Introduction to Particle Systems and Modeling Methods

Stefan Luding
MSM, TS, CTW, UTwente, NL

Stefan Luding, s.luding@utwente.nl
MSM, TS, CTW, UTwente, NL

Granular Materials

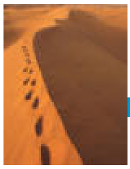
Real:
- sand, soil, rock,
- grain, rice, lentils,
- powder, pills, granulate,
- micro- and nano-particles

Model Granular Materials
- steel/aluminum spheres
- spheres with dissipation/friction/adhesion

Why Granular Materials

Numberless applications:
- constructions, industry (silos), agriculture, …
- everyday life (e.g. coffee powder, sugar, salt, …)

Challenges for Physics, Mechanics, Materials- and Computational Science and Engineering
- many particle systems, non-linear, non-equilibrium

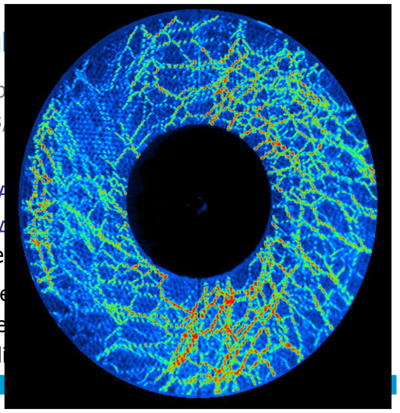


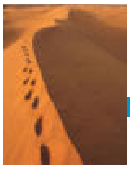
- segregation (mixing), pattern formation
- force chains (wide distributions)
- localization (shearbands, fracture)

Why Granu

Numberless app
- constructions,
- everyday life

Challenges for P
and Comp
- many particle
  - segre
  - force
  - locali

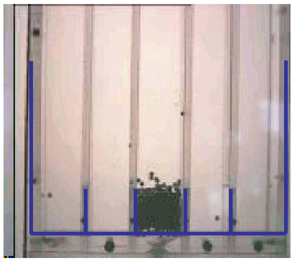




Clustering
- vibrated (weak) box with compartments

Experiments:
Twente, NL,
D. Lohse et al. 2001, …

Clustering
- (strongly) vibrated box with compartments



What is the problem ?

- Excluded volume effects … crystallization
- Granular medium with ALL densities realized
- Dissipation & Friction & Adhesion
- Out of equilibrium, chaotic
- Non-equipartition of energies
- Temperature and pressure dependence
- sintering, fracture, damage, …
- etc.

How to approach ?

Experiments …
Continuum theory (materials, micropolar, …)
Statistical Physics
\+ Kinetic theory + dissipation + friction
Numerical Modeling

- Monte Carlo (stochastic methods)
- Molecular dynamics-like simulations (MD++)
- Finite Element Method (FEM)

Numerical Modeling Overview

Scales and examples:

sub-particle (atomistic – molecular dynamics)
particle & particle-contact modeling
multi-particle modeling (discrete element method)
system modeling (silo, reactor, …)
using e.g. FEM to solve continuum theory
process and plant modeling

Methods discussed:

particle methods (stochastic-deterministic)
finite element model (FEM)

Deterministic or Stochastic Models ?

Method	Abbrev.	Theory
Molecular dynamics (soft particles)	MD	…
Event Driven (hard particles)	ED	(Kinetic Theory)
Monte Carlo (random motion)	MC	Stat. Phys.
Direct Simulation Monte Carlo	DSMC	Kinetic Theory
Lattice (Boltzmann) Models	LB	Navier Stokes

Deterministic or Stochastic Models ?

Method	Determ./ Stochast.	Discrete Time	Discrete Space	Discrete Events	Flexible	Fast
MD (soft p.)	D	X			*****	*
ED (hard p.)	D			X	*	***
MC	S	?			*	**
DSMC	S	X			***	****
LB	S	X	X		*	*****

DCCSE – steps in simulation

see:
pcse.tudelft.nl/index.php?page=introduction

1. Setting up a model
2. Analytical treatment
3. Numerical treatment
4. Implementation
5. Embedding
6. Visualisation
7. Validation

DCCSE – steps in simulation

see:
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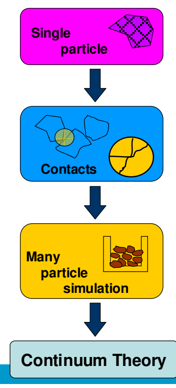
1. Setting up a model	1. Particle model
2. Analytical treatment	2. Kinetic theory
3. Numerical treatment	3. Algorithms for MD
4. Implementation	4. FORTRAN or C++/MPI
5. Embedding	5. Linux – research codes
6. Visualisation	6. xballs X11 C-tool
7. Validation	7. theory/experiment

Approach philosophy

- Introduction
- Single Particles
- Particle Contacts/Interactions
- Many particle cooperative behavior
- Applications/Examples
- Conclusion



Deterministic Models …

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What is Molecular Dynamics ?

