Rheology of Granular Flow

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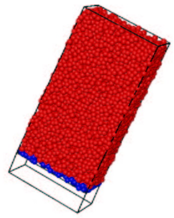
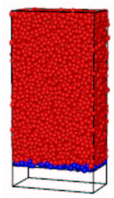


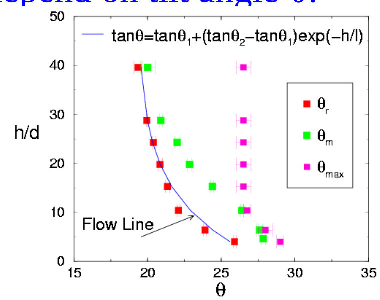
Chute flows



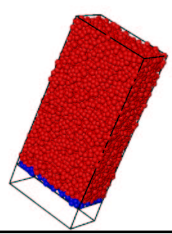
Packings

Flow down an inclined plane

- Simplest dynamical system to relate stress and structure
- Three distinct regimes of flow depend on tilt angle θ:
  - *$\theta < \theta_r(h)$: No motion*
  - *$\theta_r < \theta < \theta_{max}(h)$: Steady state flow*
  - *$\theta > \theta_{max}(h)$: Avalanching flow*



- *Steady state* flow depends on material properties: μ and ε
- Dimensional analysis expect $\sigma \propto \dot{\gamma}^2$
- For constant density this leads to $\langle v \rangle \propto h^{3/2}$



Physical Interests in Granular Systems

Granular materials are ubiquitous in everyday life

Ceramics in a die
Sand on a beach
Grains

- **STATICS**
  - Grains in a pile
  - Silos
  - Coffee-grounds
  - Pills in a bottle
- **DYNAMICS**
  - Rock debris flows
  - Avalanches
  - Coal on a conveyor belt
  - Flow in a hopper

- *Storage, transport, and handling of granular materials is of immense industrial importance*

Current Issues in Granular Matter

- Theoretical understanding of the basic phenomena is needed:
  - Granular matter: macroscopic particles of different shape, size, and material properties
  - Friction and plastic deformation dissipate energy
  - Standard methods of statistical mechanics *not* applicable
  - Need constitutive equations for continuum calculations
- There are few *well-controlled* experiments to test theoretical models

Granular Simulations - Recent Developments

- An efficient, highly parallel molecular dynamics code has been developed to simulate granular materials
  - Mono or polydispersed particulates
  - Arbitrary materials properties: hardness, coefficient of restitution, and friction coefficients
  - Arbitrary shaped container: smooth or rough wall
- Maximum number of particles in range 1-2 million
- Variety of analysis codes have been developed

• Results for gravity driven flow and geometry of frictional sphere packings will be focus of this presentation

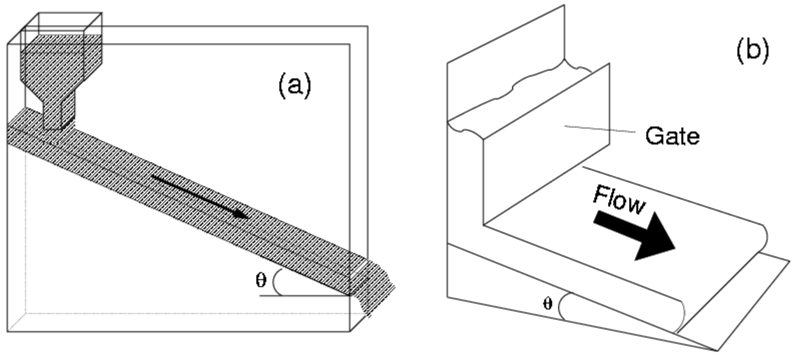
Simulation Technique

- Molecular Dynamics - Solve Newton's Equation
  - translational and rotational degrees of freedom
- Interaction forces depend on particle-particle overlap δ

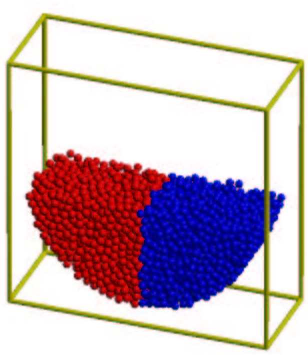
  μ - particle friction coefficient (Coulomb criterion)

