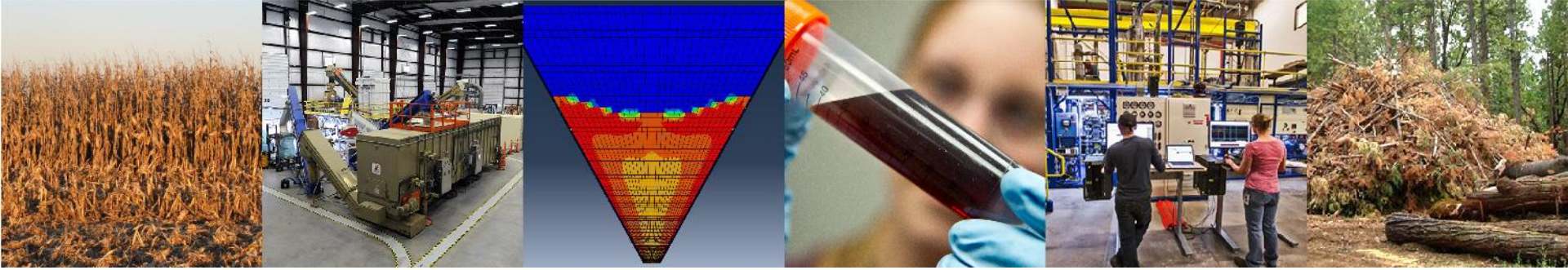


# *Feedstock Physical Performance Modeling*
## *WBS 1.2.2.501*

**FCIC Kick-Off Meeting**

**Dec. 11, 2017**


**Tyler Westover, Hai Huang, Yidong Xia (INL)**

**Jonathan Stickel, Hariswaran Sitaraman (NREL)**

**George Fenske, Oyelayo Ajayi (ANL)**

**Carl Wassgren (Purdue University)**

**Bryan Ennis (E&G Associates)**

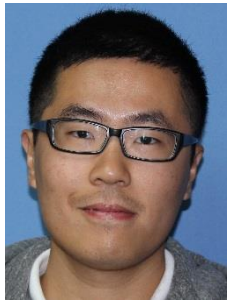
**Kerry Johanson (Material Flow Solutions)**


fcic
FEEDSTOCK CONVERSION INTERFACE CONSORTIUM

# The Fundamental Modeling Team

Tyler Westover, Ph.D.

Hai Huang, Ph.D.



Yidong Xia, Ph.D.

Jonathan Stickel, Ph.D.

Hariswaran Sitaraman, PhD.

Mohammad Rahimi, PhD.

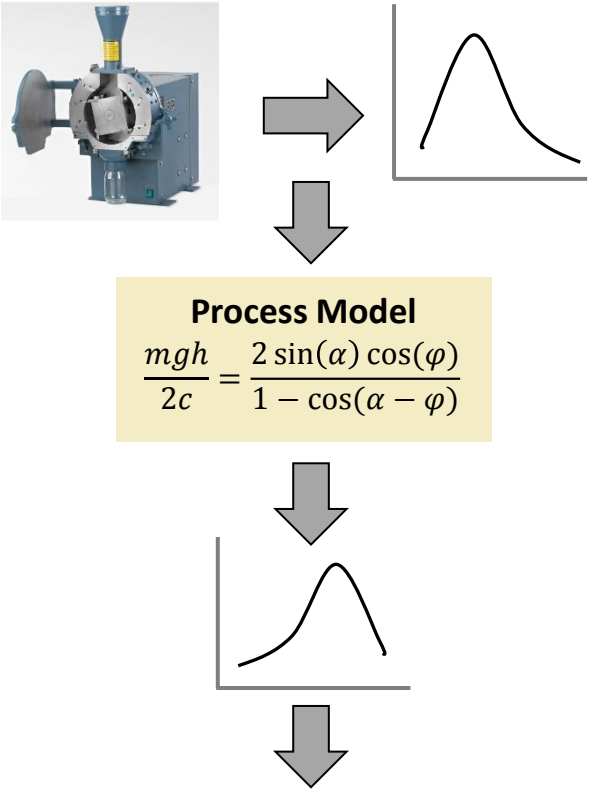
James Lischeske

George Fenske, Ph.D.

Oyelayo Ajayi, Ph.D.

# Motivation

1. **Developing reliable engineering design guides**
   - All current design guides use Mohr/Coulomb flow model, which is unreliable for biomass
   - Will develop new guides based on advanced models
   - Will propose rapid tests that industry can use near-term
2. **Iterating process models / Identifying relationships**
   - Modifying equipment after installation is expensive & slow; modifying models is cheaper & faster
   - Numerous examples: buildings, automobiles, pumps, etc.
   - Properties vary in location, direction & scale (100's of uncontrollable combinations)
   - Variables cannot usually be physically isolated
   - Physical tests have limited ability alone to determine relationships
   - Cause & effect cannot always be physically determined
3. **Transferring models between equipment & scale**
   - Transfer key discoveries from lab to industry




**Potential dominant physical/mechanical properties**

1. Cohesion
2. Friction/shear strength
3. 3D Young's moduli
4. Plastic hardening
5. Particle size and shape
6. Particle roughness
7. Moisture content
8. Bulk density
9. 3D Poisson ratios
10. Elastic recovery
11. Chemical composition
12. Particle durability

# *Objectives & Approach*

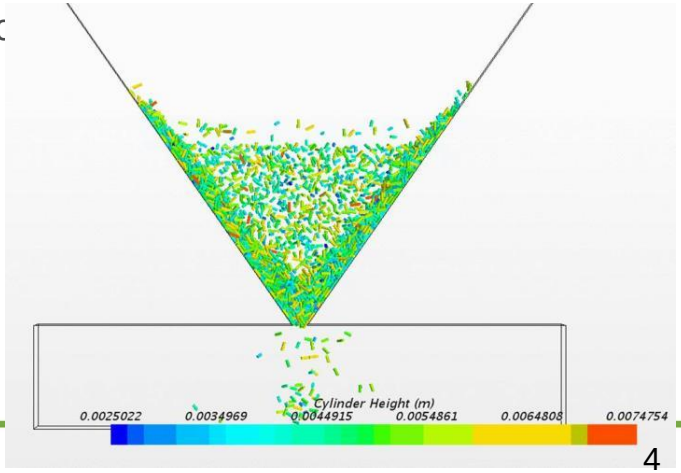
**Objective:** Use mechanistic modeling to identify the causes of feed-handling failures and validate predictions to lead to improved process designs that enhance the reliability of industrial IBRs

