
# GPU based DEM for bulk particle transport simulations.

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# Outline

- Introduction
- DEM
- Computational simulation
- Collision detection
- GPU Implementation
- Experimental validation
- Conclusion

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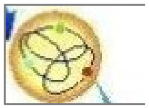
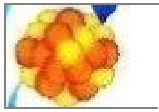
# Introduction

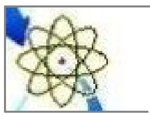
**Forces**



$10^{-13}$ cm Proton — Color (Quarks)

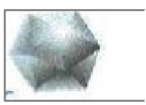


$10^{-11}$ cm Nuclei — Strong (residual)



$10^{-8}$ cm Atom — EM, Weak

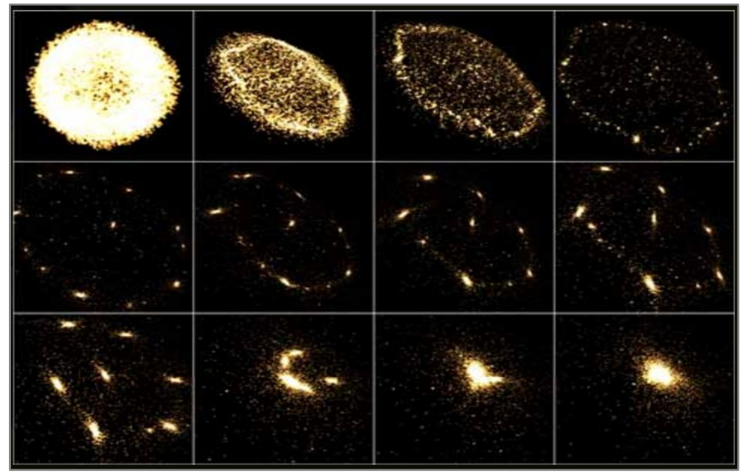
$10^{-7}$ cm Molecule — Gravity, EM*



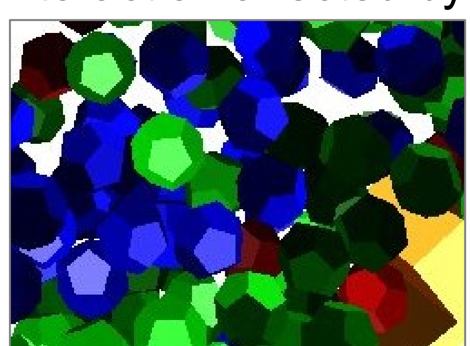
1 cm Grain — Gravity

100 cm Rocks

The physical size of the particle does not affect interaction

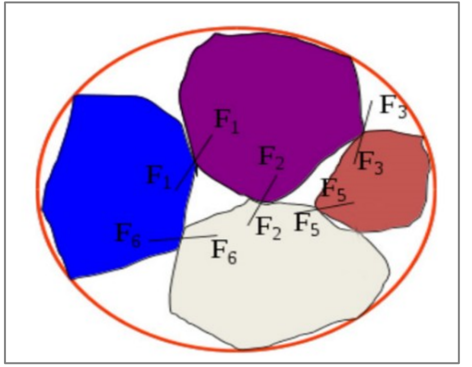


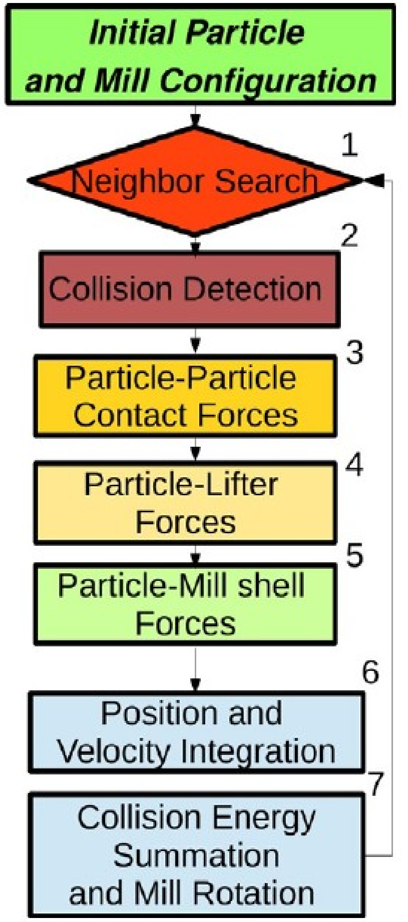
Interaction affected by physical contact



# Discrete Element Method

- Most popular and successful approach first described by *“CUNDALL: A discrete numerical model for granular assemblies. Geotechnique 29, (1979), 47–65.”*
- Similar force ranges and particle sizes
- Motion of particle depend on the net sum of forces per time step
- Binary contact is assumed to resolve contact forces
- Explicit integration
- Embarrassingly parallel
- Particles are commonly treated as spheres



