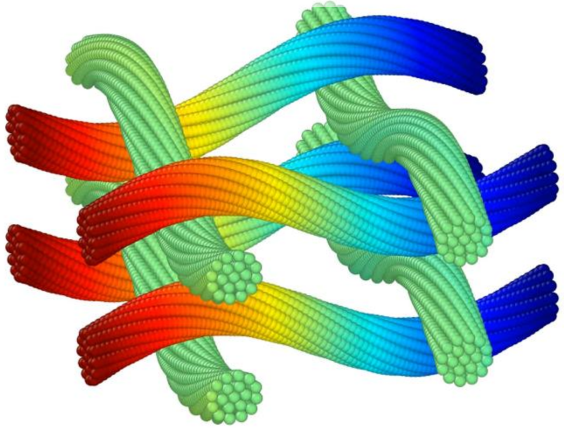
Weave Density and Conductivity for a 2D Weave

Thermal conductivity increases with decreased fiber path and yarn density

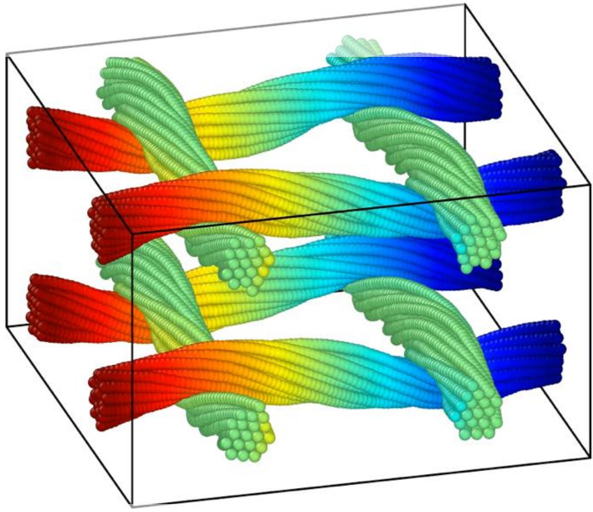
Yarns are fully carbon, not blended

Weave	Yarn Conductivity [normalized]
As-generated	1
Tightened	1.09
TT compressed	1.11
IP compressed	1.14

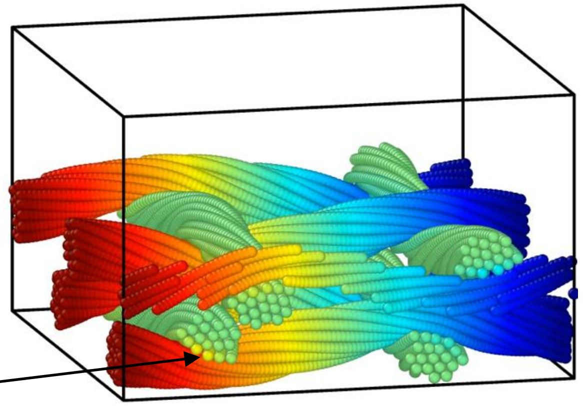
(a) In-plane thermal conductivity of different 2D plain weave variants



(b) As-generated

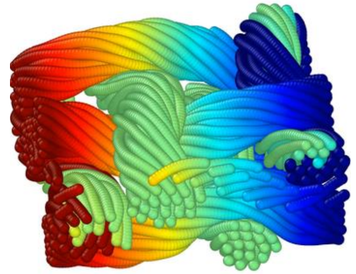


(c) Tightened



Yarn-to-yarn conduction via contact

(d) TT Compressed

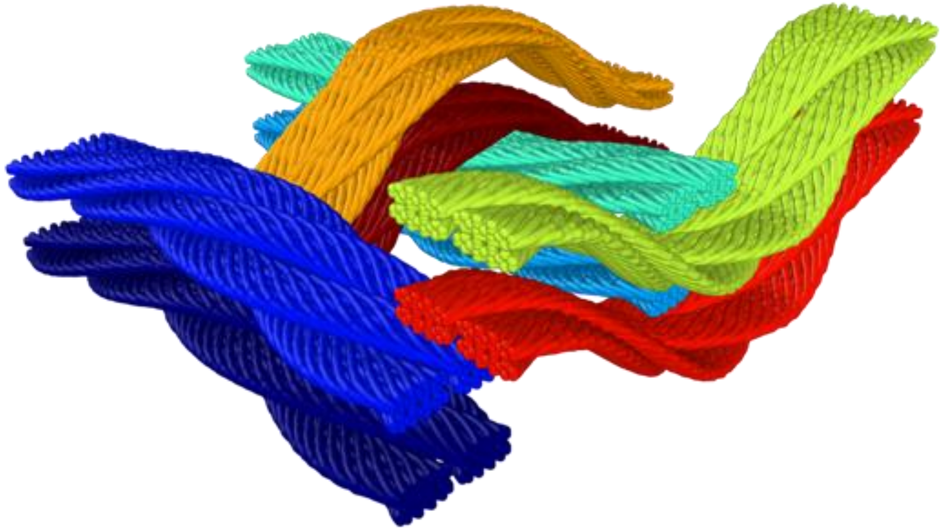


(e) IP Compressed

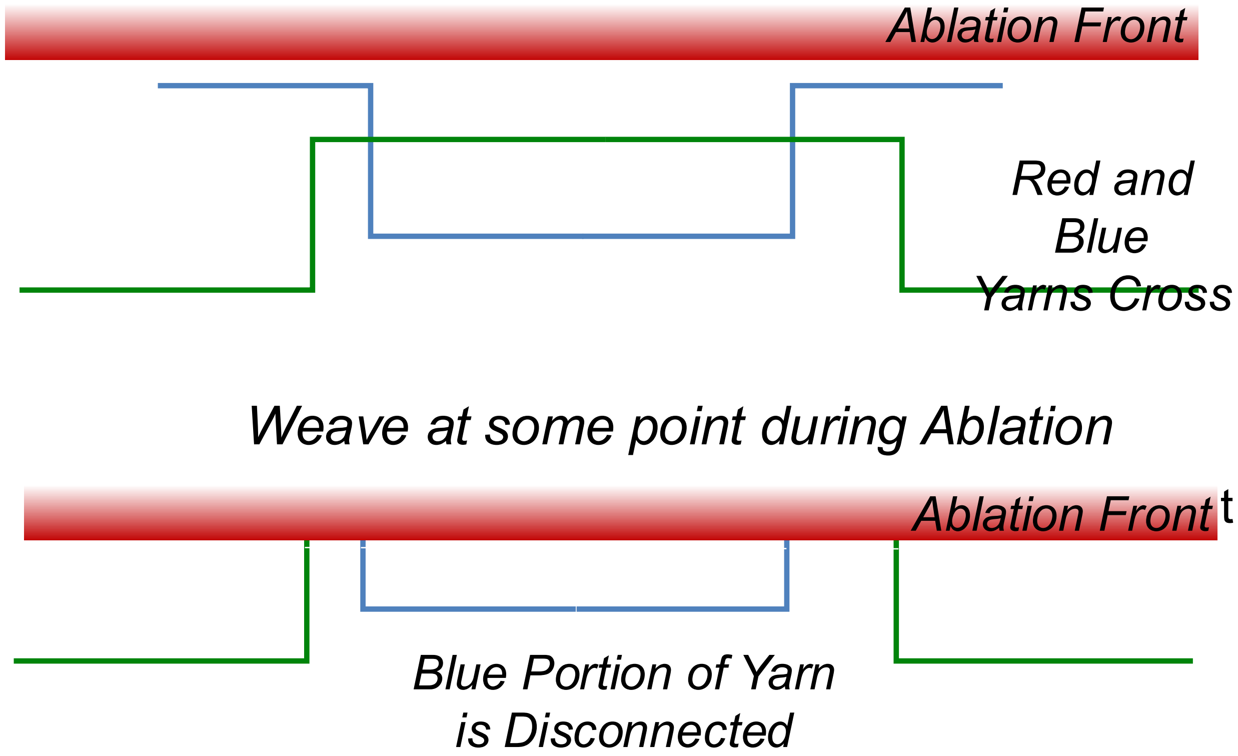
An illustration - ablative disconnection of yarns