**3-Year Goal:** Robust computational simulations and characterization methods to enable 50% improvement in operating reliability relative to base case, and reduced wear for coupled hopper/feed auger systems and compression screw augers at scales of 1 to 50 tonne/hr

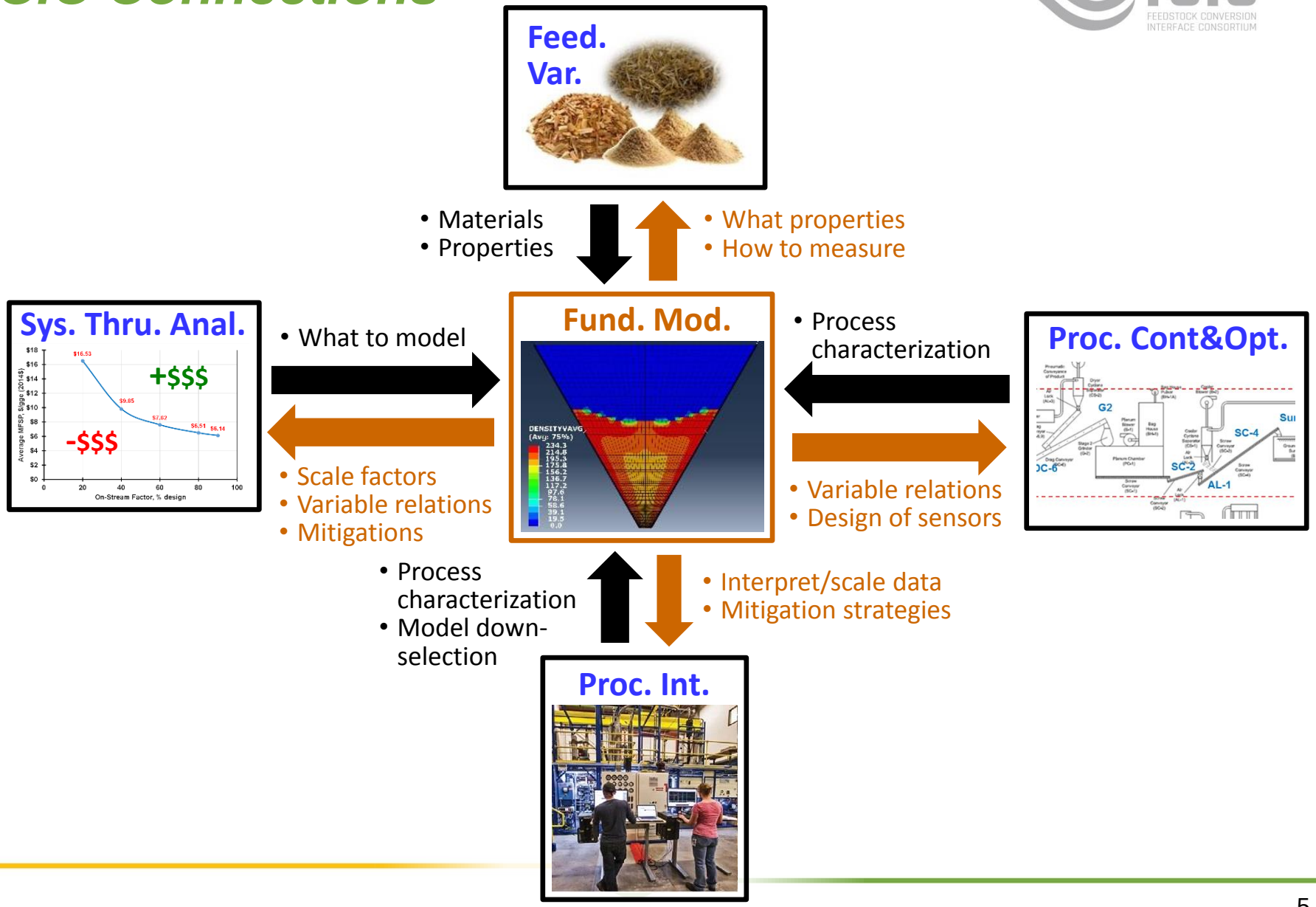
**History:** This project began 1 year ago combining simulations and physical experiments and was annexed separately into FCIC

**Technical Approach**

- Particle models (discrete element method, DEM)
- Reduced-order continuum models (averages over many partic
  - Plasticity/elasticity models for general flow & comminution
  - Comp. fluid dynamics (CFD) for specific cases
  - Analytical models for specific wear mechanisms



# FCIC Connections

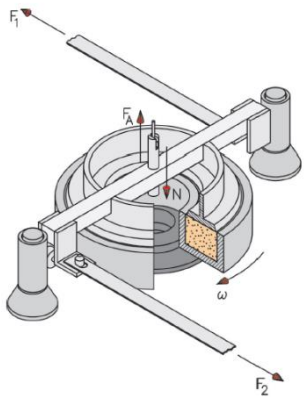


# Tasks and Connections

| Task Name | Inputs | Outputs | Specific driving questions |
|---|---|---|---|
| **Task 1: Baseline of current industry design practices** | Literature design methods | Effectiveness of current methods | What is the cause of current problems? |
| **Task 2: Flow of elastoplastic bulk solid biomass** | **FV:** Properties<br>**PI:** Flow data | Flow models / functional parameter relationships:<br>**FV, PI, PCO, SWA** | What to measure?<br>How to measure?<br>Which models work?<br>How to interpret/use?<br>How to transfer or scale? |
| **Task 3: Flow of highly compressed feedstocks (i.e. negligible elastic behavior)** | Same as #2 | Same as #2: **FV, PI, PCO, SWA** | Same as #2 |
| **Task 4: Mechanics of grinding (<u>not currently funded</u>)** | **FV:** Properties | Comminution …. (same as #2):<br>**FV, PI, PCO, SWA** | Same as #2 |
| **Task 5: Adhesion, corrosion, erosion, and fatigue wear modeling (<u>not currently funded</u>)** | **FV:** Properties<br>**PI:** Wear data | Wear … (same as #2):<br>**FV, PI, PCO, SWA** | Same as #2 |

