Computer Simulation of Granular Matter:

A Study of An Industrial Grinding Mill

By John Drozd
Outline

• Introduction and motivation.
• Event driven algorithm and formulae.
• Crushing forces.
• Discussion and analysis
  – Verification
  – Parameters
  – Steady state
  – Mean square displacement
  – Circulation
• Conclusions and recommendations.
Granular Matter

- Granular matter definition
  - Small discrete particles vs. continuum

- Granular matter interest
  - Biology, engineering, geology, material science, physics.
  - Mathematics and computer science.

- Granular motion
  - Energy input and dissipation.

- Granular experiments
  - Vibration
Small Amplitude Surface Waves \[\downarrow\] 3-Node Arching \[\downarrow\] Large Amplitude Surface Waves

C. Wassgren et al. 1996
Other Phenomena in Granular Materials

- Shear flow
- Vertical shaking
- Horizontal shaking
- Conical hopper
- Rotating drum
- Cylindrical pan
Cylindrical Pan Oscillations

Oleh Baran et al. 2001
Harry Swinney et al. 1997
FIG. 1. Standing wave patterns: (a) squares, (b) stripes, (c) and (d) alternating phases of hexagons, (e) flat layer, (f) squares, (g) stripes, and (h) hexagons. Patterns (a)–(e) oscillate at $f/2$, (f)–(h) at $f/4$. The dimensionless layer depth $N$ is 5.42. The brightness indicates the height of the layer. The experiments use lead spheres sieved between 0.5 and 0.6 mm.
Vibratory Drum Grinder

Raw Feed

Grinding Media, Rods

Vibrator Motor

Reactor Springs

Isolation Spring

Ground Product
Goal

• Find optimum oscillation that results in a force between the rods which achieves the ultimate stress of a particular medium that is to be crushed between the rods.

• Minimize the total energy required to grind the medium.

• Mixing is also important.
Typical Simulation
Event-driven Simulation Without Gravity

event #1

$t = 0$

event #2

$t = 17$

event #3

$t = 23$
Event-driven Simulation With Gravity

particles colliding in free flight

vertical oscillation of container
Lubachevsky Algorithm

- **Time values**
  - Sum collision times

- **Heap data structure**
  - Disk with smallest time value kept at top

- **Sectoring**
  - Time complexity $O(\log n)$ vs $O(n)$
  - Buffer zones
Rod 1 collides with Rod 2 with a collision time = 58
Rod 2 collides with Rod 3 with a collision time = 124
Rod-Rod Collisions

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

\[ v_{ij}^2 t_{ij}^2 + 2 b_{ij} t_{ij} + r_{ij}^2 - \sigma^2 = 0 \]

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

- Adjust velocities

\[ \delta \vec{v}_i = -\delta \vec{v}_j = -\left(b_{ij} / \sigma^2\right) \vec{r}_{ij} = -\vec{v}_{ij}^{||} \]
A Smooth Disk Collision
Coefficient of Restitution

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

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

- 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
Rod-Container Collisions

\[(x + v_x t)^2 + \left( y + v_y t - \frac{1}{2} g t^2 - \bar{y} \right)^2 = (R - r)^2 \]
Typical Simulation
Circulation

• The net circulation $\Gamma$ of the whole system was calculated by first calculating the angular velocity $\omega$ of the vortex about the center of mass of the system and then using the formula

$$\Gamma = \int \Omega \, dA = \int 2\omega \, dA = 2\omega \pi r_{\text{max}}^2$$

• where $\Omega = \nabla \times V = 2\omega$ is the angular velocity of rotation or vorticity of the system and $r_{\text{max}}$ is the distance from the farthest disk to the center of mass of the system.
Circulation

- The angular velocity of the vortex was calculated using the formula

\[ \omega = \frac{1}{N} \sum_i \frac{1}{a_i} (\vec{v}_i - \vec{v}) \cdot (\hat{k} \times \hat{a}_i) \]
Typical Time Averaged Velocity Field
Net Circulation (\(\Gamma\)) vs Time (\(t\))
Measuring Disk Disk Forces as Collision Energies

• For a disk-disk collision, the collision energy can be calculated as

\[ E_c = \frac{1}{2} m_{\text{eff}} v_{n,\text{rel}}^2 \]