  ε -coefficient of restitution (determine inelasticity)
- Dry limit - purely repulsive forces which act only on contact $\mathbf{F}=\mathbf{F}_n + \mathbf{F}_t$
  - $\mathbf{F}_n = f(\delta/d)\,(k_n\delta\mathbf{n} + \gamma_n m_{eff}\,\mathbf{v}_n)$, $f(\delta/d) = 1$ or $(\delta/d)^{1/2}$
  - $\mathbf{F}_t = f(\delta/d)\,(-k_t\Delta\mathbf{s}_t - \gamma_t m_{eff}\,\mathbf{v}_t)$, $\Delta\mathbf{s}_t$ is integral over relative displacement of two particles in contact
  - Coulomb proportionality $|\,\mathbf{F}_t\,| \leq \mu|\,\mathbf{F}_n\,|$

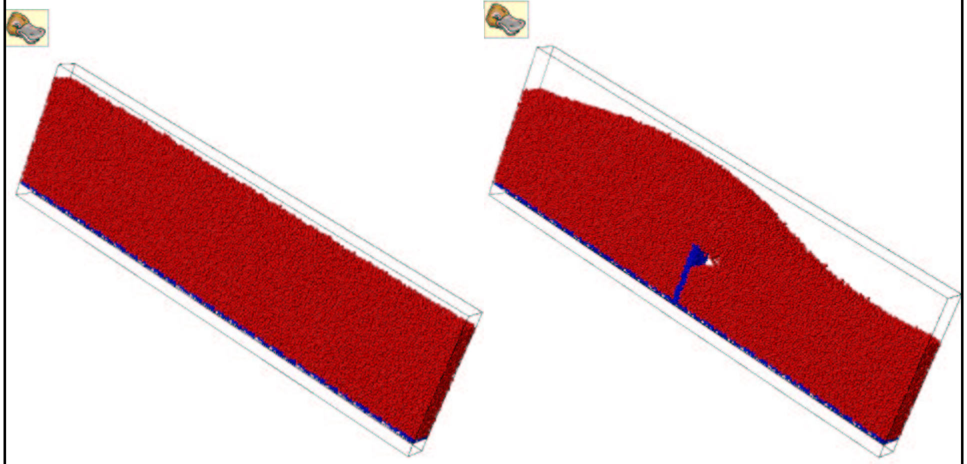
Experimental Geometries



Rotating Drum

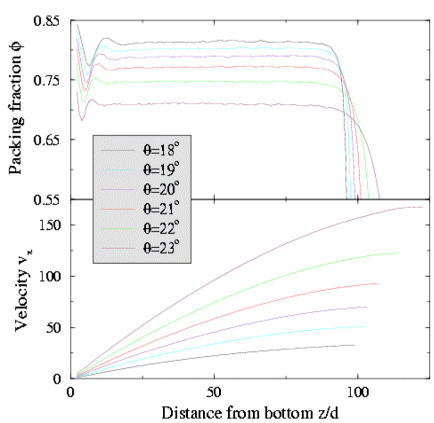


Gravity Driven Flow

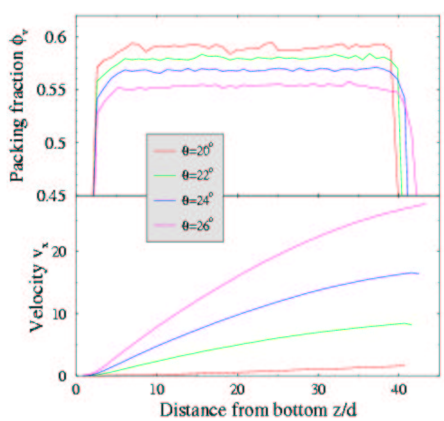


Dependence on inclination angle

2D: N=10,000; μ=0.50; ε=0.92

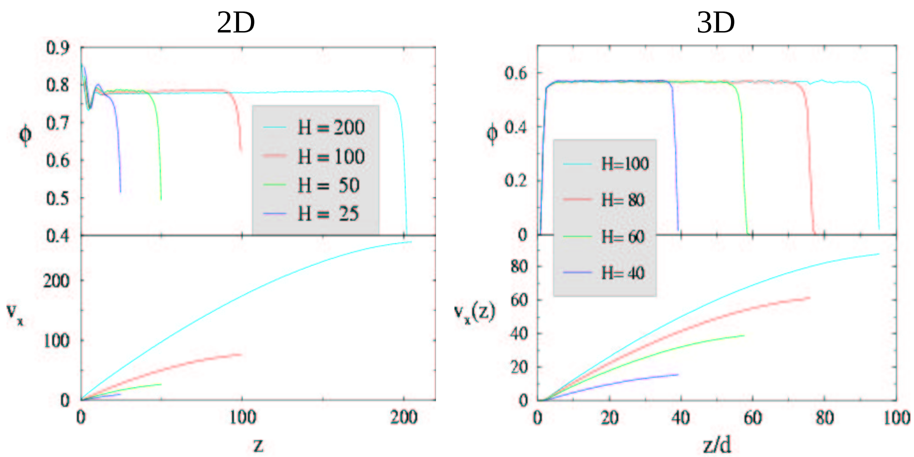


3D: N=8,000; μ=0.50; ε=0.88



• **Steady state:** constant volume fraction in the bulk, away from the free top surface and the bottom plate

Dependence on system size



