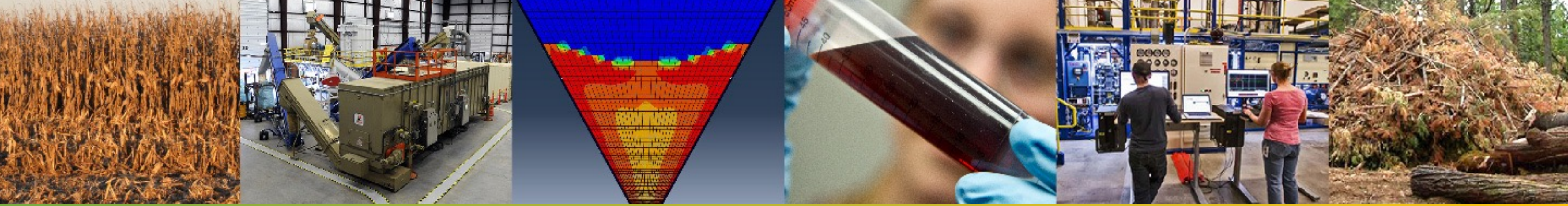
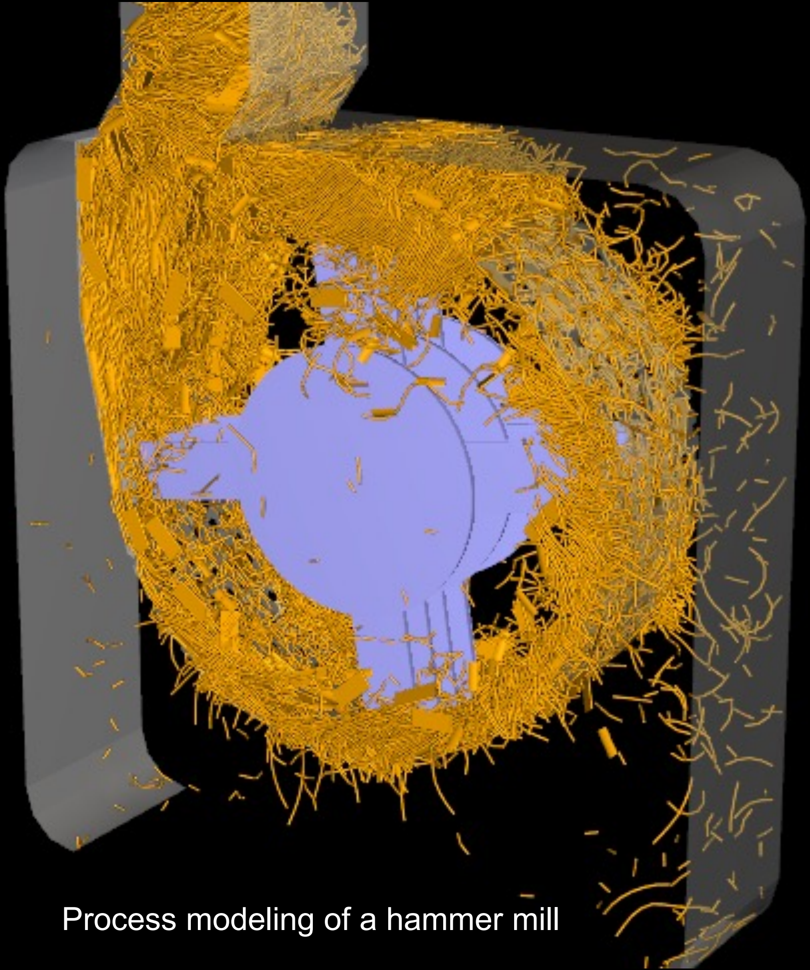


Experiment-informed computational models for granular feedstock preprocessing and handling unit operations


Process modeling of a hammer mill

Presented by
Yidong Xia, Ph.D., Senior Computational Scientist
Idaho National Laboratory

Idaho National Laboratory

2023 NETL Multiphase Flow Science Workshop

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FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Process Upsets & Downtime

Relevance to TEA (Techno-Economic Analysis) and LCA (Life Cycle Assessment) :

- Commercial-scale conversion of biomass in biorefineries has remained limited.

- A primary challenge in the design of a biorefinery is the storage, transport, and reactor feeding of the biomass feedstocks.

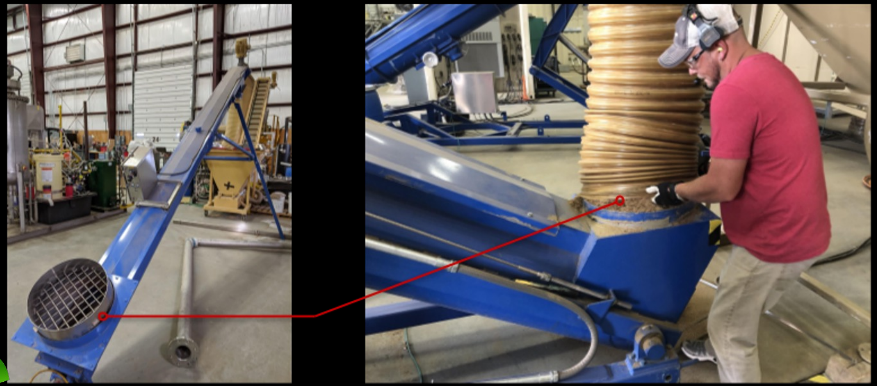
- Milling and handling have been prone to process upsets such as jamming and clogging, resulting in increased downtime and ultimately higher costs.

Typical biomass materials


Loblolly pine particles


Corn stover particles

Typical feedstock feeding and preprocessing issues

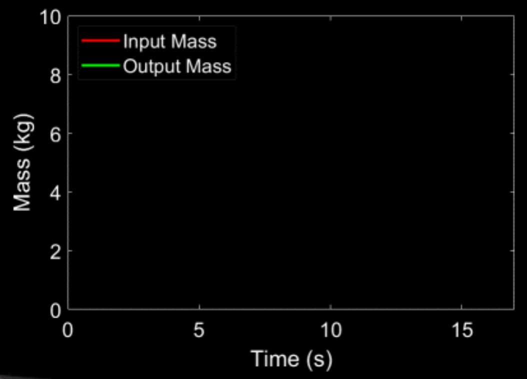

Material clogging in screw conveyor

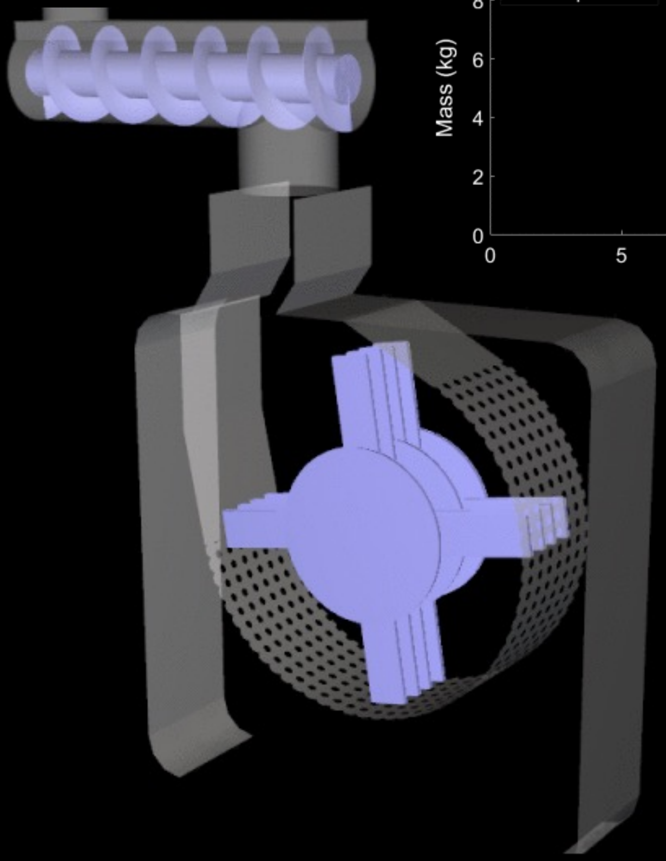

Material jamming in hammer mill grinder

How Can Modeling Assist Quality-by-Design (QbD)?

An experiment-informed hammer milling model

Example





Modeling facilitates massive testing for QbD

- **CMA:** input PSD, particle shapes, etc.
- **CPP:** rotor speed, blade size, input mass rate, screen sieve size.
- **CQA:** output PSD, output mass rate etc.

Feedstock materials	Corn stovers
	Pine residuals
Morphology	shape & size
Water/moisture content	internal
	surface
Density	Intrinsic
	Envelope
Stiffness	Intrinsic
	Effective
Friction	Sliding
	Rolling
Adhesion	Other types

Description

- Developed a hammer milling model (particle flow & deconstruction) for assisting QbD

Value of new tool

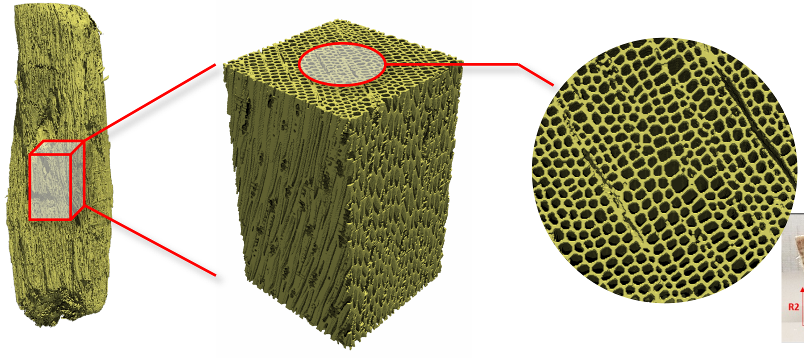
- First-of-its-kind virtual laboratory
- Enabled fast massive testing and real-time performance diagnosis

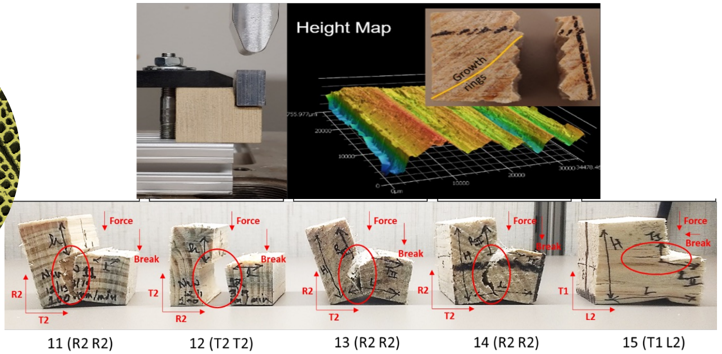
Potential Customers & Outreach

- Feedstock preprocessing industry partner, biorefinery designers

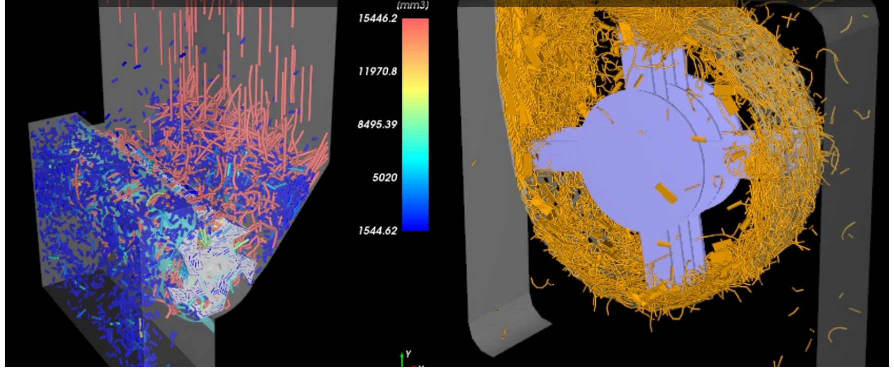
Virtual Feedstock Processing Laboratory Based on Multiscale Multiphysics

