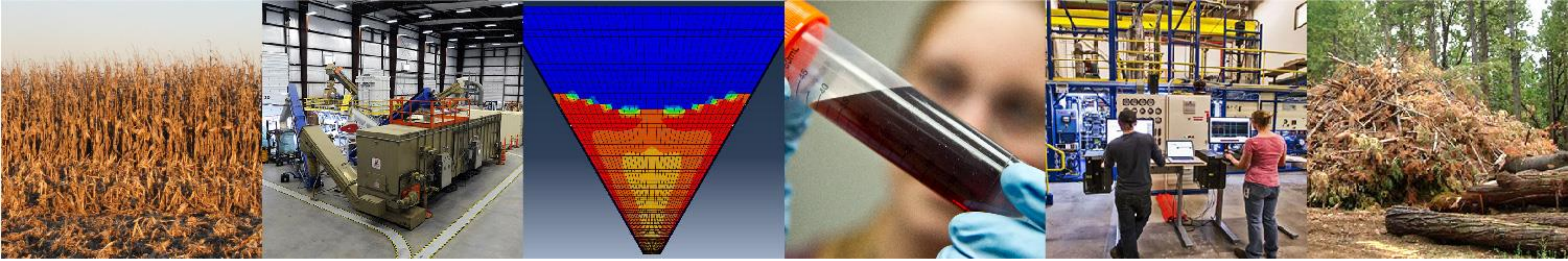


DOE Bioenergy Technologies Office
BETO 2019 Project Peer Review

Feedstock-Conversion Interface Consortium (FCIC)
WBS 1.2.2.50x: Feedstock Physical Performance Modeling

March 4-8, 2019
Technology Session Area Review

Principal Investigator: Tyler Westover

FCIC
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Goal Statement

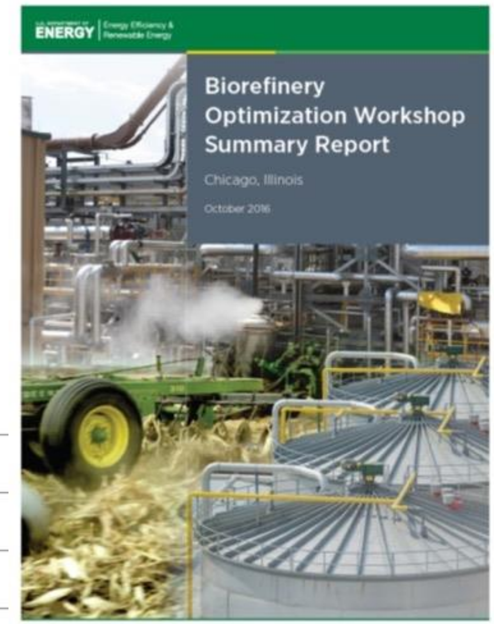
1-Year Project Goal (shared with Variability Project, 1.2.2.40x):

– Develop accurate & complete methods to measure physical & mechanical properties of bulk corn stover and loblolly pine materials for physics-based computational simulations
  - *Specific application*: Achieve agreement $R^2>0.8$ between model predictions and lab measurements for a custom lab-scale flow test apparatus

Outcomes:

– Physics based models provide:
  - Relationships between **specifications** and **flowability**
  - Identification of properties needed for QA/QC (**variability**)
  - Means to scale lab/pilot feeding data to industry operations (**equipment performance data**)

– Above items lead to increased **equipment uptime**

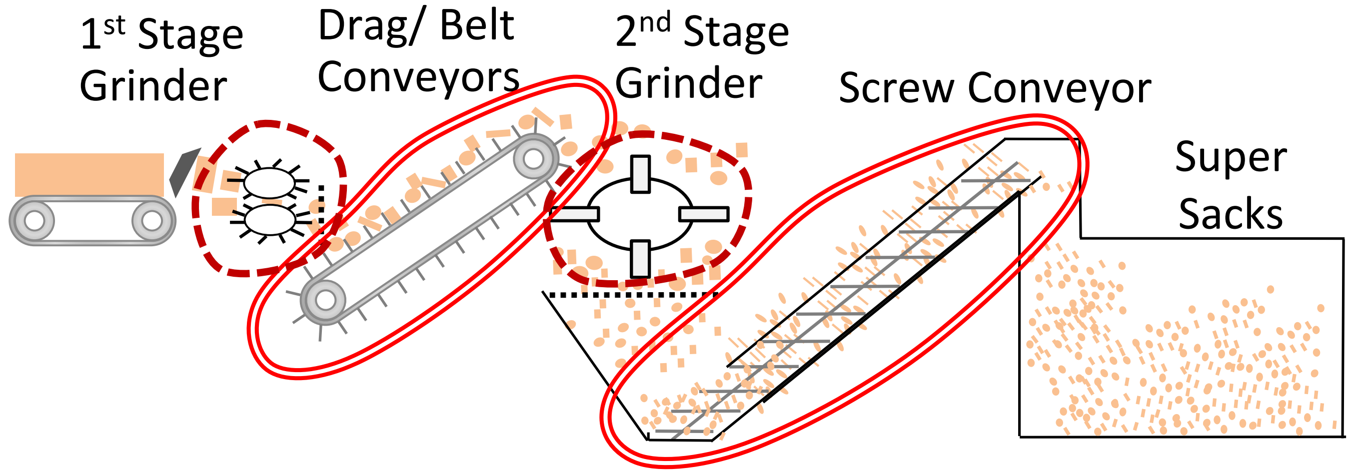


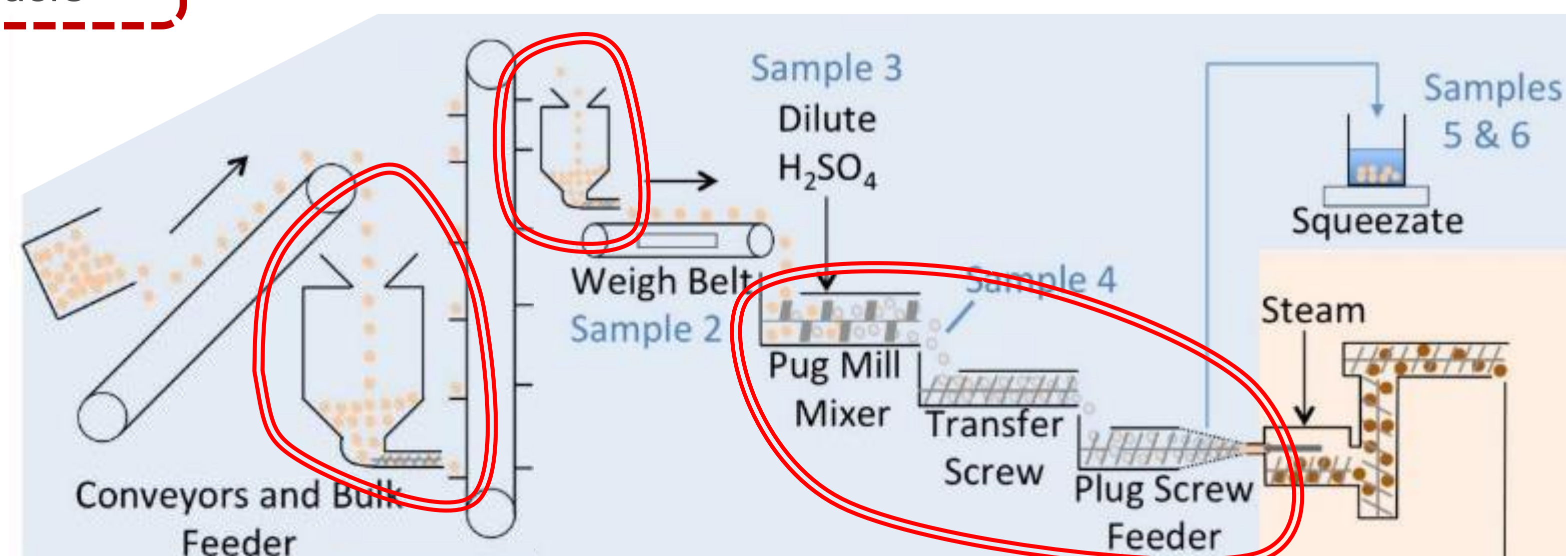
https://energy.gov/eere/bioenergy/downloads/biorefinery-optimization-workshop-summary-report

1 – Project Overview

Near-term target areas of impact:
- Belts
- Conveyors
- Hoppers
- Mixers
- Feeders

Future target:
- Grinders





1st Year focus: Fundamental material behavior, not specific equipment or operation

1 - Project Overview (Cont.)

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Goal of the Consortia

- Identify and address the impacts of feedstock variability – chemical, physical, and mechanical – on biomass preprocessing and conversion equipment and system performance, to move towards 90% operational reliability.

Biomass Quality

- Feedstock Variability and Specification Development — *Allison Ray (INL)*
- **Feedstock Physical Performance Modeling** — *Tyler Westover (INL)*

Upstream-Downstream Process Integration

- Process Integration — *Ed Wolfrum (NREL)*

System Readiness Evaluation

- System-wide Throughput Analysis — *Dave Thompson (INL)*
- Process Control and Optimization — *Quang Nguyen (INL)*

Characterizing Biomass & Mining Data

Improving Operational Performance

Implementing Integrated Control Strategies

Quad Chart Overview

Timeline

- Start date: 10/01/2017
- End date: 09/30/2018
- **Percent complete: 100%**

	Total Costs Pre FY18**	FY 18 Costs (total)
Total DOE funded	$0	$1,500,000
INL	$0	53%
NREL	$0	37%
ANL	$0	10%

Partners: ● Purdue University
● Clemson University
● E&G Associates
● Material Flow Solutions, Inc.

