Discrete element simulations of dense granular matter: from techniques to data analysis

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support

Some recent granular projects

- Relevance of energy fluctuations in dense granular matter: granular temperature and out-of-equilibrium statistical physics
- Nonlinear/linear wave propagation: 1D/2D/3D; from solitary to plane waves
- influence of microstructure on impact mechanics
- topological properties of the force chains

Why are granular systems so different?

- We do not understand how forces propagate through granular system
 - Therefore we do not know how to build good silos!
- To understand better how forces propagate consider simple systems and simple geometries



Experiment: 2D Angular Couette flow

- Experiments with photoelastic discs
- Colors show the forces which particles
 experience
- Note extreme nonuniformity of force field



 Behavior very different from `usual' materials

Overview

- Discrete element method (DEM)
 - Discuss different approaches towards modeling of the interaction of granular particles
- Data analysis
 - Extracting useful information from simulations
- Recent applications involving force and energy propagation, impact, and spatial structure of the relevant fields
- Important: interdisciplinary nature of the research in the field involving experiments, simulations, analytical work carried out by physicists, engineers, mathematicians
 - requires developing common `language' and joint approach to consider complex problems

DEM Techniques

- Level of complexity of simulation techniques
 - `Event driven' simulations
 - particles are considered as infinitely hard spheres/disks interacting infinitely fast
 - advantages: efficient, since no time stepping is involved
 - disadvantages: `technical' problems with inelastic collapse and difficulties when volume fraction (the part of the space occupied by granular particles) becomes large (review: Herrmann &Luding, Continuum Mech. Thermodyn. (1998) 10: 189–231)
 - `Soft' particle simulations
 - particles are considered as (elastic) objects interacting during finite time with the particles in their surrounding
 - advantages: applicable to dense systems and enduring contacts
 - disadvantages: computationally expensive, requiring small time step, since each interaction/collision has to be resolved
 - require careful simulation techniques in order to be able to simulate large systems for long times (General reviews: Allen & Tildesley, Computer Simulation of Liquids; Haile: Molecular Dynamics Simulation)

DEM Models

- Level of complexity of interaction models
 - spherical, elastic, frictionless particles interacting infinitely fast only when in contact
 - relatively easy to implement, can be connected to continuum fluid-mechanics like theories
 - certain part of physics is lost...
 - spherical particles with inelasticity and friction interacting with repulsive or attractive interactions when in contact
 - relatively easy to implement
 - typically use relatively simple force interaction laws
 - More complex approaches:
 - resolving details of individual contacts (linear/nonlinear elasticity theory) (see Johnson, Contact Mechanics)
 - aspherical particles

...

long range interactions

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DEM Software

- `In-house' software developed by individual researchers
 - typically using simplified interaction models and relatively small system sizes
 - simplicity allows for fine-tuning and flexibility (no black-box effect)
- Publicly available software packages
 - LAMMPS, NAMD, ...
 - professionally written, complex interaction methods
 - efficient, allowing for simulations of large systems
 - may be extremely complex; certain lack of flexibility
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Computational Techniques

- Serial versus parallel
- parallelization becomes more and more important due to necessity to simulate large systems
 - multi-cpu and multi-core programming
 - Open MPI, Open MP, distributed and shared memory machines...
 - trade-off between speed and (human) effort involved

- Split the system into cells
- Make the list of particles in each cell
- check for interactions between particles in a given cell and each neighbor cell
- if there is an interaction, calculate the interaction forces
- update the positions, velocities, acceleration of particles
- recalculate the lists as appropriate



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Equations

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = m_i \mathbf{g} + \mathbf{F}_{i,j}^n$$
$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = -\frac{1}{2} d_i \mathbf{n}_i \times \mathbf{F}_{i,j}^t$$

$$\mathbf{n}_i = rac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$



Forces

• Normal: linear force model

$$\mathbf{F}_{i,j}^{\ n} = k_n x \mathbf{n}_i - \gamma_n \bar{m} \mathbf{v}_{i,j}^{\ n}$$

$$\mathbf{v}_{i,j} = (\mathbf{v}_i - \mathbf{v}_j) - (\omega_i d_i/2 + \omega_j d_j/2)\mathbf{e_z} \times \mathbf{n}_i$$

$$\bar{m} = \frac{m_i m_j}{m_i + m_j}$$

 γ_n - damping: proportional to the coefficient of restitution

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 γ_n - damping: proportional to the coefficient of restitution Connection of material properties and DEM parameters: see Schaffer, Dippel, Wolf, J. Phys. I France, 6, 5 (1996); Latzel, PhD Thesis, U. Stuttgart (2003); Kondic, Phys. Rev. E, 60, 751 (1999)