XCT-informed microstructural deconstruction model and upscaling



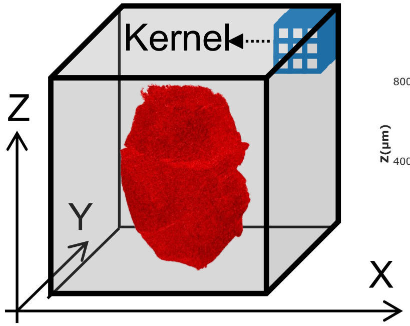


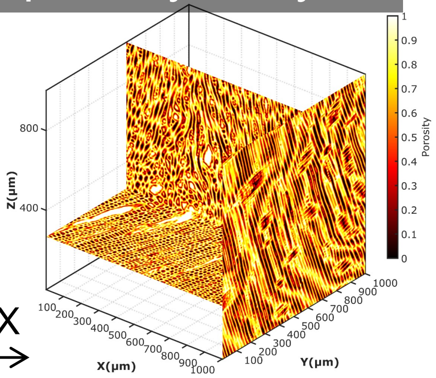
Modeling of various milling techniques

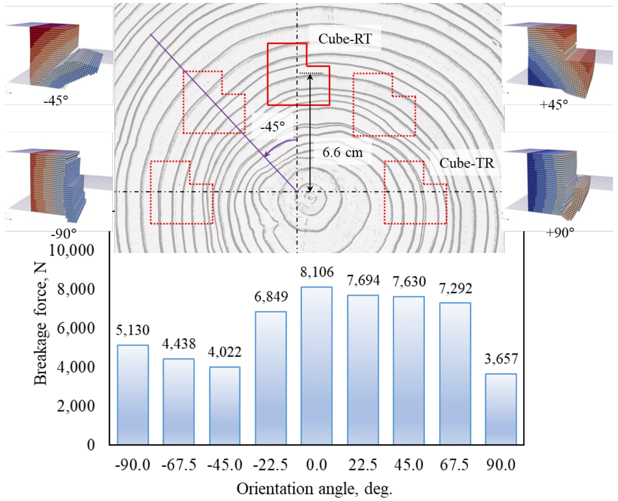


Microscale (um) → **Laboratory scale (cm)** → **Pilot scale (m)**

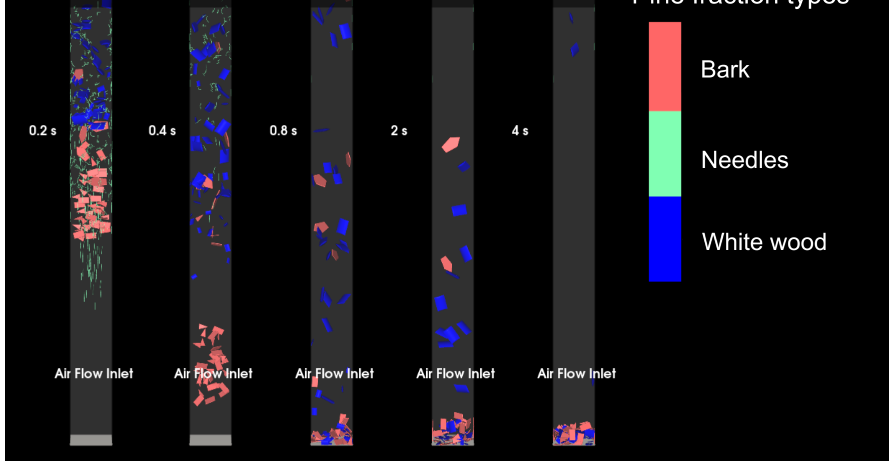
Advanced micro-porosity analysis







Air classification modeling



Flow Models: Limitations & Best Practices

Knowledge

Identified particle- & bulk-scale models suitable for the flow of milled biomass and recommended best practices (part 1)

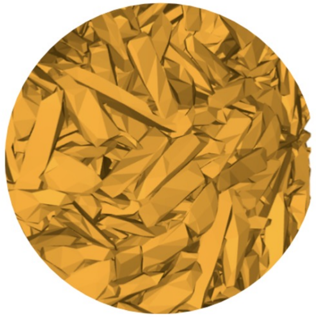
Current Knowledge Gap

- Lack of computational models suitable for biomass flow
- Lack of experimental data for new model development
- Lack of open-source model platforms for user coverage

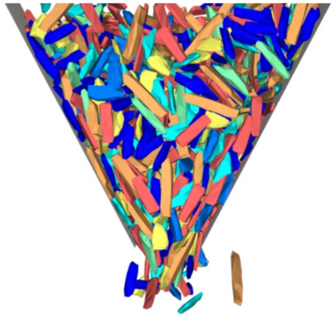
Achievement

- Identified limitations of existing models as knowledge base
- Recommended potential flow models & codes for biomass

Chipped loblolly pine particles (3-4 mm sieve size)

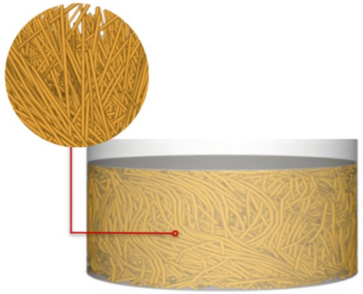


Custom polyhedral particles of arbitrary shapes

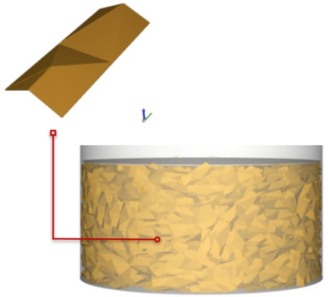


A v-shape hopper discharge of polyhedral particles

Milled corn stover particles (e.g. fiber & shell shapes)



Flexible fiber particles of arbitrary aspect ratio



Flexible thin shell of arbitrary aspect ratio

Yidong Xia, Jonathan Stickel, Wencheng Jin, Jordan Klinger. A review of computational models for the flow of milled biomass I: Discrete-particle models, *ACS Sustainable Chemistry & Engineering*, 8, No. 16 (2020): 6142-6156. https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.0c00402

Flow Models: Limitations & Best Practices

Knowledge

Identified particle- & bulk-scale models suitable for the flow of milled biomass and recommended best practices (part 2)

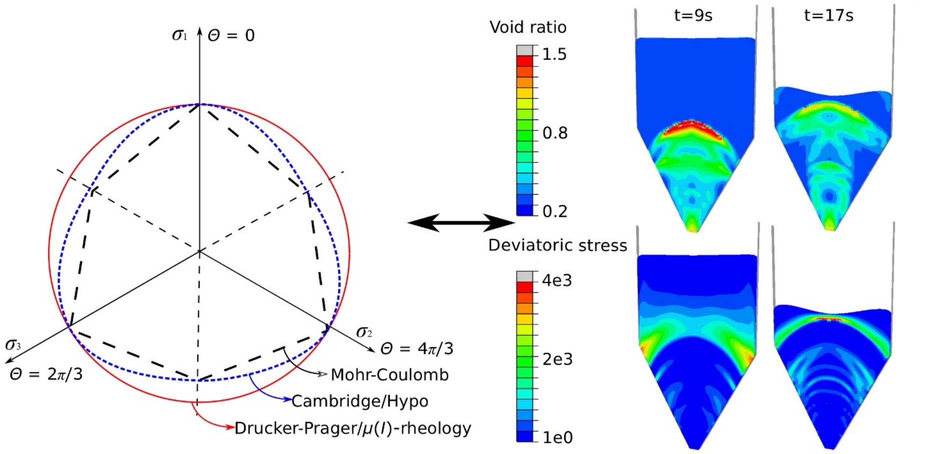
Current Knowledge Gap

- Lack of computational models suitable for the flow of milled biomass
- Lack of experimental data for supporting new model development
- Lack of open-source model platforms for user coverage

Achievement

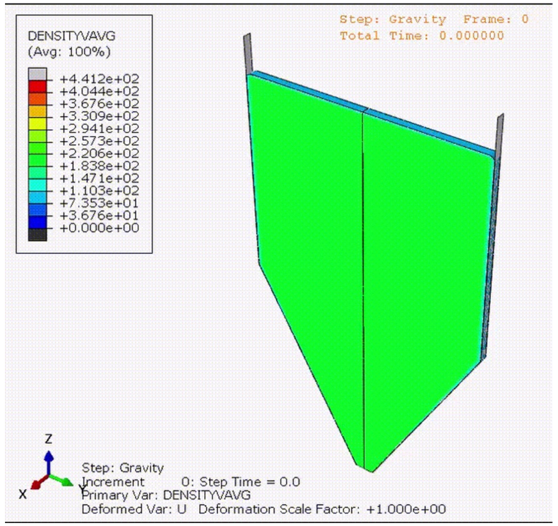
- Identified limitations of existing models as knowledge base
- Recommended potential flow models & codes for biomass materials

Wencheng Jin, Jonathan Stickel, Yidong Xia, Jordan Klinger. A review of computational models for the flow of milled biomass II: Continuum-mechanics models, *ACS Sustainable Chemistry & Engineering*, 8, No. 16 (2020): 6157-6172. https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.0c00412



Constitutive model review

Application in milled biomass flow modeling



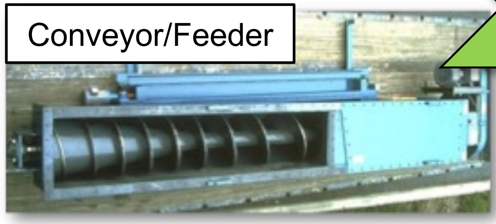
Approach

Goal: Develop first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat.

Process upsets in handling are a major challenge for lowering costs of biomass.

Hopper

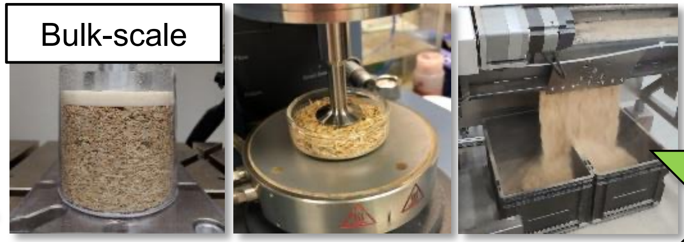
Conveyor/Feeder



Experimental: multi-scale material characterization for state-of-the-art **knowledge** and **design charts**

Particle-scale

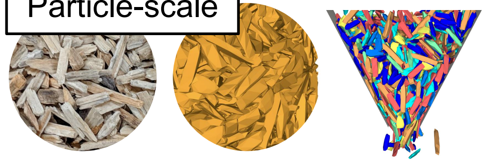
Bulk-scale



Pilot/demonstration-scale

Computational: experiment-validated multi-scale biomass mechanics & flow simulators as **open-source toolkits**

Particle-scale

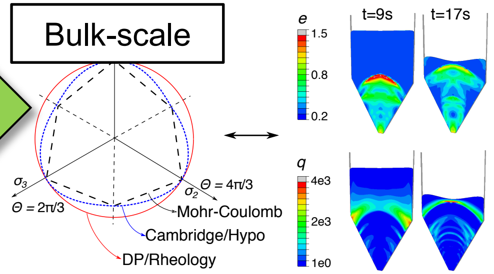


Chipped loblolly pine particles

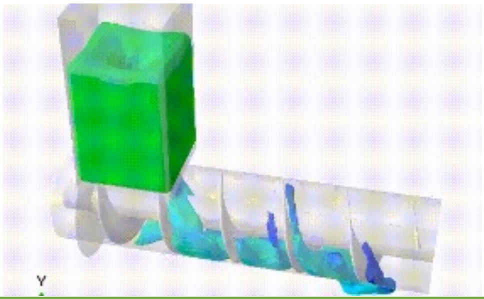
Polyhedral particles of arbitrary shapes

A v-shape hopper discharge simulation

Bulk-scale



Pilot/demonstration-scale



Outcome: efficient & effective design charts and simulators for bioenergy industries and other applicable areas

Preprocessing
CQAs (e.g., particle shape, PSD, feed rate)

CMAs & CPPs (e.g., particle shape, PSD, feed rate)
Material Handling
CQAs (controlled flow rate)

CMAs & CPPs (e.g., particle shape, PSD, feed rate)
Conversion
CQAs

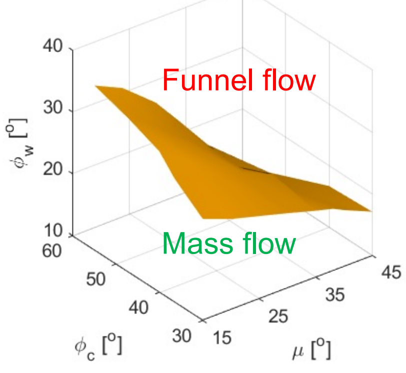
Approach (continued)

Metrics: 1) Operational reliability (e.g., design chart for consistent hopper flow at designed flow rate). 2) qualification of flow models (80% or higher agreement with experimental data.

