A comparison of two and three dimensional multi-scale simulations as applied to porous heterogeneous materials

John P. Borg
Marquette University

The Institute of Shock Physics, Imperial College

Presented at The Royal Society London
February 22, 2010

Collaborators

DTRA:
Richard Lewis

Eglin:
Lalit Chhabildas
Brian Plunkett
Bill Cooper

Sandia National Laboratories:
Tracy J. Vogler

NSWC-Indian Head:
Gerrit Sutherland

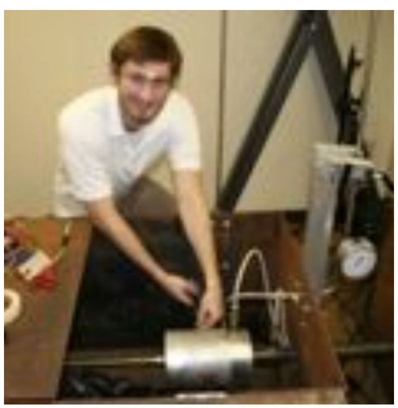
Students

Mike Morrissey
(MS-2009) Marquette Univ

Andrew Fraser
(PhD-2012) Marquette Univ

Kenneth Jordan
(PhD-2010) Marquette Univ
(SMART Fellow - NSWC-DD)

Jeff Midday
(BS-2010) Marquette Univ



Cullen Braun
(MS-2011) Marquette Univ

Cheryl Perich
(BS-2010) Marquette Univ

Computational Efforts

Objective:

Better understand complicated dynamics at the bulk scale by building up our understanding of the compaction dynamics from simple models at the particle scale.

Solution Procedure:

Two and three dimensional Hydro-code calculations:
CTH (Eulerian), EPIC (Lagrangian), EMU(periadynamics)

Outline

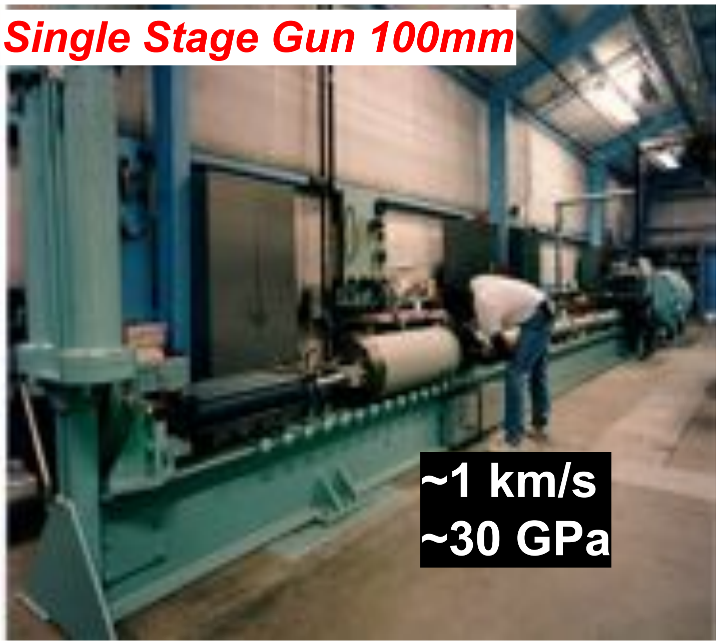
- High Strain Rate ($> 10^5$ 1/s)
  - Two-Dimensional Mesoscale simulations of Tungsten Carbide
  - Three-Dimensional WC simulations
  - Wet and Dry Sand
- Low Strain Rate ($< 10^3$ 1/s)
  - 2D and 3D simulations of Sand

Tungsten Carbide: Plane Strain Simulations

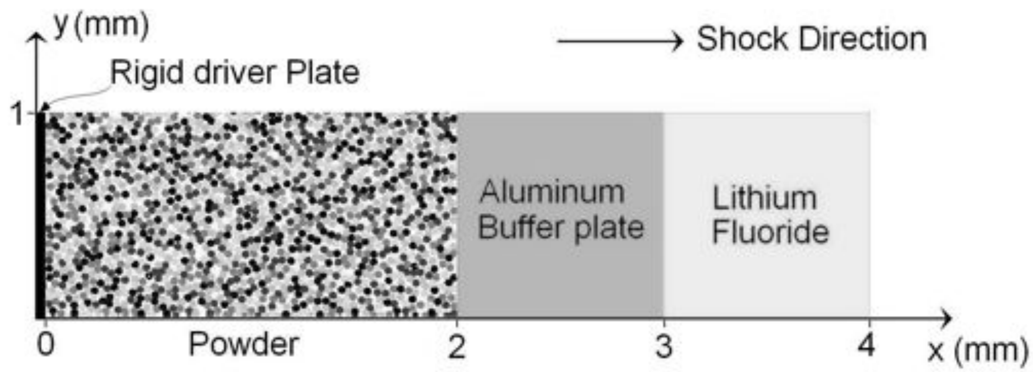
Light Gas Gun

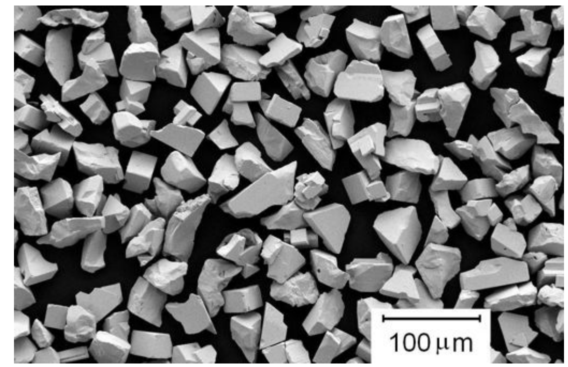
Plane Strain Impact Experiments

Strain-rate: > 10^5 s^{-1}



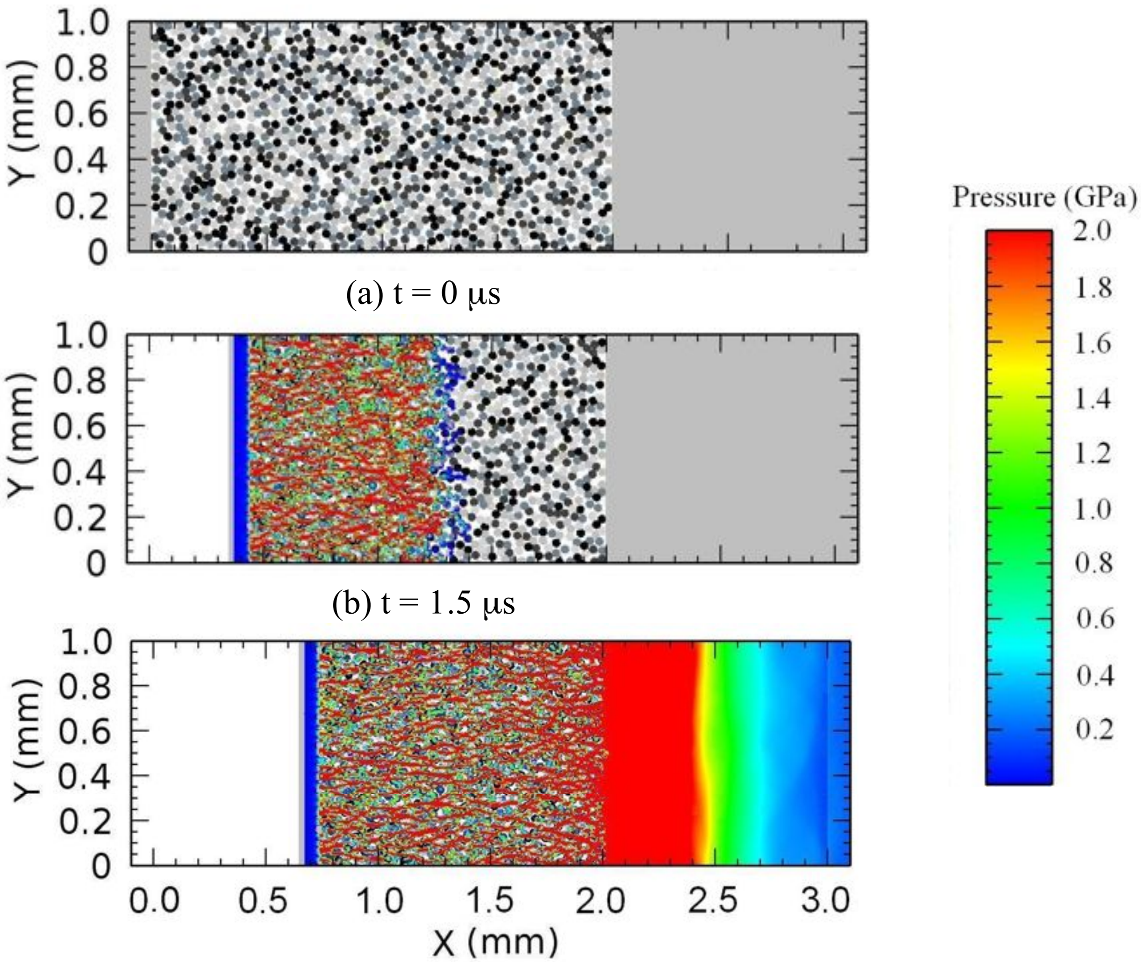
2D Mesoscale Approach

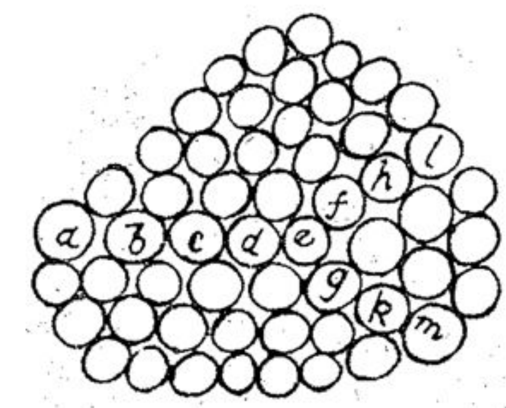




- Duplicates geometry of experiments
- 2-D and 3D simulations of porous granular materials (Baer, Benson and others)
- Calculations contain ~1,400 particles, idealized as circles (rods in 3D), with periodic y-direction BC
- CTH (explicit Eulerian finite difference code) with ~12 cells across particle diameter
- WC modeled with Mie-Gruneisen EOS, elastic-perfectly plastic strength, and failure at a specified tensile stress
- Bulk material properties obtained from open literature
- Ridged driver plate with constant velocity (simulations between 5~7,000 m/s)

2D Mesoscale Approach



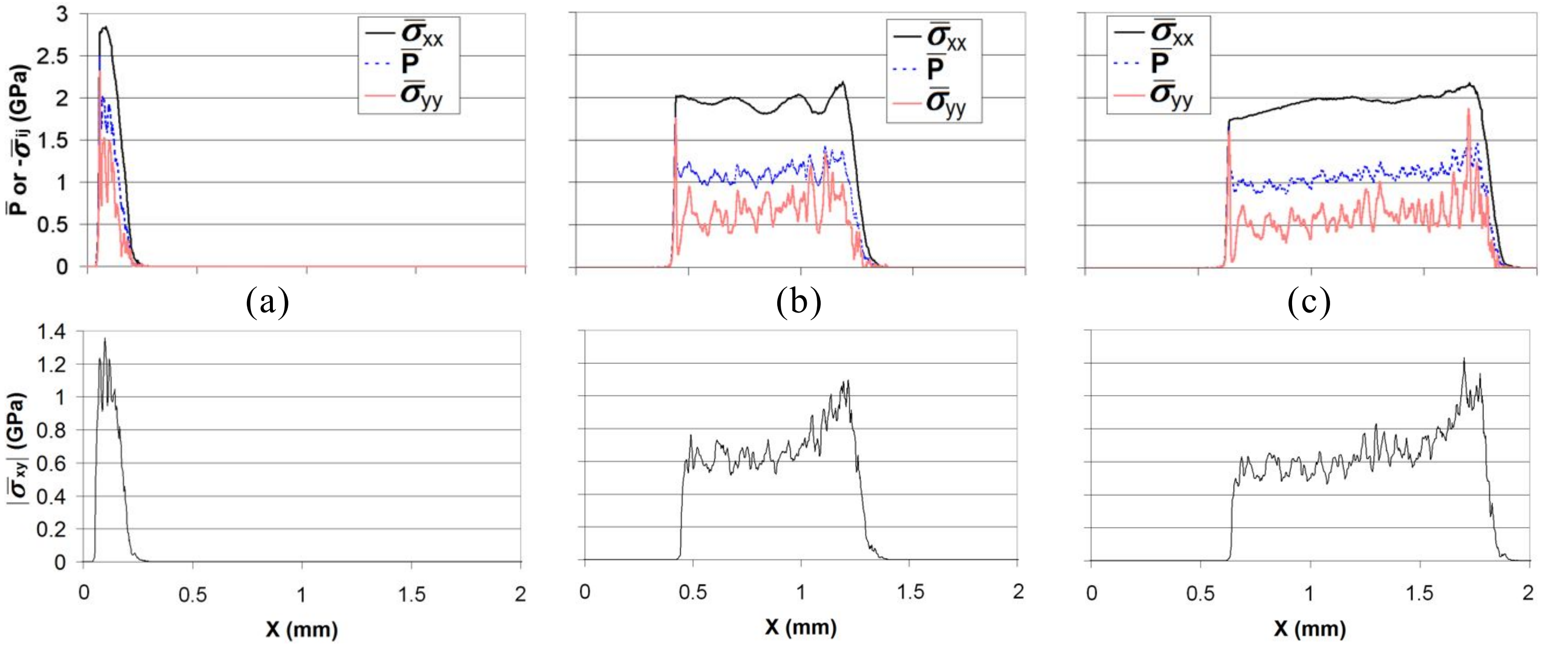


Newton (*Principia, 1687)*

- Dynamic stress bridging
- Compaction wave, 5 particle thick
- Two-dimensional flow field, $\sigma_{ij} \neq 0$

