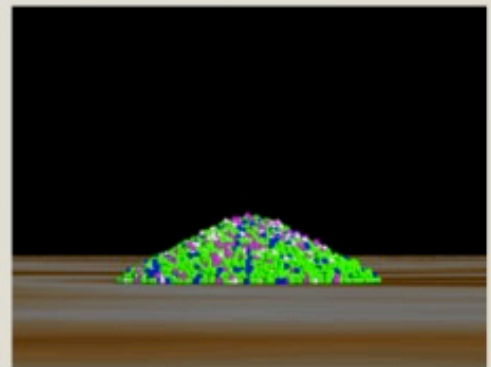
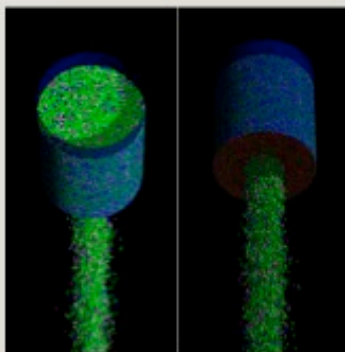


# THE SOFT-SPHERE DISCRETE ELEMENT METHOD (SSDEM)

*implementation in the N-body  
code `pkdgrav` and tests*



Stephen R. Schwartz<sup>1,2</sup>

avec:  
Patrick Michel<sup>1</sup>  
Derek C. Richardson<sup>2</sup>  
<sup>1</sup>Obs. Côte d'Azur, <sup>2</sup>U of MD

# Discrete Element Method (DEM)

- Until recently, pkdgrav simulations have used *hard-sphere* DEM:
  - Ballistic trajectories.
  - Collisions employ billiard-ball physics.
  - Suitable for dilute regime.
- Validate approach by comparing with known results and laboratory experiments.

# Simulating Gravity and Collisions

- pkdgrav: “Parallel  $k$ -D tree GRAVity code”
  - Combine parallelism and tree code to compute forces rapidly.
- Started as pure cosmology code written at U Washington.
- pkdgrav solves the equations of motion for gravity (point masses):

$$\ddot{\mathbf{r}}_i = - \sum_{j \neq i} \frac{Gm_j(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

$m$  = mass  
 $\mathbf{r}$  = vector position

- Introduce collision constraint (requires collision search):

Separation

Sum of radii

$$|\mathbf{r}_i - \mathbf{r}_j| = s_i + s_j.$$

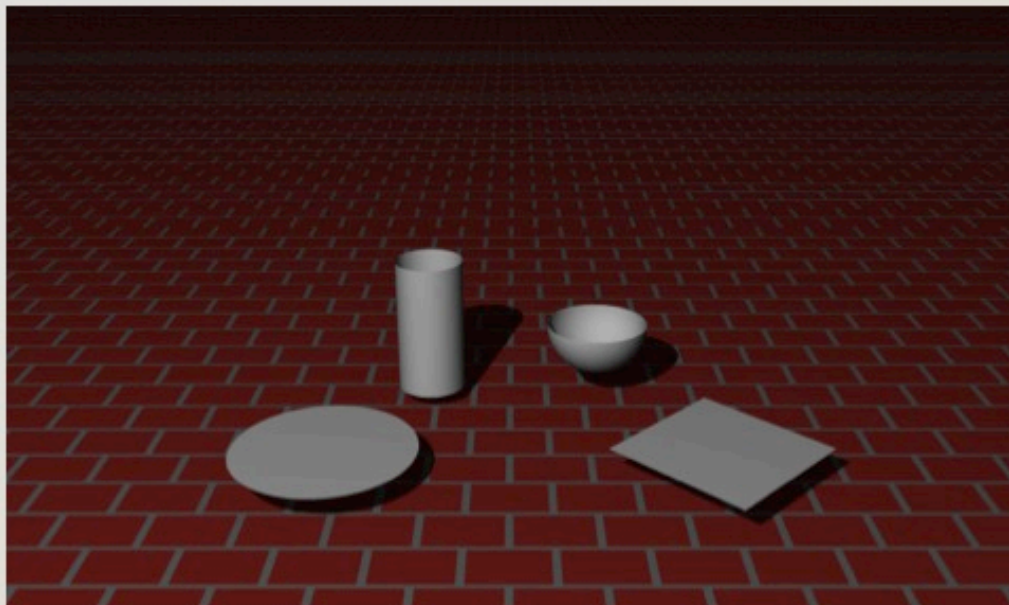
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Simulating Walls

- Need confining surfaces (walls) for these simulations, e.g. to model apparatus or rock faces.
- New constraint:  $|\mathbf{r}_{\text{impact}} - \mathbf{c}| = s$ , where  $\mathbf{c}$  is contact point.
- Often consider just uniform gravity:  $d^2\mathbf{r}_i/dt^2 = -\mathbf{g}$ .

Richardson et al. (2011)

# Example Configuration



Ray-traced with POV-Ray

wall type plane  
transparency 1

wall type disk  
origin -1 0 0.2  
orient 0 0 1  
radius 0.5

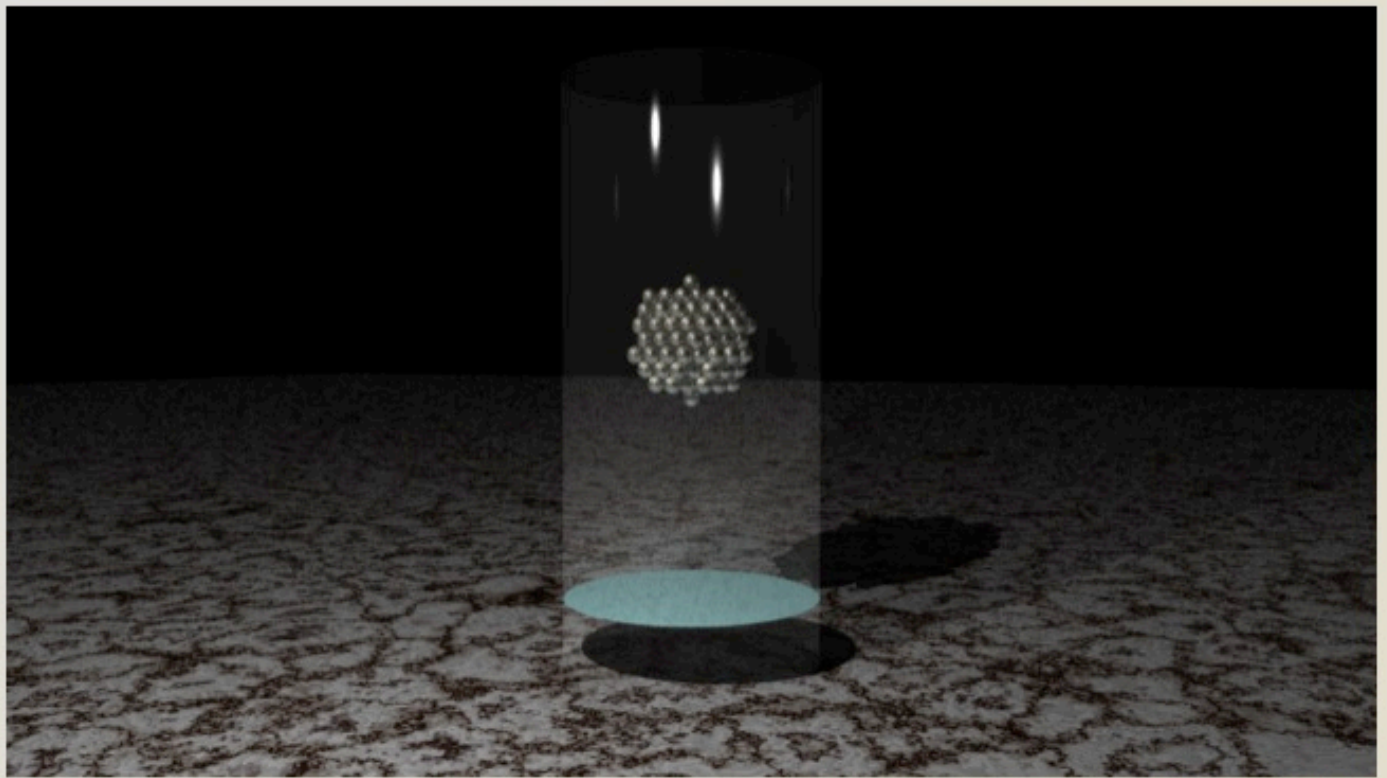
wall type cylinder-finite  
origin -0.5 1 0.5  
radius 0.2  
length 0.8

wall type shell  
origin 0.5 1 0.5  
radius 0.3  
open-angle 90

wall type rectangle  
origin 0.5 0 0.2  
vertex1 -0.6 0.6 0  
vertex2 0.6 0.6 0



# HSDEM Demo



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

**D. C. Richardson**

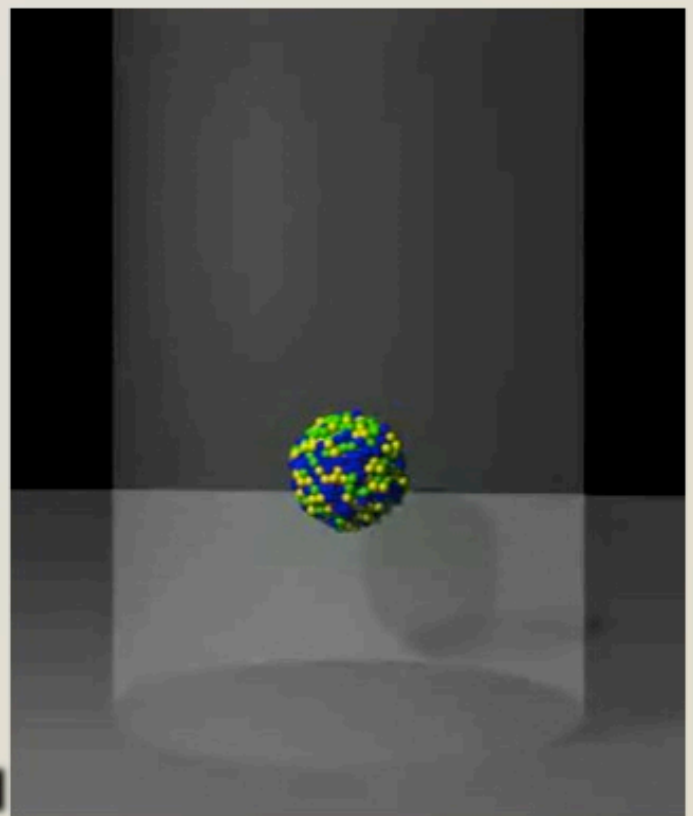
# HSDEM Test: Model Atmosphere

- 1,000 particles in cylinder.
- NO dissipation.
- Particles masses 1, 3, 10.
- Expect vertical profile:

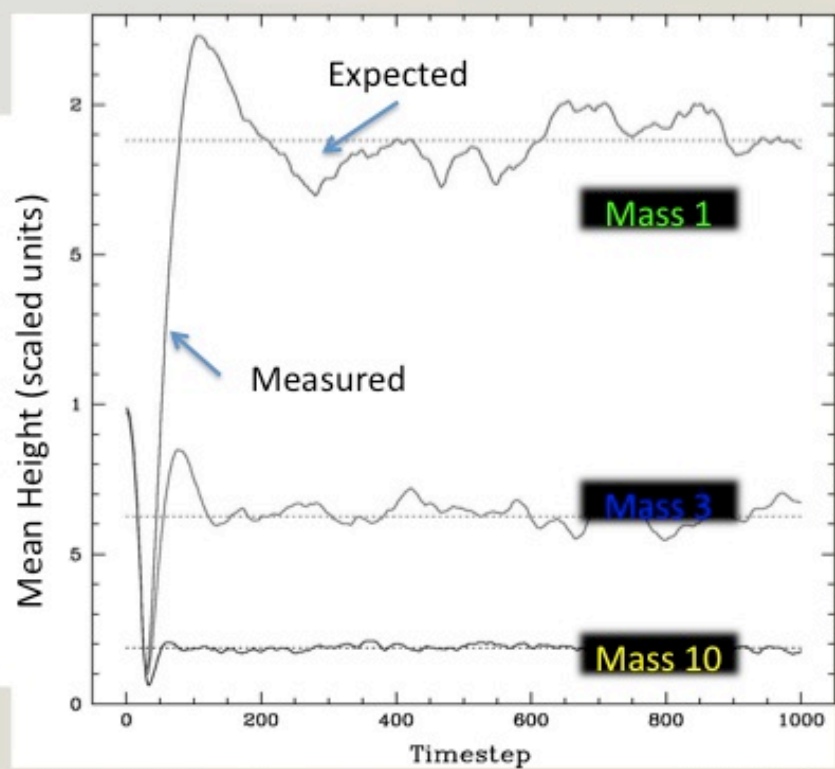
$$P_m(z) \propto \exp\left(-\frac{z}{h_m}\right),$$

- where  $h_m = (2/5) \langle E \rangle / mg$ ,  
and  $\langle E \rangle = E/N$  is the mean  
particle energy (KE + PE).

Green, blue, yellow = mass 1, 3, 10



# Model Atmosphere: Mean Heights



D. C. Richardson

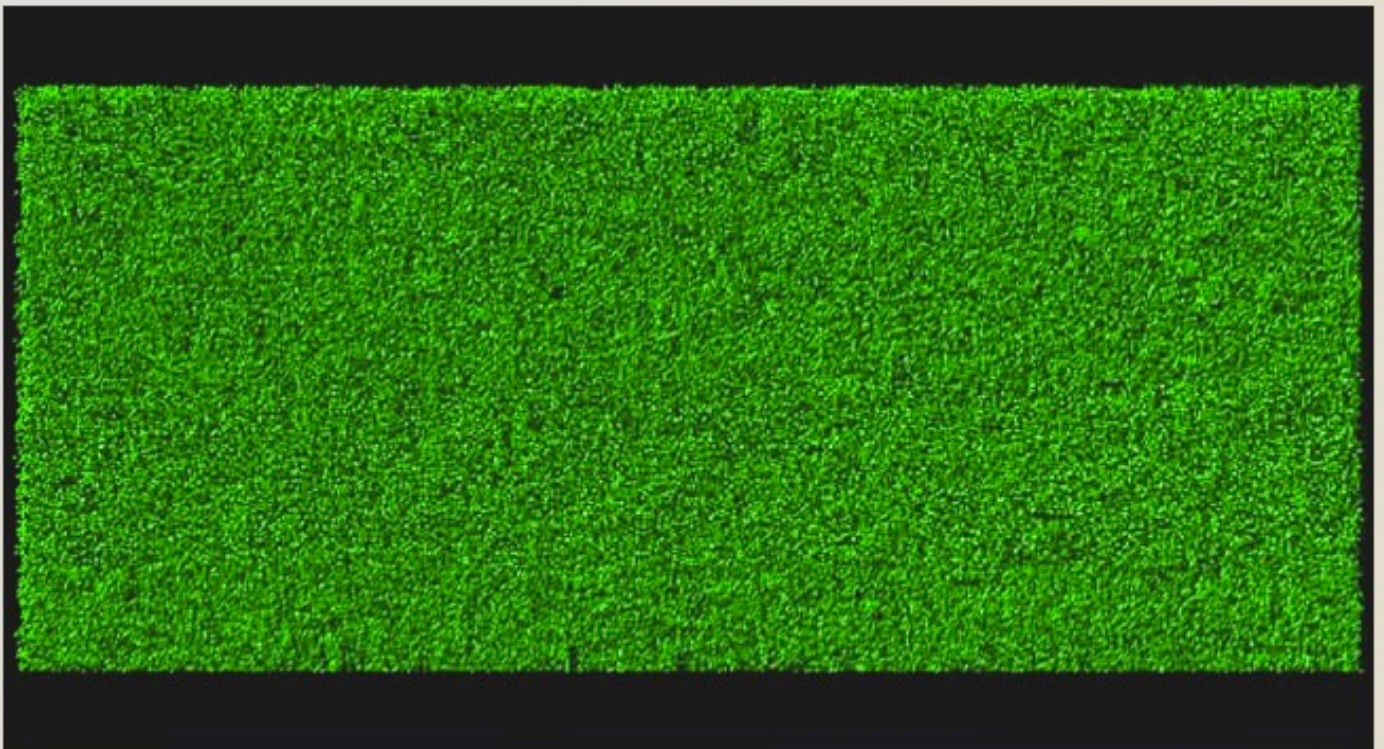
Timestep

*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*



# Cohesion in Planetary Rings?

Perrine et al. (2011)