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

3D Weave unit cell

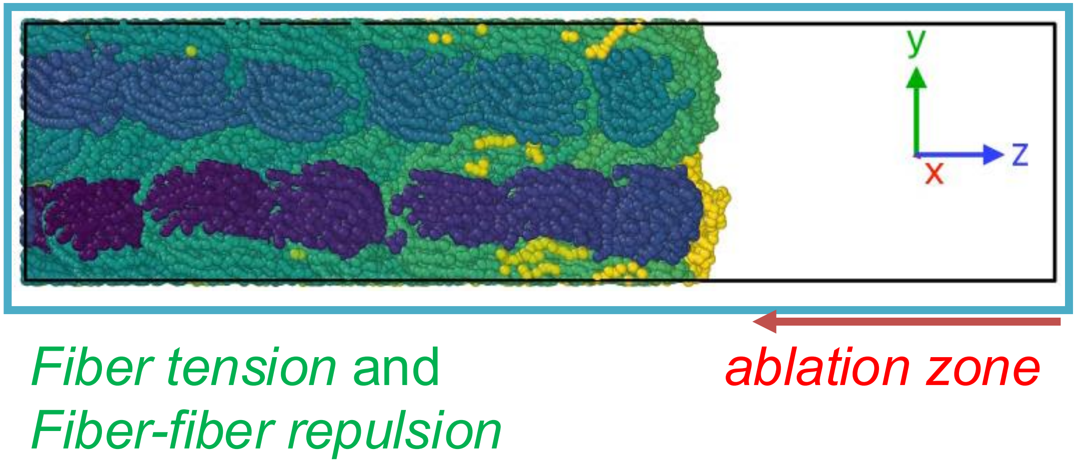


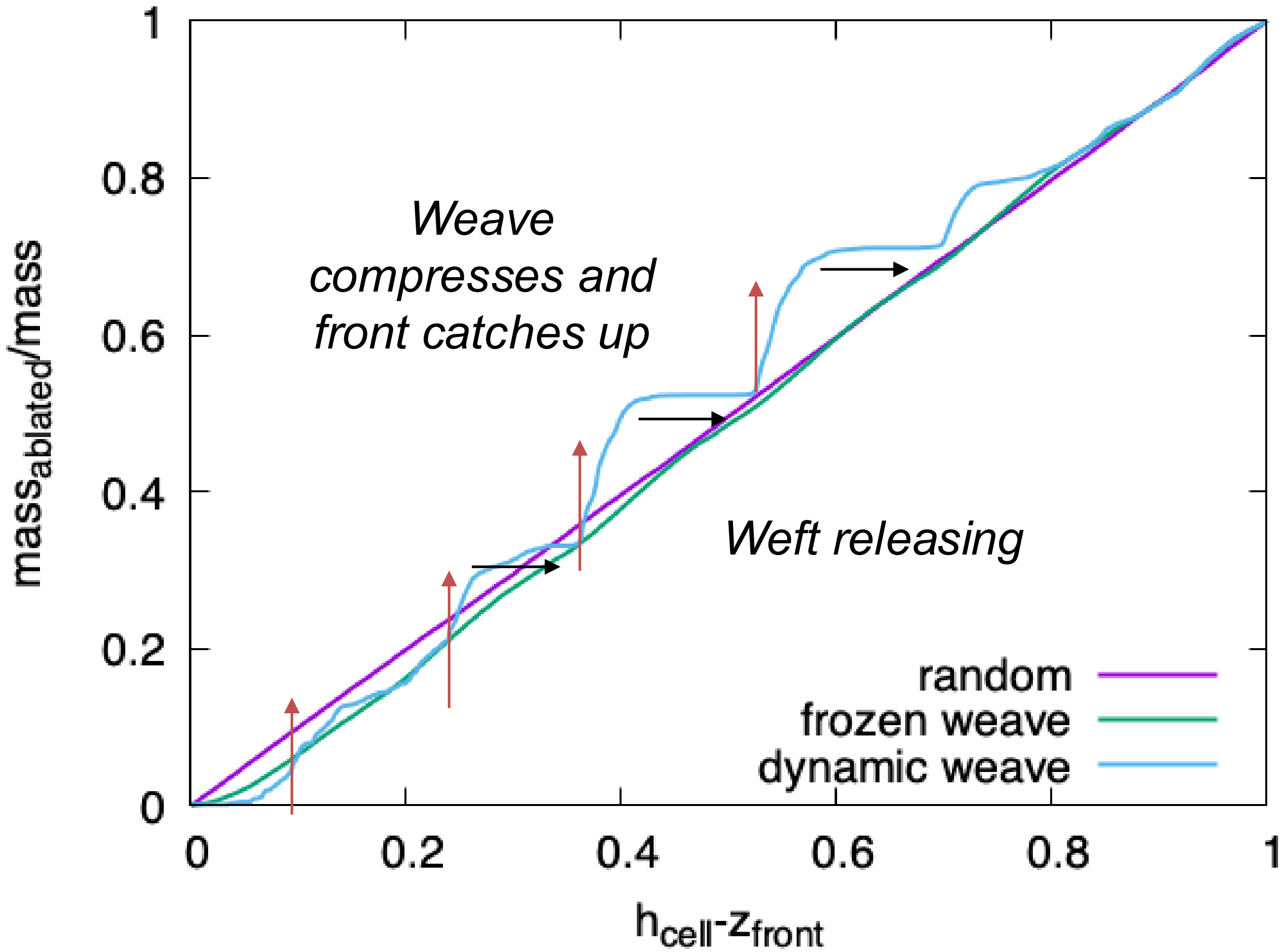
Weave before Ablation



Augmentation from loss of weave connectivity

The yarn length scale appears in the ablative behavior of woven TPS





- Large portions of weft fibers ablate at high rate due to the 3D, layered weave
- Area between blue and green curves constitutes enhanced ablation

The mechanics of this behavior is important. Lab experiments can validate the model mechanics.

Thank you, any questions?

