Introduction to Particle Systems and Modeling Methods

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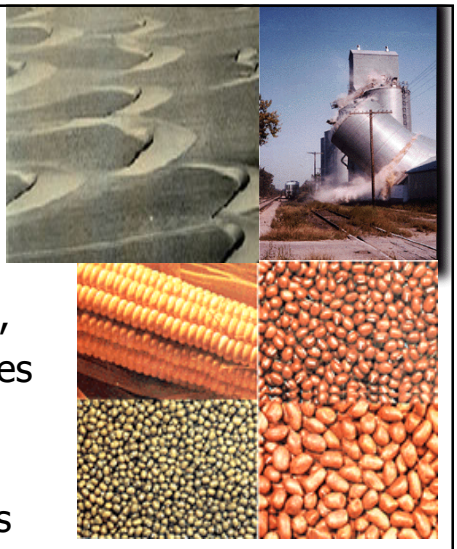
Granular Materials



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)

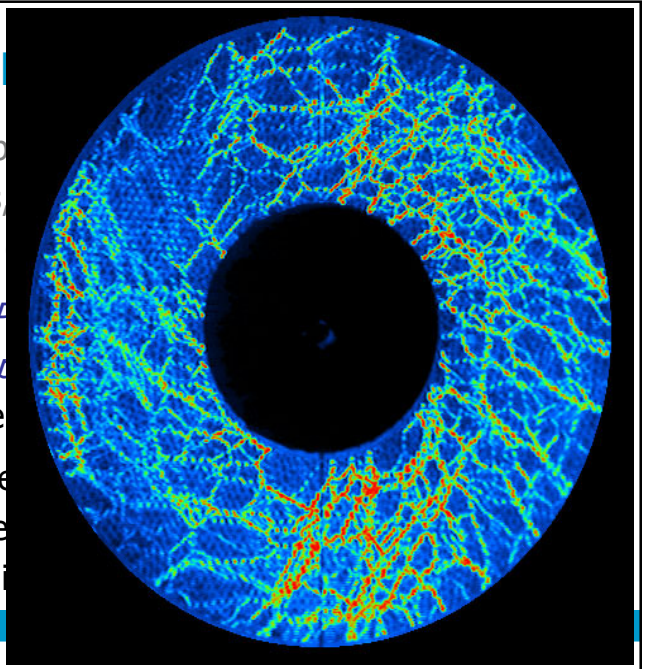
Why Granul

Numberless app

- constructions,
- everyday life

Challenges for P
and Comp

- many particle

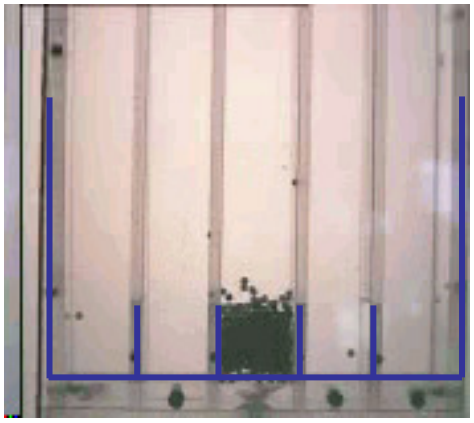


- segre
- force
- locali

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

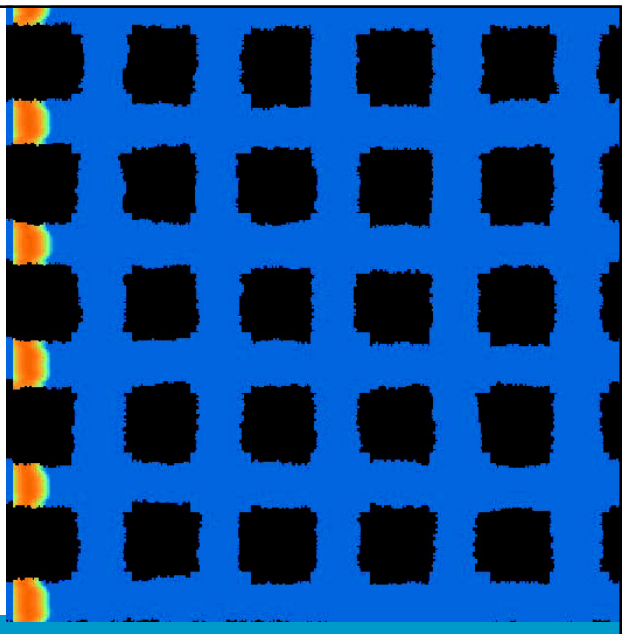
1. Setting up a model
2. Analytical treatment
3. Numerical treatment
4. Implementation
5. Embedding
6. Visualisation
7. Validation

DCCSE – steps in simulation

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

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

Flow in porous media



Deterministic Models …

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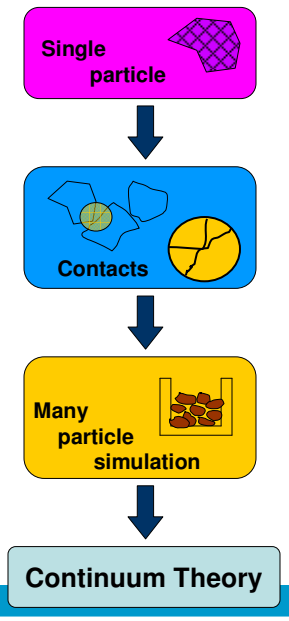
Approach philosophy

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



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

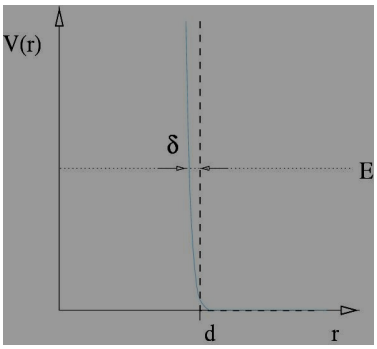
$$m\ddot{\mathbf{x}}_i = \sum_{j\neq i} \mathbf{f}_{j\to i}$$

What is Molecular Dynamics ?

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

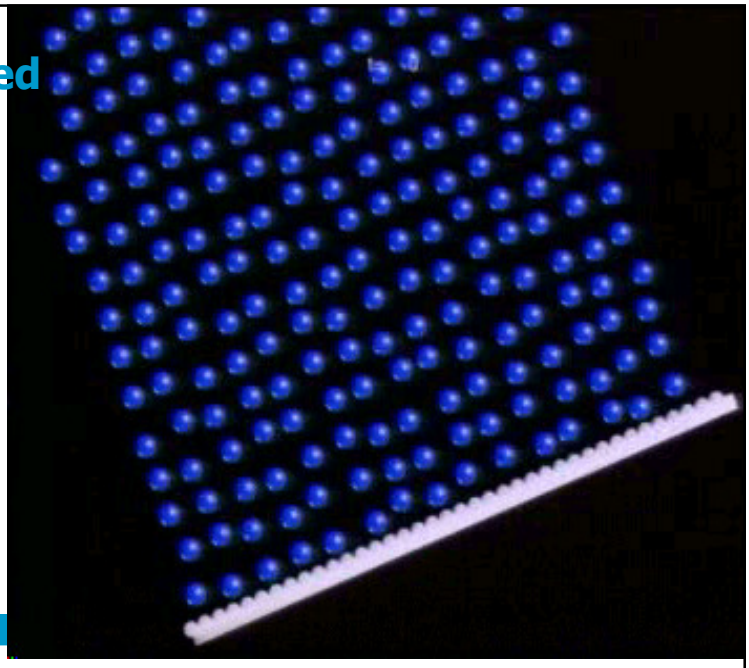
2. Compute all forces $\mathbf{f}_{j\to i}$

