DEM for Non-Spherical Particulate Systems

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2019 NETL Workshop on Multiphase Flow Science
August 6-8, 2019

Outline

1. Background and Motivation
2. Objectives of Research
3. Geometry Definition
4. Collision Detection
5. Collision Resolution
6. Results and Discussion
7. Summary & Conclusions

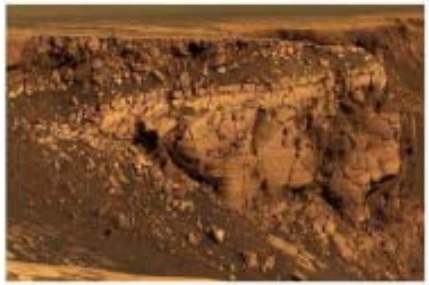
Model Development

Background and Motivation

- **Modelling of particulate systems have mostly been carried out by approximating the particles as spheres**
  - **Easier and more cost-effective to simulate**
- **However, with advancements in computational capability, building non-spherical particle models may provide improved fidelity and accuracy.**

Non-spherical Particle Systems

- **Understanding the fluid - solid interaction is integral for the design and control of many processes**


Rock accumulation


ore roasting


Mineral conveying


Grain drying


Biomass/waste combustion/gasification


Garbage grinding


Tablet coating


Airborne particle inhalating

Red blood cell flowing

Different Types of Biomass Feedstock for Gasification

Objectives of Research

- **To develop a non – spherical DEM model and couple it with a fluid flow solver**

Geometry Definition

- Define non – spherical particles

Collision Detection & Resolution

- Detect collisions
- Resolve collisions using appropriate resolution models

Coupled CFD- DEM model

- Parallel implementation
- Couple developed DEM model with flow solver GenIDLEST

Validation

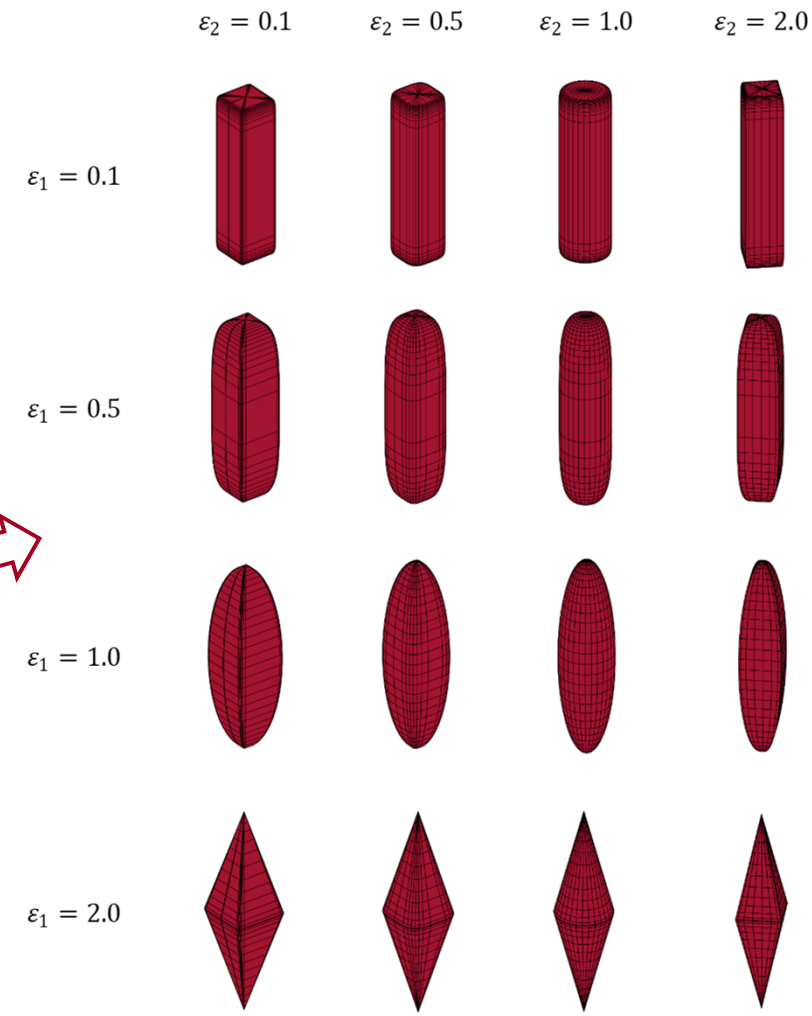
- Validate functioning of DEM model
- Validate coupled CFD-DEM model's functioning

Geometry Definition

- **Non – spherical particulate shapes**
  - **Superellipsoids are generated**
  - **Surface defined by both continuous and discrete function representations**
- **Continuous function representation (CFR) defines a surface, usually, in the particle's local coordinate system**

$$\left(\left(\frac{x}{a_1}\right)^{2/\varepsilon_2} + \left(\frac{y}{a_2}\right)^{2/\varepsilon_2}\right)^{\varepsilon_2/\varepsilon_1} + \left(\frac{z}{a_3}\right)^{2/\varepsilon_1} = 1$$

- **Disadvantage : collision detection and resolution algorithms are computationally intensive**



Geometry Definition…….

- **It is easier to model a superellipsoid with a Discrete Function Representation (DFR)**

$$x = a_1 * sgn(\cos\varphi_1) * |\cos\varphi_1|^{\varepsilon_2} * |\cos\varphi_2|^{\varepsilon_1}$$
$$y = a_2 * sgn(\sin\varphi_1) * |\sin\varphi_1|^{\varepsilon_2} * |\cos\varphi_2|^{\varepsilon_1}$$
$$z = a_3 * sgn(\sin\varphi_2) * |\sin\varphi_2|^{\varepsilon_1}$$

- **'φ_1' varies from $-\pi$ to π and 'φ_2' varies from $-\frac{\pi}{2}$ to $\frac{\pi}{2}$**

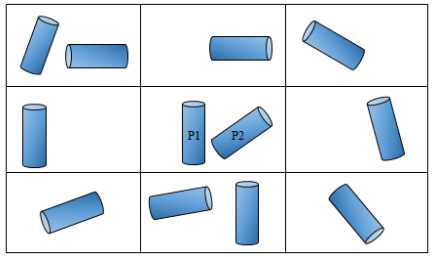
  - **DFR is preferred to CFR as the solutions when detecting collisions are guaranteed and unique**
  - **DFR is used to generate superellipsoids in this work**

Collision Detection – Particle - Particle

- **Collision detection - determining if two objects are in contact or have interpenetrated each other**
- **Three levels in the hierarchy of collision detection**

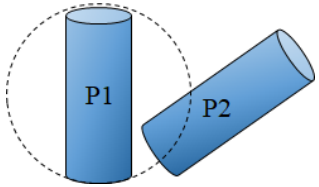
Level 1

Binning particles into separate computational cells



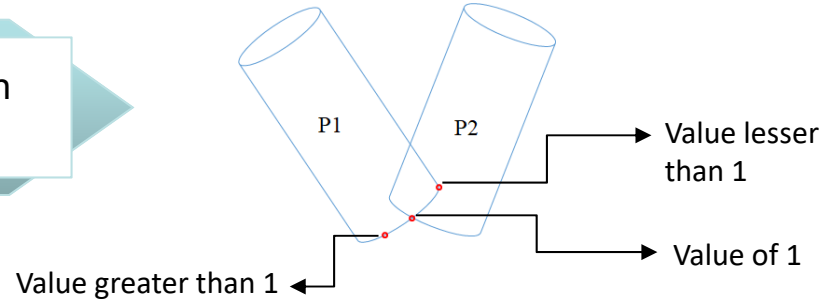
Level 2

Particles falling under a sphere of influence comprise the respective neighborhood list



