Granular Flow with Elastic Grains

Petri Fast

Henry Boateng
Valjean Elander
Chao Jin
Yan Li
Paula Vasquez
Project Overview

- Molecular Dynamics for interacting particles
- Incorporate grain elastic effects by approximations
- Taylor - Couette geometry
- Comparison with Behringer experiments
Group Work

- Two Tasks:
  - Dynamic simulation of particles
  - Quasi-static elastic model of interacting disks
- Basic numerical algorithms
- Software issues
  - Version control by CVS
  - Matlab for prototyping
  - C implementation for larger studies
Molecular Dynamics

- A straightforward application of Newton’s second law
  \[ m \ddot{x}_i = \sum_{j=1}^{N} F_{i,j} \]
- Different for molecules and grains (DEM). Force laws used to describe particles interactions
- Have to sum over all pairs of particles on the system (order \( N^2 \) work)
Cell List

- Speed up force calculation by localizing work
- Divide domain in cells
- Force evaluation only through cell neighborhood
- Parallel computing
Force Laws

- Lennard – Jones Potential
  \[ F_{i,j} = -\nabla \phi_{i,j} \]

- Contact Mechanics (Ciamarra et. al)
  Forces are functions of overlap \( \delta \)
  \[ F = F^N + F^S \]

Granular Flow with Elastic Grains
Numerical Implementation

\[ m \ddot{x}_i = \sum_{j=1}^{N} F_{i,j} \]

- Initial position and velocity inside and set boundaries.
- Implement a leap frog scheme
  - Calculate forces within a cut off radius.
  - Update translation and rotation.
- Some control is needed ...
Numerical Scheme

Leap Frog Stability Analysis

- Scheme

\[ \frac{dU}{dt} = f(U) \quad \Rightarrow \quad \frac{U_{n+1} - U_{n-1}}{2\delta t} = f(U_n) \]

- Lennard- Jones force law

\[ f_{ij} = \left( \frac{48\epsilon}{\sigma^2} \right) \left[ \left( \frac{\sigma}{r_{ij}} \right)^{14} - \frac{1}{2} \left( \frac{\sigma}{r_{ij}} \right)^{8} \right] r_{ij} \]

The time steps satisfies

\[ 0 < \delta t < \frac{1}{\sqrt{\left( \frac{48\epsilon \sigma^6}{m} \right) \left( \frac{-13\sigma^6}{d^{14}} + \frac{7}{2d^8} \right)}} \]
Some Results

Lennard _ Jones Potential

Taylor - Couette
Elasticity

Dynamic elasticity is based on three equations:

\[ \partial_j T_{ij} + f_i = \rho \partial_{tt} u_i \quad T_{ij} = 2\mu \varepsilon_{ij} + \lambda \delta_{ij} \varepsilon_{kk} \]

\[ \varepsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i) \]

Consider 2D plain stress in a domain \( \Omega \)

\[ \nabla \cdot \mathbf{T} = 0 \]

given \( \mathbf{T} \) in \( \partial\Omega \)
Elasticity

Simplify problem by introducing Airy’s Stress Function $\psi$ which reduces the problem to

$$\nabla^2 \nabla^2 \psi = 0$$

On the disk

$$\psi = a_0 + c_0 r^2 + d_1 r^3 \sin \theta + h_1 r^3 \cos \theta + \sum_{n=2}^{\infty} \left[ (a_n r^n + c_n r^{n+2}) \sin n\theta + (c_n r^n + g_n r^{n+2}) \cos n\theta \right]$$
Elasticity

Finally, stresses and displacements are related to $\psi$ by

$$T_{rr} = \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{r} \frac{\partial \psi}{\partial r}$$

$$T_{r\theta} = -\frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \psi}{\partial \theta} \right)$$

$$T_{\theta\theta} = \frac{\partial^2 \psi}{\partial r^2}$$

$$\frac{\partial u_r}{\partial r} = \frac{1}{E} \left[ (1 - \nu^2) T_{rr} - (\nu + \nu^2) T_{\theta\theta} \right]$$

$$\frac{1}{r} \left( \frac{\partial u_\theta}{\partial \theta} + u_r \right) = \frac{1}{E} \left[ (1 - \nu^2) T_{\theta\theta} - (\nu + \nu^2) T_{rr} \right]$$
Elasticity

Boundary Conditions

Consider a function of the form

\[ F = A \exp(-w*(\theta - \alpha)^2) \]

- **Given Stresses**
  - \( T_{rr}(1, \theta) = F \)
  - \( T_{r\theta}(1, \theta) = 0 \)

- **Given Displacements**
  - \( u_r(1, \theta) = F \)
  - \( u_\theta(1, \theta) = 0 \)
Some Results

Normal Stress Difference \((T_{rr} - T_{\theta\theta})\)
Some Preliminary Results

Normal Stress Difference \( (T_{rr} - T_{\theta\theta}) \)

Shear Stress \( (T_{r\theta}) \)
Conclusions

- State of the art MD method for 2D granular flow
- Develop a physically motivated force law
- Analytic solution for elastic disks under stress

- Large scales simulations to compare with experiments
- Introduce other force laws
- Improvements in the boundary description
- Construct a force law from elastic solution