Barriers addressed (Multi-year Program Plan)

- Ft-H: Biomass Material Handling & Transport
- Ct-A: Feedstock Variability
- Ct-B: Reactor Feed Introduction

Objective

Use mechanistic modeling to identify the causes of feed-handling failures and validate predictions to lead to improved process designs to enhance the reliability of industrial integrated biorefineries (IBRs).

End of Project Goal

Year 1: Achieve agreement (R^2>0.8) between model predictions and lab measurements for a custom lab-scale flow test apparatus.

Year 3 (originally planned): Robust computational simulations and characterization methods to enable 50% improvement in biorefinery operating reliability relative to base case for hopper/feed auger systems and compression screw augers at scales of 1 to 50 tonne/hr.

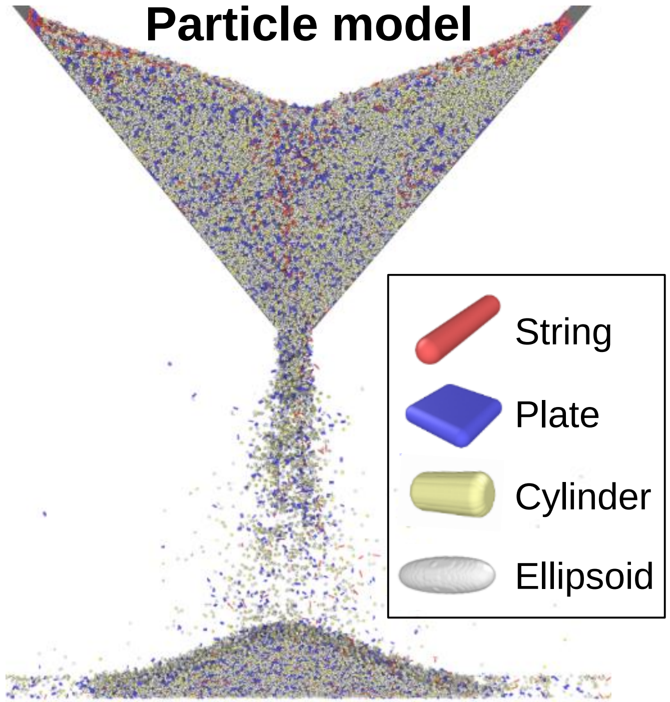
1 – Project Overview (Cont.)

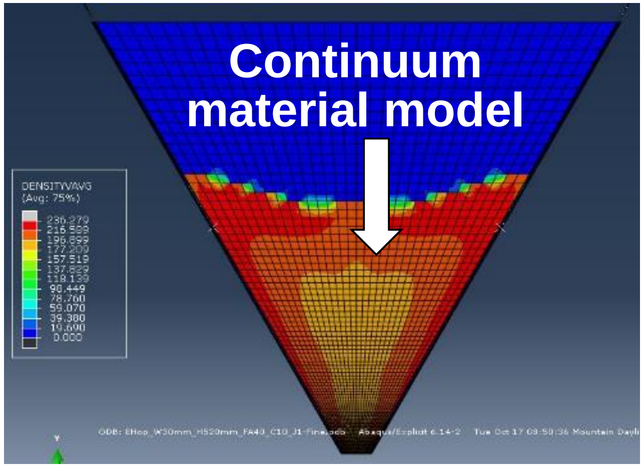
- Understanding the feeding and handling (F&H) behavior of materials is a critical enabling factor for many industries, such as petroleum, food, pharmaceutical, and manufacturing.
- Conventional design of F&H equipment is based upon technology developed for fine powders 40 years ago (not adequate for biomass).

Substantial progress in this area requires:

1. Particle (discrete element method or DEM) models that rigorously capture flow physics.
2. Continuum (structural mechanics) models that can scale to industry operations.
3. Close coupling between model development and instrumented pilot-scale flow tests.

INL, NREL, and ANL have the necessary modeling and pilot-scale test capabilities





2 – Approach (Management)

Task Management

- Bi-weekly calls with other projects in the FCIC
- Semi-annual face-to-face meeting with other FCIC projects
- Periodic inter-laboratory team meetings & visits
- Quarterly progress reports

Leverage related BETO-sponsored work

- Shared milestones, data and leadership with Feedstock Variability project (1.2.2.40x)
- Close collaboration with competitive Integrated Biorefinery Optimization Modeling projects at NREL, Purdue, Clemson and Forest Concepts
  - Sponsored interns from Purdue and Clemson
- Also collaborates with the Consortium for Computational Physics and Chemistry (CCPC; www.ccpcbiomass.org)
- Create & follow approved project management plans

Collaborate with leading bulk material handling consultants

- E&G Associates, Inc.
- Material Flow Solutions, Inc.

2 – Approach (Technical)

Tasks & Connections

Task Name	Inputs	Outputs
Task 1: Baseline industry practices	Literature	Effectiveness of current methods
Task 2: Flow of elastoplastic bulk solid biomass	**FV:** Properties **PI:** Flow data	Functional relationships: **FV, PI, PCO, SWA**
Task 3: Flow of highly compressed feedstocks	Same as #2	Same as #2
Task 4: Mechanics of grinding	**FV:** Properties	Comminution …. (same as #2)
Task 5: Mechanics of wear (reported in PI)	**FV:** Properties **PI:** Wear data	Wear … (same as #2)

80% of funds (Tasks 2 and 3)

FV: *Feedstock Variability Project (FCIC)*
PI: *Process Integration Project (FCIC)*
PCO: *Process Controls and Optimization Project (FCIC)*
SWA: *System-wide Throughput Analysis Project (FCIC)*

Bench scale
- Characterization
- Physical tests
- Particle simulations
- Continuum simulations

Pilot scale
- Physical tests
- Continuum simulations

Industry scale
- Continuum simulations

Future

2 – Approach (Technical, Cont.)

Critical Success Factors

- >85% agreement between models and verification tests.
- Acceptance of methods by OEMs and solids handling consulting firms.

Challenges

- Flow properties depend upon stress, strain rate, density, deformation history, etc.
- There are multiple layers of coupled flow mechanisms
  - Elasticity, plasticity, viscosity, creep, damping, etc.

Example: Particle Segregation During Baseline Tests

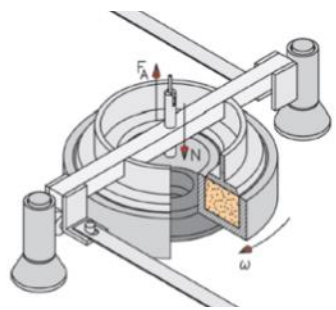
- "Hair balls" exacerbate material heterogeneity.
- Segregation introduces new transient effects with multiple time scales **!!! OUCH !!!**
- Particles with different properties have different scaling behaviors **!!! AUGH !!!**
- Well designed flow tests must avoid segregation (fortunately, industry has good understanding of segregation; other issues are not as easy).

Bridging of Biomass into plug feeder

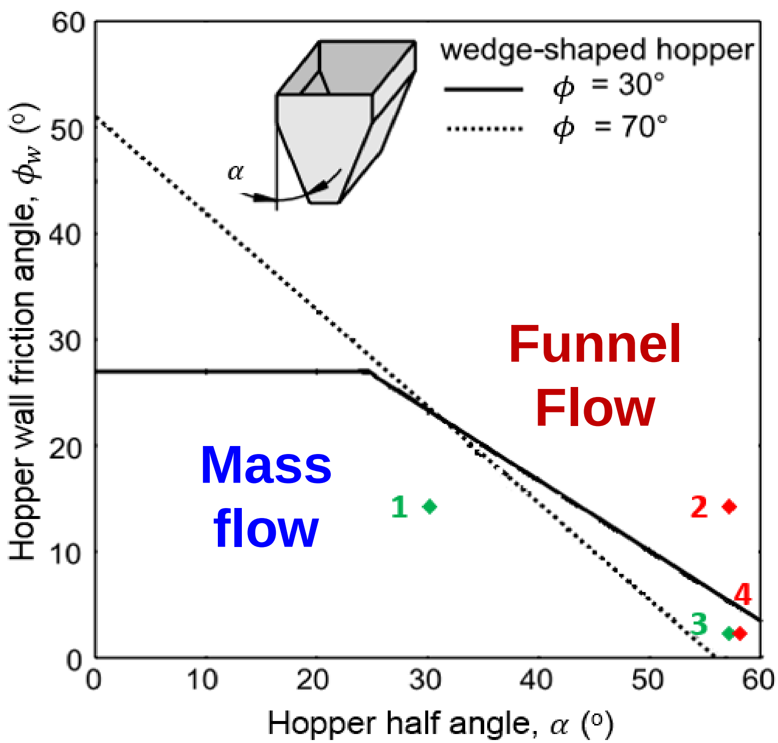
Cablevey Jam

2 – Approach (Technical, Cont.)

