Entry Systems and Technology Division
Ames Research Center

National Aeronautics and
Space Administration

Particle-based fiber models of woven materials for Earth entry thermal protection

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IS01 session, Particles23, Milan Italy
October 9, 2023

ENTRY SYSTEMS MODELING

ANALYTICAL MECHANICS ASSOCIATES

Heat shields for planetary entry

Heat shields, thermal protection systems (TPS) provide:
- thermal protection
- mechanical strength
- help slow down vehicles during entry

Mission's trajectory and entry environments set the thermal and mechanical requirements

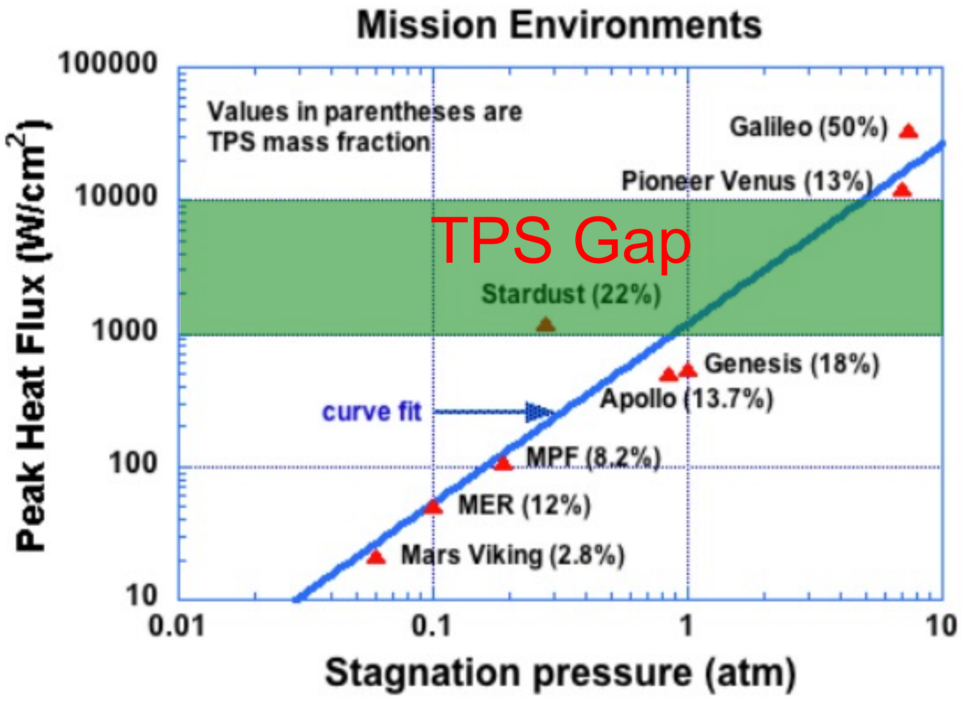
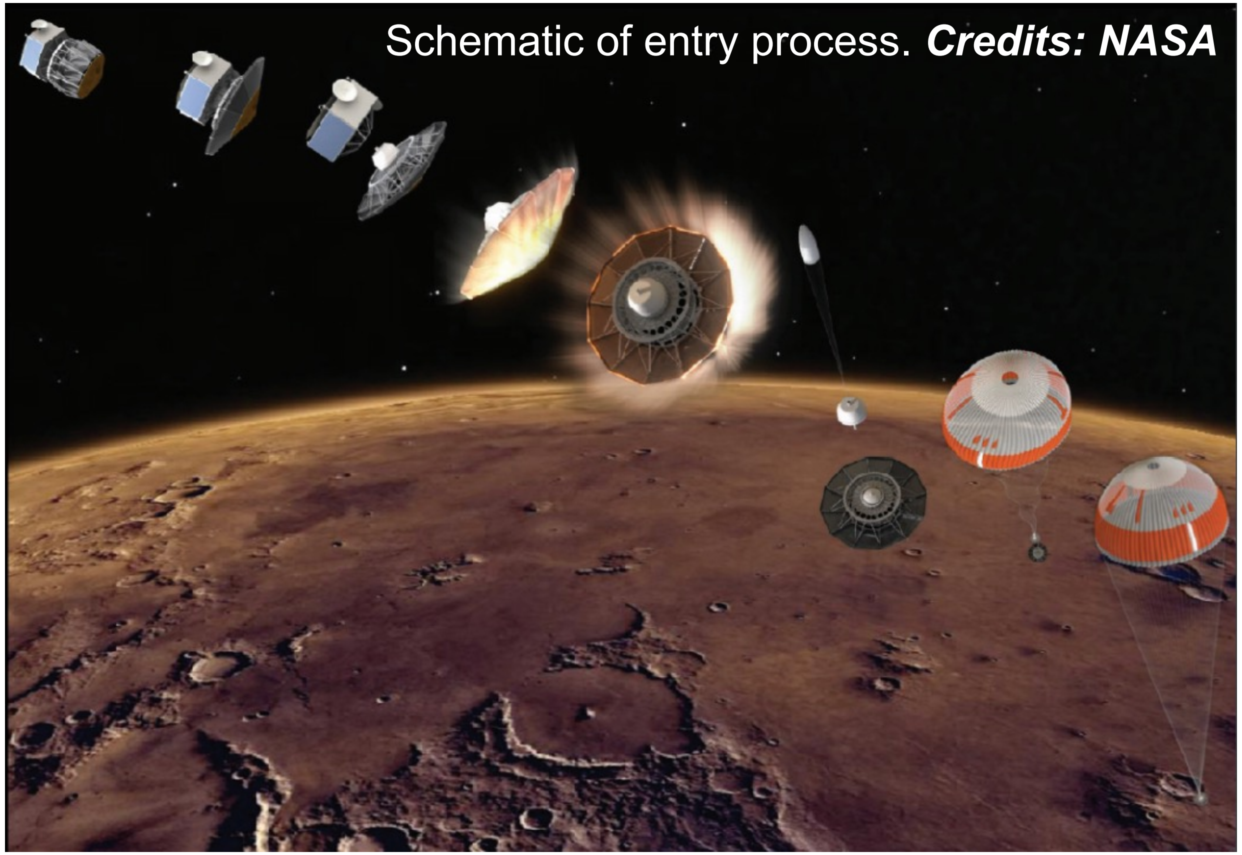


Figure 6.6 Peak heat vs. stagnation pressure for various missions. MER is Mars Exploration Rover; MPF is Mars Pathfinder. (Figure courtesy of Bernard Laub/NASA Ames Research Center)



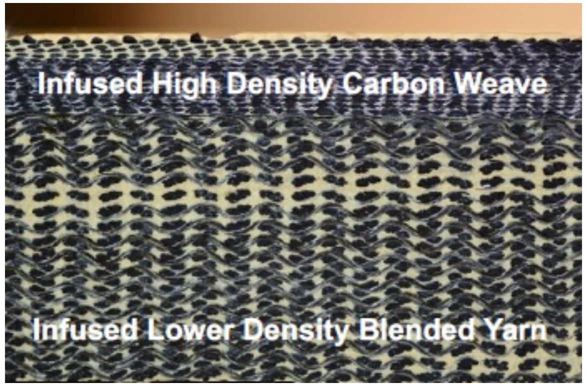
Schematic of entry process. ***Credits: NASA***

New TPS materials need to be developed to fill a gap in payload requirements and minimize risk

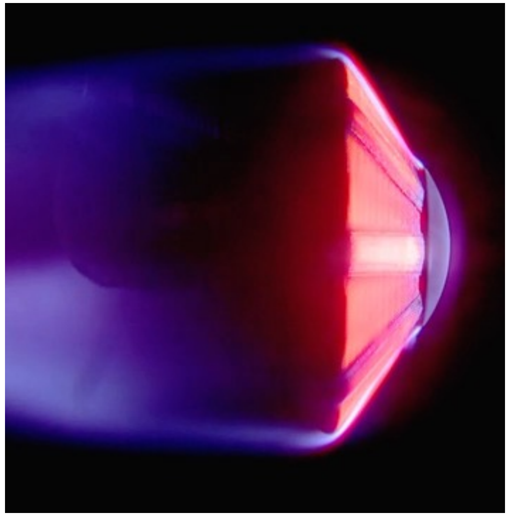
Woven Thermal Protection Systems (TPS)

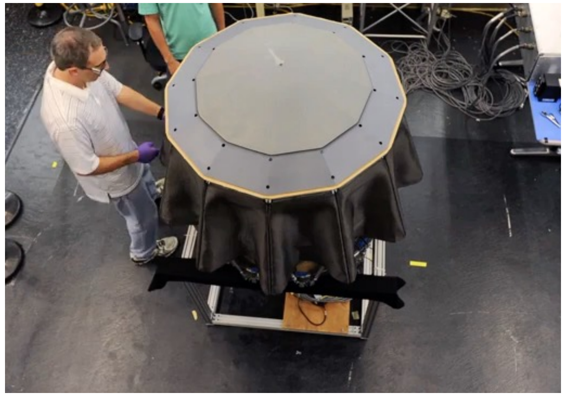
- Woven TPS are **“3D” weaves**, infusible with an ablative resin
  - Flexibility and control in **design density and structure**
  - **Different processing**, compared to carbon network TPS

3D TPS woven with carbon and phenolic fibers infused with an ablative resin



3D TPS woven with carbon fibers in an umbrella-type design





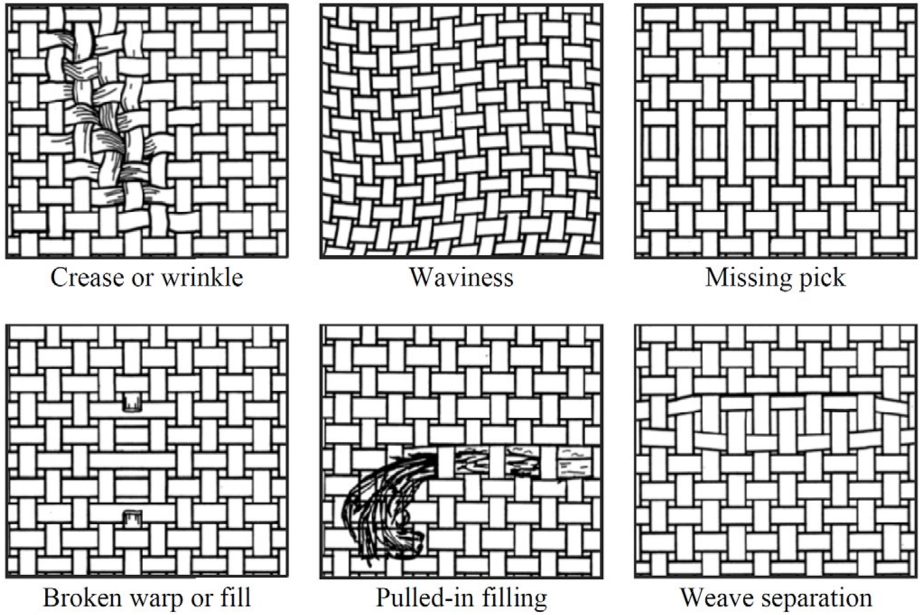
Goal: Develop computational tools and techniques to calculate material properties and characterize defects and failure

D Ellerby et al, MS&T, 2019 • A Vanaerschot et al, Composite Structures, 2017, 173, 44-52
Heat Shield for Extreme Entry Environment Technology (HEEET) • Adaptable Deployable Entry and Placement Technology (ADEPT)