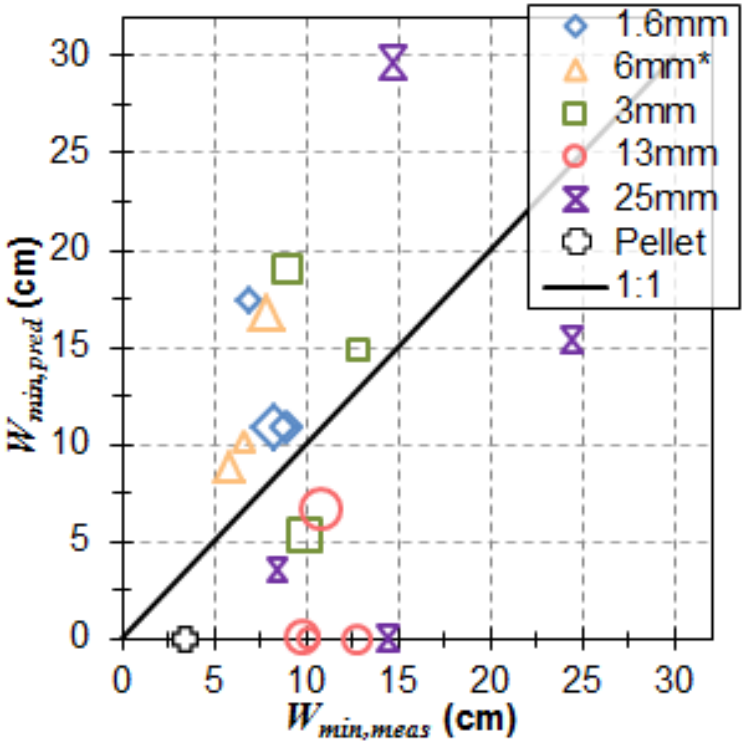
# Task 1: Baseline current design practices
## $160K: INL, NREL, ANL

- **Objective:**
  - Understand limitations and failures of current industry design practices
  - Example: Use of Mohr-Coulomb model to design bins, hoppers and feeders
  - Will also look at
    - Compression screw feeders
    - Equipment wear



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

*Motorized flow hopper at INL*




*Predicted hopper opening size to cause flow vs. measured hopper opening size. Symbol size indicates moisture content from 10% (small) to 40% (large) (Hernandez, Westover, et al. , submitted for publication).*

# Tasks and Connections

| Task Name | Inputs | Outputs | Specific driving questions |
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| **Task 1: Baseline of current industry design practices** | Literature design methods | Effectiveness of current methods | What is the cause of current problems? |
| **Task 2: Flow of elastoplastic bulk solid biomass**<br>• Particle models (discrete element method, DEM)<br>• Reduced-order continuum models | **FV:** Properties<br>**PI:** Flow data | Flow models / functional parameter relationships:<br>**FV, PI, PCO, SWA** | What to measure?<br>How to measure?<br>Which models work?<br>How to interpret data?<br>How to scale data? |
| **Task 3: Flow of highly compressed feedstocks (i.e. elastic behavior not important)** | Same as #2 | Same as #2: **FV, PI, PCO, SWA** | Same as #2 |
| **Task 4: Mechanics of grinding (<u>not currently funded</u>)** | **FV:** Properties | Comminution …. (same as #2):<br>**FV, PI, PCO, SWA** | Same as #2 |
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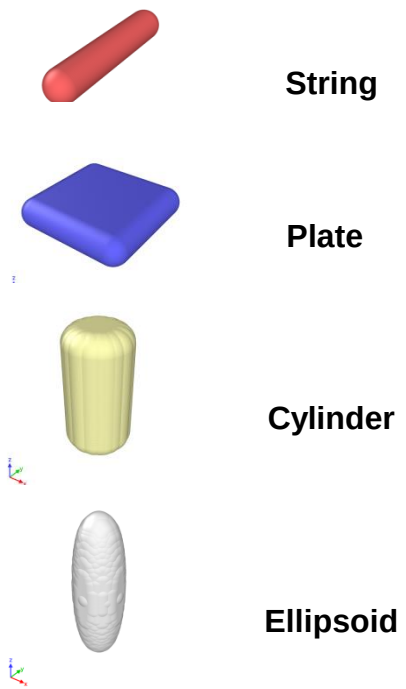
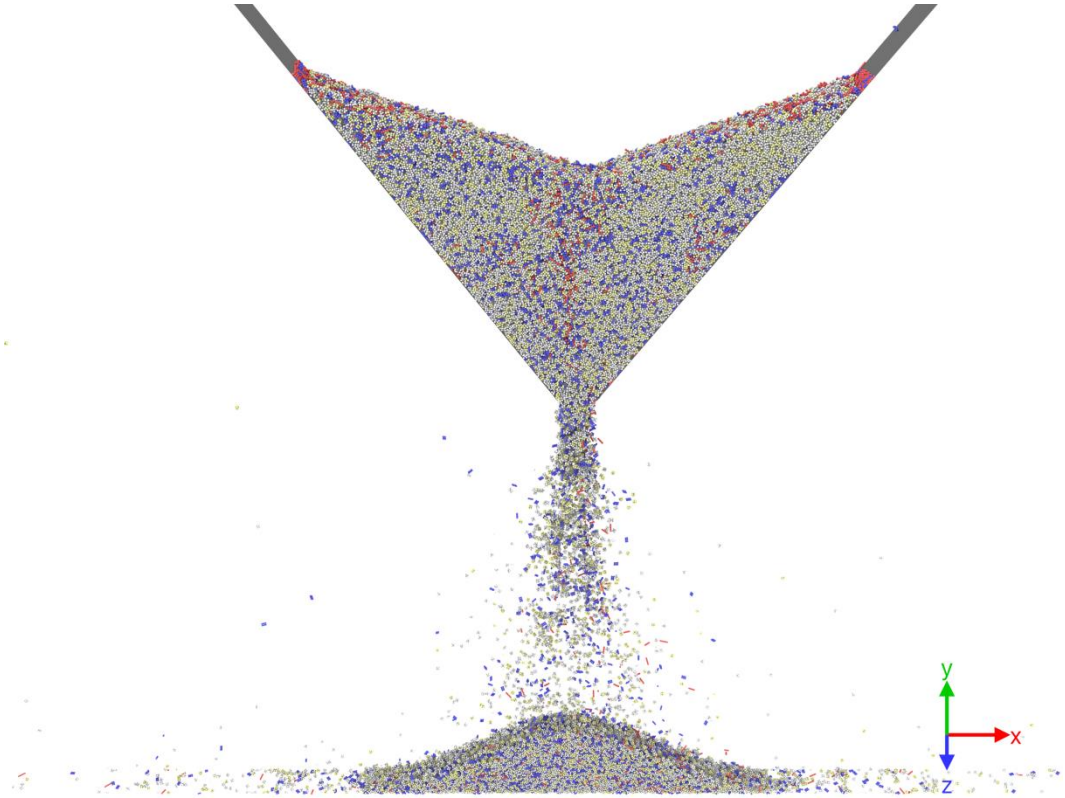
# Task 2.3: Particle Modeling