2D Mesoscale Approach

Average in lateral direction to determine bulk response



(a) (b) (c)

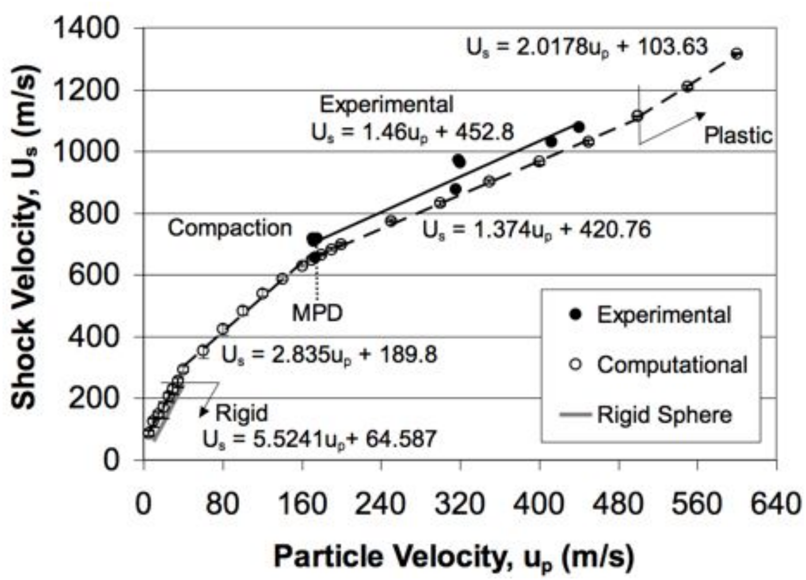
(d) t=0.2 μs

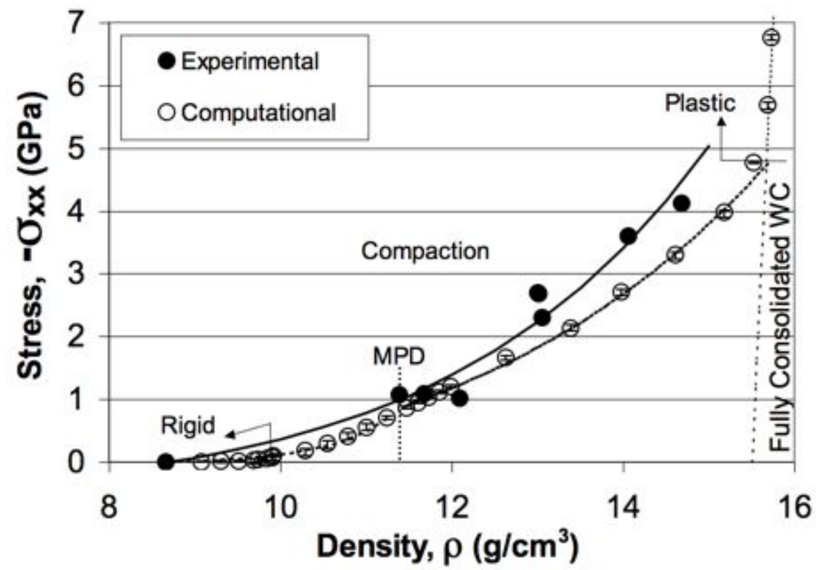
(e) t=1.5 μs

(f) t=2.15 μs

2D Mesoscale Baseline Results

Baseline Configuration:





Multiple regimes of behavior:

1. Rigid: Simple material translation - soliton wave
2. Compaction: A) Elastic: grain deformation is mostly elastic below MPD
   B) Elastic-Plastic: mixed deformation above MPD
3. Plastic

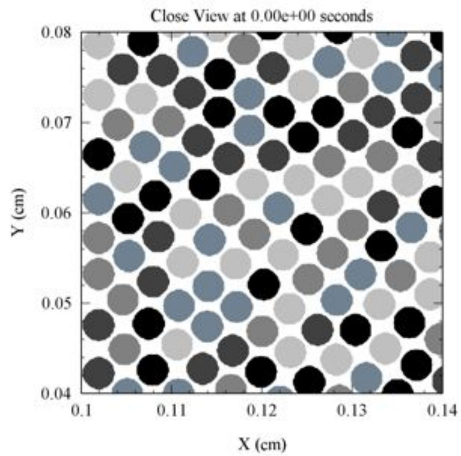
2D Mesoscale Simulation Variations

Parametric:

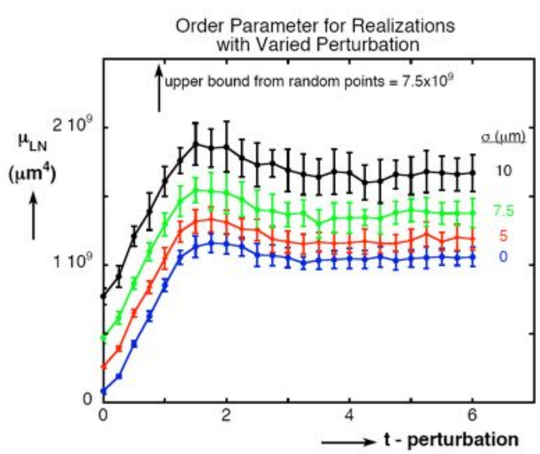
- Vary ***material realization*** holding the bulk density fixed.
- Vary the ***dynamic yield strength***.
- Vary the ***fracture stress***.

2D Mesoscale Simulation Variations

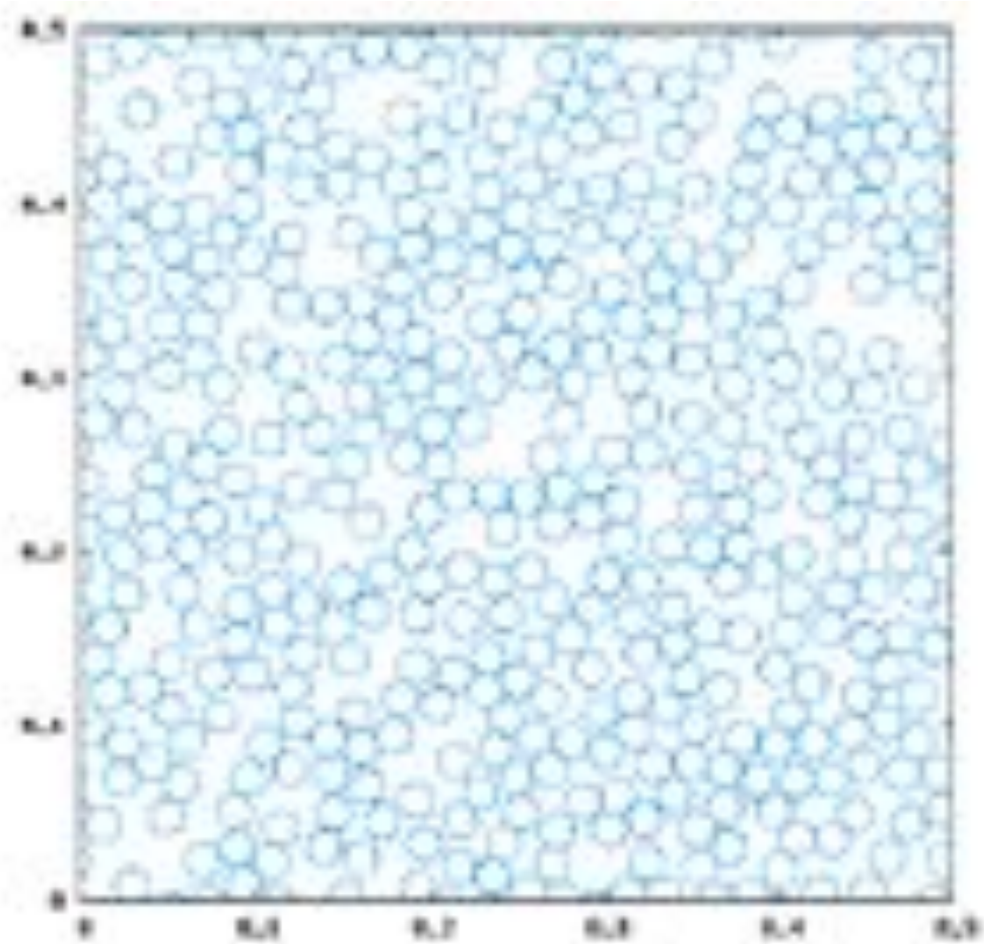
Material Realization:



Ordered Grains



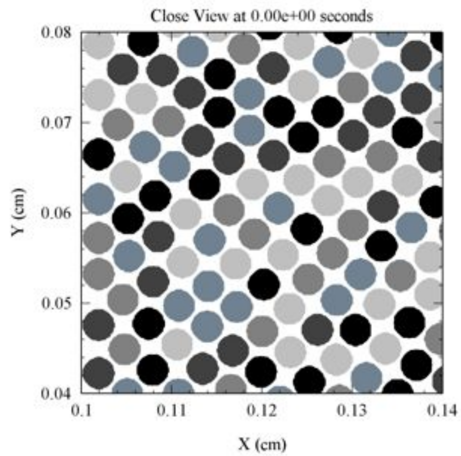
Material Perturbations

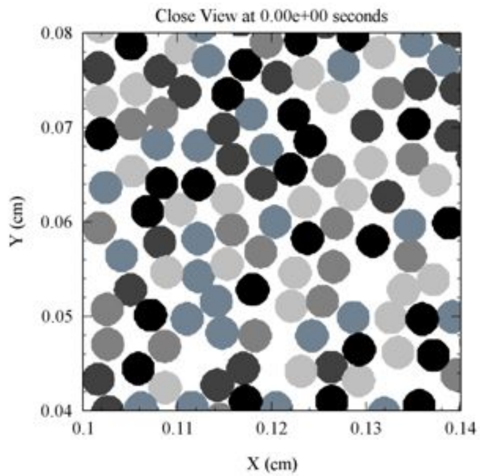


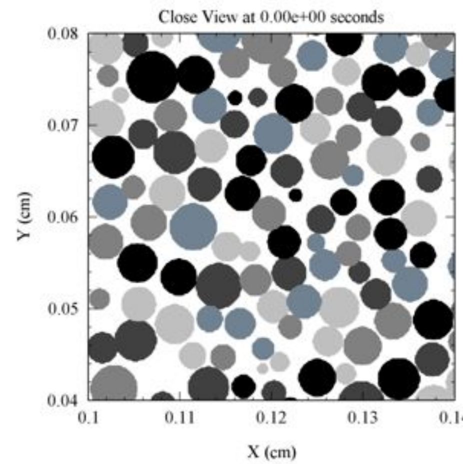
2D Mesoscale Simulation Variations

Material Realization:

Material Perturbations



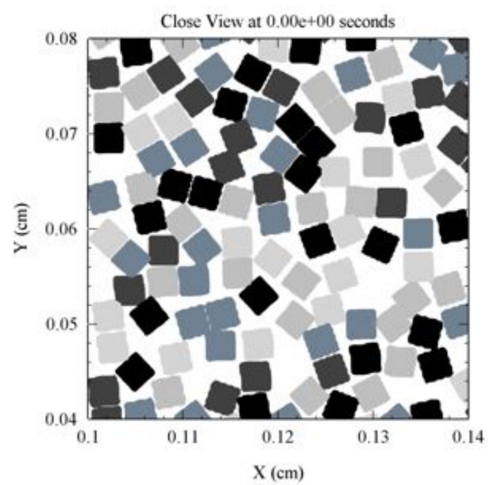


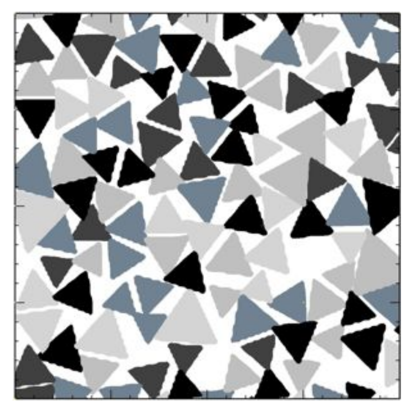


Ordered Grains

Perturbed

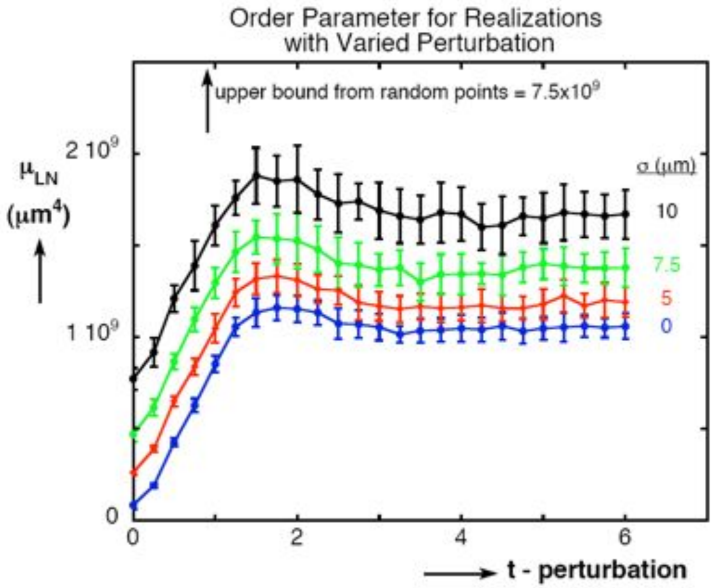
Size Distribution

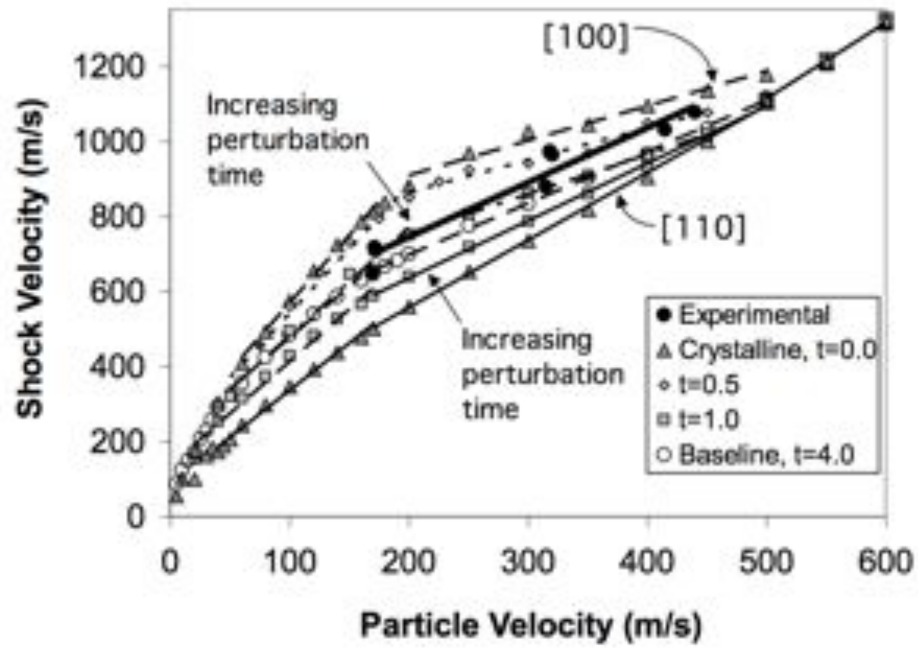




2D Mesoscale Simulation Variations

Material Realization:



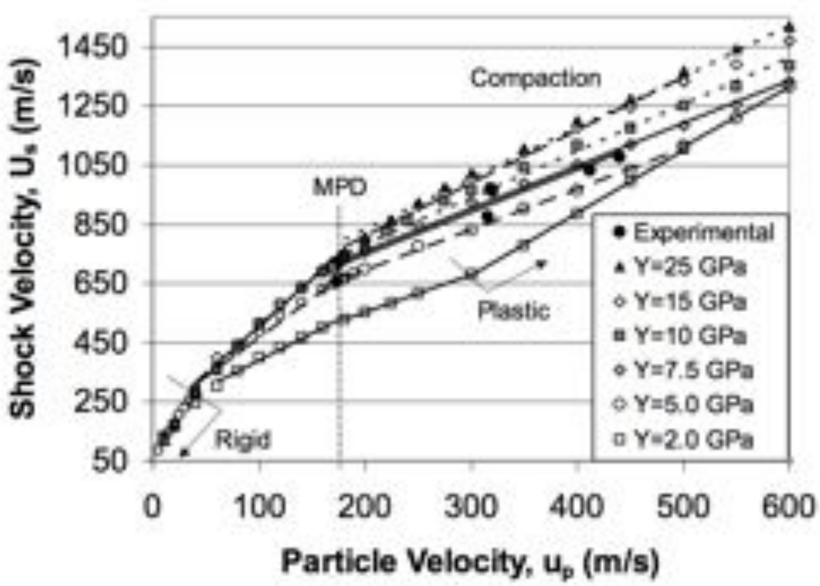


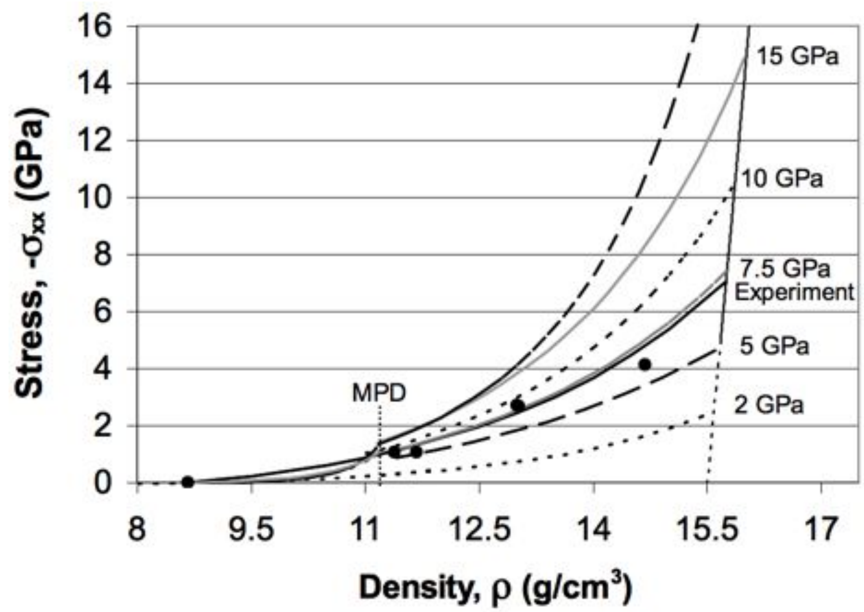
Bulk response highly dependent upon material/particle arrangement

Increasing material perturbation collapses bulk response

2D Mesoscale Simulation Variations

Variations in Dynamic Yield Strength

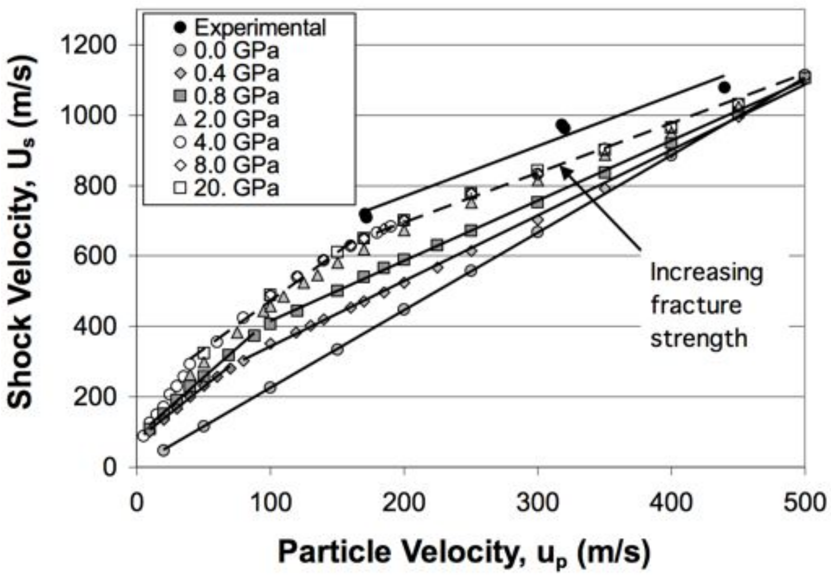


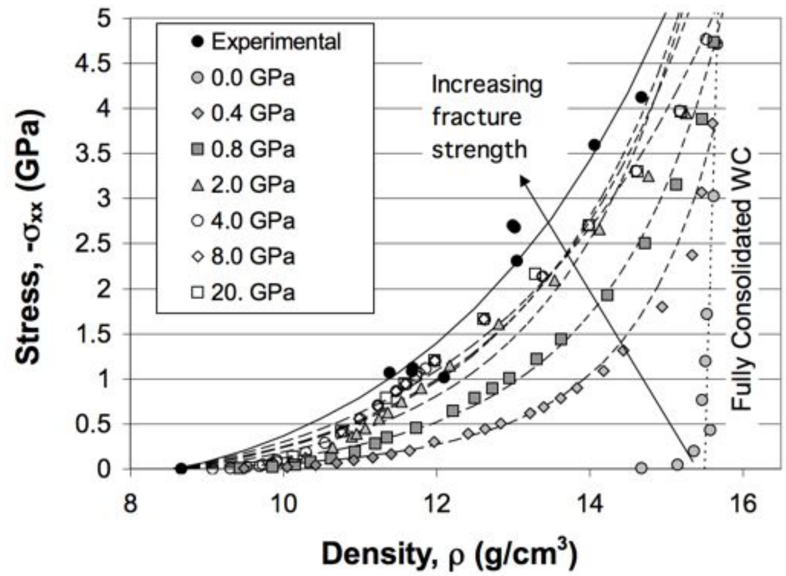


- Specified flow stress determines Hugoniot intercept
- MPD density is invariant to yield
- Rigid response is invariant to yield

2D Mesoscale Simulation Variations

Variations in Dynamic Fracture Strength





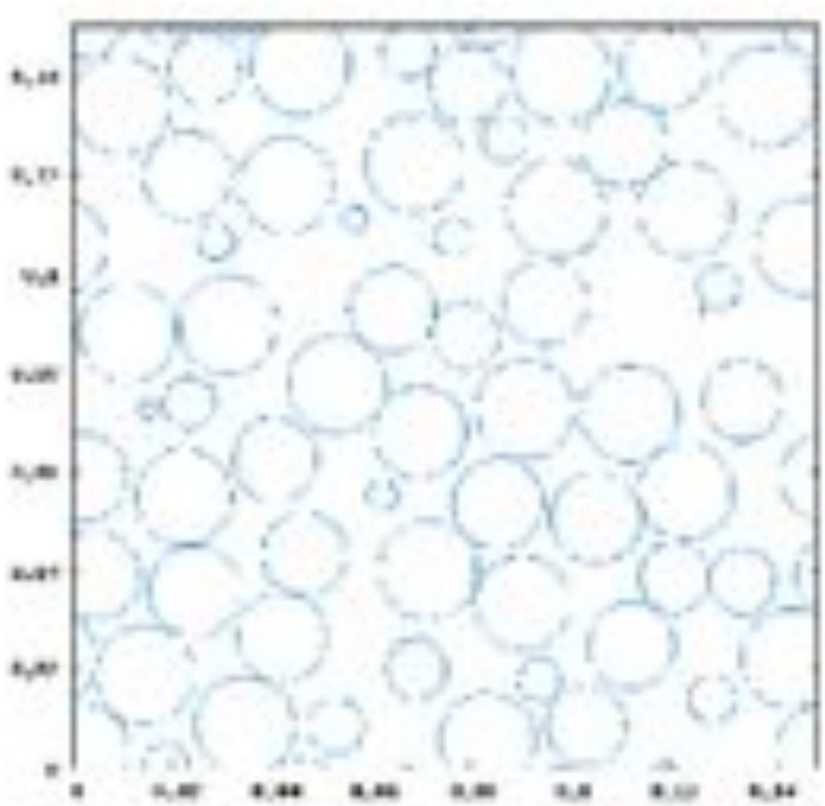
- WC spall strength is 2~1.4 GPa depending on shock level.
- Fracture strength have no effect on bulk behavior above 2 GPa.
- As fracture strength is reduced bulk stiffness is reduced.

Three-Dimensional Simulations

Loose Dry Tungsten Carbide

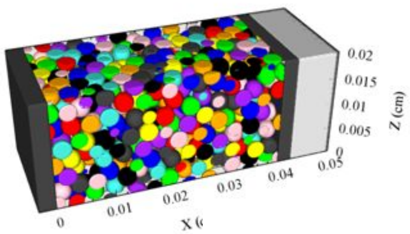
3D Mesoscale Approach

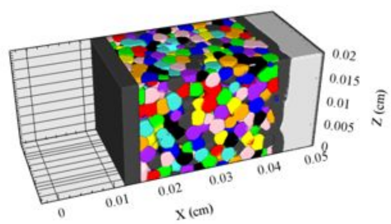
Constructing three dimensional random geometries, at high pack densities, can be challenging.