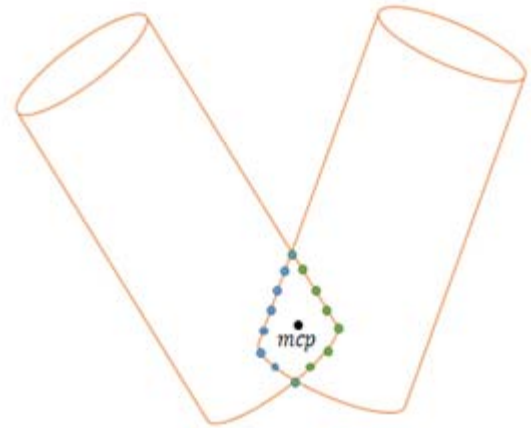
Level 3

Surface coordinates of one particle are evaluated with respect to the surface function of the other particle



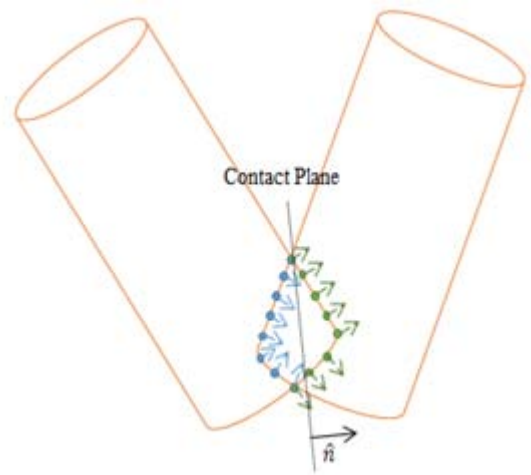
Collision Detection – Particle - Particle…contd.

- **For collision modeling, the collision detection algorithm is supplemented by information about the collision**



- **Contact point**
  - Point of application of collision force
  - Geometric center of the overlapping volume

- **Contact normal**
  - Direction of application of collision force
  - Averaged surface normal of all colliding vertices

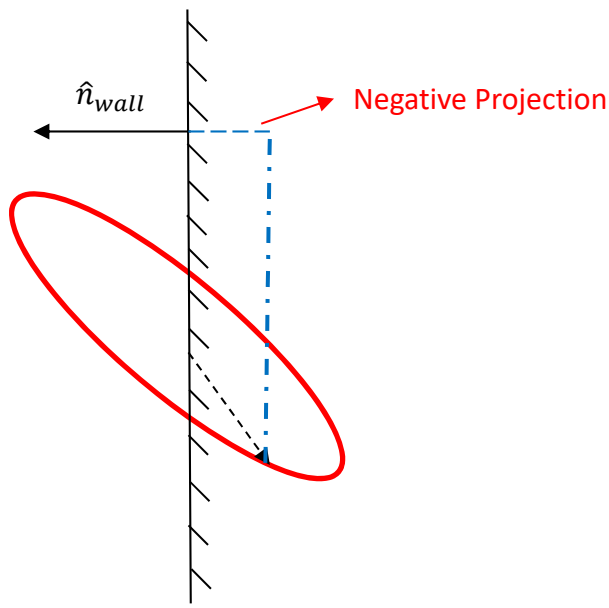


- **Penetration depth**
  - Calculation of collision force in time-driven collision model
  - Maximum projection distance between any two colliding vertices on surface normal

Collision Detection – Particle-wall

- **A novel collision detection technique is implemented**
  - **Based on computational geometry**
  - **Information about the wall normal is available**

- **The vector between wall node and each of the surface vertices is projected along the wall normal**



Collision Resolution – Hard Sphere – Normal Impact

Event – driven model :

- **A binary impulse based model is used to update the trajectories** $\vec{j_r} = \int \vec{F_r}\, dt$
- **Magnitude of impulse :**

$$j_r = \frac{-(1+COR) * (\vec{V}_{r,pre} \,.\, \hat{n})}{\frac{1}{m_1} + \frac{1}{m_2} + \left(\left(\left(\bar{\bar{I}}_1^{-1} * (\vec{r}_1 \times \hat{n})\right) \times \vec{r}_1\right) + \left(\left(\bar{\bar{I}}_2^{-1} * (\vec{r}_2 \times \hat{n})\right) \times \vec{r}_2\right)\right) \,.\, \hat{n}}$$

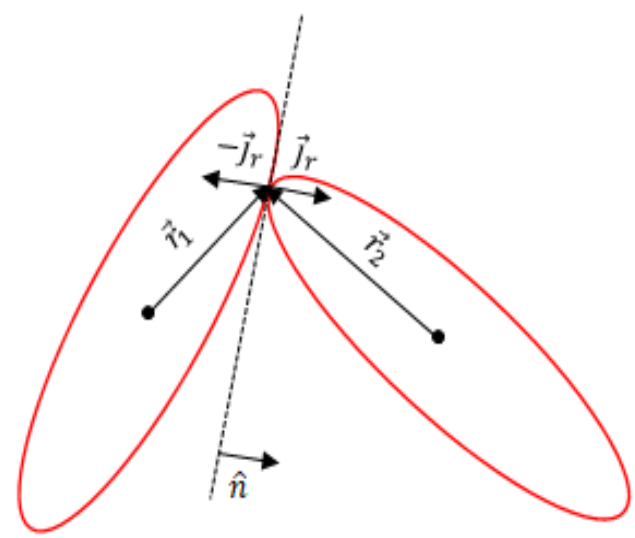
- **Post collision velocity update:**

$$\vec{v}_{1,post} = \vec{v}_{1,pre} - \frac{j_r}{m_1} . \hat{n}$$

$$\vec{v}_{2,post} = \vec{v}_{2,pre} + \frac{j_r}{m_2} . \hat{n}$$

$$\vec{\omega}_{1,post} = \vec{\omega}_{1,pre} - j_r \,.\, \bar{\bar{I}}_1^{-1} * (\vec{r}_1 \times \hat{n})$$

$$\vec{\omega}_{2,post} = \vec{\omega}_{2,pre} + j_r \,.\, \bar{\bar{I}}_2^{-1} * (\vec{r}_2 \times \hat{n})$$



Collision Resolution – Hard Sphere – Tangential Impact

- **Collisions between particles involve tangential kinematics (friction forces)**
- **Dynamic component of the total frictional impulse :**

$$j_d = \mu_d \, . \, j_r$$

- **Frictional impulse vector acting along the tangent :**

$$\vec{j_f} = -j_d \, \hat{t}$$

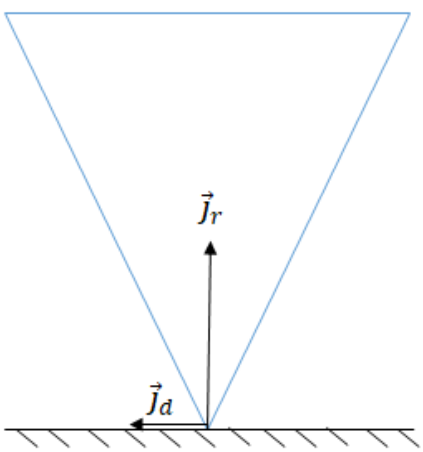
- **Post collision velocities update :**

$$\vec{v}_{1,post} = \vec{v}_{1,post} + \frac{j_d}{m_1} . \hat{t}$$

$$\vec{v}_{2,post} = \vec{v}_{2,post} - \frac{j_d}{m_2} . \hat{t}$$

$$\vec{\omega}_{1,post} = \vec{\omega}_{1,post} - j_d \, . \, \bar{\bar{I}}_1^{-1} * (\vec{r}_1 \times \hat{t}\,)$$

$$\vec{\omega}_{2,post} = \vec{\omega}_{2,post} + j_d \, . \, \bar{\bar{I}}_2^{-1} * (\vec{r}_2 \times \hat{t}\,)$$