## $290K: INL (Discrete Element Method, DEM)

- Model the motion and deformation of each particle
- Can capture all the dominant physics for robust, scalable modeling
  - DEM is difficult to scale due to high computational cost
  - Not feasible for real biomass materials (too many particles with different sizes/ shapes)
  - Instead, will model engineered materials (particles with narrower shape/size ranges)
  - DEM will be used to validate other models that are scalable

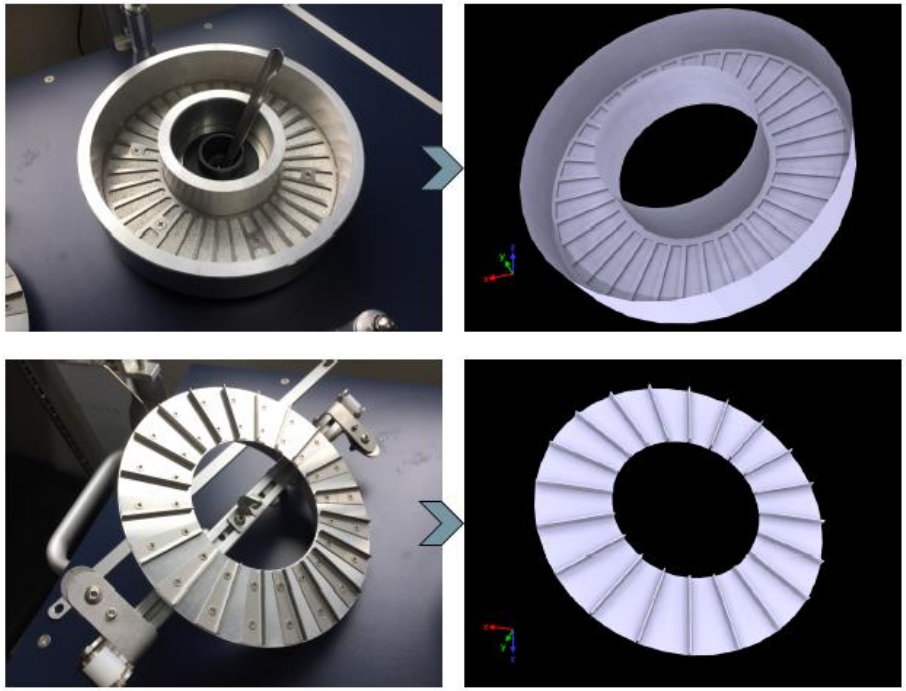
**Examples of non-spherical particle shapes:**

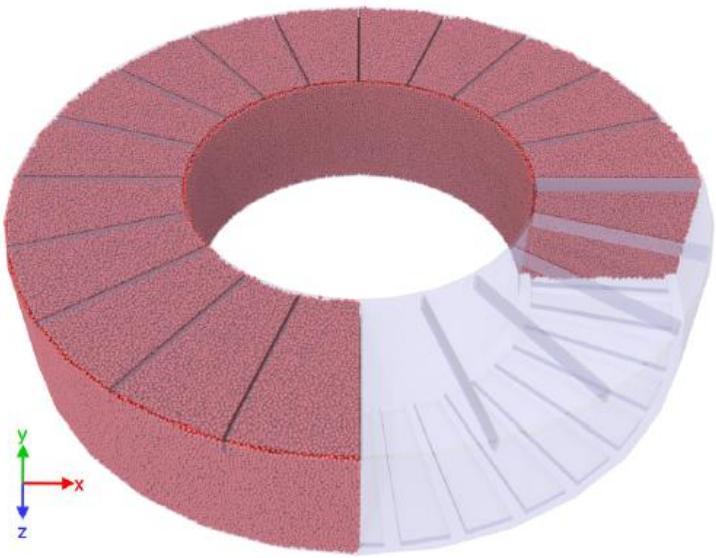


# Task 2.3: Particle Modeling
## $290K: INL (Discrete Element Method, DEM)

- Modeling of material characterization
  - Shear tests to measure friction and cohesion properties
- Can capture all the dominant physics for robust, scalable modeling
  - Will be used to validate continuum-models and guide characterization tests






Over 1 million 1mm spherical beads when fully loaded

# Task 2.3: Particle Modeling
## $290K: INL (Discrete Element Method, DEM)

Model parameters

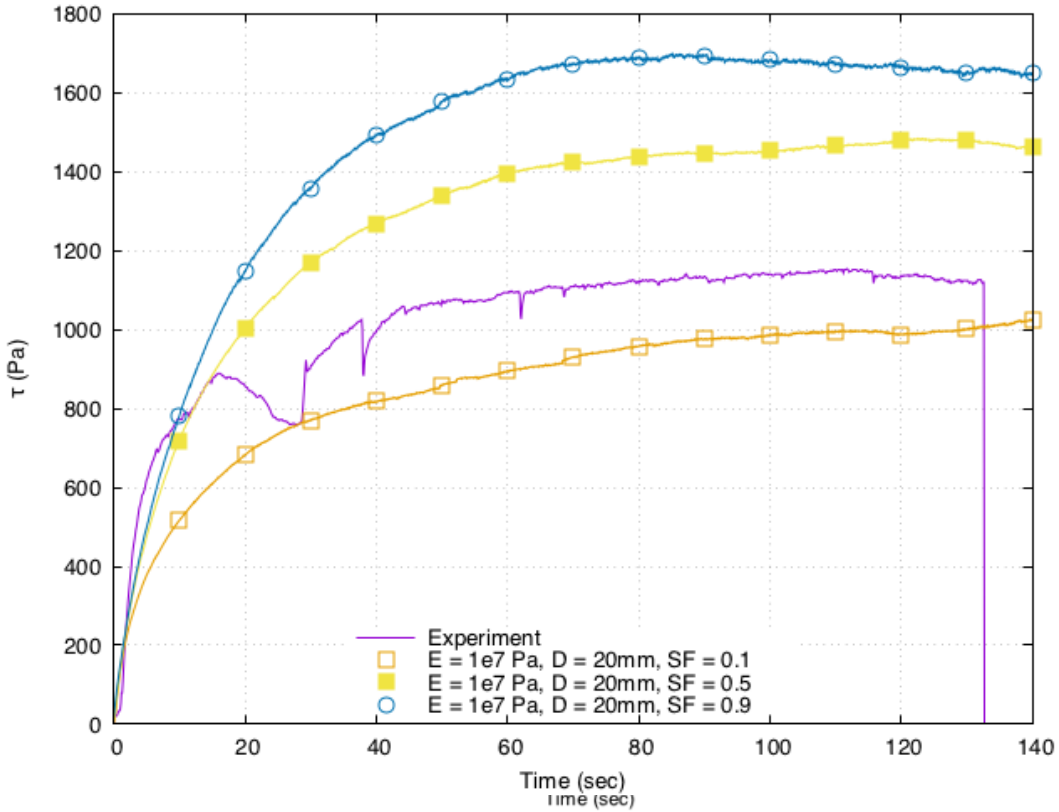
- 1 mm glass beads (ideal case)
- Includes sliding and rolling friction