- Density ϕ is independent of height of pile
- Observer co-moving atop a flowing pile would be unable to determine how deep the pack is

System size scaling

- Force balance:

$$\frac{\partial \sigma_{zz}}{\partial z} = \rho g \cos\theta \qquad \frac{\partial \sigma_{xz}}{\partial z} = \rho g \sin\theta$$

- For a given tilt angle

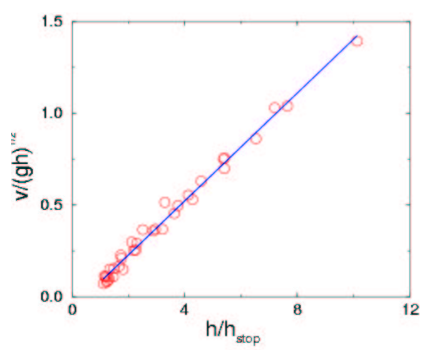
$$\sigma_{xz}(z) = \sigma_{zz}(z) \tan\theta$$

- Bagnold's momentum-collision analysis proposes that for constant density, $\left(\frac{dv_x(x)}{\partial z}\right)^2 \propto \sigma$
- Dependence of the velocity on the height of the pile

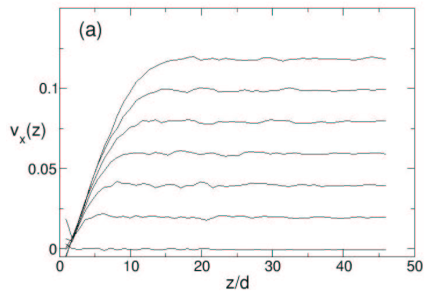
$$v_x(z) \propto [h^{3/2} - (h-z)^{3/2}]$$

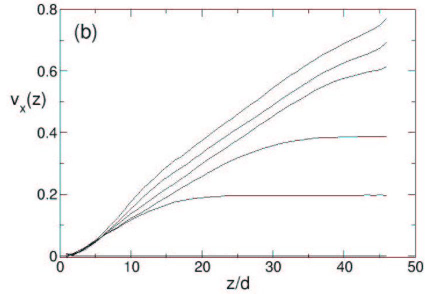
- Velocity v scales with height h as

$$\langle v \rangle \sim h^{3/2}$$



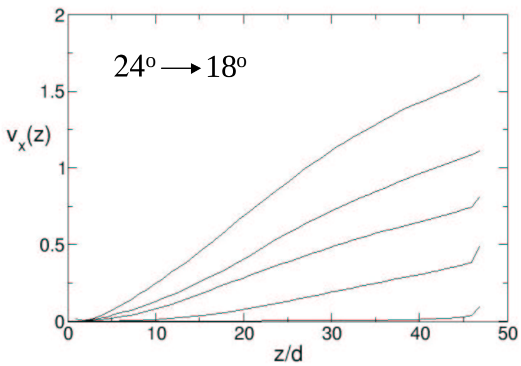
Initiation of Flow





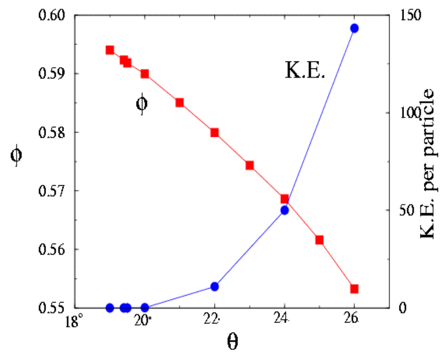
- Flow is initiated at base - top initially moves as plug
- Fluctuating region moves vertically

