Event-driven Simulation

event #1

$\text{t = 0}$

event #2

$t = 17$

event #3

$t = 23$
Collision Time Algorithm

• Tree data structure for collision times
  – Ball with smallest collision time value kept at bottom left

• Sectoring
  – Time complexity $O(\log n)$ vs $O(n)$
  – Buffer zones
collide
compute collision times
ball 1 collides with ball 6 at t=2.5
ball 2 collides with ball 7 at t=1.25
Domain Sectoring
Collision Times: $O(\log n)$ vs $O(n)$

Racking balls (use MPI or OpenMP)

We only update interacting balls locally in adjacent sectors, and we only do periodic global updates for output.
Ball-Ball Collisions

- Treat as smooth disk collisions
- Calculate Newtonian trajectories
- Calculate contact times

\[ b_{ij} = \vec{r}_{ij} \cdot \vec{v}_{ij} \]

\[ |r_{ij}(t + t_{ij})| = |r_{ij} + v_{ij}t_{ij}| = \sigma \Rightarrow v_{ij}^2 t_{ij}^2 + 2b_{ij}t_{ij} + r_{ij}^2 - \sigma^2 = 0 \]

- Adjust velocities

\[ \delta \vec{v}_i = -\delta \vec{v}_j = -\left( \frac{b_{ij}}{\sigma^2} \right) \vec{r}_{ij} = -\vec{v}_{ij}^\parallel \]
\( p_i' - p_i = C r_{ij}, \ p_j' - p_j = -C r_{ij} \)

\( p_i^2 + p_j^2 = p_i'^2 + p_j'^2, \ p_i + p_j = p_i' + p_j' \)

\Rightarrow p_i \cdot p_j = p_i' \cdot p_j'

\[ p_i \cdot p_j = (C r_{ij} + p_i) \cdot (-C r_{ij} + p_j) \]

\[ p_i \cdot p_j = -C^2 \sigma^2 + C r_{ij} \cdot p_j - C r_{ij} \cdot p_i + p_i \cdot p_j \]

\[ 0 = -C^2 \sigma^2 + C r_{ij} \cdot (p_j - p_i) \Rightarrow C = \frac{-m r_{ij} \cdot v_{ij}}{\sigma^2} = -\frac{m b_{ij}}{\sigma^2} \]

\[ p_i' - p_i = C r_{ij} \Rightarrow m v_i' - m v_i = -\frac{m b_{ij}}{\sigma^2} r_{ij} \Rightarrow \delta v_i = v_i' - v_i = -\frac{b_{ij}}{\sigma^2} r_{ij} \]

\[ \delta v_i = \left(-\frac{b_{ij}}{\sigma^2}\right) r_{ij} \frac{m_j}{m_i + m_j} (1 + \mu) \]
A Smooth Ball Collision
Numerical Tricks

Avoid catastrophic cancellation, by rationalizing the numerator in solving the quadratic formula for:

\[ a t_{ij}^2 + b t_{ij} + c = 0 \iff v_{ij}^2 t_{ij}^2 + 2b t_{ij} + r_{ij}^2 - \sigma^2 = 0 \]

For \( b > 0 \):

\[
\frac{-b + \sqrt{b^2 - 4ac}}{2a} \left(\frac{-b - \sqrt{b^2 - 4ac}}{-b - \sqrt{b^2 - 4ac}}\right) = \frac{-2c}{b + \sqrt{b^2 - 4ac}}
\]

For \( b < 0 \):

\[
\frac{-b - \sqrt{b^2 - 4ac}}{2a} \left(\frac{-b + \sqrt{b^2 - 4ac}}{-b + \sqrt{b^2 - 4ac}}\right) = \frac{-2c}{b - \sqrt{b^2 - 4ac}}
\]

When comparing floating point numbers, take their difference and compare to float epsilon:

\[
\text{if } x_1 == x_2 \rightarrow \text{if } |x_1 - x_2| \leq \text{float } \varepsilon
\]
Coefficient of Restitution

- $\mu$ is calculated as a velocity-dependent restitution coefficient to reduce inelastic collapse and overlap occurrences as justified by experiments and defined below.

\[
\mu(v_n) = \begin{cases} 
1 - B v_n^\beta, & v_n < v_0 \\
\varepsilon, & v_n > v_0 
\end{cases}
\]