Collision Resolution – Soft Sphere

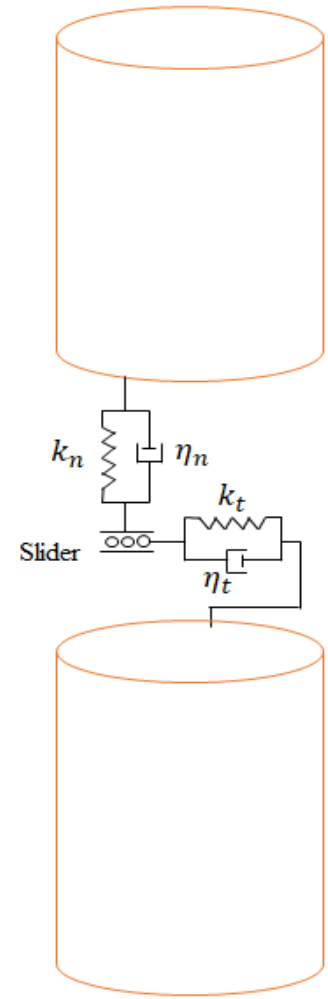
Soft sphere model :

- **Beneficial when applied to multiple particles in the computational domain**
- **Resolves multiple contacts on the particles' surfaces**
- **Particles are allowed to deform along normal and tangential directions**
- **Formulated based on the change in momentum effected by the reaction forces**

- **When a particle deforms, the collision forces can be modeled as a linear spring – dashpot system**

$$\vec{F}_n = -k_n \vec{\delta}_n - \eta_n \vec{v}_n$$

$$\vec{F}_t = \begin{cases} -k_t \vec{\delta}_t - \eta_t \vec{v}_t & \text{if } |\vec{F}_t| < \mu |\vec{F}_n| \\ -\mu |\vec{F}_n| \cdot \dfrac{\vec{v}_t}{|\vec{v}_t|} & \text{otherwise} \end{cases}$$



Collision Resolution – Soft Sphere …contd.

- **Total collision force – update linear velocity**

$$m\frac{d\vec{v}}{dt} = \vec{F}_c$$

- **Effective torque – update rotational velocity**

$$\bar{\bar{I}}\,\frac{d\vec{\omega}}{dt} = \vec{T}_c$$

Spherical DEM

Linear Velocity update:

- Normal force only
- $\vec{F}_c = \vec{F}_n$

Rotational Velocity update:

- $\vec{T}_c = \vec{r} \times \vec{F}_t$

Non-Spherical DEM

Linear Velocity update:

- Total force
- $\vec{F}_c = \vec{F}_n + \vec{F}_t$

Rotational Velocity update:

- $\vec{T}_c = \vec{r} \times \vec{F}_c$

Results and Discussion

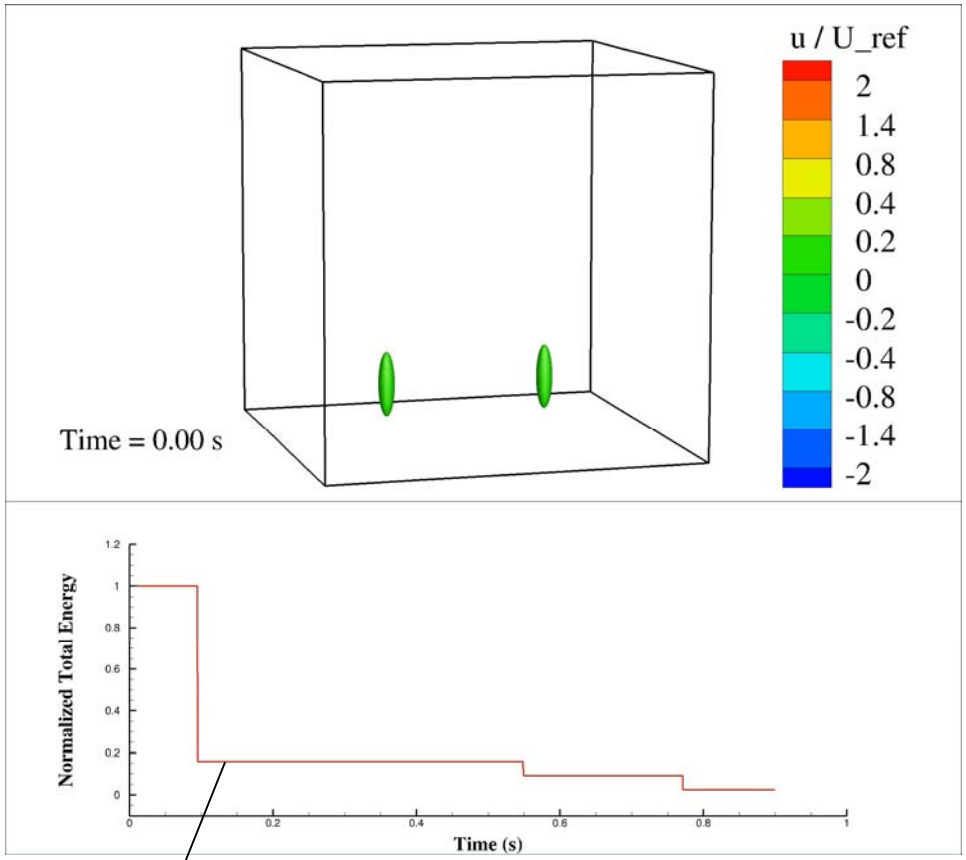
- **Following incorporation of non-spherical DEM formulations, it is necessary to validate its functioning**