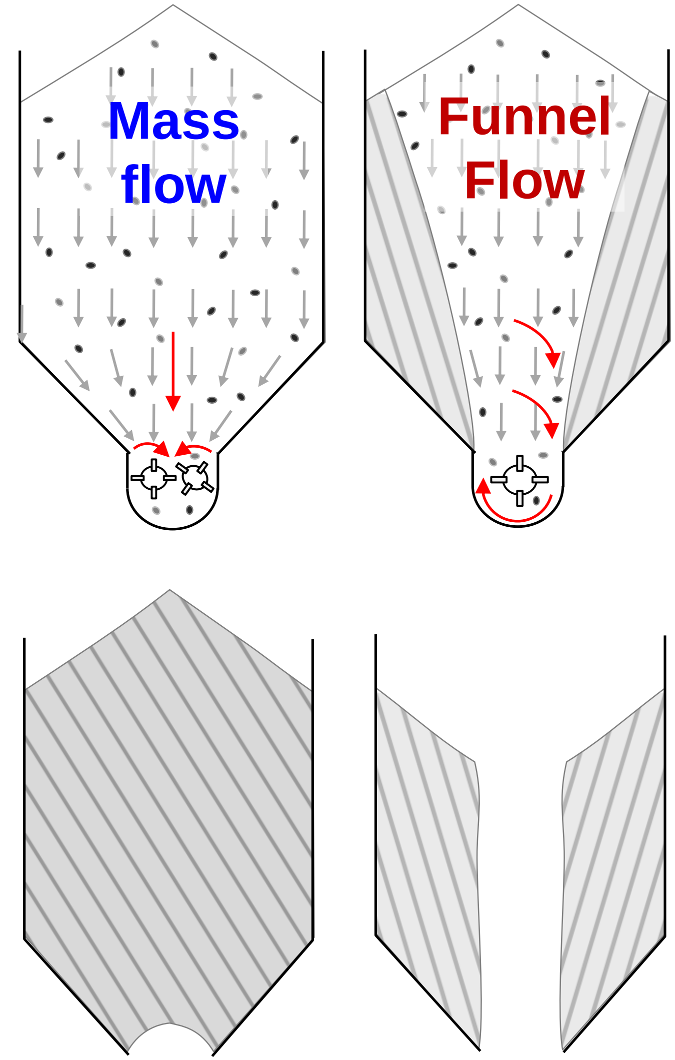
- **<u>Particulate materials</u>** exhibit a variety of flow modes, depending upon material properties and boundary conditions (<u>especially outlet</u>)
  - Mass flow: No stagnant zones; also more uniform
- Shear tests have been used for >40 years to predict the flow mode and quantitatively design equipment



Schulze Ring shear tester; www.dietmar-schulze.de/powtve



Schulze, Flow properties of powders and bulk solids, Springer, 2007.



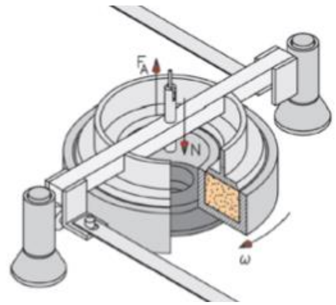
Arch

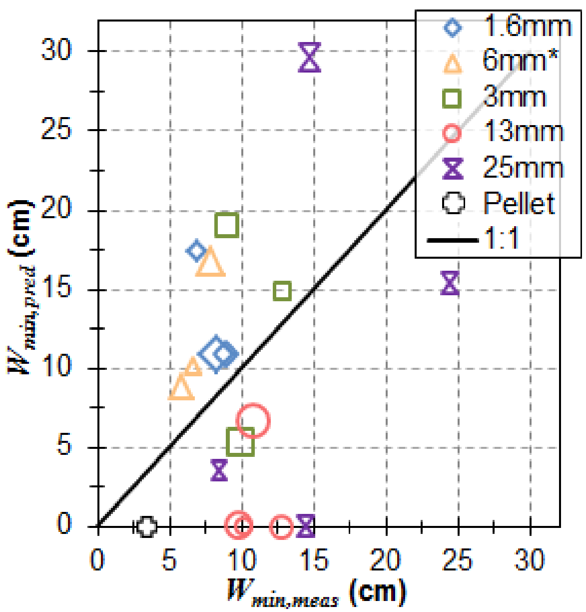
Rathole or pipe

2 – Approach (Technical, Cont.)

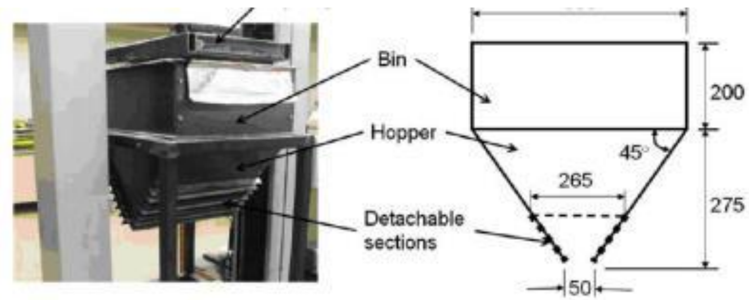
Many different tests have tried to predict biomass flow in hoppers, augers, etc.

Schulze Ring shear tester; (a leading tester world-wide)





Prior work: measured hopper opening size for flow vs. prediction based on Schulze shear test



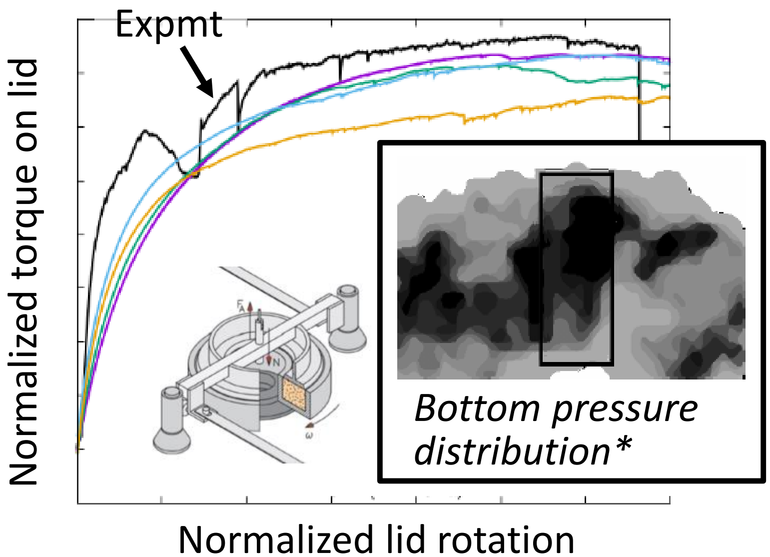
Hopper with detachable sections. *Guan & Zhang, J. Food Engineering. 94, 227 (2009).*

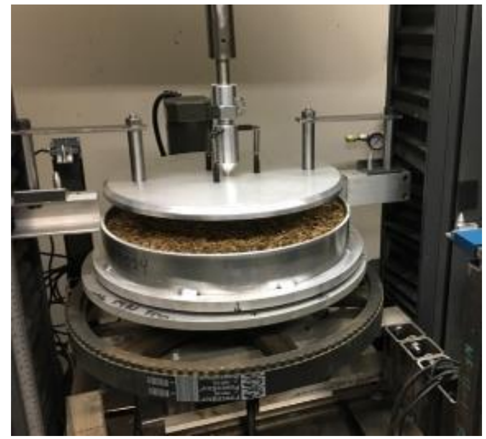
Angle of repose

Johanson "extrusion" test

- **No test has proven reliable to predict biomass flow**
- **In Year 1, we focused on three tests (next slide) to understand flow behavior, which can be applied to hoppers, augers, etc. in future years**

2 – Approach & 3 – Accomplishments (Both Technical)





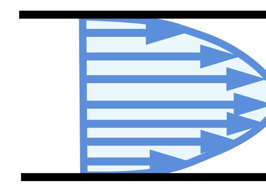
Modified Peschl shear tester (partner with E&G Associates)

Tests performed in the Feedstock Variability Project (1.2.2.40x).

- **Known issues with Schulze shear tester**
  - Non-uniform stress distribution
  - Non-ideal wall effects
- **Do these issues cause poor flow predictions?**
- **Answer sought by combination of experiments & simulations**
  - Idealized simulations match experiments
  - Results using more rigorous test (modified Peschl tester) match those from Schulze
- **Conclusion: Poor flow predictions not due to non-ideal boundary effects**

Root cause of poor flow predictions

- Biomass flow in both testers is ~ 1 dimensional
- Flow in real equipment is multi-dimensional
- Tests do not account for material anisotropy
- Tests do not account for coupling of flow mechanisms (analysis assumes simple shear)

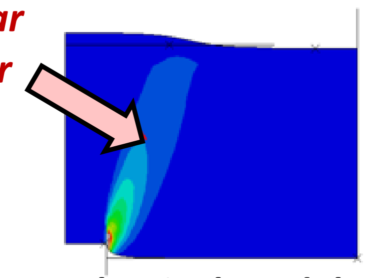


3 – Technical Accomplishments, Cont.

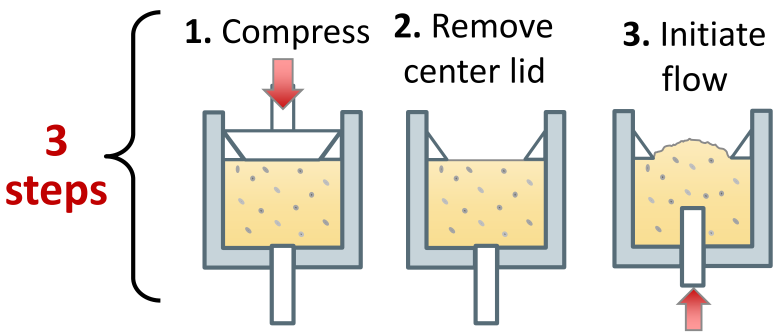
1st Year Goal: Achieve agreement (R^2>0.8) between model predictions and lab measurements for a custom lab-scale flow test apparatus (**"Direct axial shear test"**)