• where \( m_{\text{eff}} = \frac{1}{2} m_{\text{disk}} \), and \( v_{n,\text{rel}} \) is the relative normal velocity between the disks before a collision.
Measuring Disk Container Forces as Collision Energies

• For a disk-container collision, the collision energy can be calculated as

\[ E_c = \frac{1}{2} m_{\text{eff}} v_{n,\text{rel}}^2 \]

• where \( m_{\text{eff}} = m_{\text{disk}} \) and \( v_{n,\text{rel}} \) is the dot product of the velocity of the disk before the collision and a unit vector of the container surface normal \( \hat{n} \), that is calculated as

\[ v_{n,\text{rel}} = \frac{-xv_x - y\left(v_y - \frac{d\bar{y}}{dt}\right)}{\sqrt{x^2 + y^2}} \]
Measuring Forces as Collision Energies

- These collision energies can be compared to the *modulus of toughness* of the material that is to be crushed between the disks.

- The *modulus of toughness* is defined as a strain-energy density, $u$, taken to the strain at rupture $\varepsilon_R$ using the formula

\[
u = \int_0^{\varepsilon_R} \sigma_x \, d\varepsilon_x\]

\[\sigma \quad \varepsilon \quad \varepsilon_R\]

Modulus of Toughness

Rupture
Parameters for Simulation

• The program was run using the parameters \((g, \sigma, \phi, \omega_y, A_y, e_0, e_W)\) and a simulation that produced a realistic motion was selected \((\omega_y=126 \text{ rad/s} = 20 \text{ Hz}, A_y=1.5 \text{ cm}, e_0=0.4, e_W=1.0)\).

• By a realistic motion, we mean that the disks would cluster together at the bottom of the container within a relatively short period of time with few overlaps.
Total Kinetic Energy (KE/M) vs Time (t)
Power Spectrum of Total Kinetic Energy (\( P(\omega) \) )
Mean Square Displacement Plots: Mixing Times

• Fixed time origin $t_0$ formula:

$$\left\langle r^2 \right\rangle_{t-t_0} = \frac{1}{N} \sum_{i=1}^{N} \left[ (\vec{r}_i(t) - \bar{y}(t)) - (\vec{r}_i(t_0) - \bar{y}(t_0)) \right]$$

• Moving time origin $t'$ formula:

$$\left\langle r^2 \right\rangle_{t'-t} = \frac{1}{N_t} \sum_t \frac{1}{N} \sum_{i=1}^{N} \left[ (\vec{r}_i(t') - \bar{y}(t')) - (\vec{r}_i(t) - \bar{y}(t)) \right]$$
Mean Square Displacement ($< r^2 >$) versus time (t)
Phase Diagram: Amplitude (A) vs Frequency (ω_y)
Time Averaged Net Circulation ($\Gamma$) vs Frequency ($\omega_y$)
Non-dimensional Parameter \( \left( \frac{\Gamma}{(A_y^2 \omega_y)} \right) \) vs Frequency \( \omega_y \)
Circulation at Sloped Part of Curve
Circulation at Leveling Off Part of Curve
Velocity Field Snapshot for Typical Simulation

Axis of Symmetry
Number of Different Disks that Experience Mean Collision Energy \((n_i)\) \(i\) times vs Time \((t)\)
Conclusion

By quantifying the crushing forces in terms of collision energies and studying circulation and mixing, this thesis has outlined a thorough systematic approach to studying the grinding mill industrial crushing problem.
Next Steps

• Finer test matrices and calibrating results with experiments

• Compare the percentages of the medium that was crushed and compare to the \( n1, n2, \ldots \) and saturation times for various simulations using different amplitudes and frequencies of oscillation.

• Determine the frequency and amplitude for an optimum oscillation, that is, to minimize the energy required to get a well-mixed container with all the rods experiencing the mean (threshold) collision energy. This is the solution to the task outlined in this thesis.
Recommendations for Future Work

- Incorporating horizontal container oscillations.
- Incorporating rod rotations.
- Using a mixture of different sized rods.
- Using different quantities of rods and different container sizes.
- Study situations with different rod-wall boundary conditions: multiple vortices.
- Parallelization and sectoring using many numbers of rods.
Acknowledgements

• Brad Smith and Kirk Bevan
• Dr. Oleh Baran
• Dr. Ivan Saika-Voivod
• Dr. Sreeram Valluri
• Drs. Peter Poole and Robert Martinuzzi
• NSERC