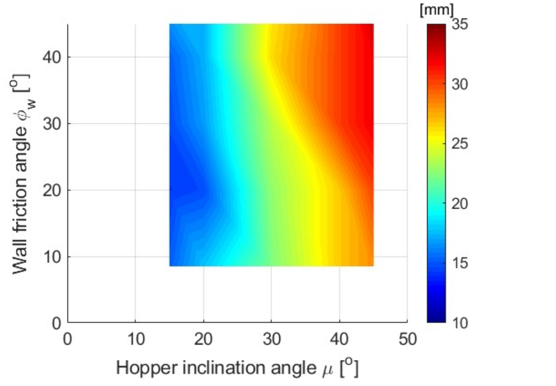
MA
Controllable attributes
Particle size distribution
Morphology (aspect ratio, shape, etc.)
Particle density/porosity
Surface energy
* Moisture content; * Ash content
Physical properties
Initial & critical state void ratio/density (bulk scale)
Critical state friction angle (bulk scale)
Elasticity (bulk scale)
Contact laws (particle scale)
* Time consolidation; * Scale-up effect

CPPs of Hopper
Feeding mass rate
Outlet mass rate
Depth
Side inclination angle
Outlet aperture size

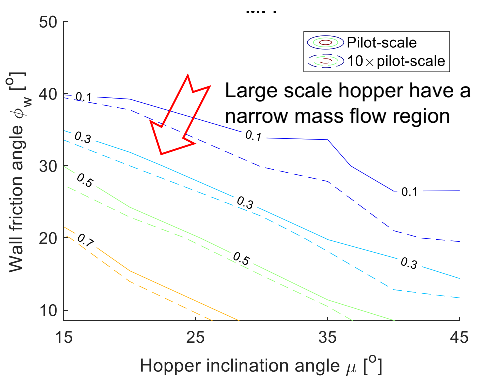
- Flow pattern design chart (Wedge-shaped)



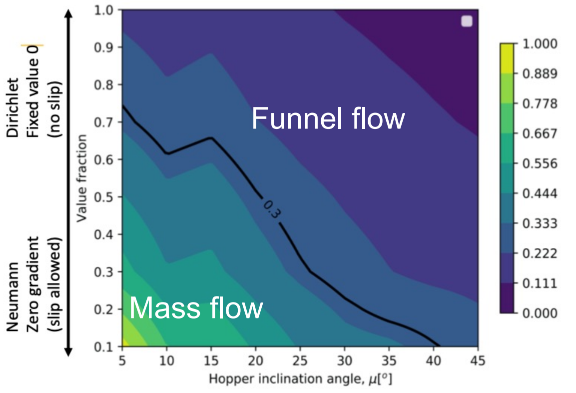
- Critical arching distance design chart (Wedge-shaped)



- Flow pattern shift (Wedge-shaped, scale dependence)



- Flow pattern design chart (Conical)



CMA: Internal friction angle ϕ_c
CQA: Flow pattern, critical arching distance

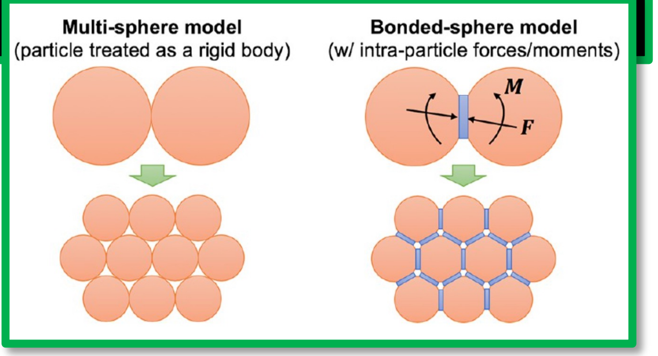
CPP: Inclination angle μ, Wall friction angle ϕ_w

Attributes denoted by * means not being currently studied in modeling

Early DEM Models for Biomass Particle Flow

Multi-sphere (rigid) and bonded-sphere (flexible) DEM particle models

- Advantages: simple surface contact detection
- Biomass applications: Pines (Xia et al, 2019) switchgrass (Guo et al. 2020)
- Limitation: (1) Limited shape complexity; (2) Expensive for certain shapes like long fiber-like particles, corn stover



Yidong Xia, Zhengshou Lai, Tyler Westover, Jordan Klinger, Hai Huang, Qiushi Chen, "Discrete element modeling of deformable pinewood chips in cyclic loading test", *Powder Technology*, Vol 345, 1 March 2019, Pages 1-14. https://doi.org/10.1016/j.powtec.2018.12.072

Yuan Guo, Qiushi Chen, Yidong Xia, Tyler Westover, Sandra Eksioglu, Mohammad Roni, "Discrete element modeling of switchgrass particles under compression and rotational shear," Biomass & Bioenergy, Vol. 141, No. 105649, Oct. 2020. https://doi.org/10.1016/j.biombioe.2020.105649

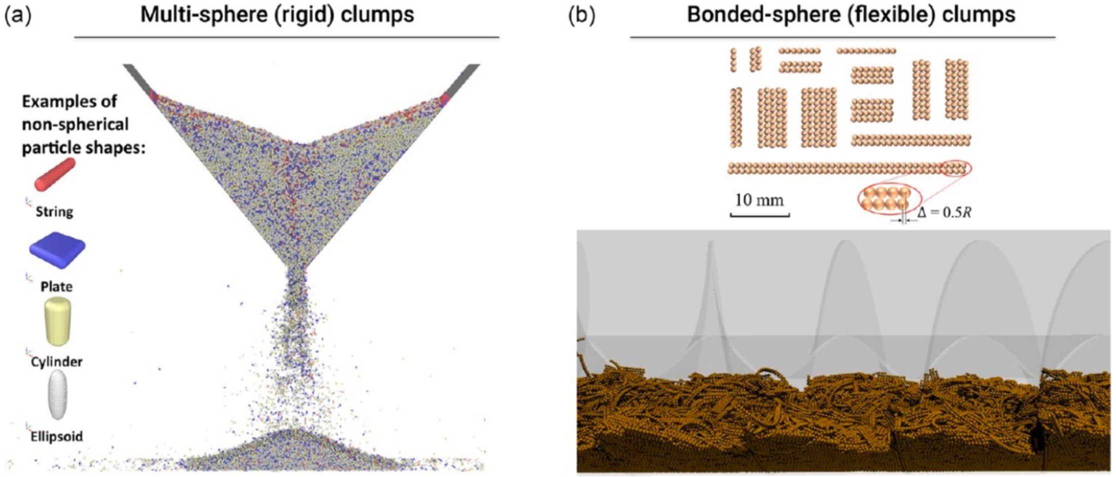


Figure 4. Composite-sphere models for milled biomass: (a) multisphere models for hard wood chips and (b) bonded-sphere models for flexible chopped switchgrass fragments.

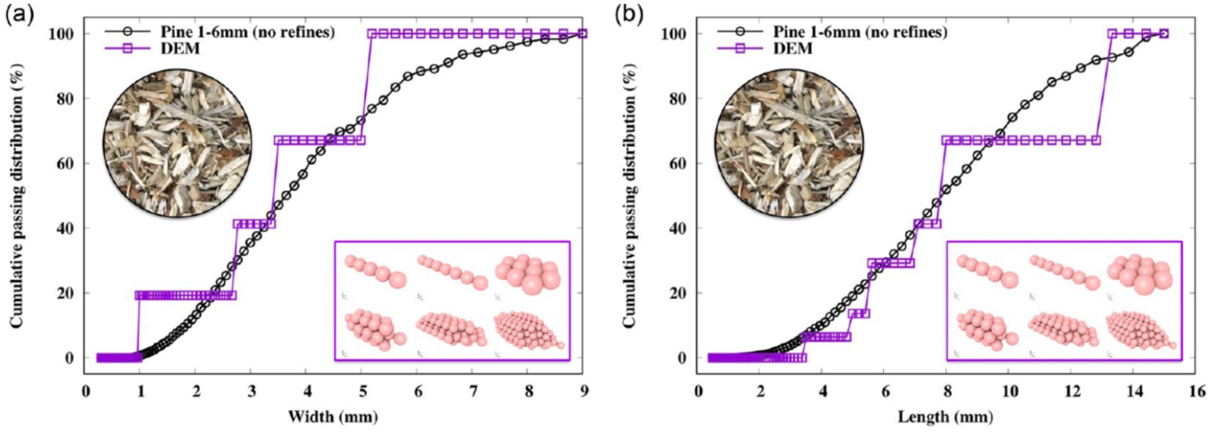
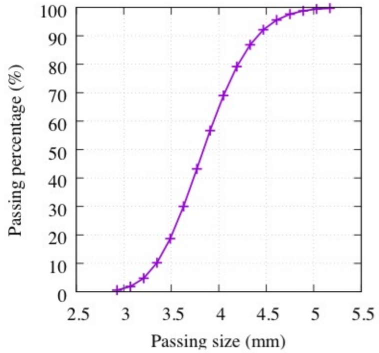


Figure 5. Approximation of (a) width and (b) length distributions of the physical loblolly pine particles (smooth curves) using the bonded-sphere DEM model with six shape templates and thus finite width and length distribution (staircase lines) (adapted with permission from Xia et al.,[45] Copyright 2019, Elsevier). Each bonded-sphere shape template represents real pine particles for a certain range of sizes. As a result, the cumulative distributions of the DEM particles show steps with each step corresponding to the size of a shape template.

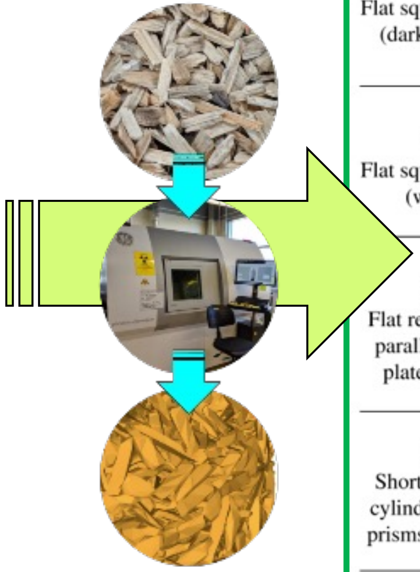
Shape Specification for Biomass Particles

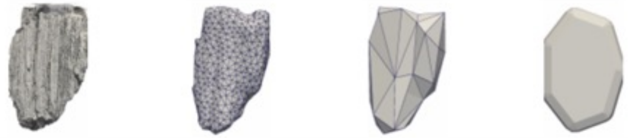
Tools



	Types	Shape description	No. of particles	% No. of particles
(a)		Flat square flakes (dark brown)	38	6.2%
(b)		Flat square flakes (white)	153	25.1%
(c)		Flat rectangular parallelepiped plates/flakes	116	19.0%
(d)		Short needles, cylinders, rods, prisms (4 faces)	171	28.1%
(e)		Medium needles, cylinders, rods, prisms (4 faces)	107	17.6%
(f)		Long needles, cylinders, prisms (4 faces)	24	3.9%

Nano-CT



Types	Example particle	EX-POLY / HIGH-POLY / LOW-POLY / SPHERO-POLY
(a) Flat square flakes (dark brown)	2.5 x 5.2 x 9,9 (mm^3)	
(b) Flat square flakes (white)	2.2 x 5.6 x 8.6 (mm^3)	
(c) Flat rectangular parallelepiped plates/flakes	2.5 x 3.8 x 11.6 (mm^3)	
(d) Short needles, cylinders, rods, prisms (4 faces)	2.6 x 4.8 x 14.1 (mm^3)	
(e) Medium needles, cylinders, rods, prisms (4 faces)	3.1 x 4.9 x 16 (mm^3)	
(f) Long needles, cylinders, prisms (4 faces)	3.6 x 4.6 x 18.7 (mm^3)	

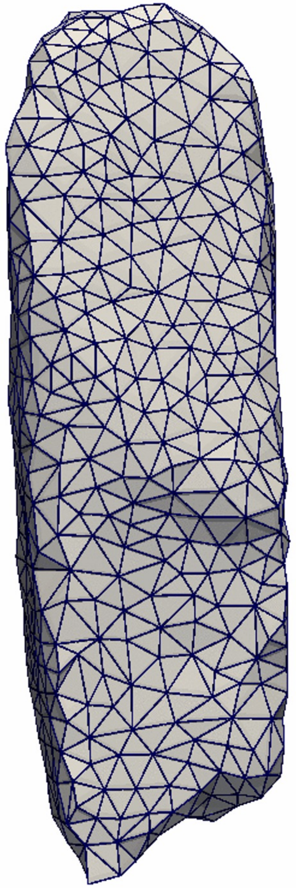
Yidong Xia, Feiyang Chen, Jordan Klinger, Joshua Kane, Tiasha Bhattacharjee, Robert Seifert, Oyelayo O. Ajayi, Qiushi Chen, "Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation." Biosystems Engineering, 205 (2021): 187-211. https://doi.org/10.1016/j.biosystemseng.2021.03.007

A Closer Look at the Fractured Pine Particles

15 micrometer resolution

"Extreme"-resolution polyhedron

Coarse-graining for DEM modeling



"High"-resolution polyhedron

Polyhedral DEM for Pine Particle Physics

Tools

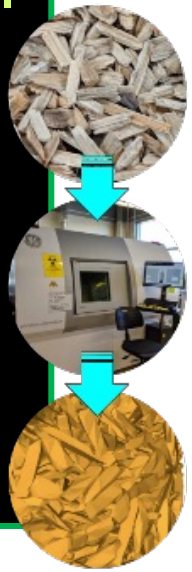
XCT-informed polyhedral DEM for fundamental flow physics of bulk fractured pine particles

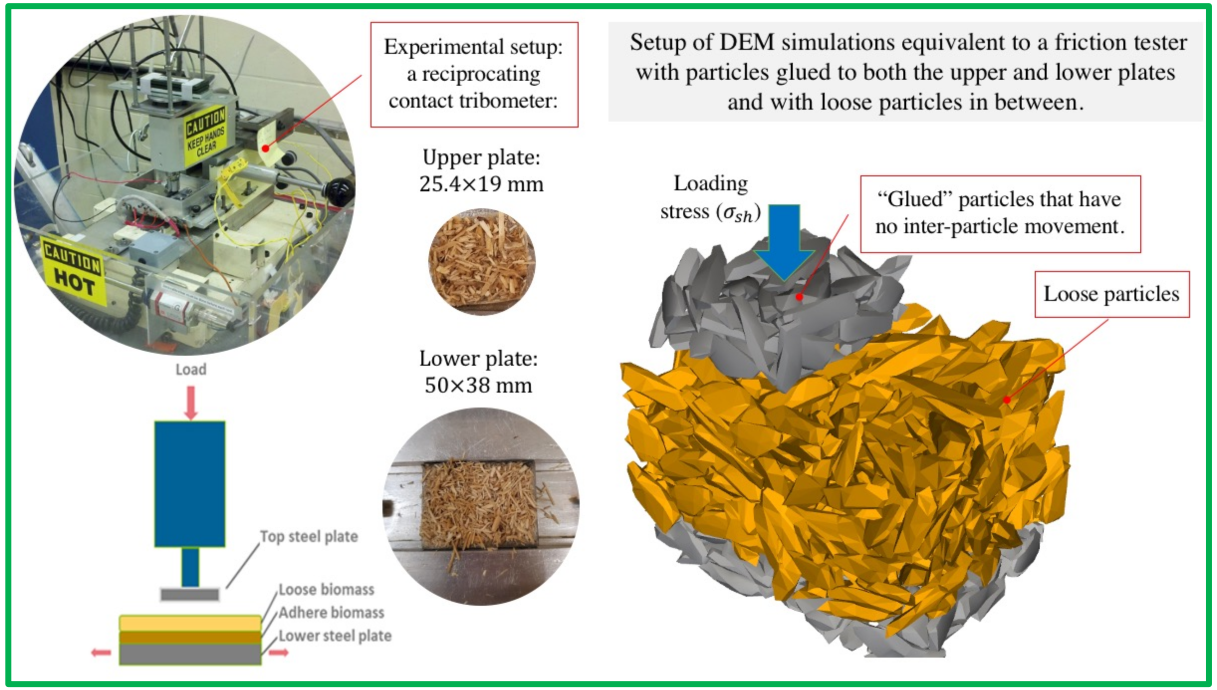
Description

- For study of the influence of particle morphologies (shape, size, etc.) and contact force models as CMAs in stress consolidation.