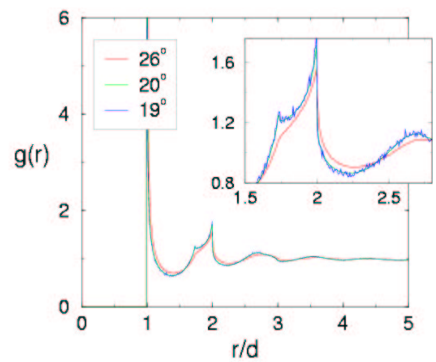
Cessation of Flow



- Cessation of flow begins at base and moves vertically even though velocity fluctuations are greatest at bottom of pile

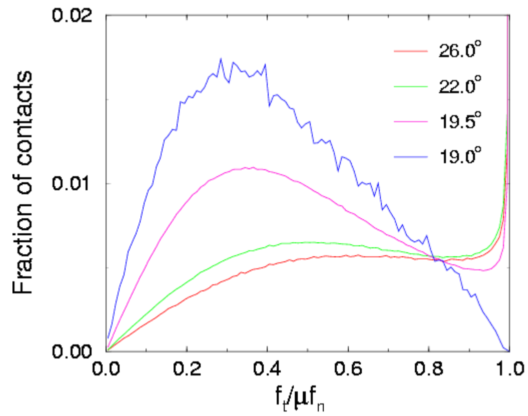
Jamming Transition





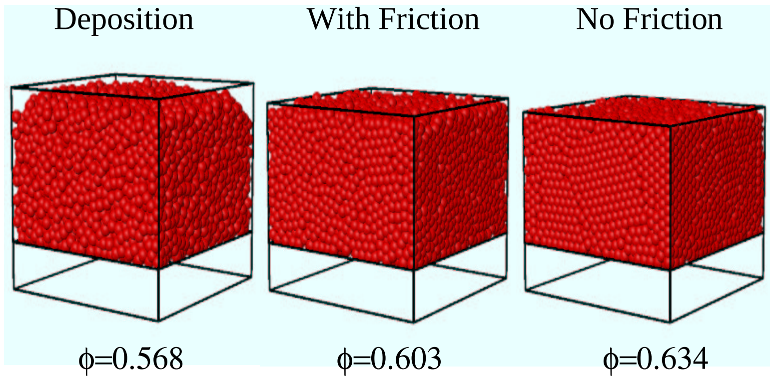
- System compacts and cools as θ is reduced
- Flow ceases at the angle of repose θ_r=19.4°
- Emerging amorphous phase is seen as a splitting of the second peak in g(r)

Plastic-Elastic Transition



- Force ratio: friction force / maximal force = $f_t/\mu f_n$
- Flowing states have a predominance of plastic contacts, i.e. contacts exactly at yield
- Once $\theta<\theta_r$ plastic contacts relax and convert to elastic ones

Effect of Friction on Packing



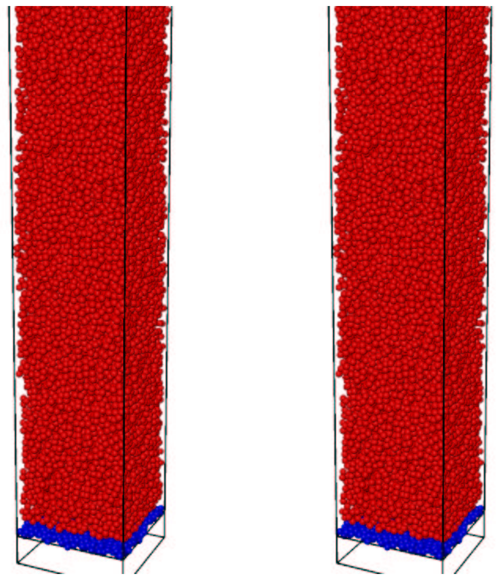
- Loose random packing generated by J Cesarano (Sandia)
- Reducing particle friction increases particle contact
  - leading to denser, more ordered structures

Granular Packing

- Nature of granular packing depends strongly on its history
- Coordination number for a stable packing:
  - z_n=6 for frictionless spheres
  - z_f=4 for frictional spheres
  - packings with z_n=6 or z_f=4 are *isostatic*
- We studied the packing of granular materials which have settled under the influence of gravity - poured into a container
  - dependence on hardness k_n
  - coefficient of friction μ