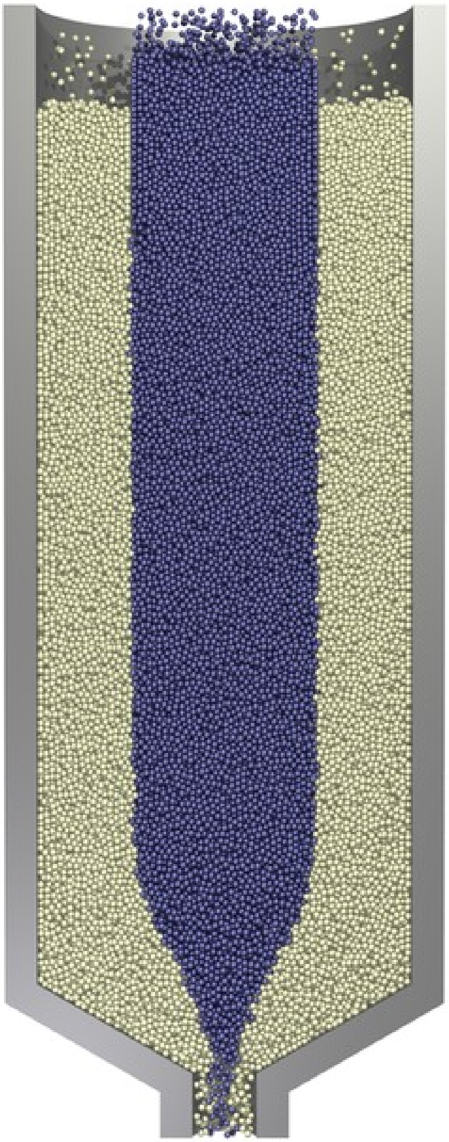







# If only they had simulated...

# Some of them did...

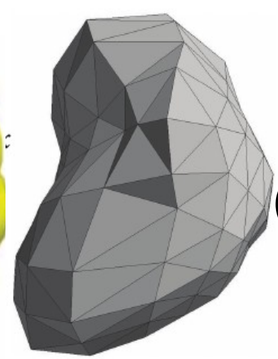


- "**Large-scale simulations** of an experimental device, featuring **440,000** spherical particles"

***(1) It is meant to be bulk material simulation!***

***Large is relative.***

- "The DEM simulations in this study required **over a month** of time on **90 processors**, since the contact models are stiff and a small timestep is required."



***(2) Shape, no wonder the mars rover got stuck.***

C. H. Rycroft, G. S. Grest, J. W. Landry, and M. Z. Bazant, Analysis of Granular Flow in a Pebble-Bed Nuclear Reactor, Phys. Rev. E 74, 021306

# DEM limitation

- Particle numbers

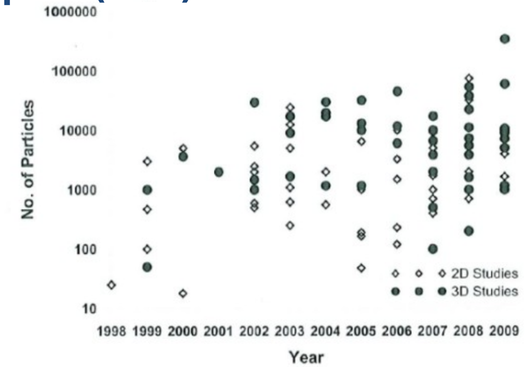
Ex. fine sand
□ 200 ∟ m
1 $cm^3$

150 000
particles

vs

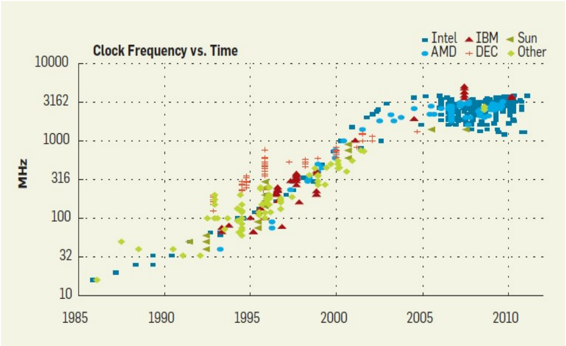
**DEM challenges for the geomechanic applications is number of elements**

**Numbers of particles vs time in DEM papers (CPU)**

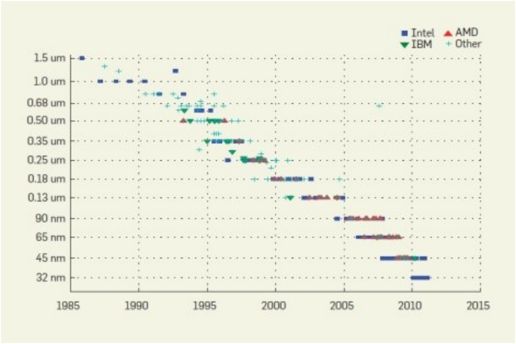



*Particulate DEM, A geomechanics Perspectives, O'Sullivan 2011*

**Clock frequency vs time**




**Size of transistor vs time**




GPU approach needed if we want to increase particles and model the industrial-scale

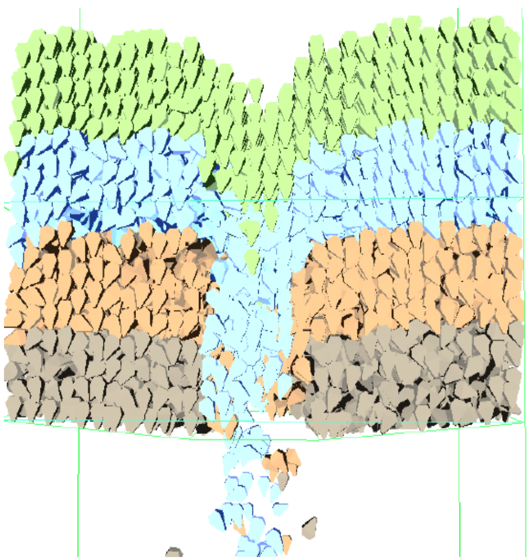
# Aim

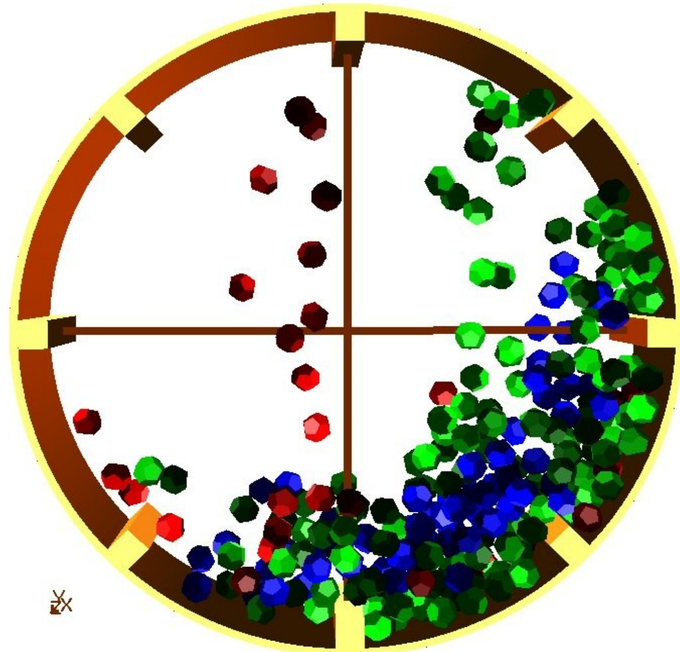
- Provide a GPU based framework that can be used to solve bulk flow problems encountered in engineering industry.
- Run on typical workstations using consumer hardware while being able to efficiently utilize multi GPU configurations.
- Needs to provide physical quantities that are relevant to aid in the design process.
- Needs to be modular in terms of:
    - Collision detection.
    - Collision resolution (physics).
- Allow for accurate particle shape representation when needed.
- Allow for large number of particles to be simulated.