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

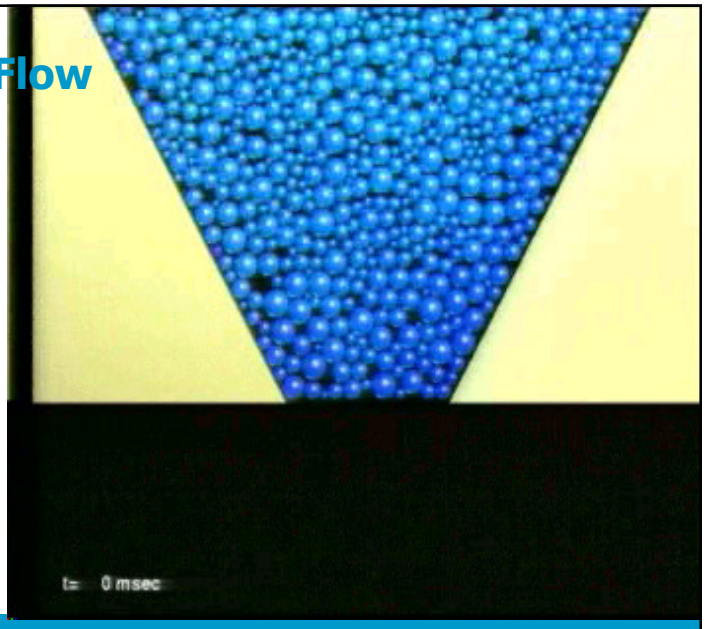


$$m\ddot{\mathbf{x}}_i = \sum_{j\neq i} \mathbf{f}_{j\to i}$$

Inclined plane



Hopper Flow



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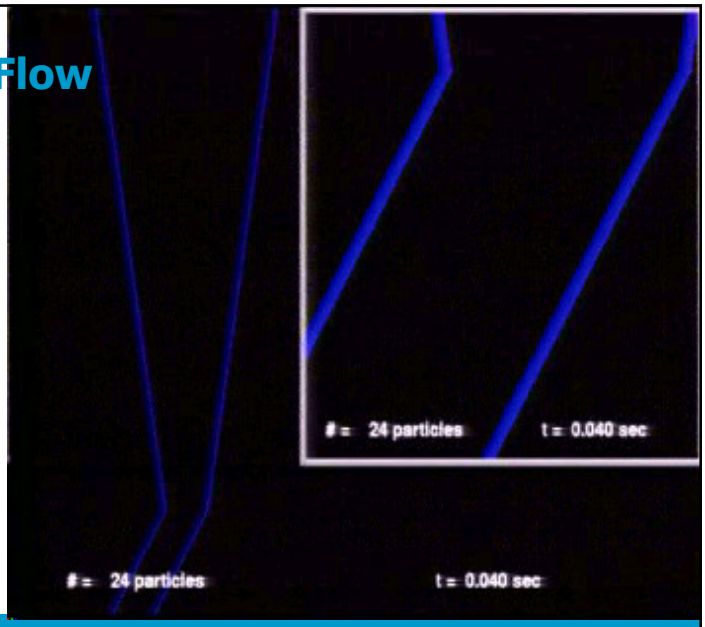
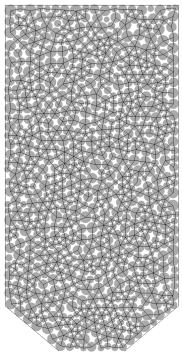
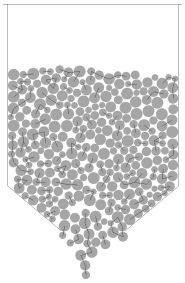


