


Eulerian-Eulerian Two-Fluid Modeling of Non-Spherical Particles Using DEM as a Closure Method to Determine the Deviation from the Kinetic Theory

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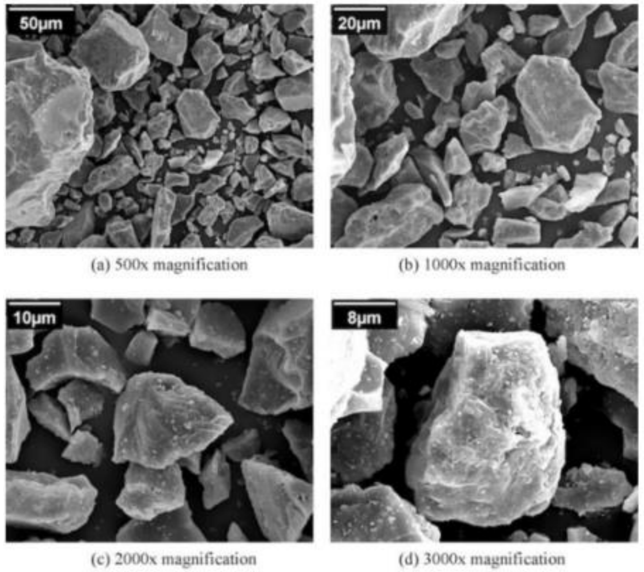
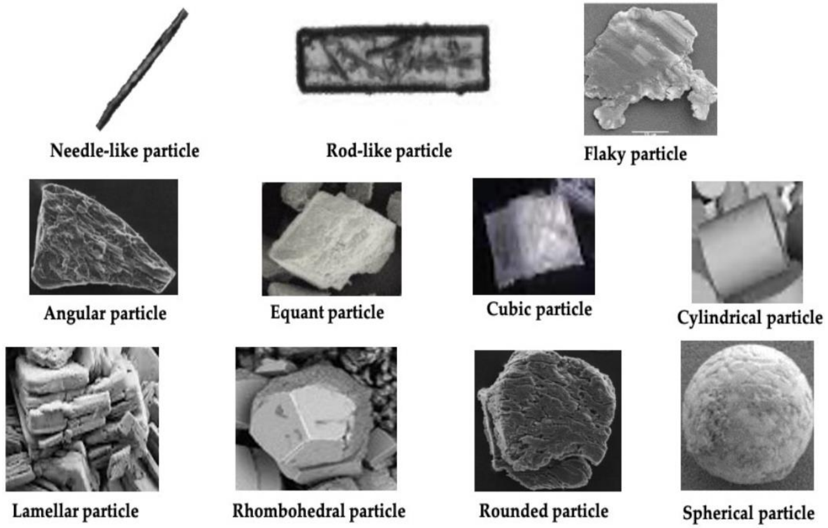
Motivation

- Particle shape has an essential effect on the macroscopic properties of the granular materials, such as packing limit, collisional dissipation energy, shear friction, and flowability
- Most of the computational method assumes spherical particles, although most particles in engineering processes have an irregular shape
  - API
  - Regolith
  - Biomass
- To address the gap between theory and real granular material, the discrete element method (DEM) is applied to investigate the macroscopic properties of granular flows and their applications
- Most industrial processes require the simulation of millions/billions of particles
  - An Eulerian-Eulerian approach is more appropriate for industrial applications



[1]



[2]

[1] Alshibli, K.A. and A. Hasan, *Strength properties of JSC-1A lunar regolith simulant.* Journal of Geotechnical and Geoenvironmental Engineering, 2009. **135**(5): p. 673-679.
[2] Ulusoy, U. A Review of Particle Shape Effects on Material Properties for Various Engineering Applications: From Macro to Nanoscale. *Minerals* **2023**, *13*, 91. https://doi.org/10.3390/min13010091

Material Modeling: LIGGGHTS Discrete Element Method (DEM)

DEM is a Lagrangian method that solves for the motion of each individual particle.

- Tracks position and collisions (particle-particle interactions)
- ***Spherical particles:*** kinetic theory is used to described the mechanical properties of the solid phase.
- ***Non-spherical particles:*** DEM simulations are used to develop constitutive relationships that are incorporated into the large-scale Eulerian-Eulerian gas-granular solvers
  - Normal friction shear stress and cooling rate are required as inputs for Loci/GGFS.

STL/Geometry Particle Properties:
- Shape
- Smooth/Rough
- Flexible/Rigid
- Materials

→

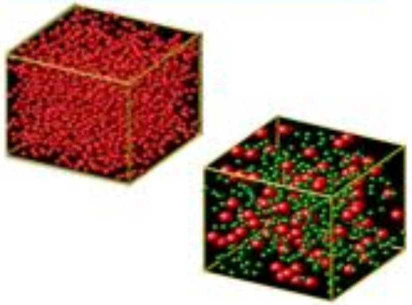
LIGGGHTS DEM Simulations:
- Measure Particle-Particle Interactions
- Obtain Deviation from Theory

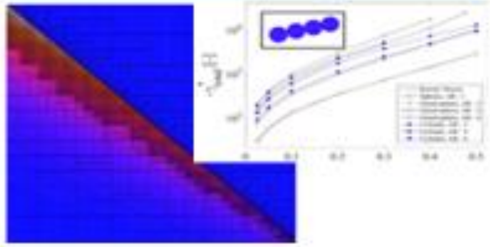
→

DEM Mixture Data:
- Functional Scaling Relations
- Generate Database for use with Multi-dimensional Interpolator

→

CFD Simulations:
- Use Sphere Theory for Polydispersity
- Use DEM Data to Introduce Deviations from Theory in Models

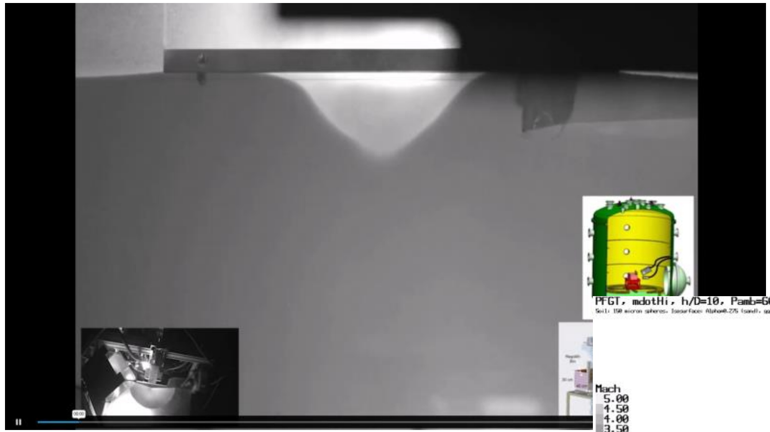




CFD Modeling: Loci/GGFS (Gas-Granular Flow Solver)