1. Specify interactions between bodies

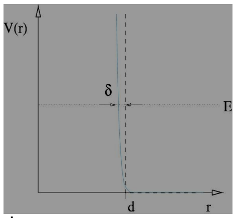
2. Compute all forces

$$\mathbf{f}_{j \to i}$$

3. Integrate the equations of motion for all particles

$$m\ddot{\mathbf{x}}_i = \sum_{j \neq i} \mathbf{f}_{j \to i}$$

What is Molecular Dynamics ?



1. Specify interactions between bodies (for example: two spherical atoms)

2. Compute all forces $\mathbf{f}_{j \to i}$

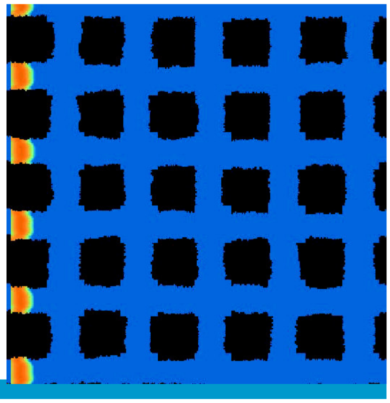
3. Integrate the equations of motion for all particles (Verlet, Runge-Kutta, Predictor-Corrector, …) with fixed time-step dt

$$m\ddot{\mathbf{x}}_i = \sum_{j \neq i} \mathbf{f}_{j \to i}$$

Applications & Examples

1. Flow in porous media (fluids)
2. Granular Flow (pipe & hopper)
3. Vibration & Segregation
4. Granular Gases (Diffusion & Clustering)
5. Shear cells (slow, dense flow)
6. Membranes (topology & fluctuations)
7. Adhesion and Sintering (attractive forces)
8. Sound propagation (wave theory)
9. Electro-spray (charged particles = long-range forces)
10. Particle-Fluid coupling

Flow in porous media



Approach philosophy

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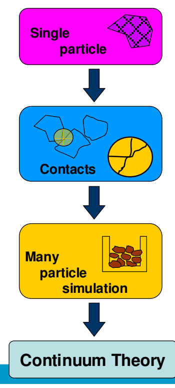
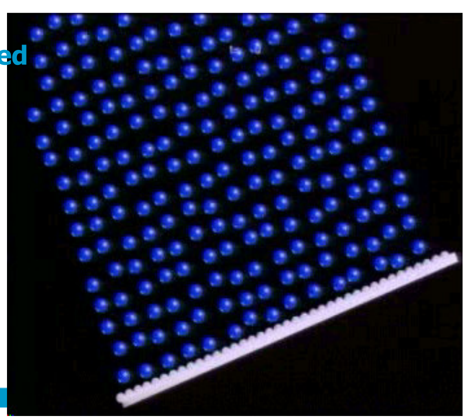
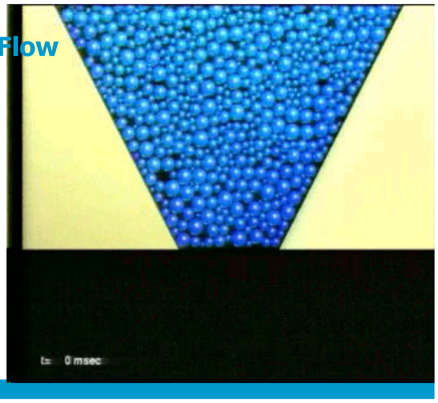