Upcoming

- Report on bonded particle, finite volume and finite element methods for woven composites
- Using simulations to parse the role of microstructure and fiber type in networked TPS, specifically PICA

Conclusions

- Explicit **connectivity and porosity in phenolic** captures drop in conductivity
- **Yarn microstructure,** twist and stretch breaking, decreases thermal conductivity
- **Weave compression** increases thermal conductivity
- 3D weave pattern can lead to augmented **ablation**

Acknowledgements

Entry Systems Modeling (ESM) Project

TPS Certification by Analysis

Core Team Members

ARC

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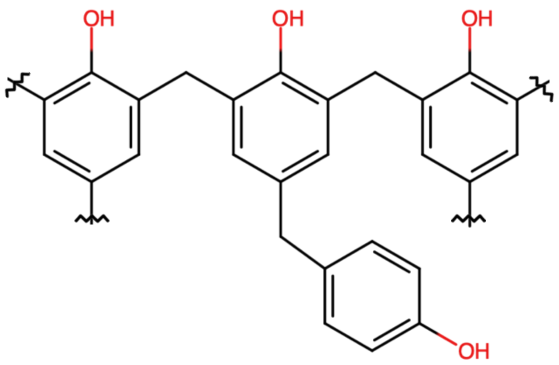
Aaron Allred, CU Boulder
Chloe Zeller, UMN
Michael Olaya, U Mass Lowell
Victoria Arias, UIUC
Joseph Ferguson, Stanford U.
Alexandre Quintart

Phenolic-Containing Thermal Protection Materials

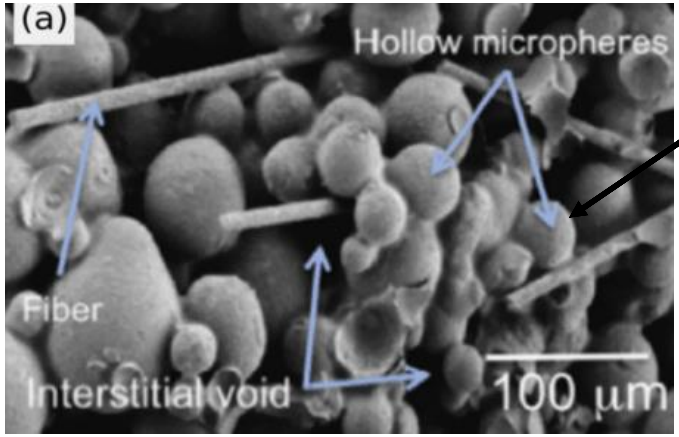
Phenolic resin provides excellent ablative properties at a low density

Support structure:

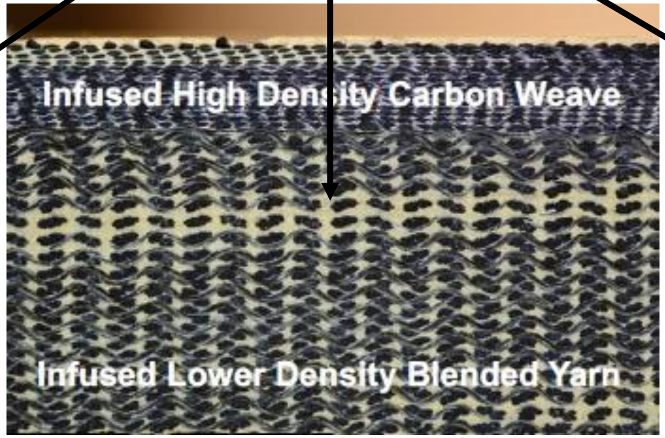
- Glass fiber (AVCOAT),
- Carbon fiber network (PICA)
- Carbon fiber weave (3MDCP, HEEET)



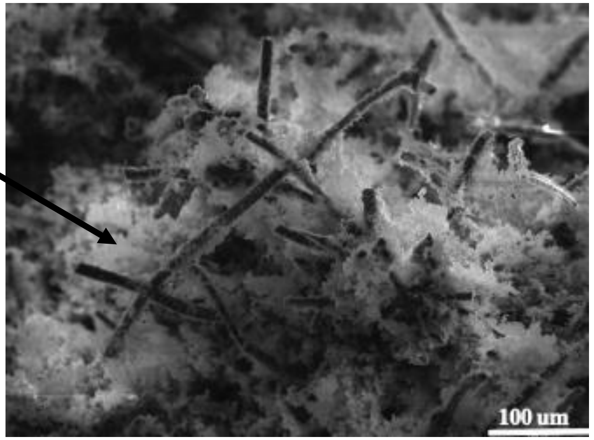
Phenolic resin



Phenolic hollow spheres, fiberglass, epoxy, (Avcoat)



3D woven carbon-phenolic blended yarns infused with phenolic resin

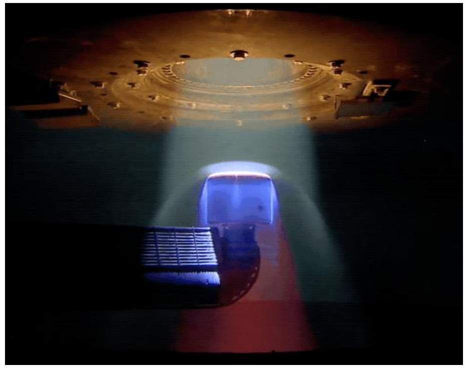


Phenolic Impregnated Carbon Ablator

Sawant, S. et al. *IJHMT* **2019**, *133*, 1176–1195.
D Ellerby et al, MS&T, 2019; Bessire, B. et al. *ACS Appl. Mater. Interfaces* **2017**, *9* (25), 21422–21437
Agrawal, Chavez-Garcia, *J. Spacecraft Rockets*, (4) 50, 2013

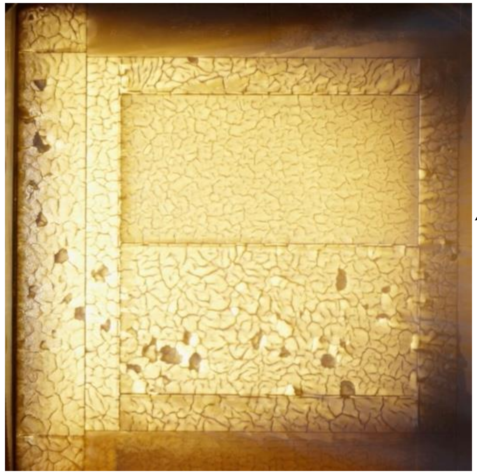
Thermal Response of Phenolic-Containing Materials

Phenomena we want to capture:
- Entry
- How does fracture affect entry, from
  - MMODs, manufacturing, entry stresses