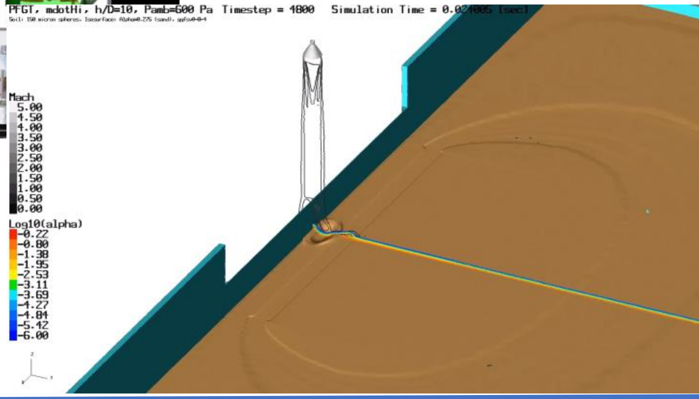
Features of Loci/GGFS:

- Unstructured Implicit Finite Volume—2nd Order Accuracy Space/Time
- Adaptive-Mesh-Algorithm Refinement
- Moving-Mesh 6-DOF for complex moving geometry.
- State-of-the-art gas-particle, particle-particle, and turbulence models
- Full (Garzo-Hrenya-Dufty, GHD) and pseudo-polydisperse granular model capabilities with GPGPU acceleration
- **Irregular shape effects:**
  - Discrete Element Method-informed irregular-shaped particle-particle interaction models
  - Nonspherical gas-particle models (Drag/etc)
- Highly-parallelizable framework with excellent scalability
- Forward-Automatic Differentiation (FAD) for Runtime Uncertainty Quantification and Sensitivity Analysis
- GPGPU-enabled solvers



(Above) A 12-second vacuum chamber experiment with 150 micron single-size glass-sphere particle mixture that was used for validation of Loci/GGFS. The movie shows the crater formation viewed through the transparent viewing pane which is centered on the plume. *Jeff West, Manuel Gale, NASA/Marshall*

(Below) Validation (first 2 seconds) simulation performed with Loci/GGFS of experiment on shown on the left. *Jeff West, Manuel Gale, NASA/Marshall*



Insight Lander Simulation with 250M Cells on 3k Cores. Courtesy of MSFC/ER42 ESSCA

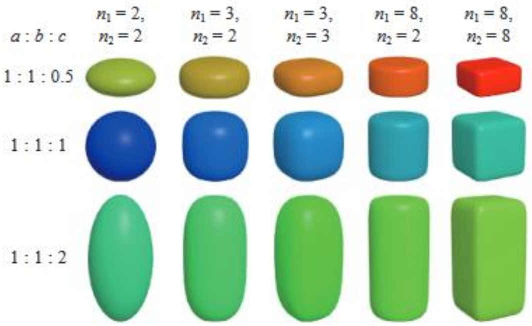
DEM Non-Spherical Particles using the Superquadric and Multisphere Method

Superquadric method

- The particle shape is defined with the following equation [1]:

$$f(x) = \left(\left|\frac{x}{a}\right|^{n2} + \left|\frac{y}{b}\right|^{n2} \right)^{\frac{n1}{n2}} + \left|\frac{z}{c}\right|^{n1} - 1 = 0$$

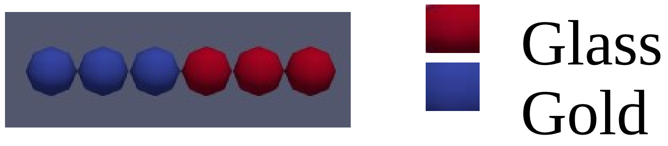
- The superquadric equation can describe ellipsoidal particles, cylindrical particles, and box-like particles
- Use an iterative method for collision detection
- Other shapes cannot be simulated with this method



[3]

Multisphere method

- The particle is represented as a clump of spherical particles
- An STL file of the particle is used to generate the clump
- Bimaterial multisphere can be simulated
- Simple collision detection compared to the Superquadric method
- For flat and elongated particles, a considerable number of spheres is needed for an accurate representation

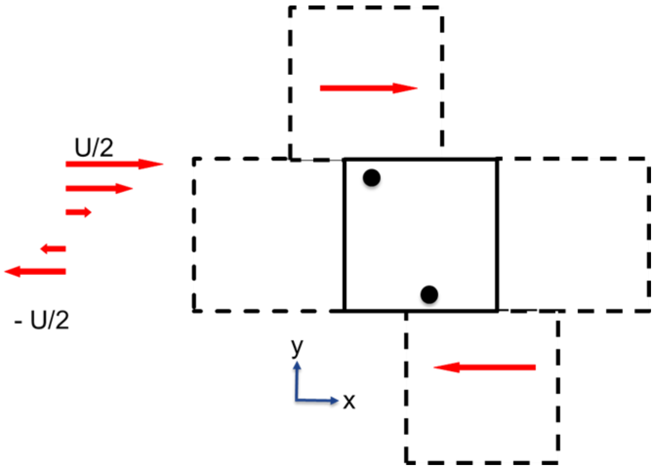


[1] Barr, *Superquadrics and Angle-Preserving Transformations.* IEEE Computer Graphics and Applications, 1981. **1**(1): p. 11-23.
[2] Podlozhnyuk, A., Pirker, S. & Kloss, C. Efficient implementation of superquadric particles in Discrete Element Method within an open-source framework. *Comp. Part. Mech.* **4**, 101–118 (2017).
[3] Wang ,S., Marmysh D., Ji, D.Construction of irregular particles with superquadric equation in DEM, Theoretical and Applied Mechanics Letters, Volume 10, Issue 2, 2020, 68-73,ISSN 2095-0349

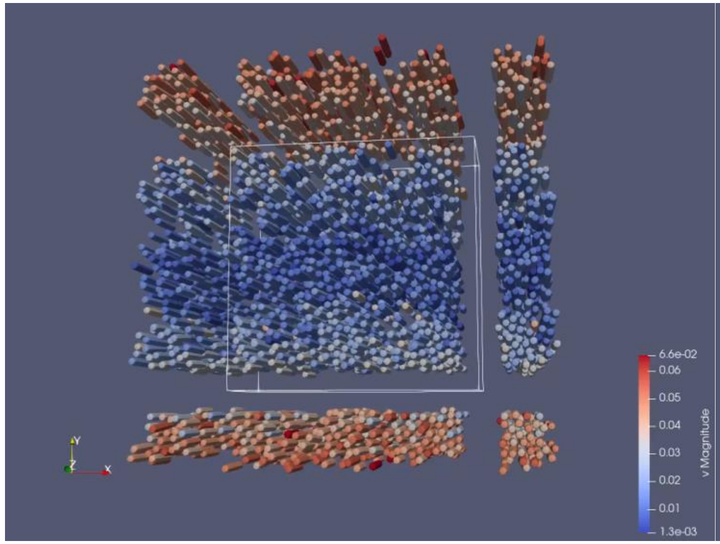
DEM Simulation Set-Up

- Cooling simulations are used to determine the collisional dissipation rate
- Lees-Edwards [1] boundaries are used to produce a shear flow in the shear simulations
  - The shear properties are determined at steady state
- MPI parallelization in both simulations
- Mechanical properties are determined as a function of the solid volume fraction