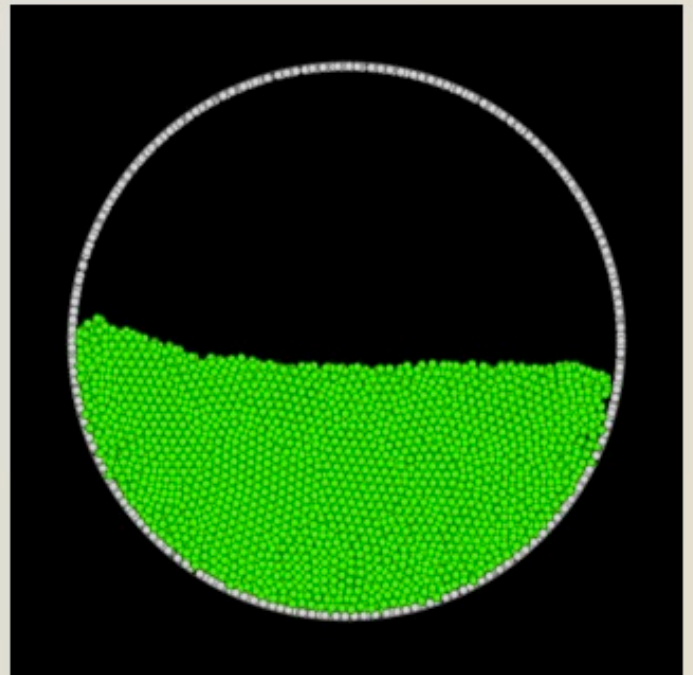


# HSDEM Test: Tumbler

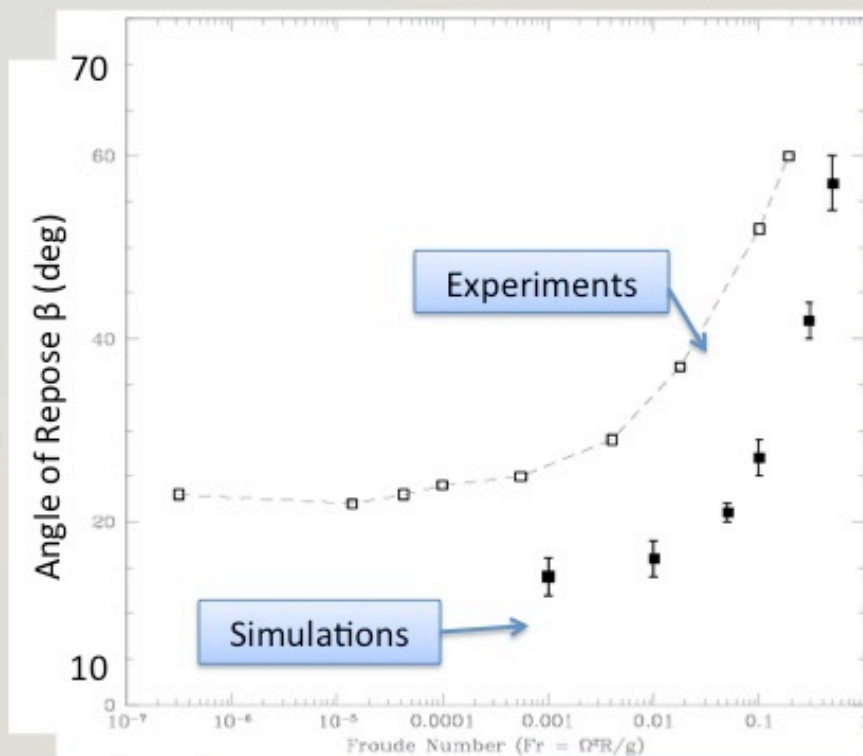
- Experiments show angle of repose is a function of the Froude number,

$$Fr = \frac{\Omega^2 R}{g}.$$

- 3-D simulation,  $Fr = 0.5$ .
- Particles glued to cylinder.



# Tumbler: Dynamic Angles of Repose



D. C. Richardson

$10^{-7}$  Froude Number ( $Fr = \Omega^2 R / g$ ) 1

Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire

# HSDEM Successes and Failures

- HSDEM works well in hot, dilute “gas” regime, less well in cold, dense regime.
  - E.g., dynamic repose angles too low in tumbler experiments.
- What is missing is “stickiness” and “true” surface friction.

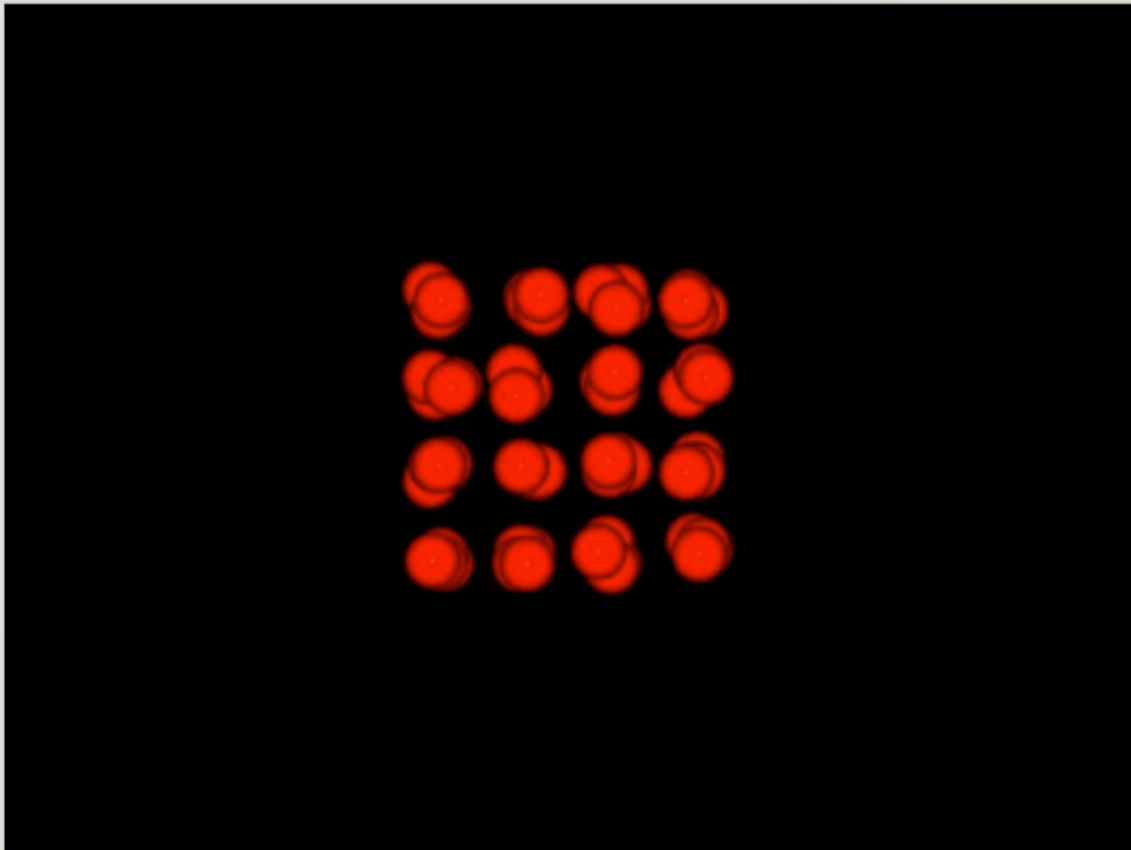
# SSDEM as a Tool for the Simulation of Granular Physics

## Strategy:

- Allow the spherical particles used in pkdgrav to penetrate each other so that we can simulate the contact forces that occur when grains collide.
- Use the instantaneous momentum state and overlap history of the particles to solve for and to apply a robust treatment frictional forces.



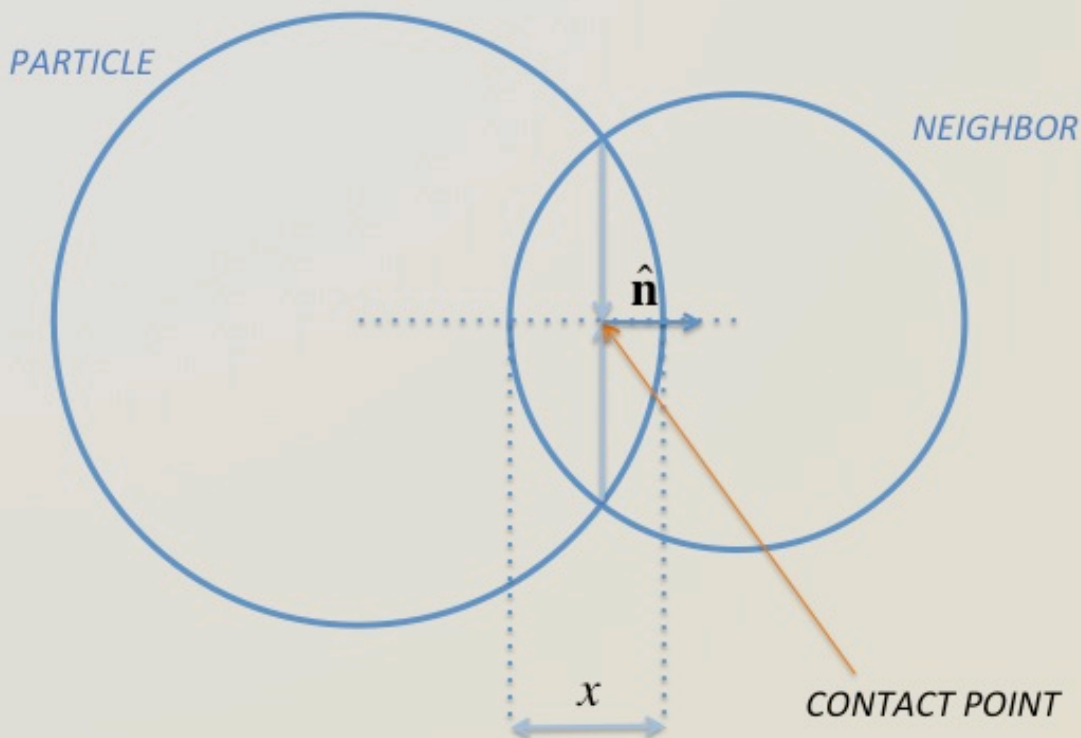
# Self-Collapse in SSDEM



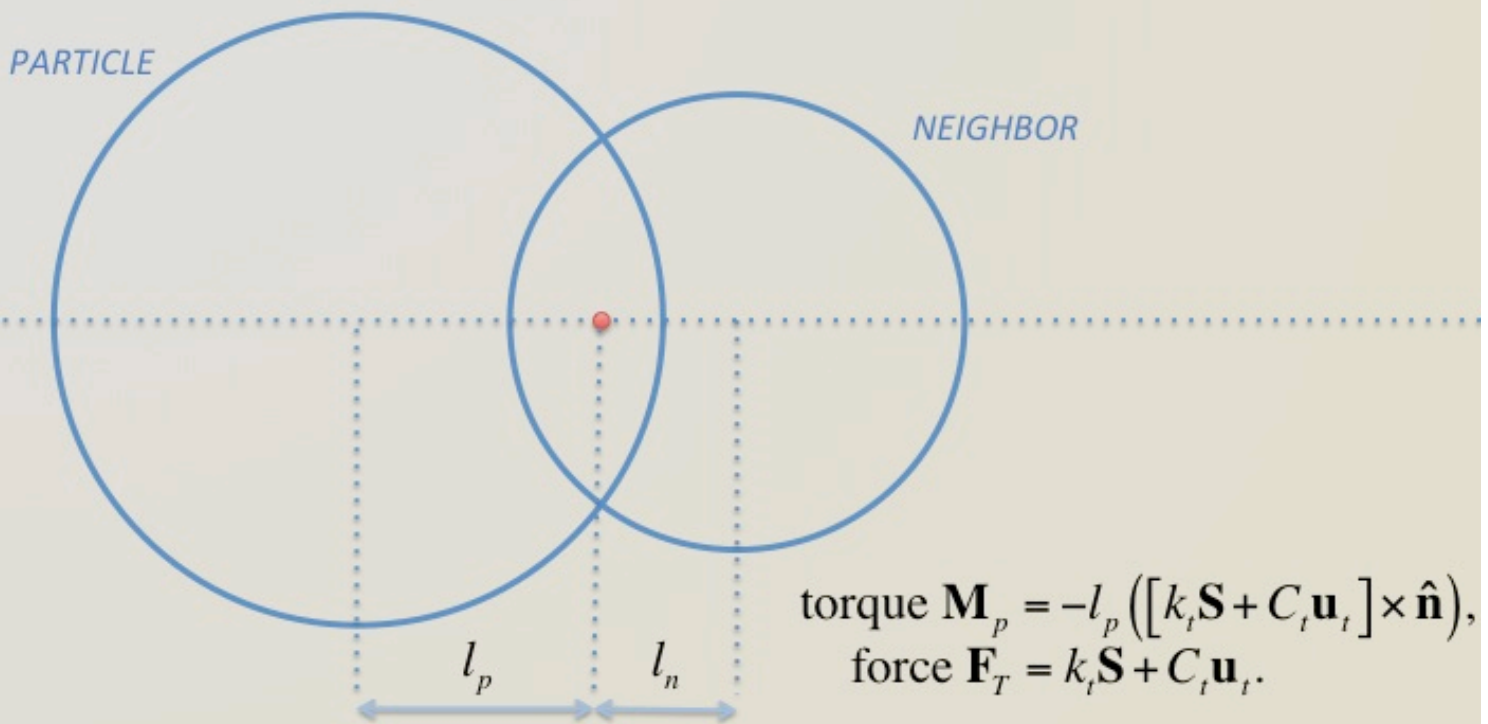
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# SSDEM: Normal Restoring Force

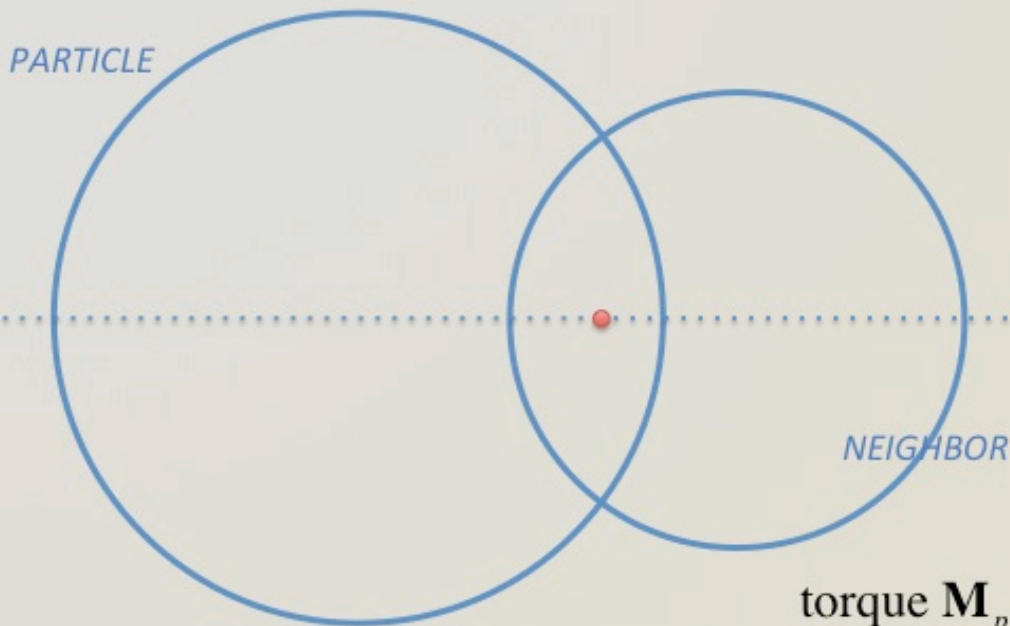
$$\mathbf{F}_N = -(k_n x) \hat{\mathbf{n}} + C_n \mathbf{u}_n.$$



# SSDEM: Basic Tangential Force

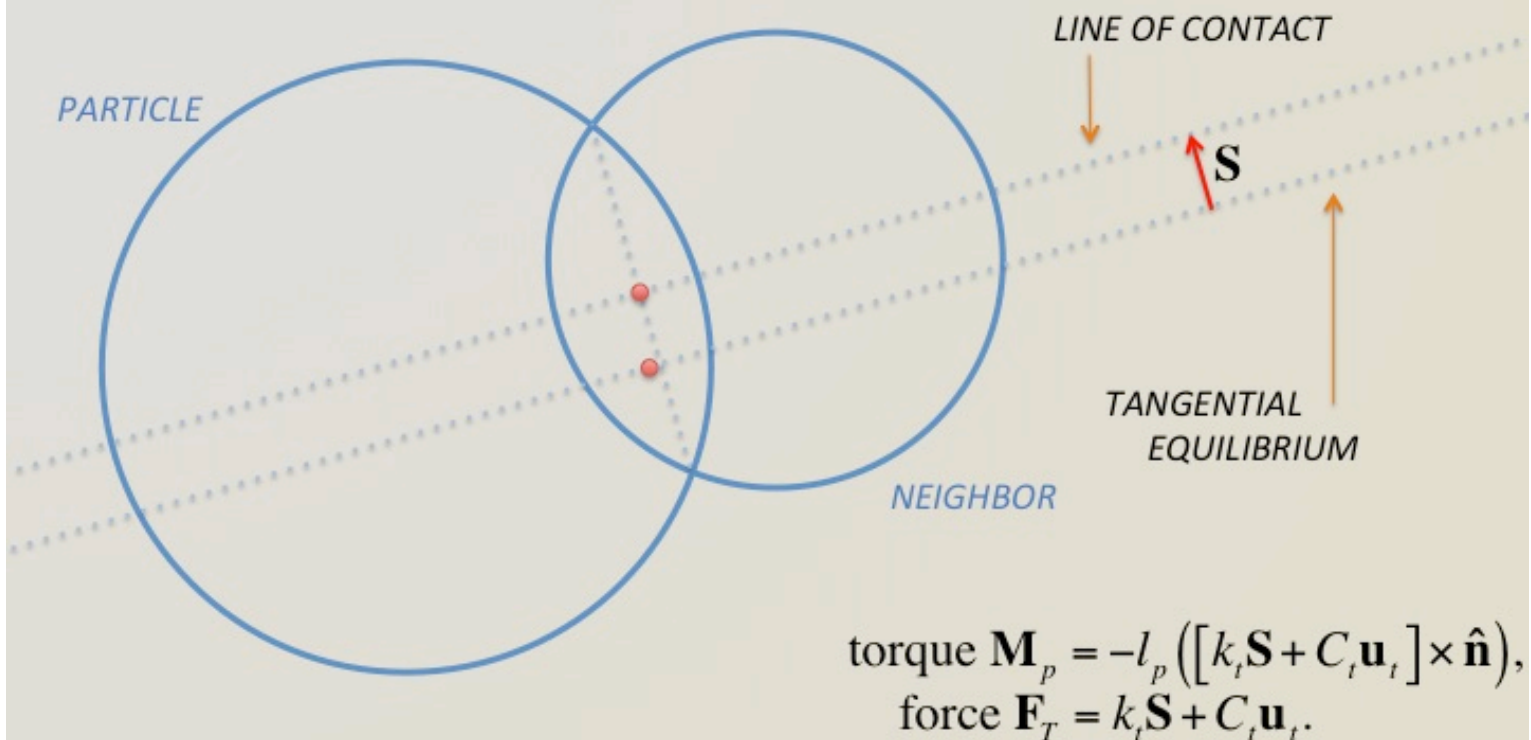


# SSDEM: Basic Tangential Force



$$\begin{aligned}\text{torque } \mathbf{M}_p &= -l_p \left( [k_t \mathbf{S} + C_t \mathbf{u}_t] \times \hat{\mathbf{n}} \right), \\ \text{force } \mathbf{F}_T &= k_t \mathbf{S} + C_t \mathbf{u}_t.\end{aligned}$$