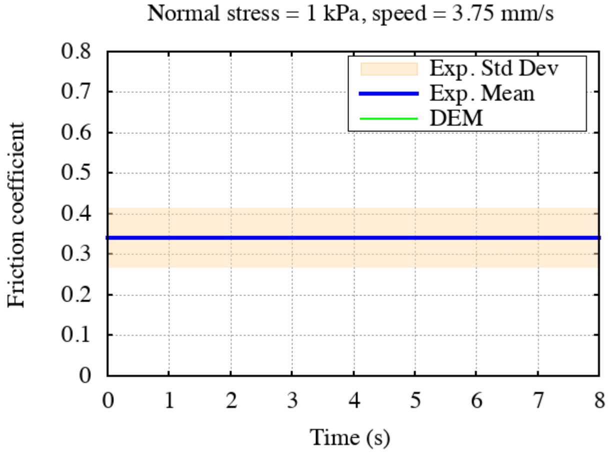
Value of new tool

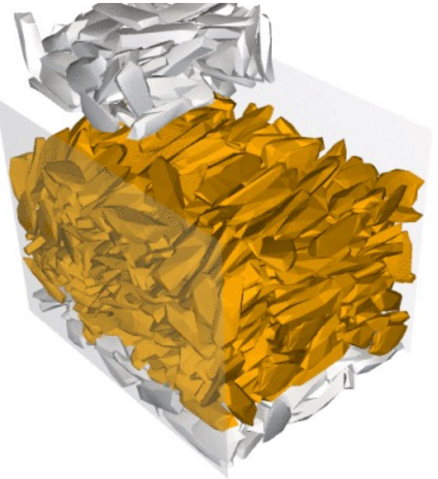
- First-of-its-kind virtual laboratory for biomass particle mechanics.





Yidong Xia, Feiyang Chen, Jordan Klinger, Joshua Kane, Tiasha Bhattacharjee, Robert Seifert, Oyelayo O. Ajayi, Qiushi Chen, "Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation." Biosystems Engineering, 205 (2021): 187-211. https://doi.org/10.1016/j.biosystemseng.2021.03.007

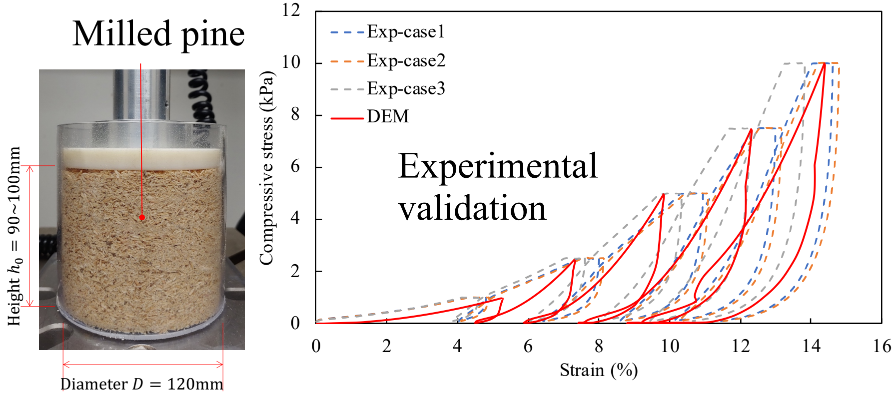




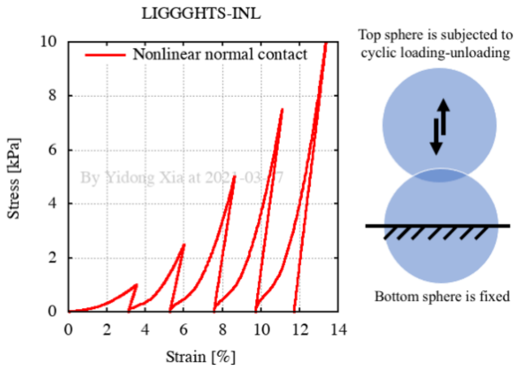
LIGGGHTS-INL open-source DEM

Coarse-grain DEM for bulk feedstock flow

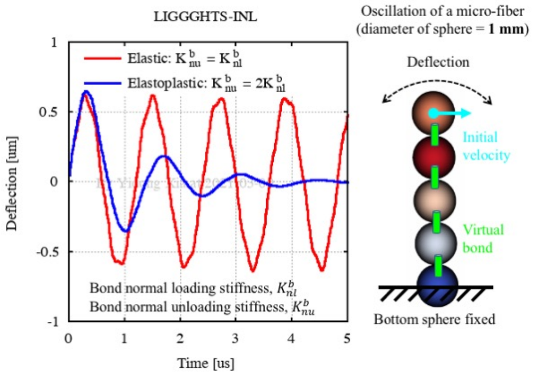
A coarse-grained DEM with hysteretic nonlinear force-displacement contact laws



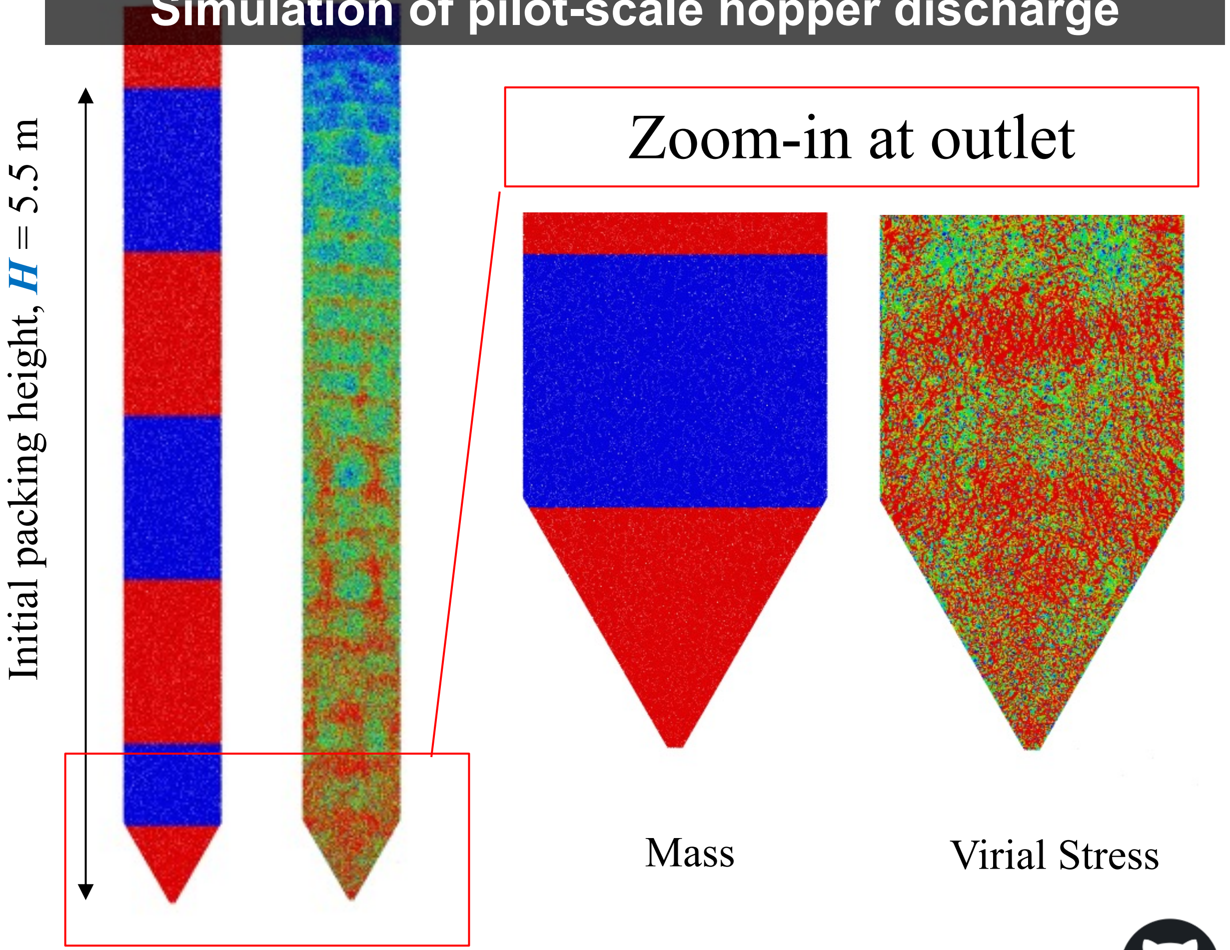
Hysteretic nonlinear contact model



Hysteretic nonlinear flexible fiber model



Simulation of pilot-scale hopper discharge

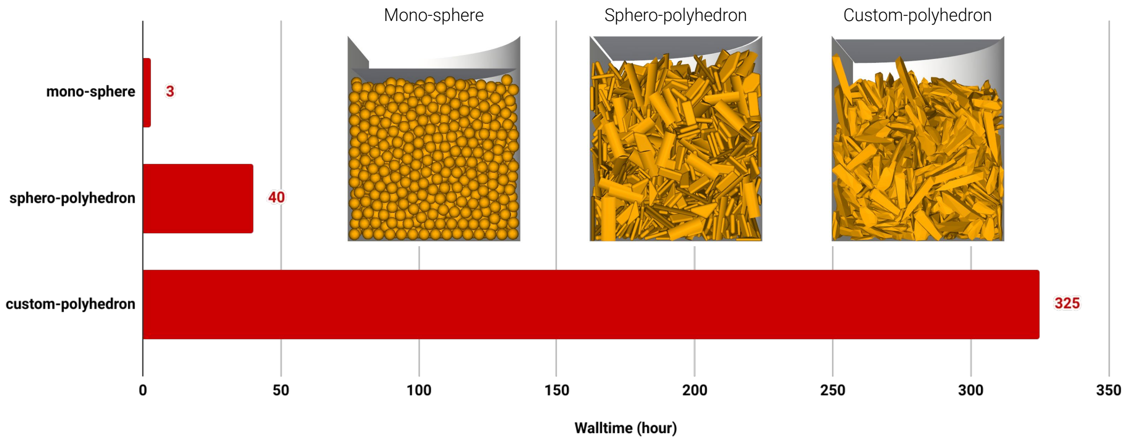


https://github.com/idaholab/LIGGGHTS-INL

GitHub

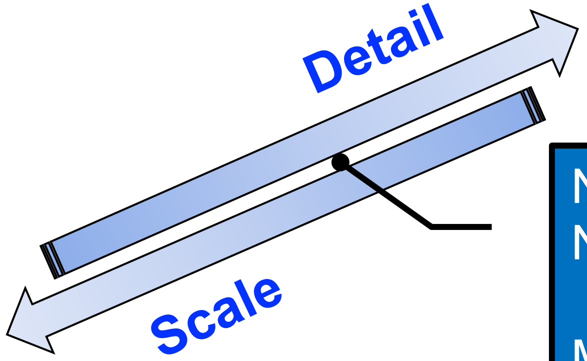
Powder Technology 385 (2021) 557-571
https://doi.org/10.1016/j.powtec.2021.03.008

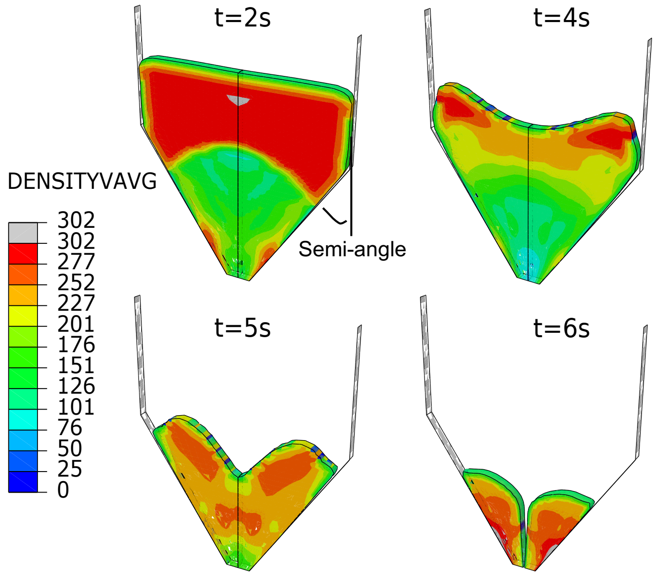
Limitations of Particle-based Models



DEM particle axial shear simulation:

- Size: ~50mm (~2000 particles)
- Resource: 4 CPU cores
- Cost: **300 hours** with polyhedral DEM model
- Cost: **3 hours with** coarse-grained DEM model





FEM pilot-scale hopper simulation
[Jin et al, 2020]:

- Size: ~1000mm;
- Resource: 32 CPU cores
- **Cost: 2 hours**

No access to HPC?
Not a problem.