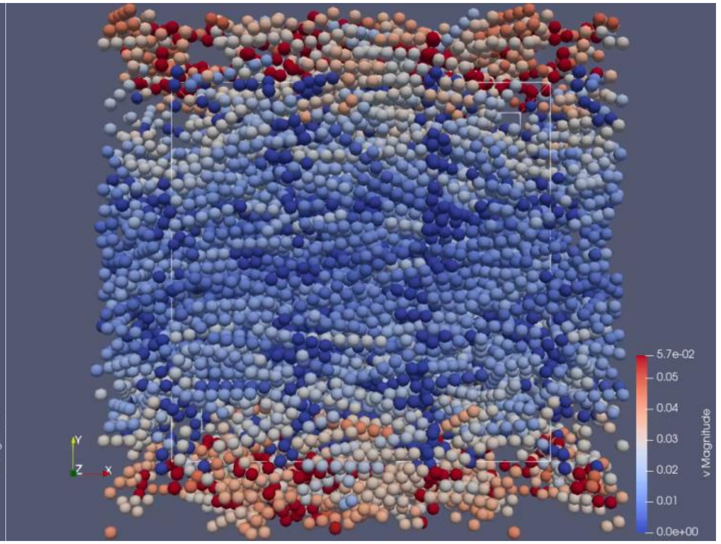
Lees-Edwards boundaries



Superquadric method



Multisphere method



[1]Lees, A. W. & Edwards, S. F. 1972 The computer study of transport processes under extreme conditions. *J. Phys. C: Solid State Phys.* **5**, 1921–1929.

Verification Case with the Multisphere Method

- The pressure and normal shear stress for smooth inelastic sphere in a shear plane are given by[1]:

$$\sigma_{yy}^{N}=\frac{\sigma_{yy}}{\rho d_p^2\gamma^2}=\frac{5\pi}{4608}\frac{F(v,e)}{\eta(1-\eta)vg_0}(1+4\eta v g_0)$$

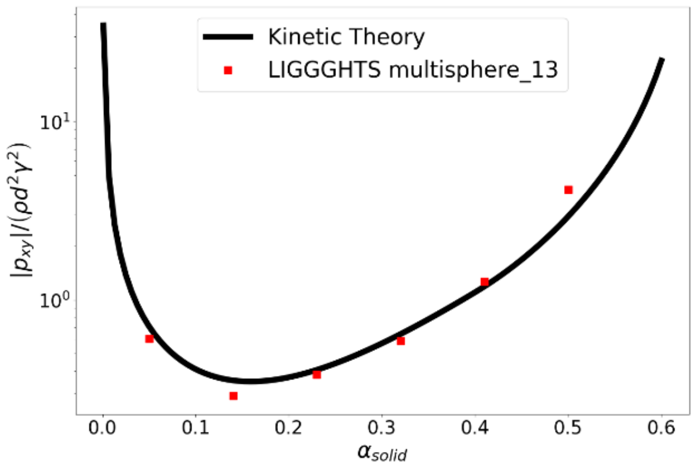
$$\sigma_{xy}^{N}=\frac{\sigma_{xy}}{\rho d_p^2\gamma^2}=-\frac{5\pi}{4608}\frac{F(v,e)}{v}\sqrt{\frac{5}{2}\frac{F(v,e)}{\eta(1-\eta)g_0}}$$

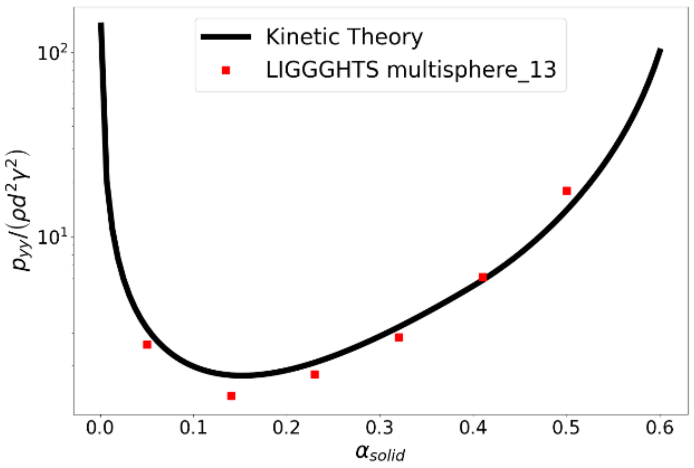
- Collisional dissipation rate

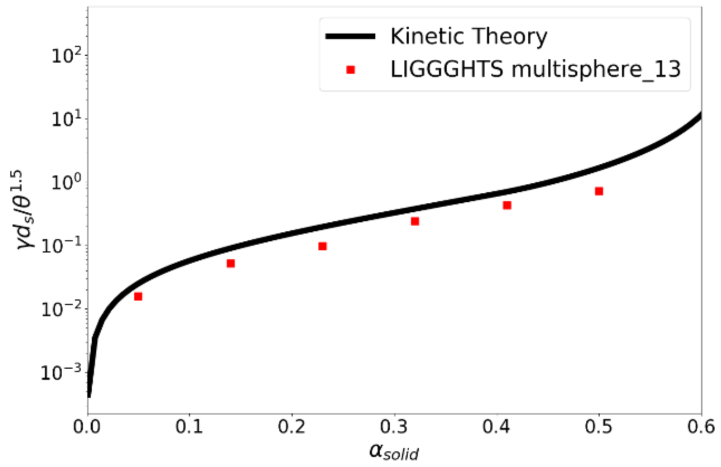
$$\Gamma=\rho\frac{12}{\pi^{\frac{1}{2}}}v^2g_0(1-e^2)\frac{T^{3/2}}{d_p}$$

Case a multisphere representation of a sphere

Results match the kinetic theory





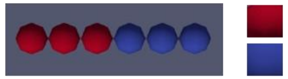


[1] Lun, C. K. K., Savage, S. B., Jeffrey, D. J. & Chepurniy, N. 1984 Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flow field. *J. Fluid Mech.* **140**, 223–256