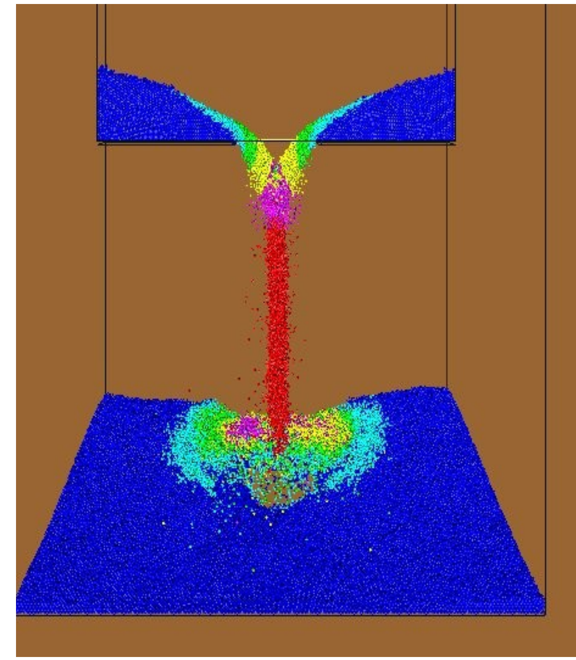

GPU-DEM

Because shape and speed matter!

POWERED BY NVIDIA







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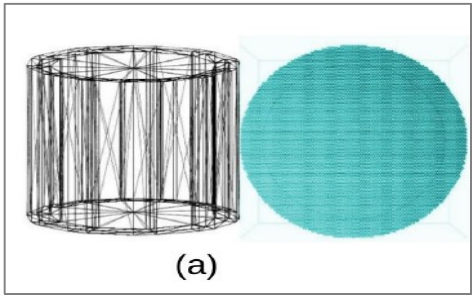
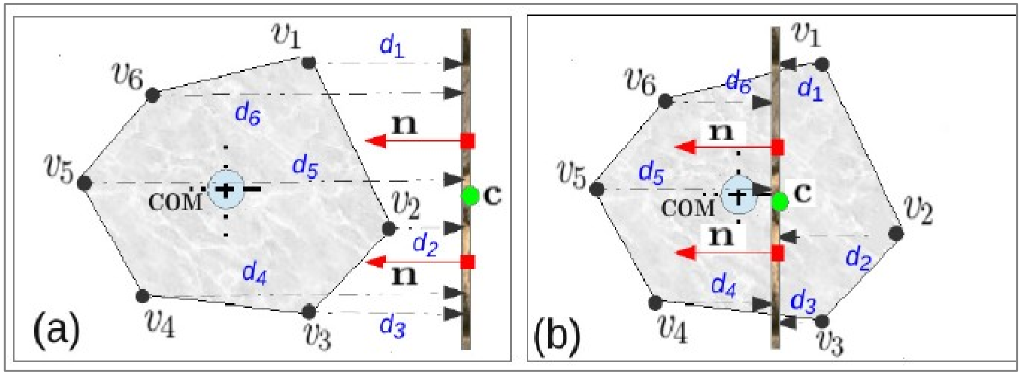
# Collision detection

- Current methods use triangulation/particles, which require thousands of checks to determine collision.

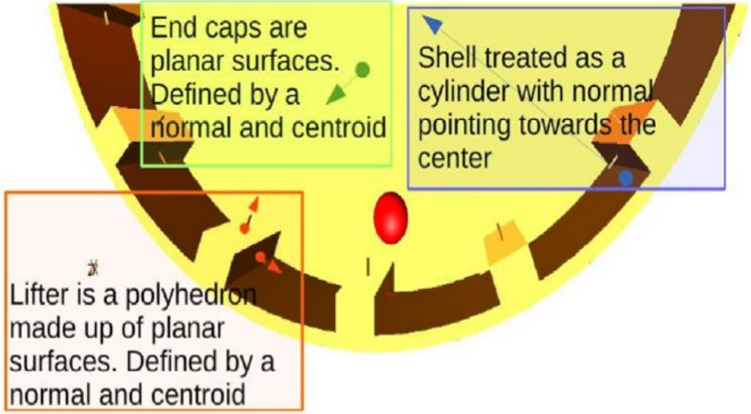



- We employ a ray based approach, which does not require a mesh.



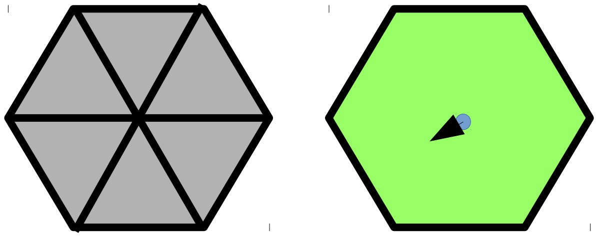

$$d = \mathbf{n} \cdot (\mathbf{v} - \mathbf{c})$$

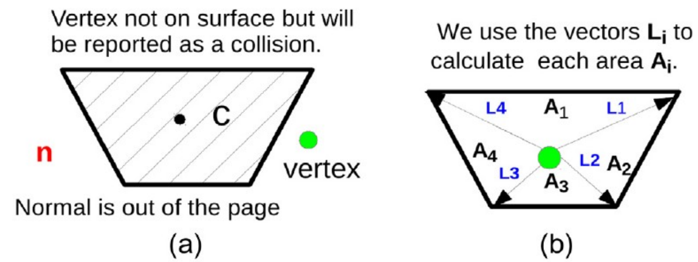
- For higher order surfaces we use analytical expressions.




$$d = f(\mathbf{v})$$

- Mathematically only a change in normal implies a new surface.