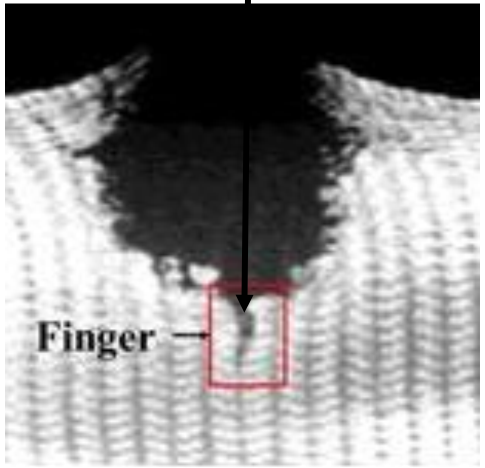


PICA ablating in the ArcJet. NASA

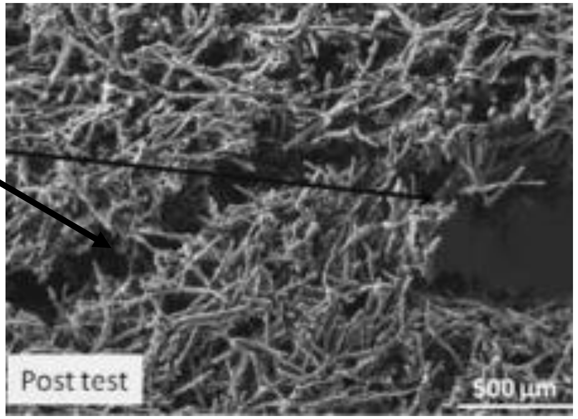
Phenolic drives fracture



Avcoat fracture in ArcJet. NASA



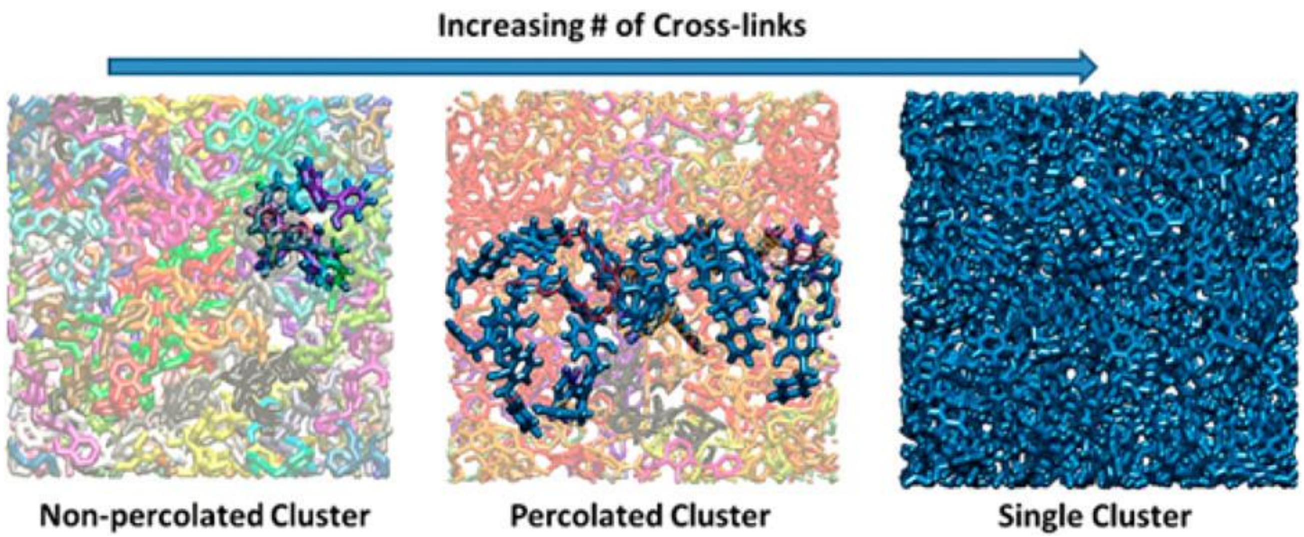
Impact of a woven TPS

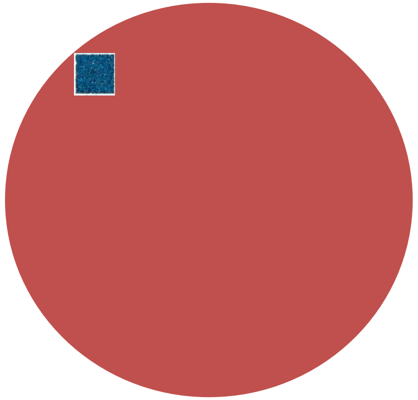


SEM of fractured PICA

Libben, et al (2019)
Agrawal, Chavez-Garcia, *J. Spacecraft Rockets*, (4) 50, 2013

Particle and Meshfree Methods





Molecular dynamics

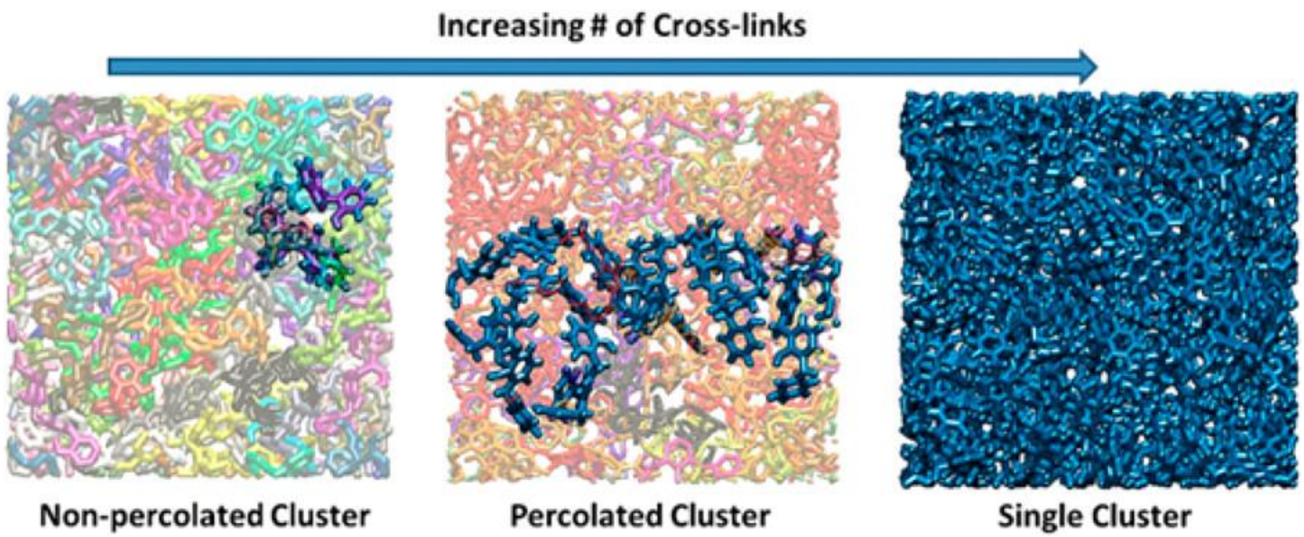
- Simulate each atom with classical statistical mechanics
- bridge RXN competition
- Role of crosslinking on conductivity, modulus, CTE
- Cross link density effect on fracture behavior

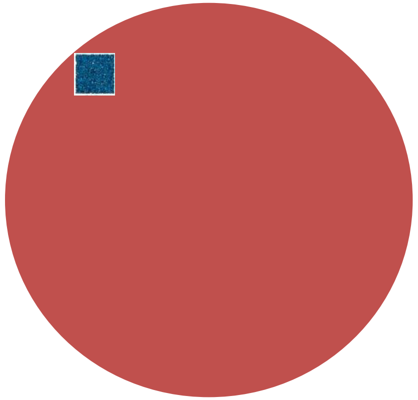
Bonded particle

- Between statistical and continuum mechanics
- 10^4-10^{10} monomers/particle
- Bond modes of deformation follow experimental parameterization

Abbott, A. et al. ACS Fall 2022
Monk, J. D. et al. *Polymer* **2015**, *62*, 39–49.
Monk, J. D. et al. *Macromol.* **2015**, *48* (20), 7670–7680.
Santos, et al. Particles, 2023