- Here $v_n$ is the component of relative velocity along the line joining the disk centers, $B = (1-\varepsilon)v_0^{-\beta}$, $\beta = 0.7$, $v_0 = \sqrt{g\sigma}$ and $\varepsilon$ varying between 0 and 1 is a tunable parameter for the simulation.
Figure 172. Coefficient of Restitution as a Function of Impact Velocity for the Impact of Spheres on Thick Plates.
Collision rules for dry granular media as modelled by inelastic hard spheres

\[
\begin{pmatrix}
\dot{r}_1' \\
\dot{r}_2'
\end{pmatrix} = \begin{pmatrix}
\dot{r}_1 \\
\dot{r}_2
\end{pmatrix} + \left(1 + \mu(v_n)\right) \begin{pmatrix}
-m_2 & m_2 \\
m_1 & -m_1
\end{pmatrix} \begin{pmatrix}
\dot{r}_1 \cdot q \\
\dot{r}_2 \cdot q
\end{pmatrix} q
\]

The velocity dependent coefficient of restitution \( \mu(v_n) \) determines the energy loss:

\[
\mu(v_n) = \begin{cases} 
1 - (1 - \mu_0) \left(\frac{v_n}{v_0}\right)^{0.7}, & v_n < v_0 \\
\mu_0, & v_n > v_0
\end{cases}
\]

\[
\mu_0 = \frac{(v_2' - v_1') \cdot \hat{q}}{(v_2 - v_1) \cdot \hat{q}} < 1, \; v_0 = \sqrt{ga}, \; a = \text{radius of particle}
\]

Energy is dissipated. C. Bizon et. al., PRL 80, 57, 1997.
Polydispersity means Normal distribution of particle radii

"Do Binary Hard Disks Exhibit an Ideal Glass Transition?"

\[ P = D(\rho k_B T)(1 - \rho / \rho_c)^{-1} \]
The density in the glassy region is a constant. In the interface between the fluid and the glass does the density approach the glass density exponentially?

Interface width seems to increase as $\mu_0 \to 1$

$$|\rho - \rho_c| = A \exp(\lambda y)$$

How does $\lambda$ depend on $(1 - \mu_0)$?
Density vs Height in Fluid-Glass Transition

\[ |\rho - \rho_c| = A \exp(\lambda y) \]
Length Scale in Transition

\[ |\rho - \rho_c| = A \exp(\lambda y) \]

\[ \lambda = (1 - \mu_0)^{0.44} \]

Slope = 0.42 poly
Slope = 0.46 mono

"interface width diverges"
Y Velocity Distribution

Poiseuille flow

Plug flow snapshot

Mono-disperse (crystallized) only

300 (free fall region)
250 (fluid region)
200 (glass region)
150

y
x
z

Mono kink fracture
Granular Temperature

300 (free fall region)

250 (fluid region)

235 (At Equilibrium Temperature)

200 (glass region)

150
Fluctuating and Flow Velocity


\[ \delta V \propto V^{2/3} \]


"questionable" averaging over nonuniform regions gives 2/3
\[ \delta v = \langle v_x^2 \rangle - T_g = (v_y - v_c)^\lambda \]

\( \lambda \approx 1 \) in fluid glass transition

For \( \mu_0 = 0.9, 0.95, 0.96, 0.97, 0.98, 0.99 \)

Subtracting of \( T_g \) and \( v_c \) and not averaging over regions of different \( \langle v_x^2 \rangle \)

Down centre

Slope \( \lambda = 1.0 \)
FIG. 1. Experimental setup: The granular material (between two concentric cylinders) is fluidized by an upward air flow and sheared by rotation of the inner cylinder, which is connected to the motor through a flexible spring (S). Shear forces are determined from the spring displacement. Particle motions in the top layer are measured through the glass outer cylinder with a fast CCD camera.
Velocity Fluctuations vs. Shear Rate

\[ \dot{\gamma} = \partial_x v_y \]
\[ \sigma_{xy} = \eta \dot{\gamma} \]

\[ \text{Slope} = 0.406 \pm 0.018 \]

From simulation

Must Subtract \( T_g \)!

Slope = 0.4

FIG. 4. Connection between the local rms velocity fluctuations and local shear rate (same symbols as for Fig. 2). Local fluctuations are found to increase approximately as a power law of the local velocity gradient, with a power of 0.4 (dashed line).