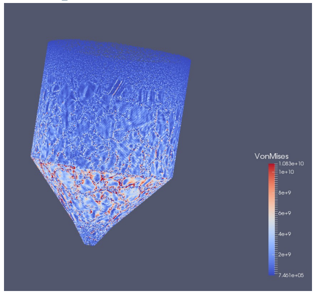





- Thus surface triangulation is not needed for collision detection, a point and normal is sufficient.

- Justification from DEM community is it is needed for calculating wear, stress/pressure, tallies etc.

- However it is actually only a “virtual” mesh that is needed. Furthermore since they are not intrinsic properties they can be processed in parallel/post with the DEM step.



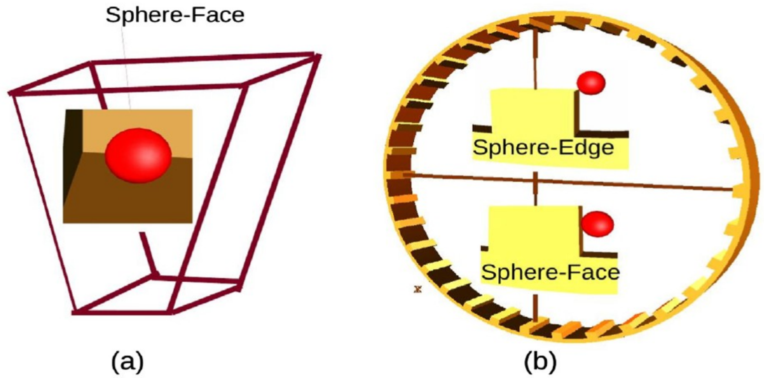
# GPU Data Storage

- SOA approach: 2.6 GB per 10 million particles, unpadded since memory is a premium.

- Spatial binning grid requires 8 bytes per cell (8 GB for a $10m^3$ area).
  - Largest particle dictates cell size.
  - ~-15% 1:2 ratio .
  - Smaller ratio than this requires parameter change so cannot compare.

  - Can have a coarser grid to decrease memory usage but performance drops by 2.8X and 15X for a factor of 2 and 4 cell-size reduction.

- World Geometry is split into: macro (cylinder,cone), surface (internal concave) and volume (convex) objects. Stored in constant memory*.




  - Objects can rotate and translate imparting the resultant dynamics on particles.

  - All objects can deform rigidly in real-time.

# GPU Computation

- We split world collision detection into (Kernel_Planar) and (Kernel_Marco) to ensure there is no divergence. We launch kernels per world object in multiple streams.
- NN search using spatial binning, requires the cells to be set using memset after each iteration. This is expensive and also scaled with the domain not particles.
- However, we can run the opposite of the binning kernel, to set bin values to zero. 10X faster than memset and scales with number of particles/distn.
- We only grid the region where particles are contained in for silo/flow problems where the domain moves. (First and last particle hash gives the extent of the region).
- Particle, World and Volume CD are in different streams to allow concurrent execution
- On a single GPU we can do 32 million particles using 8.7GB memory 0.2 seconds per step. **35 minutes** for **1 second** simulation time. Cundall No = 1.6E8
- Multi-GPU: Brute-force sorting on GPU 0, then send N/k particle to each GPU.+ buffer. Only useful when domain does not change much, eg filling, mass flow . Waiting for Pascal...

# GPU Optimizations

- For the past 3 years chose “sensible” algorithms for the GPU.
  - Code is many of times faster than CPU codes, and about 3X faster than comparable GPU codes.

    – As always predicting the real world is the essential proof, pushing to 10's of millions of particles started taking time, about 3 days for an industry relevant simulation.

  - Although it is a new performance level for DEM, I didn't like waiting.

    – Finally this year after extensive validation (documented in journal publications) that shows good agreement to experiment, new ideas kept on the back burner were implemented.

    – Short story in two weeks got a 4X speed-up ! That is more than any full algorithmic changes can yield...

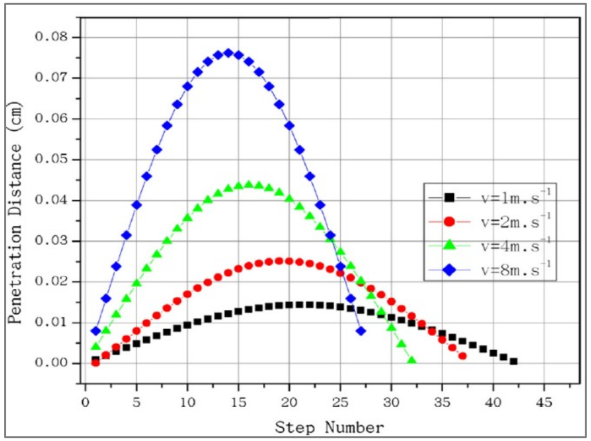
# What had to change from typical "particle simulations" .