# SSDEM: Basic Tangential Force





## SSDEM: Extra Frictional Forces

- **Static Friction:**

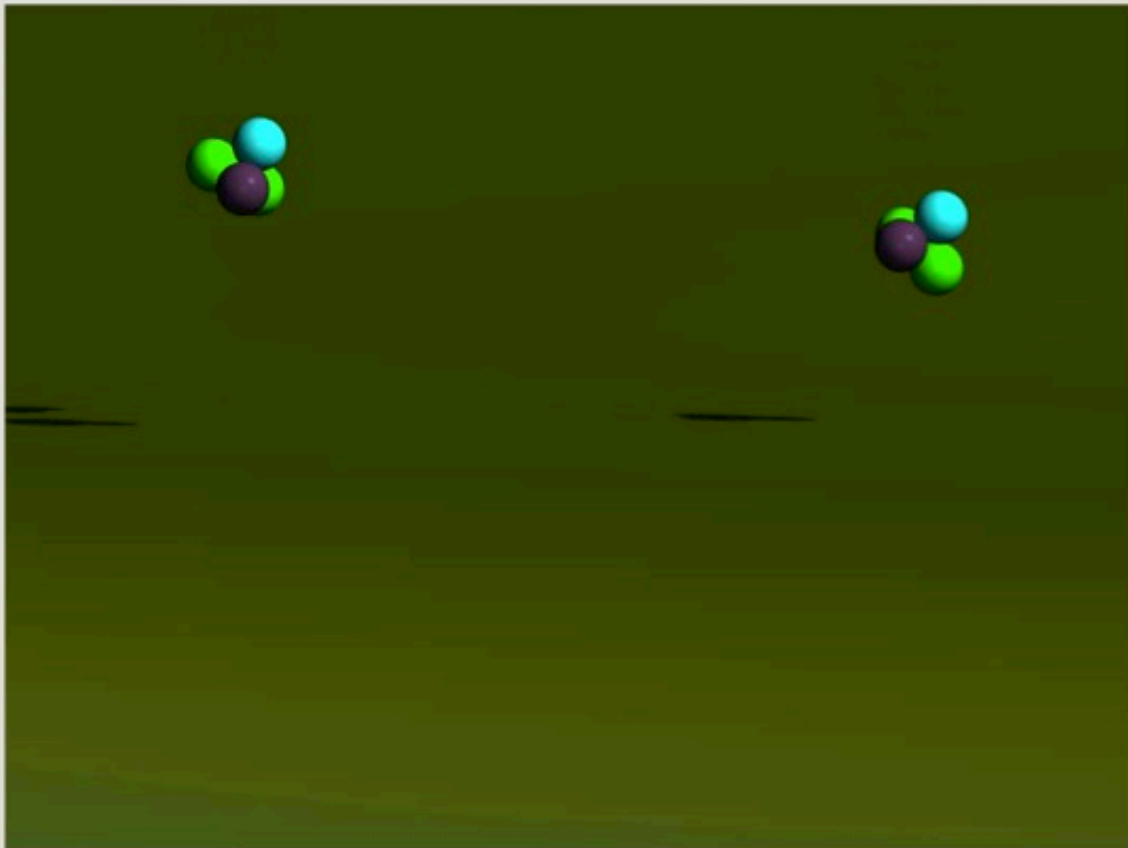
- There is a maximum allowed static frictional force, whose magnitude is given by:

$$\mathbf{F}_N = -(k_n x) \hat{\mathbf{n}}, \quad \hat{\mathbf{n}} \equiv (\mathbf{r}_p - \mathbf{r}_n) / |\mathbf{r}_p - \mathbf{r}_n|.$$

- If  $\mathbf{F}_T$  exceeds this threshold, the elastic component of the tangential force gets reset to zero and contact memory is lost (slip-stick).

- **Rolling Friction:** Damping of rotation along rolling axis.
- **Twisting Friction:** Damping of rotation along the normal axis, which connects the particles' centers.

# Why Include Twisting Friction?



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

## Soft-sphere Discrete Element Method (SSDEM)

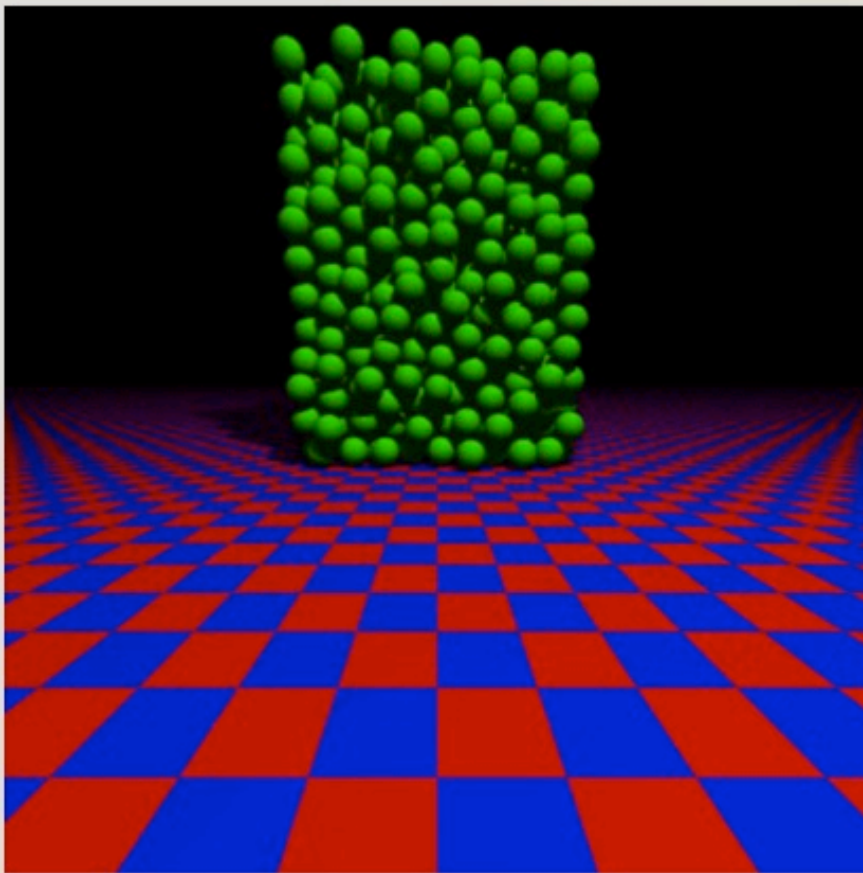
- HSDEM fails in dense and/or near-static regimes.
- In soft-sphere approach, allow particles to overlap, then apply restoring forces with optional damping/friction.
- Disadvantage: need small timesteps to resolve forces.
- Soft-sphere implementation:

Schwartz et al.  
(2012), in prep.

## SSDEM: Boundaries

- Create boundary conditions (walls) in order to model the physical conditions of laboratory set-ups or specific mechanical devices (sample return missions!)
- Easier in SS than in HS, since collisions do not have to be predicted – only need to check for overlap and find the contact point.

## Boundaries: Pile Formation on a Floor



$$\varepsilon_N = 0.80$$

$$\varepsilon_T = 0.65$$

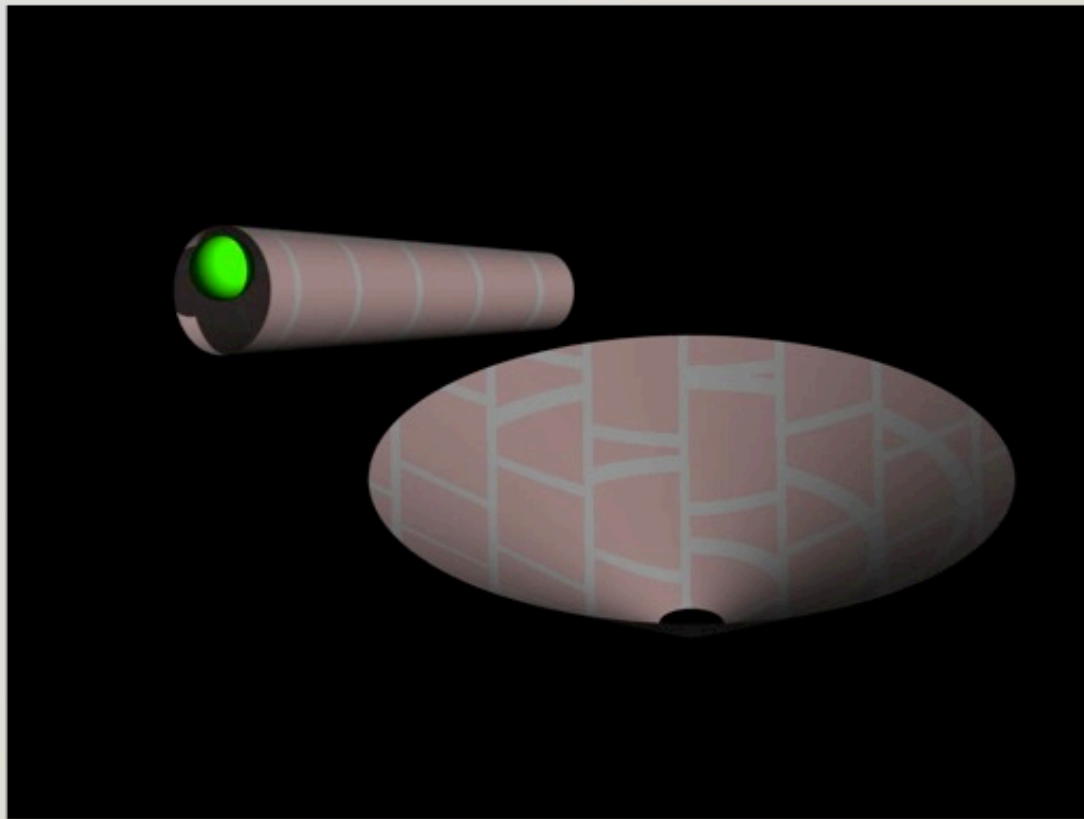
$$\mu_S = 0.20$$

$$\mu_R = 0.10$$

*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*



# Boundaries: The Tapered Cylinder



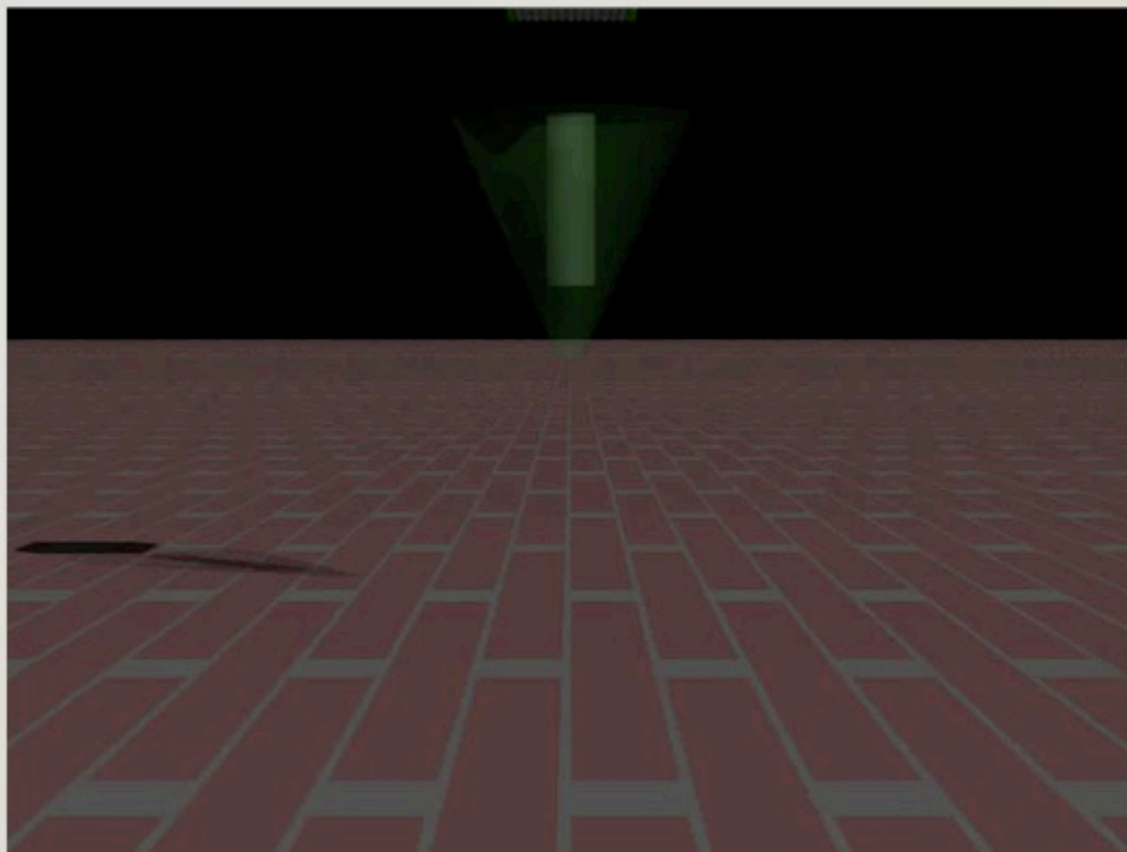
$$\varepsilon_N = 0.80$$

$$\varepsilon_T = 0.65$$

$$\mu_S = 0.20$$

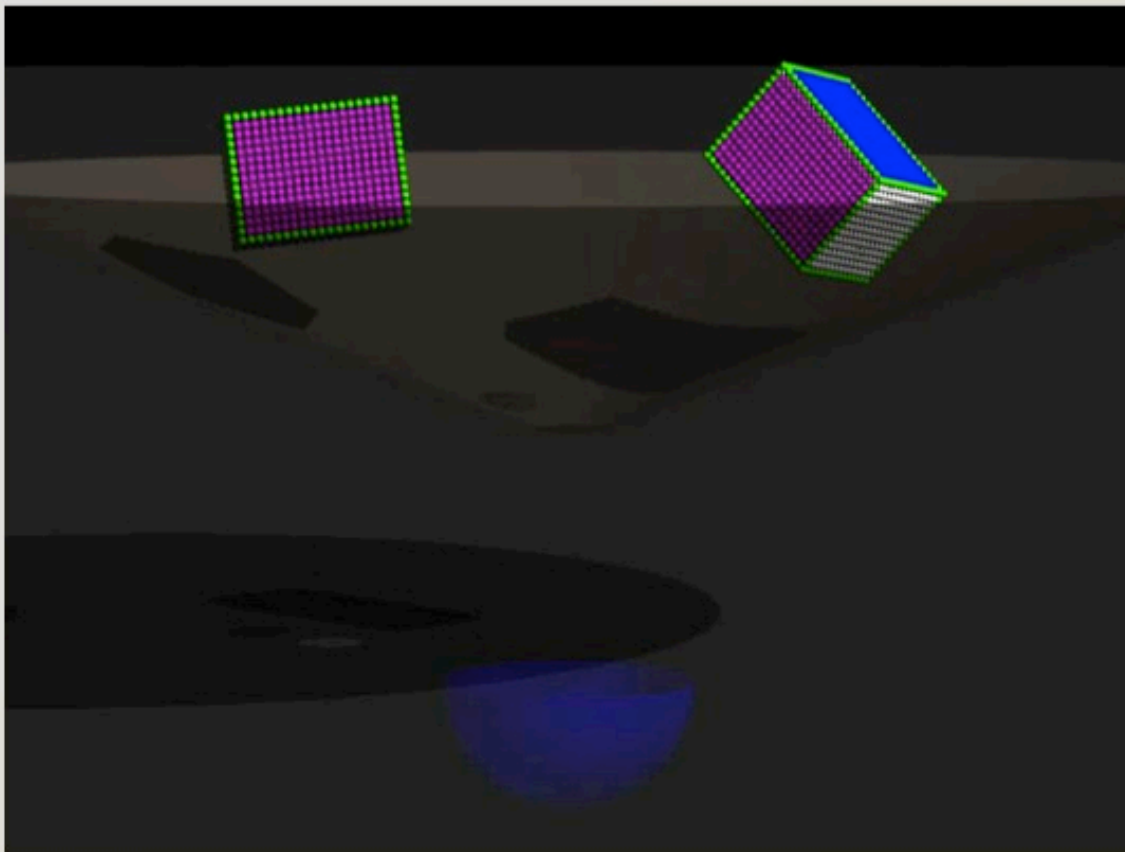
$$\mu_R = 0.10$$

# Boundaries: Motion, Forcing



$$\begin{aligned}\varepsilon_N &= 0.80 \\ \varepsilon_T &= 0.65 \\ \varepsilon_{T,w} &= 0.25 \\ \mu_S &= 0.20 \\ \mu_R &= 0.10\end{aligned}$$