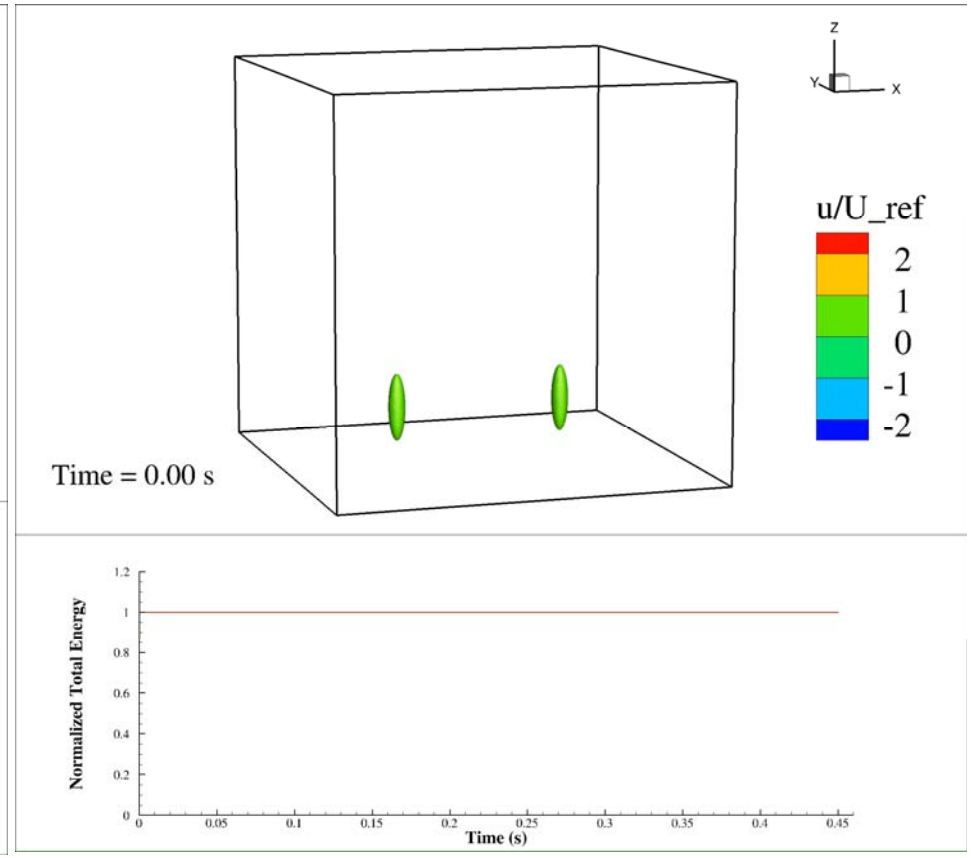
Total Energy Validation	• Validate by observing total energy of system • Different COR specified • Both Hard Sphere and Soft Sphere
Coupled CFD-DEM Validation	• Couple with flow solver GenIDLEST • Compare to experimental measurements in fluidized bed • Generate spheres (subset of superellipsoids) and compare averaged results
Scalability of Model	• Evaluate parallel scalability • Speedup and Efficiency of DEM model
Performance Metrics	• Dependency of DEM collision model on particle geometry definition

Total Energy Validation

- **Validation of DEM models at two different COR (0.4 and 1.0)**
- **Ellipsoids are generated , supplied with an initial velocity equal in magnitude and opposite in direction**
- **Gravitational and fluid forces are deactivated**