Most simulations shown here require only a good personal workstation to complete within a reasonable amount of time.

Continuum Flow Theories and Models

Knowledge

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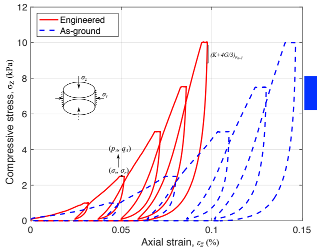
Advanced continuum particle flow theories & models to predict biomass in storage & slow flow conditions.

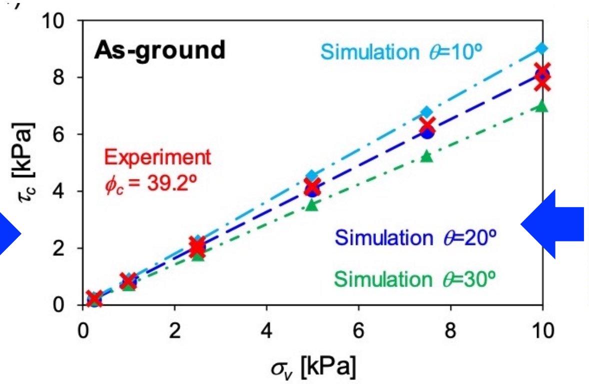
Current Knowledge Gap

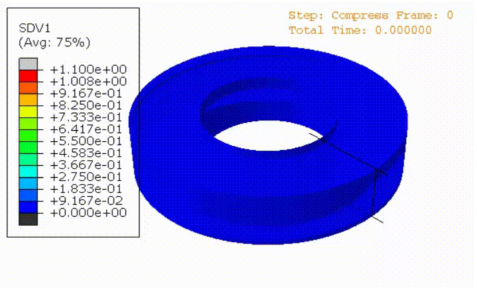
- The state-of-the-art continuum flow models based on different theories & mathematical frameworks have not been evaluated for modeling biomass.
- Lab tests cannot provide direct measurement of constitutive model parameters due to the compressibility of particles

Achievement

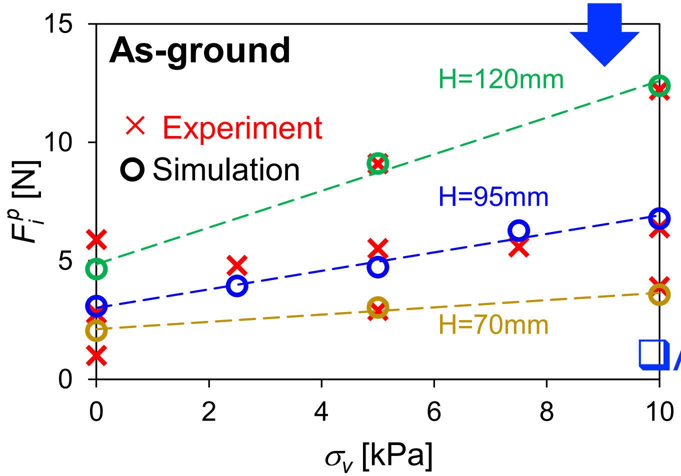
- Established a work-flow to calibrate the model parameters by coupling standard laboratory tests with numerical simulations
- Implemented and evaluated four advanced continuum particle flow models for biomass granular material, and identified the hypoplastic model with critical state theory is the best one

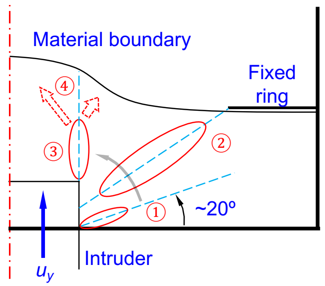


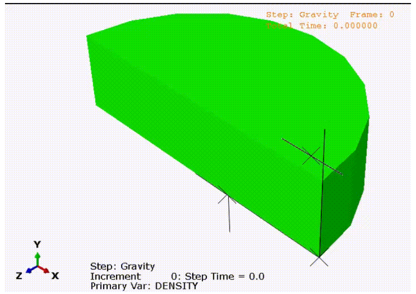




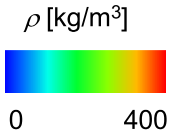
❑ Experiments ❑ Calibrated FEM model ❑ Ring shear simulation







❑Axial shear validation



W. Jin et al. A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine, *Powder Technology*, 368:45-58, 2020. https://doi.org/10.1016/j.powtec.2020.04.038

Continuum Model for Flow Design Guidance

Tools

Reformulated continuum particle flow models predict biomass & guide design of pilot-/industrial-scale hopper & conveyor.

Description

The validated hypoplastic model accurately capture the flow behavior in a pilot-scale hopper and capture flow behavior in the Acrison feeder at industrial-scale

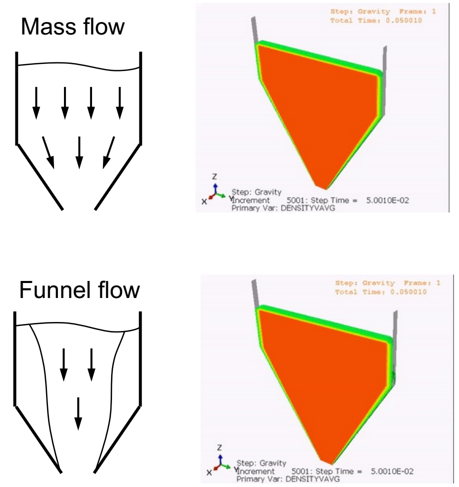
Value of new tool

Industry-scale simulation using the constitutive model will identify the CMAs that control material flow and provide a tool to optimize equipment design and to guide equipment operation for biorefinery engineers

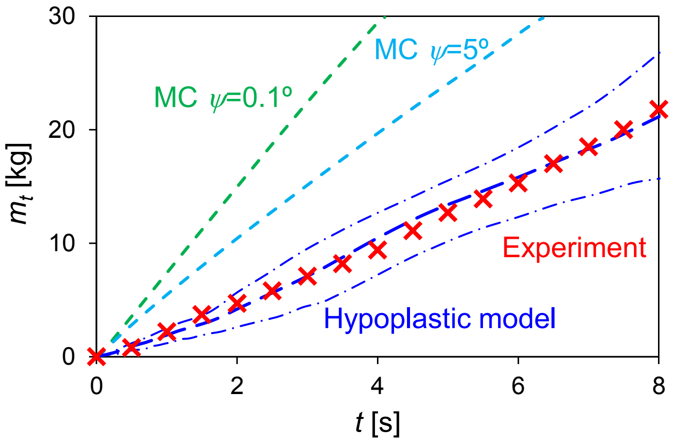
Sensitivity analysis using the constitutive model will provide CMAs working envelops for conventional flow equipment as a tool and the tool will guide biomass preprocessing steps

Y., Lu, W. Jin, J. Klinger, T. Westover, S. Dai. Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model, *Powder Technology* (2021). https://doi.org/10.1016/j.powtec.2021.01.027

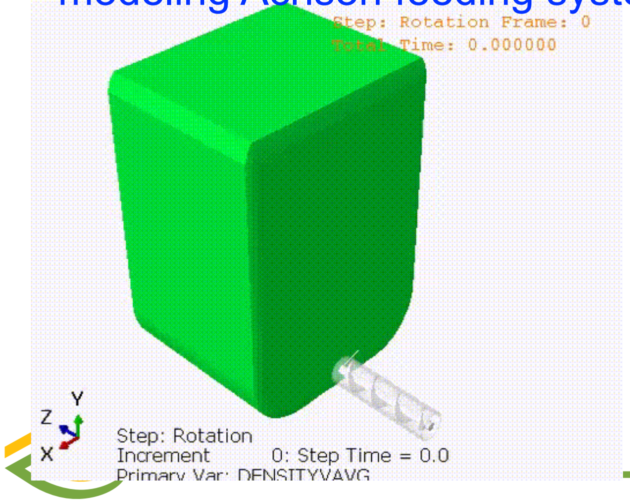
❑ Hopper flow pattern prediction



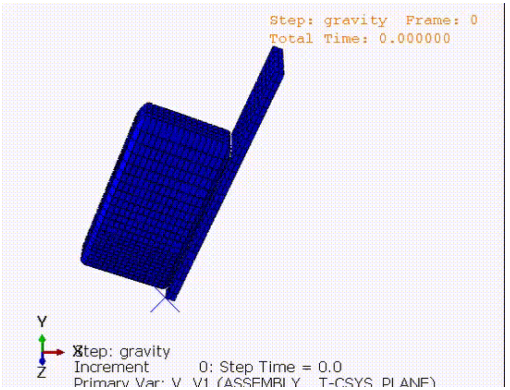
❑ Quantitative flow rate validation



❑ Engineering Application - modeling Acrison feeding system



❑ Inclined plate flow modeling

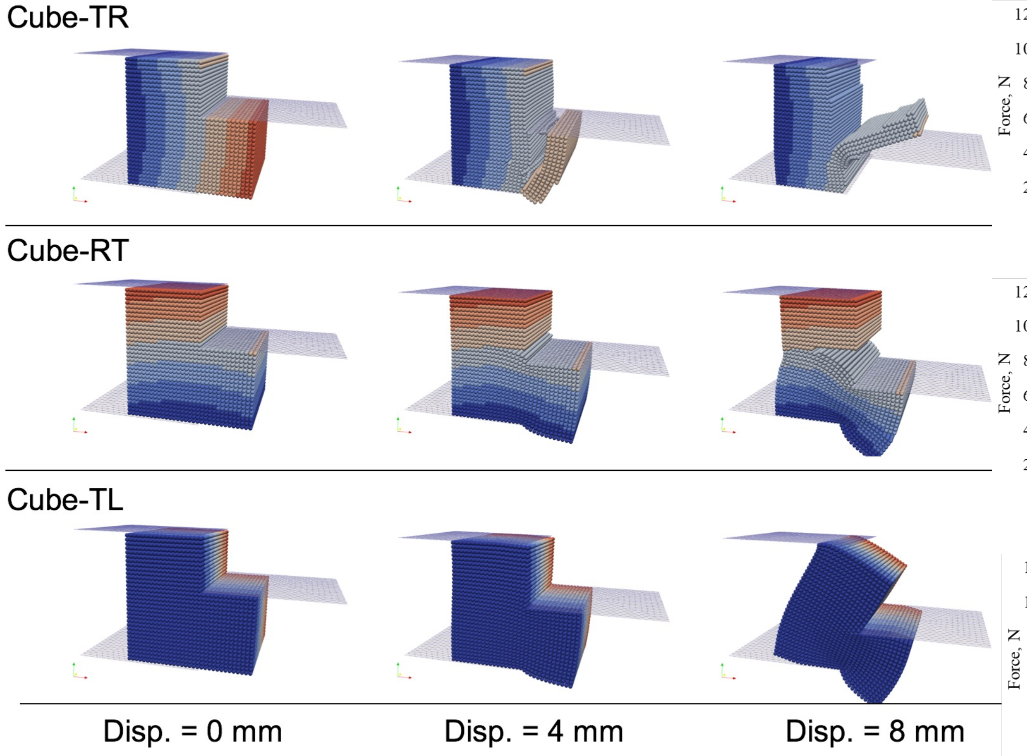


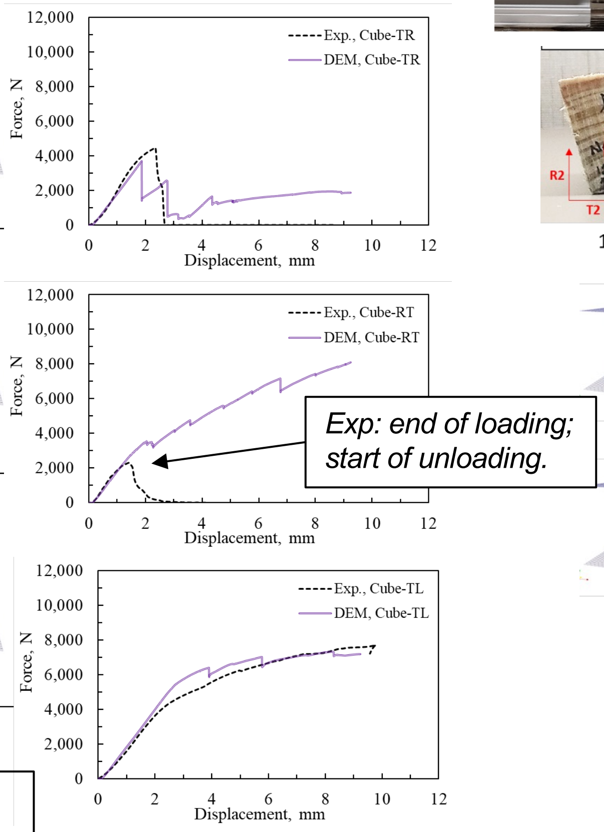
This work is performed jointly with the "Bio-crude Production and Upgrading to Renewable Diesel"