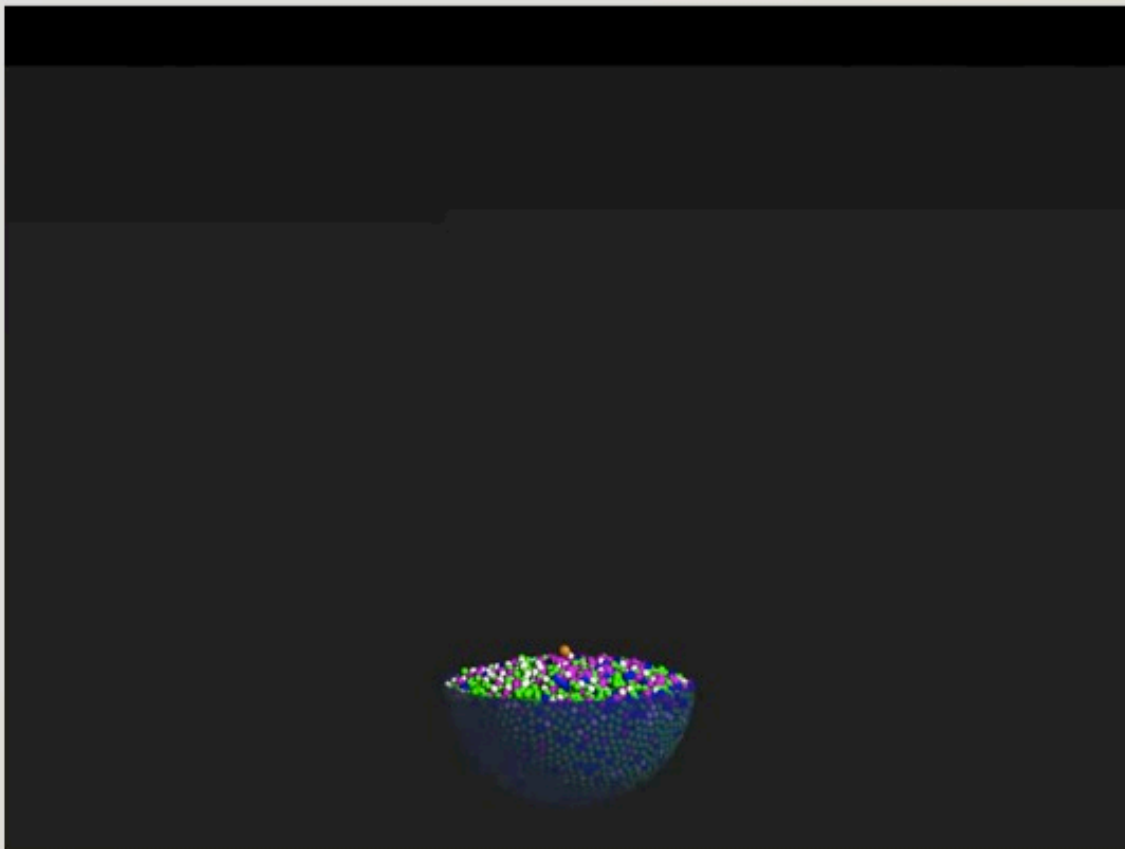
# Filling a Shell with Particles



$$\begin{aligned}\varepsilon_N &= 0.80 \\ \varepsilon_T &= 0.65 \\ \varepsilon_{T,w} &= 0.25 \\ \mu_S &= 0.20 \\ \mu_R &= 0.00\end{aligned}$$

*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

## Impactor at 30°



$$\varepsilon_N = 0.80$$

$$\varepsilon_T = 0.65$$

$$\varepsilon_{T,w} = 0.25$$

$$\mu_S = 0.20$$

$$\mu_R = 0.033$$

Target Spheres:

$$R_{cm} = 1.01$$

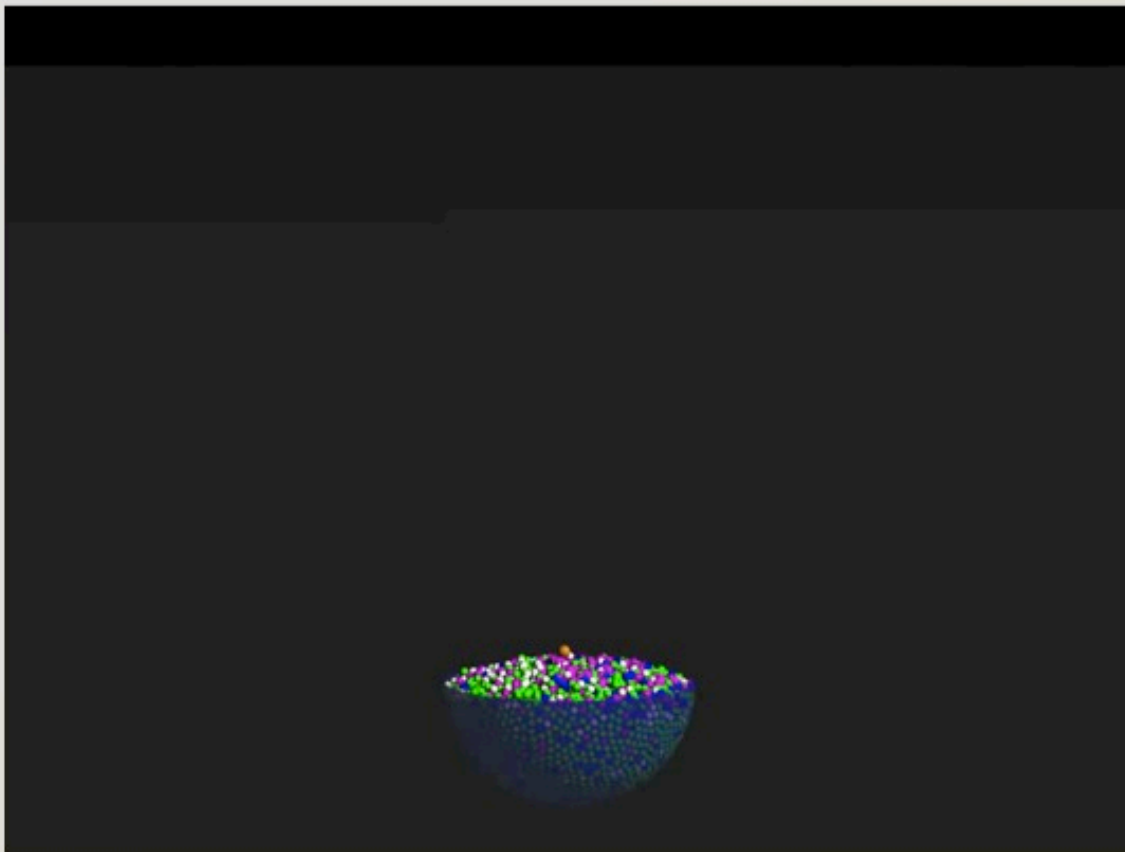
$$\rho_{g/cc} = 2.1$$

Projectile:

$$R_{cm} = 1.52$$

$$\rho_{g/cc} = 2.1$$

## Impactor at 30° (10x speed)



$$\varepsilon_N = 0.80$$

$$\varepsilon_T = 0.65$$

$$\varepsilon_{T,w} = 0.25$$

$$\mu_S = 0.20$$

$$\mu_R = 0.033$$

Target Spheres:

$$R_{cm} = 1.01$$

$$\rho_{g/cc} = 2.1$$

Projectile:

$$R_{cm} = 1.52$$

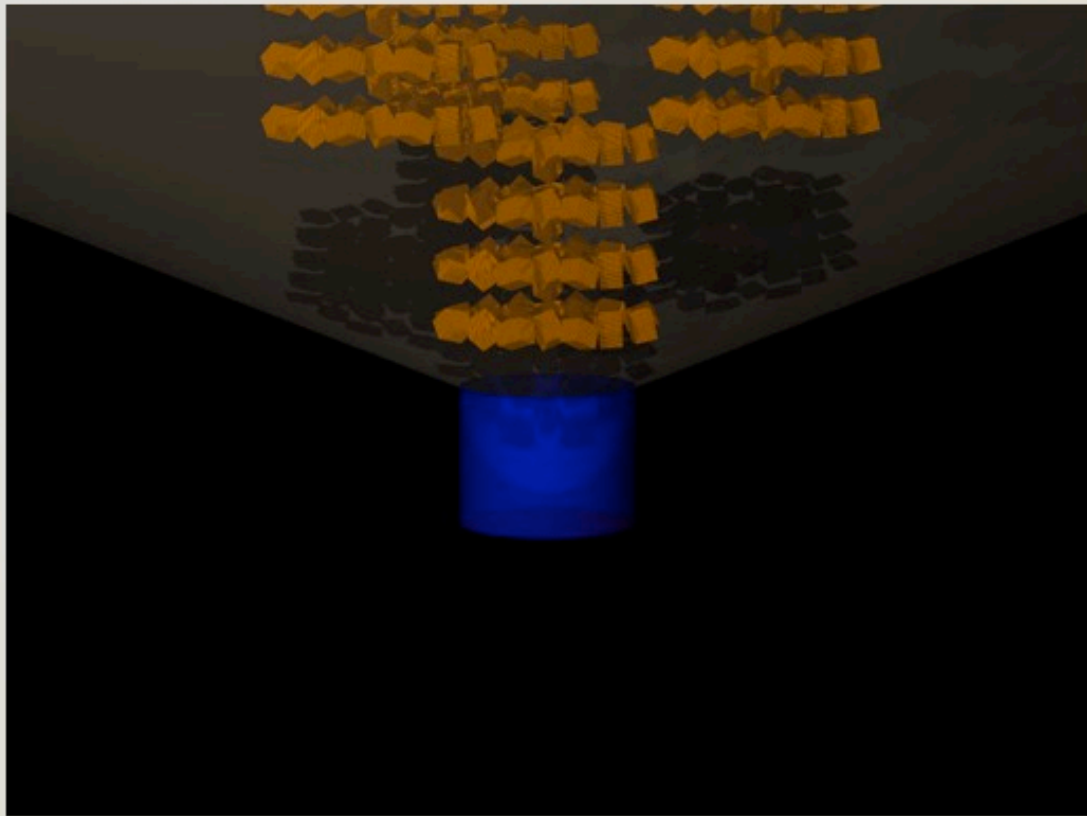
$$\rho_{g/cc} = 2.1$$



## SSDEM: Laboratory Experiments

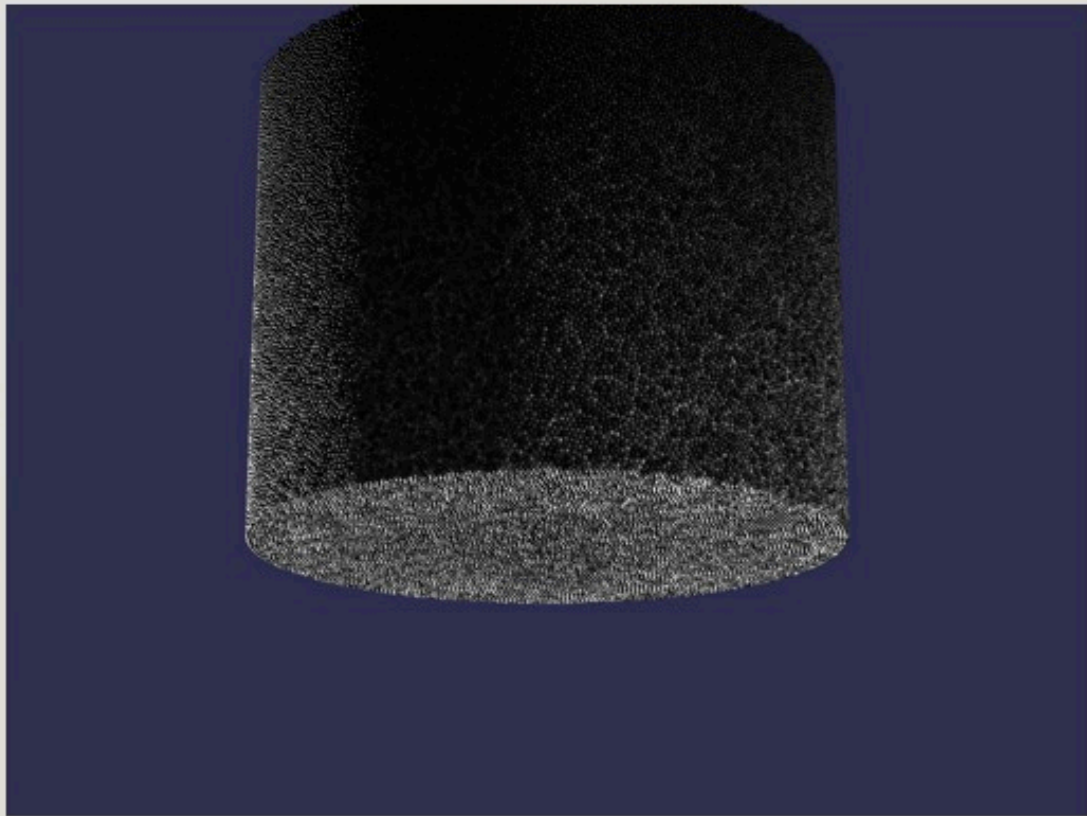
- Validate and tune code by comparing with laboratory experiments.
  - **Cylindrical Hopper**
  - **Sintered Glass Bead Agglomerates**
    - Combine soft-sphere with cohesive “Springs”

## SSDEM Test: Hopper ( $N = 1.5 \times 10^6$ )



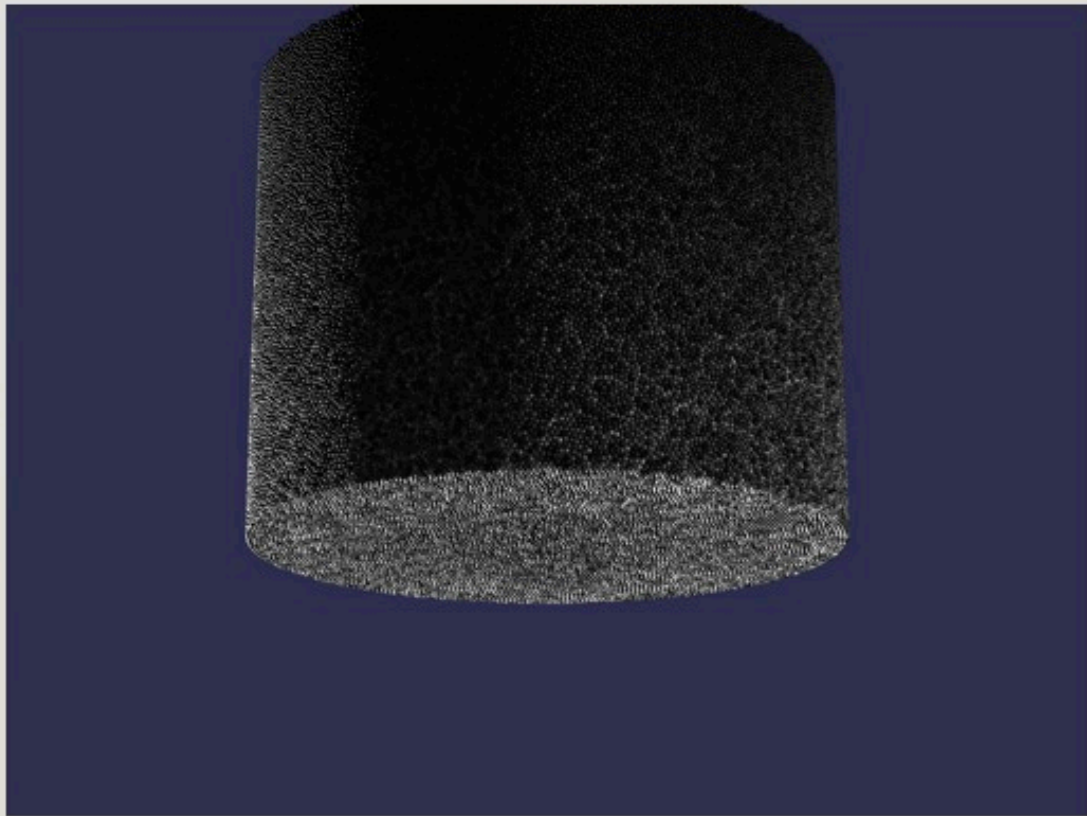
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Hopper: Force Networks (Real Time)