Total energy validation - HS model



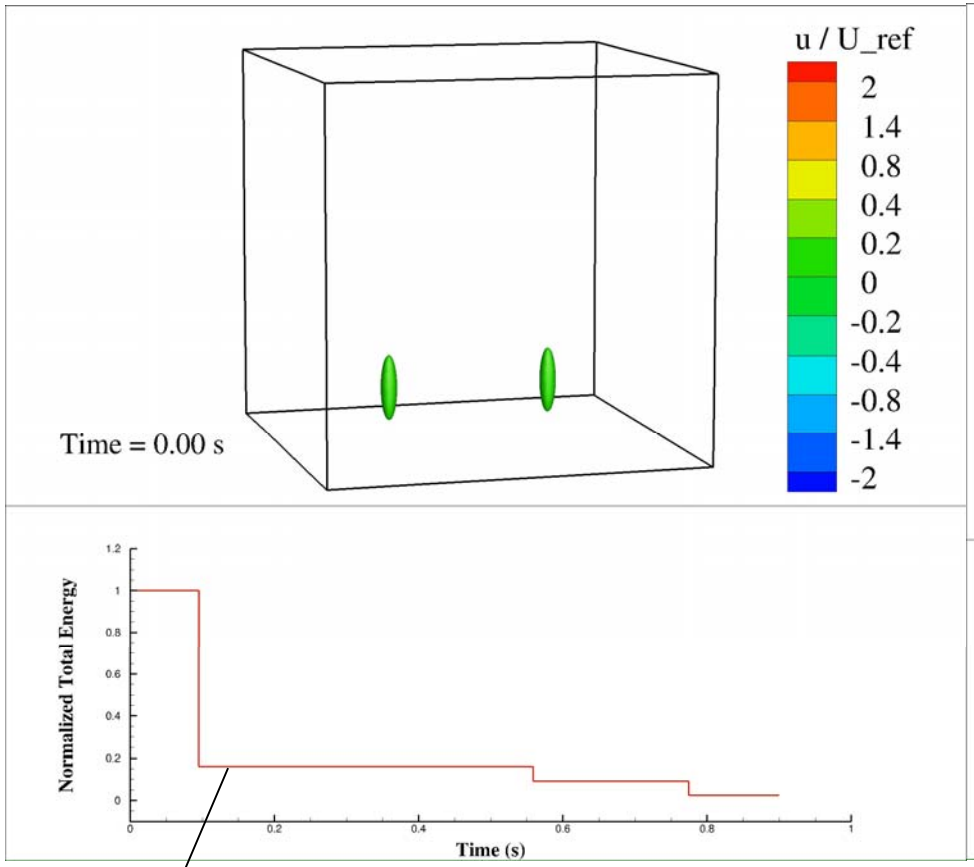


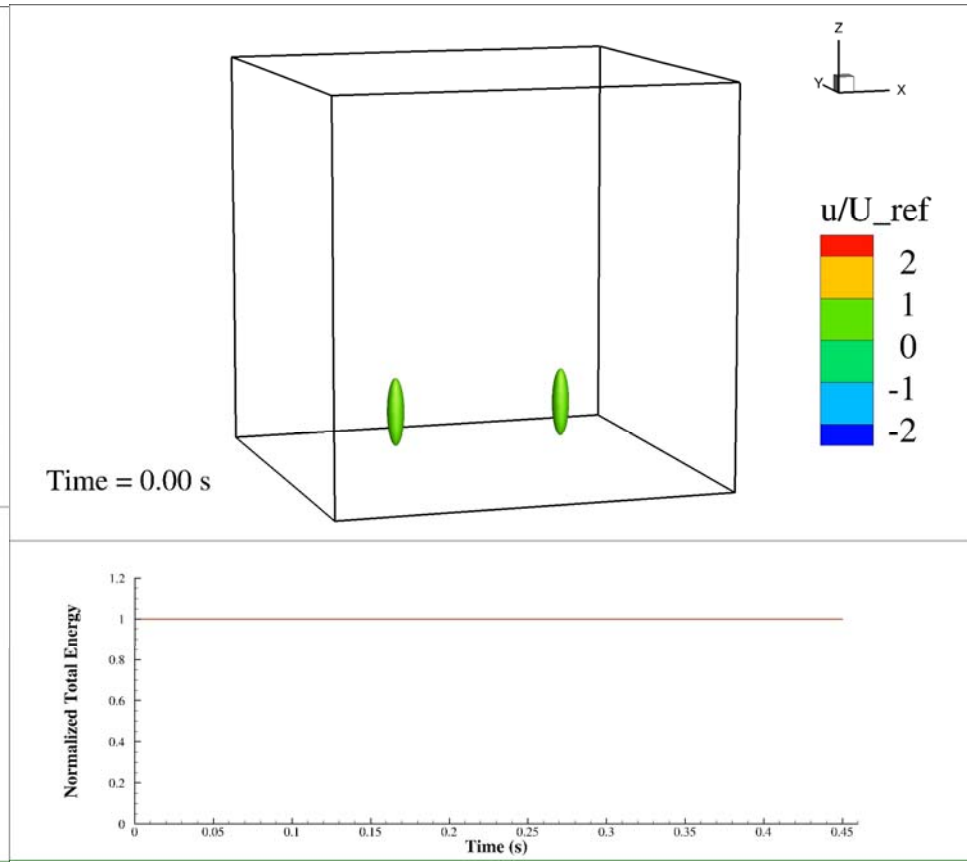
$$\sqrt{\frac{0.16}{1}} = 0.4$$

COR of 0.4

COR of 1.0

Total energy validation - SS model



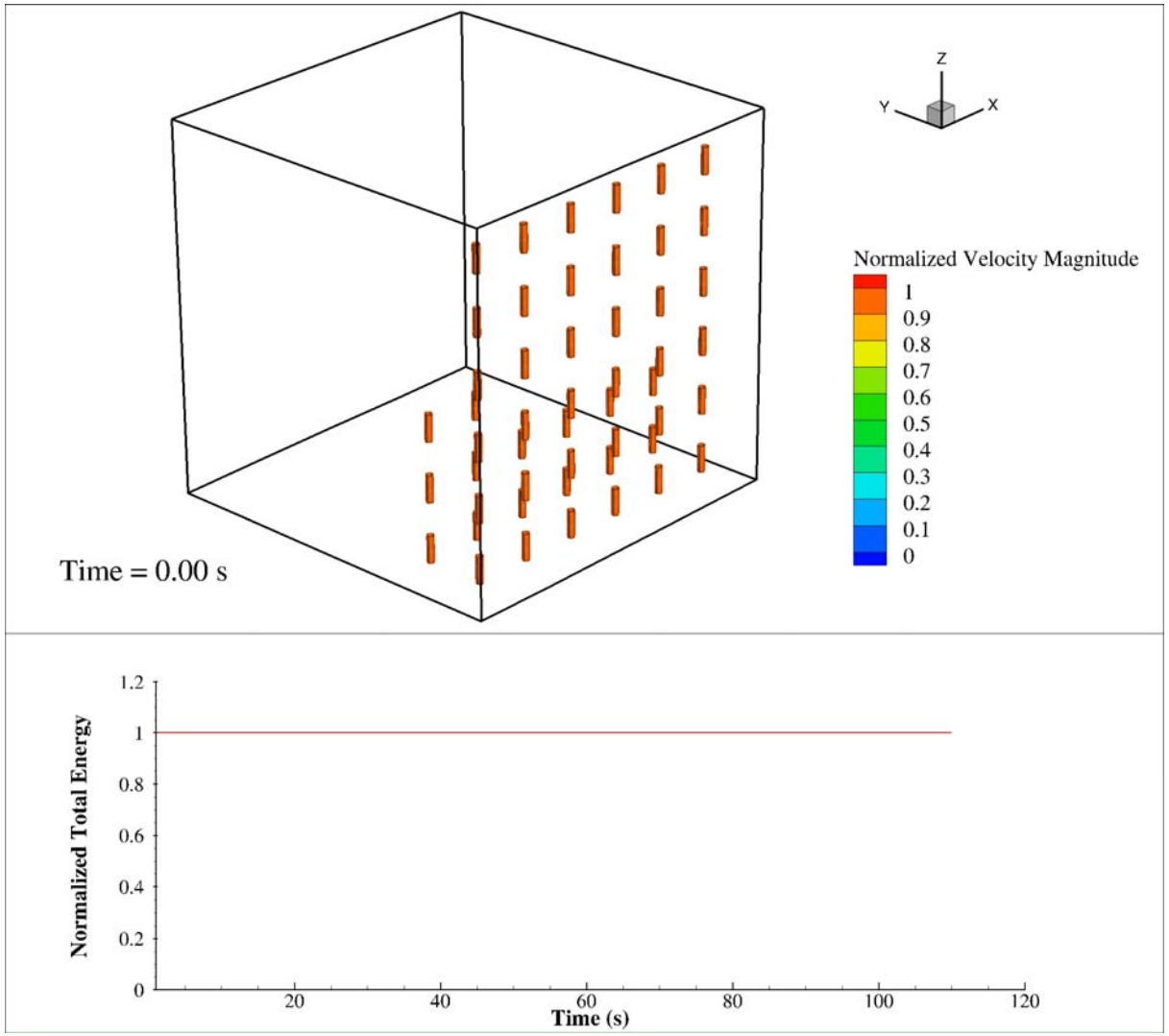


$$\sqrt{\frac{0.16}{1}} = 0.4$$

COR of 0.4

COR of 1.0

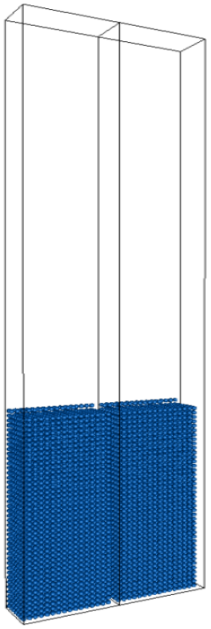
Total energy validation - HS model– multiparticulate system



Coupled CFD-DEM Validation

- **Primary purpose of non –spherical DEM model**
  - **couple the model with a fluid solver - GenIDLEST**
  - **Validate coupled model with experiments**

- **GenIDLEST – implementation to calculate fluid forces for spherical particulate systems**
- **The experiments conducted by Muller et al.[1] on a fluidized bed have been employed**
- **Simulations - run for 10 seconds and results were averaged for the last 5 seconds**

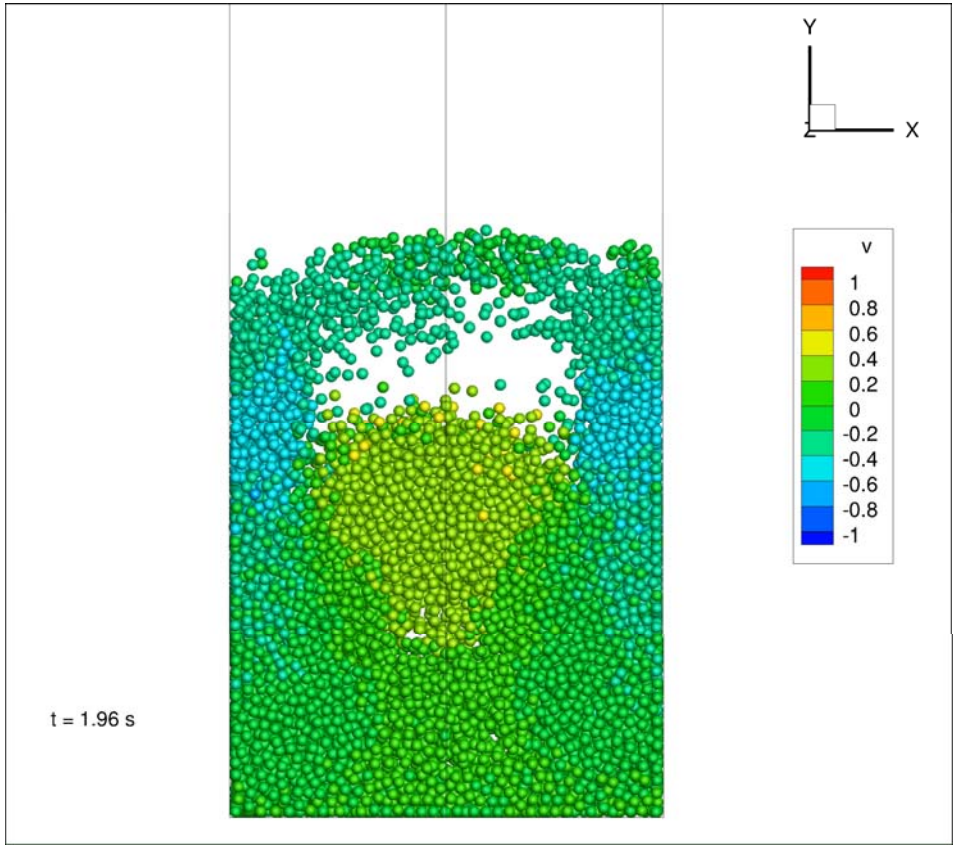


Particle Property	Value
Diameter	1.2 mm
Density	1000 kg / m^3
Friction coefficient	0.1
COR	0.98
Stiffness	8 N/m