- Gaming approximates contact duration crudely by impulse calculations

$$\mathbf{v}^{new} = \mathbf{v}^{n} \pm \mathbf{j}/m, \quad \omega^{new} = \omega^{n} \pm \mathbf{I}^{-1}(\mathbf{r} \times \mathbf{j})$$

- Physics simulations resolves the contact duration from constitutive contact models

$$\mathbf{F}_{\mathrm{N}}^{\mathrm{elastic}} = (\mathrm{K_r}\delta^{\frac{3}{2}})\mathbf{n} \qquad \mathbf{F}_{\mathrm{N}}^{\mathrm{diss}} = -\mathrm{K_D}\delta^{\gamma}\mathbf{vrel}_{\mathrm{n}}$$



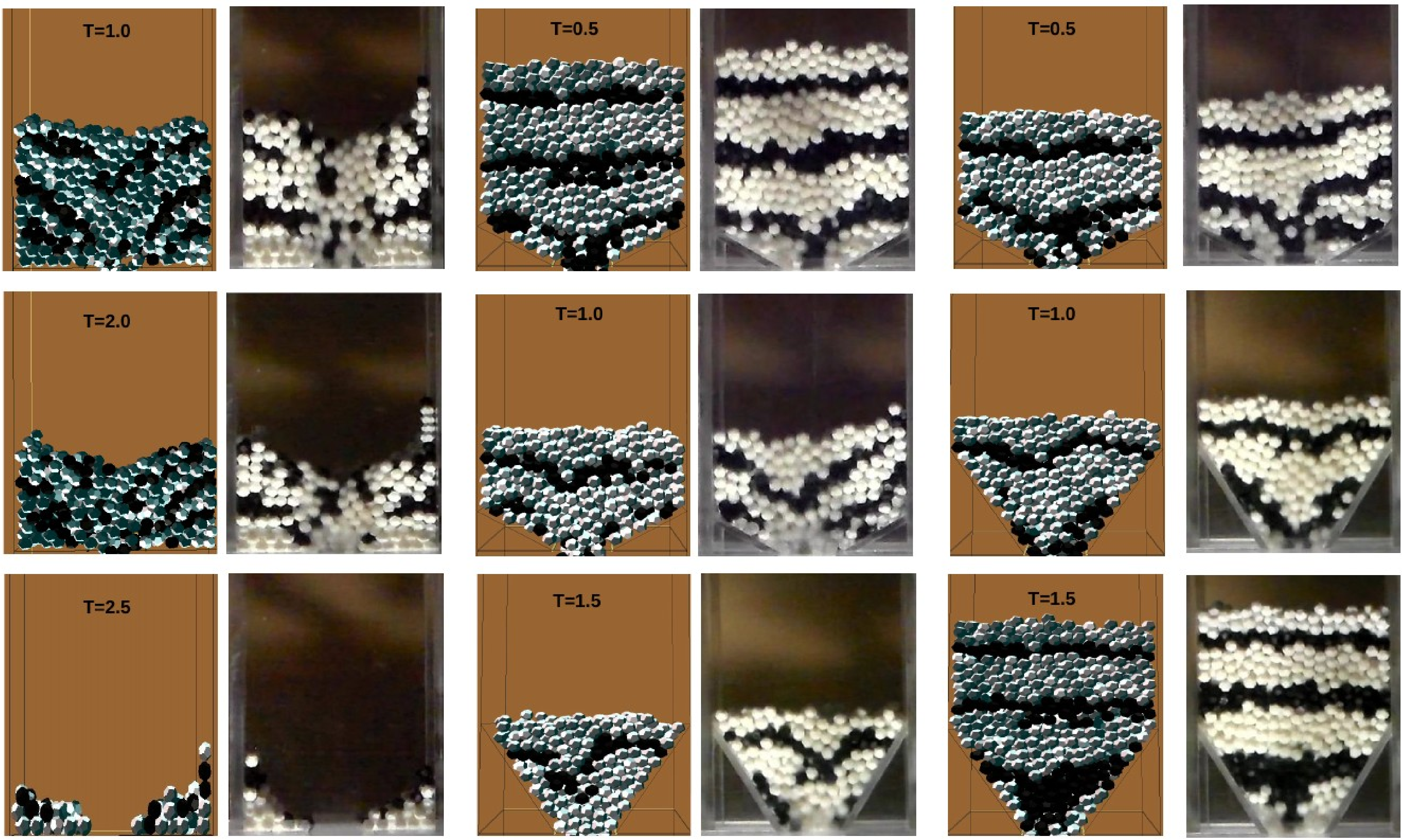

- Contact is resolved in a single time-step!
- Contact is resolved over multiple steps!

- Gaming is qualitative and estimates visual acceptable behavior
- Physics simulations are quantitative and estimate physical quantities such as energy, impact and shear and normal forces

# DEM vs Experiment Spherical Particle Flow

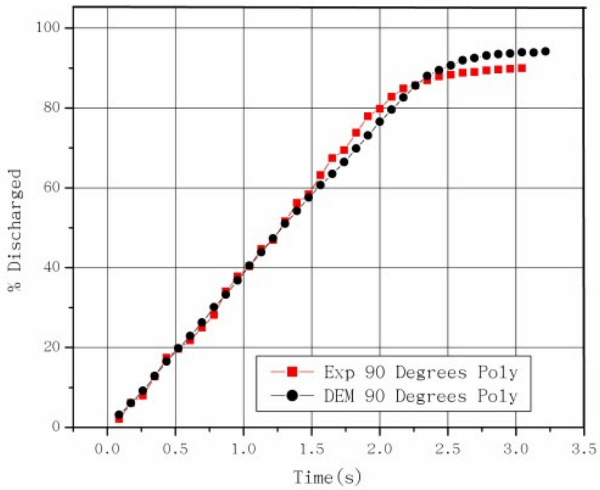

(a) (b) (c)

# DEM vs Experiment Polyhedra Particle Flow

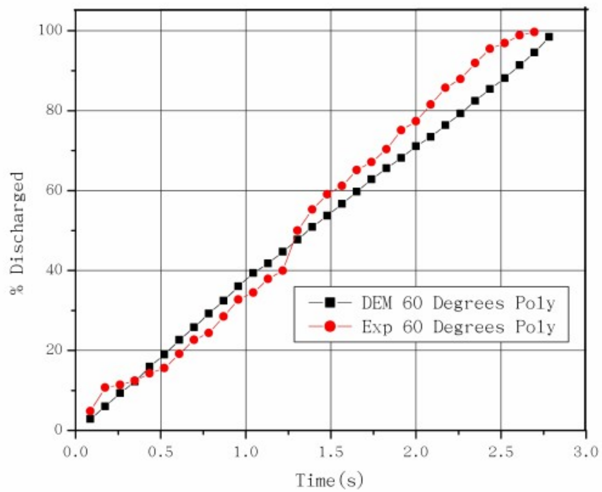



(a) (b) (c)