Weave features and defects affect performance

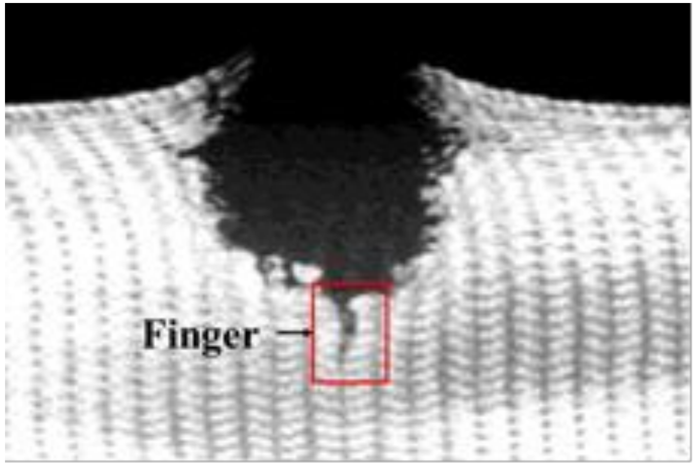
Hypothesis:
Thermal conductivity variation is explained by the connection between microstructure and manufacturing

Weave features or defects



Crease or wrinkle
Waviness
Missing pick
Broken warp or fill
Pulled-in filling
Weave separation

Impact from micrometeoroids and orbital debris (MMOD)



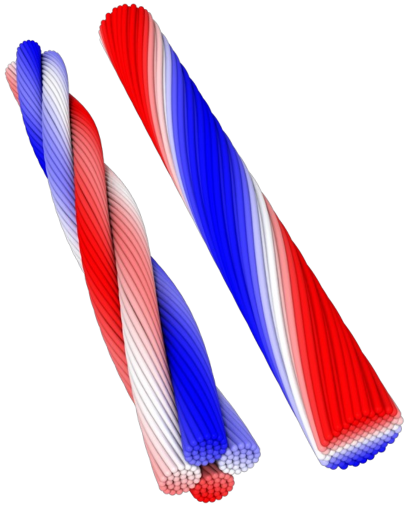
Objective:
Develop fiber/yarn model that captures single-yarn and single component thermal conductivity

SY Park et al, Advanced Composite Materials: Properties and Applications, 2017 • BJ Libben et al, First International Orbital Debris Conference, 2019

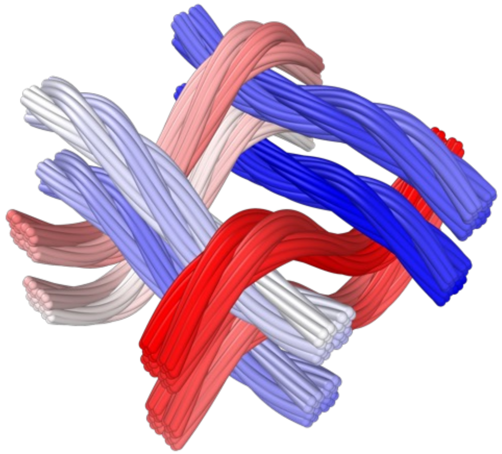
Yarn- and Weave-level Features

Features in woven TPS

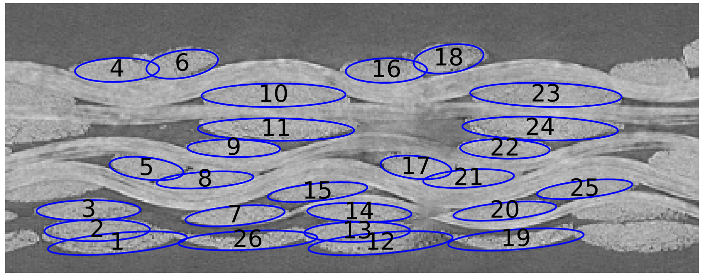
- Ellipsoidal cross sections
- Yarn stretch breaking
- Ordered and random fiber packing
- Fiber blends with different radii
- Packing density
- Weave density
- Matrix fill



Single- or multi-ply yarns with twisting



3D structure

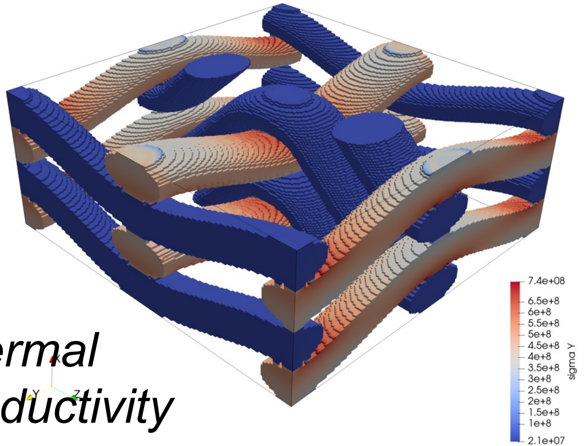


Fiber and yarn packing

TPS Modeling

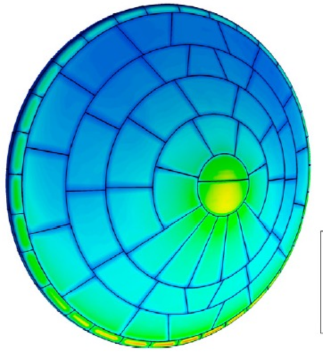
- **Meshed methods** are crucial for TPS design sizing
- **Particle-based methods** bridge the scale gap to model chemistry, microstructure and damage

Finite Element Method



Thermal conductivity

Material Response

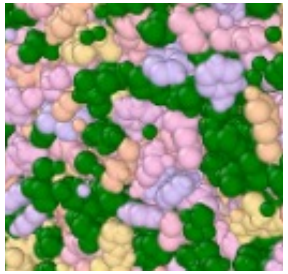


heat shield recession

microscale mesoscale

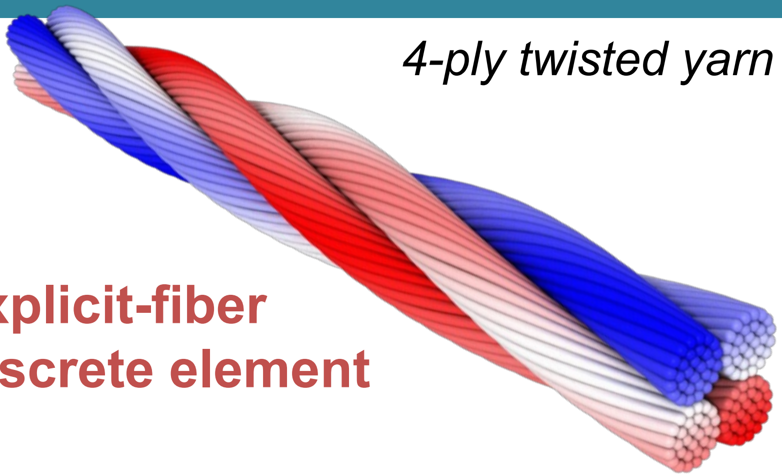
phenolic resin chemistry

Molecular dynamics



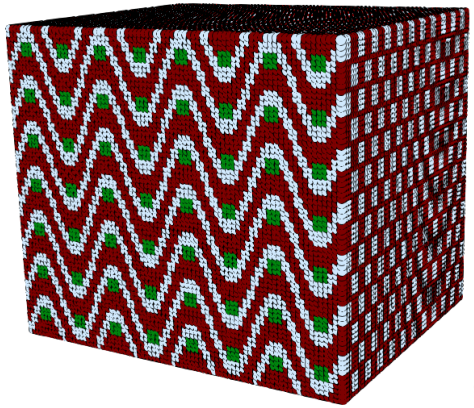
4-ply twisted yarn

Explicit-fiber Discrete element



fracture during impact

Peridynamics

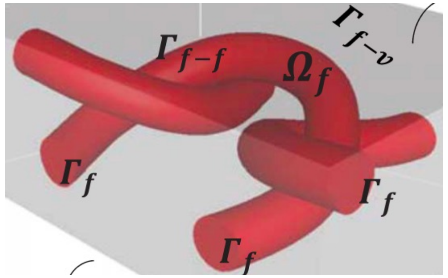


Phenomena Captured by Explicit-Fiber Modeling

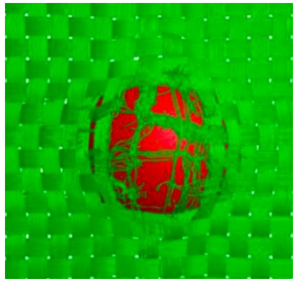
Physics incorporated with explicit-fiber models
- Role of geometry and directionality
- Fiber-fiber friction
- Rupture
- Dynamic collective motion

Explicit-fiber models capture certain experimental observations where continuum models are unable

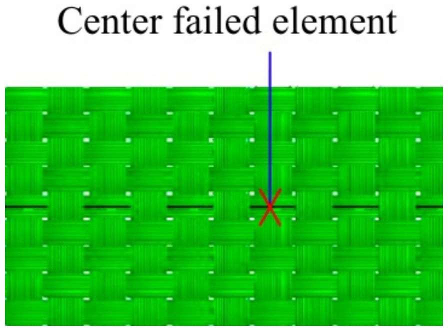
<u>Explicit-fiber applications in the literature</u>



*Strength of knit vs purl**



*Impact with friction^*



Friction with localized failure +

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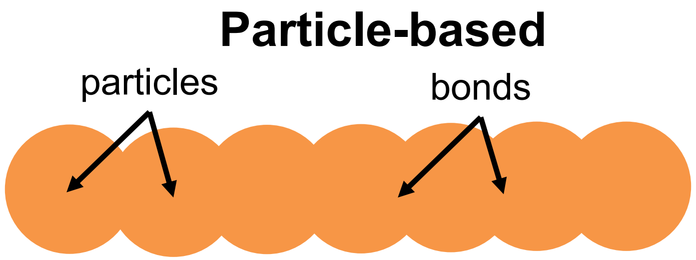
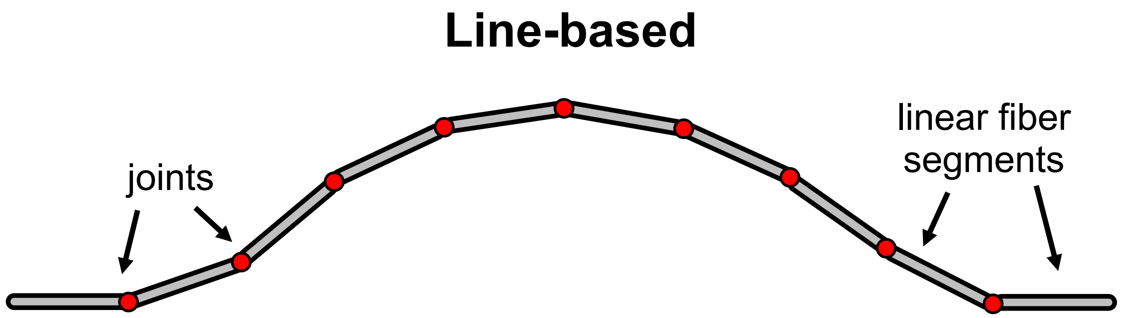
*Liu, D. *et al*. *J. App. Mech.* **2019**, *86* (11). • #Ghaedsharaf, M. *et al*. *Composites Part B* **2021**, *218*, 108938.
+Wang, Y. *et al. Int. J. Impact Eng.* **2016**, *97*, 66–78. • ^Wang, Y.; *et al. Int. J. Impact Eng* **2016**, *97*, 66–78.