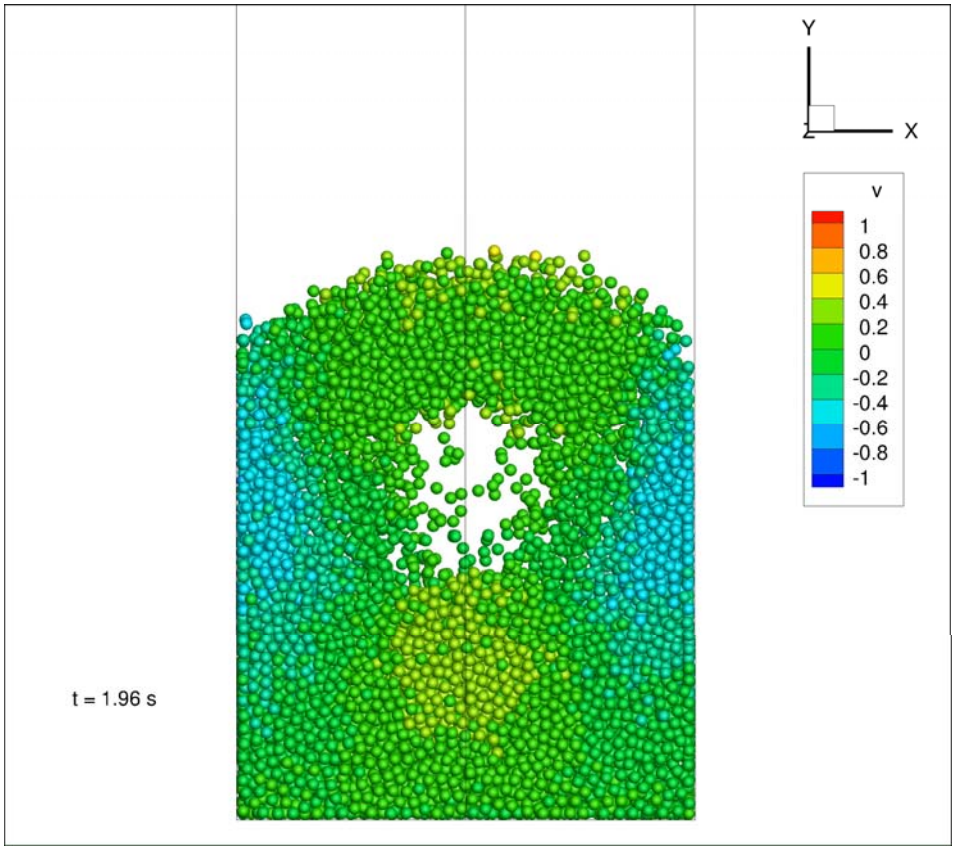
Fluid Property	Value
Density	1.205 Kg / m^3
Viscosity	1.8 x 10^{-5} Kg / m s

[1] Müller, C. R., Scott, S. A., Holland, D. J., Clarke, B. C., Sederman, A. J., Dennis, J. S., & Gladden, L. F. ,*"Validation of a discrete element model using magnetic resonance measurements", Particuology, 7*(4), 297–306,2009