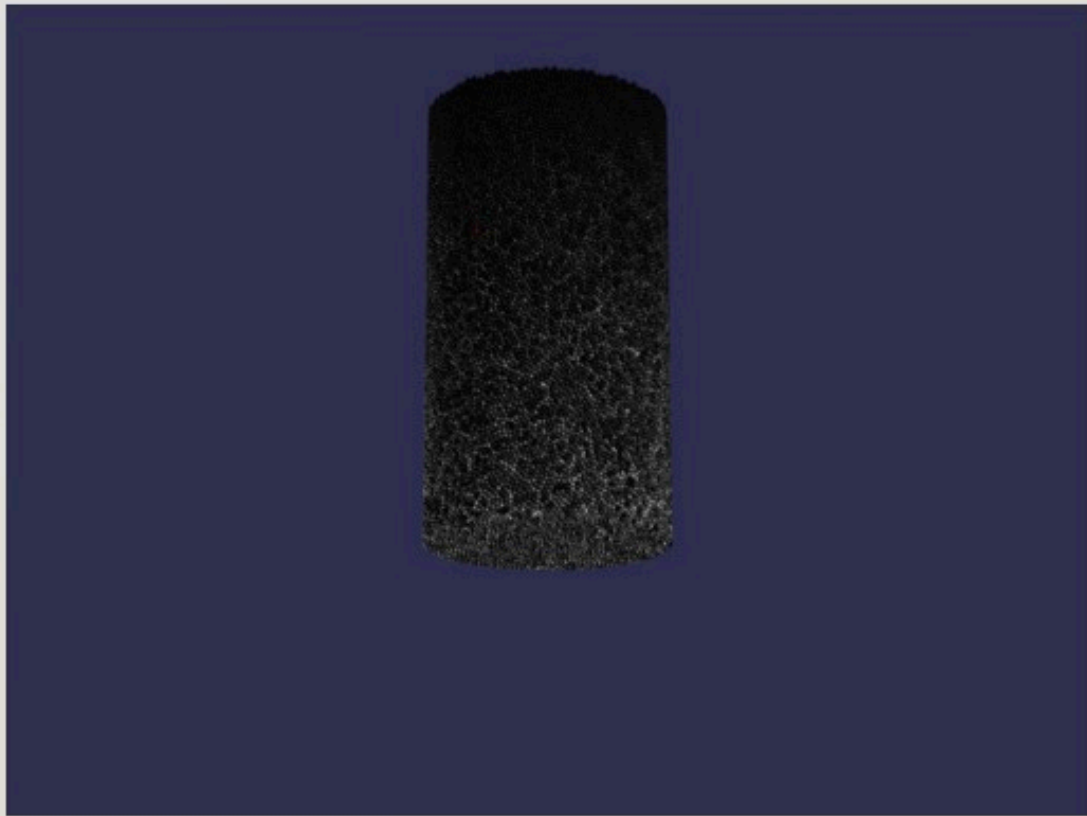
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Hopper: Force Networks (Peek Inside)



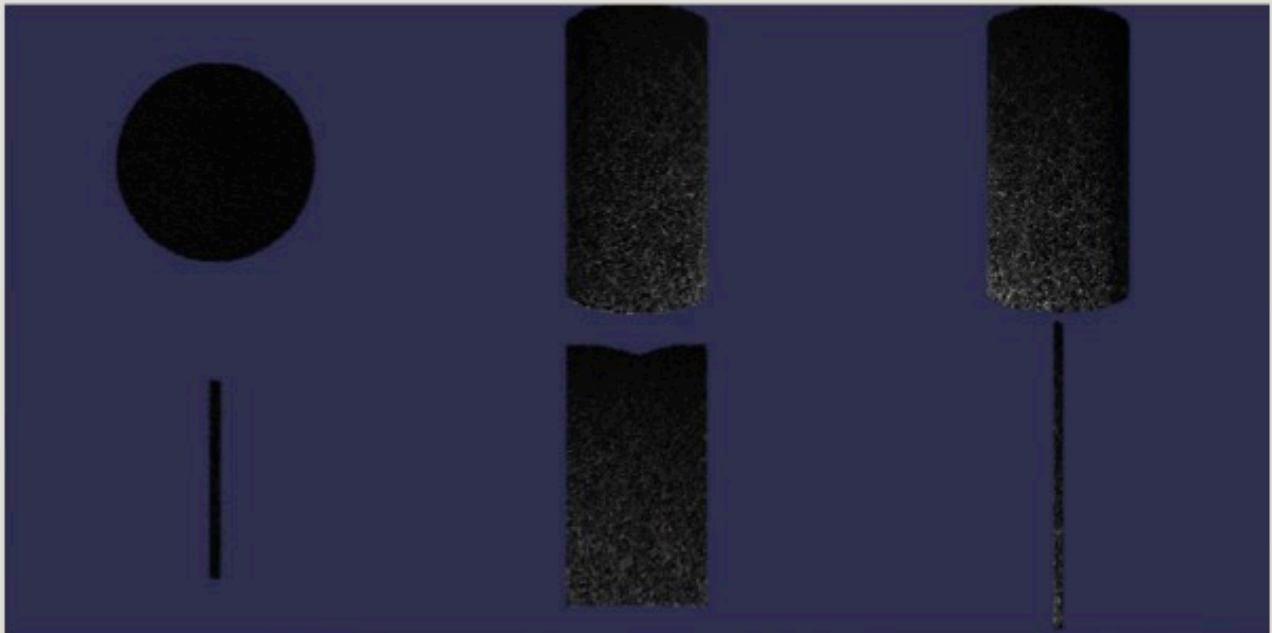
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Hopper: Force Networks (Real Time)



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Hopper: Force Networks (Animation of a Slice)



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*



## Hole Size/Flow-rate Correlation

- Beverloo et al. (1961) find an empirical correlation between the size of the aperture in a cylindrical hopper and the flow-rate through the aperture:

$$W \propto (D_0 - kd)^{5/2}$$

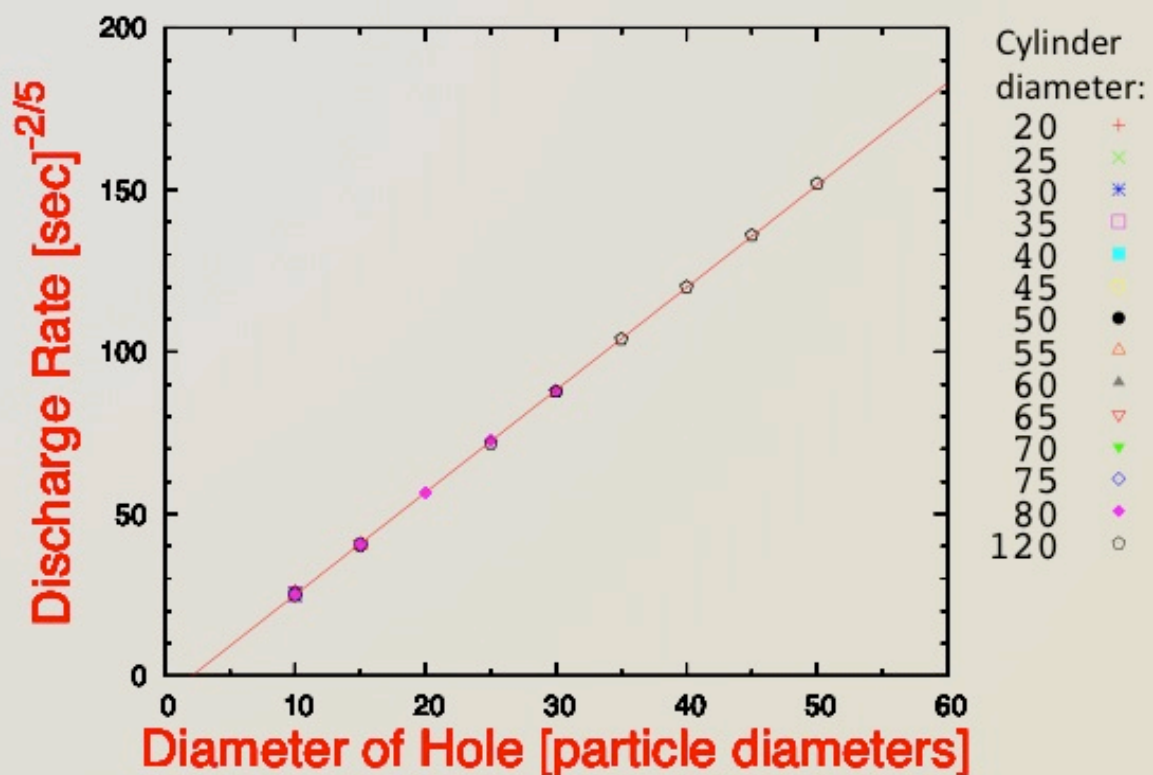
$W \equiv$  flow-rate

$D_0 \equiv$  hole diameter

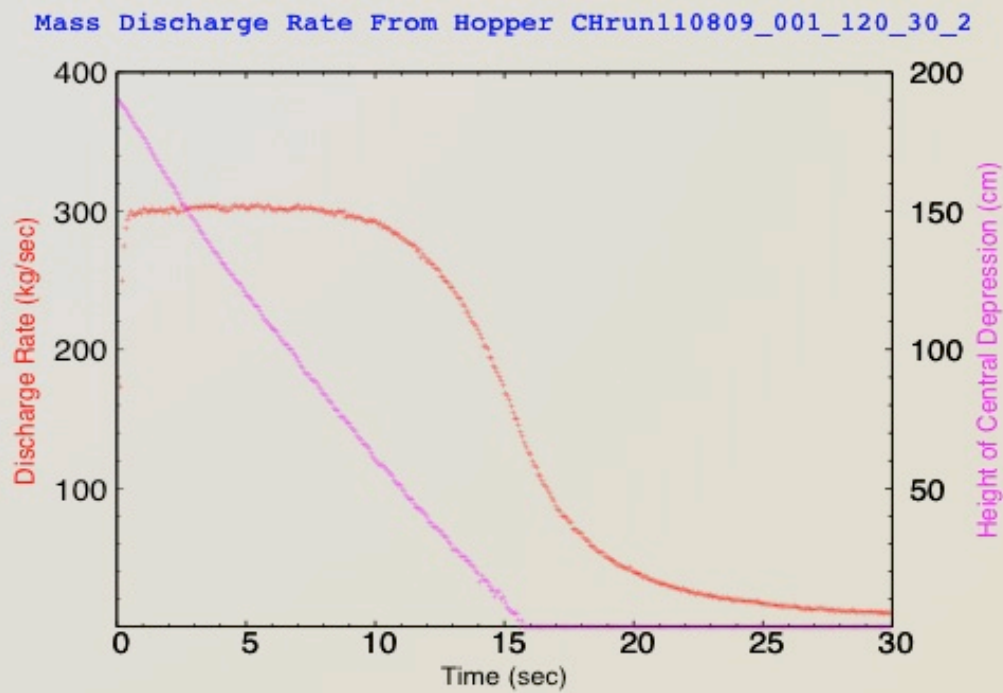
$d \equiv$  particle diameter

$k \equiv$  material constant

# Hole Size/Flow-rate Correlation

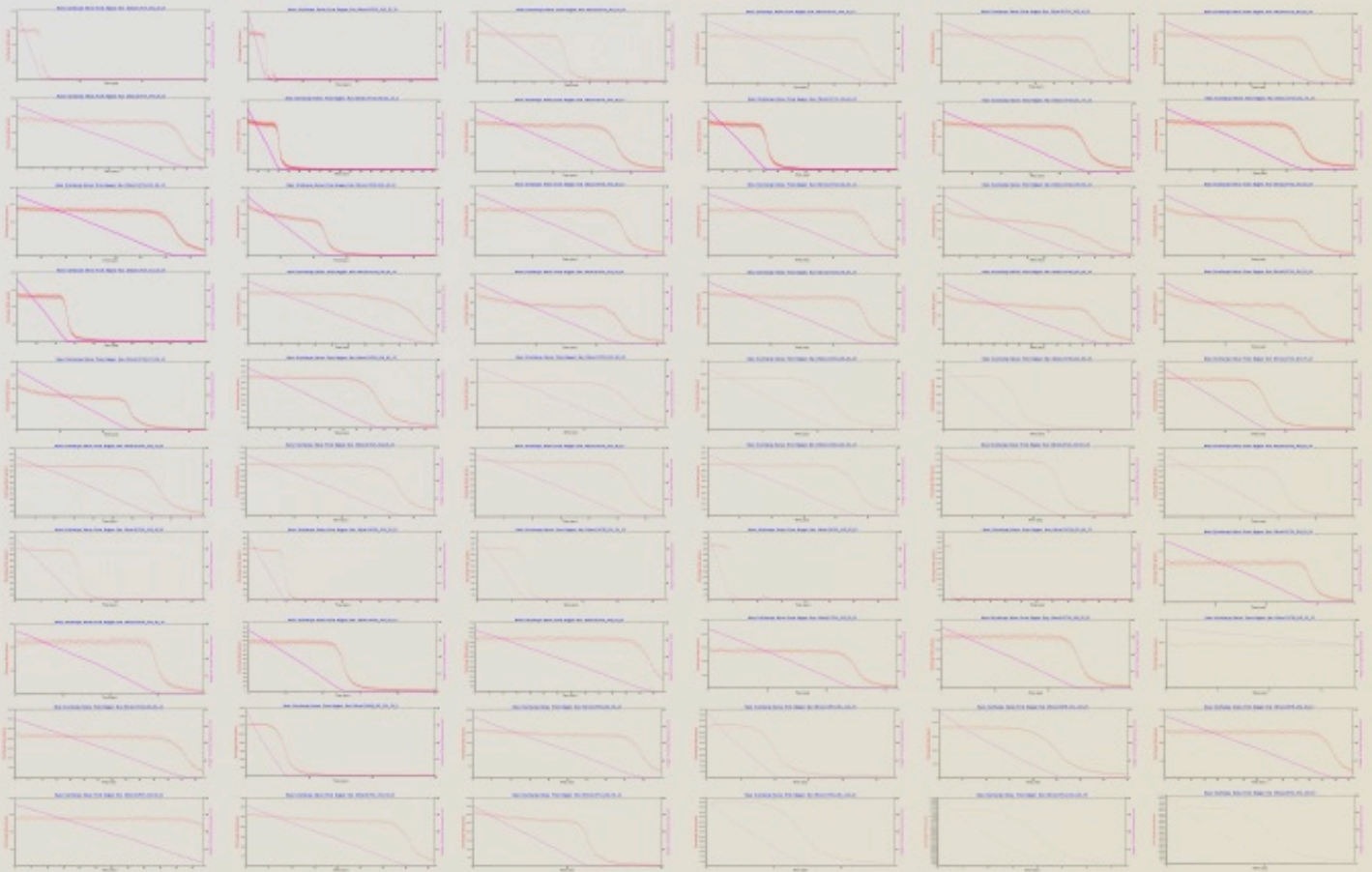


# Flow Rate From Hopper



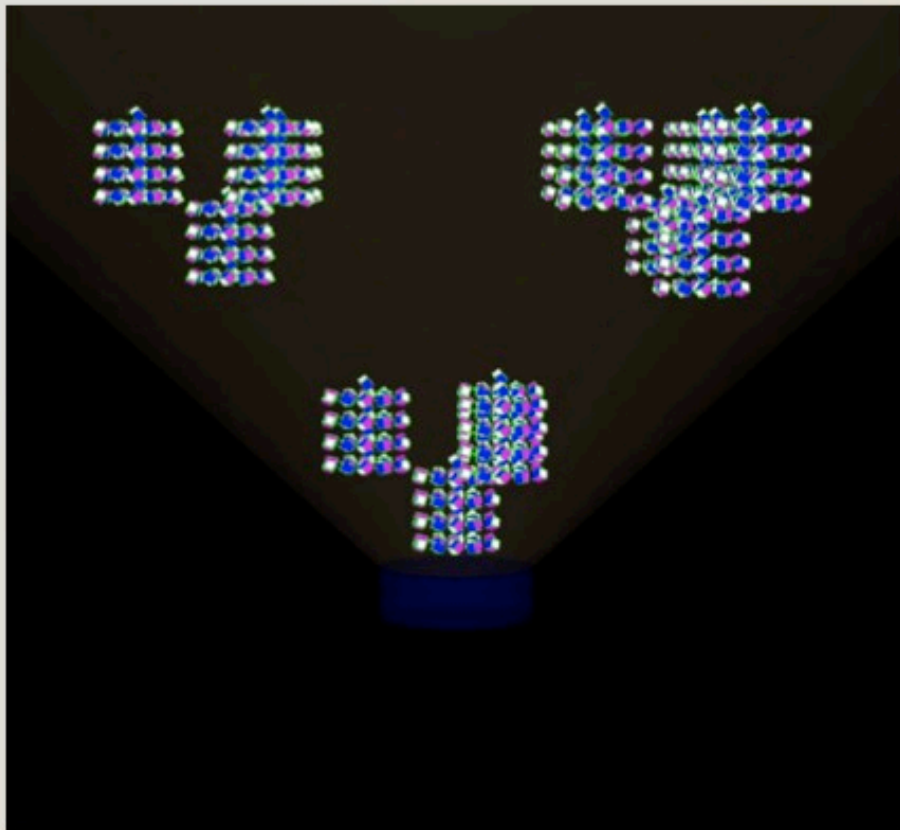
Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire

# 60 Hoppers: Height and Flow-rate vs. Time



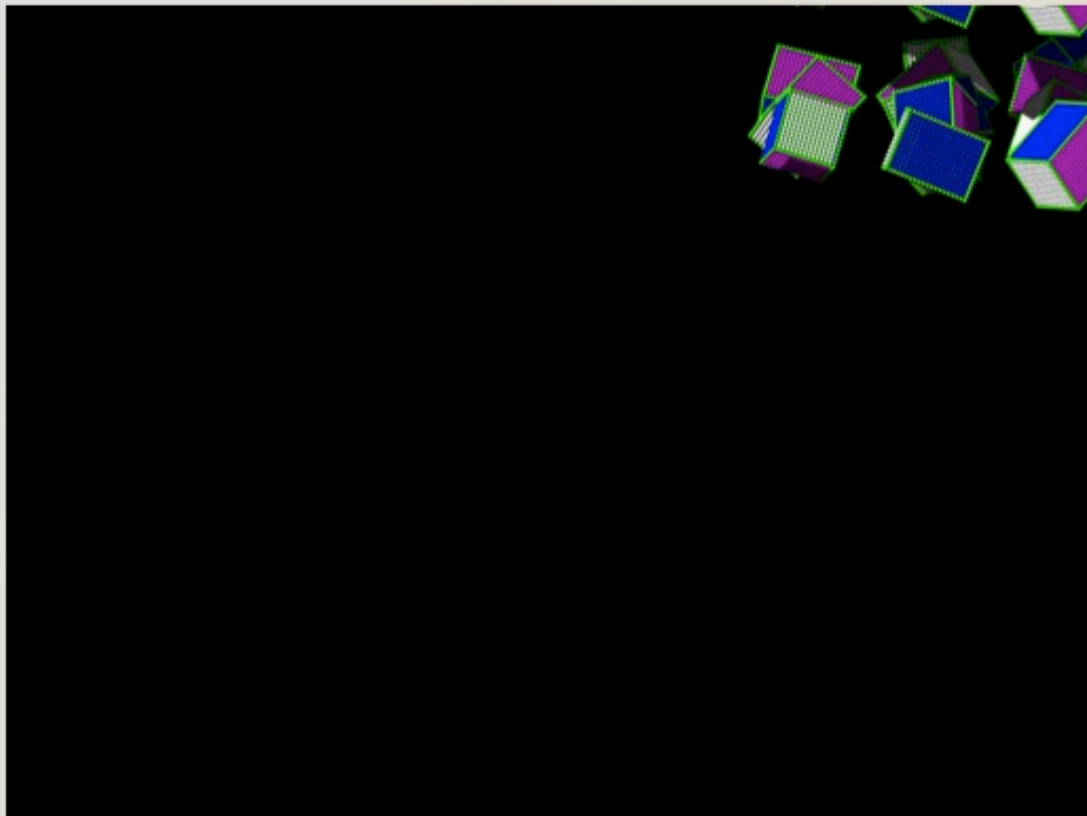
Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire

# Hopper: $N = 6+$ Million



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Hopper: $N = 6+$ Million



*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*



## Cohesion Models in Gravitational Aggregates

*N*-body code (pkdgrav) is used to simulate forces between particles:

- Gravity
- Collisions
- Strength
  - No Deformation (rigid aggregates)
  - **Elastic Deformation equivalent to Hooke's Law** (springs)

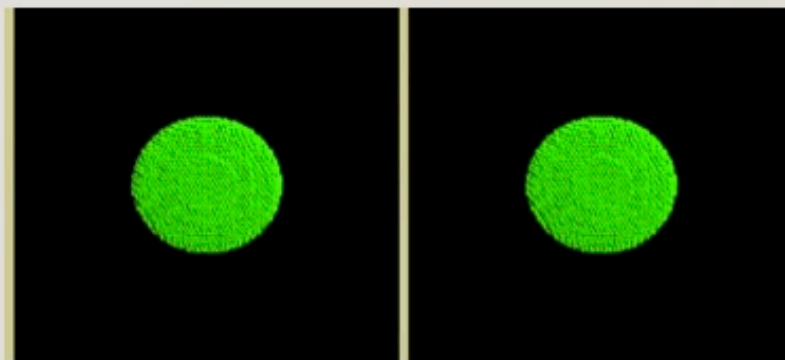
## Modeling Weak Cohesion

- Add simple Hooke's law restoring force between nearby particles.



- Deform elastically up to maximum strain (spring rigidity set by Young's modulus).
- Other force laws can be implemented, e.g. van der Waals.

# Spin Tests With and Without Cohesion



## No COHESION

$Y = 0 \text{ Pa}$

$L = 0 \text{ Pa}$

Spin period  $P = 2.00 \text{ h}$

## COHESION

$Y = 250 \text{ Pa}$

$L = 125 \text{ Pa}$

Spin period  $P = 1.71 \text{ h}$

## COHESION COLOR LEGEND:

green	3 or more springs
yellow	2 springs only
orange	1 spring only
red	no springs left

# Oblate Spheroid, $Y=500$ , $L=250$ Pa

## COLOR LEGEND:

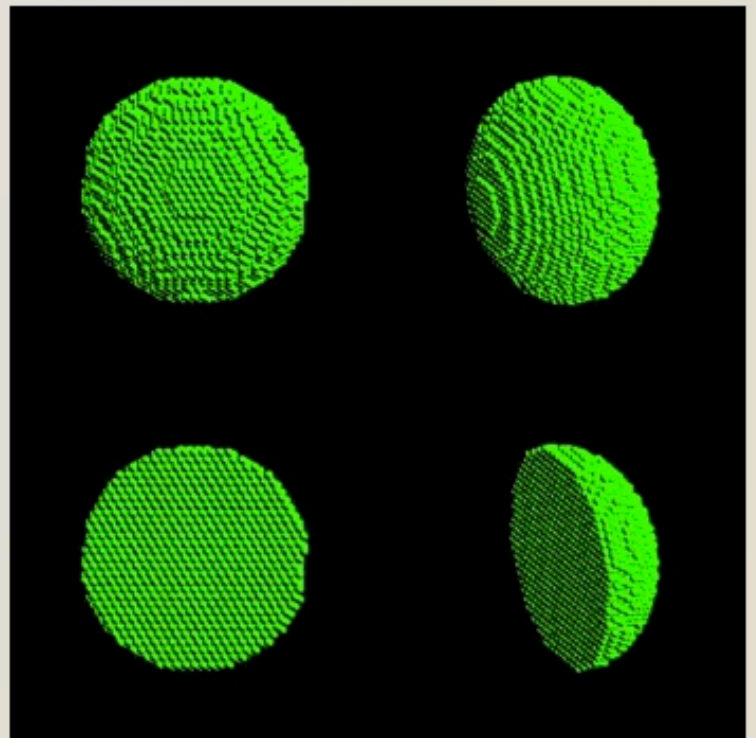
green	3 or more springs
yellow	2 springs only
orange	1 spring only
red	no springs left

Y Std Deviation = 0

L Std Deviation = 0

Spin period  $P = 1.52$  h

Shape  $\alpha = 0.79$



## Elastic (Springs) Model

- Neighboring particles “connected” by springs.
- Each spring is defined by:
  - An equilibrium separation (length at zero strain)
  - A Young’s modulus
  - A maximum stress/strain beyond which spring breaks
  - A damping term
- *Particles are effectively tracers of a continuum solid that deforms under stress until failure.*

## Spring Damping

- Damping force applied along axis of spring.
- Opposes any extension or contraction of spring.
- Simulates viscosity of the continuum solid.
- Defined in code as a fraction of the critical damping, which is given by:

$$\gamma_{CRIT} = \sqrt{4\mu Y(\pi r_{eff}^2) / x_0}$$

$$F_{DAMP} = -\gamma(v - v_{neighbor})$$



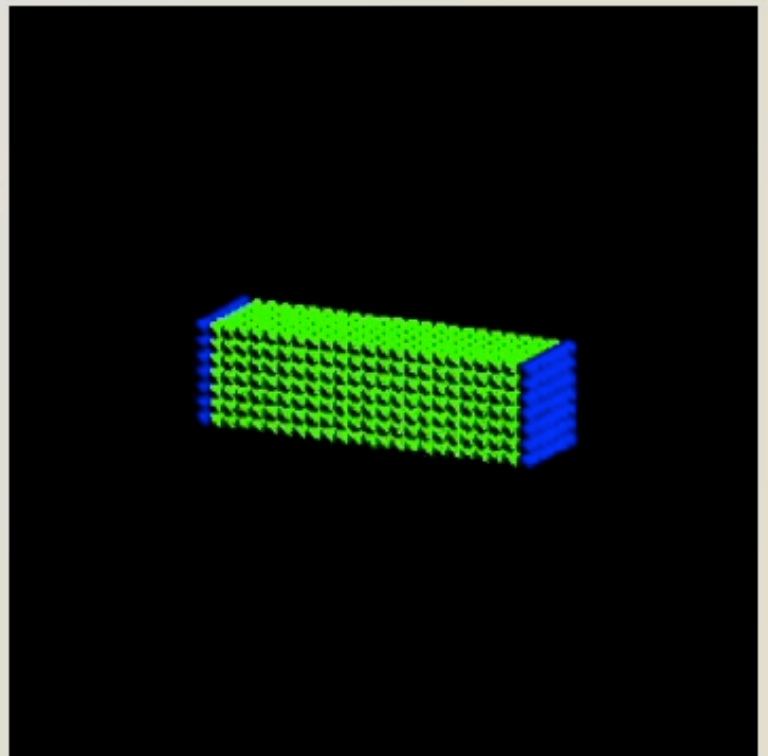
# Spring Strength Distribution

- Can provide strength distributions to give a more realistic outcome.
  - We use a simple stress test to analyze this effect.

## 24x7x7 Cuboid, $Y=250$ Pa, $\epsilon_{MAX}=0.5$

### COLOR LEGEND:

blue	moving wall particle
green	3 or more springs
yellow	2 springs only
orange	1 spring only
red	no springs left

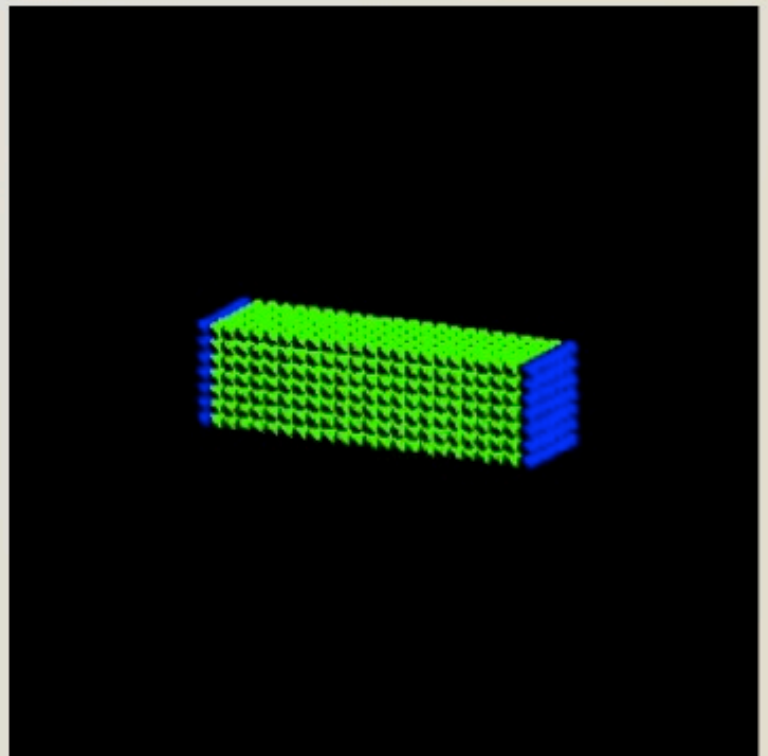


$Y$  Std Deviation = 0 Pa  
 $\epsilon_{MAX}$  Std Deviation = 0.0

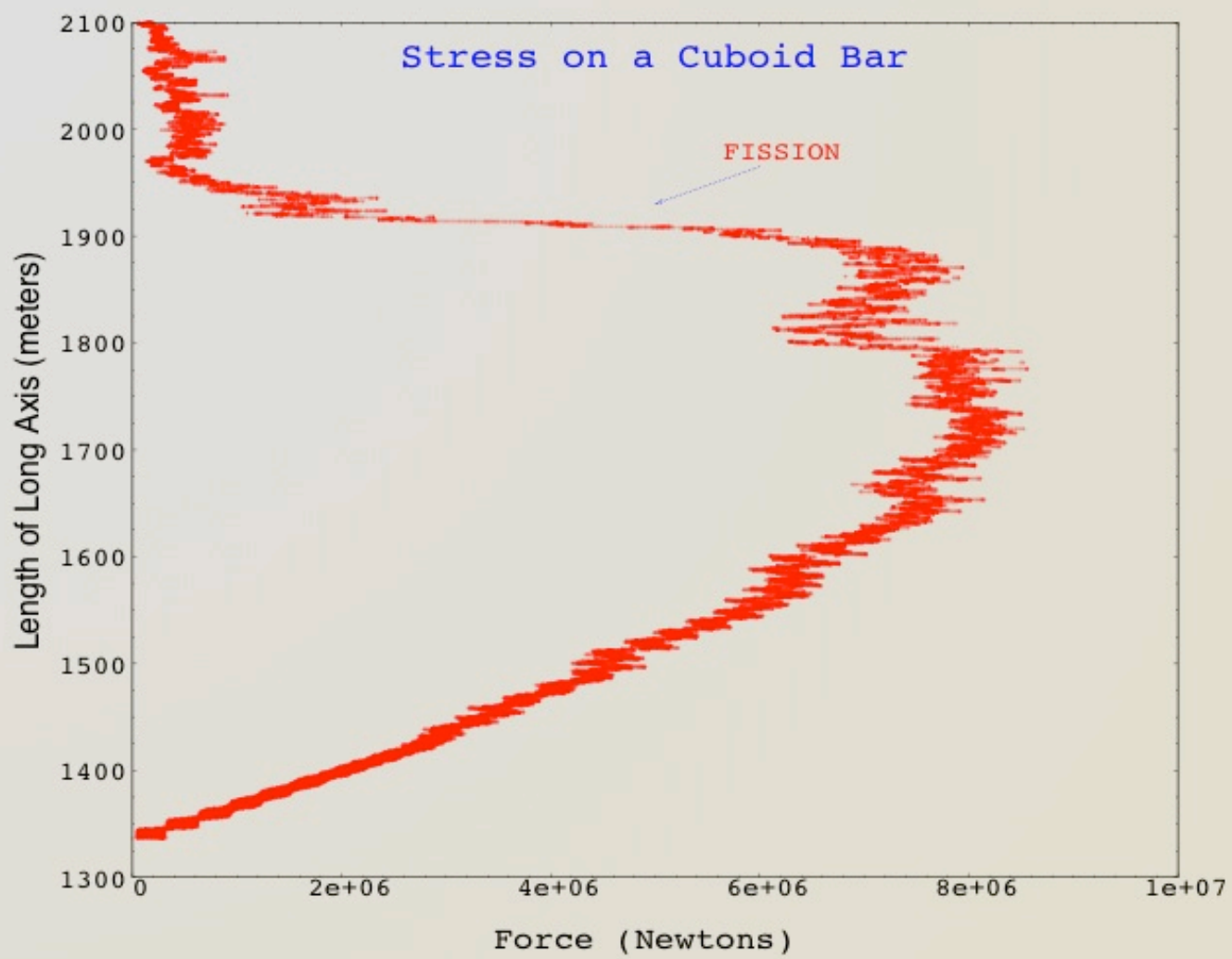
24x7x7 Cuboid,  $\langle Y \rangle = 250$  Pa,  $\langle \epsilon_{MAX} \rangle = 0.5$

COLOR LEGEND:

blue	moving wall particle
green	3 or more springs
yellow	2 springs only
orange	1 spring only
red	no springs left



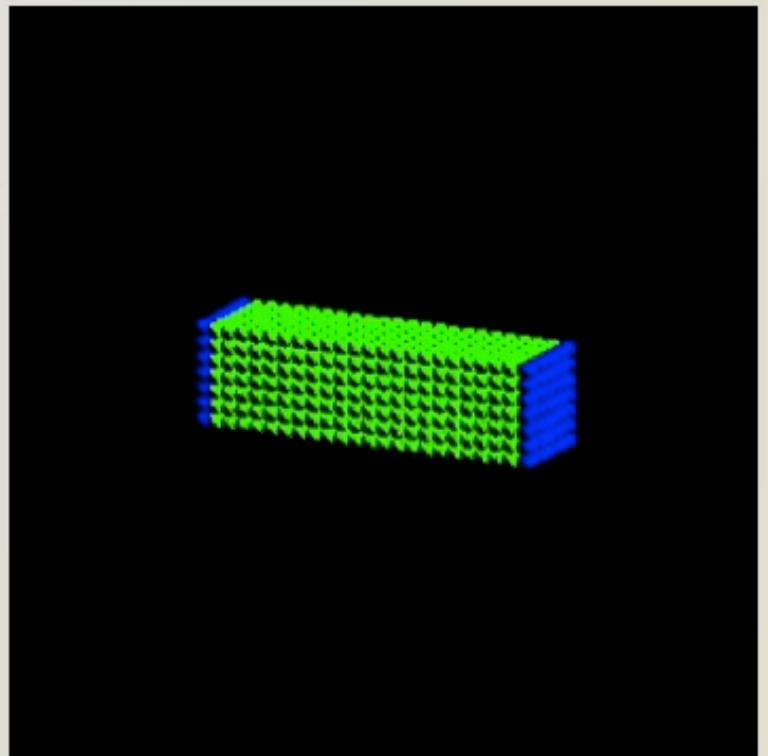
$Y$  Std Deviation = 50 Pa  
 $\epsilon_{MAX}$  Std Deviation = 0.1



24x7x7 Cuboid,  $\langle Y \rangle = 250$  Pa,  $\langle \epsilon_{MAX} \rangle = 0.5$