Particle-based and fiber-based models





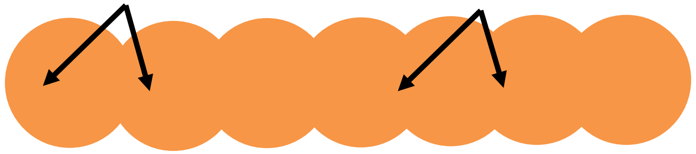
- Takes advantage of DEM literature
- More points per length
- Implemented in open-source, parallel code (LAMMPS)

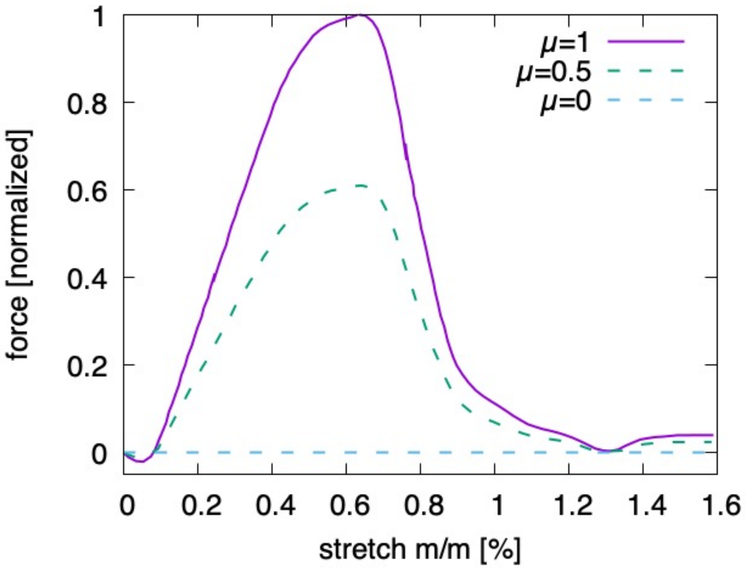
- Intuitively model fibers
- Comparable to beam and truss elements
- Fewer, more expensive material points
- Implemented in an in-house, parallel code (HYDRA)

Chen, X. et al. *Granular Matter* **2021**, *24* (1), 29. • Wang, Y. and Sun, X. *Composites Sci. Tech.* **2001**, *61* (2), 311–319.
Y. Mahadik et al., *Composites: Part A* **41**, 1192 (2010). • Daeleman, L. et al., *Composites Sci. Technol.* **137**, 177 (2016).

Fiber-based model details

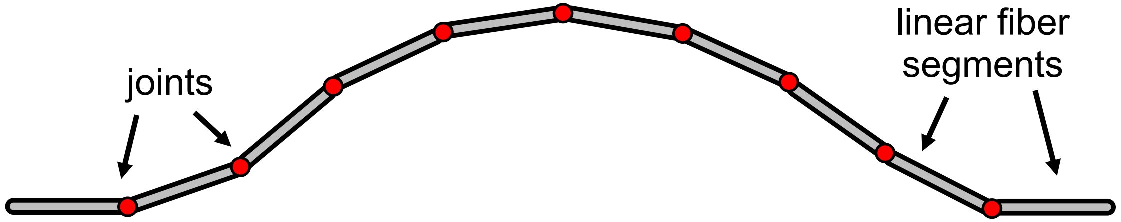
Particle-based

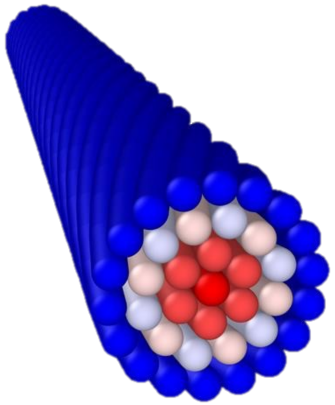




Role of friction in stretch-broken, twisted fiber deformation

Line-based

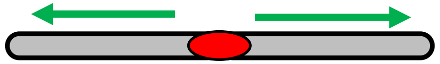




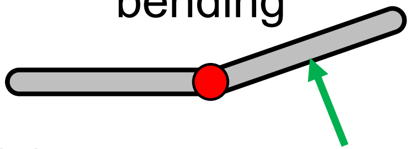
Tension Distribution
high:red, low:blue

contact energy
friction

stretching



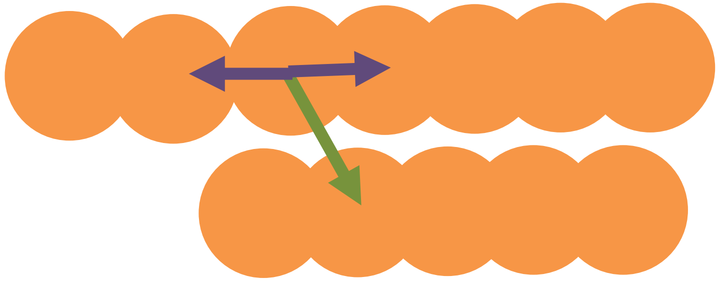
bending



Line-based methods have been applied to study the role of **stretch-broken, twisted and frictional yarns**

Particle-based and fiber-based models

Particle-based



Thermal model

$$Q_{\text{bond}} = \frac{\hat{k}_{\text{bond}} l_{0,\text{bond}}}{l_{\text{bond}}^2} (T_j - T_i)$$

$$Q_{\text{contact}} = k_{\text{particle}} A_{\text{contact}} (T_j - T_i)$$

Hookean spring + damping

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

Failure criteria (B>1)

$$B = \max\left\{0, \frac{f_{\text{r}}}{f_{\text{r},c}}, \frac{f_{\text{s}}}{f_{s,c}}, \frac{\tau_b}{\tau_{\text{b},c}}, \frac{\tau_{\text{t}}}{\tau_{\text{t},c}}, \frac{T_i}{T_c}\right\}$$

- **Inter[3]-fiber, contact forces**
  - Spring-dashpot-slider
    - Hookean and mass-damped
    - sliding and rolling friction
  - *Cohesion*
  - Contact area-based thermal conduction
- **Intra[1,2]-fiber, bonded forces**
  - stretch, bending, twist, shear
    - Hookean spring + damping (f_r)
  - Rupture at a critical force (B)
  - Rod-based thermal conduction
- **Methodology**
  - Meshless
  - MD engine, LAMMPS

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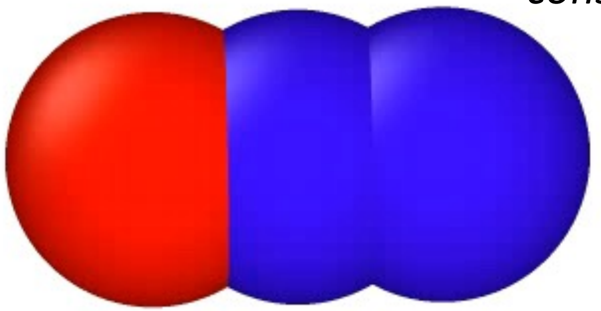
[1] Chen, X. et al. *Granular Matter* **2021**, *24* (1), 29. • [2] Wang, Y. and Sun, X. *Composites Sci. Tech.* **2001**, *61* (2), 311–319.
[3] Silbert, L. E. et al., *Phys. Rev. E* **2001**, *64* (5), 051302. • [4] Plimpton, S. J. et al., LAMMPS … . *Comp. Phys. Comm.* **2022**, *271*, 108171

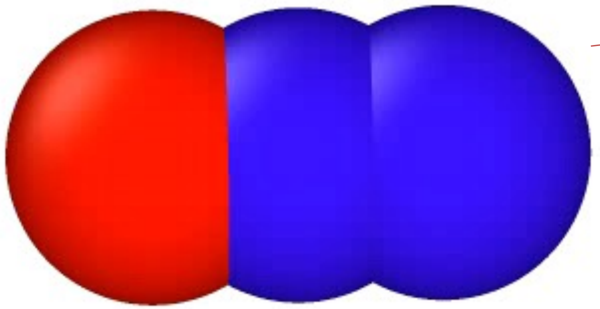
Strain-dependent Thermal Conduction

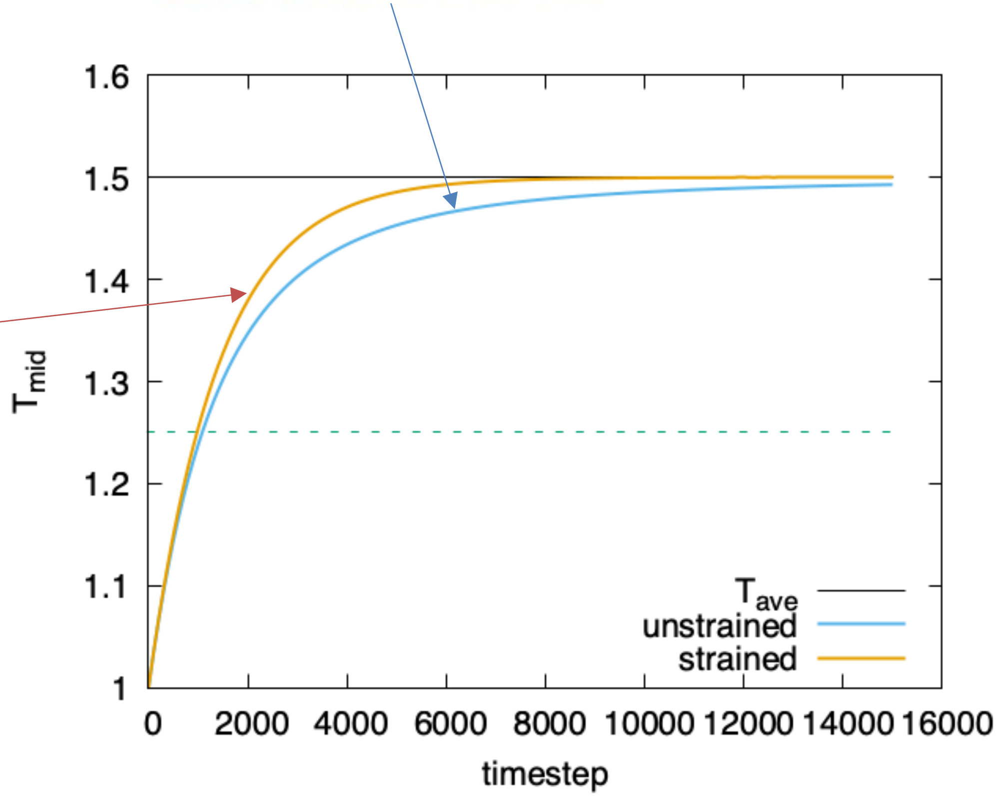
- **Thermo-mechanical** processes can be modeled
- As fiber length increases, the fiber cross-section decreases
- Strain slows approach to steady-state