Silo Flow

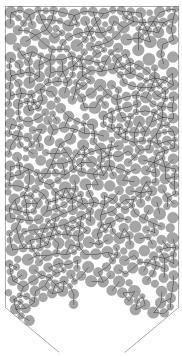
Initial



Outflow

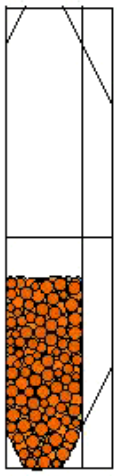


Jamming



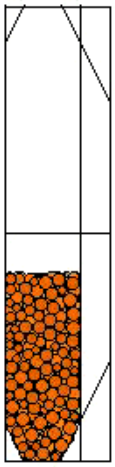
Silo Flow with friction

t = 0.200 s



$\mu = 0.5$

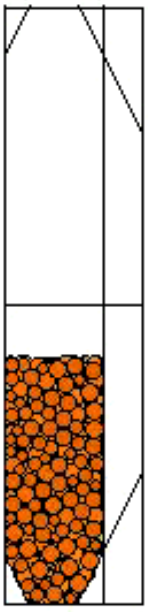
t = 0.100 s



$\mu = 0.5$

$\mu_r = 0.2$

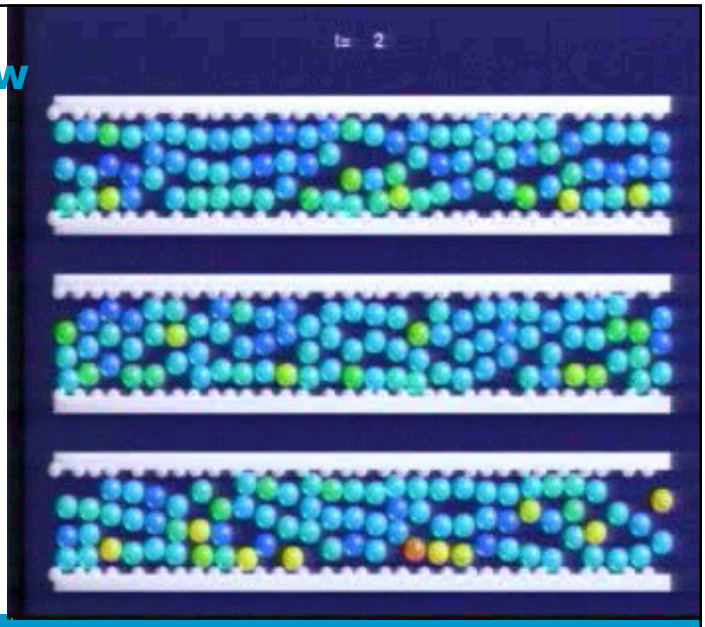
t = 0.100 s



$\mu = 0.5$

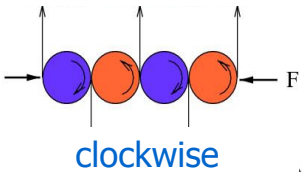
$\mu_r = 0.2$

Pipe Flow

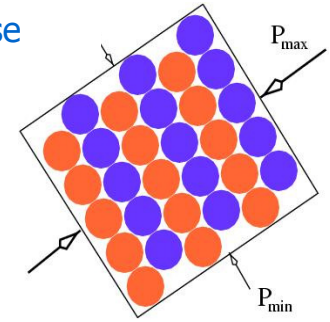


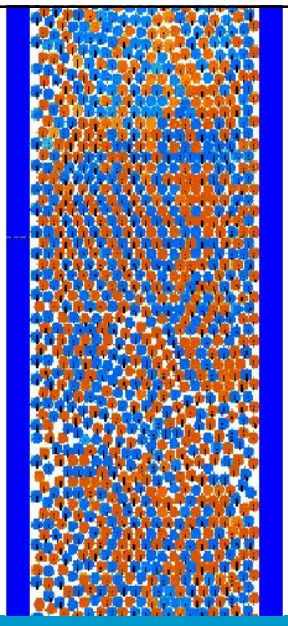
Rotational order

counterclockwise



clockwise



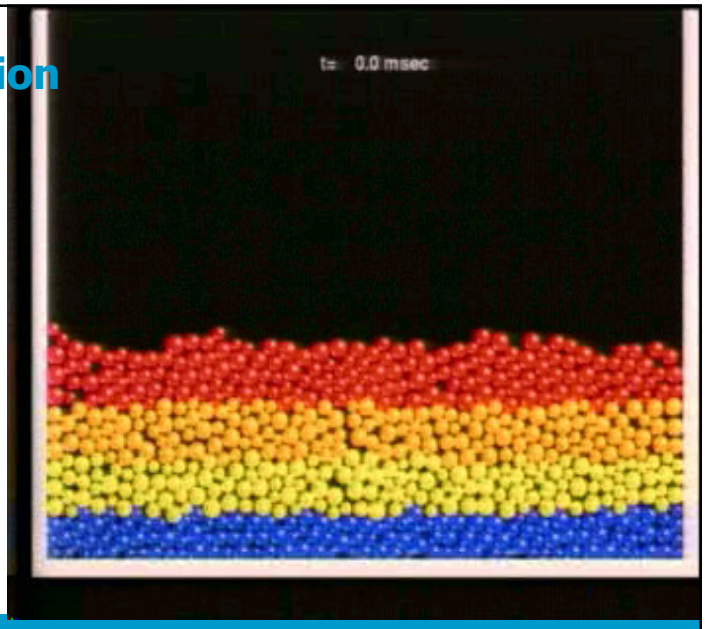


Simulation of Contacts
Between Many Bodies Using
Methods from Molecular Dynamics

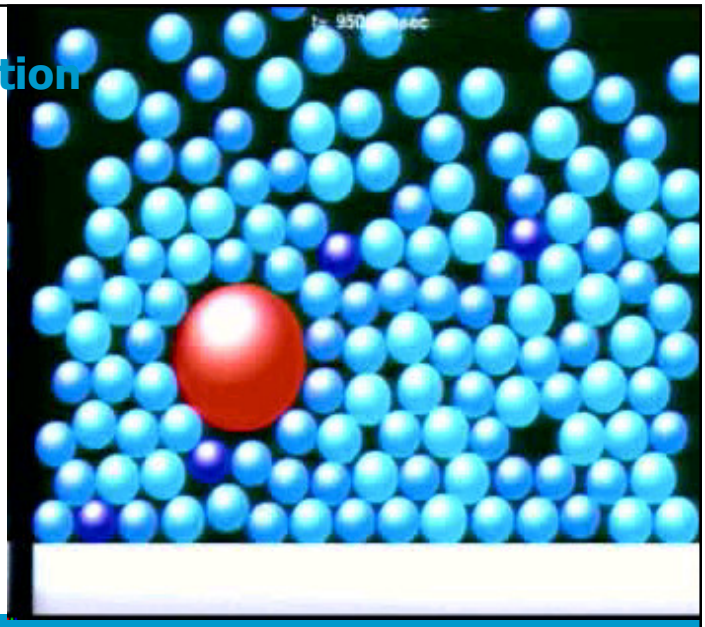
by

B. Muth, P. Eberhard and S. Luding

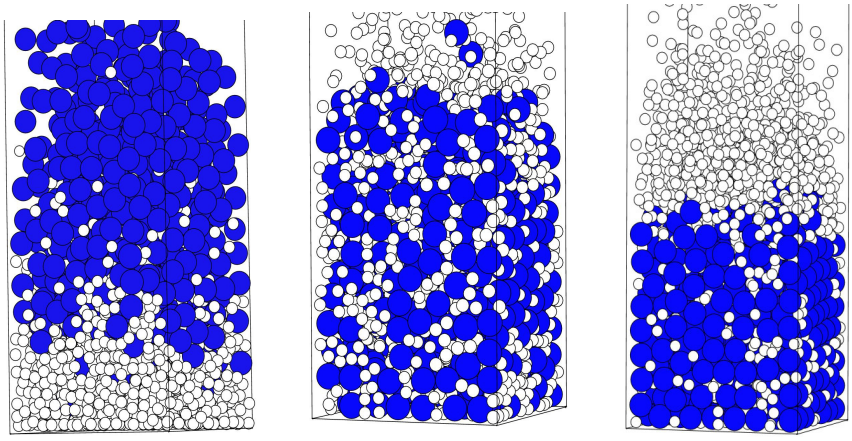
Convection



Segregation

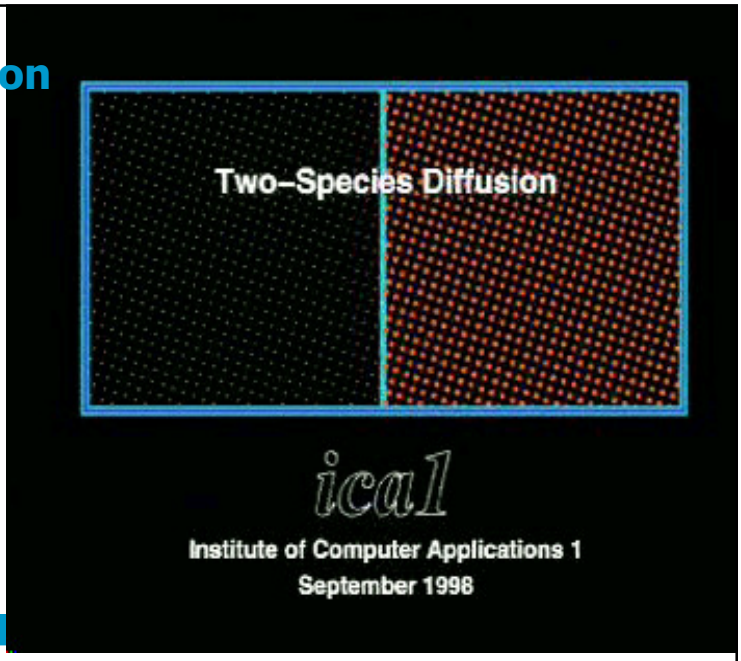


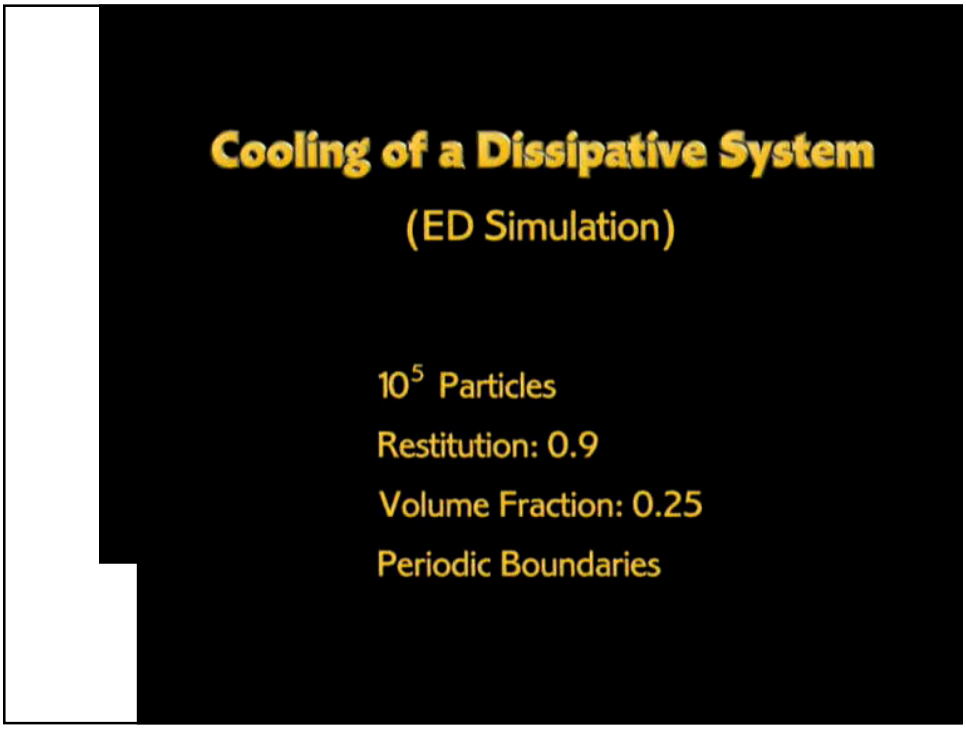
Segregation – Mixing – Reverse segregation



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

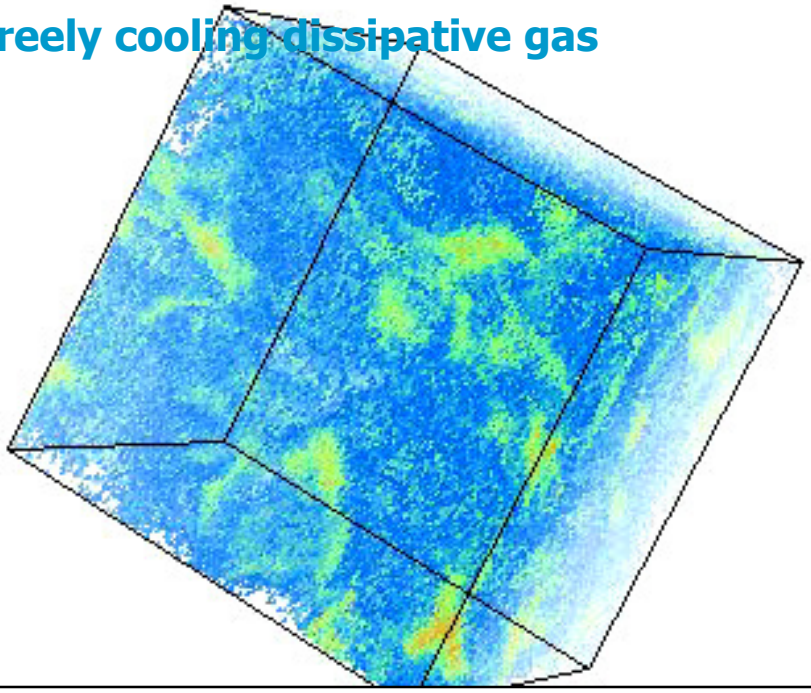
Diffusion


Two–Species Diffusion
ica1
Institute of Computer Applications 1
September 1998


Cooling of a Dissipative System
(ED Simulation)
10^5 Particles
Restitution: 0.9
Volume Fraction: 0.25
Periodic Boundaries