Computational Approaches to Phenolic models





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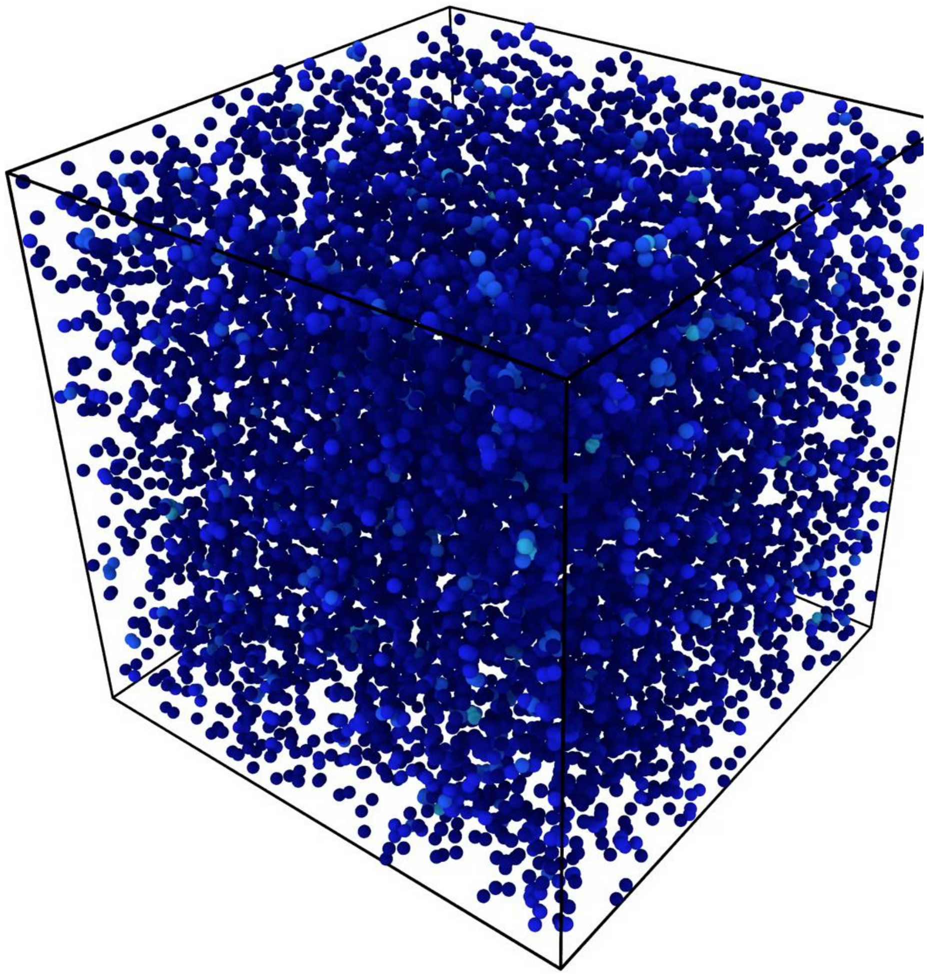
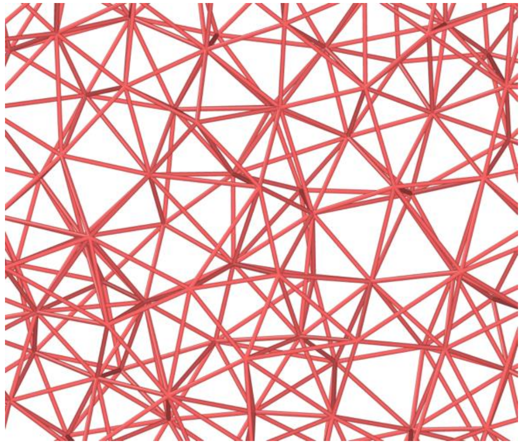
Monk, J. D.;et al. *Macromol.* **2015**, *48* (20), 7670–7680.
Santos, et al. Particles, 2023

Resin Configuration Generation

1. Generate random packing:
   a) 20,000 particles in Start from a low volume fraction
   b) Vary triclinic box dimensions to satisfy a very low pressure tensor
   c) Discrete element modeling (DEM) with frictionless Hertzian contacts
2. Add bonds:
   a) contacting and next-nearest neighbors (within ~1.5D); 10-17 bonds/particle
   b) Vary bonding radius R_b=7.5, 8.5µm ($\langle N_{\text{bonds}} \rangle$=11, 13.4 respectively)



Granular packing to form random network

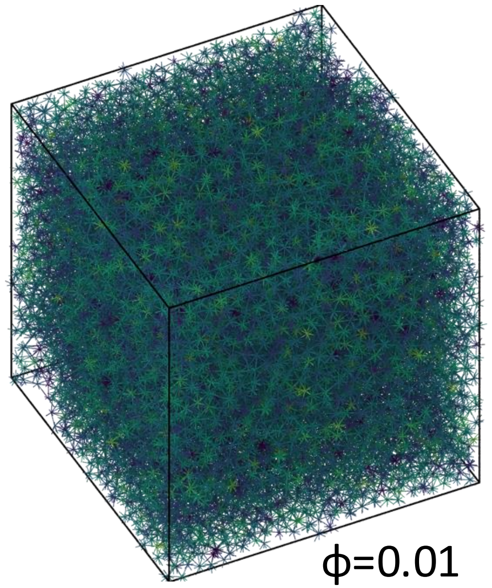


Visualization of a slice of the bond network.

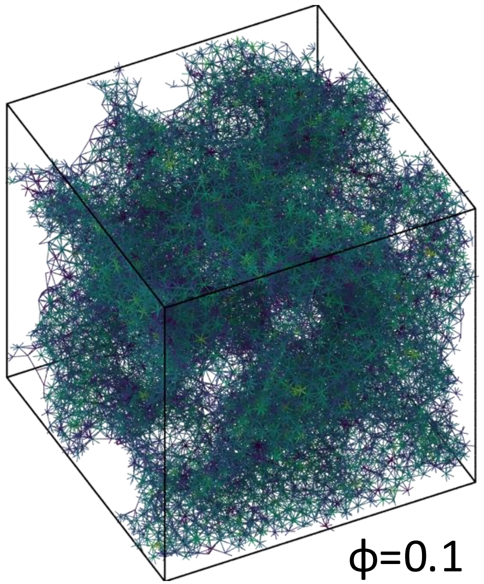
Plimpton S. (1995). *J. Comput. Phys.*, 117, 1-19.
Mindlin, R. D. (1949). *J. Appl. Mech., ASME* 16, 259-268.
Luding, S. (2008). *Granular matter*, 10(4), 235.
Santos, A.P. *et al.* (2020). *Phys. Rev. E*, *102* (3), 032903
CIF22, ESPUR
Clemmer, J. T. et al. (2022) *Phys. Rev. Lett*, *129* (7), 078002

Explicit Porosity and Network Connectivity

1. Generate random packing:
   a) 20,000 particles in Start from a low volume fraction
   b) Vary triclinic box dimensions to satisfy a very low pressure tensor
   c) Discrete element modeling (DEM) with frictionless Hertzian contacts
2. Add bonds:
   a) contacting and next-nearest neighbors (within ~1.5D); 10-17 bonds/particle
   b) Vary bonding radius R_b=7.5, 8.5μm ($\langle N_{\mathrm{bonds}} \rangle$=11, 13.4 respectively)
3. Add Porosity explicitly
   a) Delete spherical segments of material
   b) Vary pore radius R_p=3μm, 9μm (0.5D and 1.5D)
   c) Vary porosity ϕ=0.01, 0.1