Comparison of Temporal Progression of Simulation

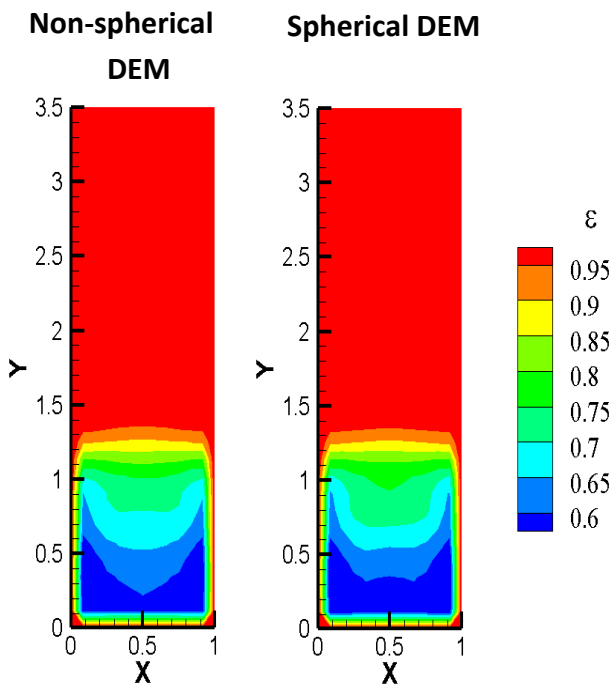


Non-spherical DEM

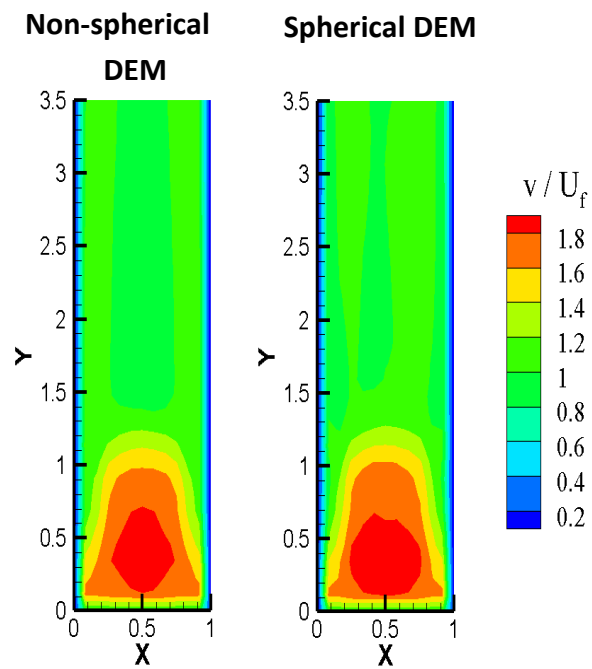


Spherical DEM

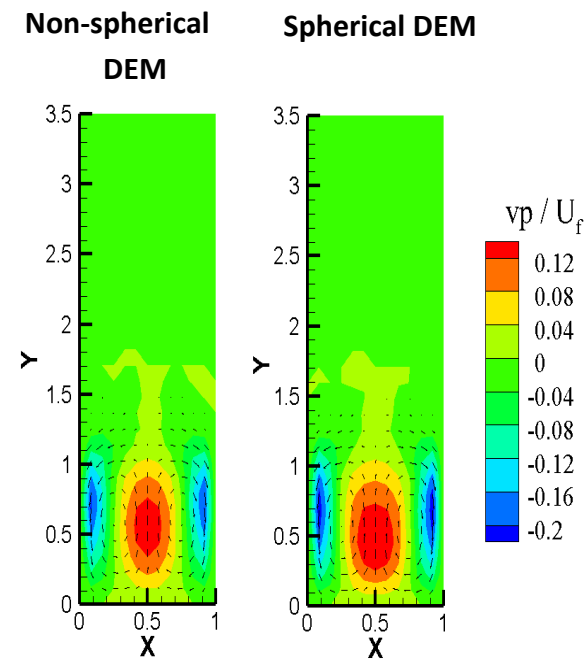
Comparison of Averaged Results



Averaged void fraction

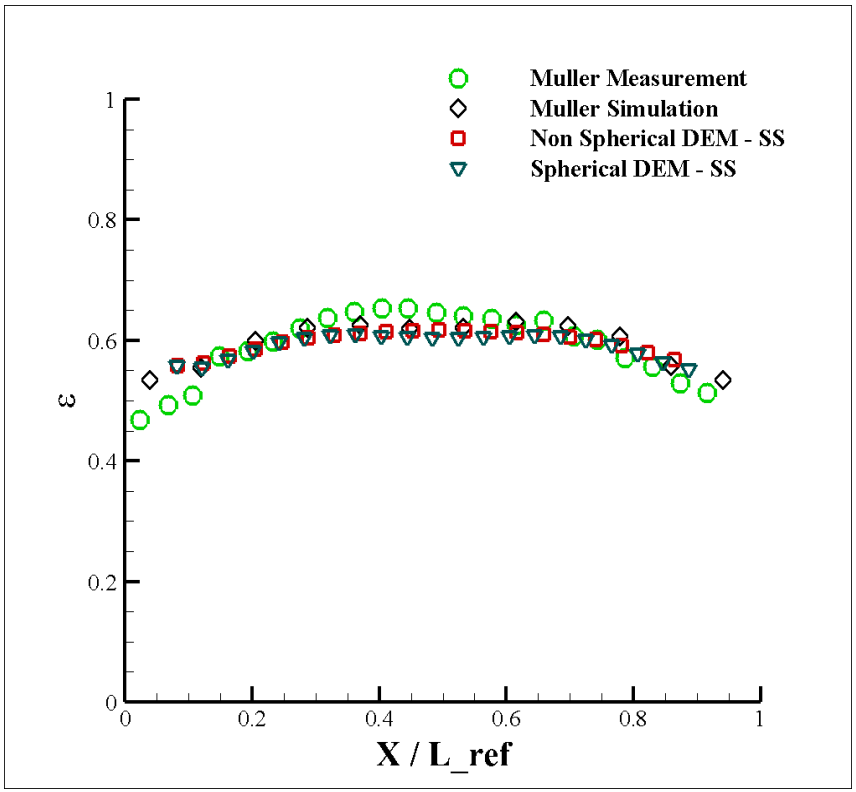


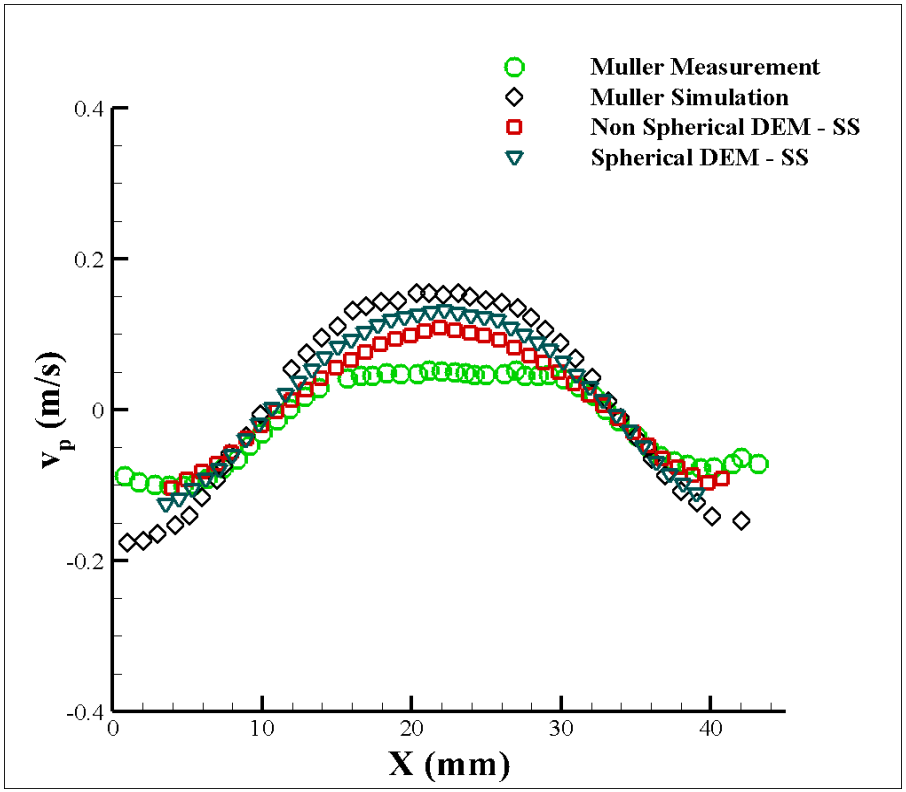
Averaged non dimensionalized fluid velocity



Averaged non dimensionalized particle velocity

Comparison With Experiments

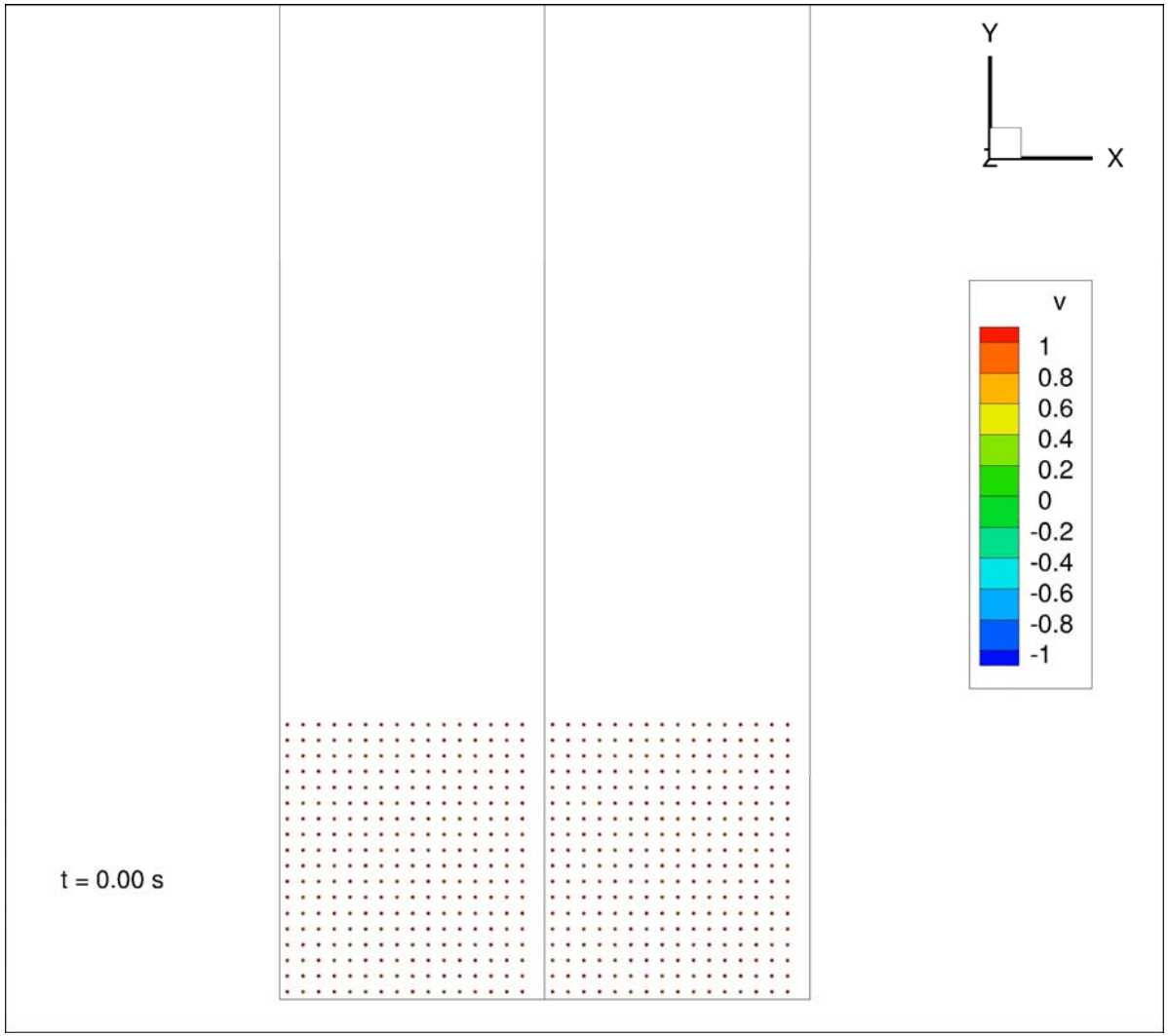




Averaged void f le velocity values at 16.4 mm from distributor plate

Model	Wall clock time taken for DEM computations on two computational cores
Spherical DEM	1207040 seconds (or) 13.97 days
Non – spherical DEM	1661787 seconds (or) 19.23 days

Fluidization of Ellipsoidal Particles (work in progress….)