Simulated Pouring - Movie

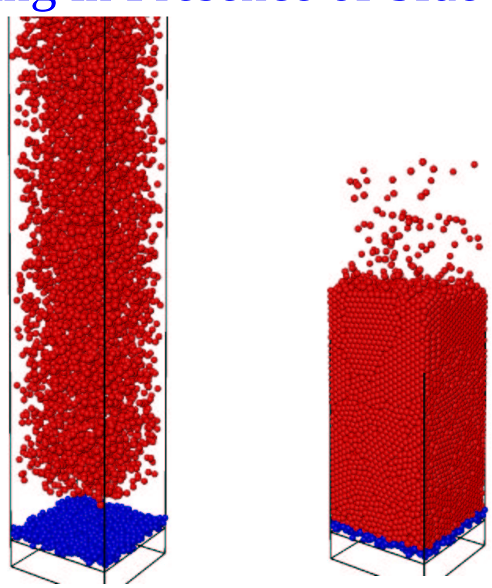
No Friction



Friction

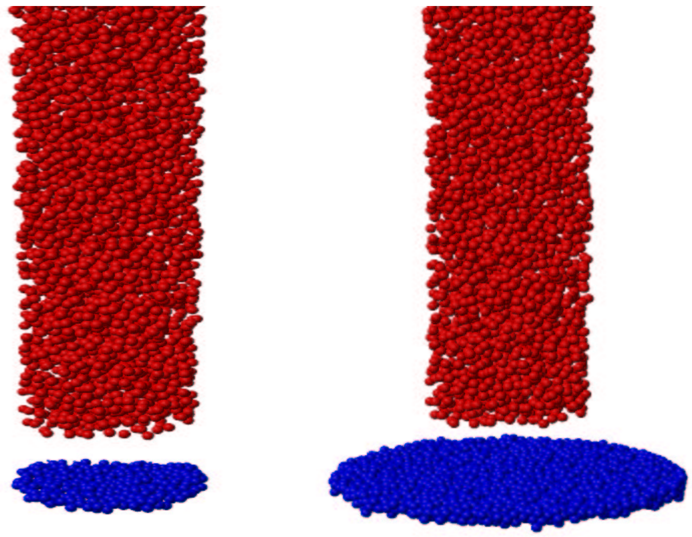
Packing in Presence of Side Walls

Friction

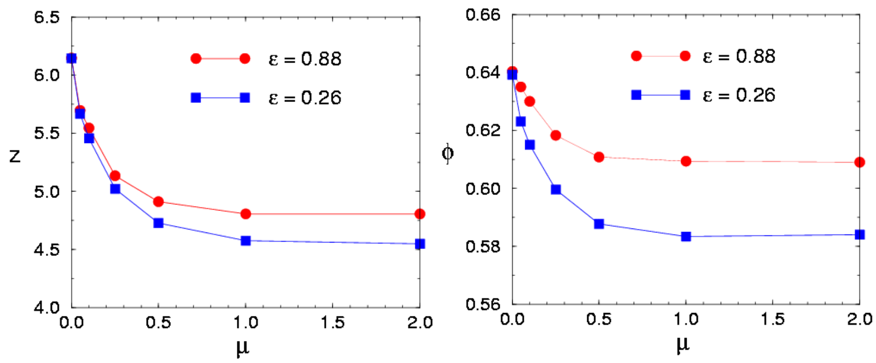


No Friction

Pouring in Presence of Walls



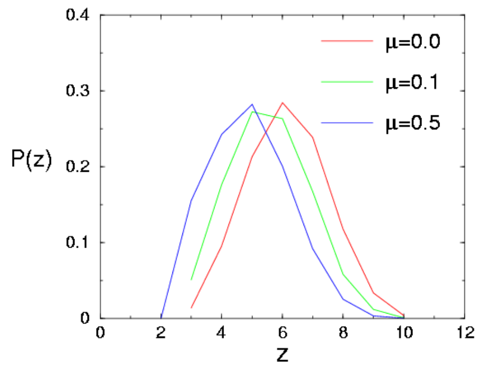
Effect of Friction on Packing



$k_n = 2 \times 10^5 mg/d$

- Coordination z and density ϕ decrease smoothly as coefficient of friction μ increase
- Similar results obtained on cessation of flow on inclined plane