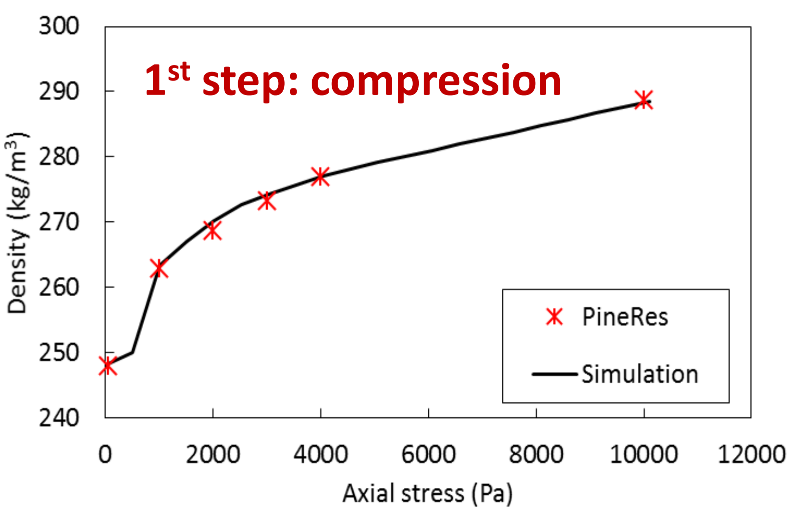
- **Includes effects of material anisotropy**
- **!!! Much more difficult to simulate !!!**

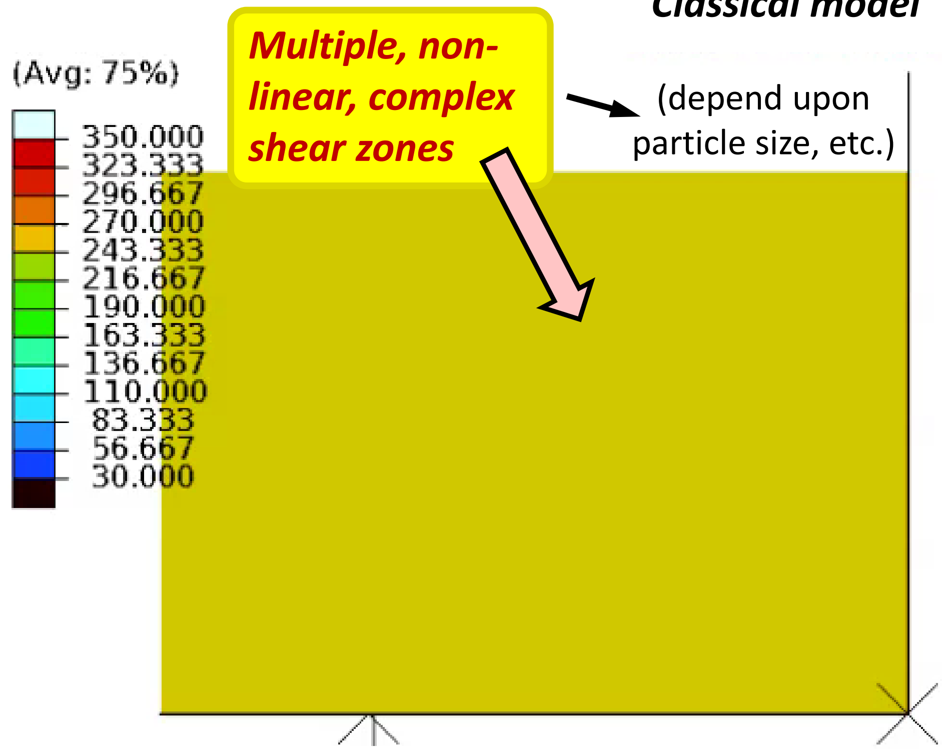
Linear shear zone



Classical model



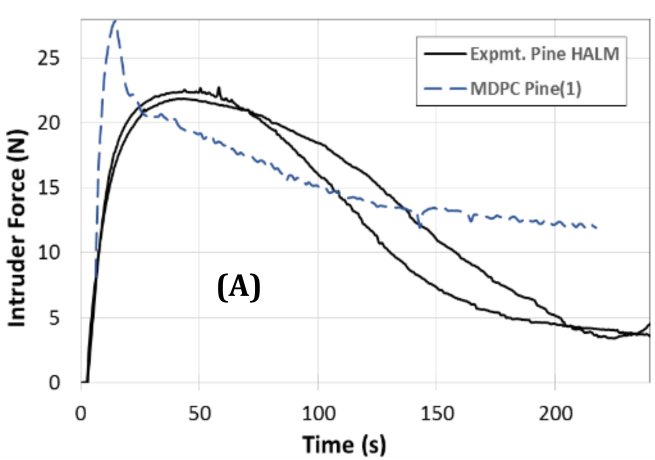


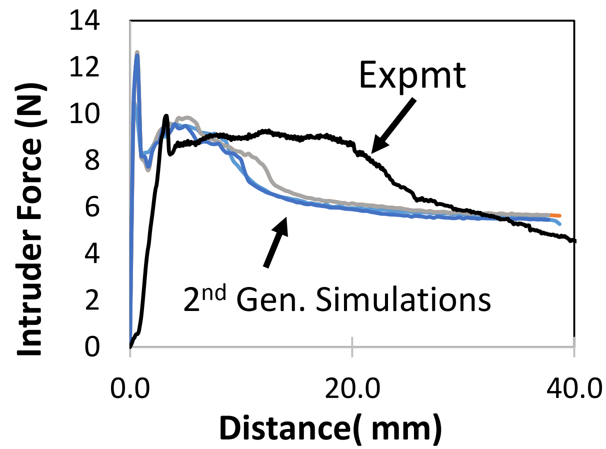


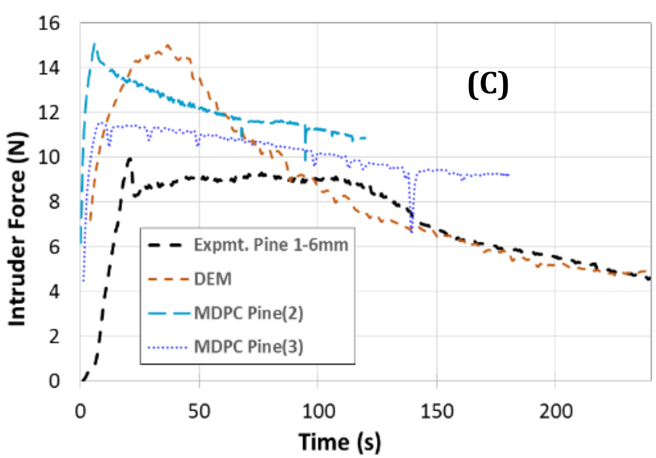
Drucker-Prager Cap Model: Radial cross-section, Step 3

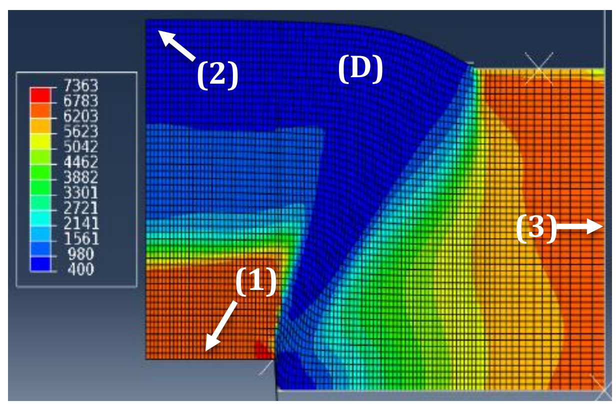
3 – Technical Accomplishments, Cont.

Experimental and simulation results from direct axial shear test.









Panels (A)-(C): Force on intruder vs. time/distance

Agreement between experiments & simulations exceeds goal of 80% but still needs improvement (see next slides).

*Agreement for experiments & continuum simulation**

Parameter	% Agreement
Shear strength (50% weight)	
Material [Pa]	98%
Pressure (average) [Pa]	
Intruder top (1)	98%
Point 2	100%
Point 3	24%
Overall	**86%**

*Agreement for continuum & DEM simulation**

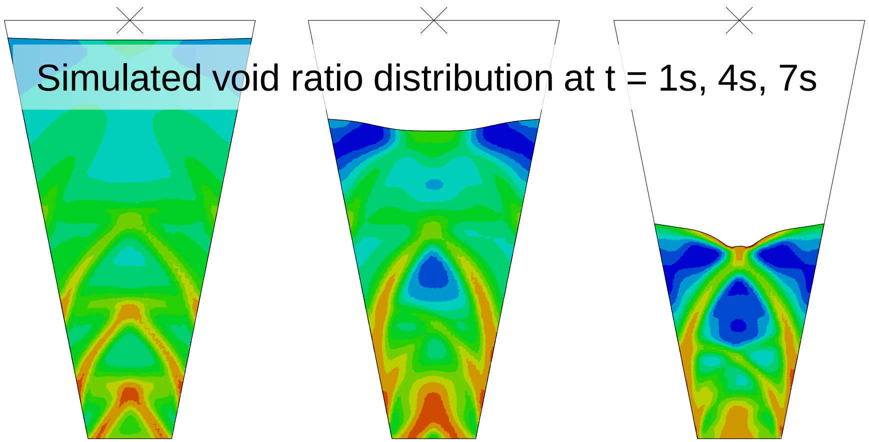
Parameter	% Agreement
Shear strength (50% weight)	
Material [Pa]	95%
Pressure (average) [Pa]	
Intruder top (1)	95%
Point (2)	100%
Point (3)	74%
Overall	**91%**

*Does not include compression step or Schulze shear test – both had >90% agreement

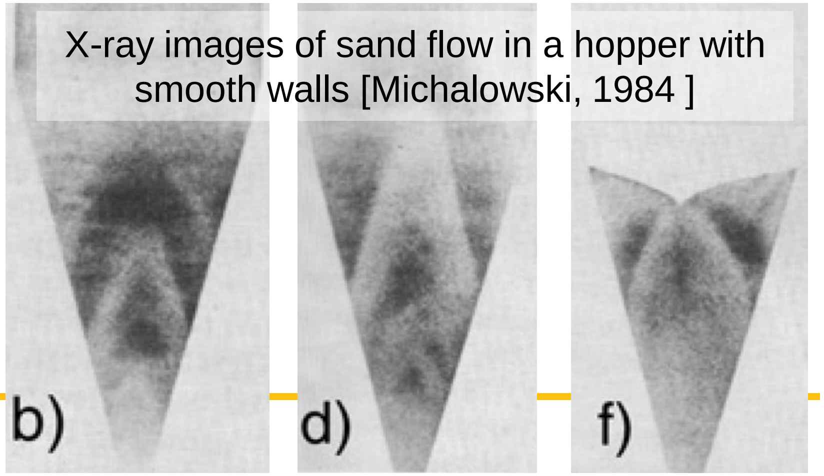
3 – Technical Accomplishments, Cont.