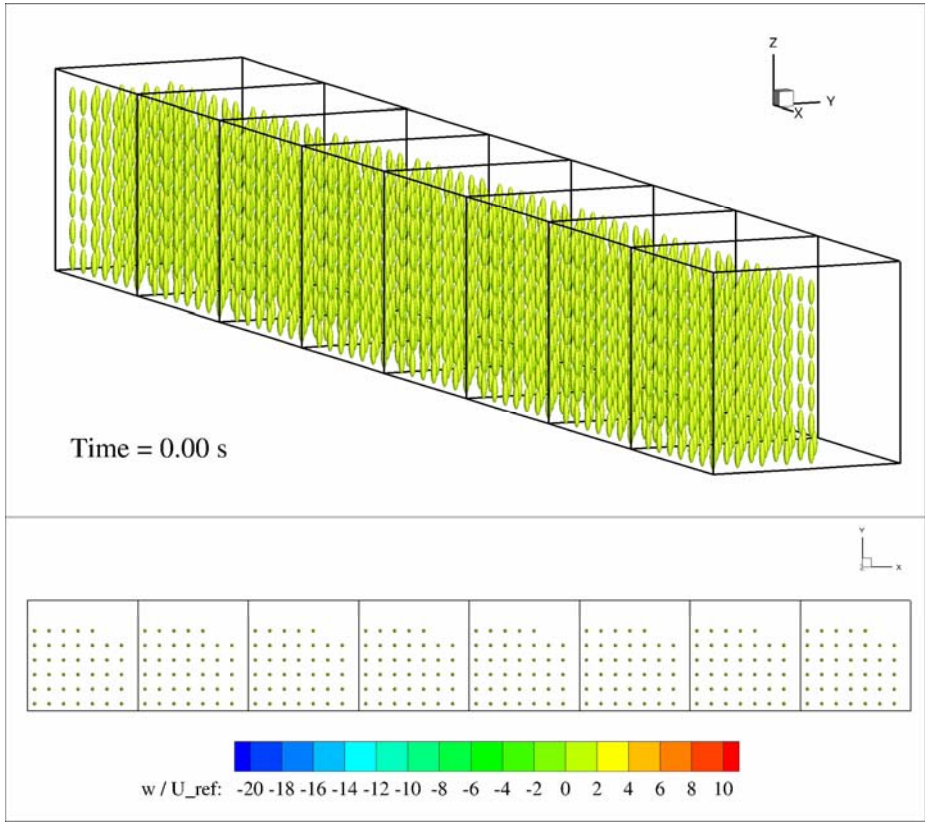


- 4000 ellipsoidal particles in the domain with aspect ratio 4.
- Spherical drag model

Scalability of the Model

Particle Property	Value
Major axis length	4 mm
Minor axis length	1 mm
Density	2650 kg / m^3
Friction coefficient	0.5
COR	0.5
Stiffness	40 N/m

No. of processors	Wall clock time taken for 1 sec. (in seconds)	Speedup	Efficiency (%)
1	16731	-	-
2	8646	1.934	96.7
4	4463	3.749	93.72
8	2331	7.179	89.73

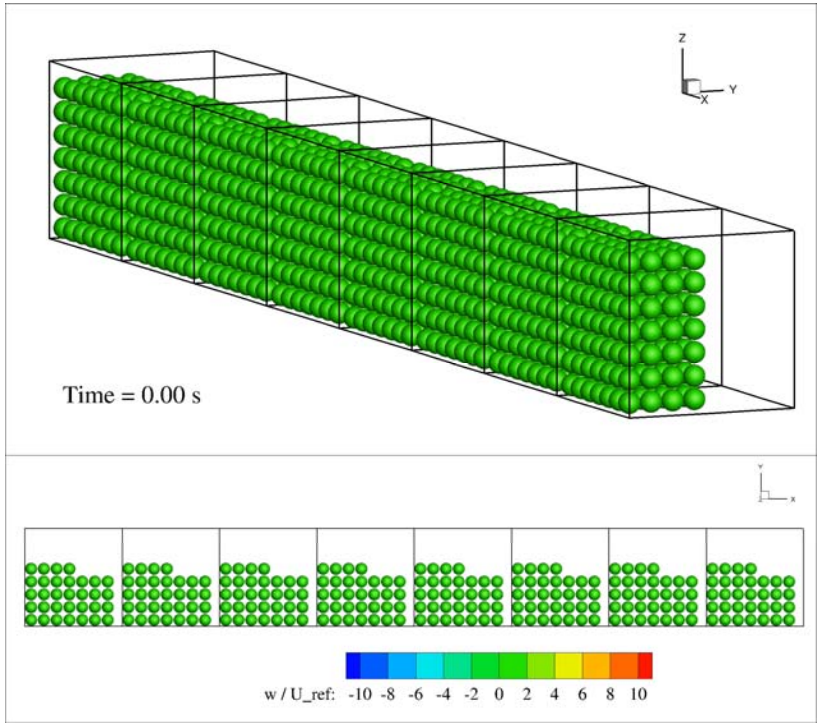


Total 2000 ellipsoids with 400 surface vertices each. Soft sphere model used

Performance Metrics

No. of surface vertices on each particle	Wall clock time (in seconds)	No. of particle - particle collision instances	No. of particle – wall collision instances	Total no. of collision instances	Wall clock time per collision instance per processor (in micro seconds)
400	7645	62415940	10567446	72983386	13.1
900	18972	80681123	12208878	92890001	25.5
1600	37098	86898067	13750284	100648351	46.07

Model	Wall clock time (in seconds)	No. of particle - particle collision instances	No. of particle – wall collision instances	Total no. of collision instances	Wall clock time per collision instance per processor (in micro seconds)
NSP - DEM	7645	62415940	10567446	72983386	13.1
Spherical DEM	2592	60685720	10224988	70910708	4.56



Summary & Conclusions

Development of the model:

- A new framework to simulate non spherical particle dynamics has been developed
- In an event - driven model, an impulse based collision resolution technique is employed
- In a time - driven model, a linear spring – dashpot model is utilized

Validation of the model:

- Temporal progression of energy is monitored at various coefficients of restitution
- Coupled CFD- DEM model is validated by comparing to results from experiments

Scalability and Performance:

- The scalability of the model is evaluated in terms of efficiency and speedup
- Metrics that delineate the wall clock time utilized per collision per processor have been documented

Thank you !

Support of the National Energy Technology Lab and Advanced Research Computing at Virginia Tech

QUESTIONS?