constant velocity strain and T on edges



constant T on edges, no strain

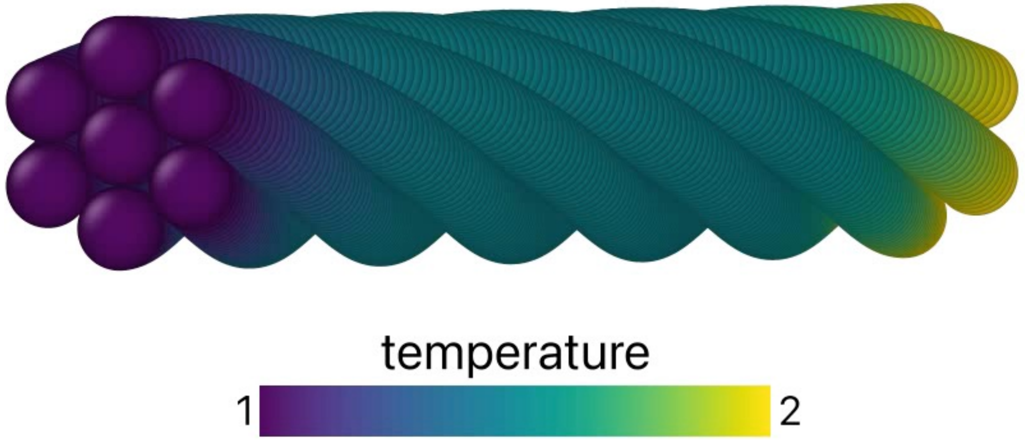




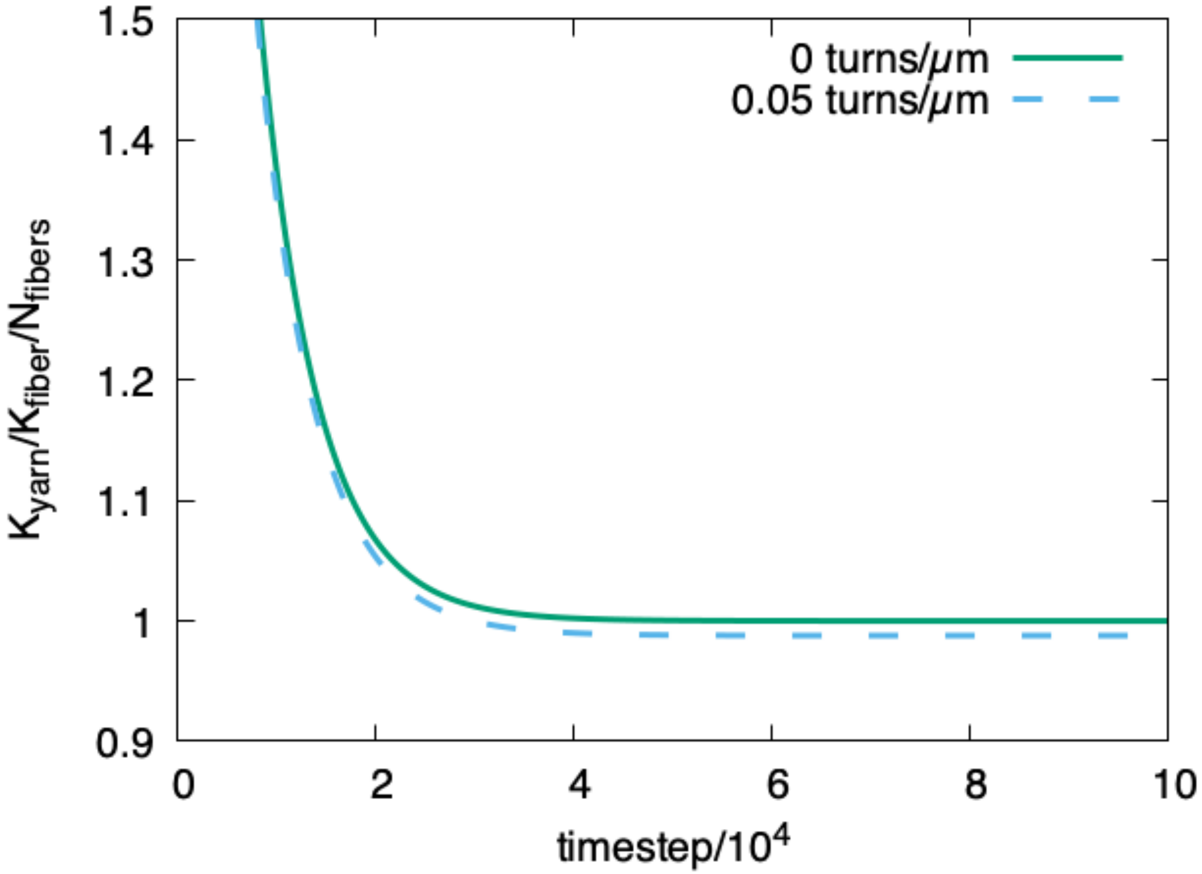
7-fiber yarn thermal conductivity and twist

These parameterization tools can be used to investigate the role of yarn processing, like twist, on material properties

7 twisted Kynol phenolic fibers



- Twisted yarn has lower conductivity because outer bonds are slightly longer
- Lead to modified development conductivity model (material-based conductivity)



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

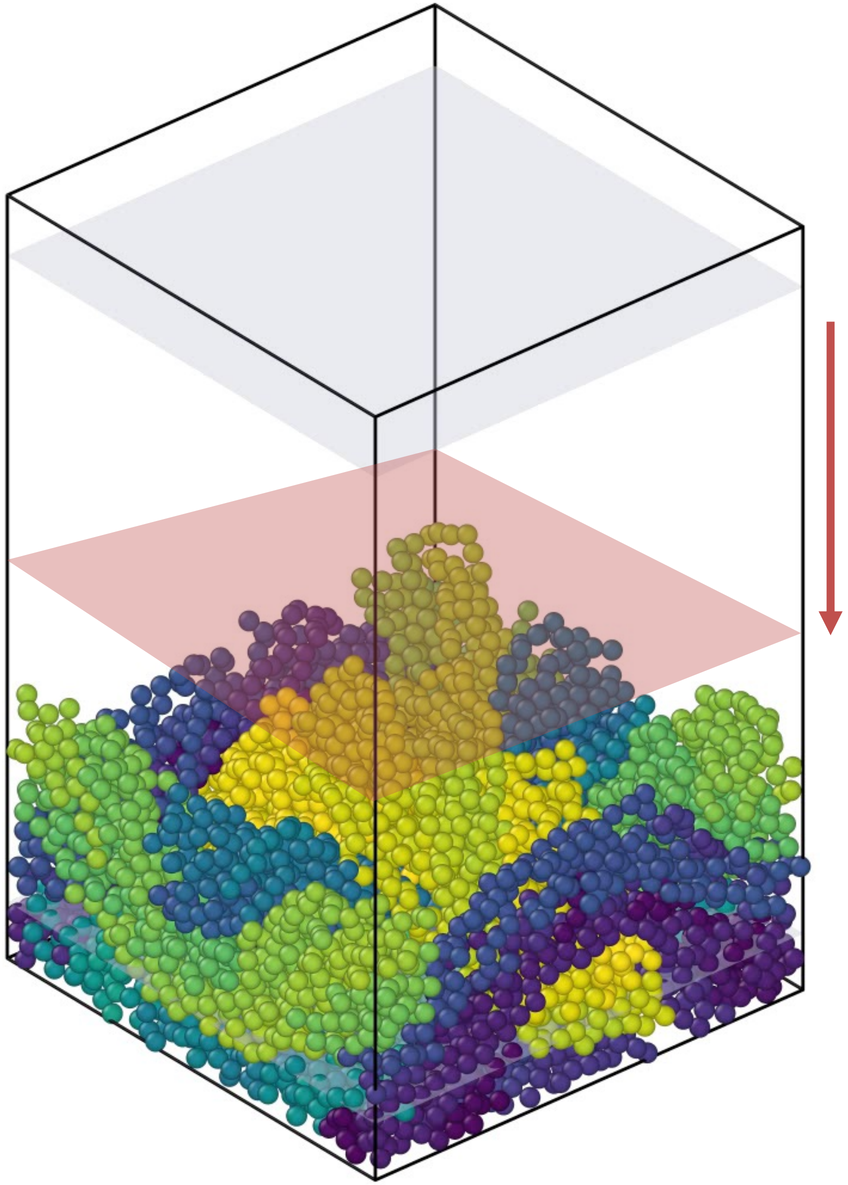
Red and Blue Yarns Cross

Weave at some point during Ablation

Blue Portion of Yarn is Disconnected

Model of Weave Ablation and Connectivity

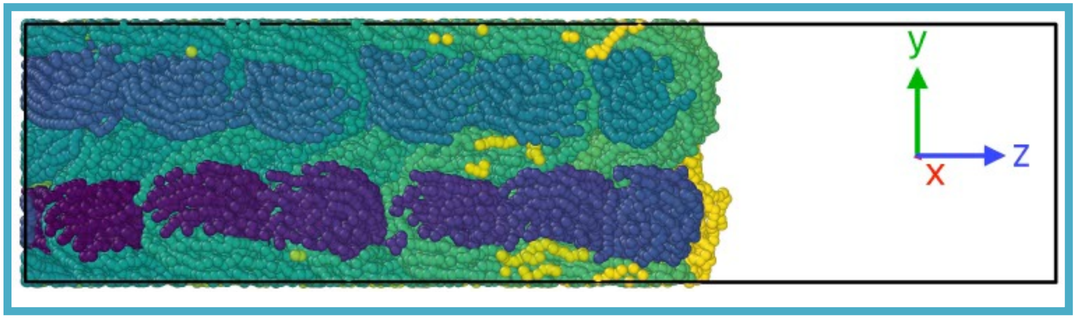
- Weave is constructed from a particle-based model
- Ablation front moves into the material and removes particles
- Forces applied such that disconnected portions of fibers are ejected from the surface into the ablation zone



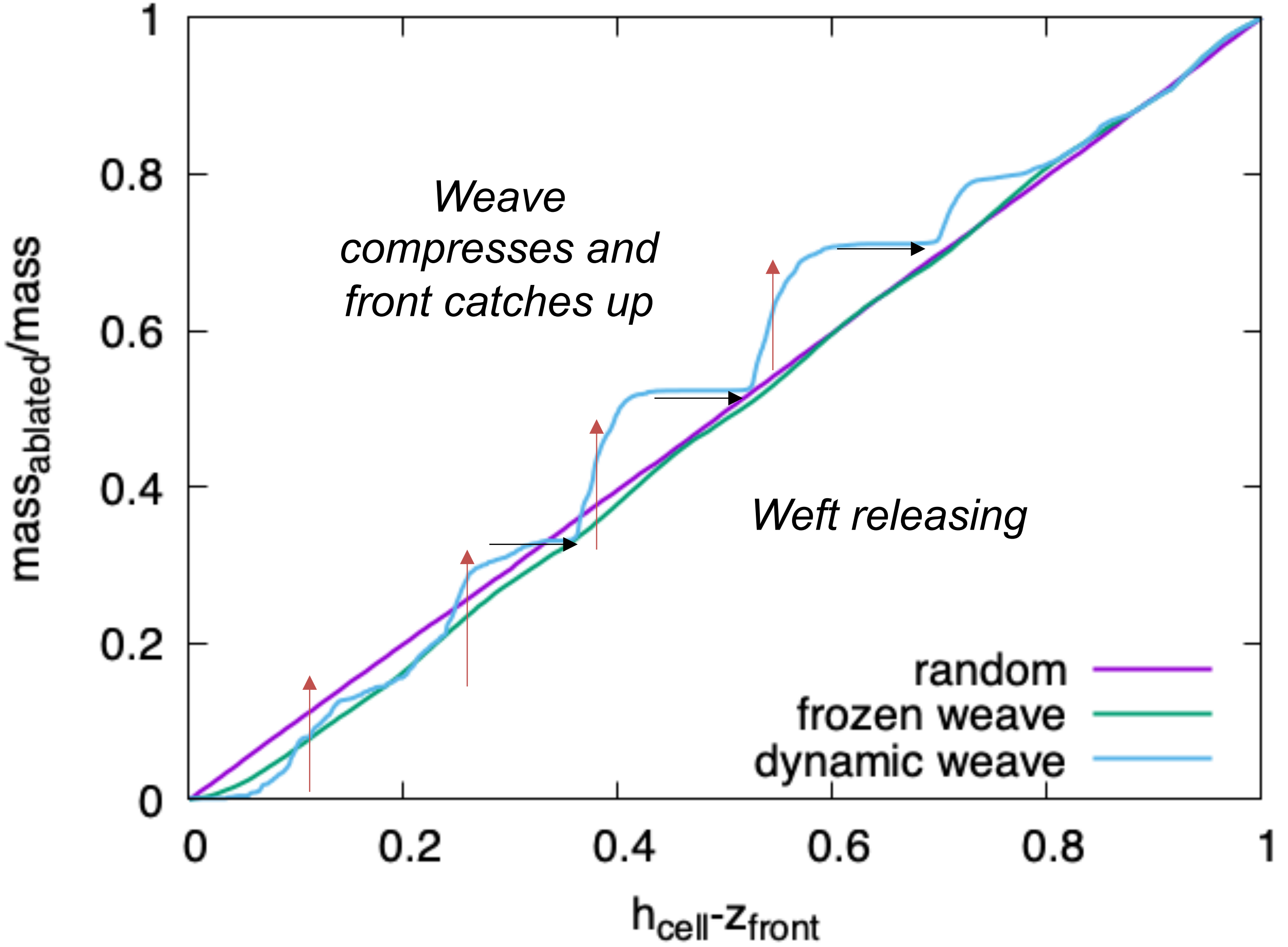
ablation zone

Fiber tension: harmonic bonds
Fiber-fiber repulsion: viscoelasticity

Augmentation from Loss of Weave Connectivity



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



Conclusions

- Particle- and line-based fiber models were implemented to model:
  - Fiber-fiber contact mechanics
  - Intra-fiber stretching, bending and failure
- Simulated twisted yarns had:
  - decreased thermal conductivity
  - concentrated stress in central fibers
- Weave connectivity can cause enhanced ablation