Continuum non-local hypoplastic model

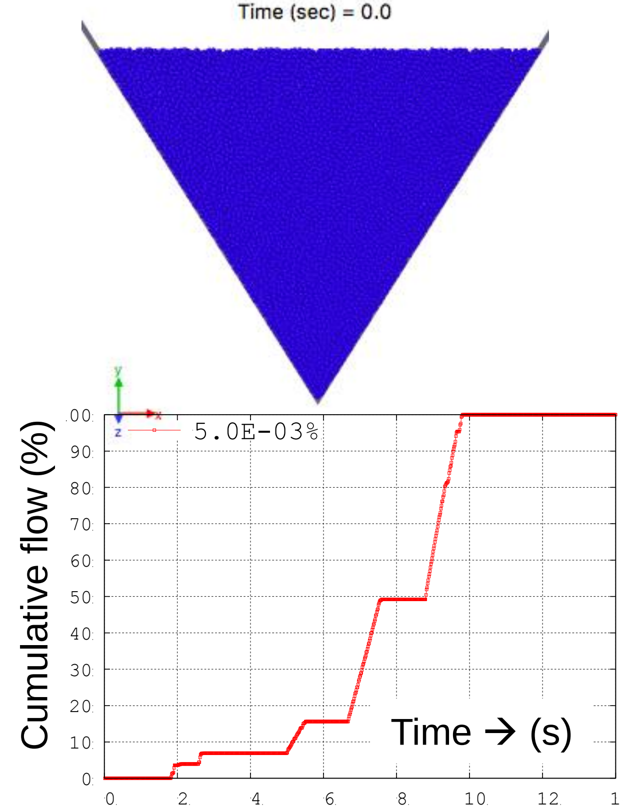
- Accounts for observed shear banding (including particle size effects)



Simulated void ratio distribution at t = 1s, 4s, 7s



X-ray images of sand flow in a hopper with smooth walls [Michalowski, 1984]



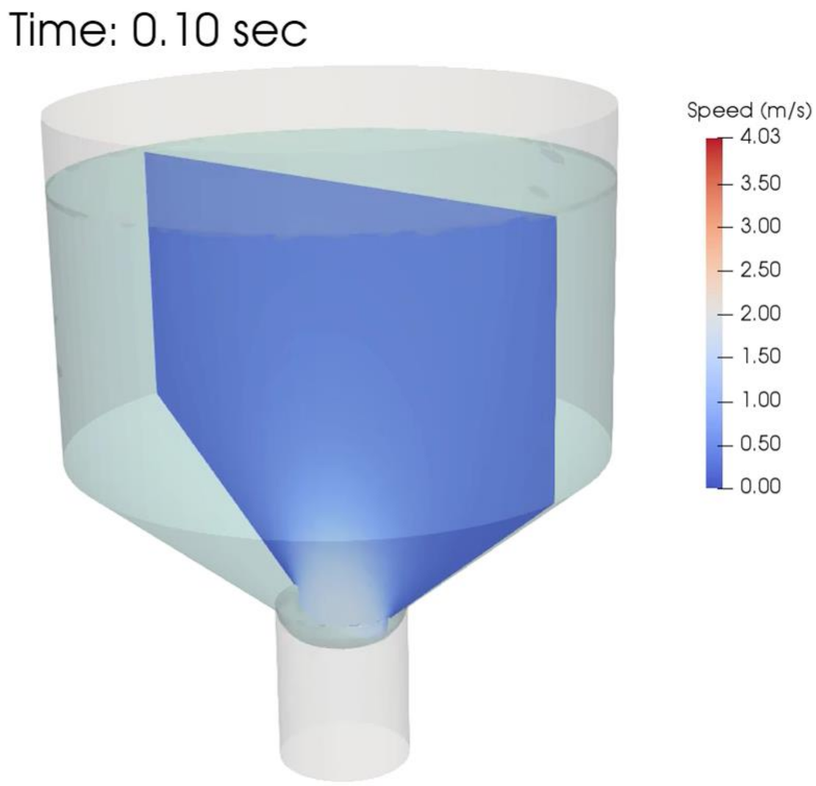
Particle (DEM) simulation of spherical beads flowing in a hopper.

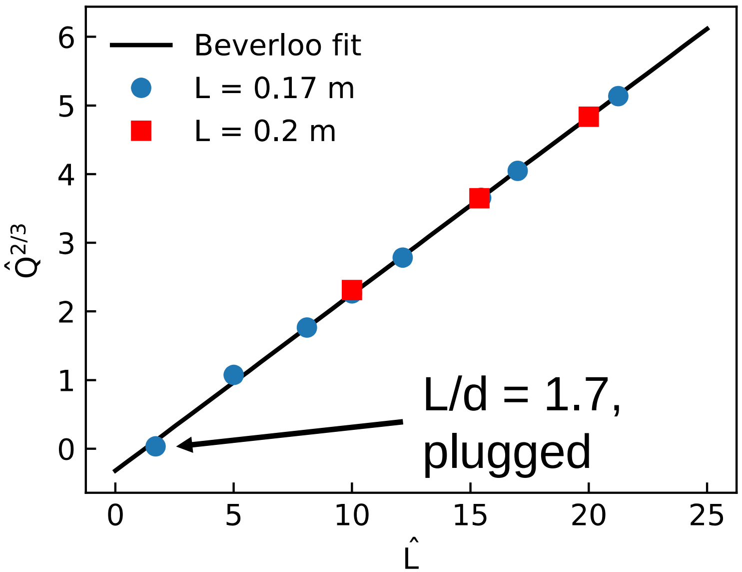
- **Episodic starts & stops are a result of shear banding (particle agglomerates with multiple time scales).**
- **This is what continuum models need to capture (very difficult)**

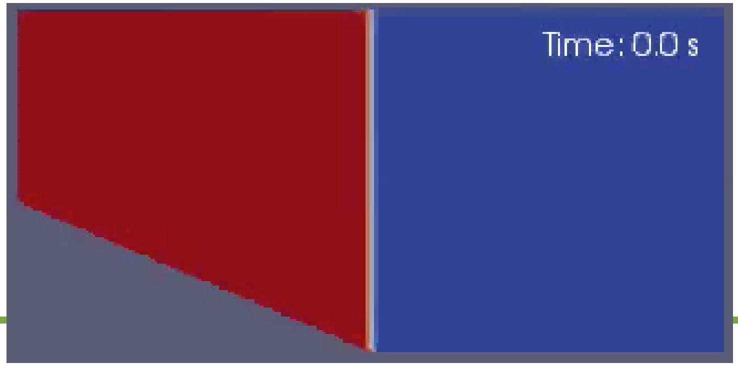
3 – Technical Accomplishments, Cont.

Continuum non-local granular fluidity model implemented in OpenFOAM CFD

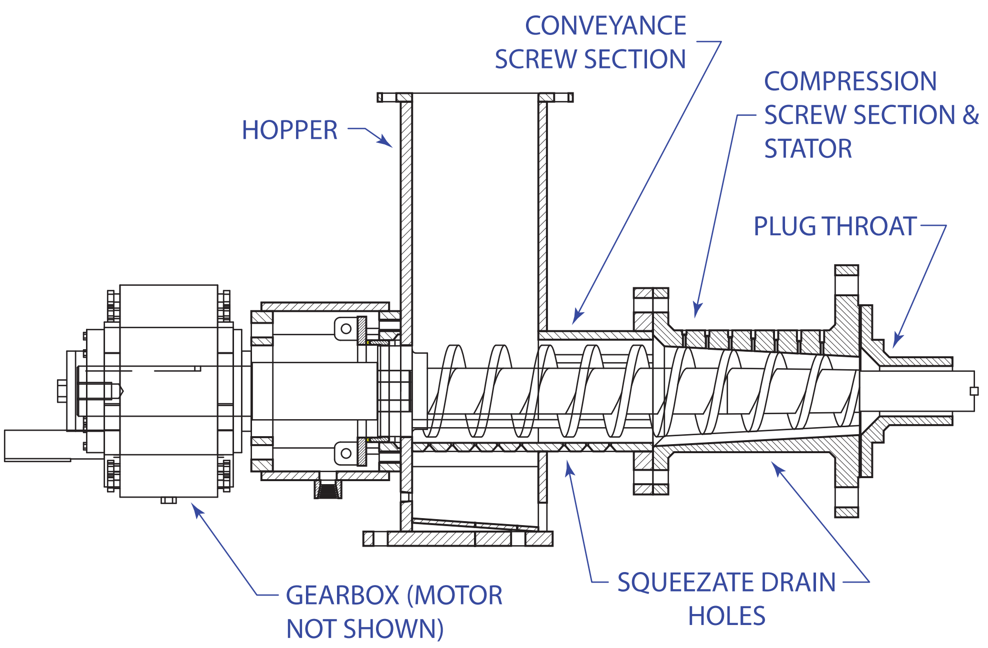
- Viscosity is a function of pressure and a new scalar field parameter “fluidity”.
- Beverloo scaling of silo discharge and stop height on inclined planes were reproduced in 2D test simulations.
- Successful simulation of 3D conical hopper flow on HPC (32 cpus).