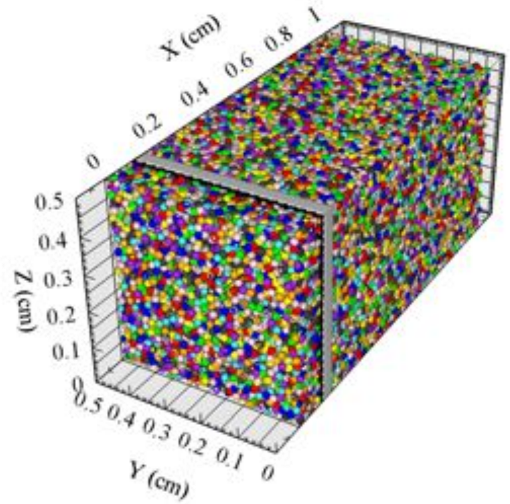


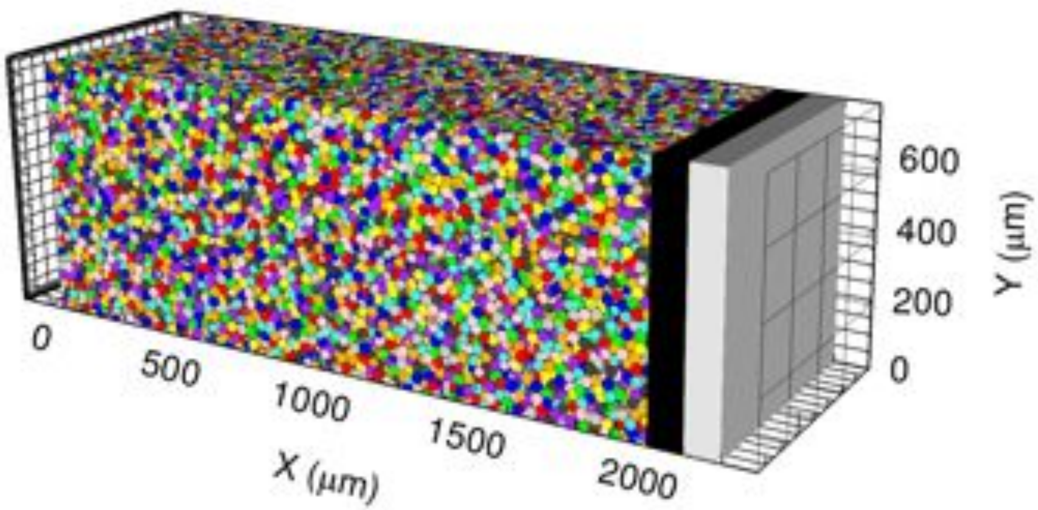
3D Geometries

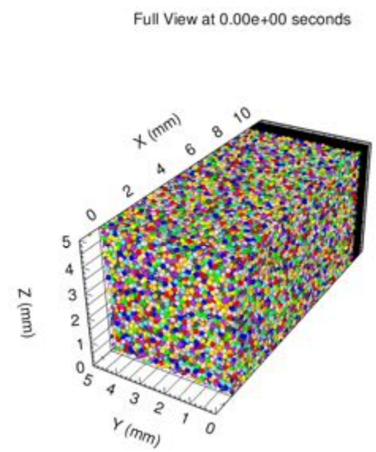
Initial Results exhibited geometry dependence





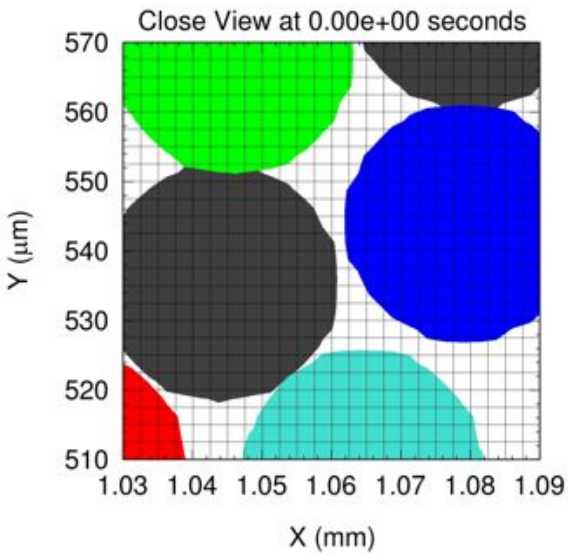






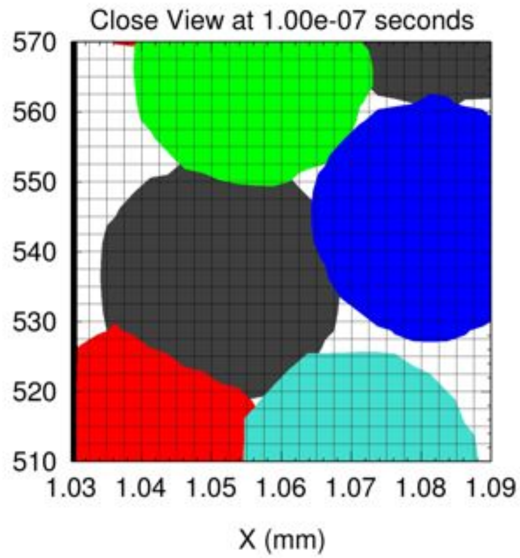
Particle Boundaries

Stiction (welding) versus Sliding

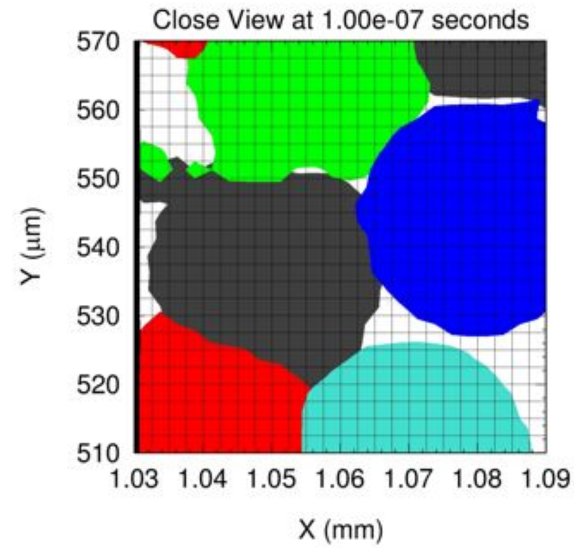


$t = 0$

Stiction



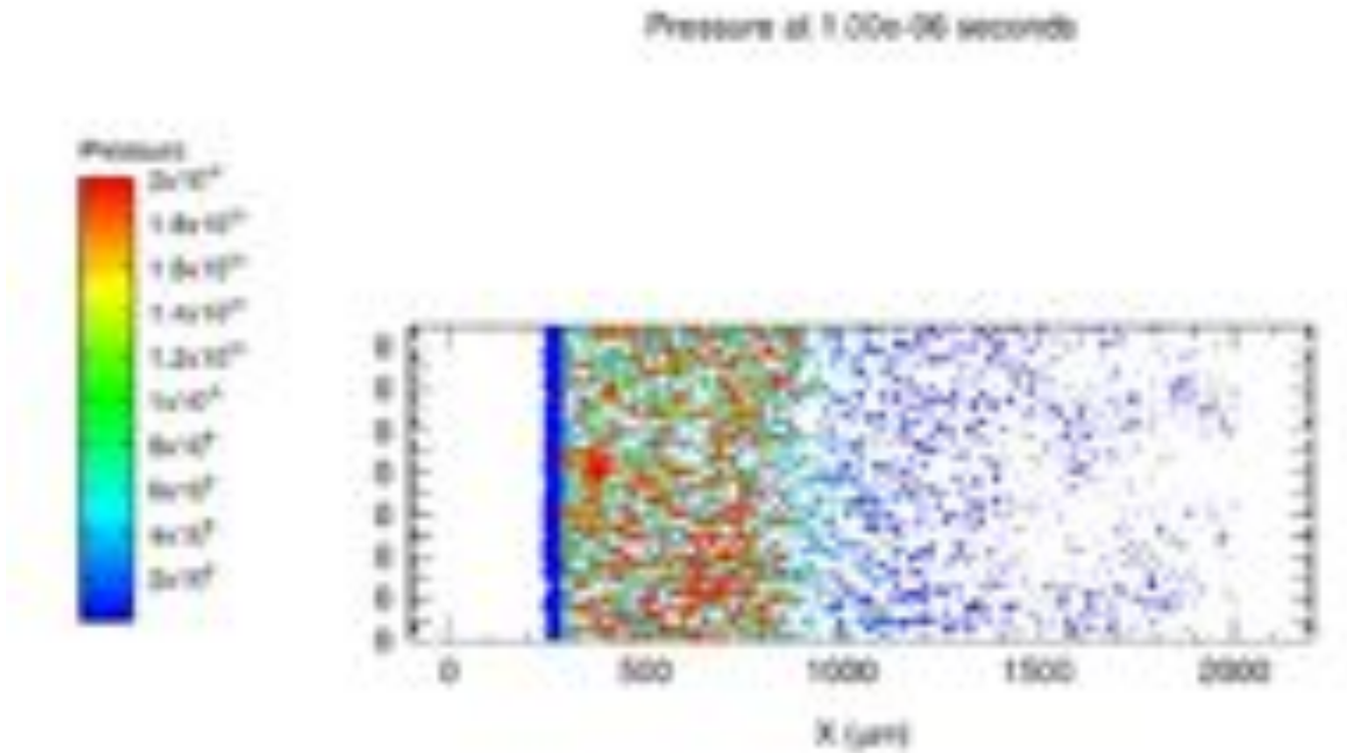
Sliding



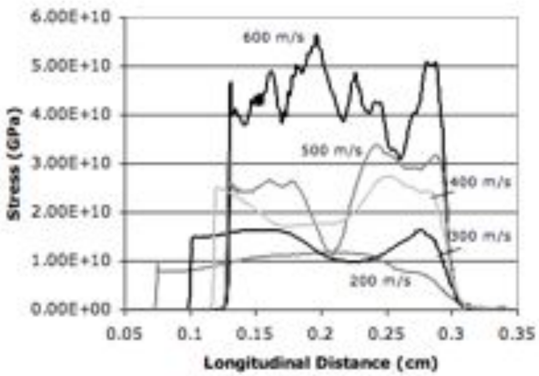
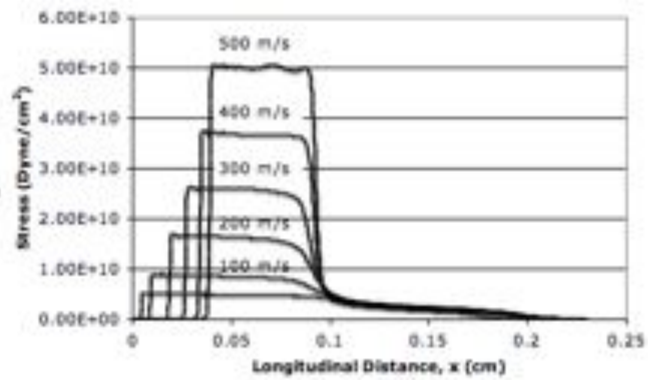
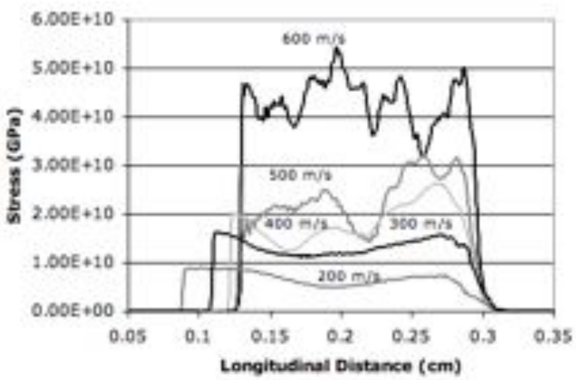
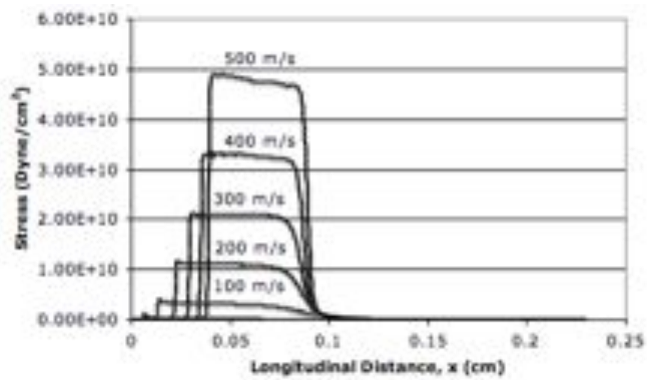
$t = 0.1$ µs

- The degree of stiction varies due to interface contact
- Since neighboring particles are assigned different material numbers, a sliding interface can be imposed.