Forces

- Tangential:
- Cundall-Strack type of model - Geotechnique, 29, 47 (1979)
- Model I: kinetic friction (active only in the presence of relative velocity)
- Model II: includes static friction

$$F_{i,j}^n = \left[k_n x - \gamma_n \bar{m} \mathbf{v}_{i,j}^n\right]$$

$$F_{i,j}^t = -min(\gamma_s \bar{m}|v_{vel}^t|, \mu_s|F_{i,j}^n|)$$

model I model II

$$\begin{aligned} \mathbf{F}_{i,j}^t &= -\min(\mu_s |F^n|, k_t \xi) \frac{\xi}{|\xi|} \\ \xi &= (\int_{t_0}^t \mathbf{v}_{i,j}^t \ (s) \ ds) \cdot \vec{t} \end{aligned}$$

Examples

 Sheared granular systems of varied volume fraction monodisperse and polydisperse



Velocity profiles



Tuesday, June 14, 2011

How do granular particles flow?

- Low volume fractions: exponential, shear banded velocity profiles
 - Predicted and explained by kinetic theory
- Large volume fractions
 - Monodisperse systems: fracture, formation of crystalline zones; temporarily and spatially nonuniform shear
 - Polydisperse systems: reasonably linear velocity profiles, similar as in Newtonian fluids (Xu, O'Hern, Kondic, PRL '05, PRE '05)

Energy Balance

 Note change of dominant energy from kinetic to elastic as system is compressed



E_l elastic energy

 $T_k \begin{array}{l} \text{kinetic granular} \\ \text{temperature} \end{array}$

y distance from the shearing wall

shearing wall: right bottom wall: left

About temperatures and other averaged quantities

- Kinetic granular temperature for dense granular systems is irrelevant from the energetic point of view.
 Can we come up with an alternative concept?
- Application of out-of-equilbrium statistical mechanics concepts to granular matter: Berthier and Barrat J. Chem. Phys. '02; Ono etal PRL '02, O'Hern etal, PRL '04, '05
- Here: consider inclusion of fluctuations of elastic energy (compression) to define `generalized' temperature (Kondic, Behringer, EPL '04)

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$$T_g = T_k + T_e = \frac{m}{2} \left[\langle v^2 \rangle - \langle v \rangle^2 \right] + \frac{k}{2} \left[\langle x^2 \rangle - \langle x \rangle^2 \right]$$

About temperatures and other averaged quantities

- Kinetic granular temperature for dense granular systems is irrelevant from the energetic point of view. 10⁵ Can we come u
- Application of concepts to gra Chem. Phys. '0 '04, '05
- Here: consider energy (compre temperature (K


About averages

calculating averages in *l*'th cell

$$E_{e,l} = \frac{1}{N_t n_l} \frac{k}{2} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} [x_{j,c}]^2$$
$$\langle E_{e,l} \rangle = \frac{k}{2} n_c \langle x_l \rangle^2 = \frac{k}{2} n_c \left[\frac{1}{N_t \bar{n}_l n_c} \sum_{k=1}^{N_t} \sum_{j=1}^{n_l} \sum_{c=1}^{n_{c,j}} x_{j,c} \right]^2$$

$$T_{e,l} = \frac{k}{2} n_c \langle \delta x^2 \rangle = \frac{k}{2} n_c \langle (x_{j,c} - \langle x_l \rangle)^2 \rangle = E_{e,l} - \langle E_{e,l} \rangle$$

What is temperature good for?

