From particle-systems to continuum theory

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msm

- Introduction MSM

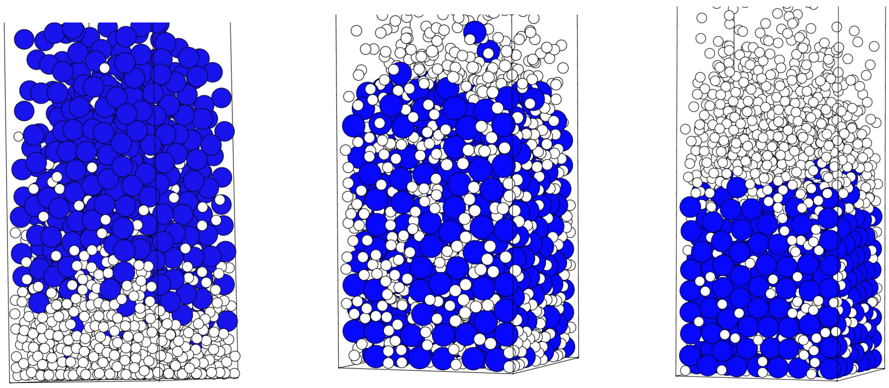
What is Multi Scale Mechanics?

www.msm.ctw.utwente.nl

Example 1: Agitation/Vibration

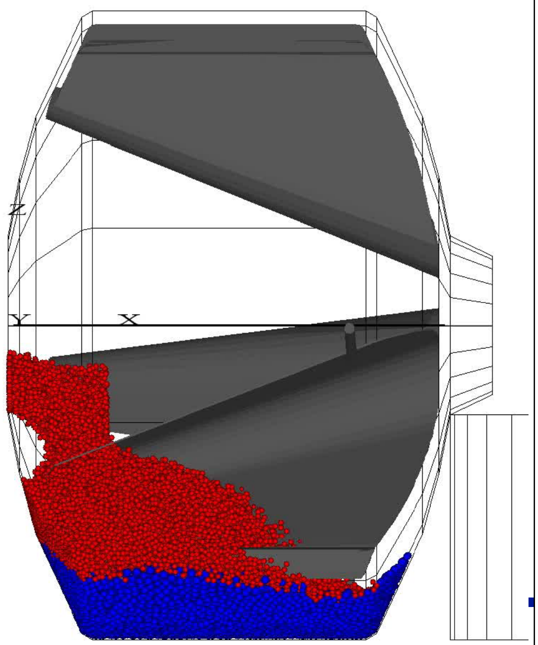
N. Rivas, MSM, 2011

Example 2: Segregation/Mixing



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

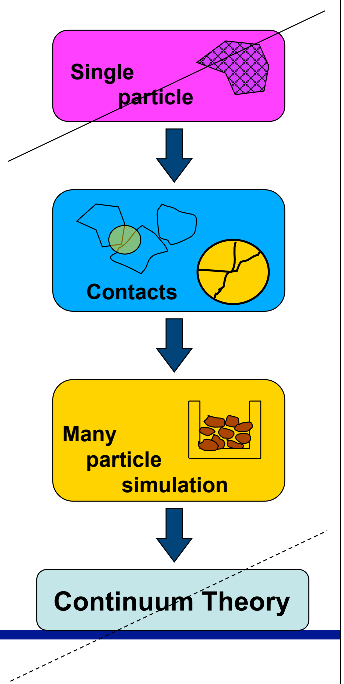
Example 2: Mixing



A. Gupta et al., MSM, 2010

Overview

- Introduction
- Contact models
- Many particle simulation
- Local coarse graining
- Continuum Theory
- … Anisotropy



Deterministic Models ...

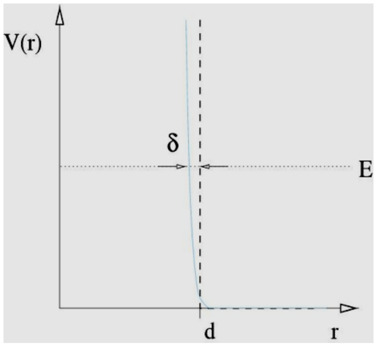
Method	Abbrev.	Theory
Molecular dynamics (soft particles)	MD	...
Event Driven (hard particles)	ED	(Kinetic Theory)
Monte Carlo (random motion)	MC	Stat. Phys.
Direct Simulation Monte Carlo	DSMC	Kinetic Theory
Lattice (Boltzmann) Models	LB	Navier Stokes

PCSE – steps in simulation ...