Compaction Wave

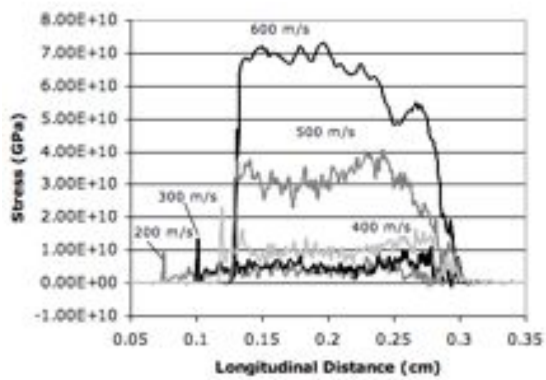
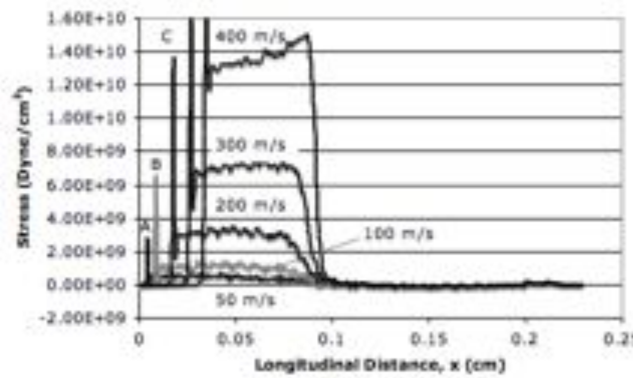
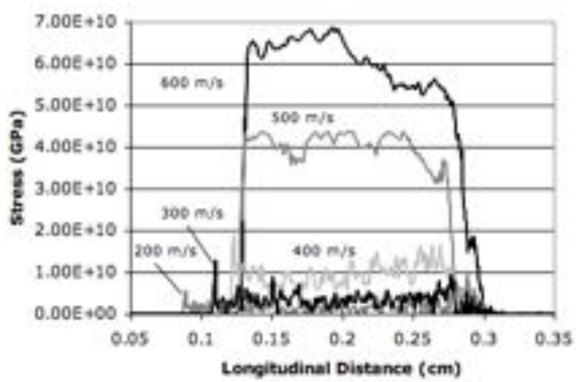
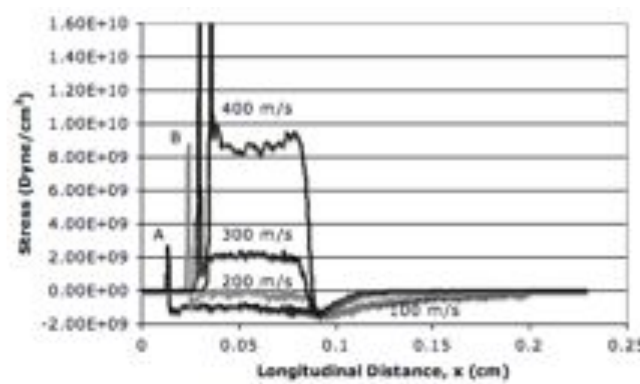


Longitudinal Stress

	2D	3D
Stiction		
Sliding		

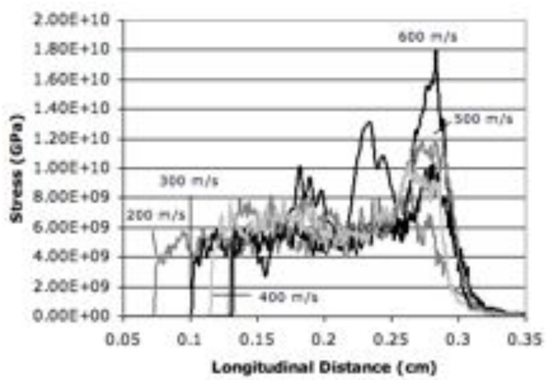
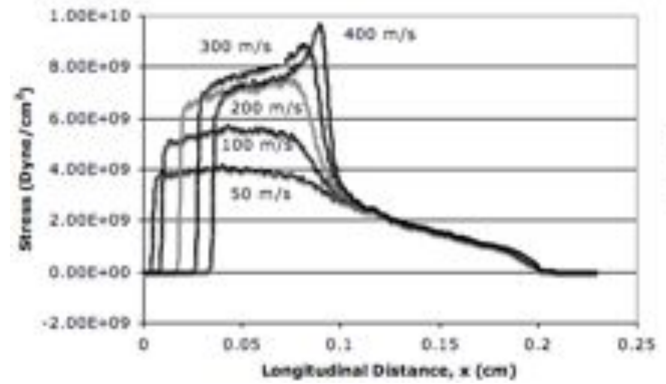
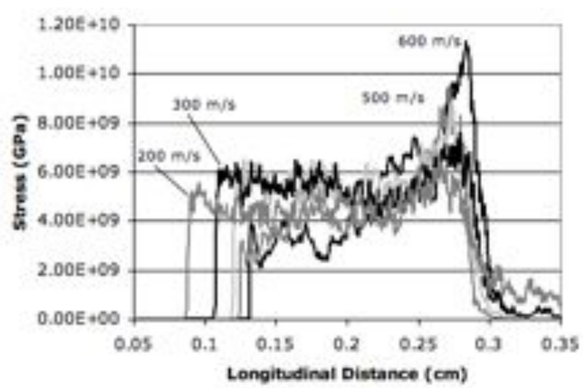
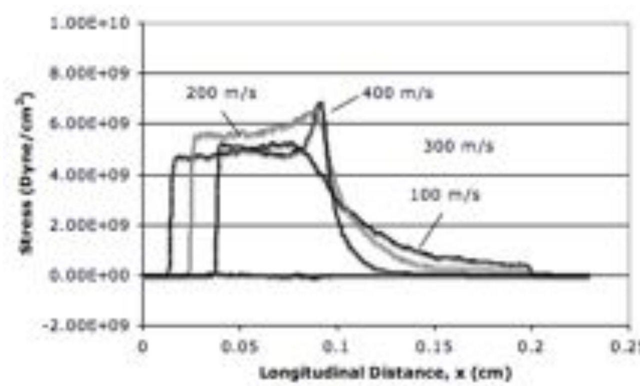
- General smooth nature of 3D simulations
- Precursor wave

Lateral Stress

	2D	3D
Stiction		
Sliding		

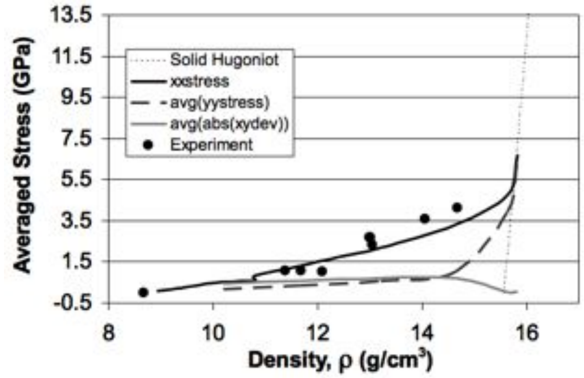
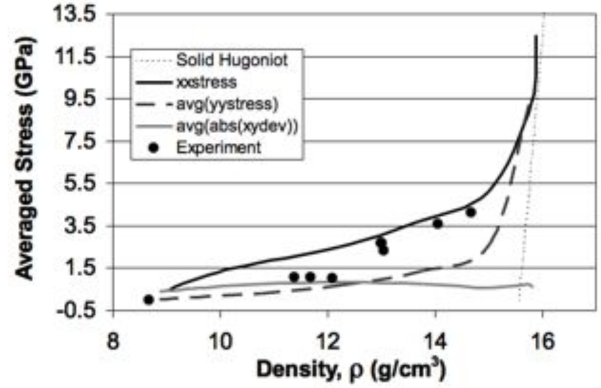
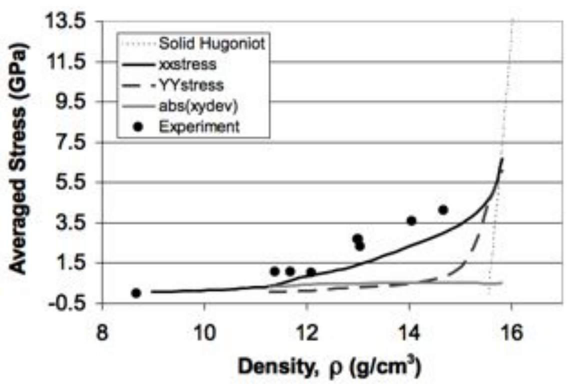
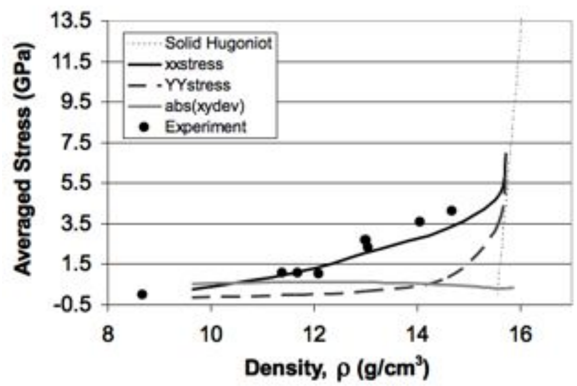
Sliding allows lateral stress to change sign

Shear Stress

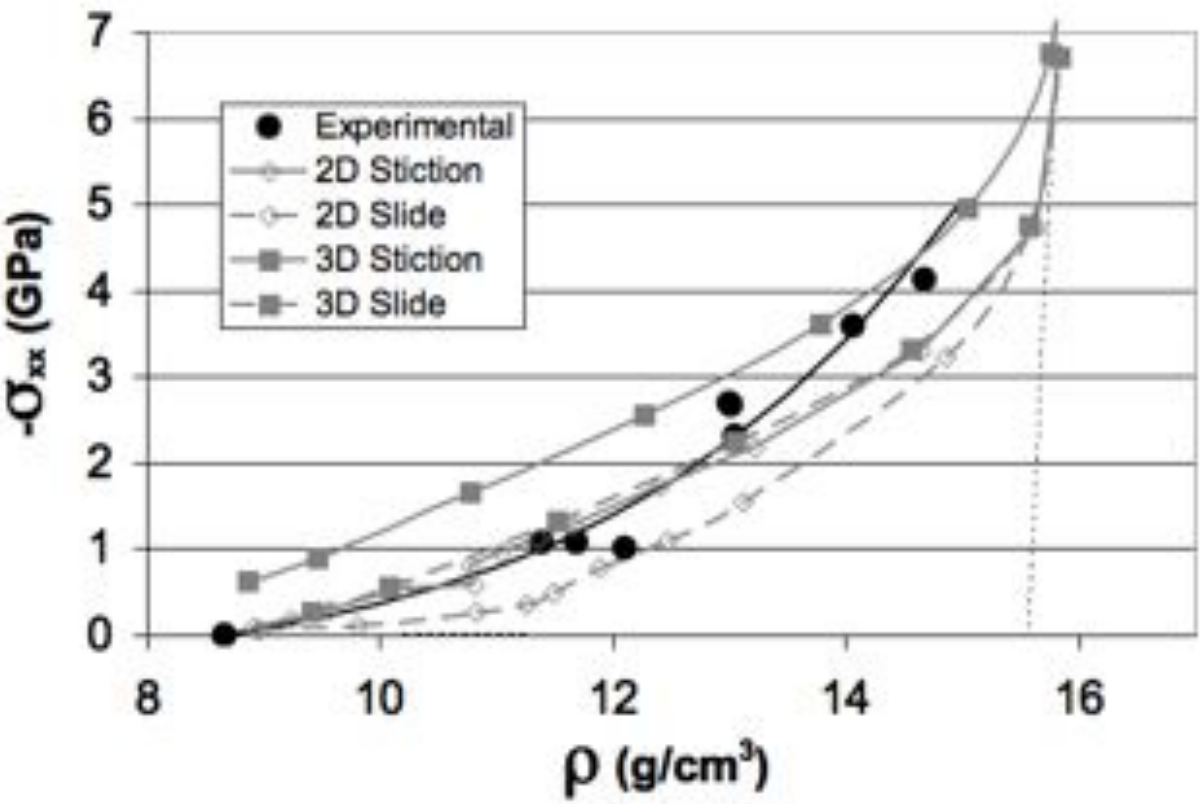
	2D	3D
Stiction		
Sliding		

- Absolute value of shear stress
- Wave profile is consistent with plateau at 5 GPa, except for 3D Stiction

Summary Stress

	2D	3D
Stiction		
Sliding		

Summary Stress



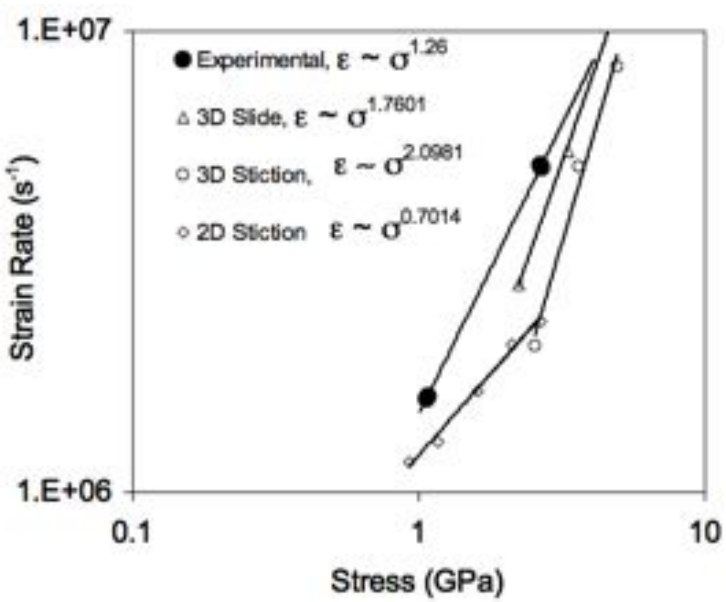
- 2D stiction and 3D sliding are nearly identical
- Both however under predict experiments at high stress
- Stiction like response better simulates the data at higher stress

But what else might differ?