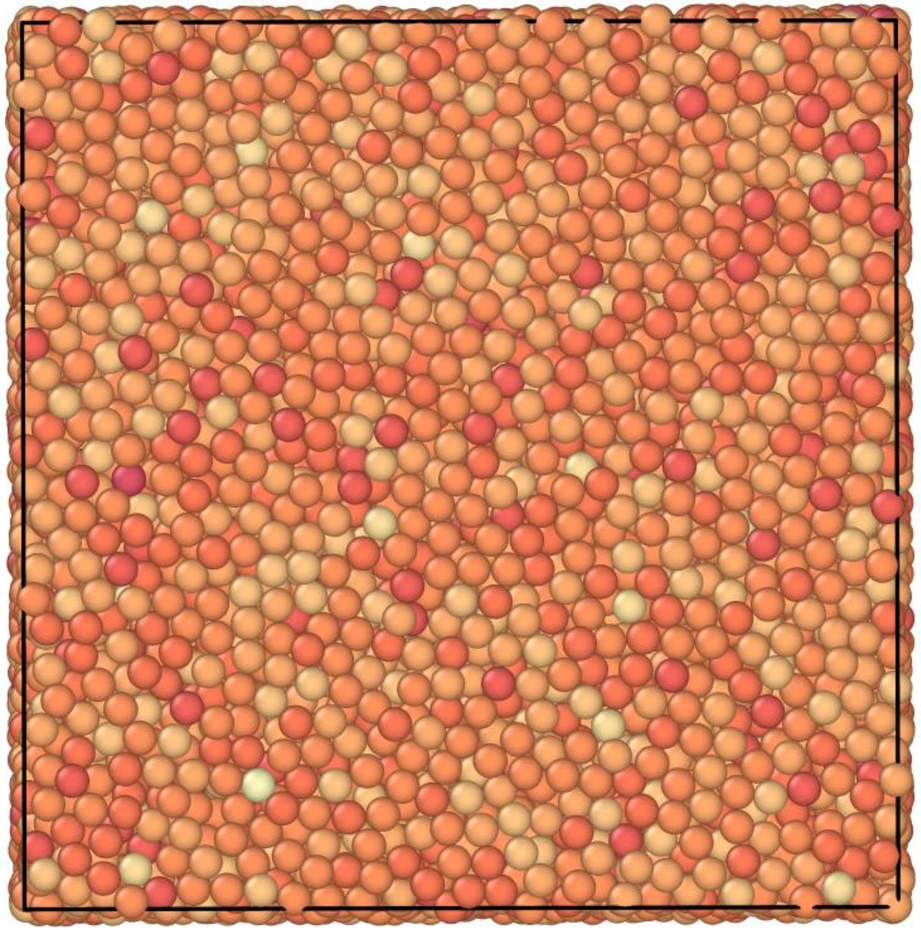


ϕ=0.01

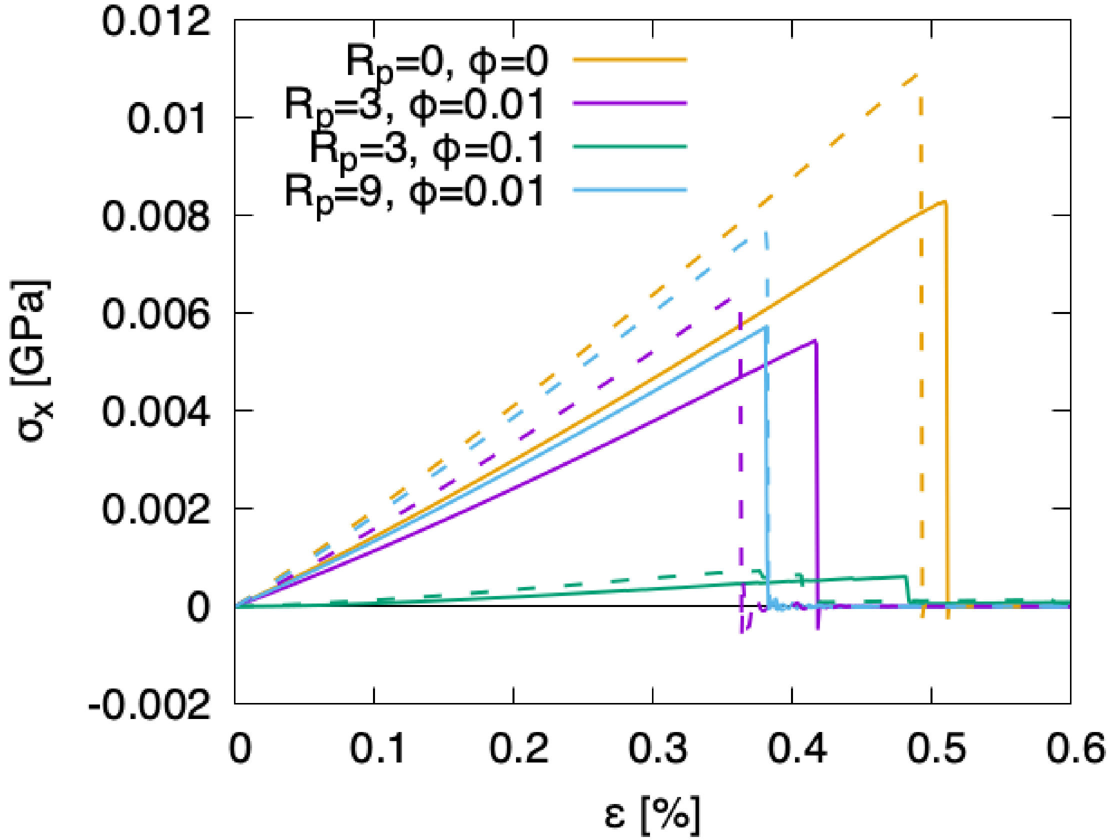


ϕ=0.1

Tensile Deformation

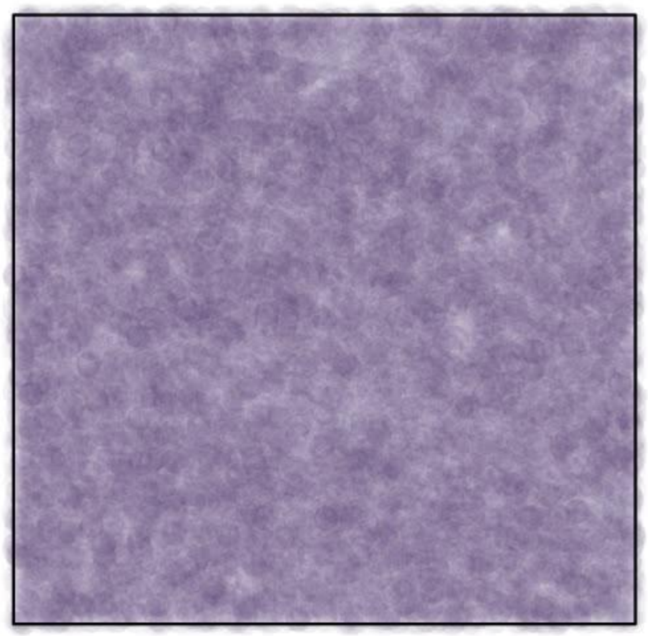


Phenolic resin bonded particle model tensile simulation, particles are colored by number of bonds (black:0 to orange:17)