- Concept of temperature is a crucial step in developing a continuum model
- Temperature allows to understand heat transfer which may be analyzed on macro scale



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Previous works on energy propagation through dense granular matter

- Extensive literature considering
- response to a localized perturbation
- Reydellet & Clement PRL '01; Geng etal PRL '01; Goldenberg and Goldhirsch, PRL 02, ...
- response to spatially independent (piston-like) perturbations
- Jia etal PRL '99, Hostler & Brennen PRE '05, Somfai etal PRE '05, Mouraille & Luding '06-'09
- response of complex granular systems
- Sen etal IJMPB '05; Baker Geophys '99; Biot JASA '55,...

Motivation

- Here: consider response to a space-time dependent perturbation?
- Why? Response to space-time dependent perturbations provides significant new insight
 - Nature of propagation should help us understand basic mathematical features of an appropriate continuum model
 - diffusive: Coppersmith etal PRE '96;...
 - wave-like: Bouchaud etal JPI '94; Blumenfeld PRL '04;...
 - elastic: Goldenberg and Golhirsch Nature '05; Geng etal PhysD '03;...

Basic System

- 2D system of soft discs modeled:
 - linear force model
 - typically dynamic friction
 - elasticity
 - polydispersity typically 10%
 - (constant) volume fraction typically 0.9
 - 40K particles
 - perturbation
 - standing-wave type, $\lambda \gg d$ $f \ll 1/\tau_c$ A = 0.6d

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Forces and Energies

 Extensive work regarding importance of force chains on signal propagation

Liu & Nagel PRL '92, Makse etal PRL '99; Somfai etal PRE '05; Hostler & Brennen PRE '05;...

• Here: average over small cells and compute spacetime averages of elastic (compression) energy

 $(E_{elas} \gg E_{kin})$

- Carry out Fourier transforms typically FT in xdirection, averaged over time $1/f \gg \Delta t \gg \tau_c$
- Consider first infinite wavelength perturbation

Infinite wavelength perturbation



- wave-like propagation as expected for low frequency excitations
- relation between frequency and the wavenumber in the direction of propagation consistent with linear dispersion
- speed of propagation consistent with the results found in literature



pagation as expected for low tations

wavenumber in the direction of propagation consistent with linear dispersion

 speed of propagation consistent with the results found in literature



pagation as expected for low tations

en frequency and the wavenumber in the direction of propagation $f = 30 \text{ Hz}, \lambda = \infty$ en frequency and the

agation consistent with the results ture





Finite wavelength perturbation - basic case (elastic energy)

6.5

8

5

 $\lambda = 250 d$

3.5

0.5

9.5

11 12.5

Still wave-like propagation, similarly to infinite wavelength perturbation

Look into FT of the propagating signal



 \mathbb{N}

ecomp:





- Well defined wavelike propagation of both elastic energy and temperature
- Are these results robust?





Particle properties: elasticity, friction





Particle properties: elasticity, friction



- no influence of elasticity
- no influence of friction
- no influence of force model



٦1

-0.8

0.6

-0.4

0.2

____0 150

 \vdash

E

11

11







- strong influence of volume fraction
- jammed/unjammed transition?



- strong influence of volume fraction
- jammed/unjammed transition?

 $\rho = 0.90$

 $\rho = 0.85$

 $\rho = 0.80$

150

100

excitations next to the perturbing boundary

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Z(

Perturbation wavelength: example



150

100







150

100







 strong influence of the wavelength of the imposed perturbation, although it is much larger than particle diameter

























 there is a frequency window where well defined signal propagation is observed
Perturbation frequency



 there is a frequency window where well defined signal propagation is observed



Continuum model

$$\nabla^{2}E - \frac{1}{c^{2}}\frac{\partial^{2}E}{\partial t^{2}} - \frac{1}{D}\frac{\partial E}{\partial t} = 0 \qquad k = \frac{2\pi}{\lambda}$$

$$q : \text{ wave number in } z \text{ - direction}$$

$$E(x, z, t) = E_{0}e^{i\omega t}e^{ikx}e^{iqz}$$

$$q = -|q|e^{i\phi/2}, \quad |q^{2}| = \mathcal{X}^{2} + (\omega/D)^{2}, \quad \tan \phi = -\frac{\omega}{(D\mathcal{X})}$$

$$\mathcal{X} = (\omega/c)^{2} - k^{2}$$

Can we explain signal properties based on this simple model?