DEM: Shear properties of Non-Spherical Particles

Cylinder A.R. = 6

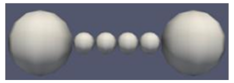
Rod A.R. = 6



Glass

Gold

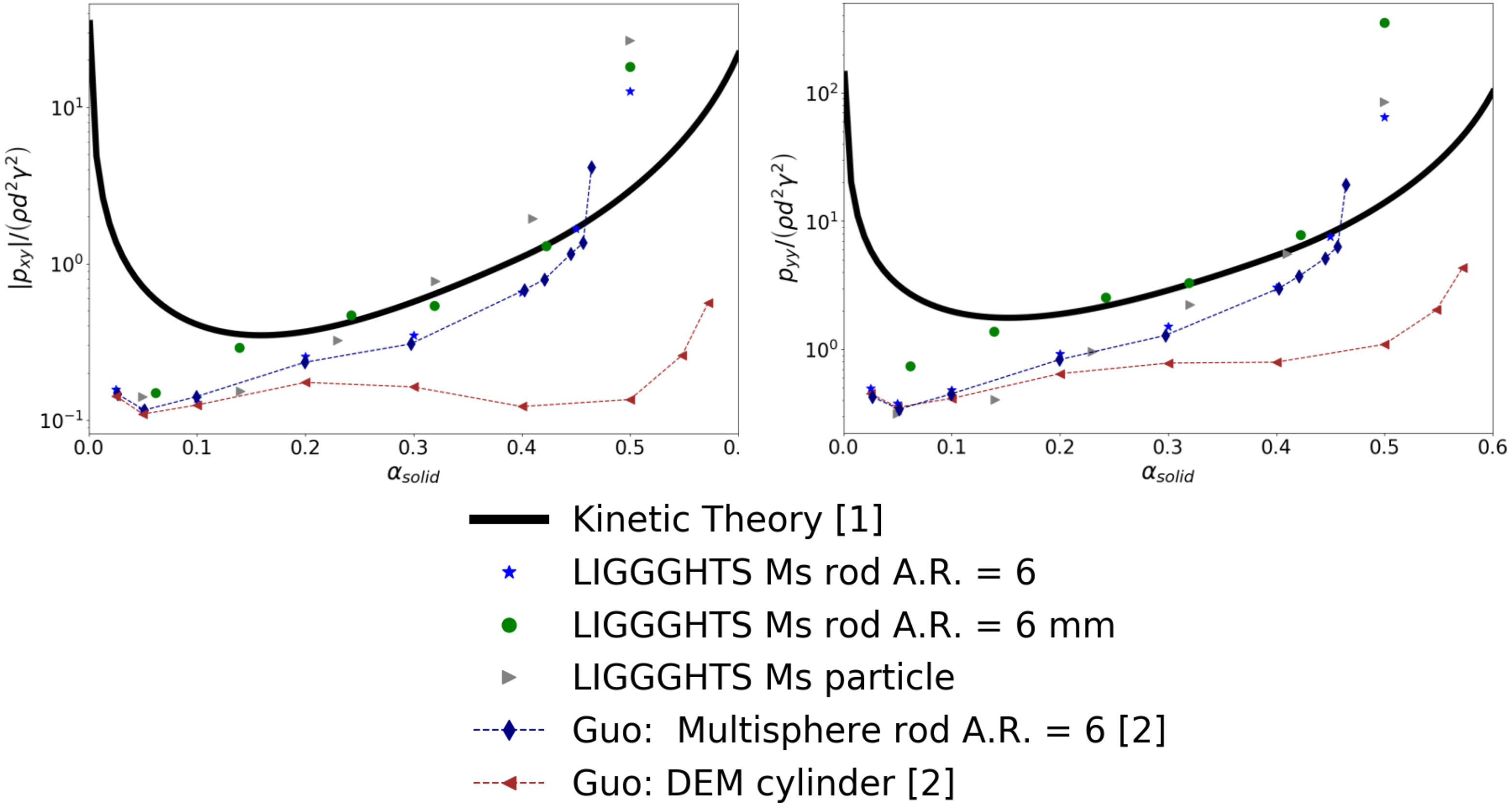
Multisphere test particle



-The results of the multisphere rod with A.R =6 match well the results reported by Guo et al. [2]

- The multi-material rod and the Ms test particle show a higher shear than the rod with A.R = 6
- Multisphere particles show higher stresses compared to the kinetic theory at high solid volume fraction

Multisphere Method



[1] Lun, C. K. K., Savage, S. B., Jeffrey, D. J. & Chepurniy, N. 1984 Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flow field. *J. Fluid Mech.* **140**, 223–256

[2] Guo, Y., et al. (2012). "A numerical study of granular shear flows of rod-like particles using the discrete element method.“. *J. Fluid Mech.* **713**,1-26

[3] Guo, Y., et al. (2013). "Granular shear flows of flat disks and elongated rods without and with friction." Physics of Fluids **25**(6).

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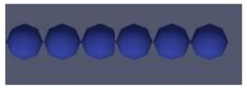
DEM: Shear properties of Non-Spherical Particles