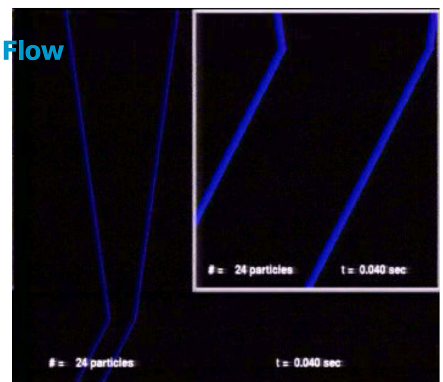
Inclined plane



Hopper Flow

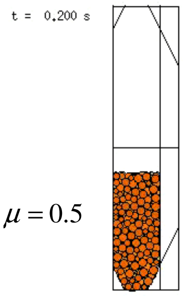


Hopper Flow

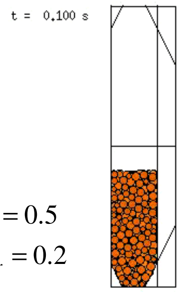


Silo Flow

Silo Flow with friction

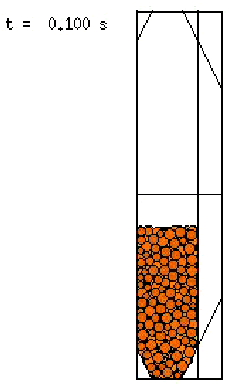


$\mu = 0.5$



$\mu = 0.5$

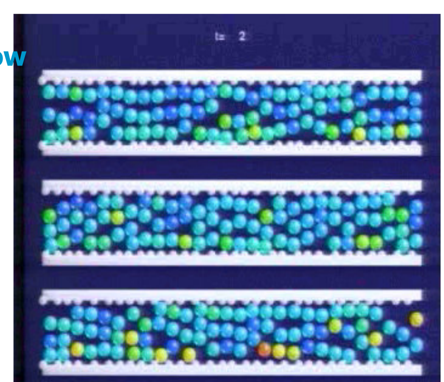
$\mu_r = 0.2$



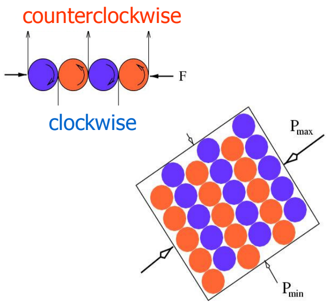
$\mu = 0.5$

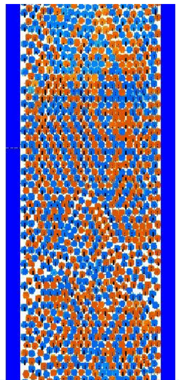
$\mu_r = 0.2$

Pipe Flow



Rotational order



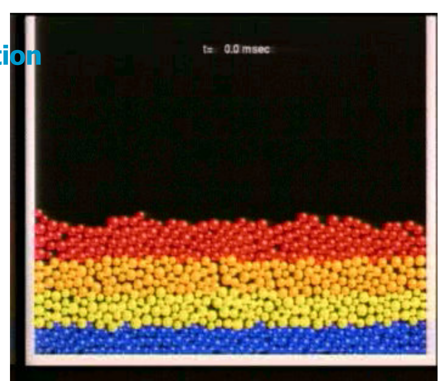


Simulation of Contacts
Between Many Bodies Using
Methods from Molecular Dynamics

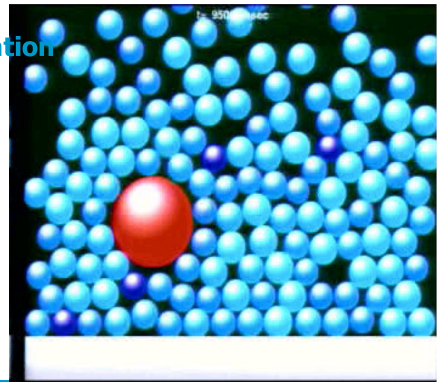
by

B. Muth, P. Eberhard and S. Luding

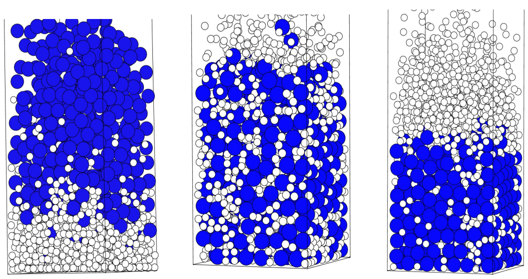
Convection



Segregation

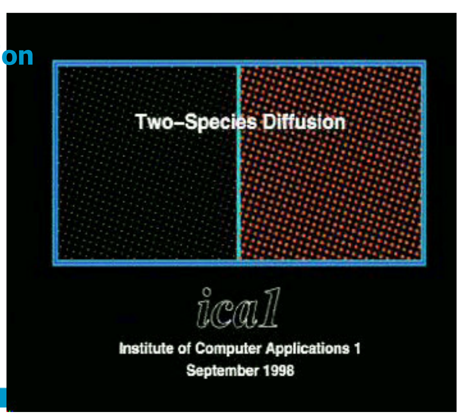


Segregation – Mixing – Reverse segregation



P. V. Quinn, D. Hong, SL, PRL 2001

Diffusion



Cooling of a Dissipative System

(ED Simulation)

10^5 Particles

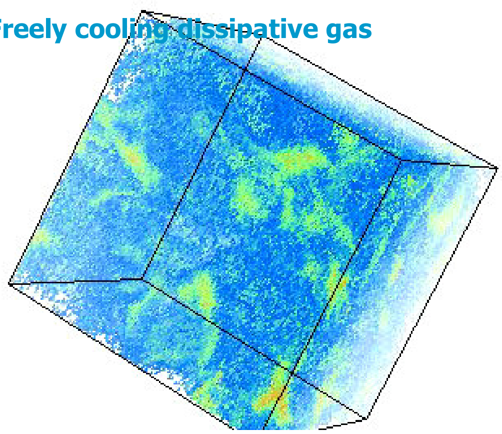
Restitution: 0.9

Volume Fraction: 0.25

Periodic Boundaries

Freely cooling dissipative gas

3D



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