| Metrics | Values |
|---|---|
| Particle type | Sphere (diameter = 0.001 [m]) |
| Particle density | 2750 kg/m$^3$ |
| Particle Young's modulus | 1 [GPa] |
| Particle Poisson's ratio | 0.2 |
| Restitution coefficient | sphere-sphere: 0.5; sphere-mesh: 0.5 |
| Sliding friction coefficient | sphere-sphere: 0.5; sphere-mesh: 0.5 (specified without much reference) |
| Rolling friction model | The constant directional torque (CDT) model |
| Rolling friction coefficient | sphere-sphere: 2e-3; sphere-mesh: 4e-3 (specified without much reference) |
| Initial surface liquid content | |
| Minimum/maximum separation distance ratio | |
| Liquid surface tension | 71.97e-3 [N/m] |
| Liquid viscosity | 8.90e-4 [Pa s] |
| Solid-liquid contact angle | sphere-water:1.0472 [rad] \| mesh-water 2.61799 [rad] |
| Time-step size | 1e-6 [s] |

# Task 2.3: Particle Modeling
## $290K: INL (Discrete Element Method, DEM)

Ring shear tests of glass beads

- Physical shear test require >100 s
- Young's Modulus = 1e7 Pa
- Fill depth = 20 cm
- Sliding friction: = 0.1 … 0.9
- Model time step ~ 1e-6 s, so ~10e9 simulation steps are needed
- Larger time steps can be used as assumed value of E decreases
  - Assuming E=1e7 is affordable
  - Need to adjust other parameters to make simulations accurate

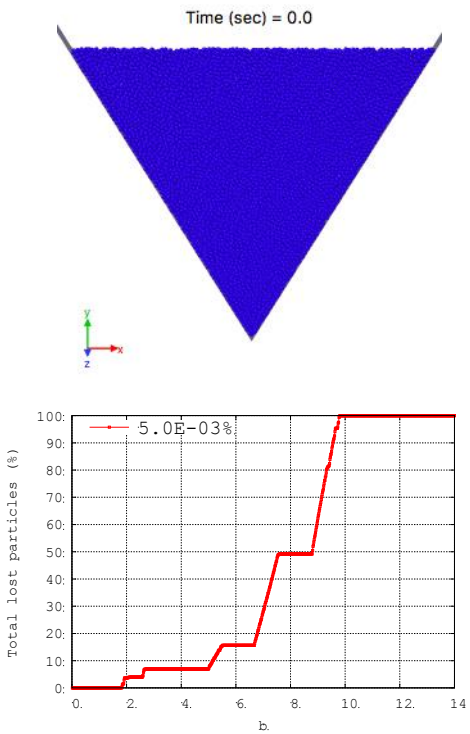



- Deformation (shear) strength strongly dependent upon sliding friction coefficient
- Model time step ~ 1e-6 s, so ~10e9 simulation steps are needed

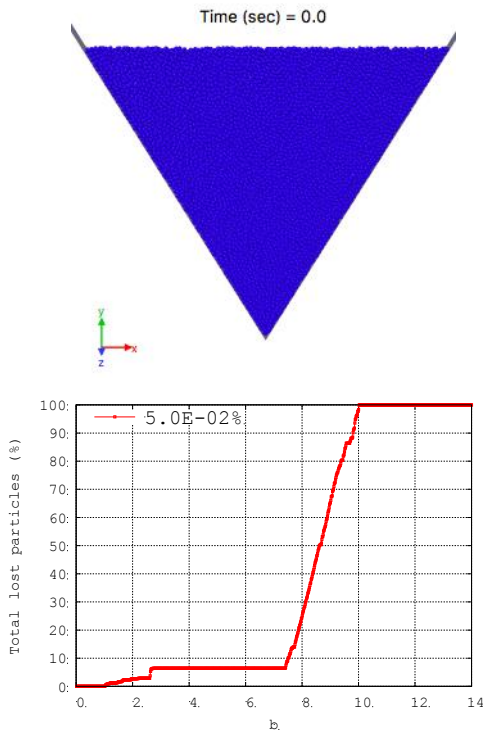
# Task 2.3: Particle Modeling
## $290K: INL (Discrete Element Method, DEM)

Effects of moister content on hoper flow:

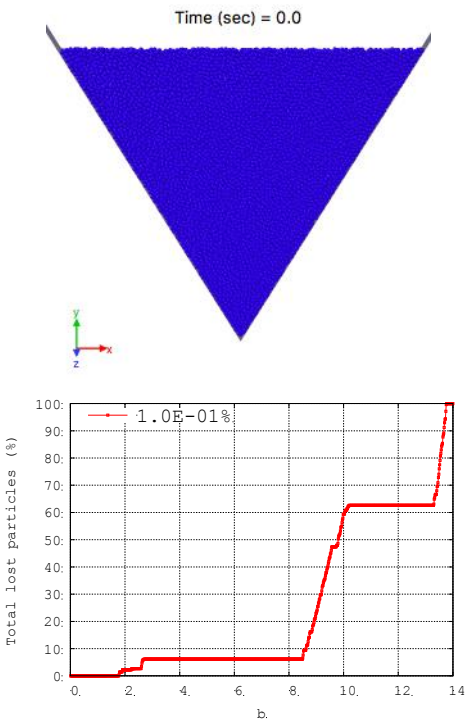
**5E-03%**




**5E-02%**




**1E-01%**

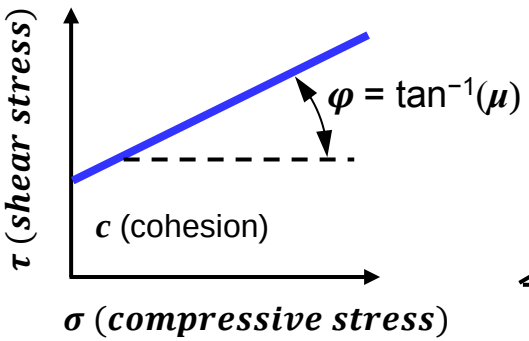


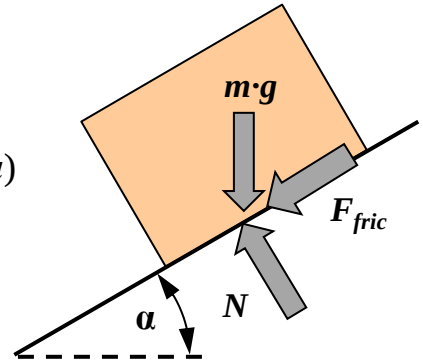

- Time sequence images of DEM simulation (wet glass beads flowing in a hopper).
- Important: material tends to flow and fall in packets (episodic flow)
- **Experiments show biomass flow is also episodic**
- **DEM can accurately capture this effect, which is very difficult for continuum models**