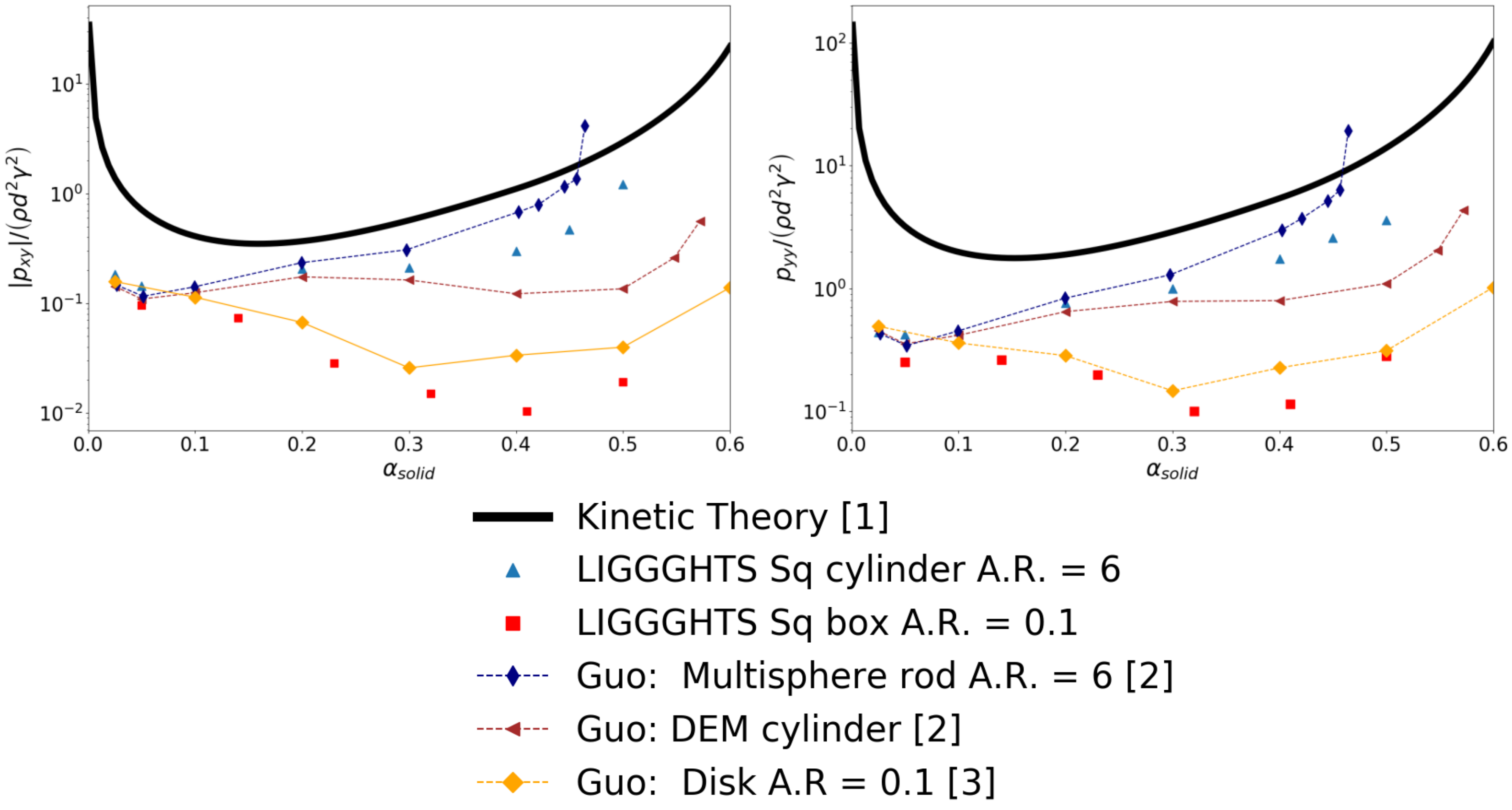
Cylinder A.R. = 6

Rod A.R. = 6



Sq. box A.R= 0.1

Superquadric Method



-The superquadric cylinder shows stresses in between the multisphere and the DEM cylinder representation of rod 6

-The box-like particles show lower stresses than the disk

-The superquadric particles generally show lower stresses compared to the kinetic theory

[1] Lun, C. K. K., Savage, S. B., Jeffrey, D. J. & Chepurniy, N. 1984 Kinetic theories for granular flow: inelastic particles in Couette flow and slightly inelastic particles in a general flow field. *J. Fluid Mech.* **140**, 223–256

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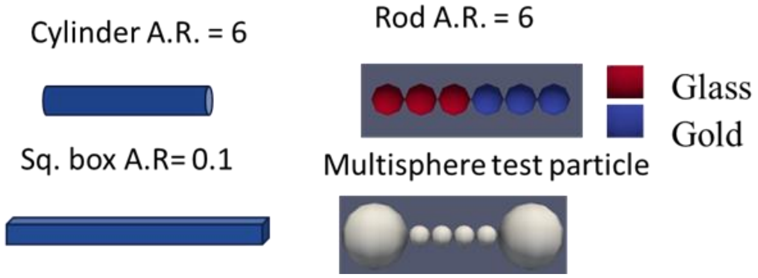
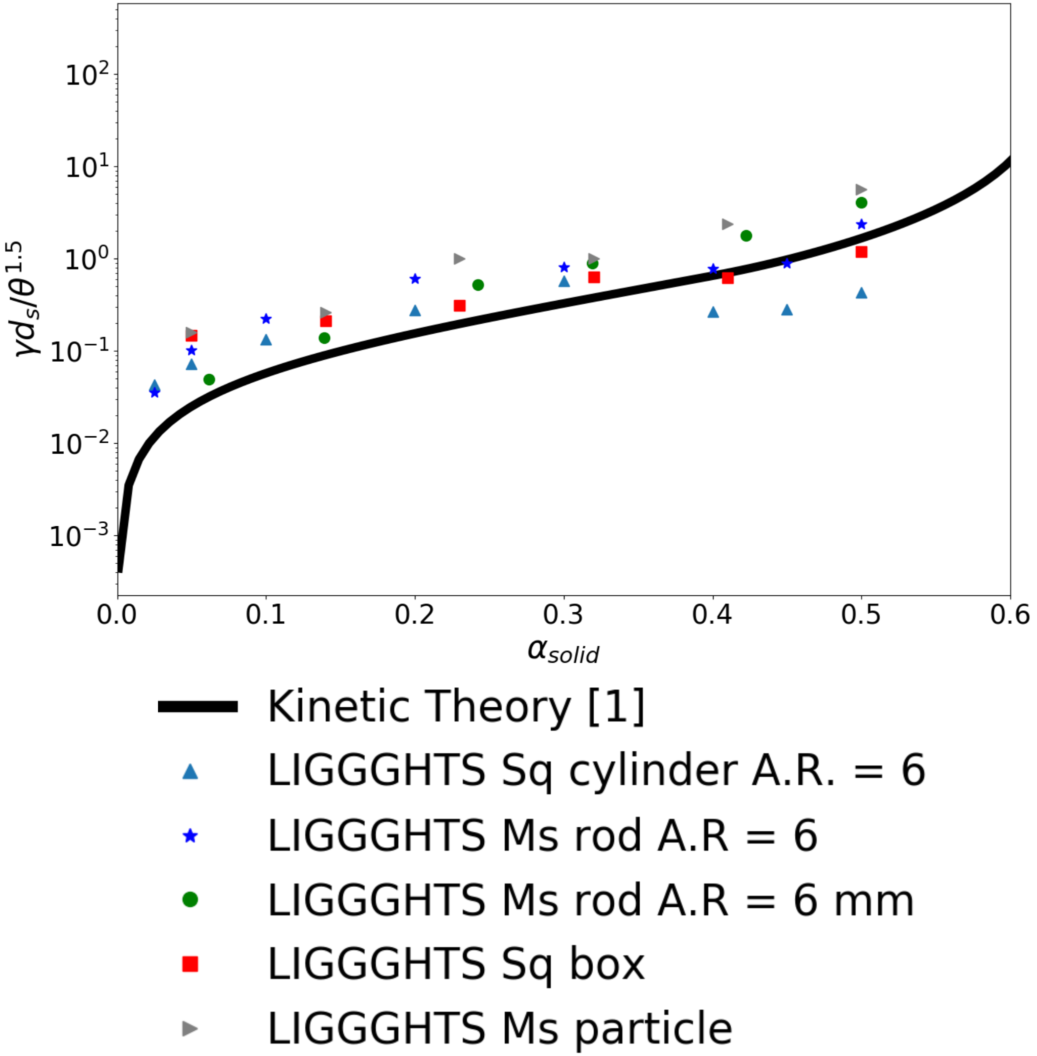
[3] Guo, Y., et al. (2013). "Granular shear flows of flat disks and elongated rods without and with friction." Physics of Fluids **25**(6).