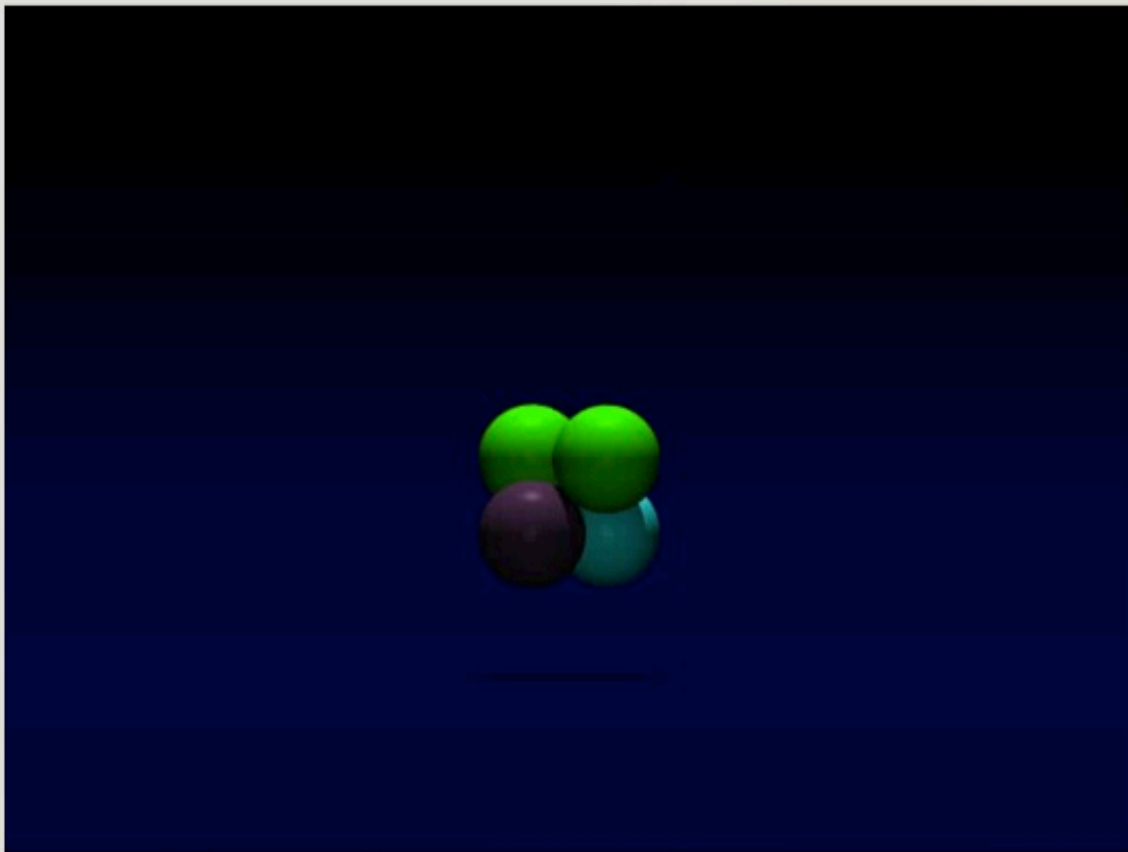
COLOR LEGEND:

blue	moving wall particle
green	3 or more springs
yellow	2 springs only
orange	1 spring only
red	no springs left



$Y$  Std Deviation = 50 Pa  
 $\epsilon_{MAX}$  Std Deviation = 0.1

# Soft Sphere Cohesive Agglomerates

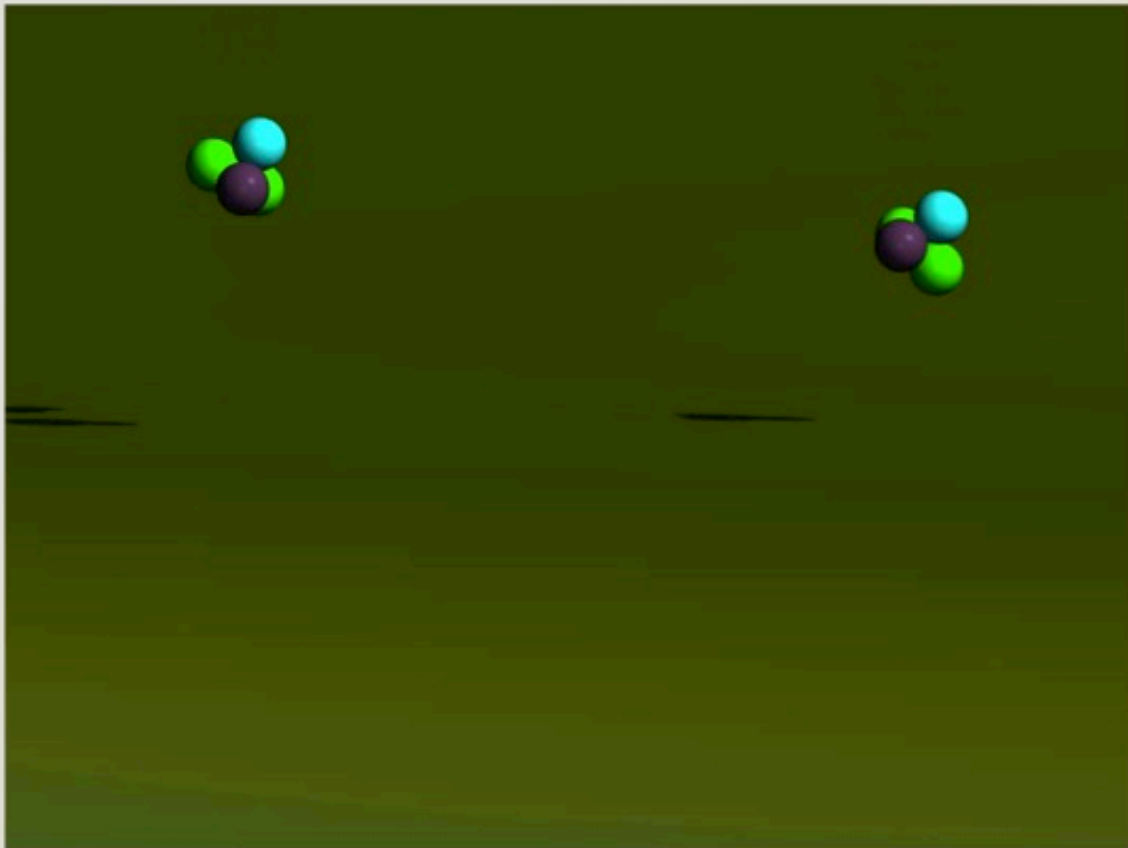


$$\begin{aligned}\varepsilon_N &= 0.50 \\ \varepsilon_T &= 0.65 \\ \varepsilon_{N,w} &= 1.00 \\ \varepsilon_{T,w} &= 0.25 \\ \mu_S &= 0.40 \\ \mu_R &= 0.00\end{aligned}$$

*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

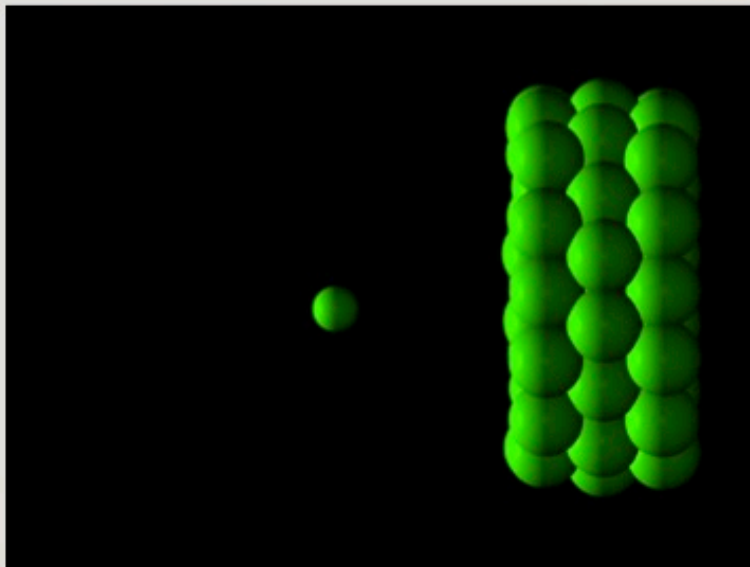


# Soft Sphere Cohesive Agglomerates

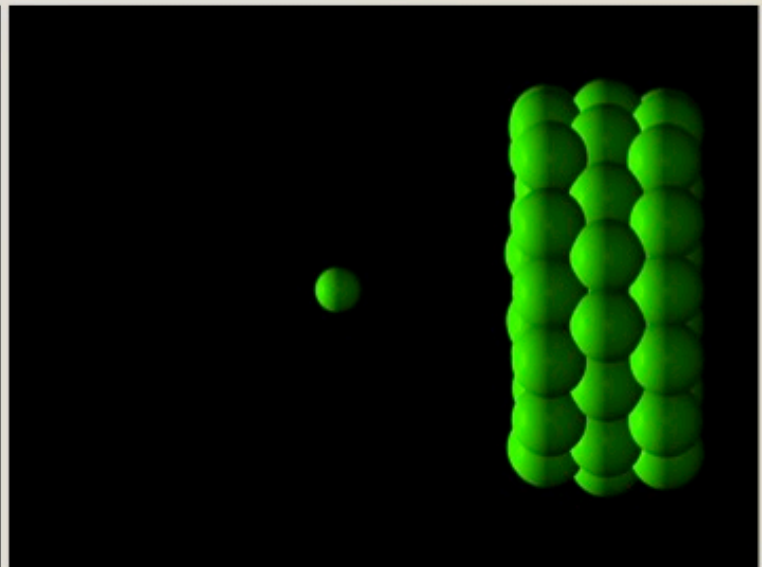


*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Soft Sphere Cohesive Agglomerates



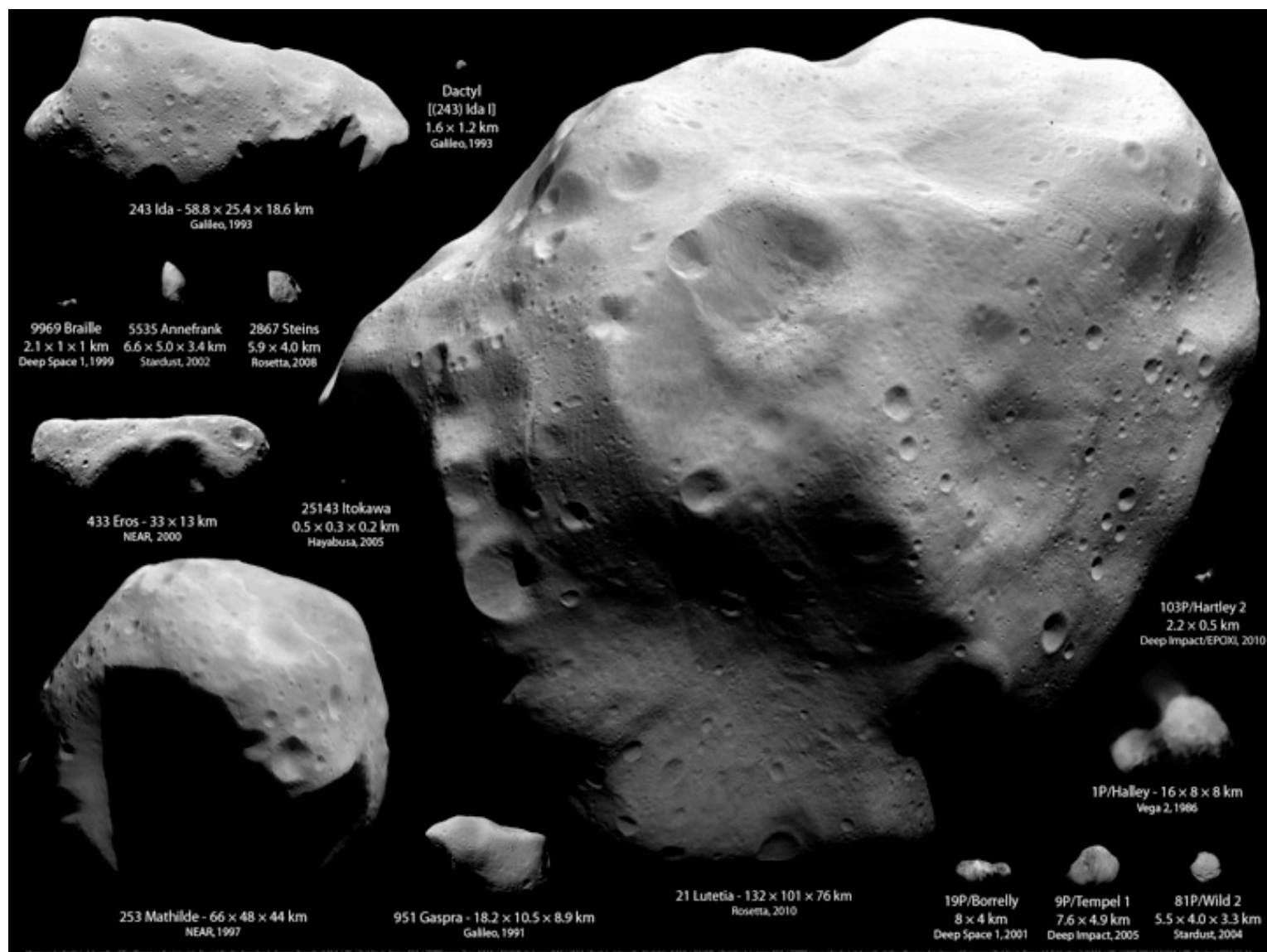
Not Using Rolling or Twisting Friction



Using Rolling and Twisting Friction

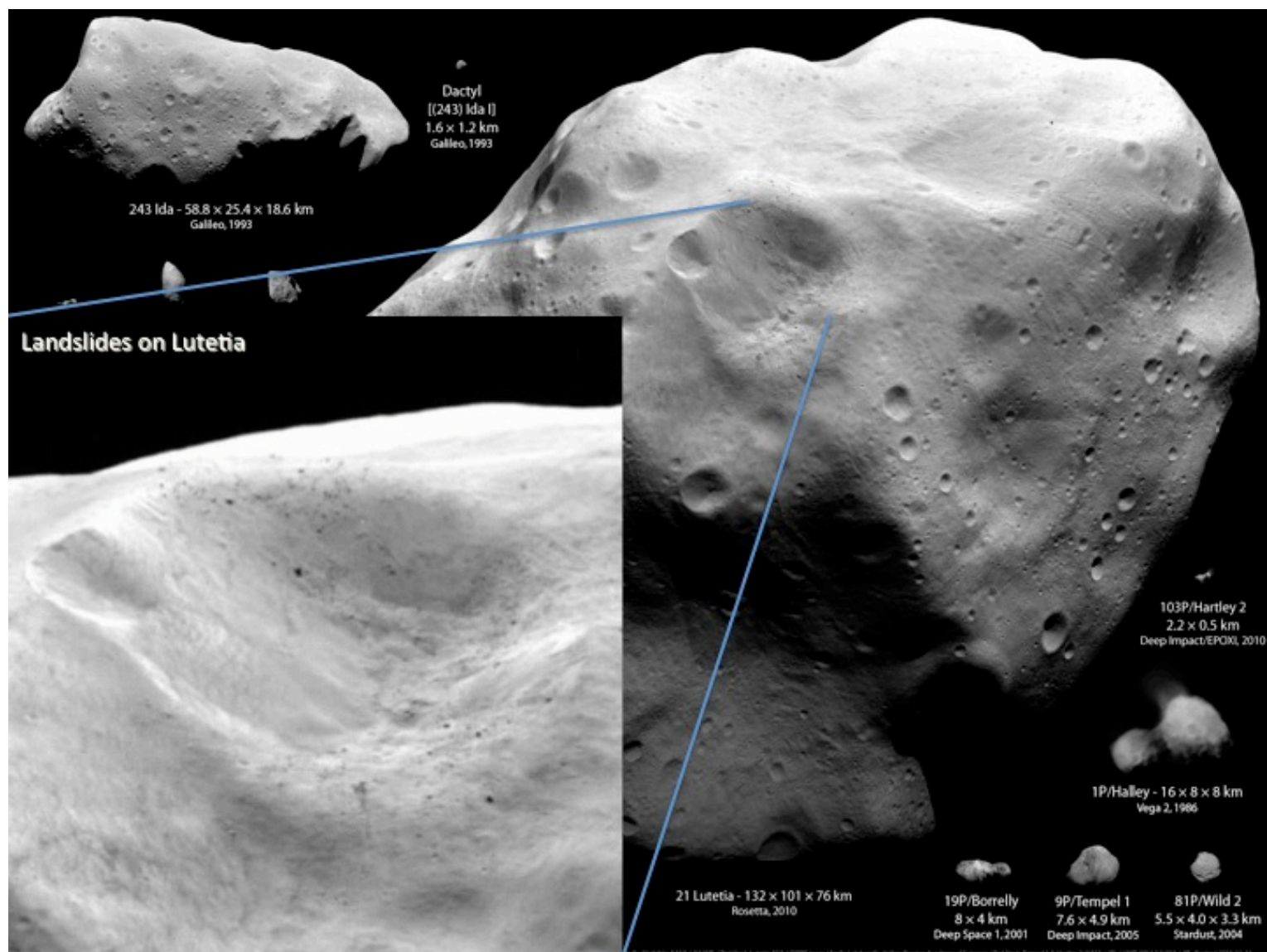
# What Can Be Learned by Applying Granular Dynamics to the Small Bodies of Our Solar System?