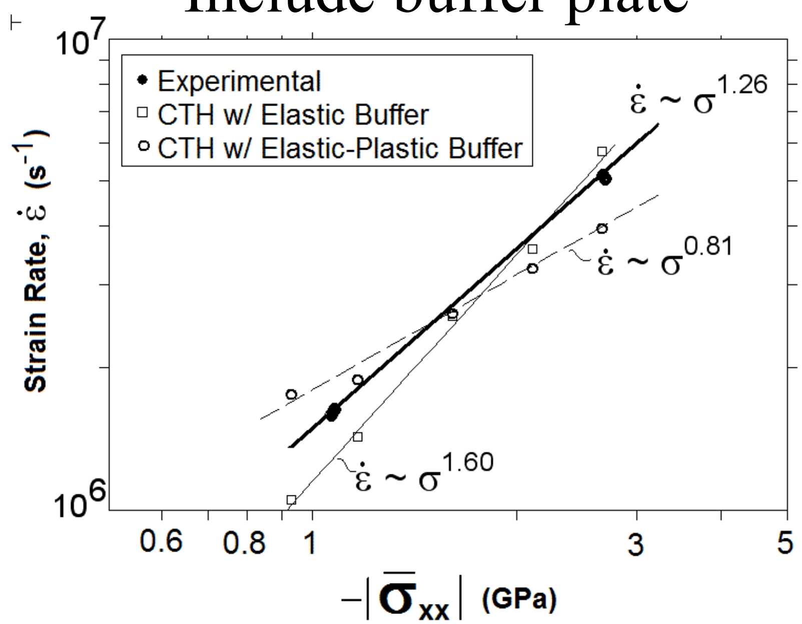
Rise Times

Swegle and Grady shock rise time relation: $\dot{\varepsilon} = \sigma^n$

n ~ 4: homogeneous metals and ceramics
n ~ 2: layered polycarbonate - aluminum, stainless steel, or glass
n ~ 1: granular materials: WC, SiO_2, TiO_2, and sugar



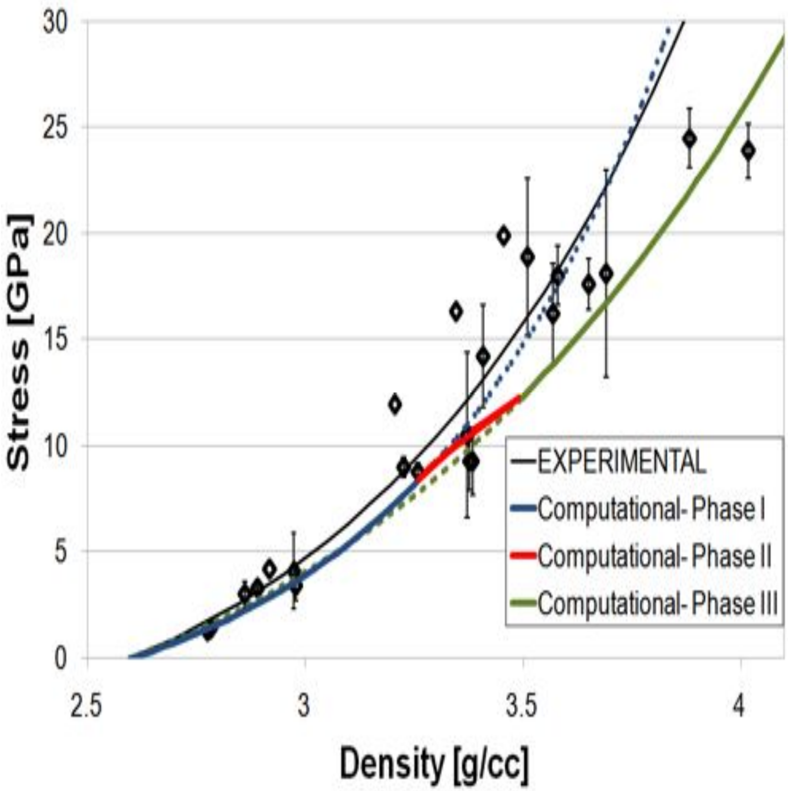
Include buffer plate



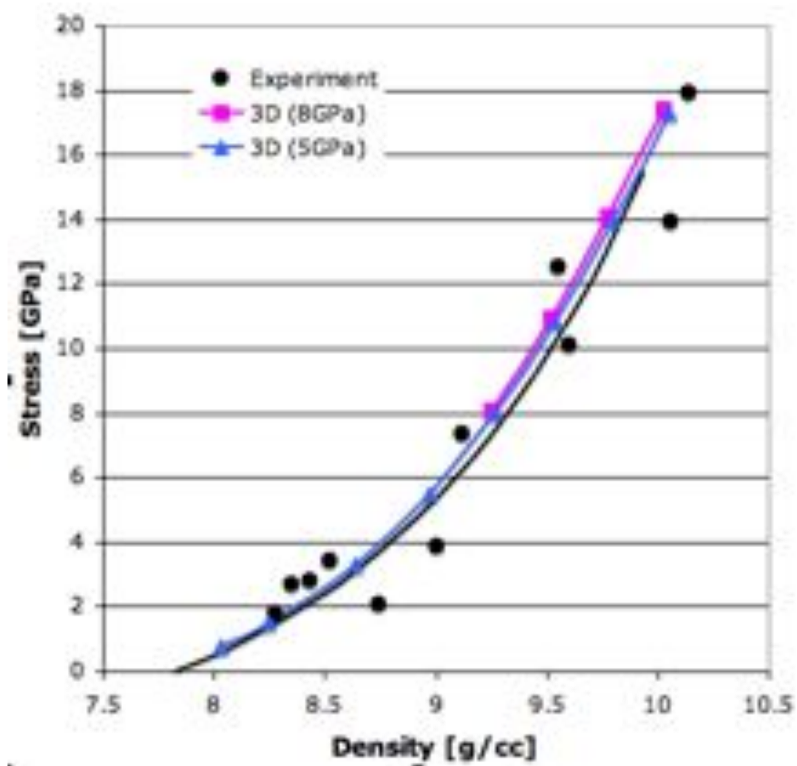
Fully Consolidated

Variations in bulk response is more pronounced for granular materials as opposed to consolidated materials.

2D Simulations



3D Simulations

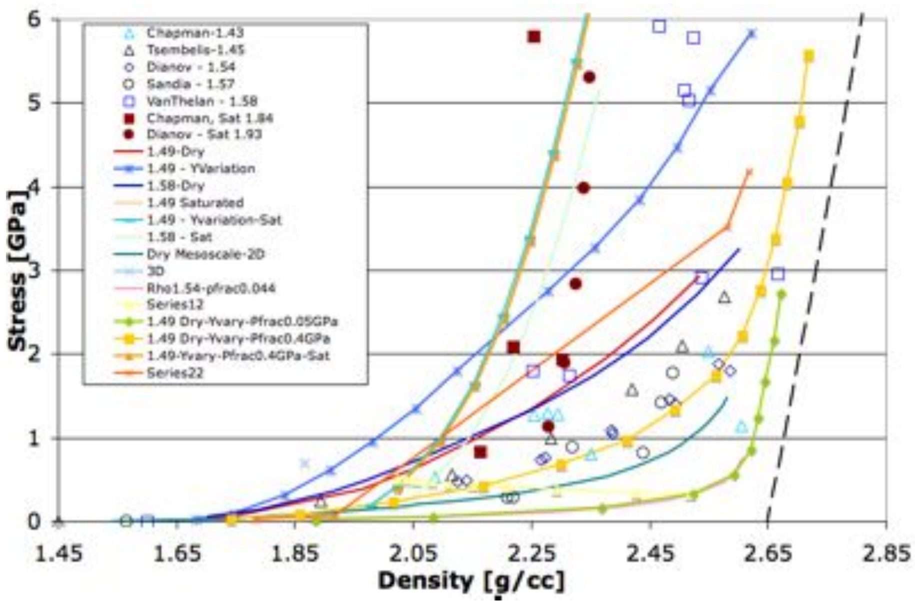


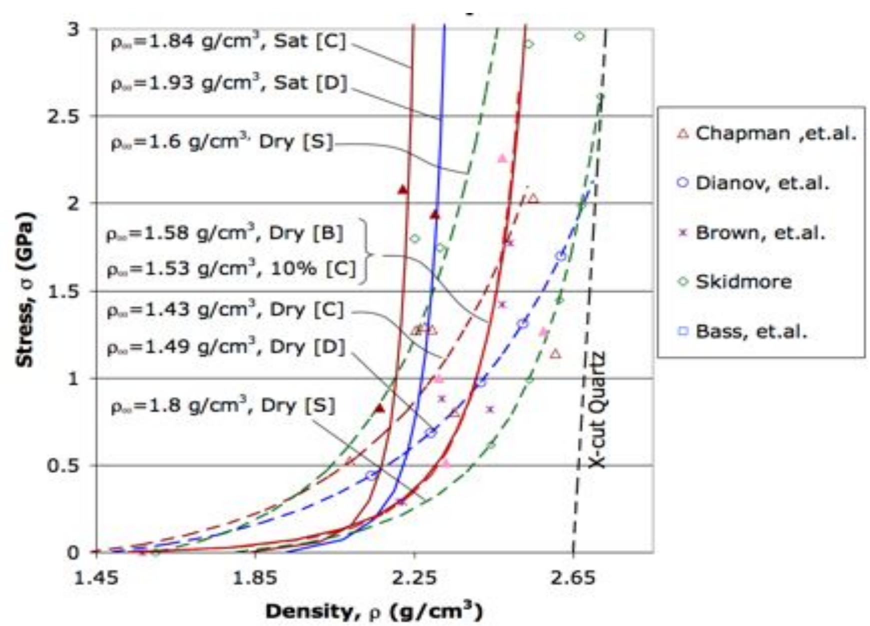
Wet and Dry Sand

How does our view of wet sand sand change?

Experimental Data

Hugoniot “sand” data is not consistent

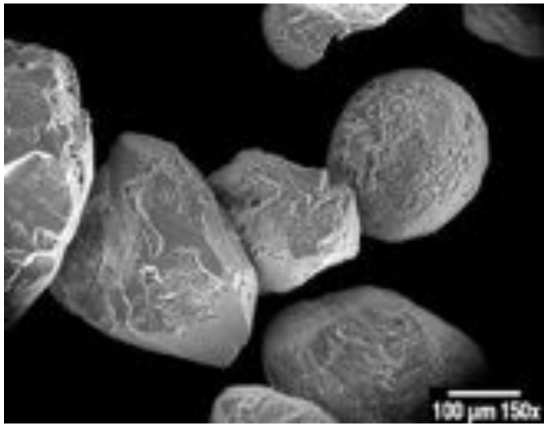


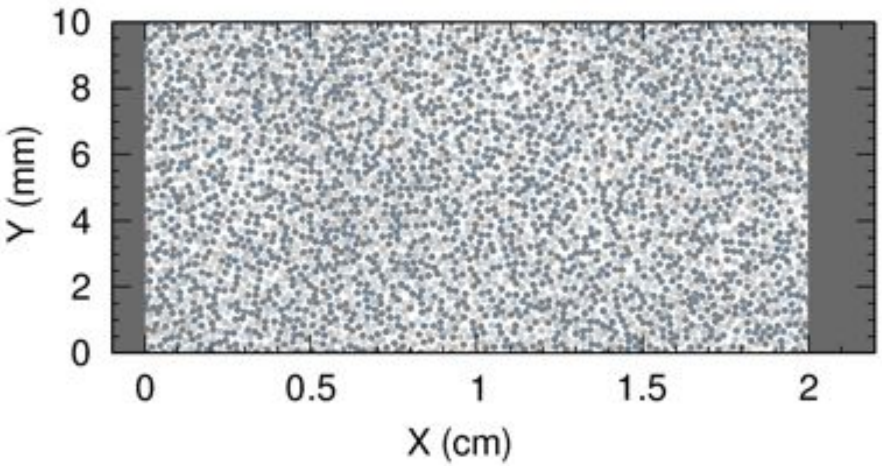


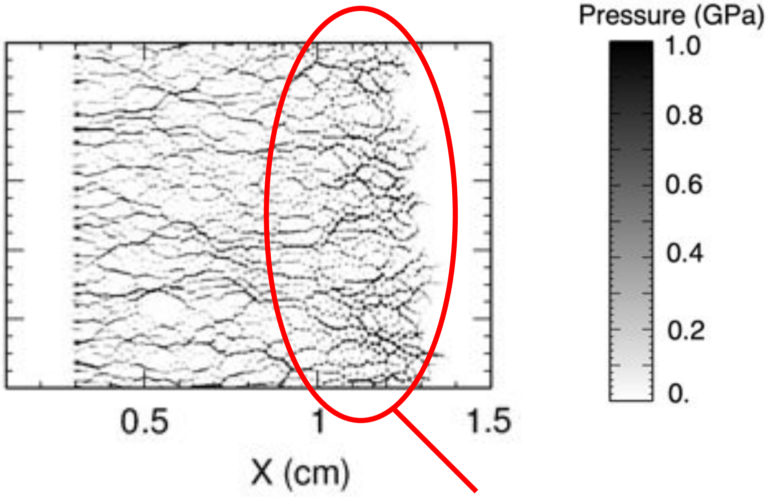
Dry Sand

Distribution of material properties

Parameter	Quartz	Water
Density, ρ [g/cm^3]	2.65	0.998
Zero stress shock speed, C_0 [*km/s*]	-	1.921
x-cut	5.610	-
z-cut	6.329	-
Hugoniot slope, s	-	1.921
x-cut	1.07	-
z-cut	1.56	-
Grüneisen coefficient, $\Gamma = V(\partial P/\partial E)_V$	0.9	0.35
Specific heat, C_V [*J/(g-K)*]	0.85	8.32
Bulk Dynamic yield strength, Y [*GPa*]	-	0.
x-cut (low, average, high)	4.1, 5.8, 7.0	-
z-cut (low, average, high)	8.2, 10.3, 12.4	-
Poisson's ratio, ν	0.15	0.5
Fracture strength, σ_s [*GPa*]	0.044 - 15 GPa	0.0001