DEM: Collisional Dissipation Rate of Non-Spherical Particles



-At low solid volume fraction, the collisional dissipation rate is higher in the non-spherical particles compared to the kinetic theory



Applying the DEM Derived Mechanical Properties to an Eulerian-Eulerian Method

Drag Laws for Non-Spherical Particles

- The drag of the sphere $C_{D,Sphere}$ was determined with the Loth's Drag Law [1] due to compressibility and/or rarified (local to the particle) conditions
- For non-spherical particles, the drag can be defined given as a function of the shape factor $\Psi = \frac{\Phi}{\mathrm{X}}$, or the ratio of sphericity to circularity and any spherical drag law [2]:

$$C_D = \frac{C_{D,Sphere}}{Re^2 \Psi^{\mathrm{Re}^{-0.23}}} \left(\frac{Re}{1.1883}\right)^{\frac{1}{0.4826}} \quad Re < 50$$

$$C_D = \frac{C_{D,Sphere}}{Re^2 \Psi^{\mathrm{Re}^{0.05}}} \left(\frac{Re}{1.1883}\right)^{\frac{1}{0.4826}} \quad Re > 50$$

with

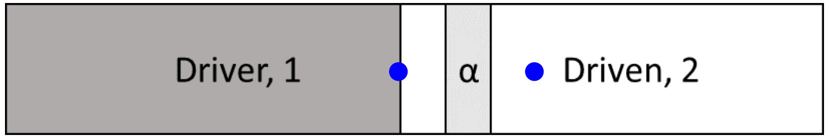
$$\boldsymbol{F}_D = \frac{1}{2} \rho C_D A |u - u_s| (u - u_s)$$

- For multiparticle systems, we use Osnes's modification [3] to account for local compressibility/Mach effects

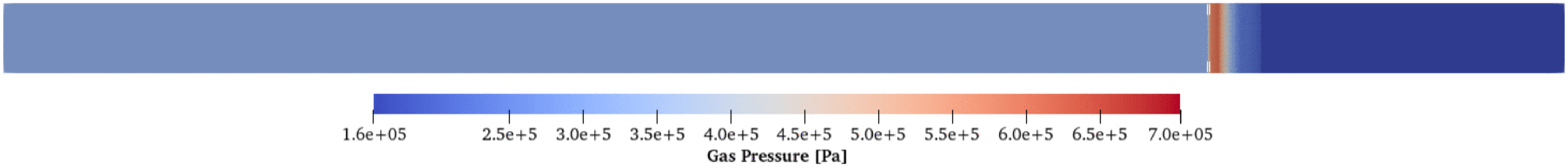
[1] Loth, Eric, John Tyler Daspit, Michael Jeong, Takayuki Nagata, and Taku Nonomura. "Supersonic and hypersonic drag coefficients for a sphere." *AIAA journal* 59, no. 8 (2021): 3261-3274.
[2] Dioguardi, F., D. Mele, and P. Dellino. "A new one-equation model of fluid drag for irregularly shaped particles valid over a wide range of Reynolds number." *Journal of Geophysical Research: Solid Earth* 123, no. 1 (2018): 144-156.
[3] Osnes, Andreas Nygård, Magnus Vartdal, Mehdi Khalloufi, Jesse Capecelatro, and Siva Balachandar. "Comprehensive quasi-steady force correlations for compressible flow through random particle suspensions." *International Journal of Multiphase Flow* 165 (2023): 104485.

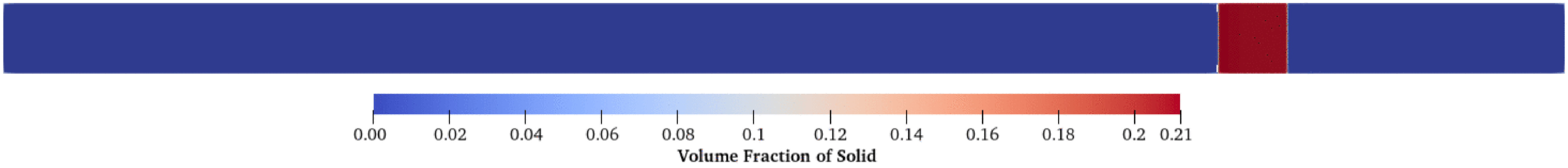
Demonstration of Non-spherical Models: Shock-Particle Curtain

- Shock Particle Curtain experiment from Wagner
  - Exercises most models required in relevant-PSI problems due to compressible gas-particle interactions
  - Well studied for model validation and model development
- $\alpha = 0.21, 0.44$ (solid volume fraction)
- Shock initial position 3 mm upstream of curtain
- Comparison of gas pressure and gas/solid velocities at $\tau = 0.334, 1.334, and\ 2.334$ (non-dimensional time until the shock passes through the curtain)
- $\tau = \frac{t-t_0}{\tau_L}, \tau_L = \frac{L_{pc}}{M_s\sqrt{\gamma\frac{p_0}{\rho_0}}}$



$$\begin{Bmatrix} \rho_{g,1} & p_{g,1} & u_{g,1} \\ \rho_{g,2} & p_{g,2} & u_{g,2} \end{Bmatrix} = \begin{Bmatrix} 2.131 & 2.177 & 0.881 \\ 1 & 0.714 & 0 \end{Bmatrix}$$