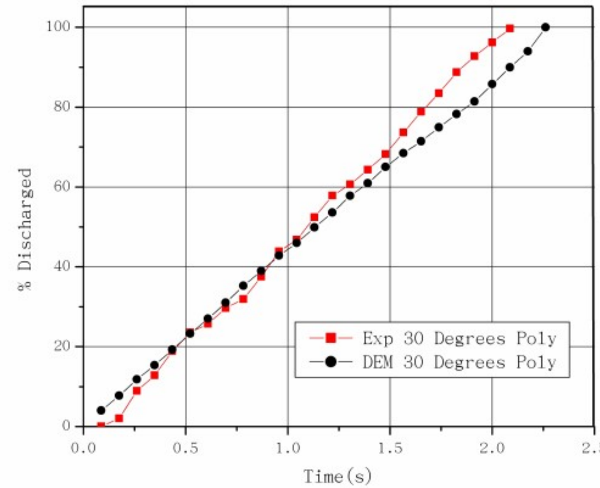
# Flow rates DEM vs Experiment



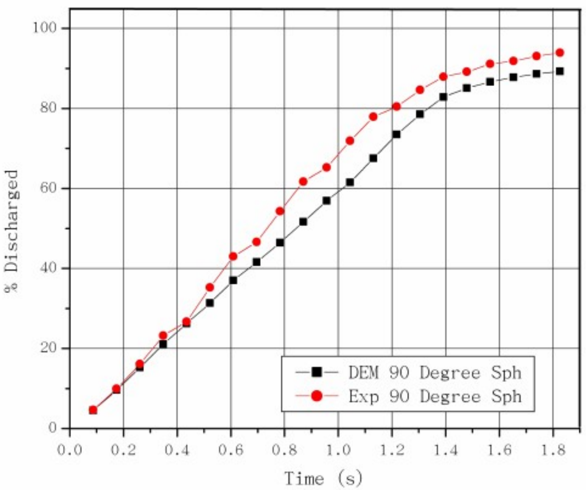
(a)



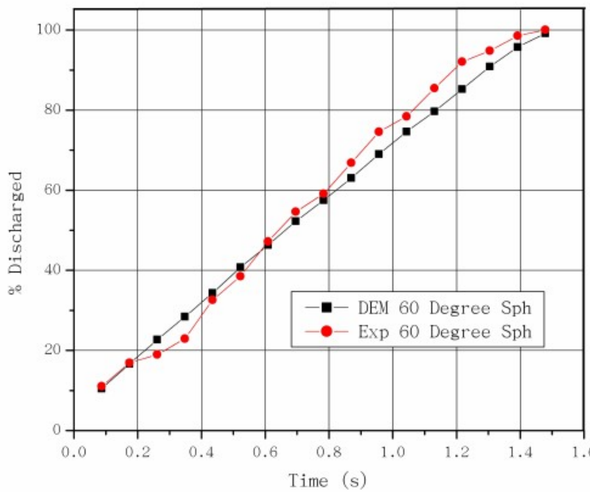
(b)



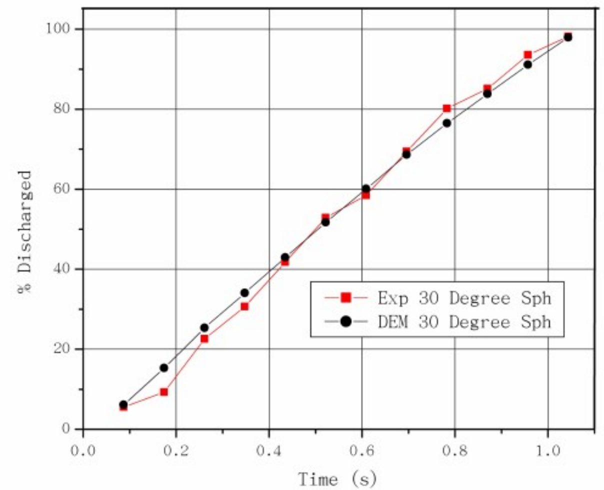
(c)



(a)

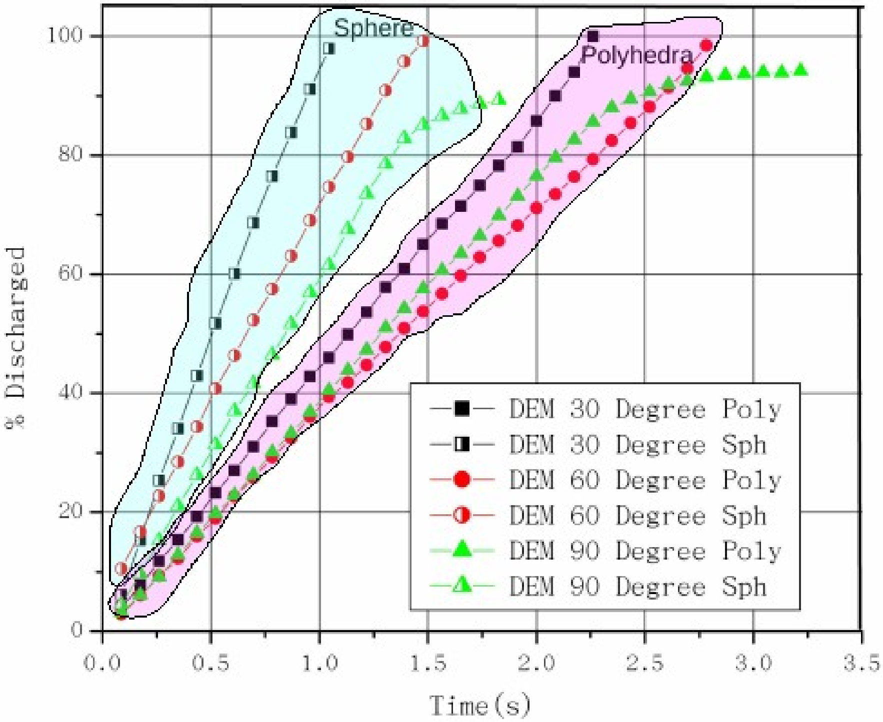


(b)