# Task 2.1: Continuum (Reduced-order) Modeling

## $560K: INL, NREL

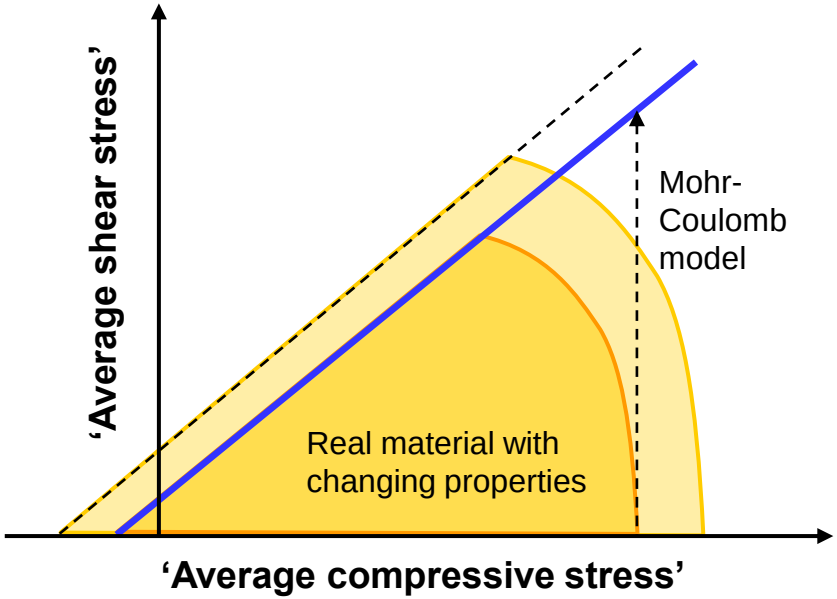
- **Assumes that particles are small and behave as a continuum**
  - Does not have direct particle effects because models average over particles
- **Simplest powder flow model is the Mohr-Coulomb Model (MCM)**
  - Used to develop all design guides for handling particulate materials
  - Basis of ~all continuum flow models
  - Assumes perfect plasticity/elasticity
  - Works very poorly for biomass



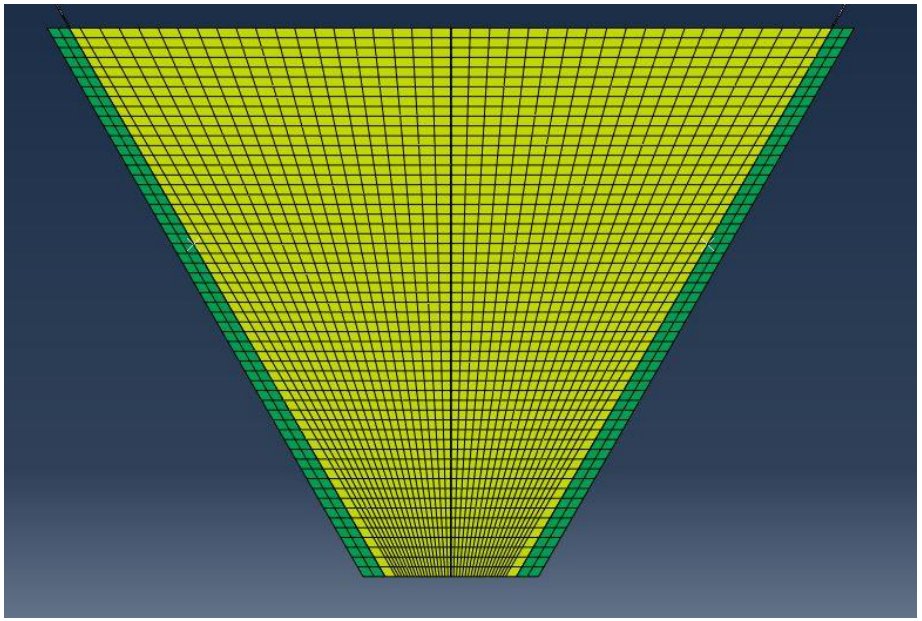

$$F_{shear} = c \cdot A + \mu \cdot N$$

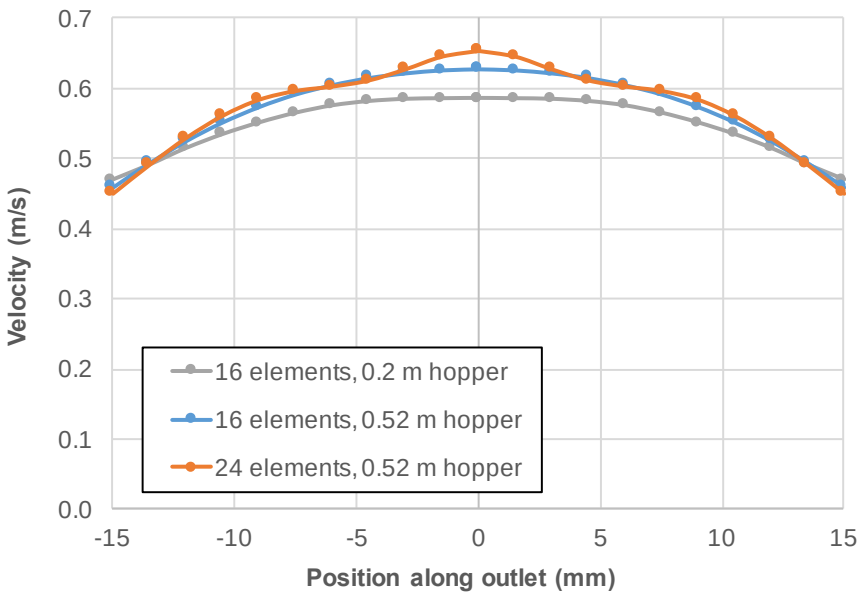
- **Requires 5 parameters**
  - Cohesion, $c$
  - Internal friction angle, $\varphi$
  - Young's modulus, $E$
  - Poisson's ratio, $\upsilon$
  - Dilation angle, $\gamma$
  - $c$, $\varphi$ have similar behavior as for rigid bodies