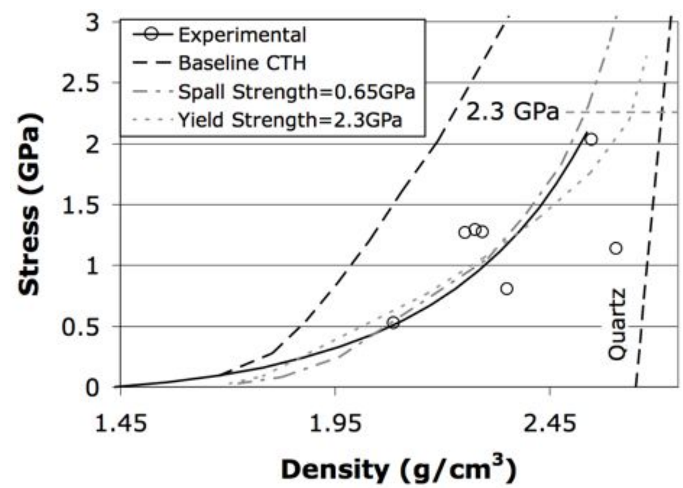




Dry Sand

Distribution of material properties

Parameter	Quartz	Water
Density, ρ [g/cm^3]	2.65	0.998
Zero stress shock speed, C_0 [*km/s*]	-	1.921
x-cut	5.610	-
z-cut	6.329	-
Hugoniot slope, s	-	1.921
x-cut	1.07	-
z-cut	1.56	-
Grüneisen coefficient, $\Gamma=V(\partial P/\partial E)_V$	0.9	0.35
Specific heat, C_V [*J/(g-K)*]	0.85	8.32
Bulk Dynamic yield strength, Y [*GPa*]	-	0.
x-cut (low, average, high)	4.1, 5.8, 7.0	-
z-cut (low, average, high)	8.2, 10.3, 12.4	-
Poisson's ratio, ν	0.15	0.5
Fracture strength, σ_s [*GPa*]	0.044 - 15 GPa	0.0001



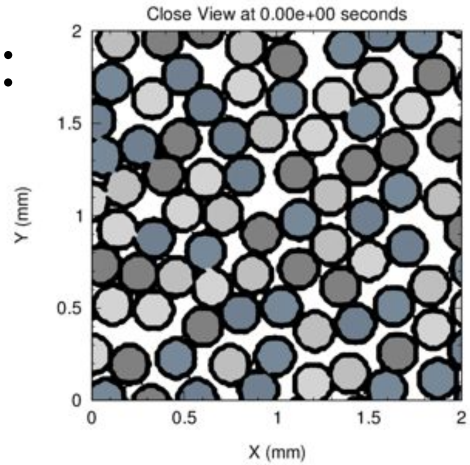
- This time 2D stiction simulations ***over predict*** bulk stiffness
- A ***reduction*** in strength is necessary to match experiment
- Distribution of strength provides some underlying skeletal strength

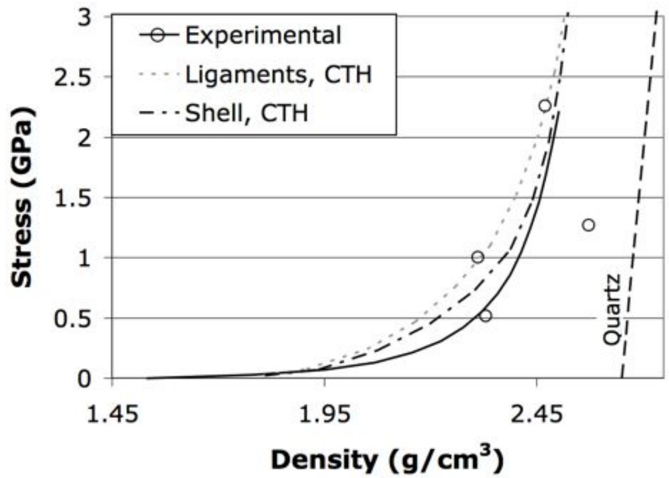
Experimental data from Chapman, Tsembelis & Proud Proceedings of the 2006 SEM, St. Louis, MO June 4-7 2006

Wet Sand

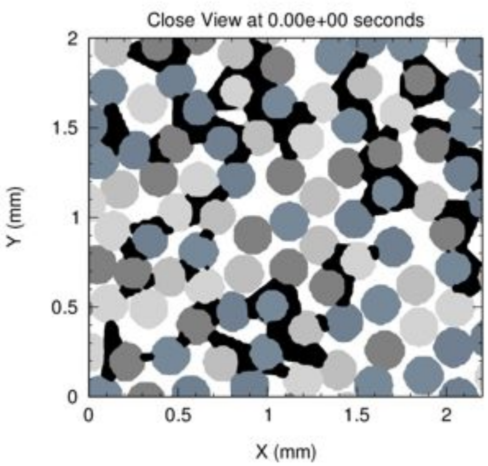
7% (by weight) moisture … but how do we insert the water?

Coating:





Ligaments

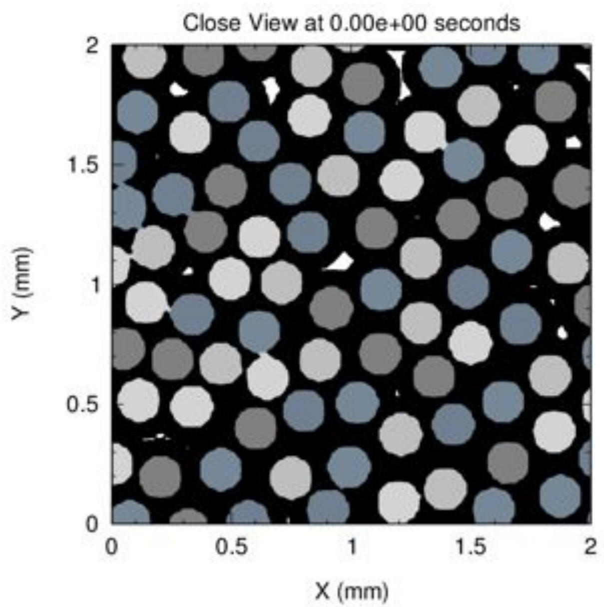


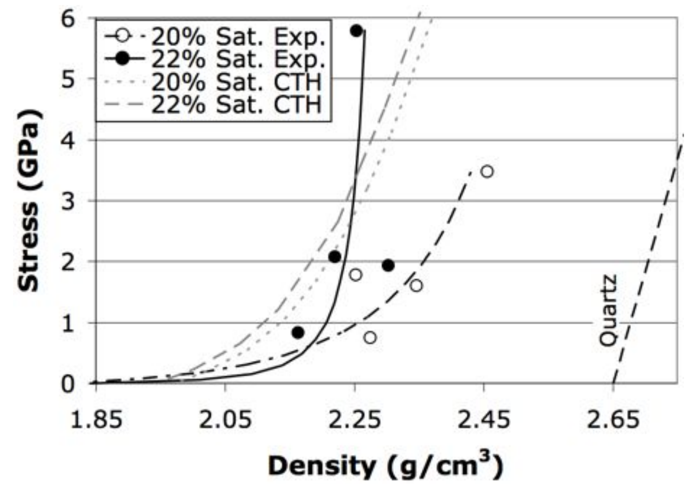
- Reduced yield strength was used.
- Bulk stiffness varies with water distribution
- Coatings induce sliding and provide less bulk stiffness

Experimental data from Chapman, Tsembelis & Proud Proceedings of the 2006 SEM, St. Louis, MO June 4-7 2006

Near Saturated Sand

22% (by weight) moisture





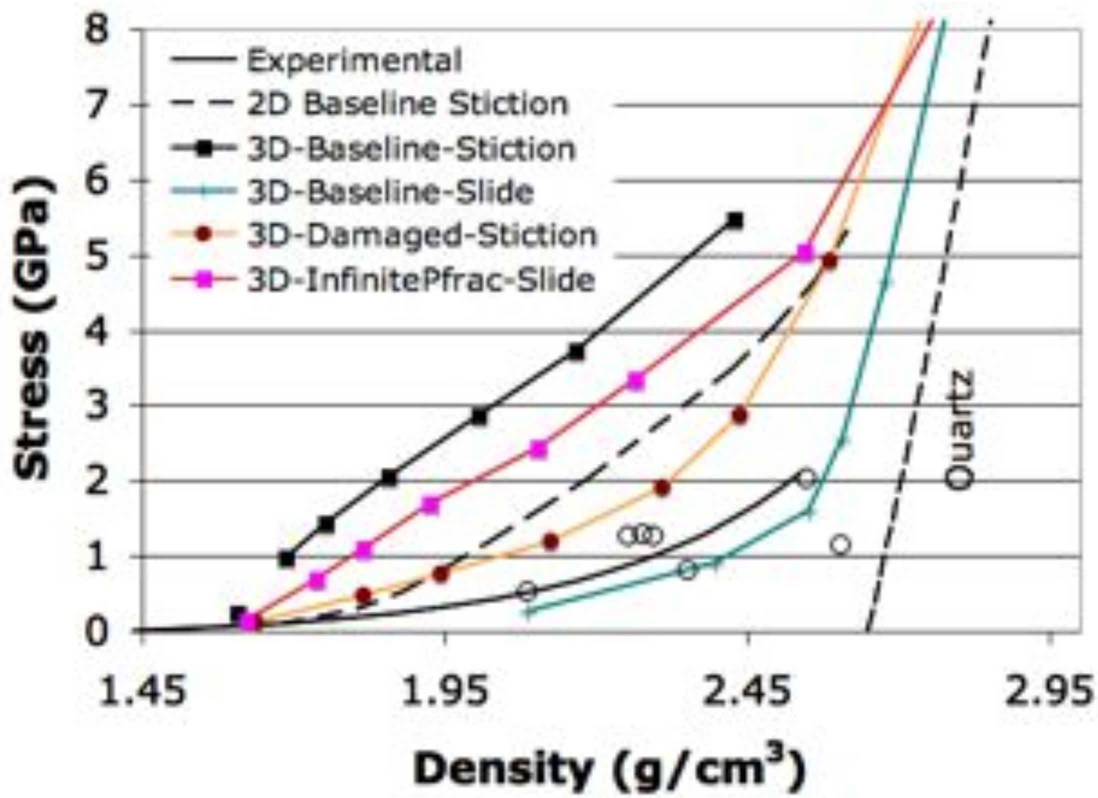
Adjusted strength calculations are now too stiff

Do not see the large variation between 20% and 22%

Experimental data from Chapman, Tsembelis & Proud Proceedings of the 2006 SEM, St. Louis, MO June 4-7 2006

3D Mesoscale Approach

Recent Results:



This time 2D stiction and 3D sliding do not correspond

Low Strain Rate

Low Strain Rate

Hopkinson or Kolsky Bar

Strain-rate: 500 to 1,600 s^{-1}

Brad Martin
Air Force Research Laboratory

Weinong Wayne Chen
AAE & MSE, Purdue University

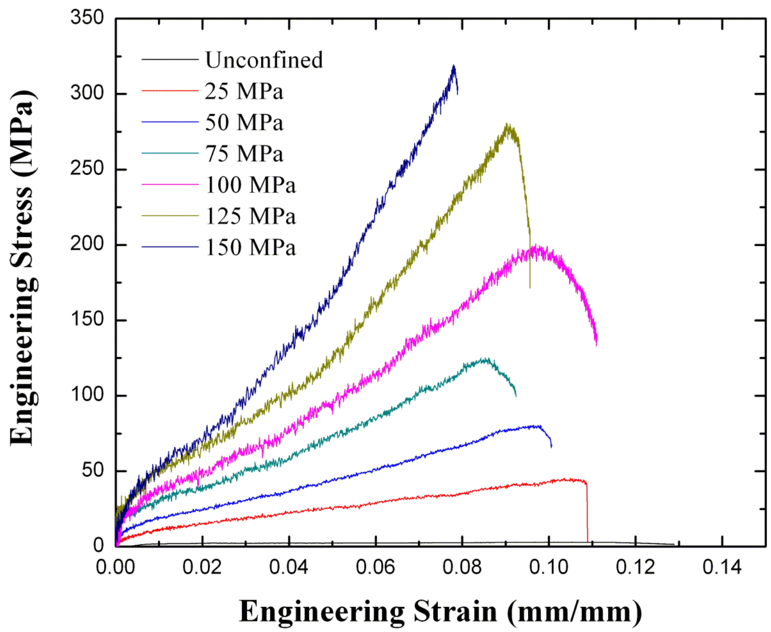
Quikrete® #1961 fine grain sand

- **Dry conditions with a 1.50 g/cc density**
- **Specimens 19.05 mm diameter and 9.3 mm thick**