Kondic, Dybenko, Behringer, PRE '09

more precise approach using Green's function solution with similar conclusions

f fixed, k increases $\rightarrow q$ decreases

 $f \text{ fixed}, k \text{ increases} \rightarrow q \text{ decreases} \checkmark$

f fixed, k increases $\rightarrow q$ decreases \checkmark

f fixed, k increases \rightarrow stronger attenuation

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k fixed, f decreases $\rightarrow q$ decreases

f increases $\rightarrow q$ increases, stronger attenuation

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f fixed, k increases \rightarrow stronger attenuation \checkmark

 $k \text{ fixed}, f \text{ decreases} \rightarrow q \text{ decreases}$

f increases $\rightarrow q$ increases, stronger attenuation ?

 $f \text{ fixed}, k \text{ increases} \rightarrow q \text{ decreases} \quad \checkmark$

f fixed, k increases \rightarrow stronger attenuation \checkmark

 $k \text{ fixed}, f \text{ decreases} \to q \text{ decreases} \quad \checkmark$

f increases $\rightarrow q$ increases, stronger attenuation ?

$$\left|\frac{2\pi}{q} \sim d \rightarrow \text{model breaks down}\right|$$

Continuum Model

- Parameters (*D*, *c*) assumed to be perturbation independent
- Values used: $\frac{c}{c*} \approx 0.025; \quad c* = \sqrt{\frac{E}{\rho(1-\sigma^2)}} \quad \text{consistent with}$ time-of-flight

$$D = v_e l/3; \quad v_e \approx c \ast \rightarrow l \approx 30 - 40d$$

Sheng '95

Jia '04

- Large correlation length! Related to force chain structure?
- Correlation length diverging close to jamming?
- More work to be done to understand this issue

Energy and stress propagation during impact on a granular system

- Discuss main features of impact
- Illustrate the effect of material properties on the impact dynamics
- Concentrate on the granular material:
 - force and energy fields in the material itself: topological and other measures

Literature

- Large number of works considering impact on granular systems
- Scaling of the penetration depth with impact velocity, size, ...
 Debouf etal, PRE'09; Walsh etal PRL'03; Uehara etal PRL'03; Ciamarra etal PRL'04;...
- Development of effective models based on
 - collisional effects (Seguin etal EPL'09)
 - fluid-like models (de Bruyn Can. J. Phys'04)
 - ballistic approach (Katsuragi&Durian Nat. Phys.'07, Tsimring&Volfson P&G'05); ...
- very few works considering influence of microstructure (Toya etal PRL'04)

Setup

- modeling inelastic, frictional spherical particles (soft particle simulations)
- details:
 - typically polydisperse granular particles, with the sizes randomly sampled in the range $1 \pm r$
 - 6,000 90,000 particles in 2D are used; linear springs are implemented, and both static and kinetic friction are considered; gravity is included
 - initial granular configuration: typically particles given random initial velocities and left to settle under gravity; in addition regular packings are considered
 - system: periodic boundaries left-right; absorbing walls top/bottom
 - impacting object large compared to a particle size (currently 5 15 average diameters), positioned at a fixed height above the granular particles and given initial velocity downwards
 - in this talk: concentrate (mostly) on shallow impacts

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Simulations

- Animations: normal force which particles and the intruder experience during impact
- Significant differences between disordered, polydisperse and ordered, monodisperse systems
- structure of the material seem to be playing an important role in determining the intruder's dynamics

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Impactor velocity (basic system)



- depth: the position of the bottom part of impactor with respect to upper boundary of the system particles at the point of impact
- basic system: increase of penetration depth with increased velocity; initial overshoot for larger velocities; elastic damping of oscillations
- considered velocities comparable to the average speed of propagation of elastic waves (speed of sound) $c \approx 2$

$$\tau_c = \pi \sqrt{\frac{d}{2gk_n}}$$

 $k_n = 4 \cdot 10^3; d \approx 4mm; \tau_c \approx 7 \cdot 10^{-4}; d/\tau_c \approx 5m/s$

Impactor velocity (basic system)



Scales

- length scale: particle diameter d
- time scale: binary collision time $\tau_c = \pi_1$
- velocity scale d/ au_c