# Continuum (Reduced-order) Modeling
## $560K: INL, NREL

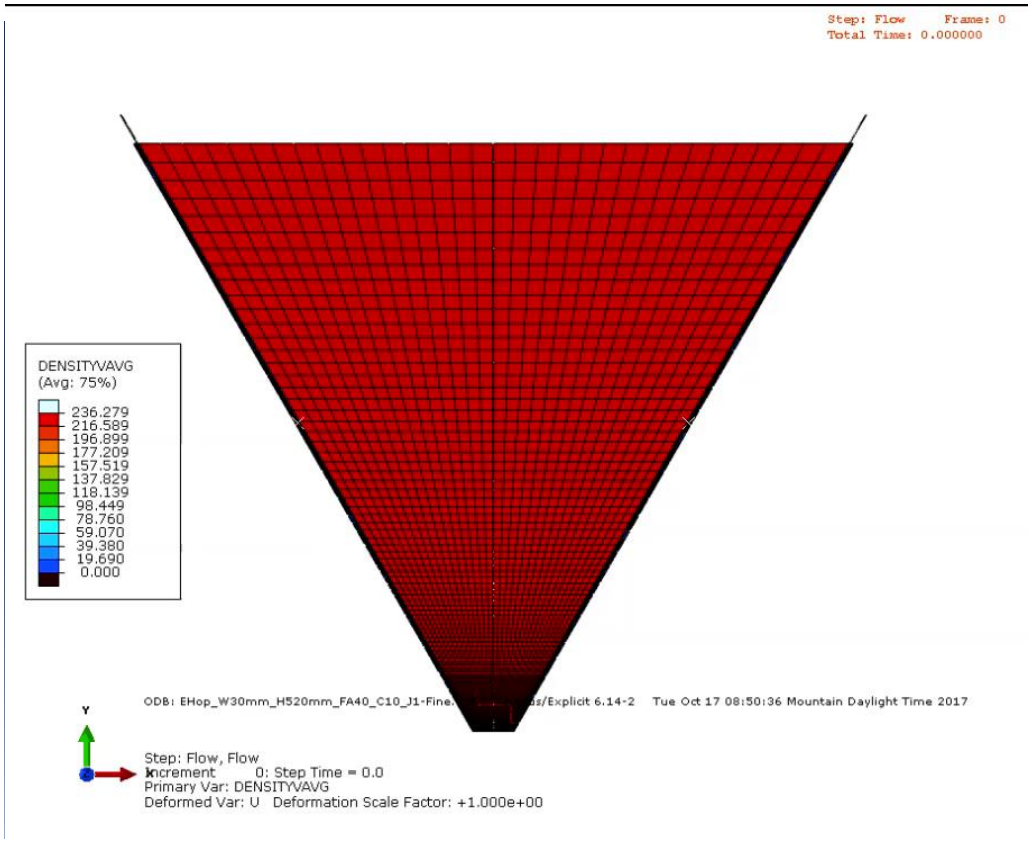
- **'Simple hopper flow'**
  - Does not account for episodic flow at outlet
  - Eulerian approach (mesh does not deform)

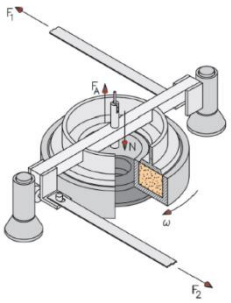





- Brick, partitioned mesh
- Mesh refinement study used 16, 24, and 32 elements across the hopper outlet

# Continuum (Reduced-order) Modeling
## $560K: INL, NREL



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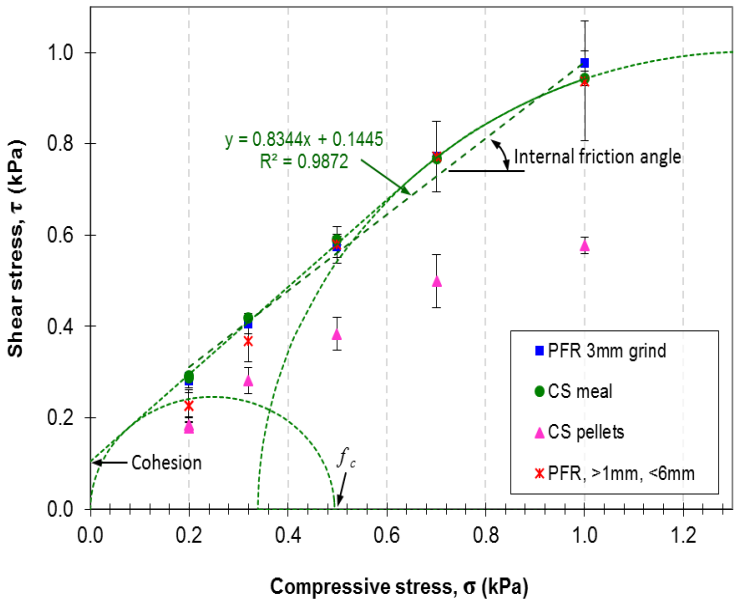
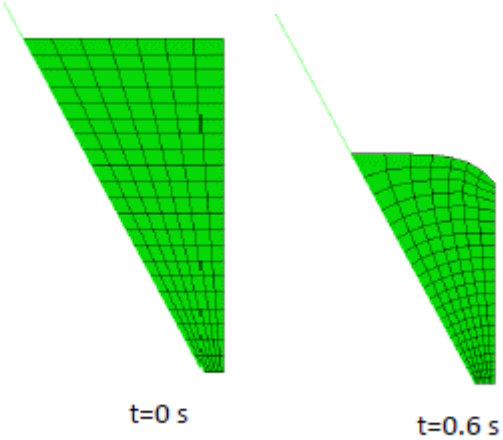



Shear characterization pine forest residue (PFR) and corn stover (CS) materials

- **Model adjusted to match flow of 3 mm PFR**
  - ***c* = 10 Pa; *φ*** = 40˚
  - Precision of shear tester is ~100 Pa
  - Need better method to measure cohesion, ***c***

# Continuum (Reduced-order) Modeling
## $560K: INL, NREL

- **More advanced models are needed to address challenging issues**
  - Non-ideal elastic and plastic behavior
  - Creep
  - Anisotropy
  - Hysteresis
  - Damping
  - Mesh deformation & ‘packet, episodic’ flow
- **A Variety of models are available but all will require modification**
  - Modified Drucker-Prager Cap (DPC) model
  - Non-local granular fluidity (NLGF) model
  - Smoothed-Particle Hydrodynamics (SPH) model