On-going and future work

- Explicit-fiber simulations
  - Full yarn parameterization of a coarse-grained model
  - Thermal conductivity change caused by defects

- Experimental verification:
  - Nanoindentation of single yarns and weaves with partners at Yale University

- Peridynamics:
  - Bridge the gap between impact and ablation and yarn-level resolution coupled with material-response

Acknowledgements

Entry Systems Modeling (ESM) Project

TPS Certification by Analysis

Core Team Members

ARC
Justin Haskins
Lauren Abbott
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Sander Visser
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Federico Semeraro
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GRC
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NASA ARC

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Keith Peterson
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Michael Olaya, U Mass Lowell
Victoria Arias, UIUC
Joseph Ferguson, Stanford U.
Alexandre Quintart

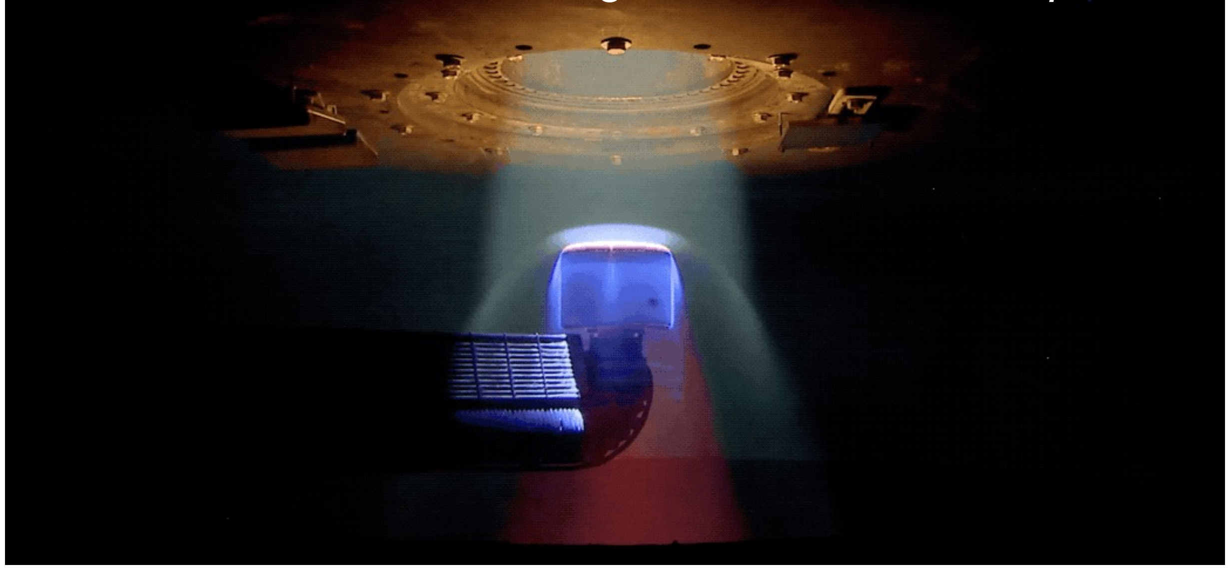
Thank you! Questions?

We seeking people with expertise in:

- Thermo-mechanical and failure of materials (peridynamics)
- Multi-scale simulations of materials for additive manufacturing

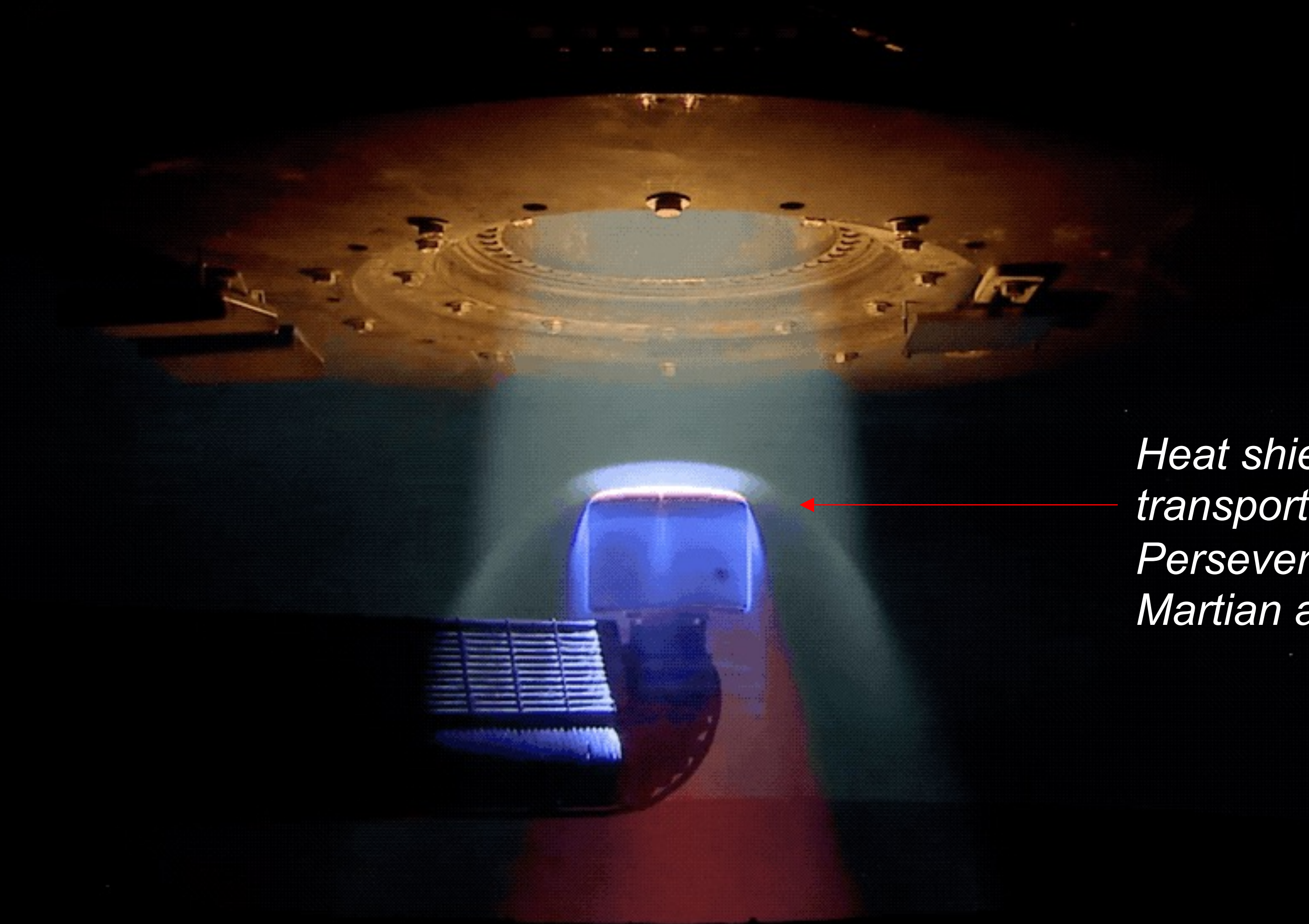
Talk to or contact me if you are interested Andrew.P.Santos@nasa.gov

Heat shield (PICA) used to transport the Mars 2020 Perseverance rover through the Martian atmosphere



Ground testing heat shields

Arc Jet facilities at NASA's Ames Research Center can deliver up to 150 MW for 15 sec of plasma (6000 K) flows up to hypersonic speeds (Mach>5)



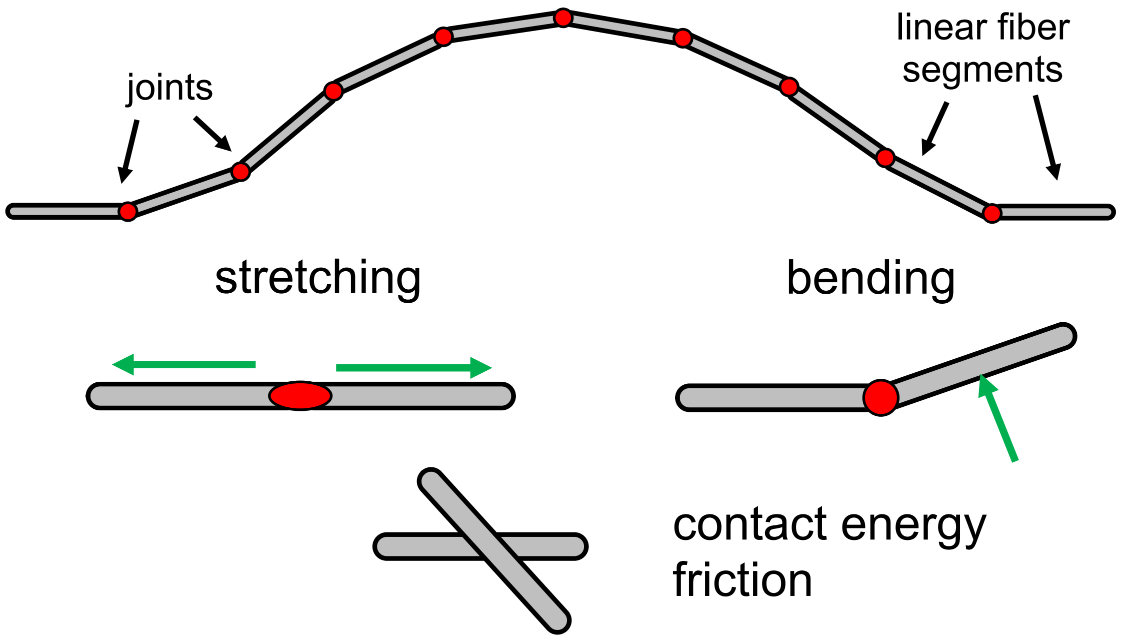
Heat shield (PICA) used to transport the Mars 2020 Perseverance rover through the Martian atmosphere

Credits: NASA

Fiber-based model details

- **Contact Forces**
  - Line integral approach
- **Friction Forces**
  - Path integral approach
- **Stretching, Bending, and Twisting**
  - All angular distortions treated through a single, unified deformation angle that couples to stress
- **Damage and Failure**
  - Cohesive law for damage accrual and failure
  - Function of fiber stretching, bending, and twisting
- **Methodology**
  - Meshless
  - Strain-based
  - In-house code implementation, HYDRA