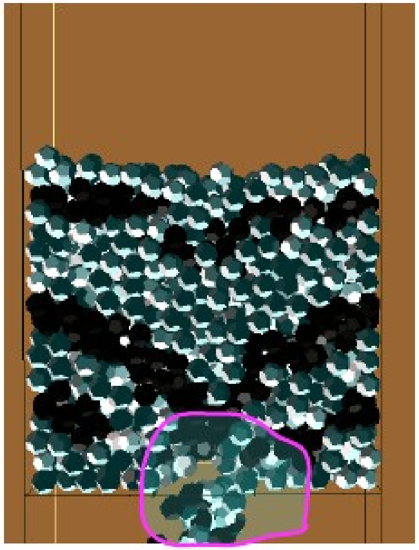


(c)

# Flow rates Spheres vs Polyhedra

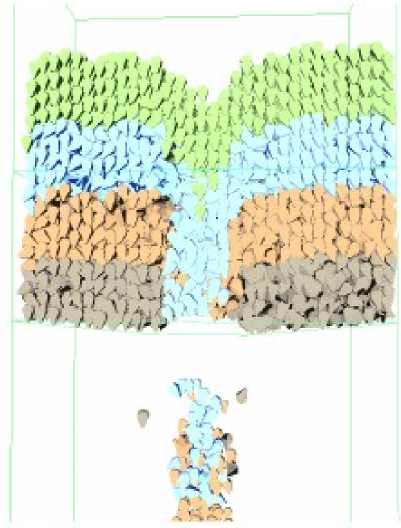



(a)



Polyhedra arching temporarily causes stop start flow.

(b)



Polyhedra (corn) stable arch causing flow to stop.

(c)

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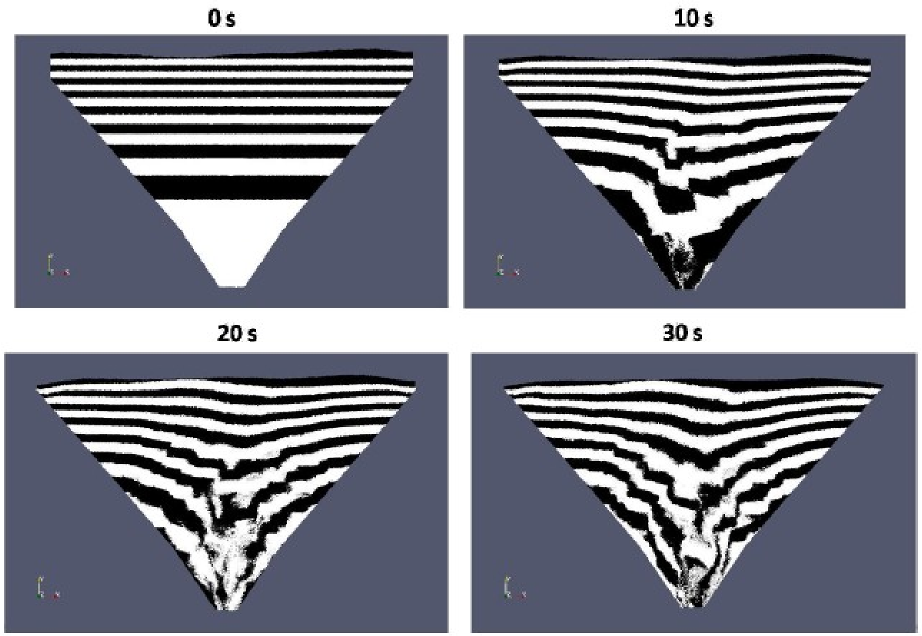
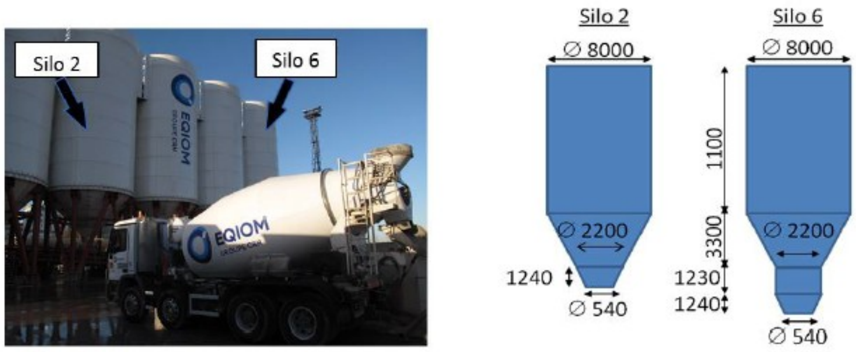
CELEBRATING 70 Years Ideas that work