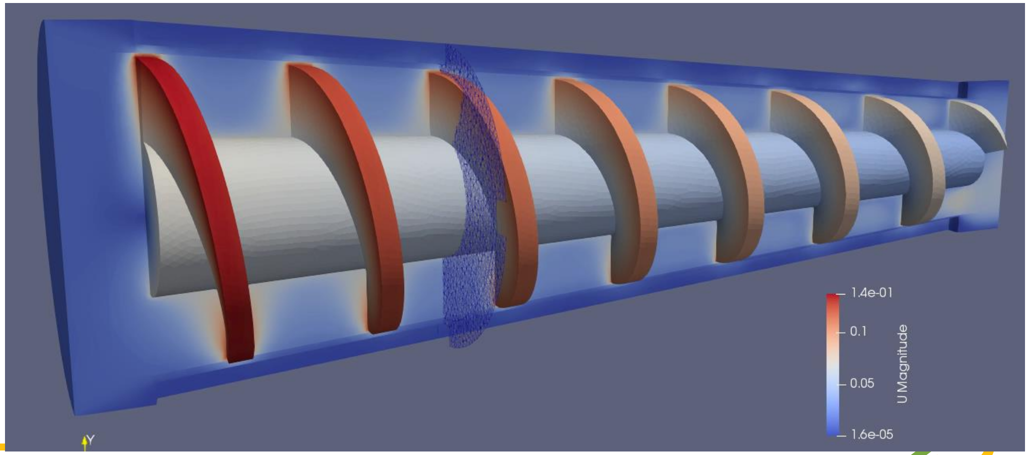






3 – Technical Accomplishments, Cont.



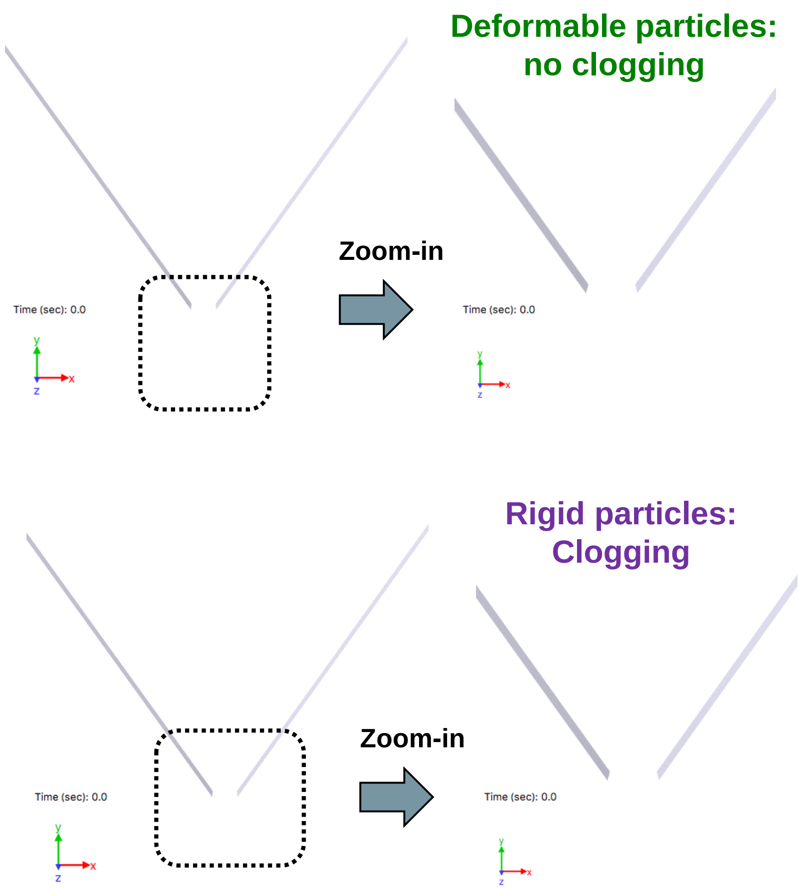


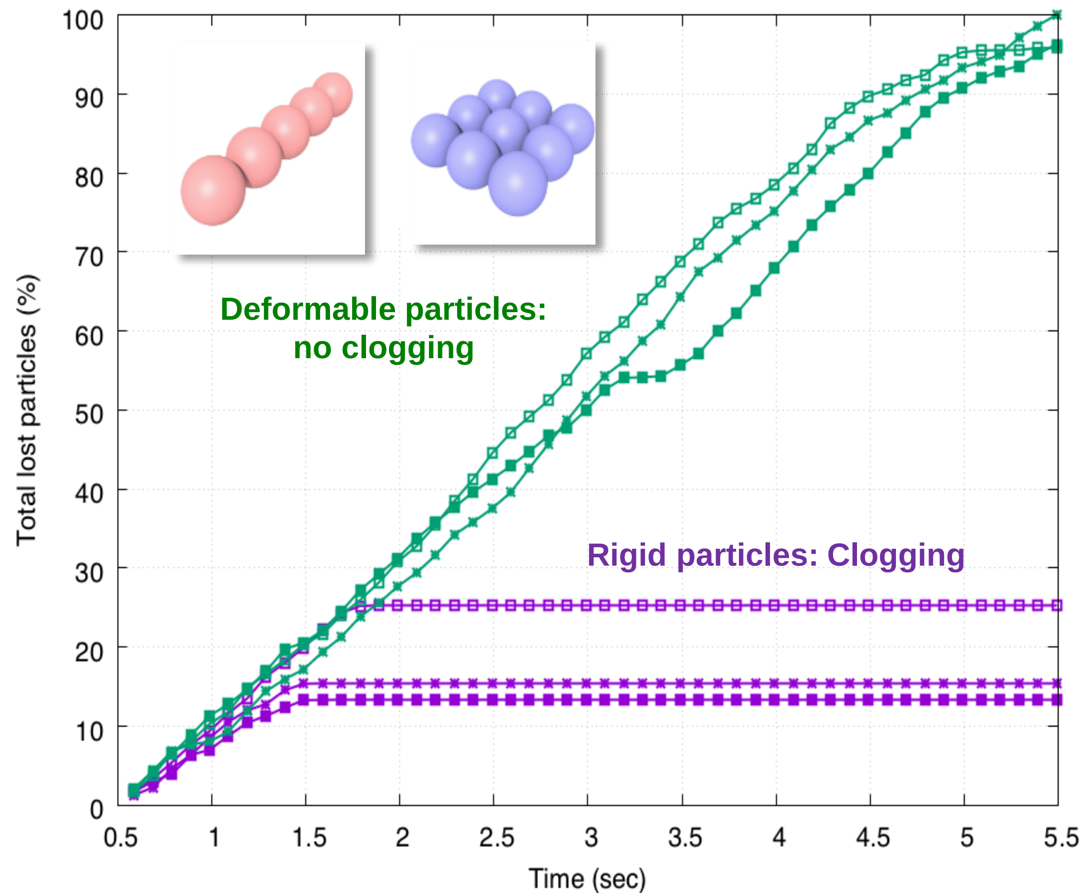
Screw-Feeder modeling (model development co-funded with 3.3.1.2)

- Defined computational mesh for compression zone:
  - Rotating screw region and non-rotating stator region
  - ~10^6 cells.
- Bingham yield-stress viscosity model with parameters inferred from literature.
- Preliminary simulations of 10 s took 48 h on 128 cpus.
- Evaluated wall shear stress on the auger surface.

3 – Technical Accomplishments, Cont.

DEM hopper flow simulation results using mixed string and sheet particles (sphere diameter = 1 mm)





Simulations using rigid non-spherical particles do NOT exhibit all critical flow behaviors.

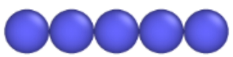
- Need to include particle deformation.
- Real biomass particles are much more complex.

3 – Technical Accomplishments, Cont.

Coupled flow modes result in complex flow, even for ideal particles

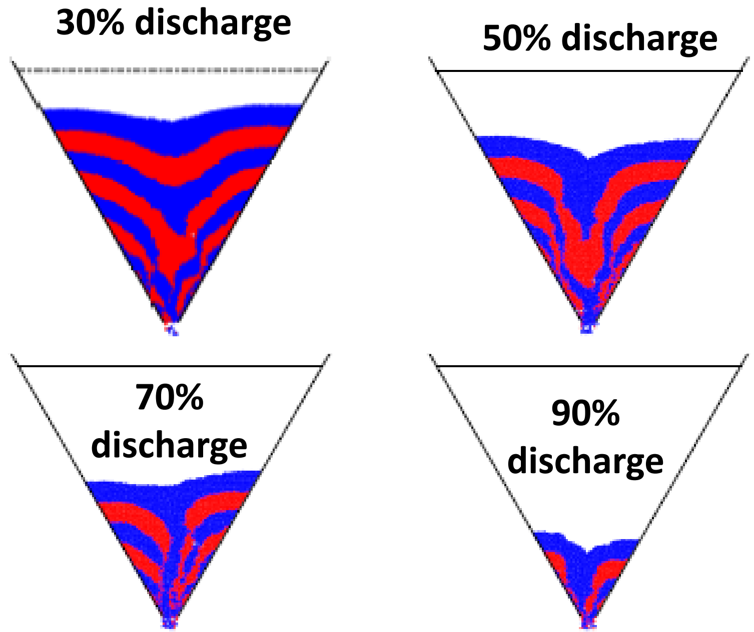
- Example: Hopper flow with “ideal” particles
  - Two particle types mixed and flowing in a hopper

Type 1: Fibers (85 wt%)



Type 2: Plates (15 wt%)

Density	430	kg/m^3
Sphere radius	0.5	mm
Young’s modulus	10	MPa
Poisson’s ratio	0.3	-
Coefficient of restitution	0.1	-
Coefficient of friction	0.5	-
Bond radius	0.5	mm
Bond normal stiffness	10	GN/m^3
Bond shear stiffness	0.6	GN/m^3