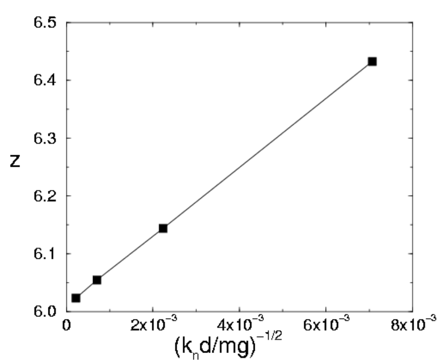
Distribution of Coordination Numbers



• Distribution shifts to lower values of z and μ increases

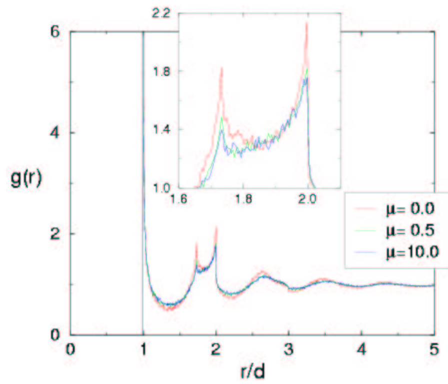
Packing of Frictionless Spheres

Effect of hardness on local coordination



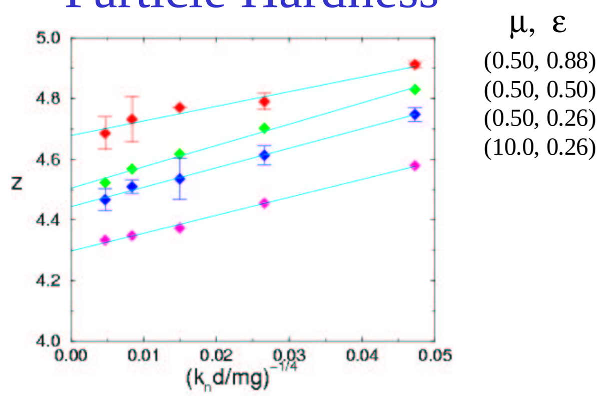
• z=6 in hard sphere limit
• Frictionless hard sphere packings are *isostatic*

Radial Distribution Function



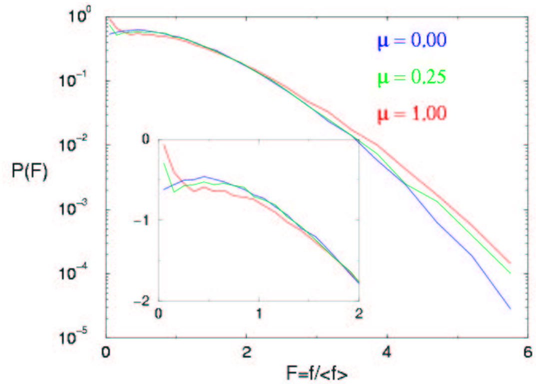
- Friction as small effect on overall pair correlations
- As μ increases, secondary peaks in g(r) diminish

Frictional Spheres - Effect of Particle Hardness



- Hard sphere limit packings are hyperstatic, $z_f > 4$
- Further crossover at extreme stiffness cannot be ruled out
    - Stiffest spheres experience stains $\delta/d<10^{-8}$

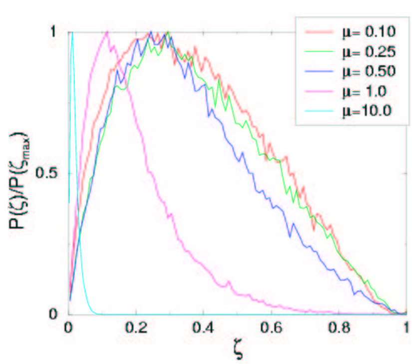
Force Distributions



- No Friction - P(F) has a maximum at f/<f> ~ 0.5
- Friction - peak occurs at small f and grows as μ increases
  - tail shifts to right as μ increases

Plastic Contacts

- Contacts for which $F_t = \mu F_n$ are plastic
  - Isostaticity condition would need to be modified if there are a finite fraction of plastic contacts



- All contacts in the static packings are below their frictional threshold $\zeta = F_t/\mu F_n$

Summary

- Efficient molecular dynamics algorithm has been developed to study large systems for long times
- For gravity-driven flow, density is uniform and shear stress satisfies simple scaling result
- Jamming transition at the angle of repose has features in common with regular glass transitions
- Packing of frictionless spheres is *isostatic* but frictional spheres are not and strongly dependent on preparation
- Current/Future simulations will study:
  - Effect of side walls and complex geometries
  - Flow in silos and hoppers
  - Slurries