# Spherical particle flow at the industrial scale

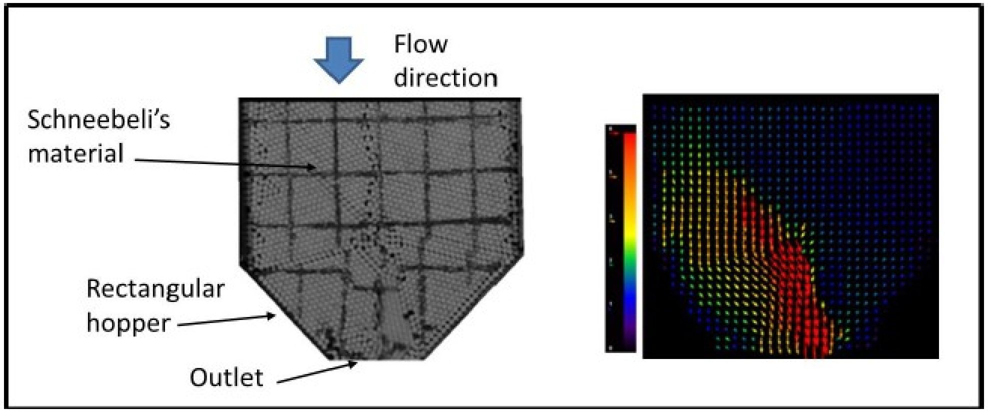



Cross-sectional views of **hopper** flow patterns at several simulation time (0, 10, 20 and 30s) for silo 2 (16777216 particles, 20 mm diameter)

Storage silo of concrete central




(a) (b)

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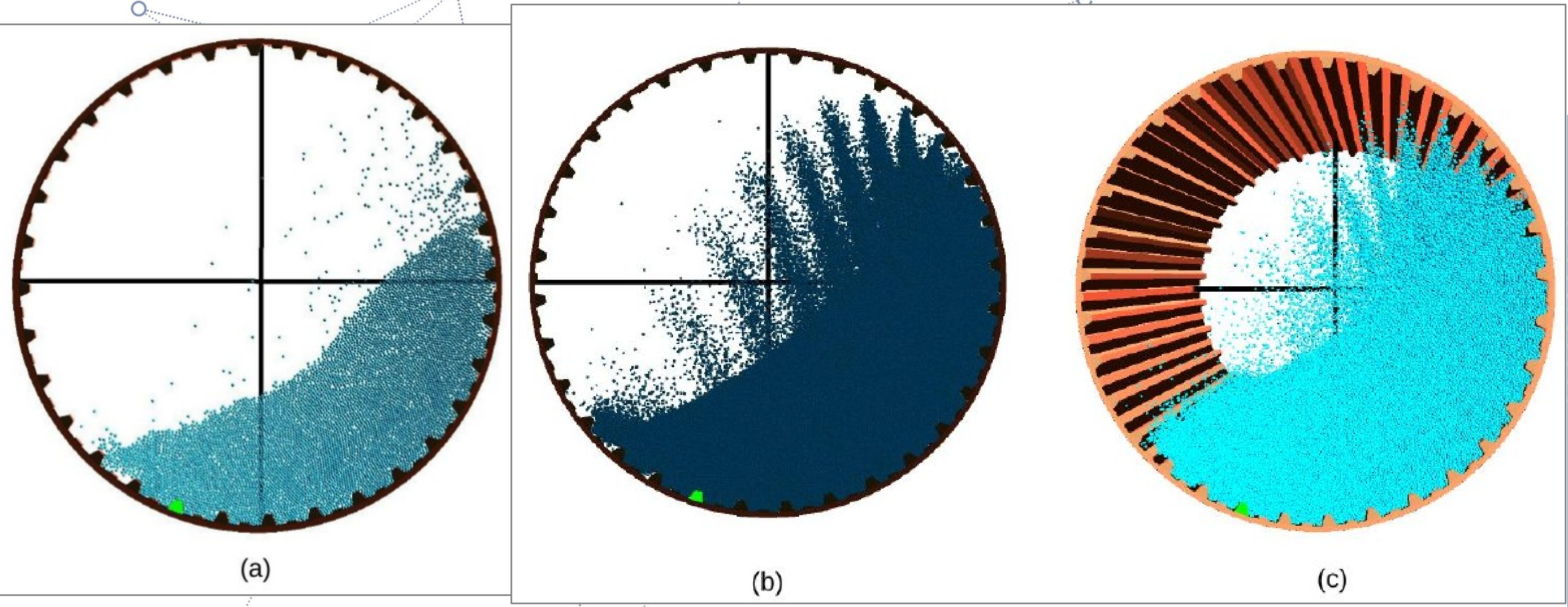
# Why do we need more particles?

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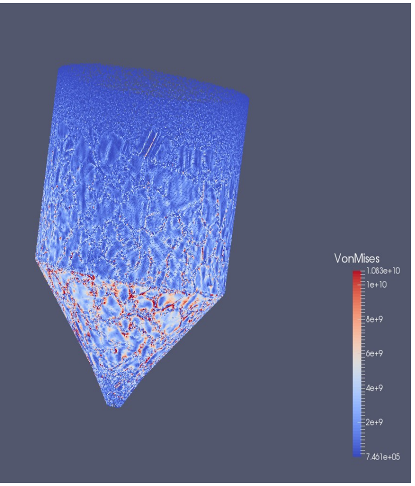
Latest LIGGGHTS benchmark
http://www.cfdem.com/media/DEM/benchmarks/LIGGGHTS_Benchmarks.pdf

10 Million Particles, **60 Cores**: 1 second = **46 hours**

Cost $ 16000 For just the CPUS! *(Price at launch in 2013)= $ 96000

## GPU 242X Faster, 27X Cheaper




Blaze-DEM GPU benchmark

10 Million Particles, 1 **GTX 980** : 1 second = **0.19 hours**

Cost $ 600

*Because the future is now!*


*Thank you for your time.*

[1] Development of a convex polyhedral discrete element simulation framework for NVIDIA Kepler based GPUs, Journal of Computational and Applied Mathematics 270 (2014) 386–400

[2] Collision detection of convex polyhedra on the NVIDIA GPU architecture for the discrete element method, Applied Mathematics and Computation 2014

[3] Discrete element simulation of mill charge in 3D using the BLAZE-DEM GPU framework, Minerals Engineering 79 (2015) 152–168.

[4] Validation of the gpu based blaze-dem framework for hopper discharge, iv international conference on particle-based methods – fundamentals and applications PARTICLES 2015

[5]  BLAZE-DEM GPU opensource framework, SoftwareX (2016).

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