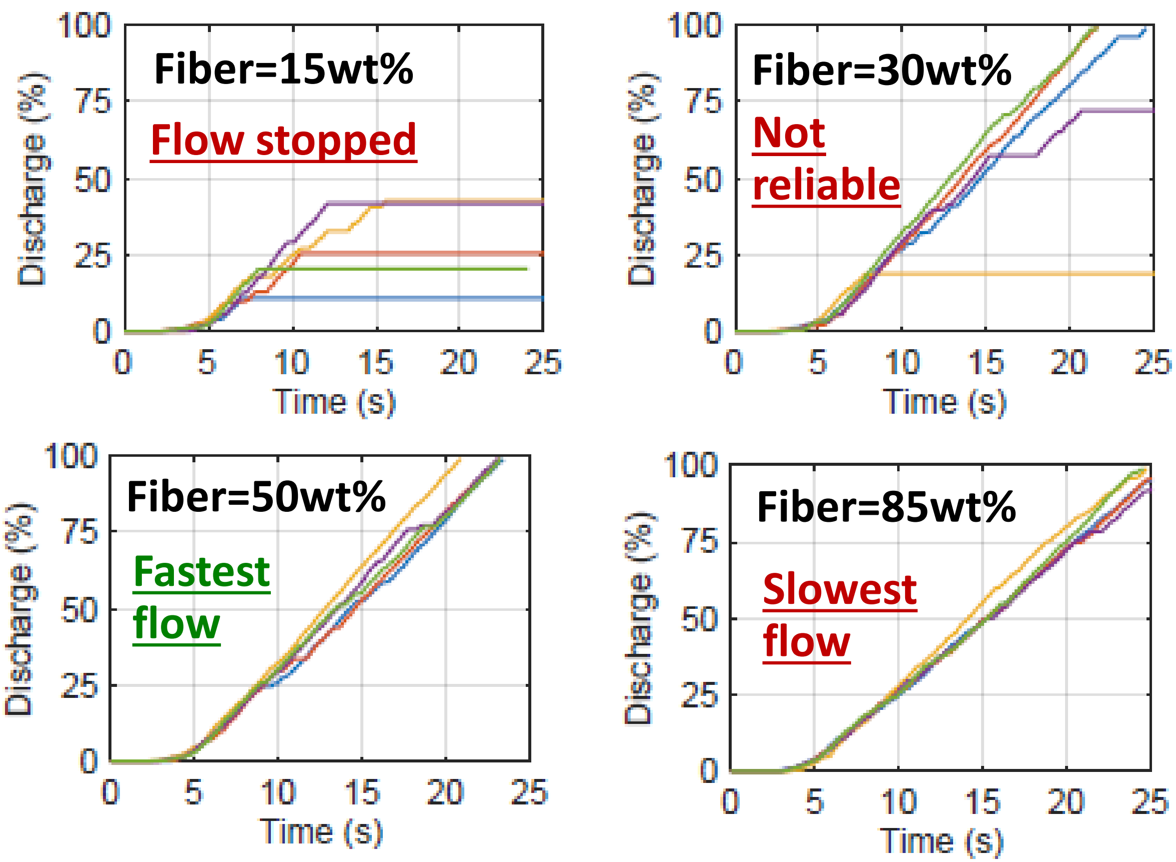
Flow patterns at different discharge levels (INL/Clemson collaboration; submitted for publication).

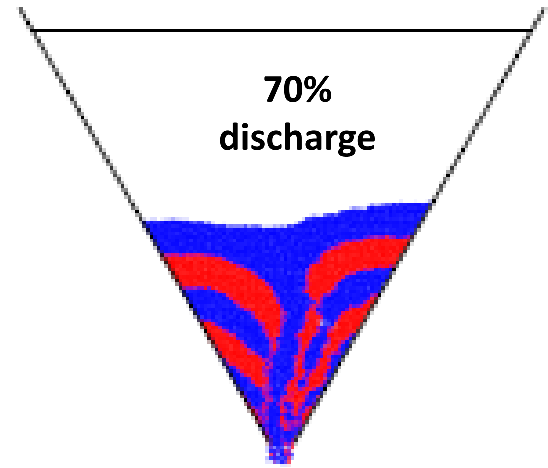
- **Oscillatory flow pattern is indicative of mode coupling**
- **Likely greater return on investment by focusing on flow modes rather than detailed particle properties.**

3 – Technical Accomplishments, Cont.

Coupling of flow modes

- Hopper flow example Continued



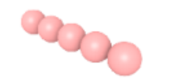
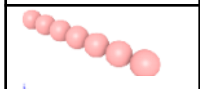
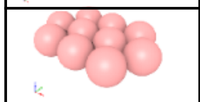
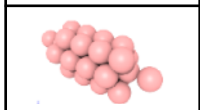
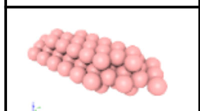
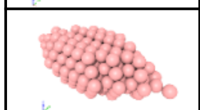


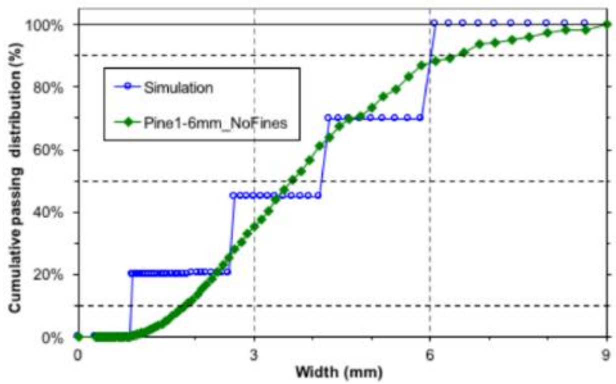
- Even for idealized particles, flow behavior is highly complex due to coupling between flow modes.
- Flow modes are geometry dependent.
- Flow behavior cannot be understood using particle characterization alone.

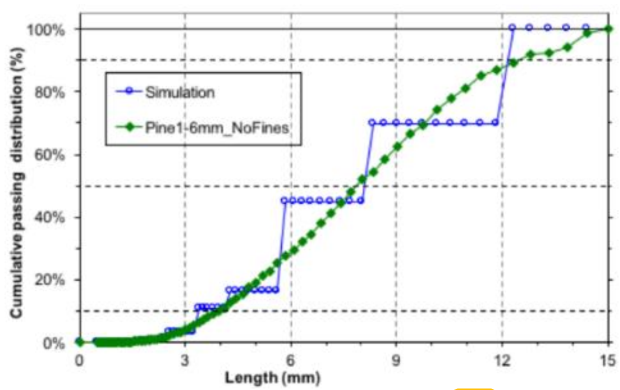
3 – Technical Accomplishments, Cont.

DEM model to mimic pine particles

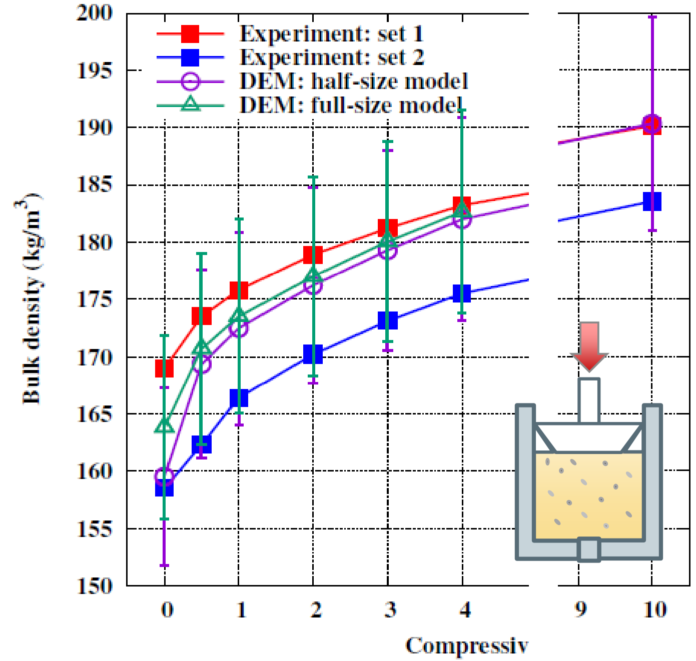
1. Create 6 DEM particle shapes and assemble distributions to match mass distributions of sieved pine chips.

Picture	# spheres
	5
	7
	10
	31
	72
	229





2. Simulated compression test compared with experiments
   - Simulation matches experiment after parameters are optimized (e.g. friction, density, cohesion, elasticity).



4 – Relevance

Enabling biofuels by developing robust feeding and handling (F&H) technologies

Directly supports BETO's Mission:

- Develop and transform our renewable biomass resources into commercially viable, high performance biofuels".
- F&H difficulties at pioneer biorefineries are leading to significant reduction in throughput versus design.