Freely cooling dissipative gas

3D



EM-course Literature (http://www2.msm.ctw.utwente.nl/sluding/publications.html)
[1] S. Luding, I*ntroduction to Discrete Element Methods: Basics of Contact Force Models and how to perform the Micro-Macro Transition to Continuum Theory*, European Journal of Environmental and Civil Engineering - EJECE 12 - No. 7-8 (Special Issue: Alert Course, Aussois), 785-826 (2008),
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/luding_alert2008.pdf]
[2] S. Luding, C*ohesive frictional powders: Contact models for tension*
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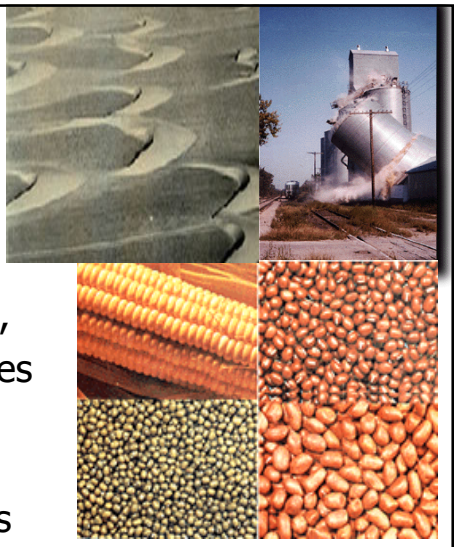
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/LudingC5.pdf]
[3] S. Luding *Collisions & Contacts between two particles,*
in: Physics of dry granular Media, eds. H. J. Herrmann, J.-P. Hovi, and S. Luding, Kluwer Academic Publishers, Dordrecht, 1998
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf]
[4] M. Lätzel, S. Luding, and H. J. Herrmann,
Macroscopic material properties from quasi-static, microscopic simulations of a two-dimensional shear-cell , Granular Matter 2(3), 123-135, 2000
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/micmac.pdf]
[5] S. Luding, *Anisotropy in cohesive, frictional granular media*
J. Phys.: Condens. Matter 17, S2623-S2640, 2005
[http://www2.msm.ctw.utwente.nl/sluding/PAPERS/jpcm1.pdf]

Granular Materials



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Deterministic Models …

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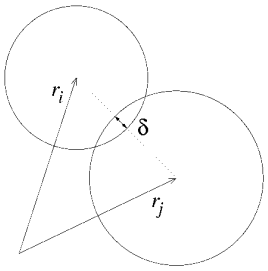
Discrete particle model

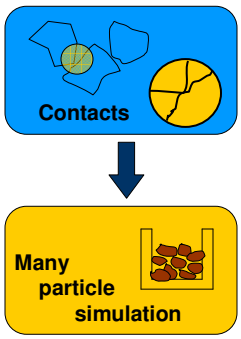


Equations of motion

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i$$

Forces and torques:

$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$

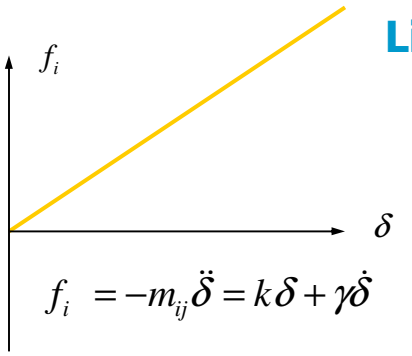


Contact if Overlap > 0

Overlap $\delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right)\cdot\vec{n}$

Normal $\hat{n} = \vec{n}_{ij} = \frac{\left(\vec{r}_i - \vec{r}_j\right)}{\left|\vec{r}_i - \vec{r}_j\right|}$

Linear Contact model



$$f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

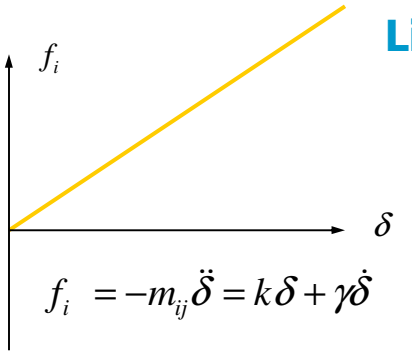
- **really simple ☺**
- **linear, analytical**
- **very easy to implement**

overlap $\delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right)\cdot\vec{n}$

rel. velocity $\dot{\delta} = -\left(\vec{v}_i - \vec{v}_j\right)\cdot\vec{n}$

acceleration $\ddot{\delta} = -\left(\vec{a}_i - \vec{a}_j\right)\cdot\vec{n}$

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf



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overlap $\delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right)\cdot\vec{n}$

rel. velocity $\dot{\delta} = -\left(\vec{v}_i - \vec{v}_j\right)\cdot\vec{n}$

acceleration $\ddot{\delta} = -\left(\vec{a}_i - \vec{a}_j\right)\cdot\vec{n} = -\left(\vec{f}_i/m_i - \vec{f}_j/m_j\right)\cdot\vec{n} \overset{\left(\vec{f}_j=-\vec{f}_i\right)}{=} -\frac{1}{m_{ij}}\vec{f}_i\cdot\vec{n}$

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Linear Contact model

$$f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

$$k\delta + \gamma\dot{\delta} + m_{ij}\ddot{\delta} = 0$$

$$\frac{k}{m_{ij}}\delta + 2\frac{\gamma}{2m_{ij}}\dot{\delta} + \ddot{\delta} = 0$$

$$\boxed{\omega_0^2\delta + 2\eta\dot{\delta} + \ddot{\delta} = 0}$$

- really simple ☺
- linear, analytical
- very **easy** to implement

elastic freq. $\omega_0 = \sqrt{k/m_{ij}}$

eigen-freq. $\omega = \sqrt{\omega_0^2 - \eta^2}$

visc. diss. $\eta = \frac{\gamma}{2m_{ij}}$

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Linear Contact model

$$f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

$$k\delta + \gamma\dot{\delta} + m_{ij}\ddot{\delta} = 0$$

$$\frac{k}{m_{ij}}\delta + 2\frac{\gamma}{2m_{ij}}\dot{\delta} + \ddot{\delta} = 0$$

$$\boxed{\omega_0^2\delta + 2\eta\dot{\delta} + \ddot{\delta} = 0}$$

- **really simple ☺**
- **linear, analytical**
- **very easy to implement**

$$\delta(t) = \frac{v_0}{\omega}\exp(-\eta t)\sin(\omega t)$$

$$\dot{\delta}(t) = \frac{v_0}{\omega}\exp(-\eta t)\left[-\eta\sin(\omega t) + \omega\cos(\omega t)\right]$$

elastic freq. $\omega_0 = \sqrt{k/m_{ij}}$

eigen-freq. $\omega = \sqrt{\omega_0^2 - \eta^2}$

visc. diss. $\eta = \frac{\gamma}{2m_{ij}}$

contact duration $\boxed{t_c = \pi/\omega}$

restitution coefficient $r = -\frac{v(t_c)}{v_0} = \exp(-\eta t_c)$

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Linear Contact model ($m_w=\infty$)

	particle-particle	particle-wall
elastic freq.	$\omega_0 = \sqrt{k/m_{ij}}$	$\omega_0^{wall} = \sqrt{k/m_i} = \omega_0/\sqrt{2}$
eigen-freq.	$\omega = \sqrt{\omega_0^2 - \eta^2}$	$\omega^{wall} = \sqrt{\omega_0^2/2 - \eta^2/4}$
visc. diss.	$\eta = \frac{\gamma}{2m_{ij}}$	$\eta^{wall} = \frac{\gamma}{2m_i} = \frac{\eta}{2}$
contact duration	$\boxed{t_c = \pi/\omega}$	$\boxed{t_c^{wall} = \pi/\omega^{wall} > t_c}$
restitution coeff.	$r = \exp(-\eta t_c)$	$r^{wall} = \exp(-\eta^{wall} t_c^{wall})$

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Time-scales

time-step $\Delta t <= t_c / 50$

contact duration $\boxed{t_c = \pi / \omega}$ $t_n < t_c$ $t_c^{wall} = \pi / \omega^{wall} > t_c$

time between contacts

$t_n > t_c$

sound propagation $N_L t_c$ ... with number of layers N_L

experiment T

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Time-scales

time-step $\Delta t <= t_c / 50$

contact duration $\boxed{t_c = \pi / \omega}$ $t_n < t_c$

different sized particles $t_c^{large} > t_c^{small}$

time between contacts

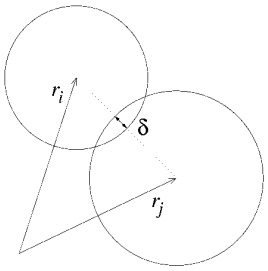
$t_n > t_c$

sound propagation $N_L t_c$ ... with number of layers N_L

experiment T

http://www.ica1.uni-stuttgart.de/~lui/PAPERS/coll2p.pdf

Discrete particle model

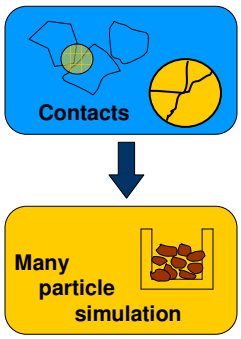


Equations of motion

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i$$

Forces and torques:

$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$

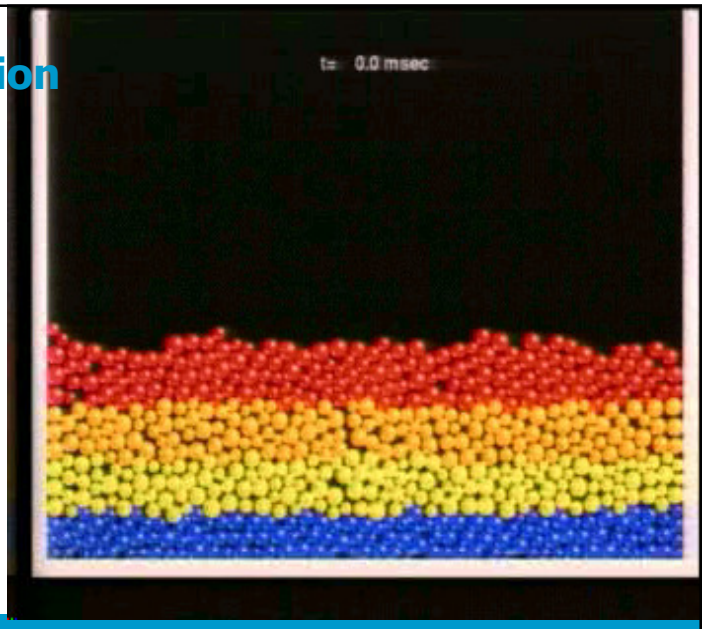


Contact if Overlap > 0

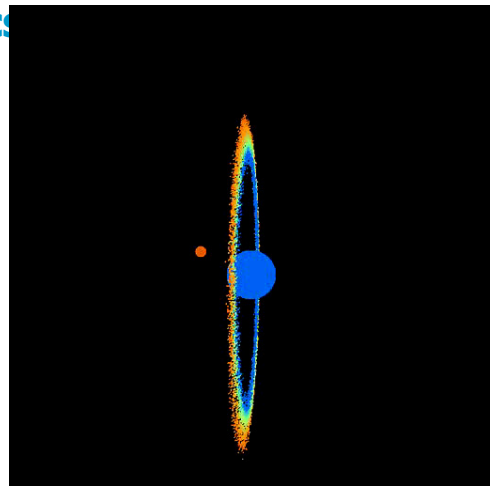
Overlap $\delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right) \cdot \vec{n}$

Normal $\hat{n} = \vec{n}_{ij} = \frac{\left(\vec{r}_i - \vec{r}_j\right)}{\left|\vec{r}_i - \vec{r}_j\right|}$

Convection

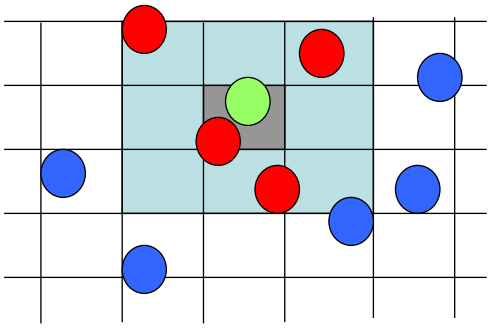


Molecular Dynamics example from astrophysics



Algorithmic trick(s) for speed-up

- Linked cells neighborhood search O(1) (*short range forces*)



- Linked cells update after 10-100 time-steps O(*N*)

Rigid interaction (hard spheres)

Stiff (rigid) interactions require dt=0

Events (=collisions) occur in **zero-time** (instantaneously)

that means: Integration is *impossible* !

1. Propagate particles between collisions
2. Identify next event (collision)
3. Apply collision matrix

Why use hard spheres ?

\+ advantages

- Event driven (ED) is faster than MD
- Analytical kinetic theory is available (with 99.9% agreement)

– drawback

- Implementation of arbitrary forces is expensive
- Parallelization is less successful

Why use hard spheres ?

+ advantages
- Event driven (ED) is faster than MD
- Analytical kinetic theory is available
  (with 99.9% agreement)

– drawback
- Implementation of arbitrary forces is expensive
- Parallelization is less successful

Algorithm (serial)

0. Initialize
- Compute all forces O(1)
- Integrate equations of motion $t+dt$
- O(N) – `goto` 1.

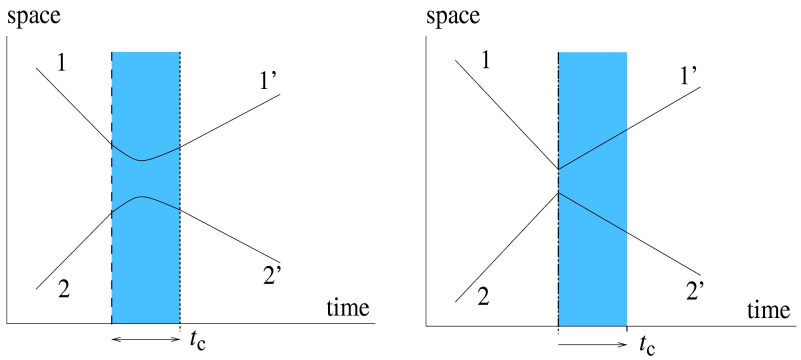
Total effort:

O(N)

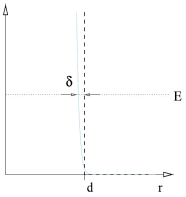
Rigid interaction (hard spheres)

1. Stiff (rigid) interactions require dt=0

   Events (=collisions) occur in **zero-time**



Rigid interaction (hard spheres)



2. Solve equation of motion between collision

- trajectory $\mathbf{x}_i(t) = \mathbf{x}_i(0) + \mathbf{v}_i(0)t + \frac{1}{2}\mathbf{g}t^2$

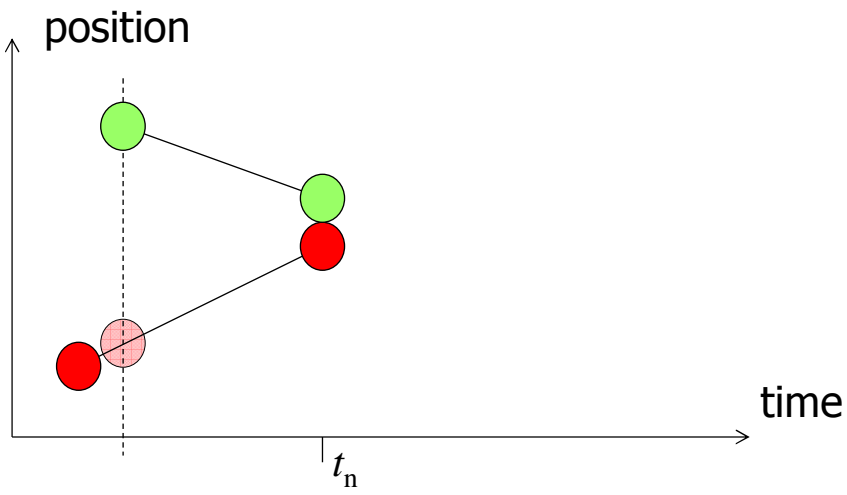
- contact $\left\|\Delta\mathbf{x}_{ij}\right\| = \left\|\mathbf{x}_i(t) - \mathbf{x}_j(t)\right\| = r_1 + r_2$

$$\left(\Delta\mathbf{x}_{ij}(0) + \Delta\mathbf{v}_{ij}(0)t\right)^2 = \left(r_1 + r_2\right)^2$$

$$\underbrace{\Delta\mathbf{x}_{ij}^{\,2} - \left(r_1 + r_2\right)^2}_{c} + \underbrace{\Delta\mathbf{x}_{ij}\cdot\Delta\mathbf{v}_{ij}}_{b}\,t + \underbrace{\Delta\mathbf{v}_{ij}^{\,2}}_{a}\,t^2 = 0$$

- event-time $t_{1,2} = \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

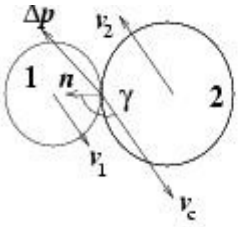
Time evolution



Rigid interaction (hard spheres)