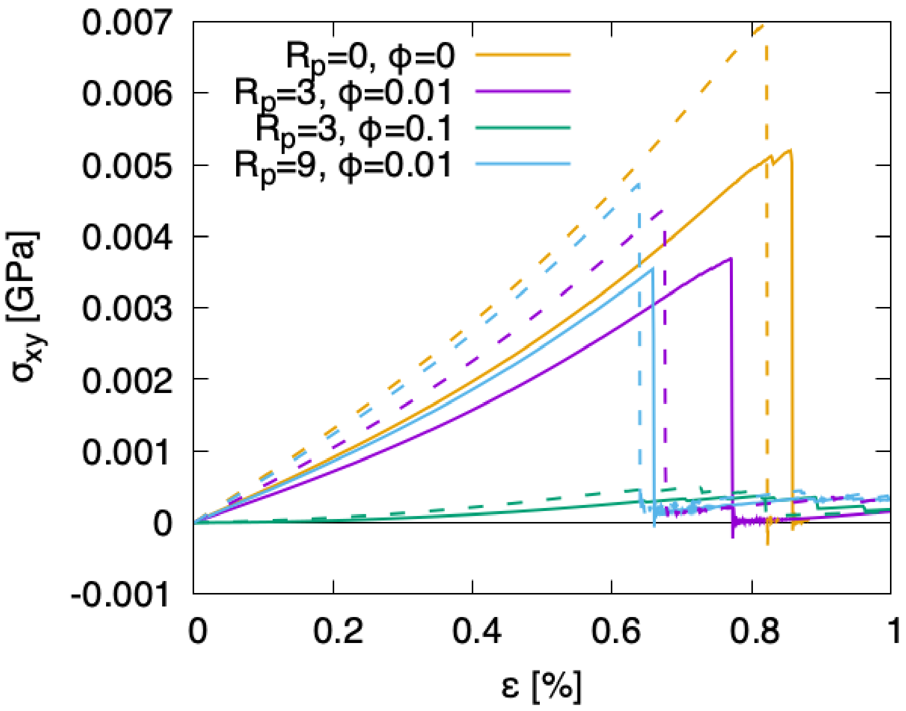


Preliminary tensile stress vs strain $\langle N_{\text{bonds}} \rangle$*= 11 (solid) and 13.4 (dashed), and porosity features.*

Shear Deformation

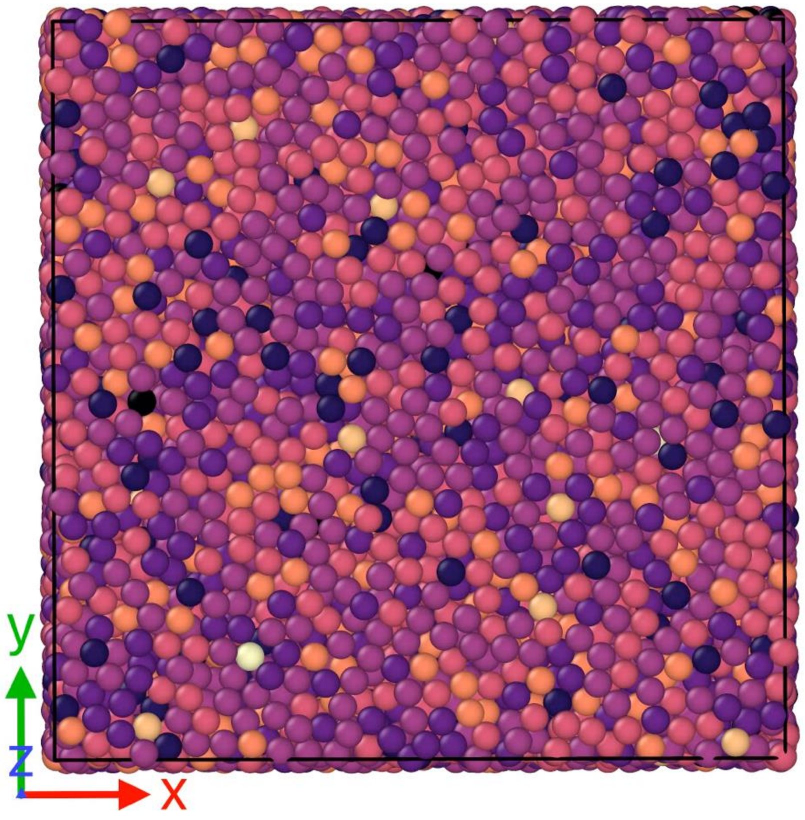


Phenolic resin bonded particle model shear simulation. Particles are colored by per-particle stress (black:-0.25 to orange:2.85 GPa. Transparency increases with number of bonds (max 17, min 0).

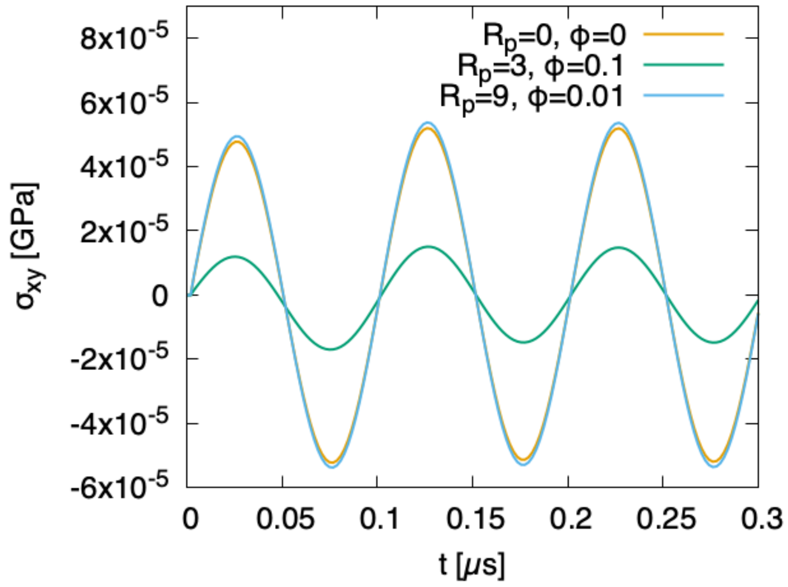


Preliminary shear stress vs strain $\langle N_{\mathrm{bonds}} \rangle$= 11 (solid) and 13.4 (dashed), and porosity features.