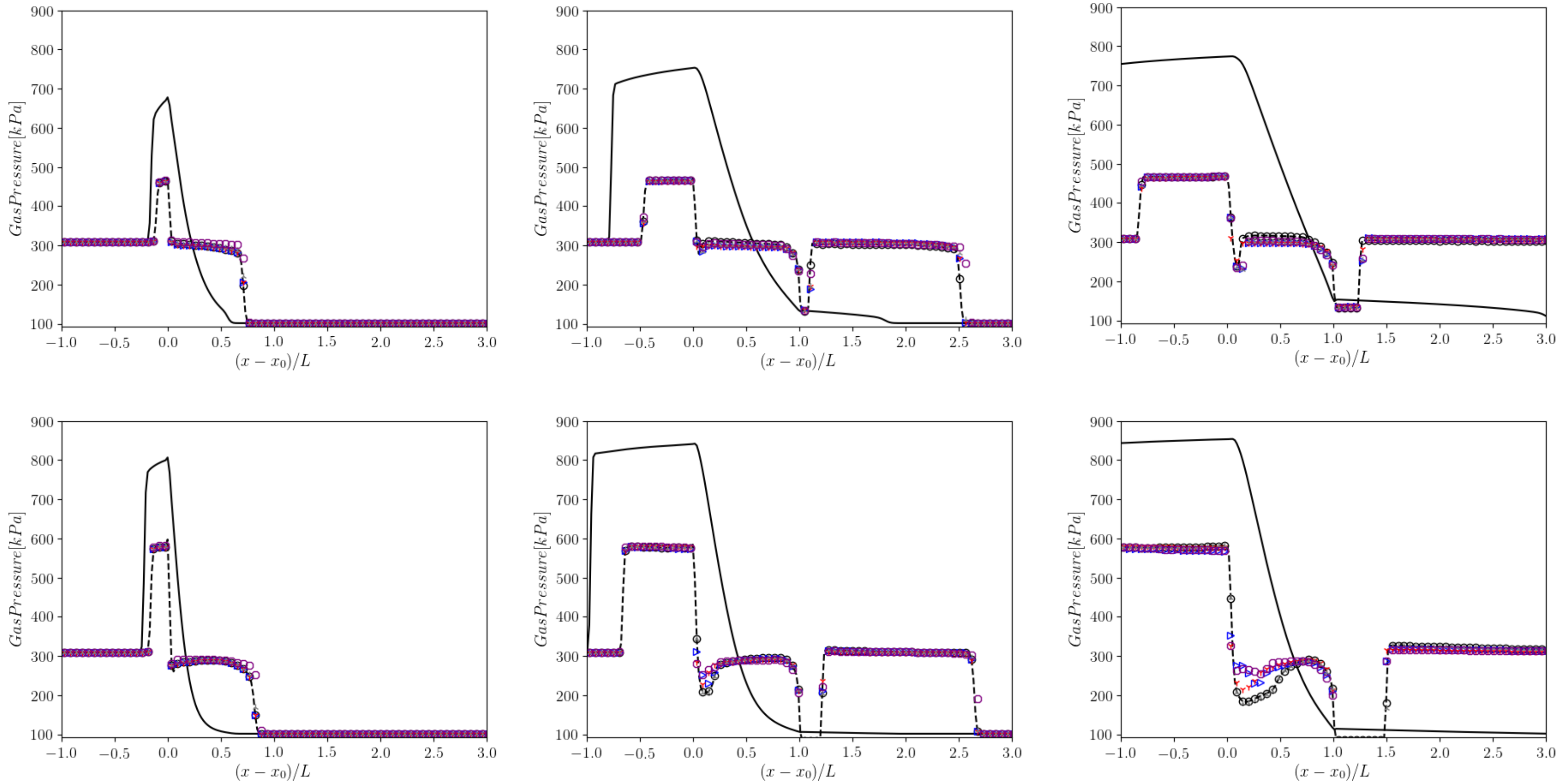
Wagner, J.L., et al., *A multiphase shock tube for shock wave interactions with dense particle fields*. Experiments in fluids, 2012. **52**(6): p. 1507-1517.

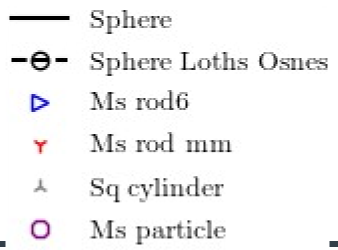
Shock Tube Results: Gas Pressure

$\tau = 0.334$ $\tau = 1.334$ $\tau = 2.334$

$\alpha = 0.21$

$\alpha = 0.44$





-The Loth's Drag Law and Osnes modification significantly impact the gas pressure
- For sphere, the permeability relationship of Ergun not account for the compressibility of the gas within the particle bed
-The pressures show that the resulting blockage is more significant in high shear cases than to spheres Loths Osnes and Sq cylinder.

The sphere case use Henderson [1] and Ergun permeability correction for multiparticle systems [2]

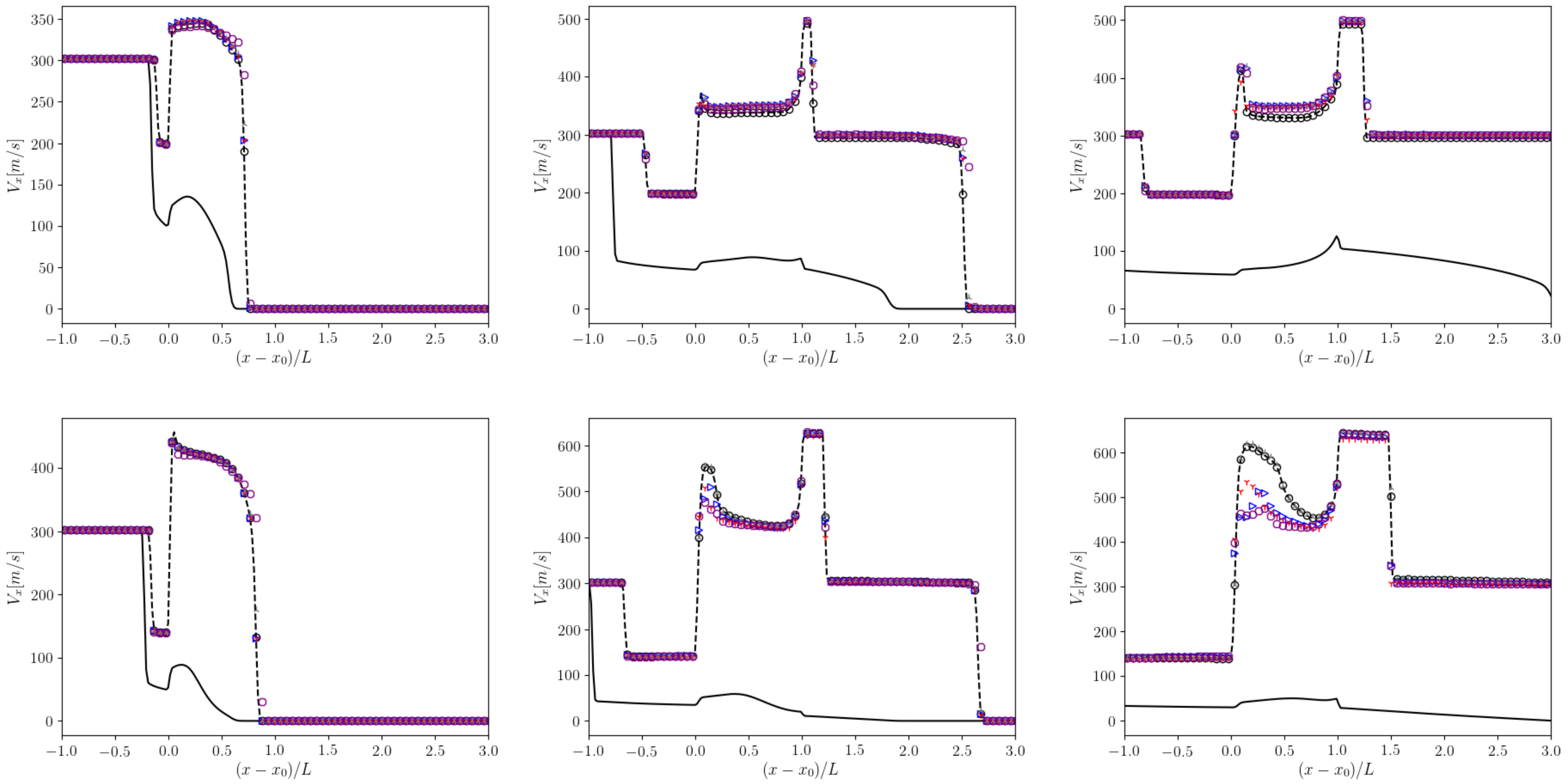
[1] Henderson, C. B., "Drag Coefficients of Spheres in Continuum and Rarefied Flows," AIAA Journal, Vol. 14, No. 6, 1976, pp. 707–708.
[2] Sabri Ergun and A. A. Orning.*Industrial & Engineering Chemistry* **1949** *41* (6), 1179-1184. DOI: 10.1021/ie50474a011