Collision rule (translational)

$$v'_{1,2} = v_{1,2} \pm (1+r)\,\Delta P / 2m_{1,2}$$

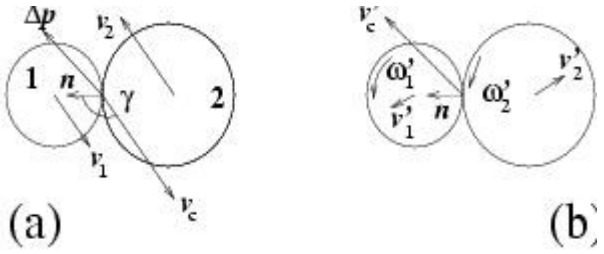


Momentum conservation + dissipation
with restitution coefficient (normal): r

Rigid interaction (hard spheres)

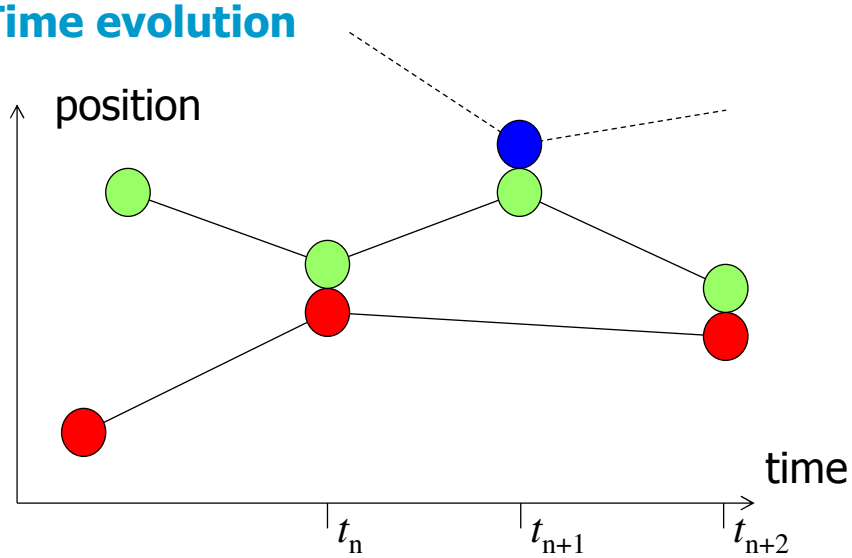
Collision rule (translational and rotational)

$$v'_{1,2} = v_{1,2} \pm (1+r)\,\Delta P / 2m_{1,2} \qquad \omega'_{1,2} = \omega_{1,2} \pm (1+r_t)\,\Delta L / 2I_{1,2}$$



Restitution coefficient (normal): r (tangential) r_t

Time evolution



Algorithm (ED serial)

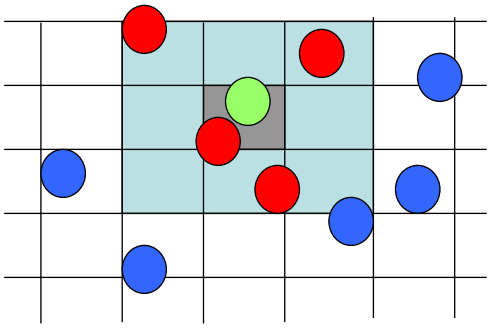
0. Initialize

- Propagate particle(s) to next event O(1)
- Compute event (collision or cell-change)
- Calculate new events and times O(1)
- Update priority queue (heap tree) O(log*N*)
- O(*N*) – `goto` 1.

Total effort: O(*N* log*N*)

Algorithmic trick(s) for speed-up

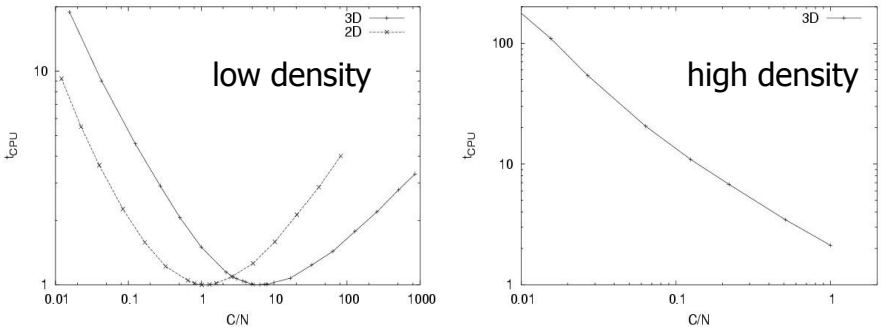
- Linked cells neighborhood search O(1) (*short range forces*)



- Linked cells update not needed !

Performance

- Short range contacts
- Linked cells neighbourhood search

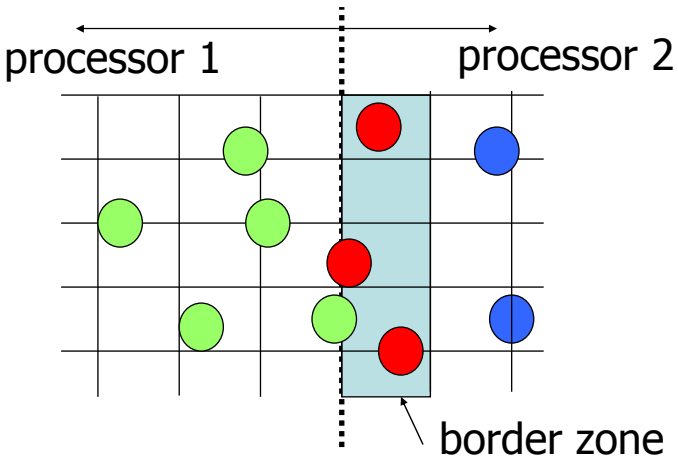


Cells per particle

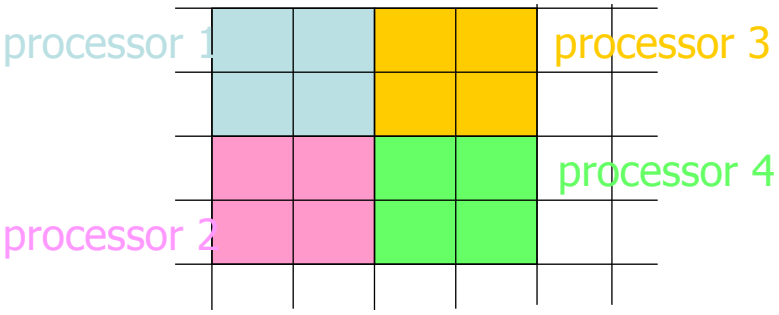
Algorithm (parallel)

0. Initialize
- Communication between processors
- Process next events t_n to t_{n+m} (see serial)
- Send and receive border-particle info
- `If` causality error `then` rollback `goto` 2.
- Synchronisation (for load-balancing and I/O)
- `goto` 1.