Experimental Results

Preliminary Variation in Confinement Pressure

Strain-rate: 500s^{-1}

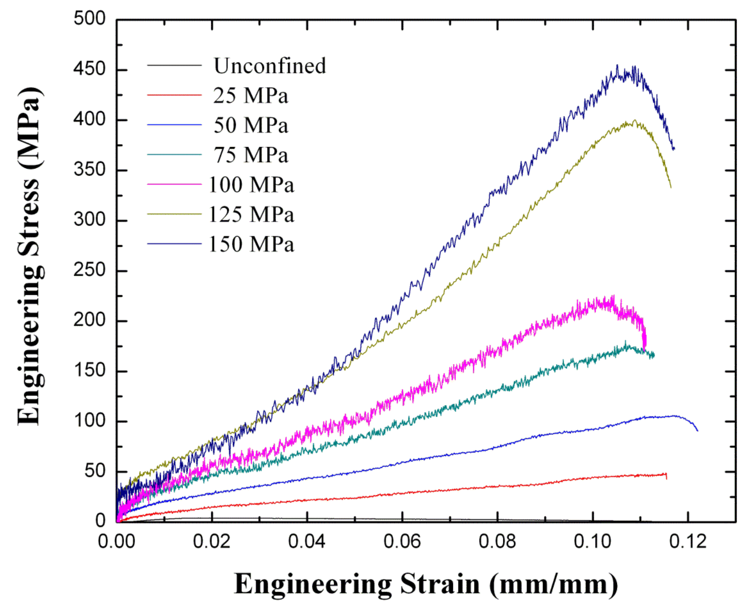


Results provided by Md. E. Kabir
(AAE , Purdue University)

Test Conditions:

- **Quikrete® #1961 fine grain sand**
- **Dry conditions with a 1.50 g/cc density**
- **Specimen 19.05 mm diameter and 9.3 mm thick**

Strain-rate: 1000s^{-1}

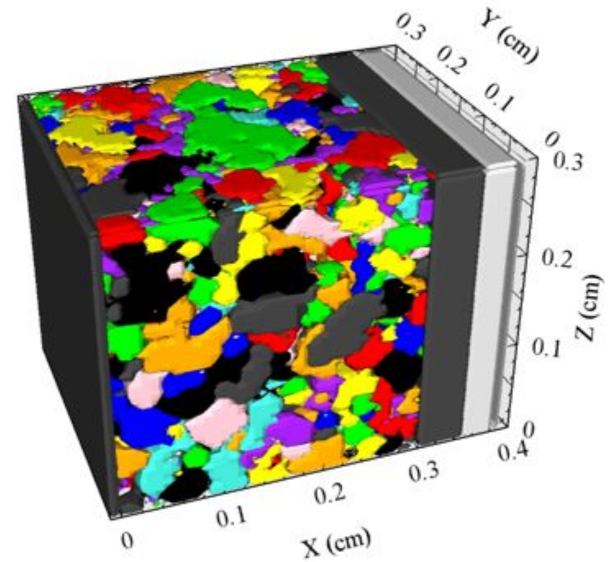


Geometry

<u>EPIC (AFRL)</u>

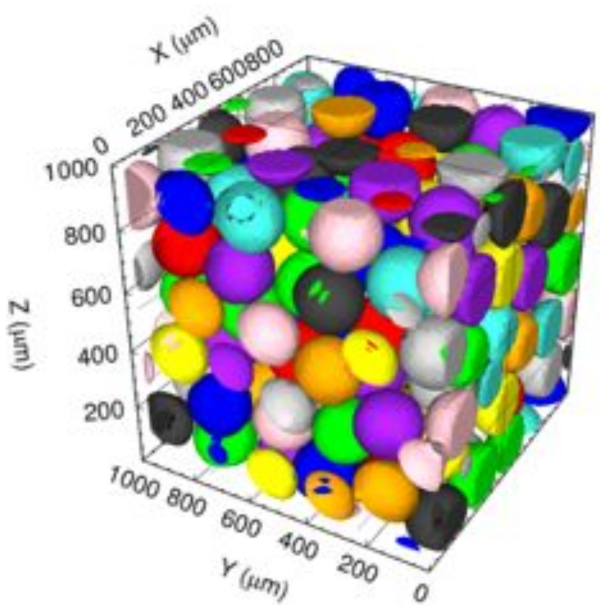
- Parallel
- Lagrangian
- Slide faces resolved

Micro CT scan



<u>CTH (Sandia)</u>

- Massively Parallel
- Eulerian
- Extensive constitutive library

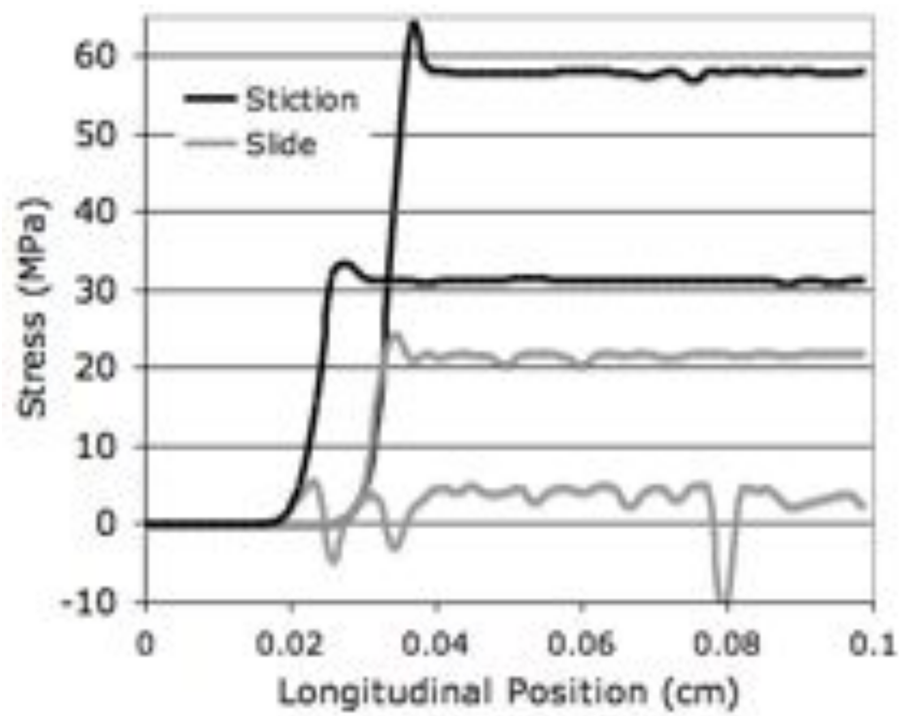


Contrived Realization

<u>EMU (Sandia- Silling and Foster)</u>

- Massively Parallel
- peridynamics
- Constitutive relation under development

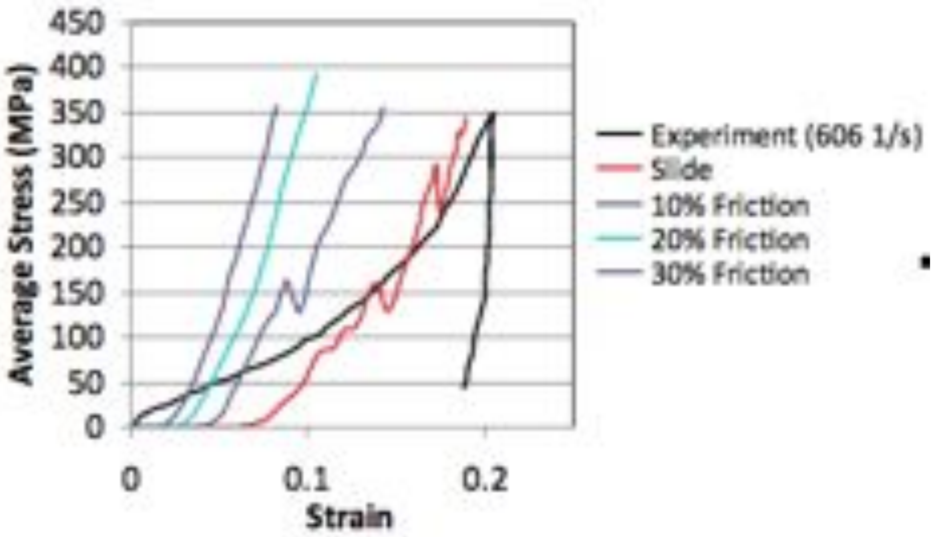
CTH Simulations



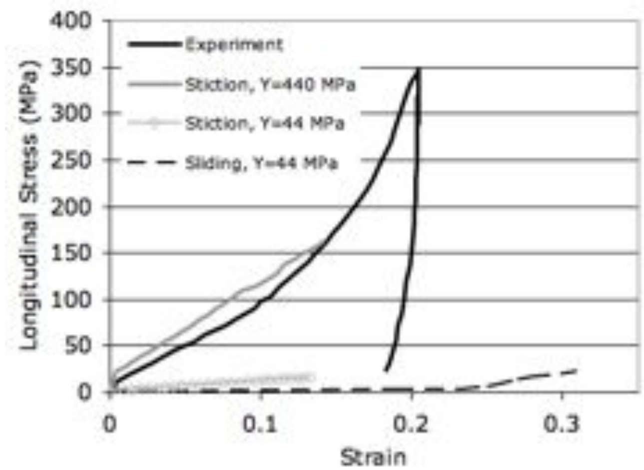
- Since the driver plate speed << bulk sound speed, the target is in equilibrium ahead of the driver plate.
- Justification for small 3D geometry.
- Average stress is extracted for a given longitudinal position (strain)

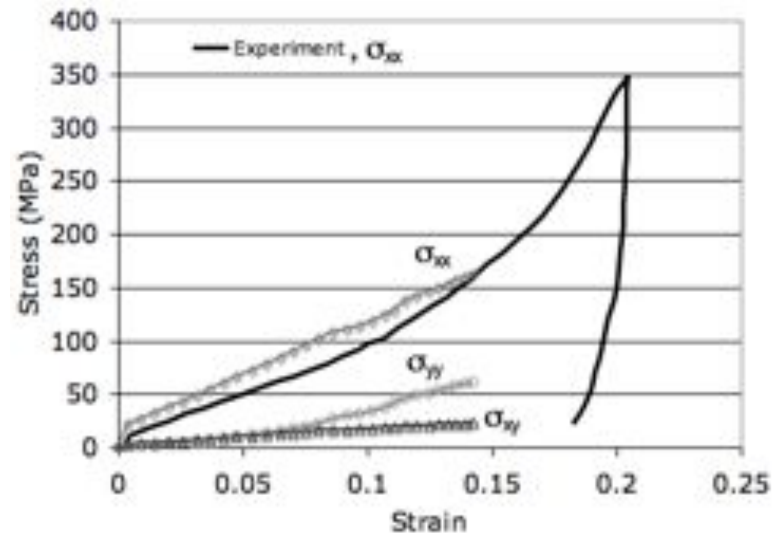
EPIC versus CTH

EPIC



CTH





- CTH best matches the high strain experimental data when there is ***Stiction***
- EPIC best matches the low strain experimental data when there is ***Sliding***

Summary

High Strain Rate

- At high strain rates, 2D stiction and 3D sliding nearly identical for WC Hugoniot response
- Baseline 3D sliding simulations worked best for Sand
- Even if Hugoniot response for 2D and 3D match, other differences remain: rise times, hot spots (?).

Low Strain Rate

- At low strain rate the role of particle boundaries varies.
  - At low strain, stiction is required to match data.
  - At higher strain, particles slide best matches data.

Review

Relevant Publications:

1. Borg, JP and Vogler, TJ, *Mesoscale Simulations of a Dart Penetrating Sand*, **Inter. J. of Impact Eng.**, 35(12) Dec. 2008 pg 1435-1440.
2. Borg, JP and Vogler, TJ, Mesoscale Simulations of a Dart Penetrating Sand, **Inter. J. of Impact Eng.**, 35(12) Dec. 2008 pg 1435-1440.
3. Borg, J.P. and Vogler, T. Mesoscale Calculations of the Dynamic Behavior of a Granular Ceramic. International Journal of Solids and Structures 45 (2008) 1676–1696
4. Borg, JP and Vogler, TJ, The Effect of Water Content on the Shock Compaction of Sand, **The European Physical Journal-Special Topics (accepted)**
5. Borg, JP and Vogler, TJ *Mesoscale Calculations of Shock Loaded Granular Ceramics.* **Shock Compression of Condensed Matter-2007**
6. Vogler, TJ and Borg, JP *Mesoscale and Continuum Calculations of Wave Profiles for Shock-Loaded Granular Ceramics*. **Shock Compression of Condensed Matter-2007**
7. Borg, J., Lloyd, A., Ward, A., Cogar, J.R., Chapman, D., and Proud, W. G., Computational Simulations of the Dynamic Compaction of Porous Media, **Inter. J. of Impact Eng**, 33, pg. 109–118, 2006
8. Borg, J.P., Chapman, D., Tsembelis, K., Proud, W. G., and Cogar, J.R. Dynamic Compaction of Porous Silica Power, **J. Applied Physics**, vol. 98 (7), pg. 073509:1-7, 2005.

Questions?

Granular Mechanics