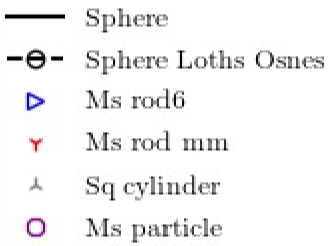
Shock Tube Results: Gas Velocity

$\tau = 0.334$ $\tau = 1.334$ $\tau = 2.334$

$\alpha = 0.21$

$\alpha = 0.44$





-At low solid volume fraction $\alpha = 0.21$, the non-spherical particle has a negligible effect on the gas velocity

-Non-spherical particles produce a lower gas velocity at a high solid volume fraction than the sphere case with Loth's-Osnes modifications

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[1] Henderson, C. B., "Drag Coefficients of Spheres in Continuum and Rarefied Flows," AIAA Journal, Vol. 14, No. 6, 1976, pp. 707–708.

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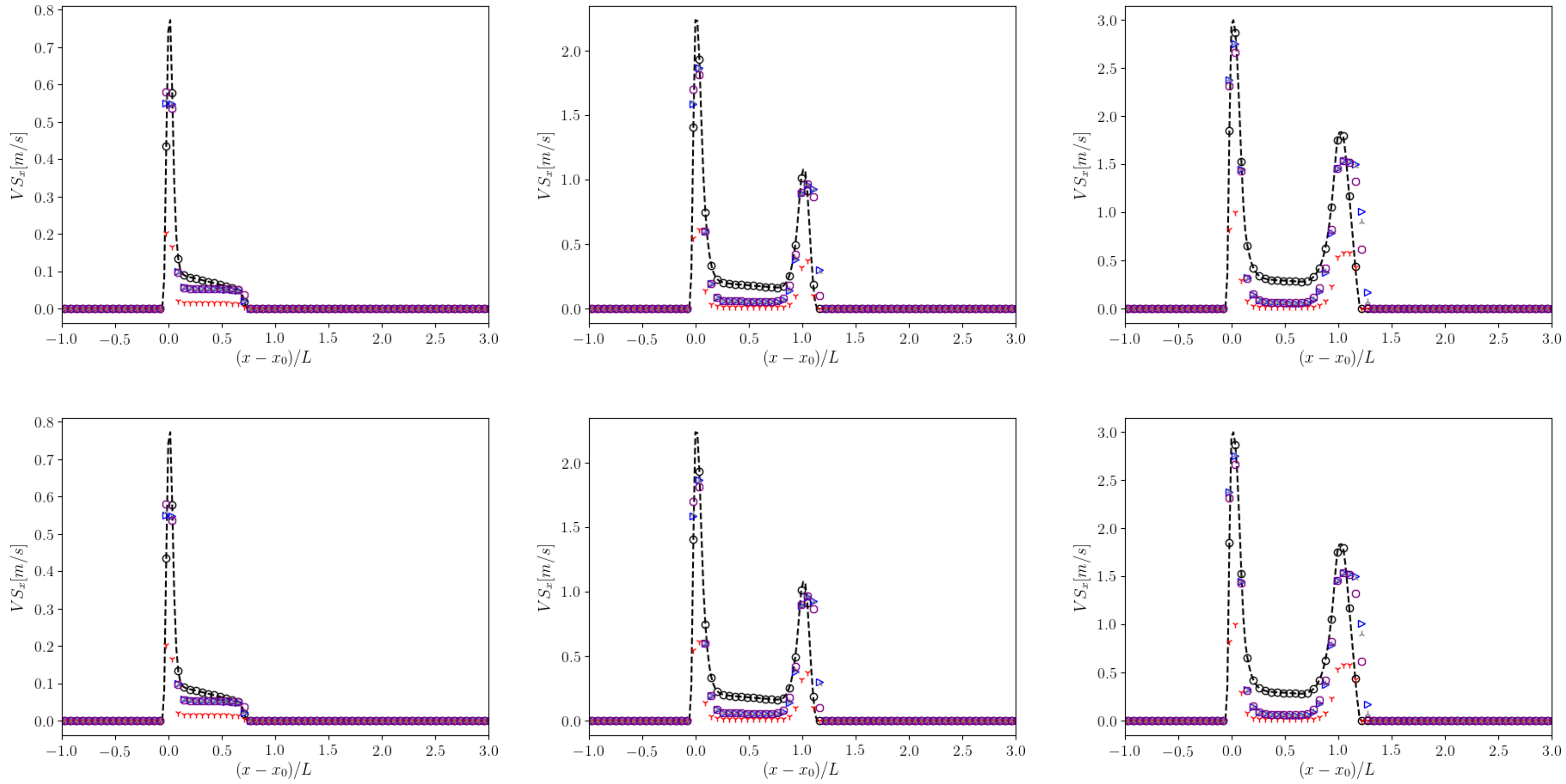
Shock Tube Results: Solid Velocity

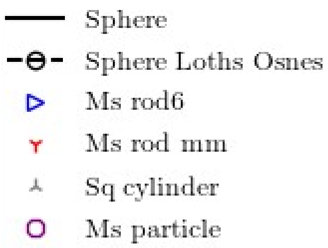
$\tau = 0.334$ | $\tau = 1.334$ | $\tau = 2.334$

$\alpha = 0.21$

$\alpha = 0.44$



-In general, the non-spherical particles shows a lower solid velocity in the particle bed compared to spheres.



Conclusions and Future Work

- We use the DEM Superquadric and the multisphere method to determine the mechanical properties of non-spherical particles
  - Compared results with existing literature and the kinetic theory
- Incorporation of the derived mechanical properties to an Eulerian-Eulerian (two fluid) method approach in a shock tube case
  - Two volume fractions were investigated
  - The gas pressure, the solid and gas velocity were compared to the sphere case
- Future work
  - Implement the polyhedral method in LIGGGHTS
  - Determine the circularity using the shear simulations
  - Verification case in the non-compressible regime
    - Fluidized bed case