Shear Stress

\[
\sigma_{xy} = \frac{1}{t_{\text{collisions}}} \left( -\frac{1}{2} (1 + \mu) \left( \dot{r}_1 - \dot{r}_2 \right) \cdot \dot{q} (\dot{q} \cdot \hat{x}) (\dot{q} \cdot \hat{y}) \right)
\approx -\frac{1}{2} f_c \langle (1 + \mu) (\dot{r}_1 - \dot{r}_2) \cdot \dot{q} \rangle \langle (\dot{q} \cdot \hat{x}) (\dot{q} \cdot \hat{y}) \rangle
\]

\text{slope} = 0.15554674 = \partial_x \sigma_{xy}

\text{ratio of slopes} = -\frac{1}{2} f_c \langle (1 + \mu) (\dot{r}_1 - \dot{r}_2) \cdot q \rangle
Viscosity vs Temperature

...can do slightly better...

\[ \dot{\gamma} = \partial_x v_y \]
\[ \sigma_{xy} = \eta \dot{\gamma} \]
\[ \eta = \sigma_{xy} / \partial_x v_y \]

Transformation from a liquid to a glass takes place in a continuous manner. Relaxation times of a liquid and its interior phase.

Shear Viscosity increases very rapidly as Temperature is lowered.

"anomalous" viscosity.
Is a fluid with "infinite" viscosity a useful description of the interior phase?

Slope $\sim 2 \neq 1$

$1.92 \pm 0.084$
Experimental data from the book:
“Sands, Powders, and Grains: An Introduction to the Physics of Granular Materials”
By Jacques Duran.
Related to Forces: Impulse Distribution

Simulation →
Impulse defined: Magnitude of momentum after collision minus momentum before collision.

Experiment → (Longhi, Easwar)

Quasi-1d Theory → (Coppersmith, et al)
Power Laws for Collision Times

1) spheres in 2d
2) 2d disks
3) 3d spheres

\[ P(\tau) = \tau^{-\alpha} \]

\[ \alpha \approx 2.81 \pm 0.06 \approx 2.75 \text{ to } 2.87 \text{ in glassy region} \]

Similar power laws for 2d and 3d simulations!
Comparison With Experiment

α: experiment 1.5 vs. simulation 2.8

Discrepancy as a result of Experimental response time and sensitivity of detector.

← Experiment
Pressure Transducer

Figure from experimental paper:
“Large Force Fluctuations in a Flowing Granular Medium”
E. Longhi, N. Easwar, N. Menon
Probability Distribution for Impulses vs. Collision Times (log scale)

\[ P(\tau) = \tau^{-\alpha} \]

\( \alpha = 2.75 \)

\( \alpha = 1.50 \)
Is there any difference between this glass and a crystal?

Answer: Look at Monodisperse grains crystallization → at later stage

α = 4.3

Disorder has a universal effect on Collision Time power law.
## Summary of Power Laws

<table>
<thead>
<tr>
<th>Radius Polydispersity</th>
<th>2d disks</th>
<th>Spheres in 2d</th>
<th>3d spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % (monodisperse)</td>
<td>4</td>
<td>4.3</td>
<td>4</td>
</tr>
<tr>
<td>15 % (polydisperse)</td>
<td>2.75</td>
<td>2.85</td>
<td>2.87</td>
</tr>
</tbody>
</table>
Conclusions

• A gravity-driven hard sphere simulation was used to study the glass transition from a granular hard sphere fluid to a jammed glass.
• We get the same 2/3 power law for velocity fluctuations vs. flow velocity as found in experiment, when each data point is averaged over a nonuniform region.
• When we look at data points averaged from a uniform region we find a power law of 1 as expected.
• We found a diverging length scale at this jamming (glass) to unjamming (granular fluid) transition.
• We compared our simulation to experiment on the connection between local velocity fluctuations and shear rate and found quantitative agreement.
• We resolved a discrepancy with experiment on the collision time power law which we found depends on the level of disorder (glass) or order (crystal).
Momentum Conservation

\[ \partial_k \sigma_{ik} +\rho g_i = 0 \]

\[ \partial_x \sigma_{yx} + \partial_y \sigma_{yy} = -\rho g \]

Weight not supported by a pressure gradient.

\[ \langle \partial_y \sigma_{yy} \rangle_x \approx 0 \]
Momentum Conservation

\[ \partial_x \sigma_{yx} + \partial_y \sigma_{yy} = -\rho \mathbf{g} \]

\( y = 100 \)

\[ \left\langle \partial_x \sigma_{xy} \right\rangle_y \gg 0 \]

Weight supported by shear stress