*Adaptive mesh: remeshes after each time step to reduce element distortion*

# Tasks and Connections

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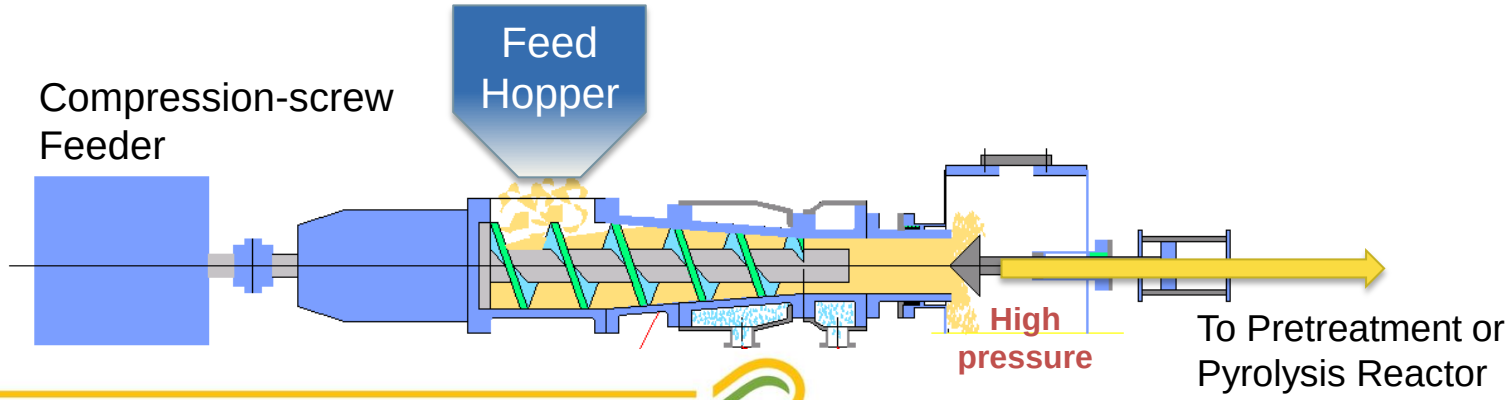
# Task 3.1 CFD Modeling (Compression Screw Feeder)

***Challenge***: Compression-screw feeding of biomass feedstock

- Direct feeding operation into pretreatment and pyrolysis reactors (>50 kPa)
- Prone to *upsets* (plugging, blowback)
- Sensitive to material properties
- Upsets often cause *shutdown* of downstream operations

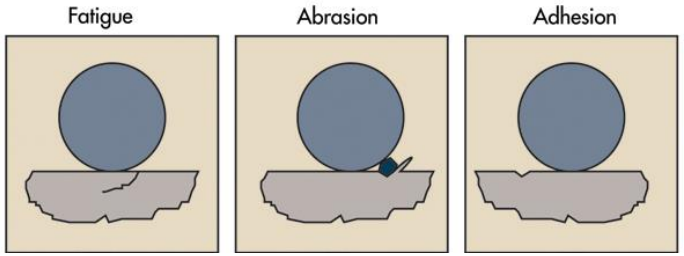
***Approach***: Predict feedstock properties and operating conditions for *reliable* operation

- Moist feedstock particles are compressed to form a single deforming material
- <u>CFD models will represent the material as a single continuum with non-Newtonian rheology</u>
- Mixture model to represent varying liquid and air content that affect the rheology
- OpenFOAM CFD software will be used to perform the simulations on NREL's HPC



# Task 5 Wear Modeling

**Goal** – develop analytic model of wear (abrasive) with capability to predict component/material wear based on biomass properties and equipment parameters




- Based on indentation plasticity and micro-fracture from kinetic energy. Corn stover isconsidered a composite material with a abrasive particles in a soft matrix
- Will model hammer milling and sliding/conveying.
- Will require material characterization data, such as composition, properties and characteristics of ash and other contaminant particles.

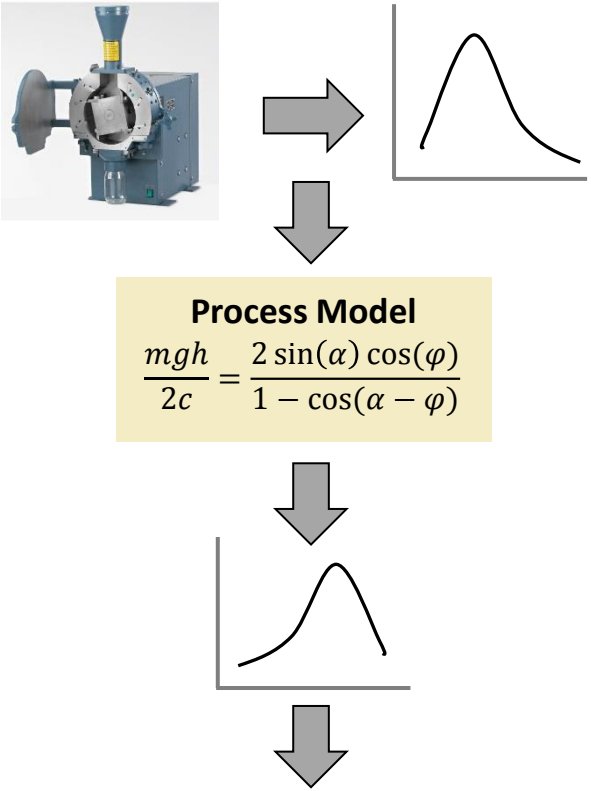
**Wear Rate (m/s)** $= (\boldsymbol{Wear\ Coeff}) \times \boldsymbol{PV}$

- Wear Coefficient considerations
  - Basic form – dependent on mechanism (abrasive, adhesive, fatigue, corrosion ….)
  - Dependent on elastic properties of ash/debris and stover (moisture)
  - Ash composition – properties, sizes, etc.,
- PV considerations – contact pressure applied to ash/debris
  - Load and speed – operational parameters
  - Load sharing between stover and ash
  - Effect of moisture (lubricant)

# Summary

**Outcomes:** Model framework and methods to measure material properties that will enable predicting the flow behavior of biomass over a wide range of industrial operations at any scale

1. Reliable engineering design guides based upon advanced rheological models (not Mohr-Coulomb)
2. Rapid flow tests for short-term industrial use
3. Detailed, robust particle models to understand mechanics
4. Reduced-order continuum models to accelerate process iteration and control and that can provide scaling between facilities and scales




**Potential dominant physical/mechanical properties**

1. Cohesion
2. Friction/shear strength
3. 3D Young's moduli
4. Plastic hardening
5. Particle size and shape
6. Particle roughness
7. Moisture content
8. Bulk density
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