Line-based



joints

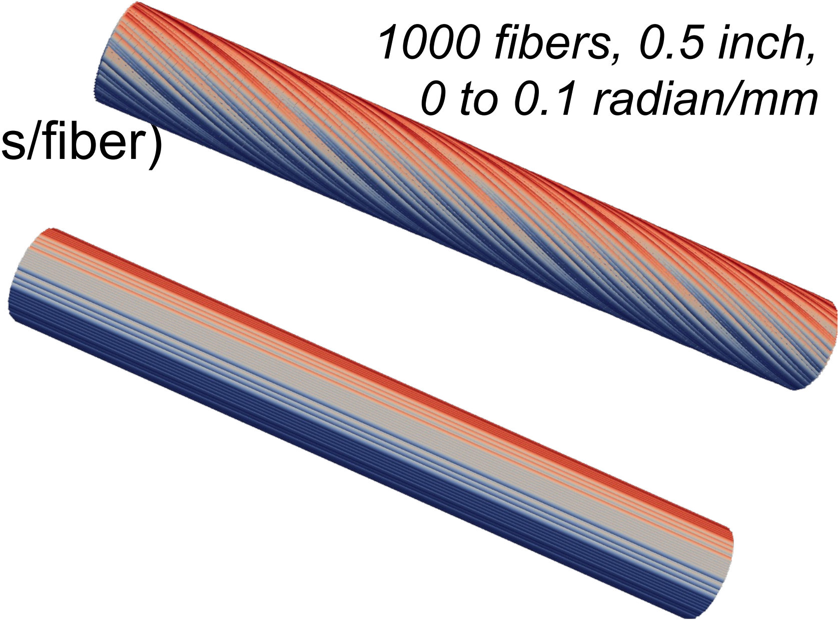
linear fiber segments

stretching

bending

contact energy
friction

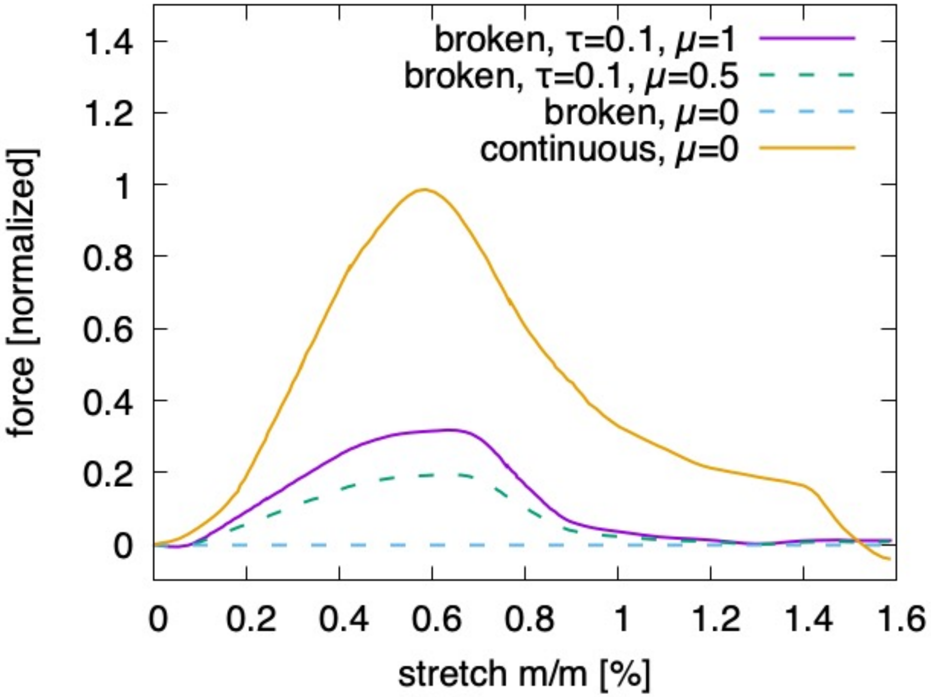
Demonstration on Twisted Yarns



1000 fibers, 0.5 inch,
0 to 0.1 radian/mm

Yarns are often:

- **stretch broken**, discontinuous fiber segments (average 2 breaks/fiber)
- **twisted** (0.1 radian per mm)
- **frictional**



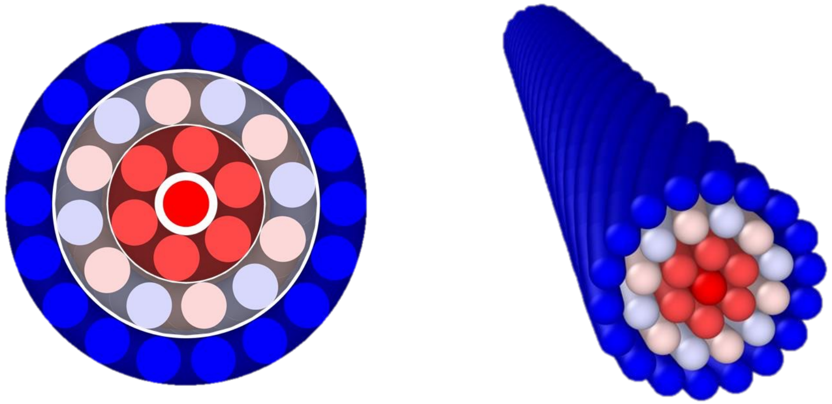
- Both fibers are pulled to 1.5% elongation
- Maximum force response is smaller for aligned fibers and large for twisted

Demonstration on Twisted Yarns

Twisted yarn composed of lumped fibers and stretched to increase stress. HYDRA imports fiber position and applies a strain to determine stress response. Lower stress response is noted for the exterior fibers during stretching compared to interior fibers:

- Twist results in exterior fibers having a longer fiber/yarn length ratio compared to interior fibers
- Longer fiber lengths more easily accommodate deformation from stretching.

Tension Distribution

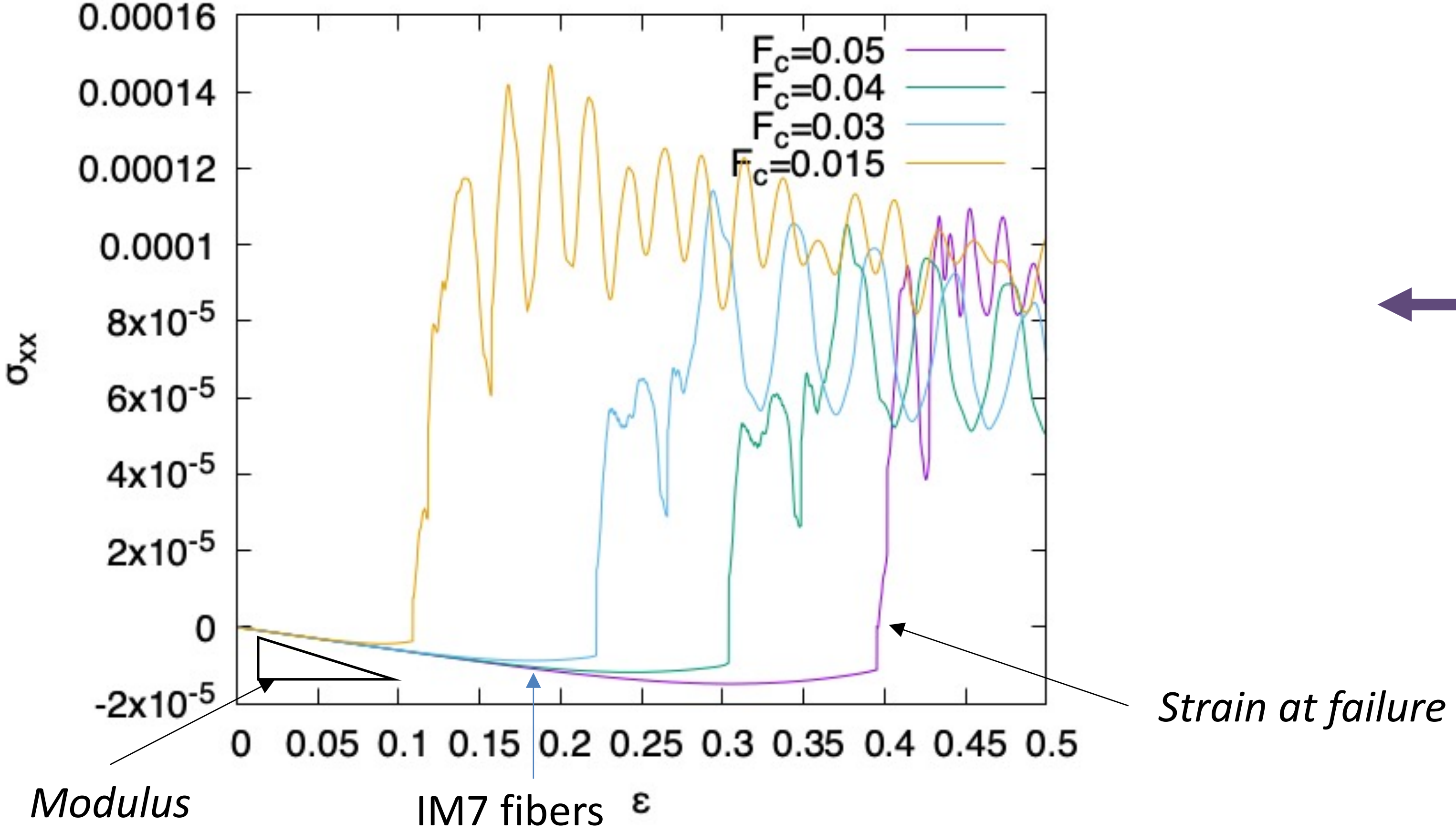


Red – high stress
Blue – low stress

Tensile modulus and failure

Tuning a critical force criteria can capture the rupture behavior due to different modes for IM7 fibers, *e.g.*, with the opportunity to compare directly to experiments