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Material parameters

- simulations allow for precise analysis of the influence of system (size, particle properties) and intruder properties (size, density, shape) on penetration
- here: concentrate on the influence of
 - friction
 - packing and polydispersity



System preparation: order versus disorder



triangular/hexagonal

random

deeper penetration into disordered polydisperse systems

 concentrate on force field structure and its influence on the dynamics of the impact

Impactor size (basic system)



large

medium

small

deeper penetration for larger impactors of same initial velocity

Impactor size (basic system)



large

medium

small

deeper penetration for larger impactors of same initial velocity

Impactor size (basic system)



large

medium

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 deeper penetration for larger impactors of same initial velocity

Influence of gravity



Influence of gravity



 strong influence of gravity on impact (keeping all other parameters the same)

Influence of gravity



 strong influence of gravity on impact (keeping all other parameters the same)

Force networks for different friction models: Normal force

polydisperse system



kinetic friction



static friction

- force networks are complicated and difficult to analyze
- we need clear and objective measure of force field for different systems

Force networks for different friction models: Tangential force

polydisperse system



• Stronger tangential forces for static friction simulations: how to quantify the structure?

Force networks for different friction models: Normal force monodisperse (ordered) system



kinetic friction

static friction

Force networks for different friction models: Tangential force monodisperse (ordered) system



kinetic friction



static friction

Current work

- impact of heavy, non-circular intruders (collaborative with experiments at Duke)
- analysis of force structure properties (connectivies, clusters, percolation)
- 3D simulations

Current work


Force field structure:

- Rigidity phase transition, Aharonov & Sparks PRE '99
- Force distributions, Radjai etal, Chaos '99
- Force networks due to localized perturbation, Goldenberg & Goldhirsch, PRL '02
- Anisotropy of force networks, Majmudar & Behringer Nature '05
- Force chain statistics, Peters etal, PRE '05
- Role of force networks in elastic wave propagation, Somfai etal PRE '05
- Scale invariance of force networks: percolation approach using MD and MC simulations: Ostojic etal, Nature '06

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Is there a simple but precise way to describe force chains?

Topological measures

- Consider topological measures of the force field
- Here: concentrate on the simplest measures specifying connectivity and holes that form as a function of force magnitude: *Betti numbers*
- Consider a very simple system: isotropically compressed system of circular disks in 2D
- Discuss how the topological measures, quantified by *Betti numbers*, change as volume fraction is modified

Exploring force field structure

looking for an objective measure of global features of the force field

 compute connectivity of the granular particles as a function of total force (normal or tangential) experienced: quantify in terms of Betti numbers measuring number of components (clusters) and number of holes (`loops') <u>http://chomp.rutgers.edu/</u>





- compute Betti numbers and observe the features of force network for different systems
- here concentrate on B0

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$$B_0 = 3$$

 $B_1 = 0$

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Topology Tools: CHomP

- CHomP: computational package by Mischaikow and collaborators used to compute Betti numbers (and many other things) of various spatial and temporal structures http://chomp.rutgers.edu/
- Here: concentrate on
 - B0: number of connected components
 - B1: number of holes
 - Structure: force field in a compressed granular system

Example of simulations













Betti numbers: BO

- polydisperse system
 dynamic friction
 average 20 realizations
 normalized by number of particles
 system-size independent
- main features of the results are rate independent



Betti numbers: BO

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- average 20 realizations
- normalized by number of particles
- system-size independent
 main features of the results are rate independent



zero threshold: showing fabric of the material
large volume fraction: huge increase of the number of
components
Is this intrinsic property of dense jammed granular
systems?

Which of material properties influence topology of force chains?



polydisperse, dynamic friction (static friction produces similar results)

Which of material properties influence topology of force chains?



polydisperse, dynamic friction static friction (static friction produces similar results)

monodisperse,

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polydisperse, dynamic friction (static friction produces similar results)

monodisperse, static friction

monodisperse, dynamic friction

B0 captures the influence of friction on the structure of force network

Summary

- discrete element simulations are very useful in analyzing granular systems
- significant information can be extracted and connected to continuum models
- computing hardware and software allows for considering problems and questions which could not be approached just few years ago
- there is a large number of relevant and important problems which should be addressed: 3D systems; cohesive particles; particles of irregular shapes, and many others