Verified simulations elucidate effects of biomass anisotropy, plasticity and elasticity to enable:

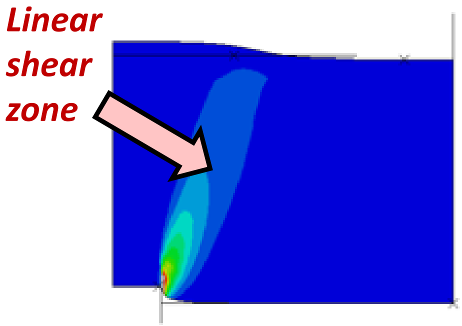
- Relating biomass properties to feeding performance.
- Improved design of equipment and processes (3 year goal).

https://energy.gov/eere/bioenergy/downloads/biorefinery-optimization-workshop-summary-report

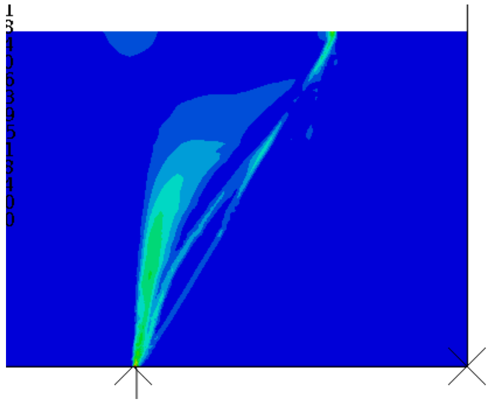
Summary

1. **Goal: Predict flow behavior of biomass in custom lab-scale flow test using physics-based simulation.**
2. **Approach: Integrated particle characterization and modeling with bulk characterization & reduced-order physics-based modeling.**
3. **Accomplishments: Achieved >85% agreement between lab scale flow test and physics-based simulations.**
4. **Project fulfills a critical need to provide feeding & handling solutions at all scales.**
5. **Key Findings**
   – "Multi-scale" and "particle-based" is not enough. Must also address
     - **Material heterogeneity.**
     - **Coupling between flow mechanisms** (not captured by classical methods).

   – Non-local models (slides 15-16) and deformable-particle simulations (slides 18-21) are steps in the right direction
   – Particle and bulk (system) characterization and physics-based simulation must progress jointly.



Classical method



Non-classical method (non-linear, complex shear zone)

Publications

1. TL Westover, D Hartley, Biomass Feeding and Handling, 2018. Chapter in book Biofuels - Past, Present and Future, edited by Dr. Madhugiri Nageswara-Rao and Dr. Jaya R. Soneji, In-Tech Publishing.
2. TL Westover, Y Xia, J Klinger, 2018. Understanding and Solving Biomass Feeding and Handling Challenges, Agri Res & Tech: Open Access J 2018; 16(2), 1-2.
3. Y. Xia, Z. Lai, T. Westover, J. Klinger, H. Huang, Q. Chen, Discrete element modeling of deformable pinewood chips in cyclic loading test, Powder Technology, 2018 (reviewed, under minor revision).
4. Z. Lai, Y. Xia, H. Huang, T. Westover, Q. Chen. Discrete element modeling the granular hopper flow of deformable-irregular particles, Powder Technology, 2018 (submitted, under review).

The Team

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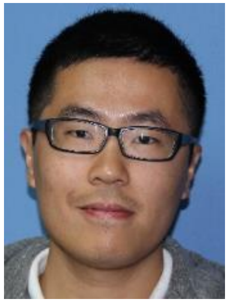

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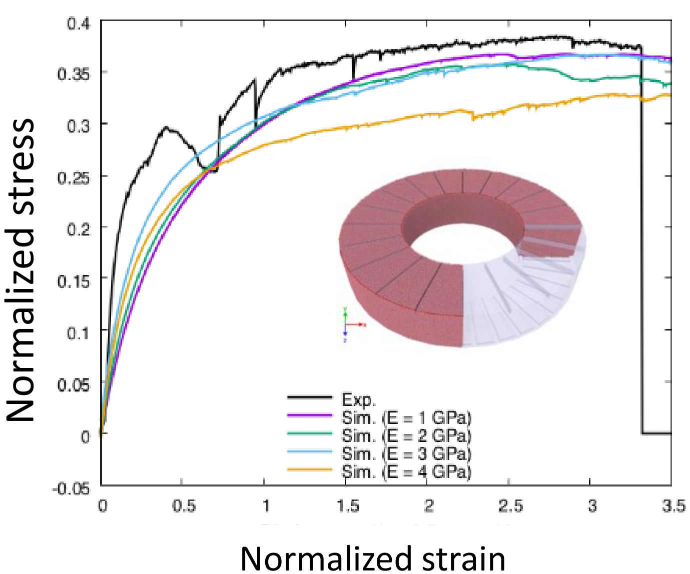
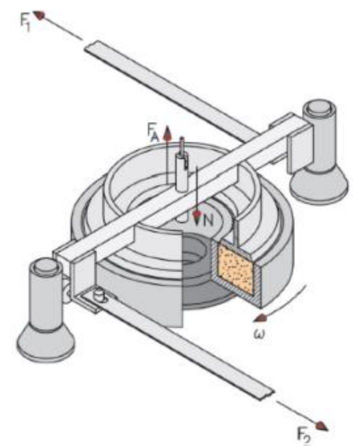
≈10 MINUTES FOR QUESTIONS

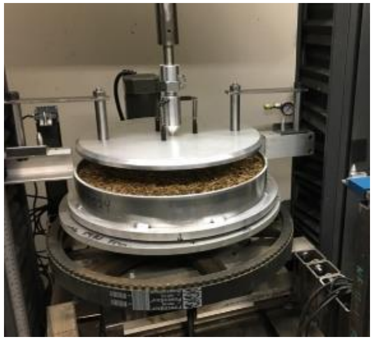
3 – Technical Accomplishments

- For decades it has been assumed that a correctly designed shear tester could provide the material properties to predict behavior
- Actually, multiple testers are needed to probe different flow modes and their coupling
- We have selected flow tests to enhance separating particle, bulk and boundary effects. Flow tests include axial shear, rotary shear, and hopper flow.





Ring shear tester.
http://www.dietmar-schulze.de/powtve.pdf



Modified Peschl shear tester (partner with E&G Associates)

Wedge-shaped hopper with adjustable walls

2 – Particle Modeling *(Technical Approach Cont.)*

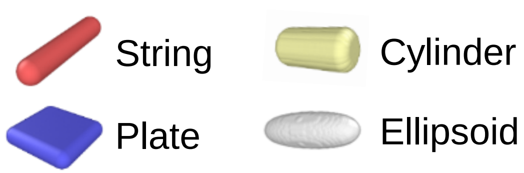
Discrete element method (DEM)

- Model the motion and deformation of each particle
- Can capture all the dominant mechanics for robust, physics-based modeling
  - Difficult to scale due to high computational cost
  - Not feasible for realistic biomass materials (too many particles, sizes, & shapes)
  - Used to validate scalable reduced-order (continuum) models
  - **Currently available models do not include all needed capabilities**

Three Available Methods

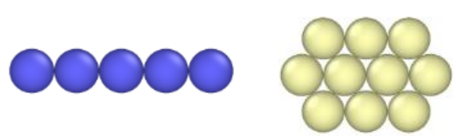
#1. Rigid particles

- *Custom particle shapes & properties (important for biomass !!!)*
- *Rigidity is problematic*



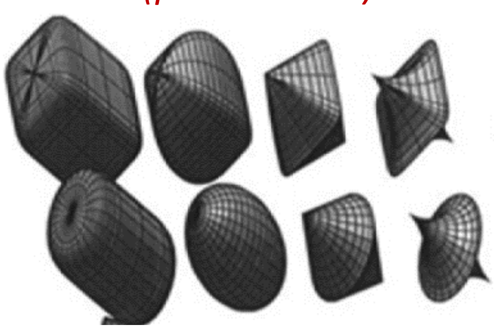
#2. Flexible coupled spheres

- *Custom properties*
- *Limited to coupled spheres (problematic)*



#3. Flexible polyhedra

- *Custom particle shapes*
- *Properties are currently limited (problematic)*



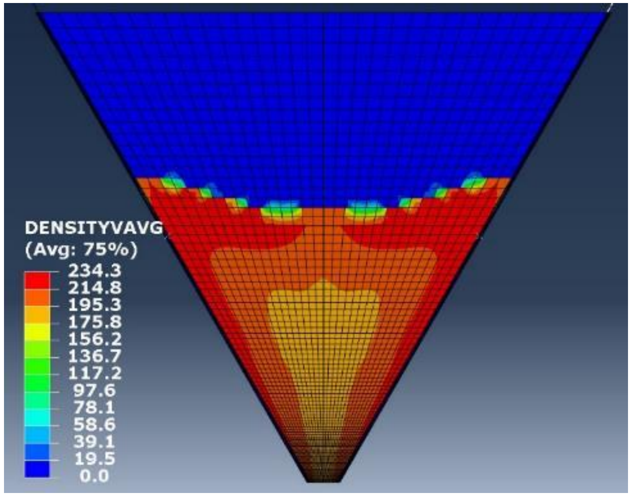
Zhong et al., Powder Technol. 2016.

2 – Continuum Modeling *(Technical Approach Cont.)*

Single inhomogeneous material deforms according to flow rules

- Elasticity (Hooke's law): $\varepsilon_{ij}^{el} = \frac{1}{E}\left[(1+\nu)\sigma_{ij} - \nu\delta_{ij}\sigma_{kk}\right]$
- Plasticity: Deformation at constant stress & volume (yield criterion, plastic potential)
- Viscosity: Deformation with dependence on strain rate
- Creep: Deformation occurs at multiple time scales
- Damping: Energy dissipation, coupling between flow modes

- **We do not actually know the flow rules for biomass, except they are likely non-linear, highly coupled and include dependencies on density, pressure, deformation history, etc.**
- **Robustness of model predictions depends upon myriad of flow rule assumptions**



INL simulation: Flow of pine media in a wedge hopper

Accomplishments

- Simulations performed using "ring" cell and rectangular cell with periodic boundary conditions.
  - *Panels (A) and (B): particle arrangements before and after application of gravity and normal load, respectively.*
  - *Panels (C) and (D): Impact of Young's modulus for the rectangular and rotational geometries, respectively.*
- Simulations used simple rigid sphere particles and reasonably mimicked physical tests
- Numerous physical tests prove that ring shear tester is not suitable to measure biomass flow properties.
- Simulations with simple particle model could not offer strong insight into flow behavior (<u>Lesson Learned</u>)