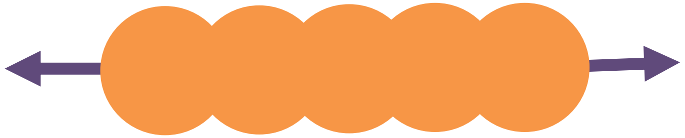
Single, short fiber simulations



Modulus

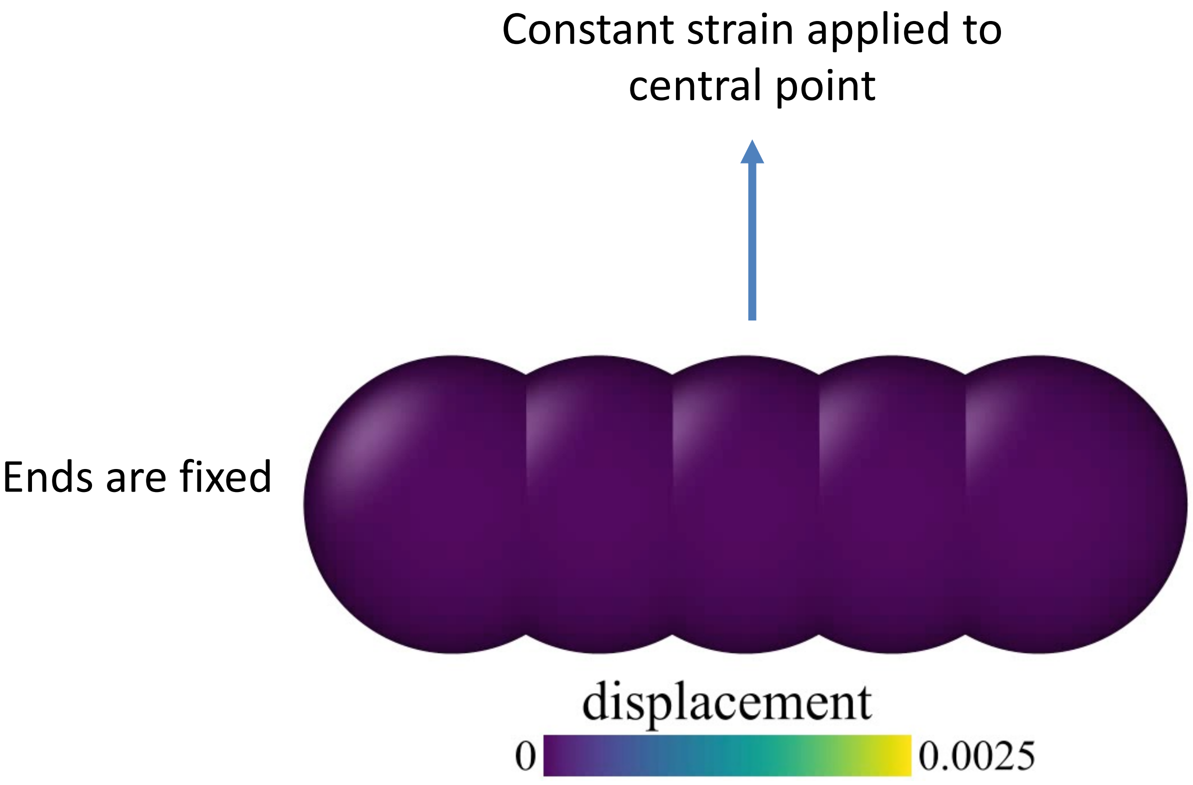
IM7 fibers

Strain at failure



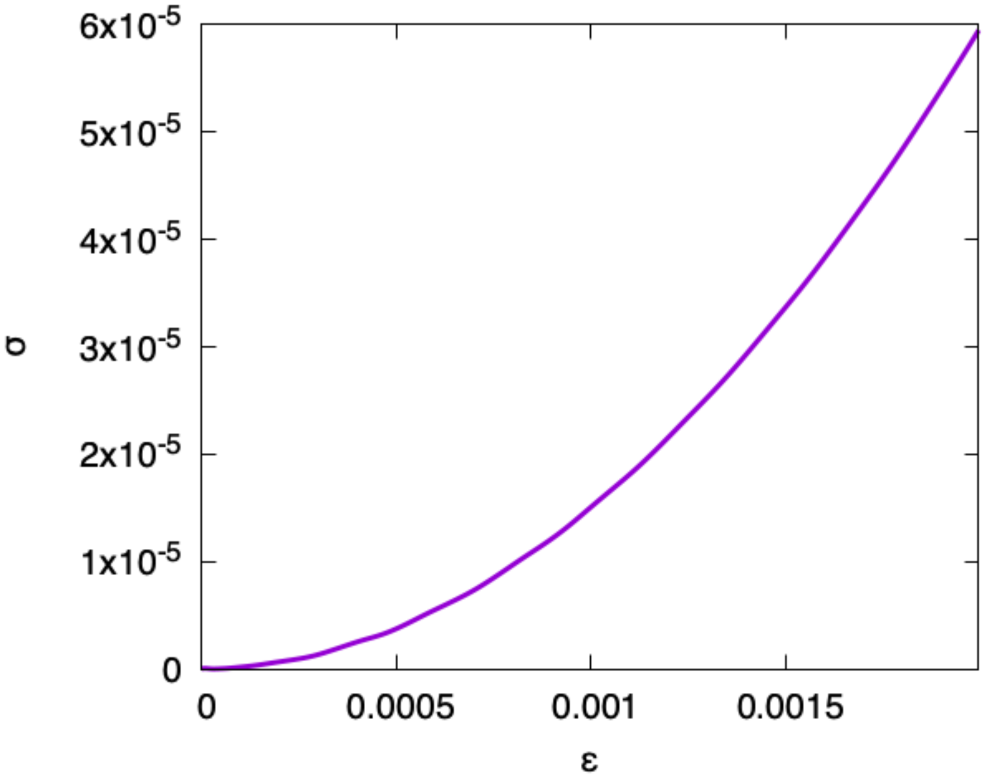
3-point bending

3-point bending can also compare directly to experiments to characterize the model shear and bending moduli


Constant strain applied to central point

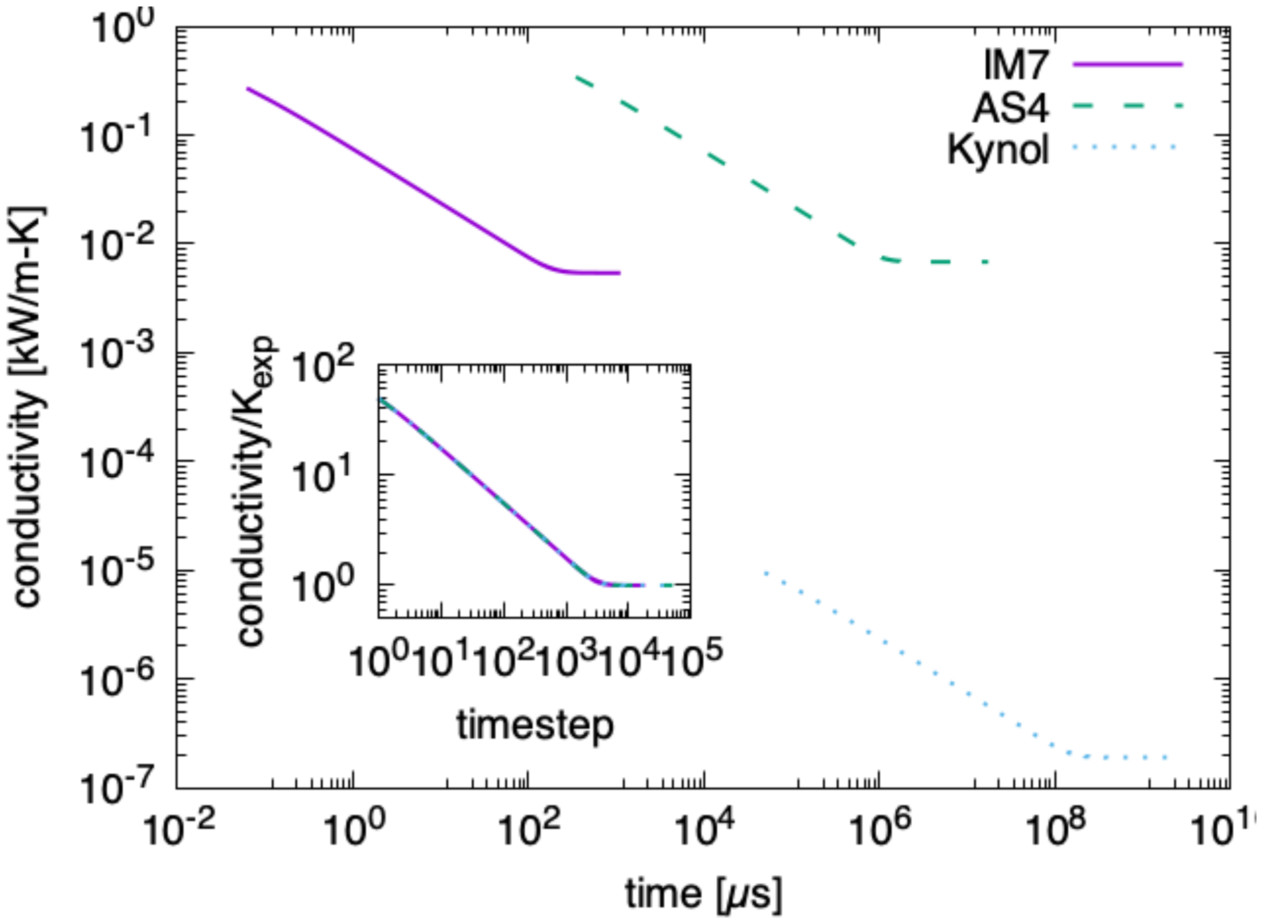
Ends are fixed

Non-linear stress-strain due to combination of tensile and shear bond stresses



Single-fiber conductivity

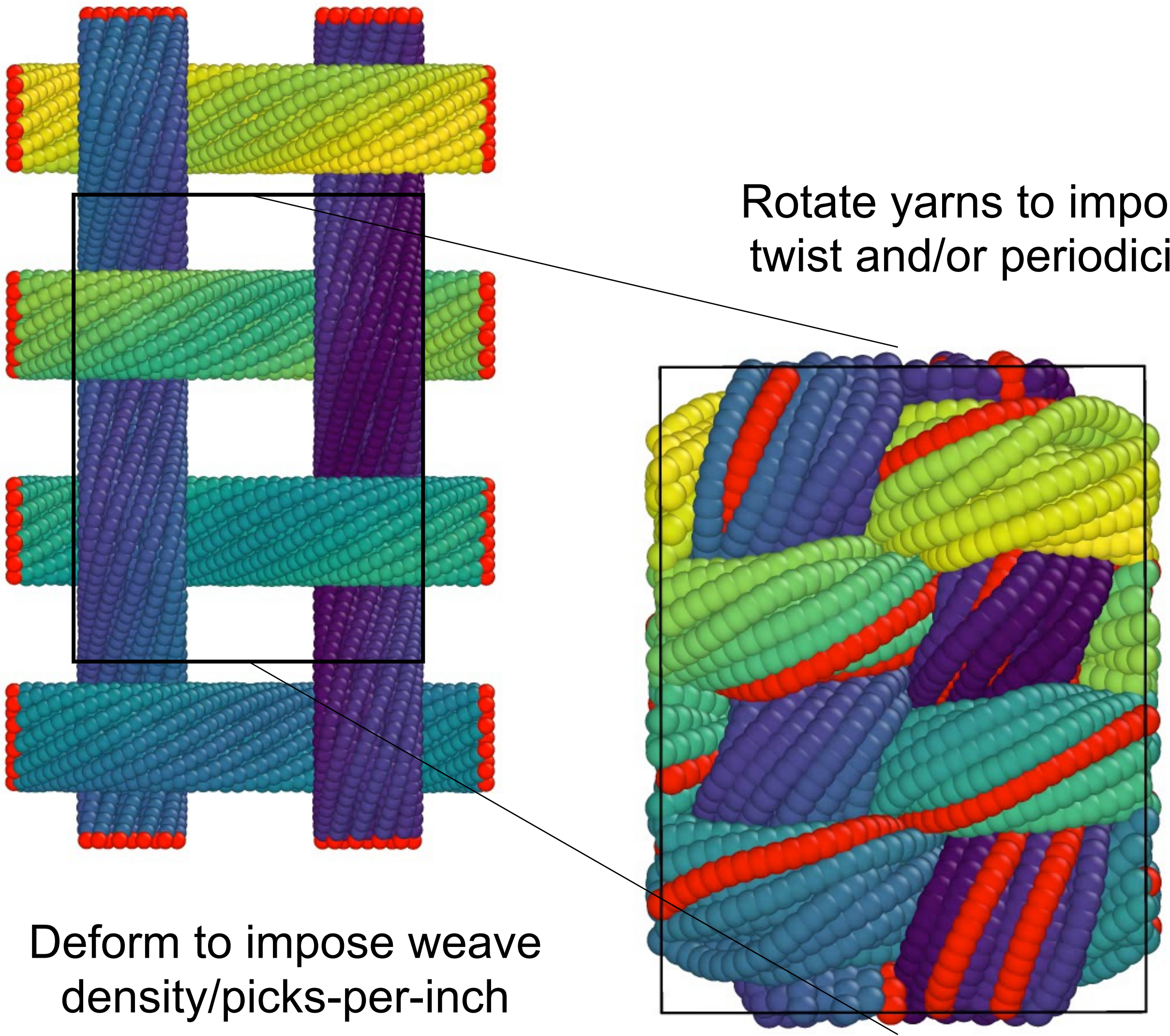
Single-fiber accessible with a timestep based on the conductivity timescale



- Conductivity is measured by setting constant temperature at fiber/yarn ends and waiting for steady-state
- Timescale is set by model conductivity, unless other processes are underway, such as tension, enables
- For single fiber, this measurement is near trivial and exact

Weave manipulation

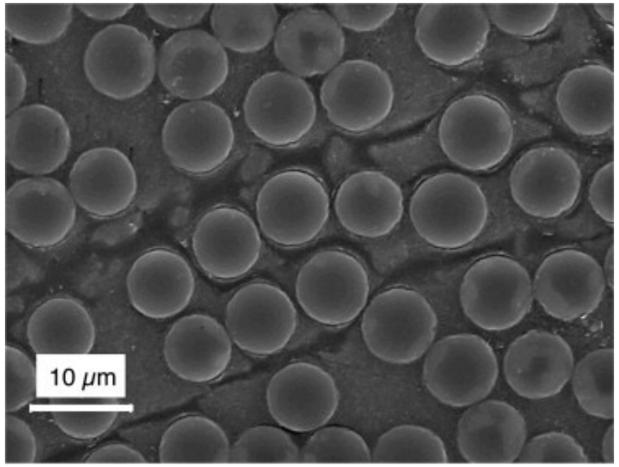
- Yarn manipulation can control the weave density
- A path to study wrinkles and other behaviors