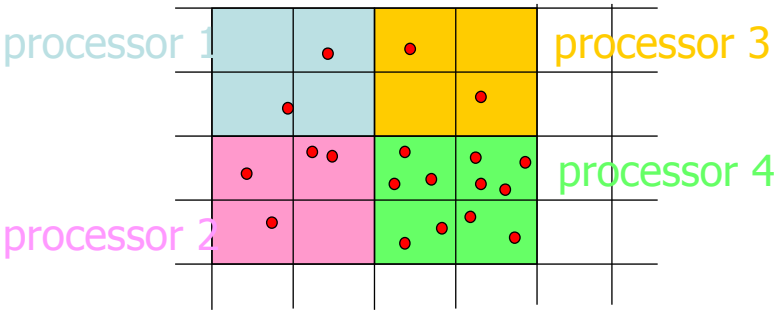
Parallelization – communication



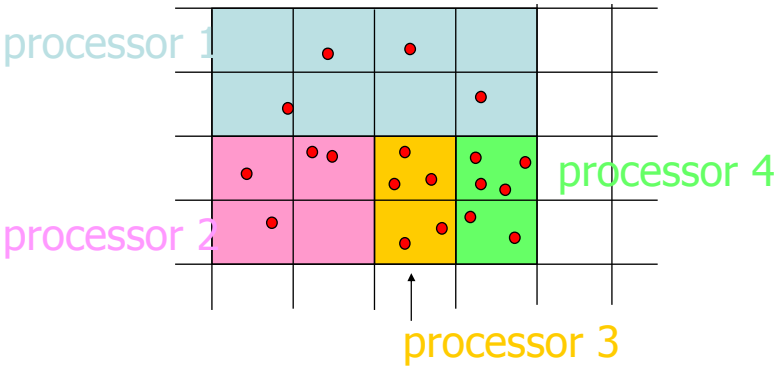
Parallelization – load balancing



Parallelization – load balancing

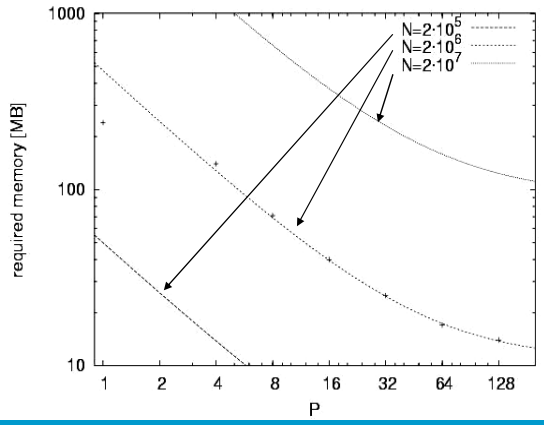


Parallelization – load balancing



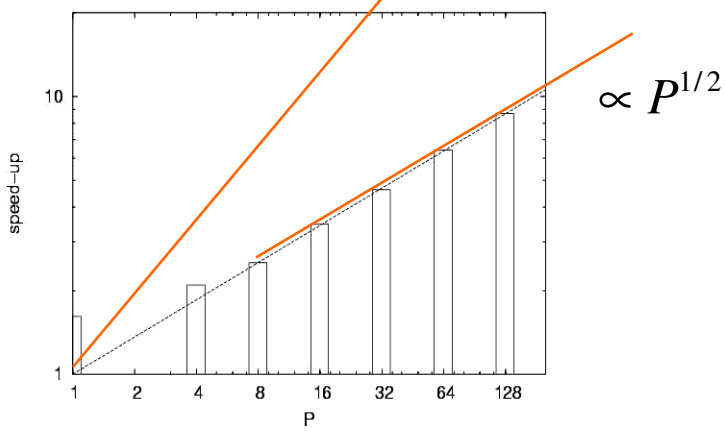
Performance (fixed N)

- Required memory per processor [MByte] $\propto N\left(\frac{c_1}{P}+\frac{c_2}{\sqrt[3]{P}}+c_3\right)$



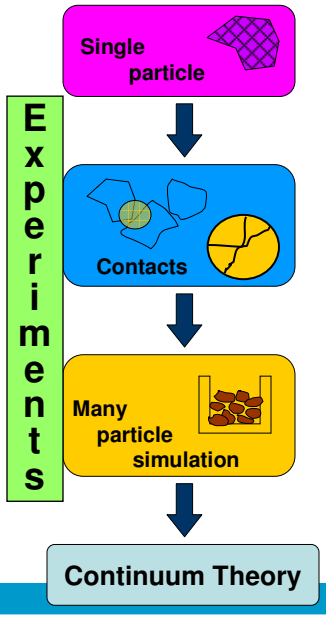
Performance (3D fixed N)

- Fixed density and number of particles $N = C = 2.10^6$

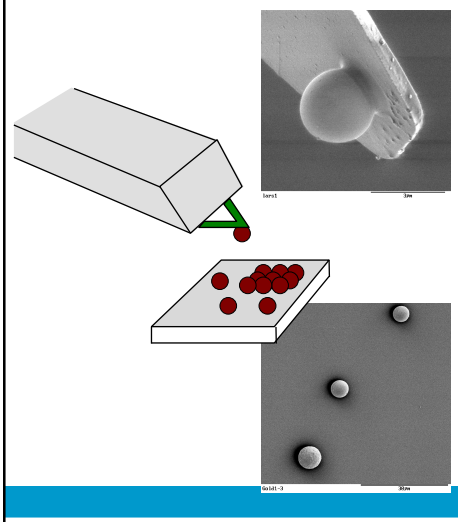


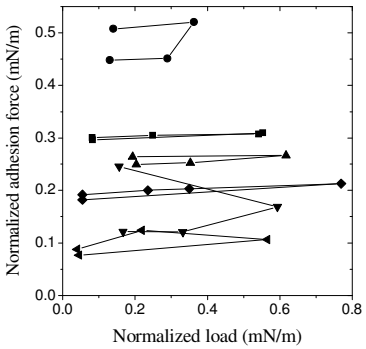
Approach philosophy

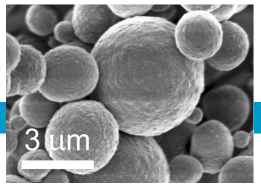
- Introduction
- Single Particles
- Particle Contacts/Interactions
- Many particle cooperative behavior
- Applications/Examples
- Conclusion



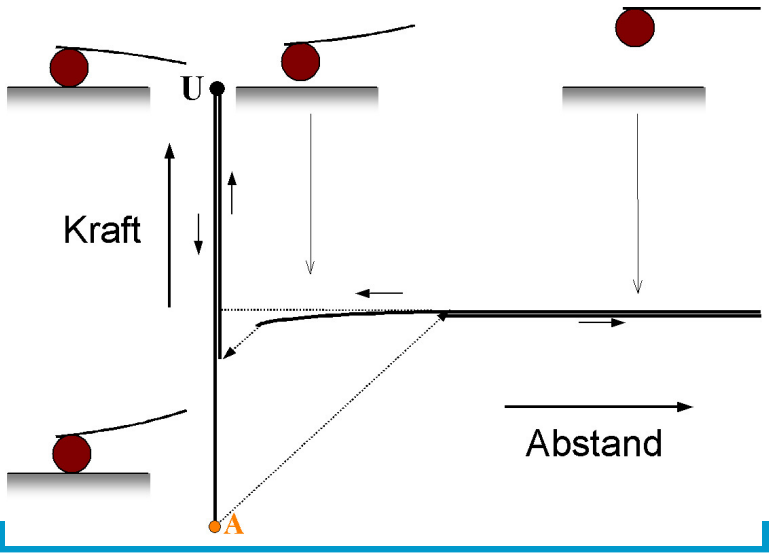
Contact force measurement (PIA)





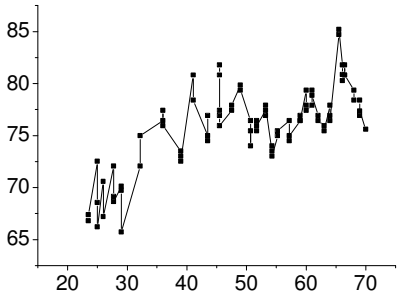


Contact Force Measurement



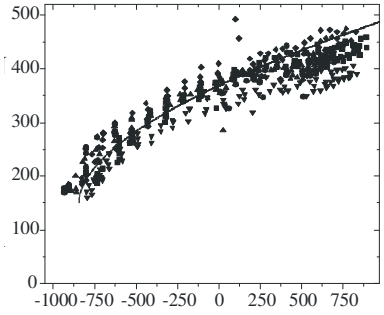
Adhesion and Friction

Adhesion force (nN)



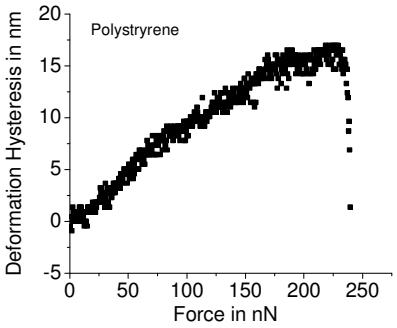
rel. humidity (%)

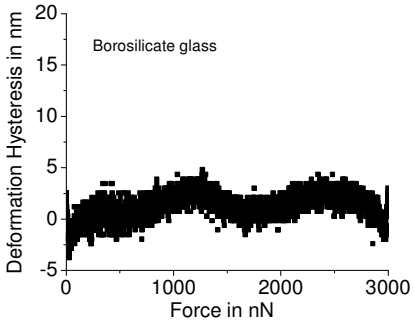
Friction force (nN)



Normal force (nN)

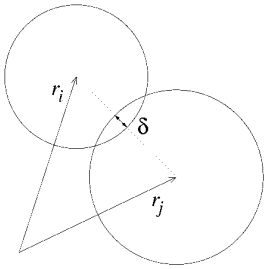
Hysteresis (plastic deformation)





Collaborations:
MPI-Polymer Science (Butt et al.)
Contact properties via AFM

Discrete particle model

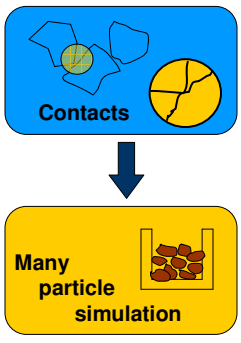


Equations of motion

$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i$$

Forces and torques:

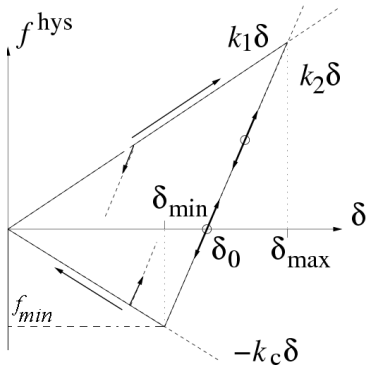
$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$



Contact if Overlap > 0

Overlap $\delta = \frac{1}{2}(d_i + d_j) - (\vec{r}_i - \vec{r}_j)\cdot\vec{n}$

Normal $\hat{n} = \vec{n}_{ij} = \frac{(\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|}$



Contact model

- (too) simple ☺
- piecewise linear
- easy to implement

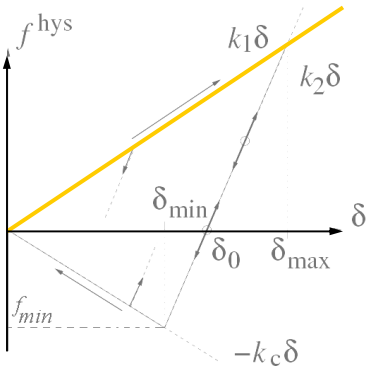
$$f_i^{hys} = \begin{cases} k_1\delta & \text{for loading} \\ k_2(\delta-\delta_0) & \text{for un-/reloading} \\ -k_c\delta & \text{for unloading} \end{cases}$$

Maximum overlap δ_{max}

stress-free overlap $\delta_0 = (1-k_1/k_2)\,\delta_{max}$

strongest attraction at: $\delta_{min} = \dfrac{k_2-k_1}{k_2+k_c}\delta_{max}$

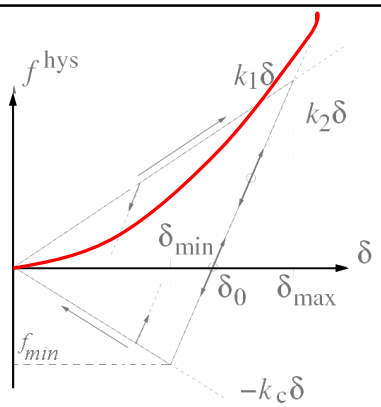
the max. attractive force: $f_{min} = -k_c\delta_{min}$



Linear Contact model

- (really too) simple ☺
- linear
- very easy to implement

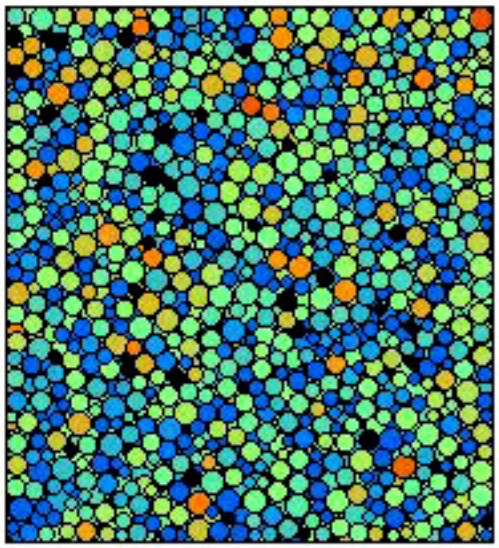
$$f_i^{hys} = \begin{cases} k_1\delta & \text{for un-/re-loading} \end{cases}$$



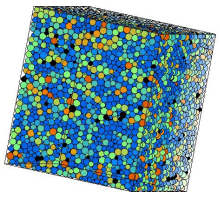
Hertz Contact model

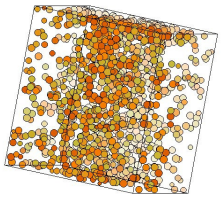
- simple ☺
- non-linear
- easy to implement

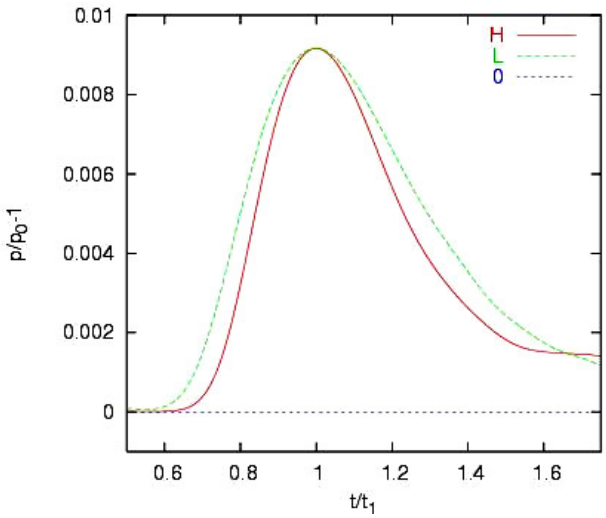
$$f_i^{hys} = \begin{cases} k_1\delta^{3/2} & \text{for un-/re-loading} \end{cases}$$



Sound







P-wave shape and speed

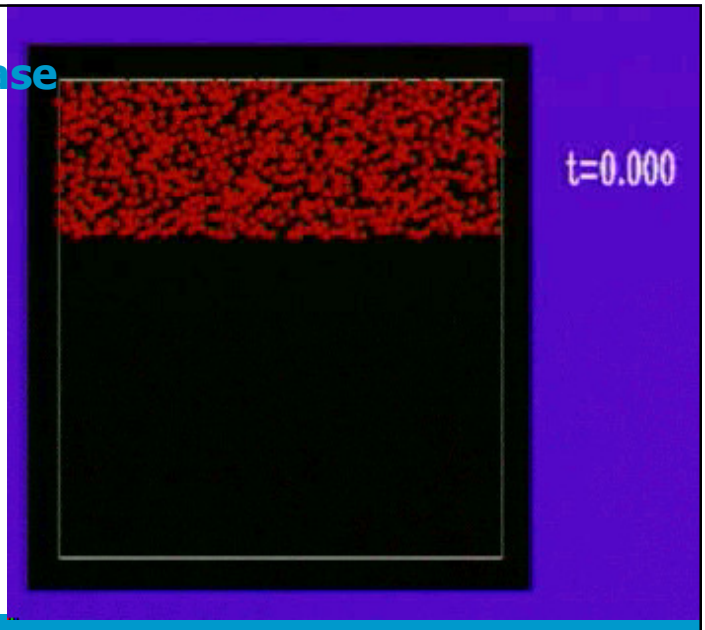
Stefan Luding, s.luding@tnw.tudelft.nl

Particle Technology, DelftChemTech, Julianalaan 136, 2628 BL Delft

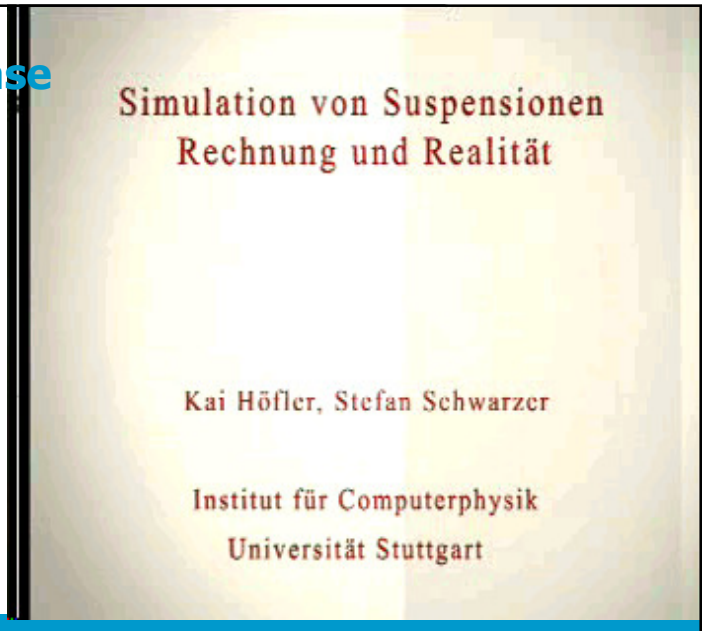
Open questions

- Agglomeration
  - population balance – cluster evolution
  - phase transitions, cooperative behavior
- Main challenges (for modeling)
  - aero-/hydro-dynamics coupling
  - cluster stability, statistics, sintering, ...

Two-phase Flows



Two phase Flows



Two phase Flows with Aggregation