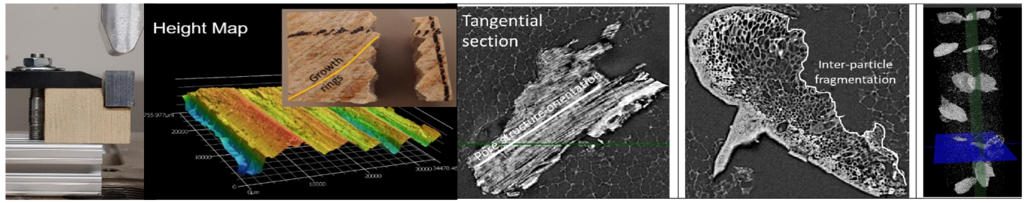
Deconstruction Mechanism Theory & Model

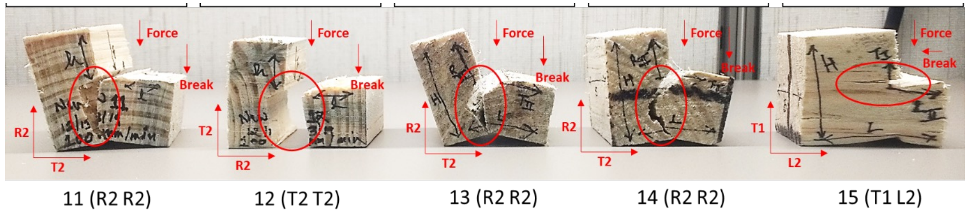
Tools

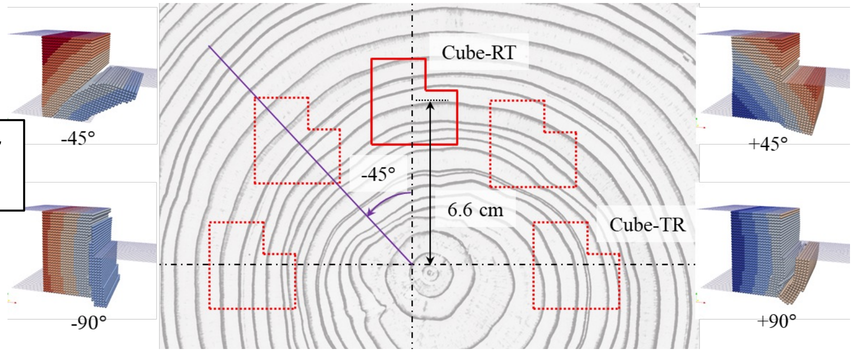
Developed experiment-validated open-source macroscale DEM model for pine structural deformation & deconstruction

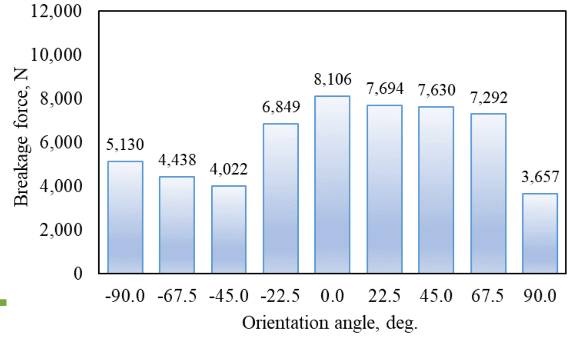










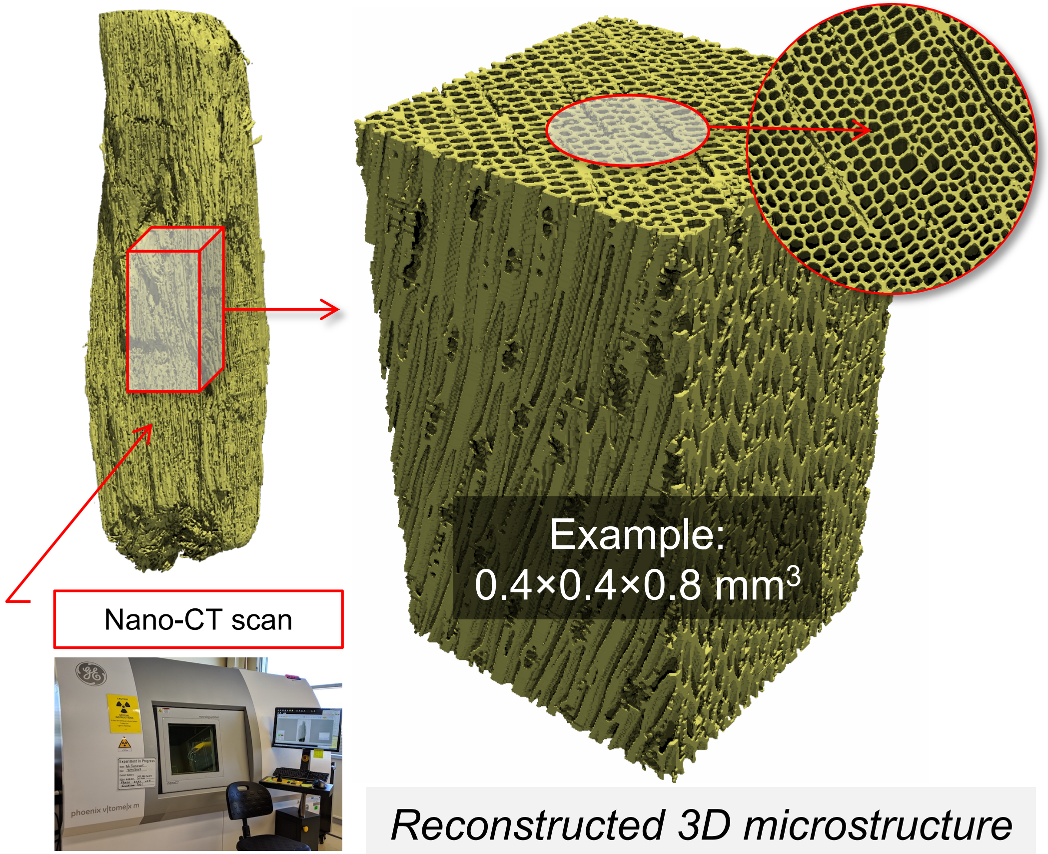


Yuan Guo, Qiushi Chen, Yidong Xia, Jordan Klinger, Vicki Thompson, "A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles." Powder Technology 385 (2021): 557-571. https://doi.org/10.1016/j.powtec.2021.03.008

Enabling Microstructural Fracture Modeling

Tools

Developed XCT-informed loblolly pine 3D microstructural topology reconstruction workflow for fracture physics & models

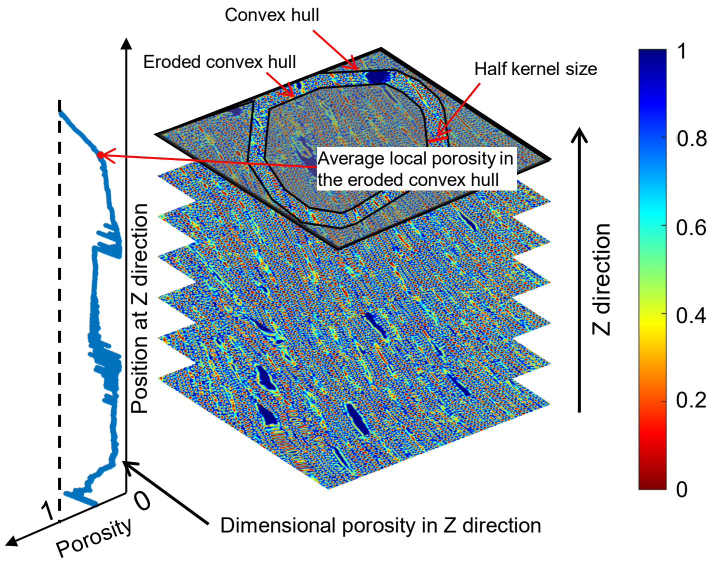


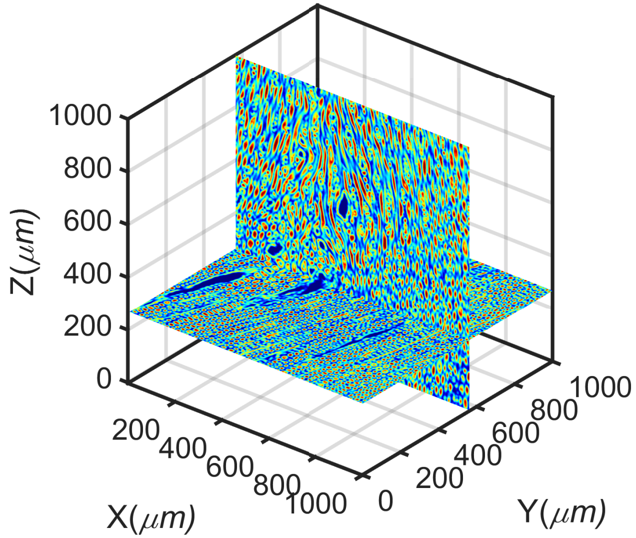
Nano-CT scan

Reconstructed 3D microstructure

Value of new tool

- First-of-its-kind virtual laboratory for biomass micromechanics
- Microstructural mechanics DEM model will be open-source
- An intermediate-scale model links mesoscale model and macroscale model in the multis-scale model plan (NREL/INL)





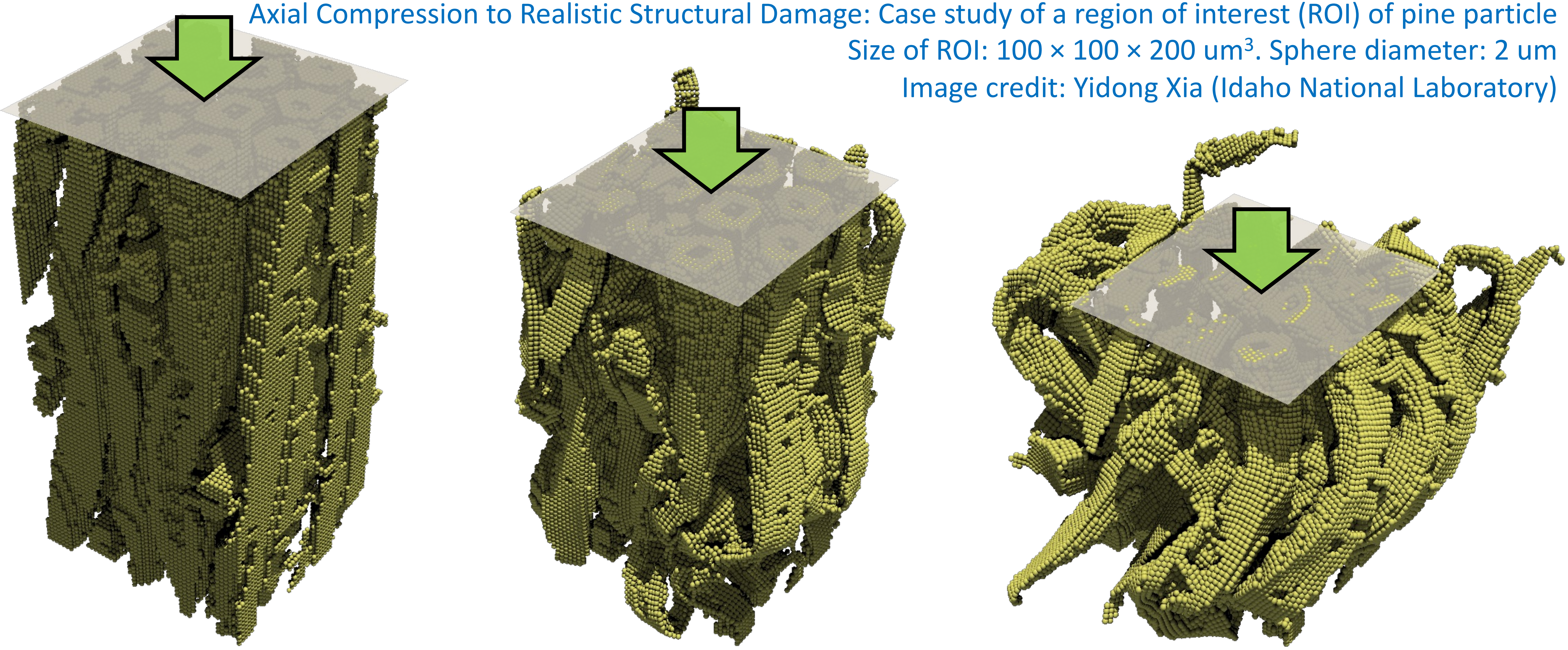
Quan Sun, Yidong Xia, Jordan Klinger, Robert Seifert, Joshua Kane, Vicki Thompson, Qiushi Chen, “X-ray computer tomography-based porosity analysis: Algorithms and application for porous woody biomass.” Powder Technology 388 (2021): 496-504. https://doi.org/10.1016/j.powtec.2021.05.006