- Their evolutionary history and make-up.
  - Gravitational reaccumulation of collisional fragments under a variety of conditions help to give rise to the diversity that we observe today.
  - Over long timescales, the action of sunlight (besides triggering outgassing on comets) can alter the orbits and spins of smaller asteroids, leading to mass loss and the formation of binary systems.
- Informed design of sample return missions.
  - Knowledge of the response from asteroid's surface to spacecraft and robotic devices will aid in our approach.





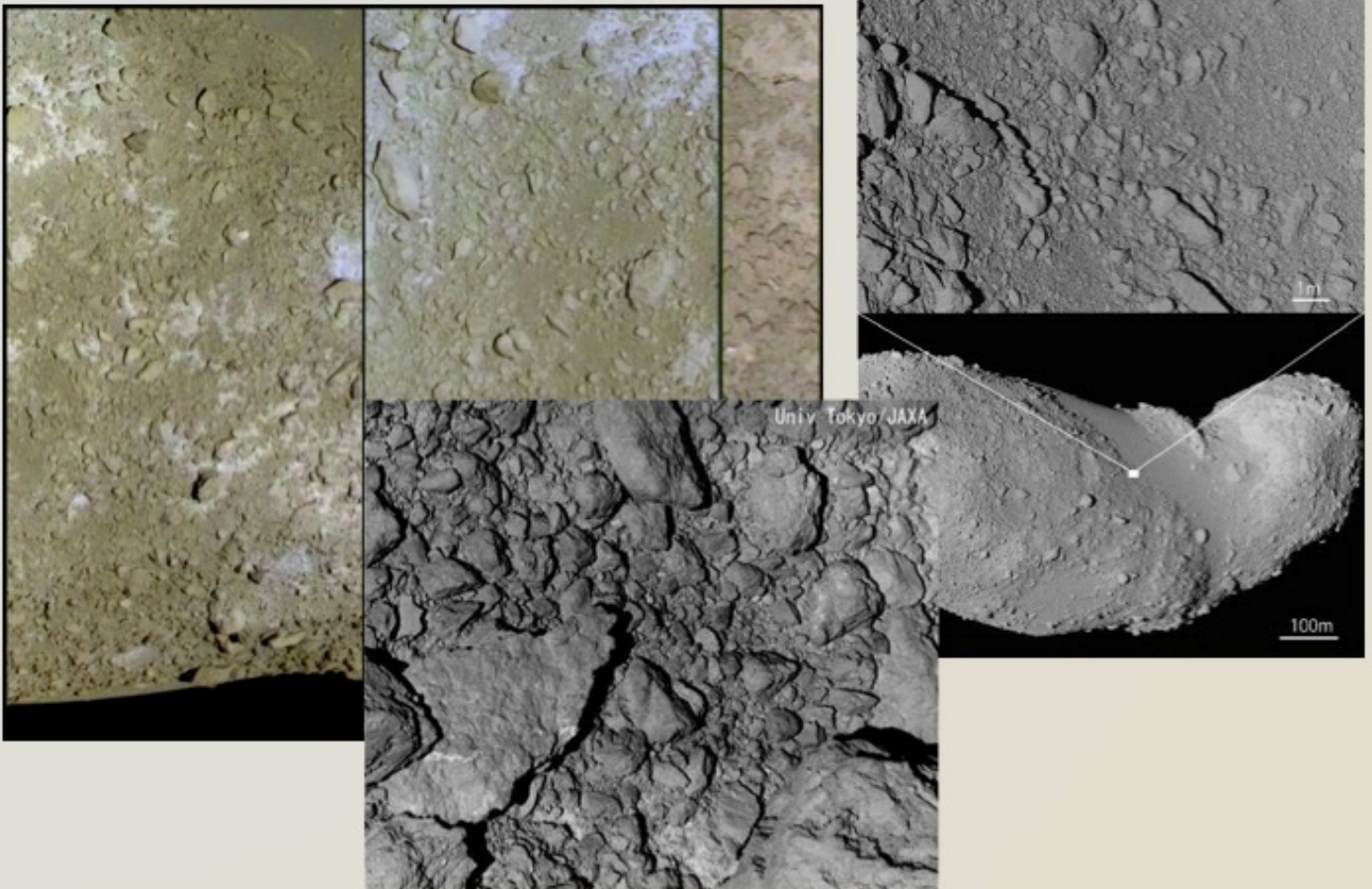






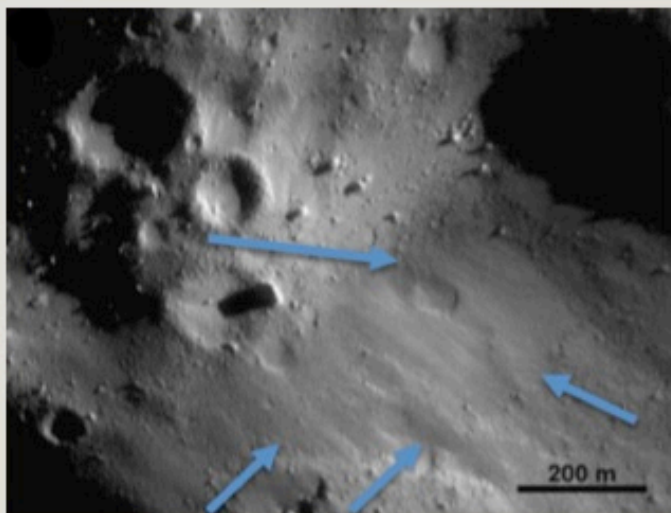


# ITOKAWA



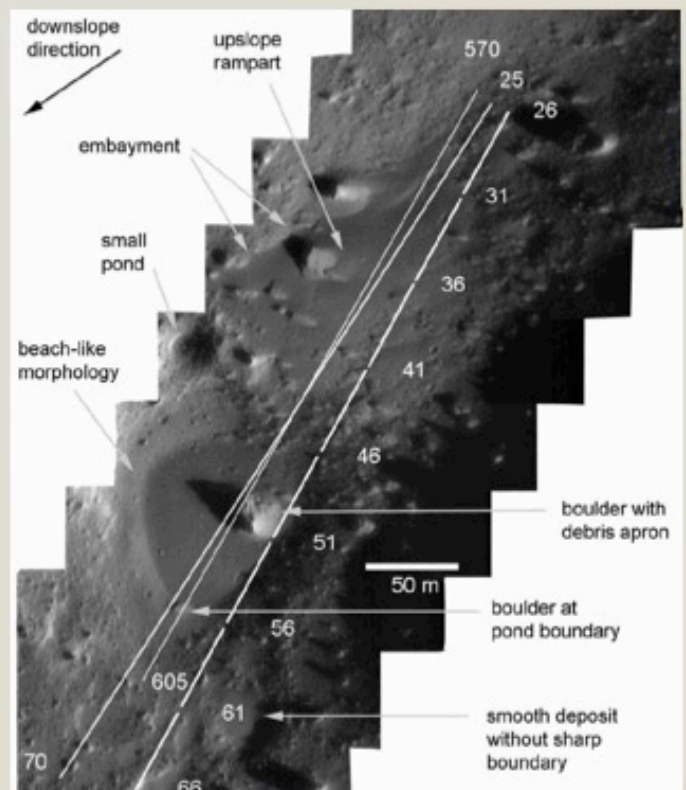
*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Eros: Evidence of Surface Flow



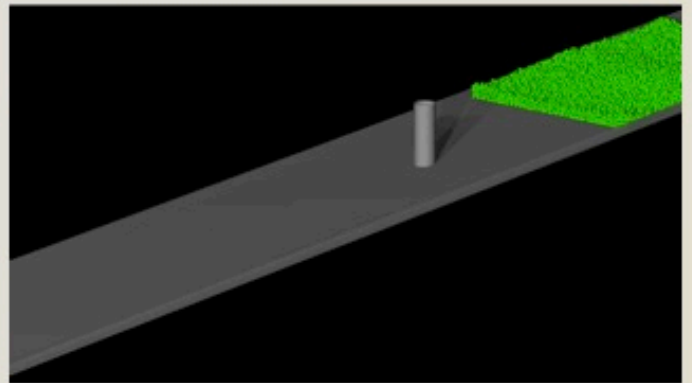
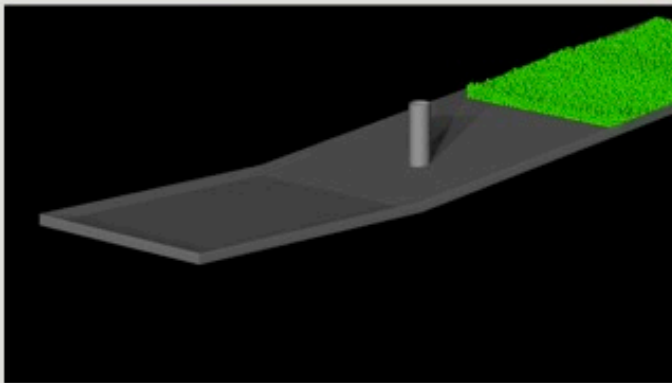
(arrows mark boundary of flow region)

Courtesy: A. Cheng

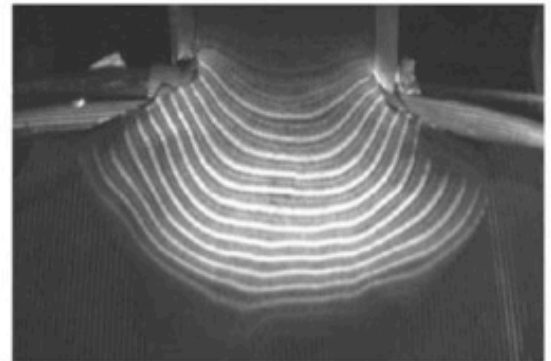
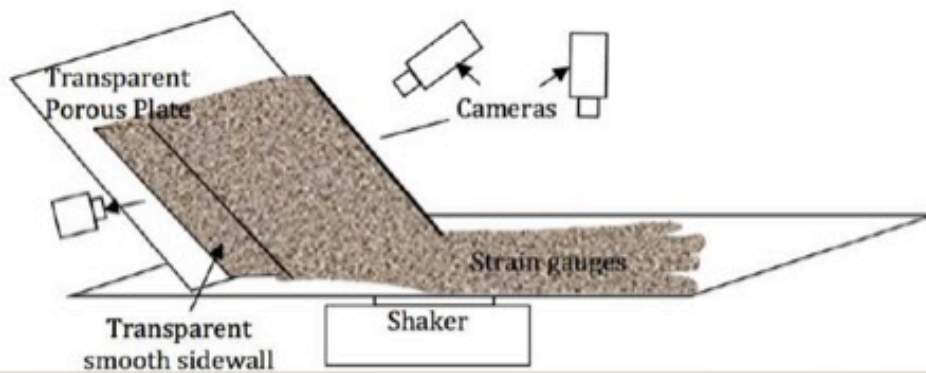


*Schwartz, S.R., SAG: 17-21 Octobre, Nice, La Maison du Séminaire*

# Landslides: Simulations

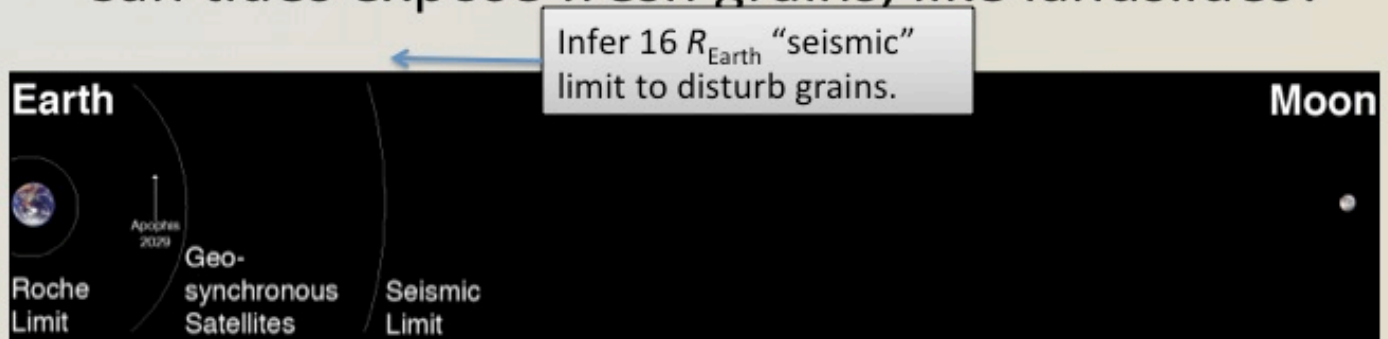


Losert lab apparatus (U Maryland Physics)

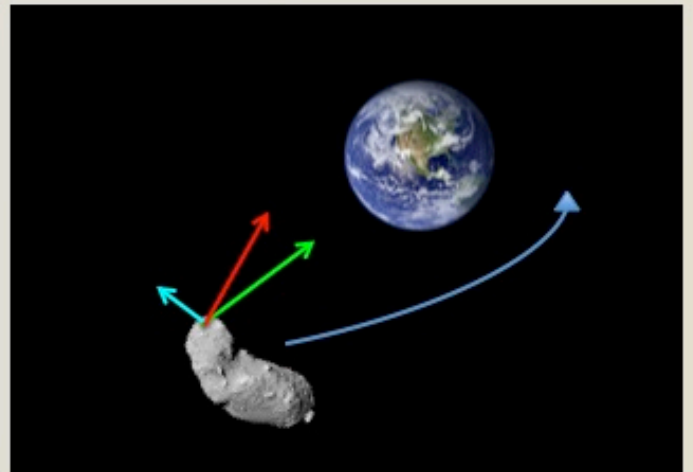
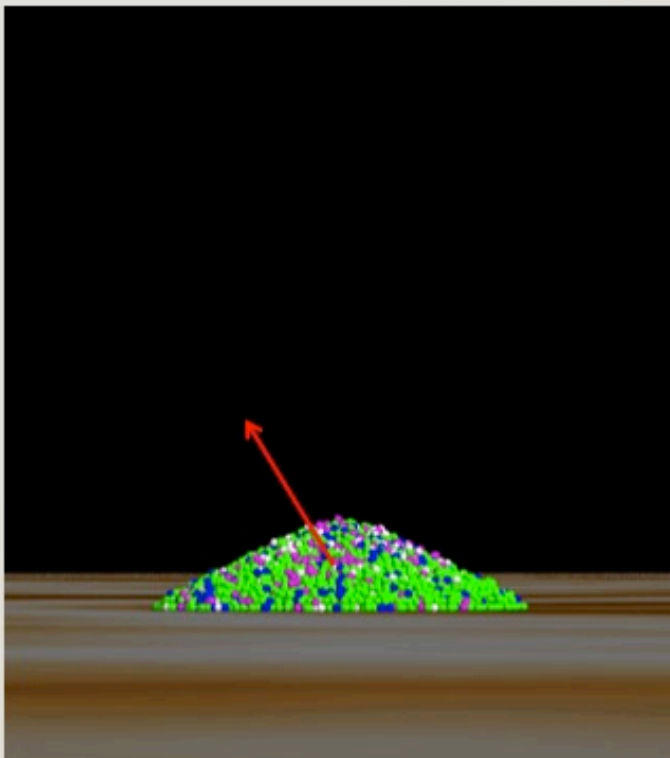


## Space Weathering (Binzel et al. 2010)

- Find “fresh” (unreddened) Q-class asteroids have high probability of recent Earth encounters (within  $\sim 1$  Myr).
- Can tides expose fresh grains, like landslides?



# Local Simulations: Concept

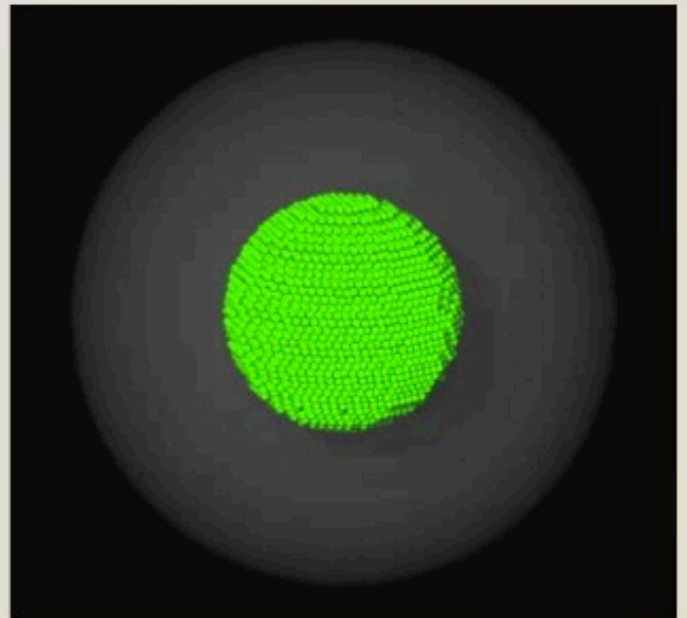


- Measure force at a point on asteroid during flyby.
- Apply to local environment.



## Local Simulations: Demo

- 12,000 particles in sphere.
- Random gravity up to 1 g.
- 14 gravity changes in 5 s of simulated time.



## Summary and Conclusions

- We have developed a tool that is capable of simulating the flow of millions of grains with a robust treatment of frictional forces, generalizable to a variety of gravitational and material regimes.
- With a comprehensive set of boundary shapes (walls), we can recreate laboratory simulations and explore design concepts of sample return missions to small bodies.
- We continue to add new functionality to the code and tune parameters to real materials.



# Extra Slides...

## Weak Cohesion in Granular Fluids