Rotate yarns to impose twist and/or periodicity

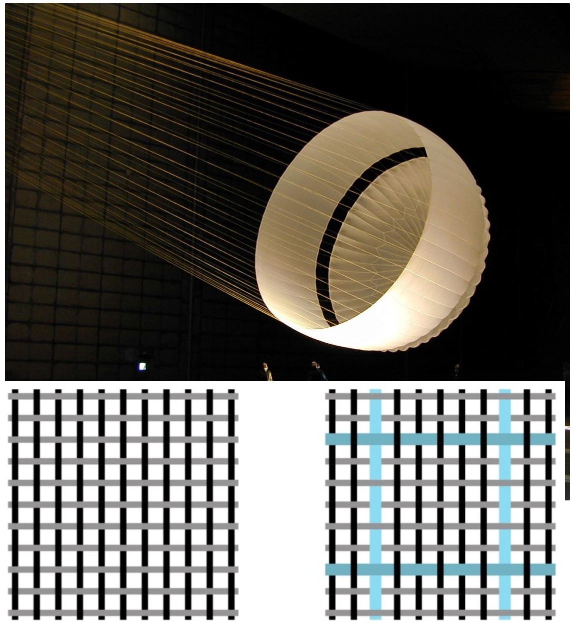
Deform to impose weave density/picks-per-inch
Maintaining accurate contacts

Woven materials



Unidirectional fiber-polymer composite [x]

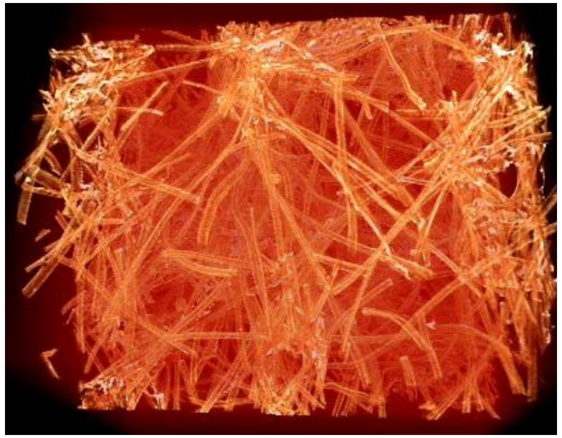
2D weave parachutes[*]



Typical fabric weave

Ripstop fabric weave

Random isotropic fiber network[*]

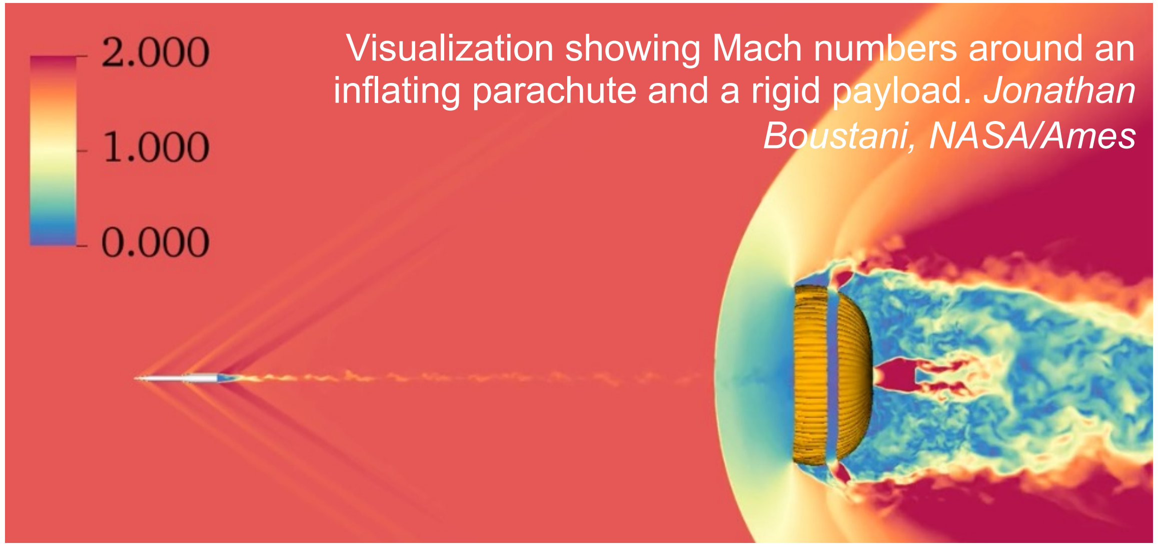


3D weaves in arts & crafts[#]

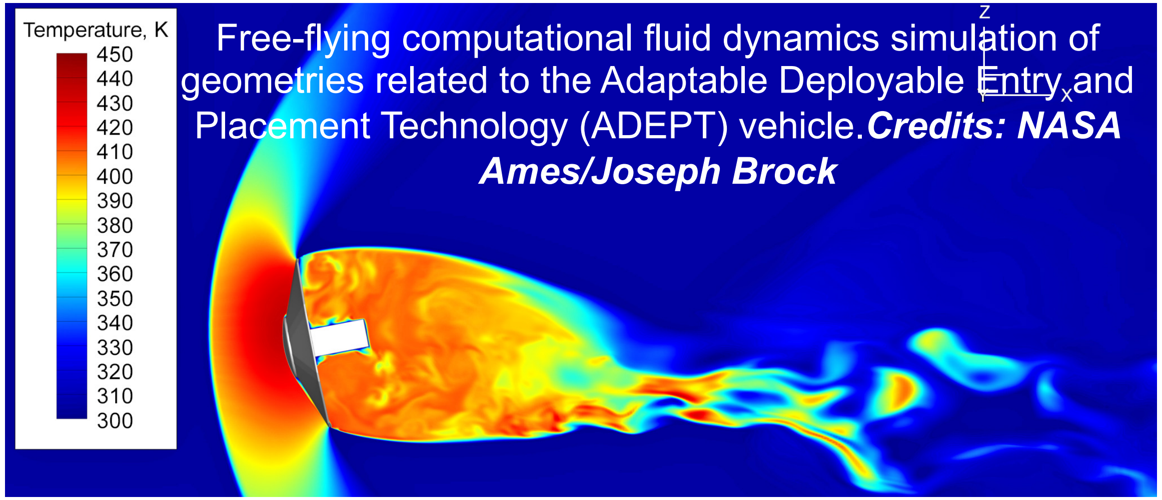
“Evidence of 3D weaving can be seen in pre-historic ages as the pre-historic humans”[^]

[#] Flower basket **1912-1989**, Japan, Bamboo • [^] Perera, Y. S. et al. *Fash. Tex.* **2021**, *8* (1), 11
[*] X-Ray CT Scan, NASA • [x] C. González et al., *Compos. Sci. Technol.* ***2007,*** 67, 2795

Flow simulations of entry



Visualization showing Mach numbers around an inflating parachute and a rigid payload. *Jonathan Boustani, NASA/Ames*



Free-flying computational fluid dynamics simulation of geometries related to the Adaptable Deployable Entry and Placement Technology (ADEPT) vehicle.***Credits: NASA Ames/Joseph Brock***

Computational fluid dynamics

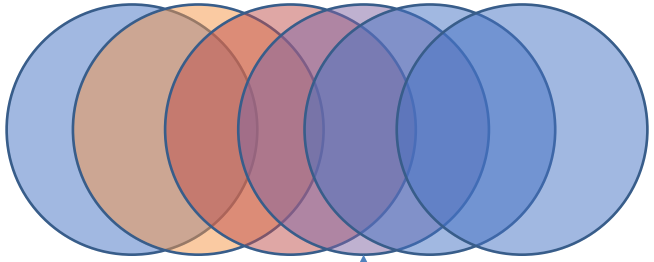
Development and simulation, on an ambitious scale, of:

- Blunt body entry dynamics
- Parachute deployment for descent

Flow environments inform the material boundaries:

- Temperature
- Heat flux, including radiation
- Pressure and shear
- Chemical environment

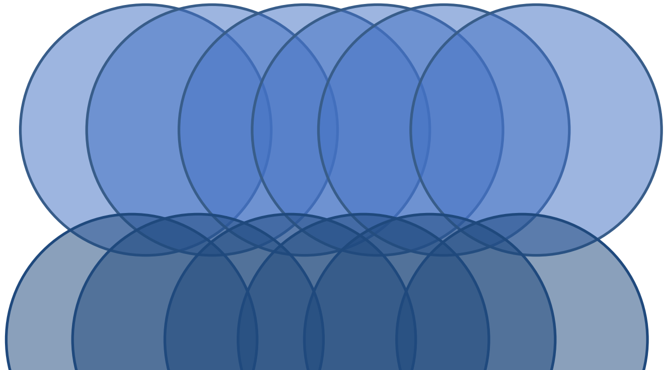
Developed bond-based thermal conduction model

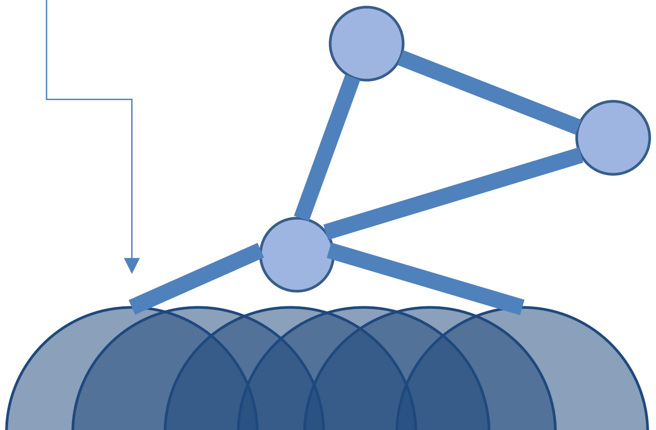


A contact-based conduction model existed in LAMMPS, which could be used if particles overlap in the fiber

Reasons for new model

- However, we want to ignore 1-2,1-3 and 1-4 (depending on coarse-graining) non-bonded interactions to:
  - Prevent repulsion
  - Reduce simulation time
- May need different conductivity for fiber-fiber contact and intra-fiber, particularly for coarse-grained models
- Planned matrix model will be a fiber/bond network, with no node-node "contact" beyond bonds





New Rod thermal Conduction Model Implementation in LAMMPS

$$\Delta T = \frac{\Delta t}{C_{\text{p,particle}} m_{\text{particle}}} \left(\boxed{Q_{\text{bond}}} + Q_{\text{contact}} \right)$$

new

$$Q_{\text{contact}} = k_{\text{particle}} A_{\text{contact}} \left(T_j - T_i \right)$$

$$Q_{\text{bond}} = \frac{k_{\text{bond}} A_{\text{rod}}}{l_{\text{bond}}} \left(T_j - T_i \right)$$

Rod conduction

$$Q_{\text{bond}} = \frac{k_{\text{bond}} \pi r_{\text{bond}}^2}{l_{\text{bond}}} \left(T_j - T_i \right)$$

$$Q_{\text{bond}} = \frac{k_{\text{bond}} \pi r_{0,\text{bond}}^2 \left({}^{l_{0,\text{bond}}} \big/ {}_{l_{\text{bond}}} \right)}{l_{\text{bond}}} \left(T_j - T_i \right)$$

Assume constant volume

$$Q_{\text{bond}} = \frac{\hat{k}_{\text{bond}} l_{0,\text{bond}}}{l_{\text{bond}}^2} \left(T_j - T_i \right)$$

Assume uniform initial bond radii

Thermal bond breaking criteria

$$B = \max \left\{ 0, \frac{f_{\text{r}}}{f_{\text{r},c}}, \frac{f_{\text{s}}}{f_{s,c}}, \frac{\tau_b}{\tau_{\text{b},c}}, \frac{\tau_{\text{t}}}{\tau_{\text{t},c}}, \boxed{\frac{T_i}{T_c}} \right\}$$