Axial Loading of Microscale ROI of Pine Particle

Axial Compression to Realistic Structural Damage: Case study of a region of interest (ROI) of pine particle

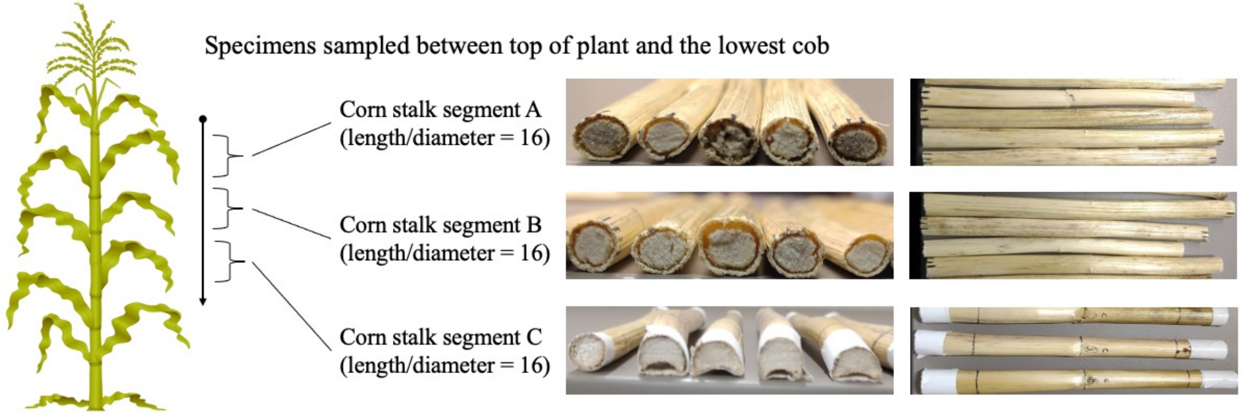
Size of ROI: 100 × 100 × 200 um^3. Sphere diameter: 2 um

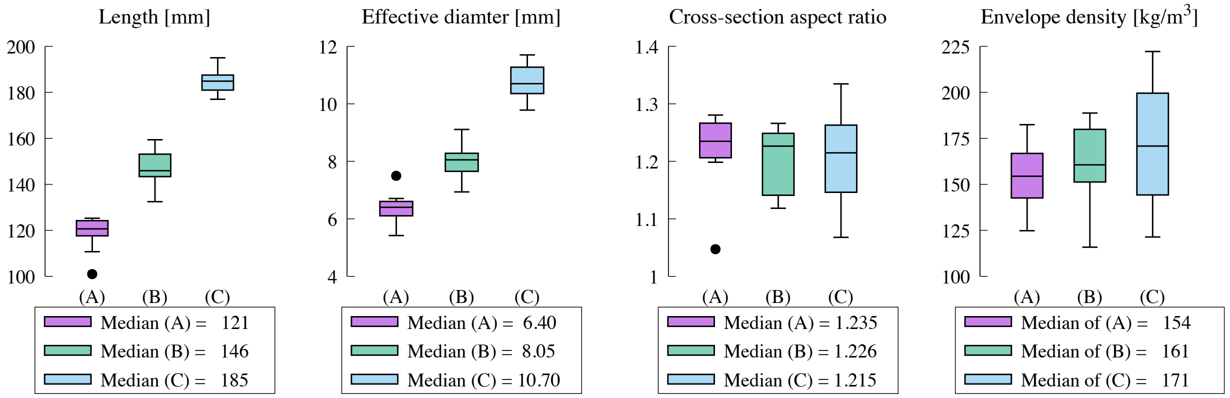
Image credit: Yidong Xia (Idaho National Laboratory)

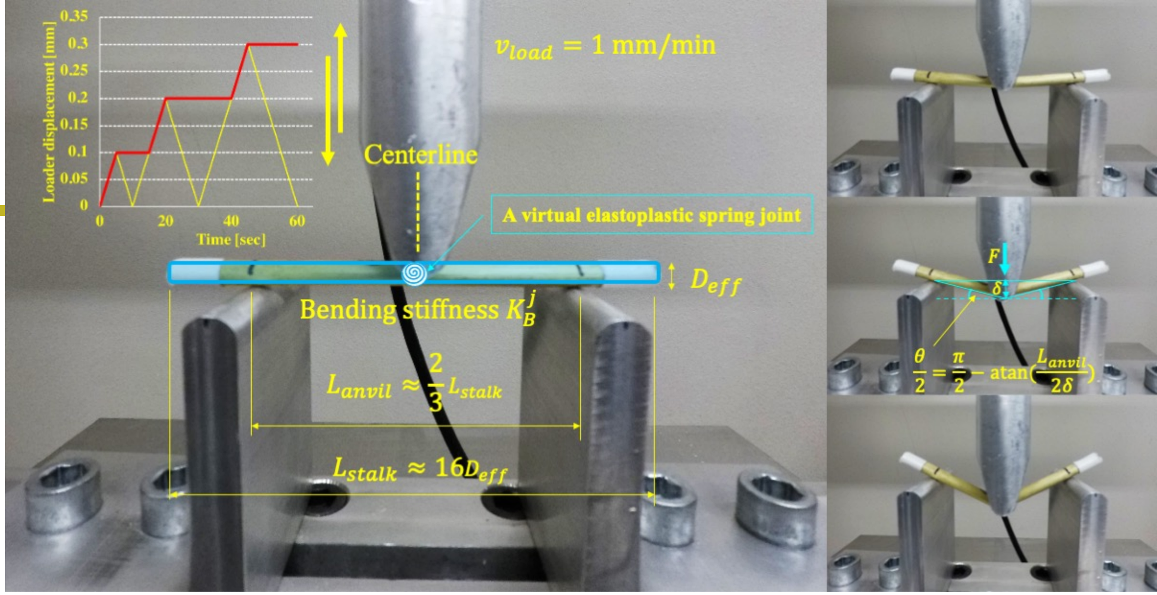


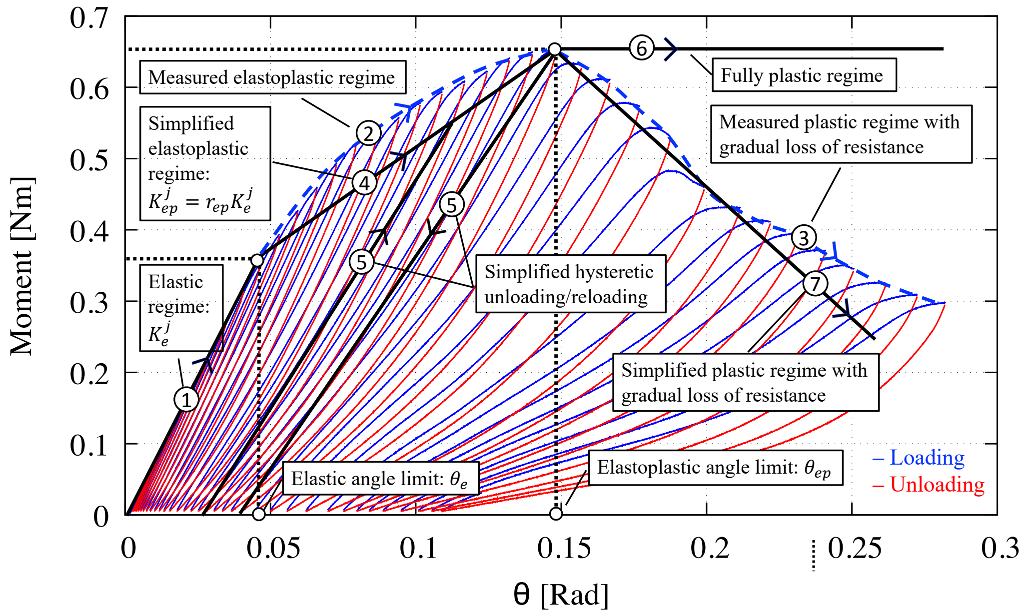
Q. Sun, Q. Chen, Y. Xia, F. Chen, J. Klinger, L. Ding, V. Thompson,
"Reverse scaling of a bonded-sphere DEM model: Formulation and application to lignocellulosic biomass microstructures." *Powder Technology* 407 (2022): 117797.

Biomechanics of Corn Stover









Yidong Xia, Jordan Klinger, Tiasha Bhattacharjee, Vicki Thompson, “The elastoplastic flexural behavior of corn stalks”, Biosystems Engineering 216 (2022): 218-228.

Preprocessing – An JRS Knife Milling Model

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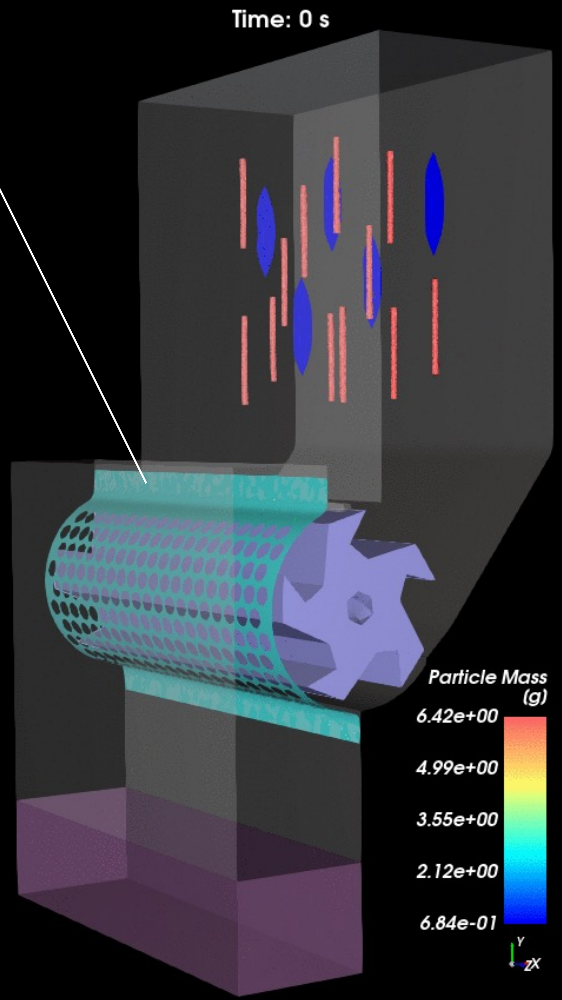
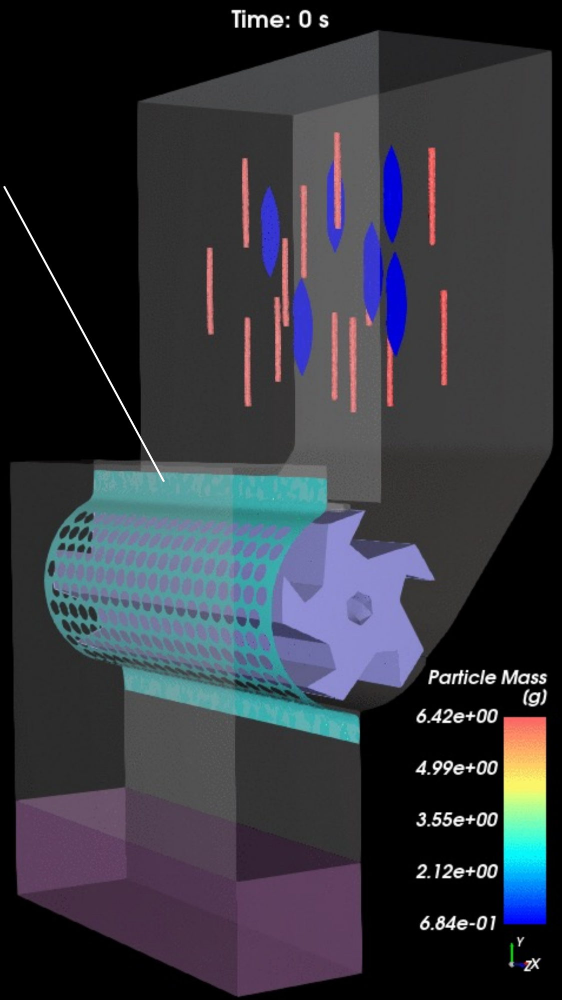
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Low rpm:
- Corn leaf comminuted
- Corn stalk deformed but not comminuted