Storage and Loss Modulus

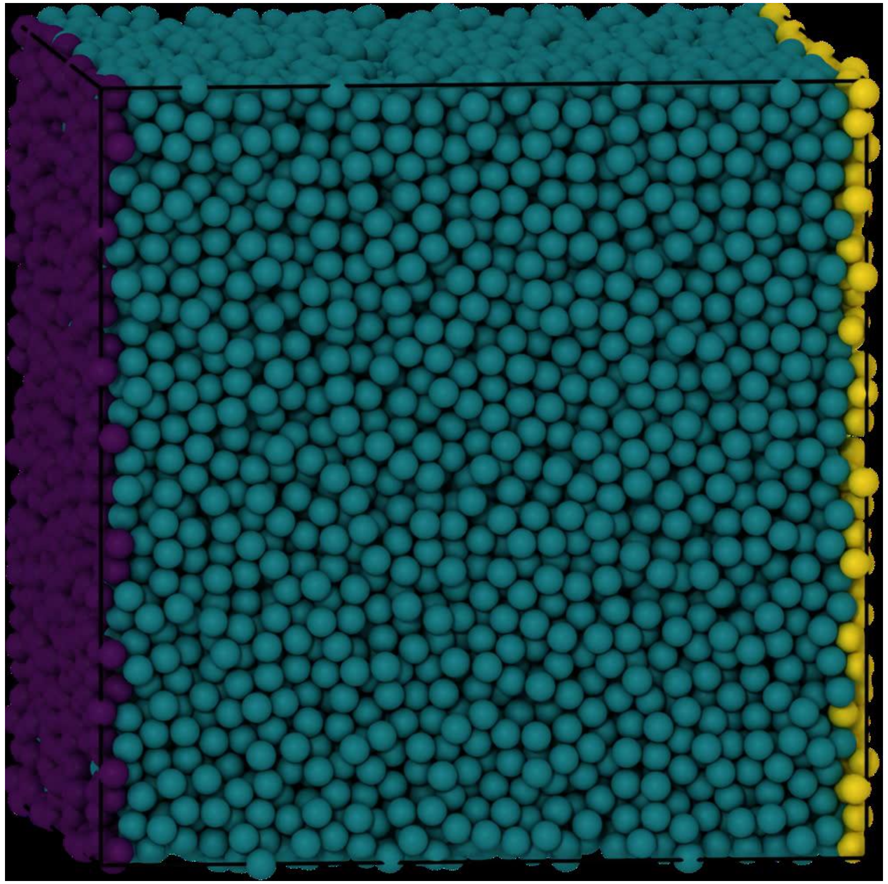


Visualization of a frequency oscillatory shear sweep (0.1 to 10 Hz) of bonded-particle resin matrix model.

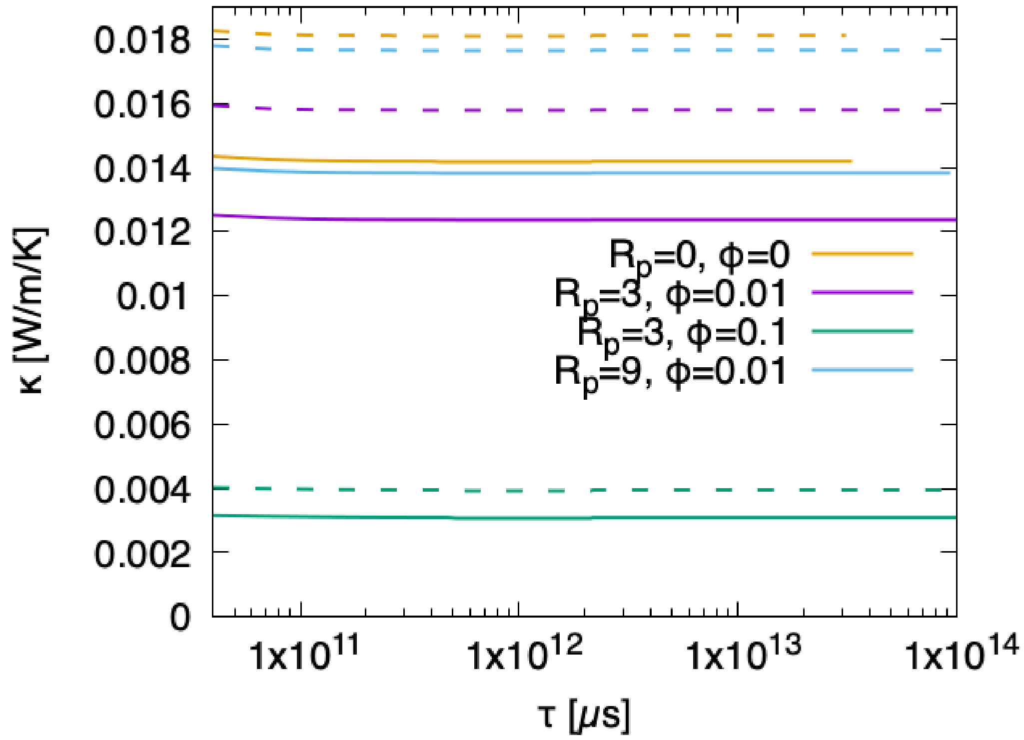


Simulation oscillatory shear stress (solid lines) wrt time for different pore structures. There is very little viscous damping, and thus near-zero loss modulus.

Thermal Conduction



Visualization of thermal gradient progression in phenolic.

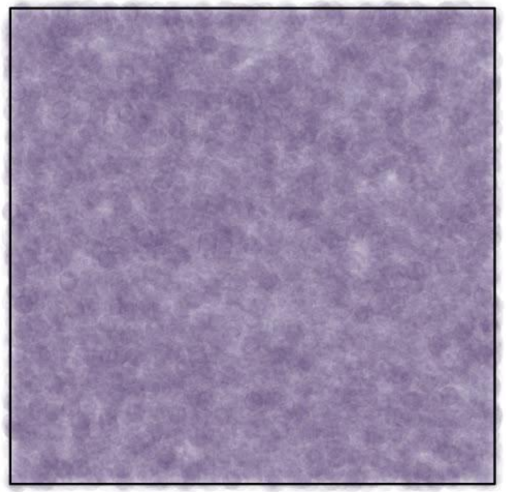


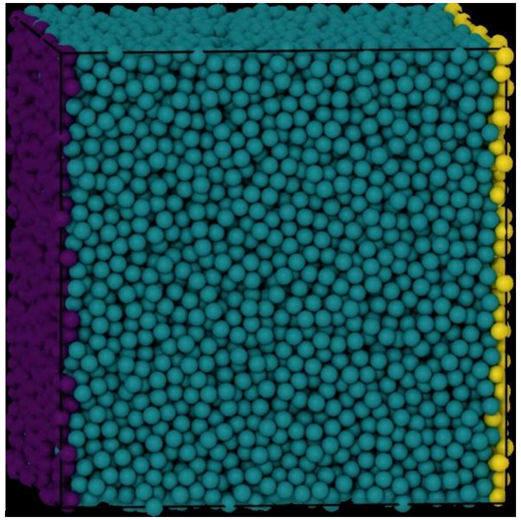
Preliminary conductivity vs time for $\langle N_{\text{bonds}} \rangle$*= 11 (solid) and 1*
(dashed), and porosity features.

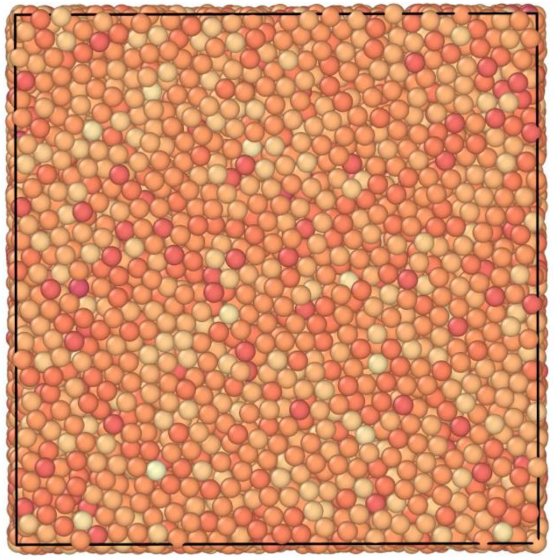
Thank you, any questions?

Conclusions

- **Parameterized** bonded particle network model of phenolic
- Studied the role of random network **connectivity and porosity**







Next Steps

- Study **infused weaves** and networks
- ***Verify*** *network behavior*
- ***In-situ*** properties of phenolic in composites