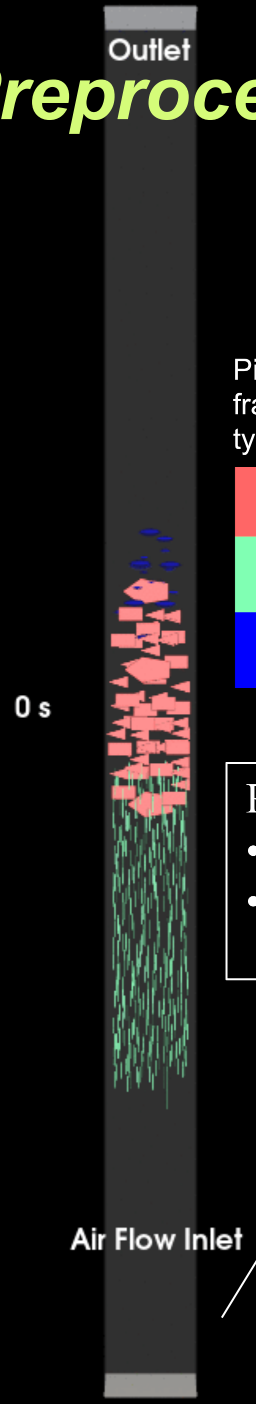


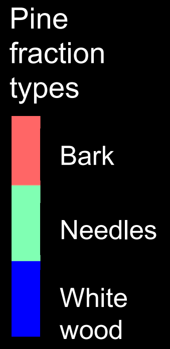
High rpm:
- Corn leaf comminuted
- Corn stalk comminuted



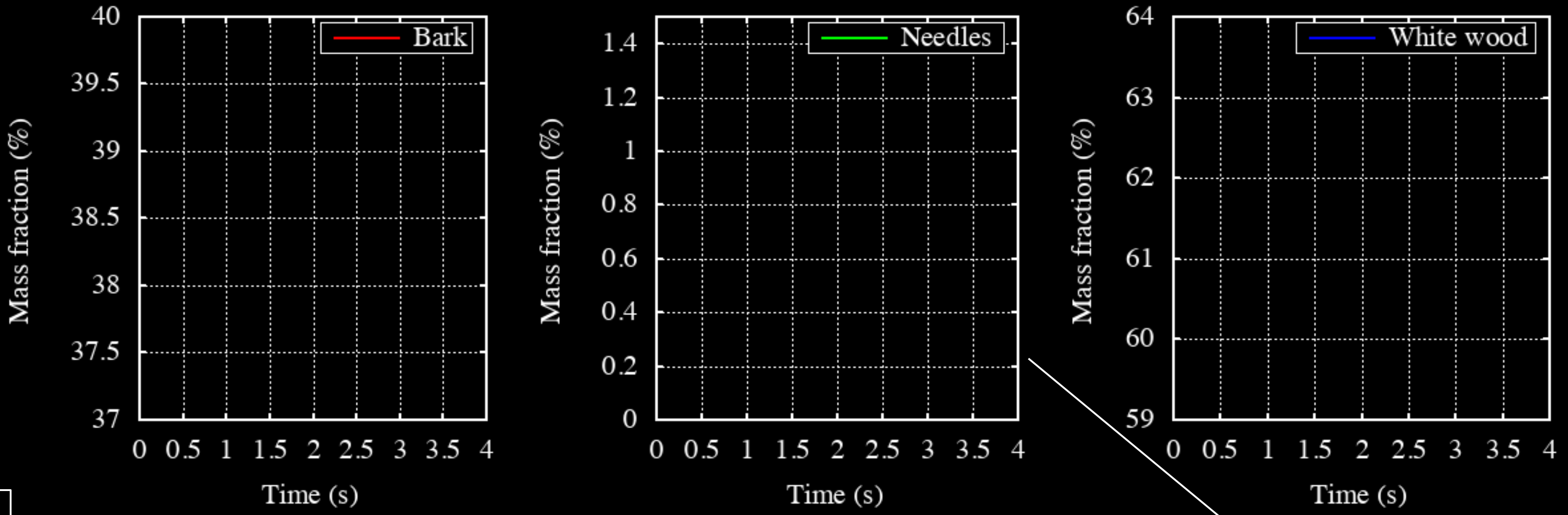
Preprocessing – An Air Classification Model

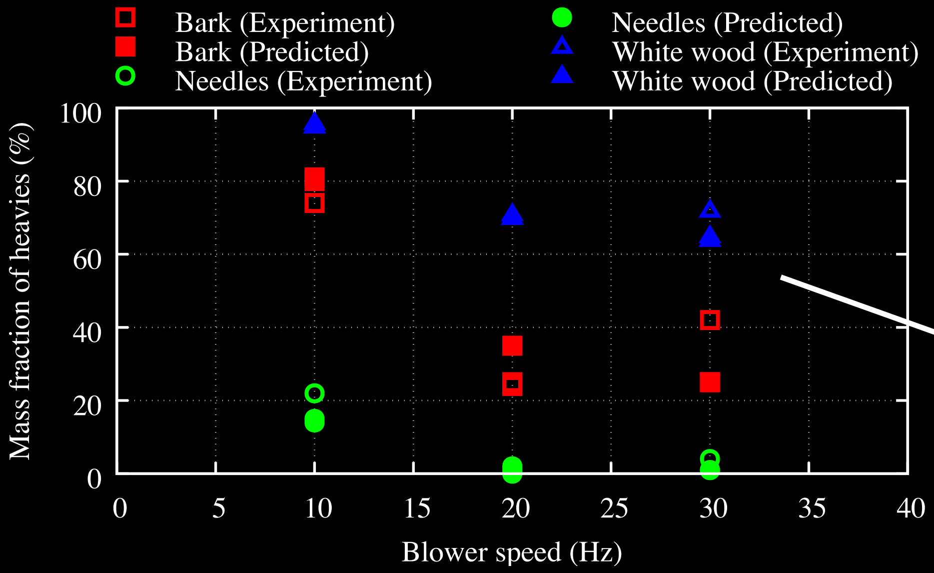
Tools





Process parameters:
- Feed rate
- Blower power, etc.





Quality attributes:
- Heavy fraction mass rate
- Output particle size distributions, etc.

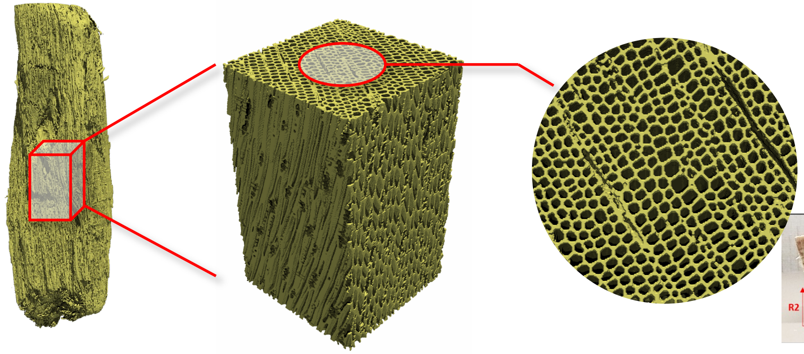
Experimental validation

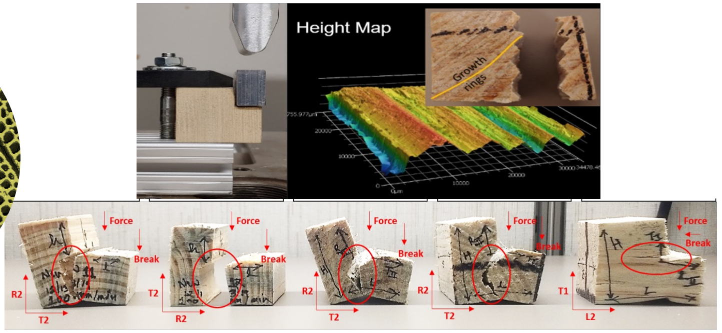
Readying Capabilities for the Emerging Needs

Understanding and being able to model the unique physical characteristics of municipal solid waste (MSW) is a prerequisite of including MSW in Virtual Feedstock Processing Laboratory.

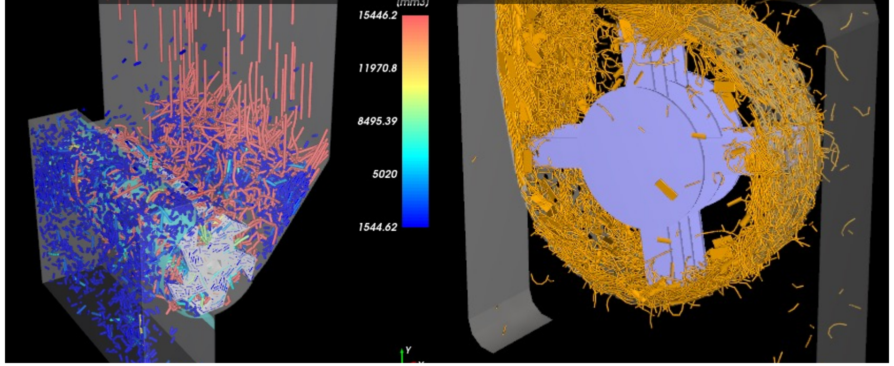
Recap: Virtual Feedstock Processing Laboratory

XCT-informed microstructural deconstruction model and upscaling



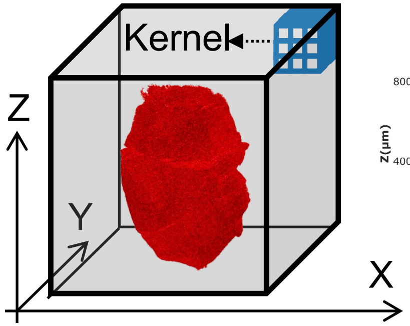


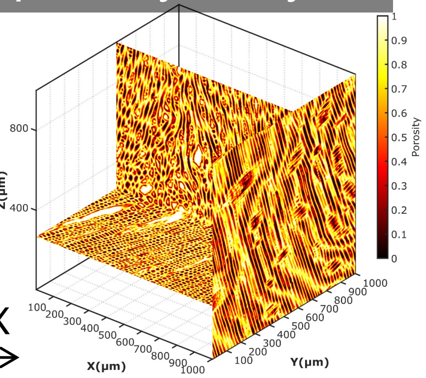
Modeling of various milling techniques

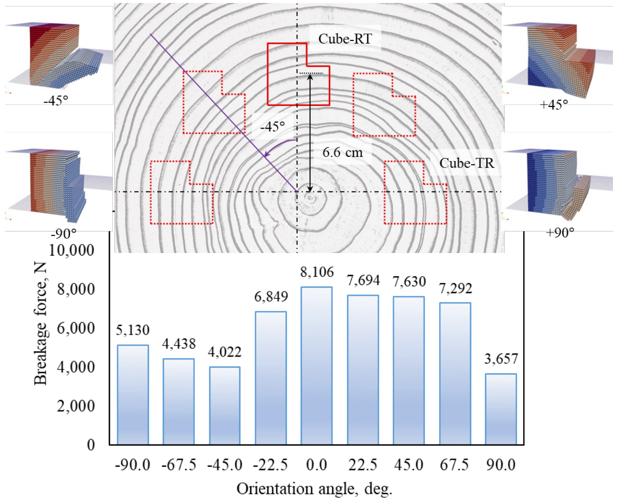


Microscale (um) → **Laboratory scale (cm)** → **Pilot scale (m)**

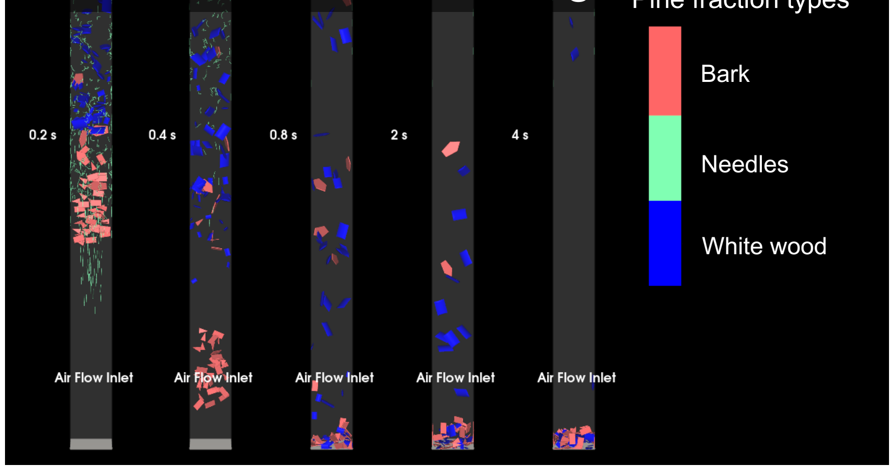
Advanced micro-porosity analysis

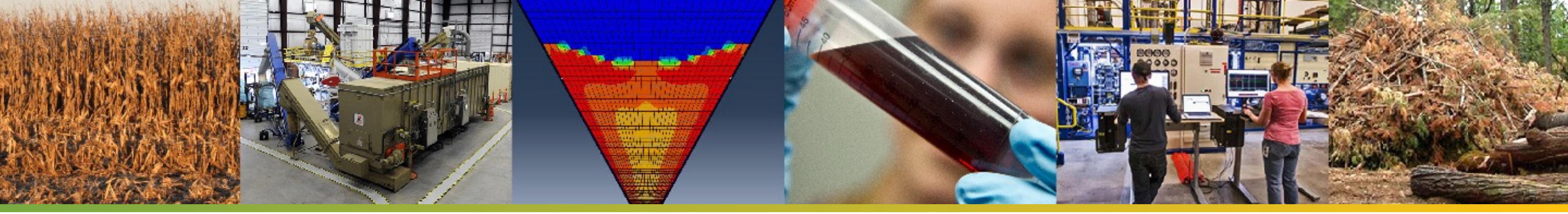






Air classification modeling





Thank you

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