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

What is Molecular Dynamics ?

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

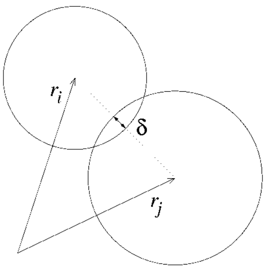


2. Compute all forces $\mathbf{f}_{j\to i}$

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

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

Discrete particle model

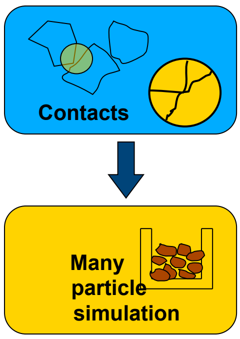


Equations of motion

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

Forces and torques:

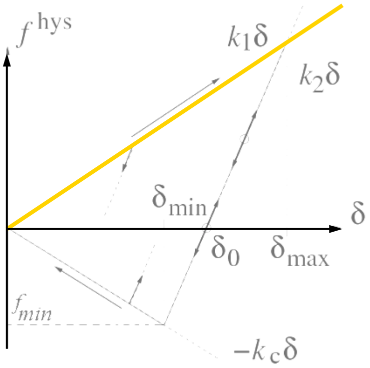
$$\vec{f}_i = \sum_c \vec{f}_i^c + \sum_w \vec{f}_i^w + m_i g$$



Contact if Overlap > 0

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

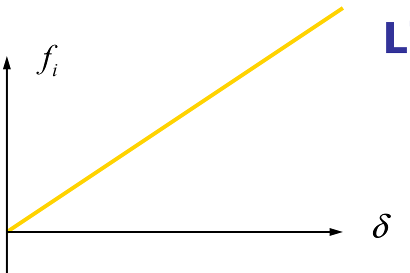
Normal $\hat{n} = \vec{n}_{ij} = \frac{\left(\vec{r}_i - \vec{r}_j\right)}{\left|\vec{r}_i - \vec{r}_j\right|}$



Linear Contact model

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

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



Linear Contact model

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

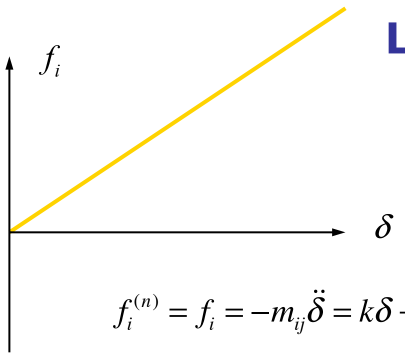
$$f_i^{(n)} = f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

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

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

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

http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



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

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

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

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

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

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

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

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

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

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

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

contact duration $t_c = \pi/\omega$

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

http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf

Linear Contact model

- comments/problems

restitution coefficient
Always >= 0

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

Forces negative
⇔ adhesion

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

=> Reconsider definition of *t_c* …

http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf

Linear Contact model

	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.	$\eta = \dfrac{\gamma}{2m_{ij}}$	$\eta^{wall} = \dfrac{\gamma}{2m_i} = \dfrac{\eta}{2}$
contact duration	$\boxed{t_c = \pi / \omega}$	$\boxed{t_c^{wall} = \pi / \omega^{wall} > t_c}$
restitution coeff.	$r = \exp(-\eta t_c)$	$r^{wall} = \exp(-\eta^{wall} t_c^{wall})$

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Time-scales

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

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

$t_n < t_c$

↑

time between contacts

↓

$t_n > t_c$

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

experiment T

Time-scales

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

contact duration $t_c = \pi / \omega$

$t_n < t_c$

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

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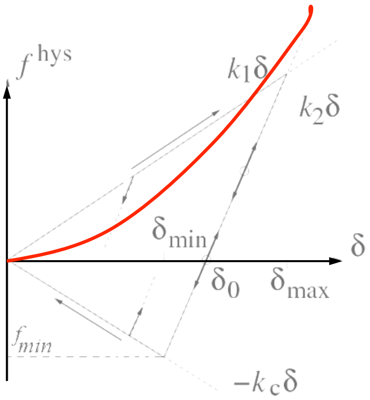
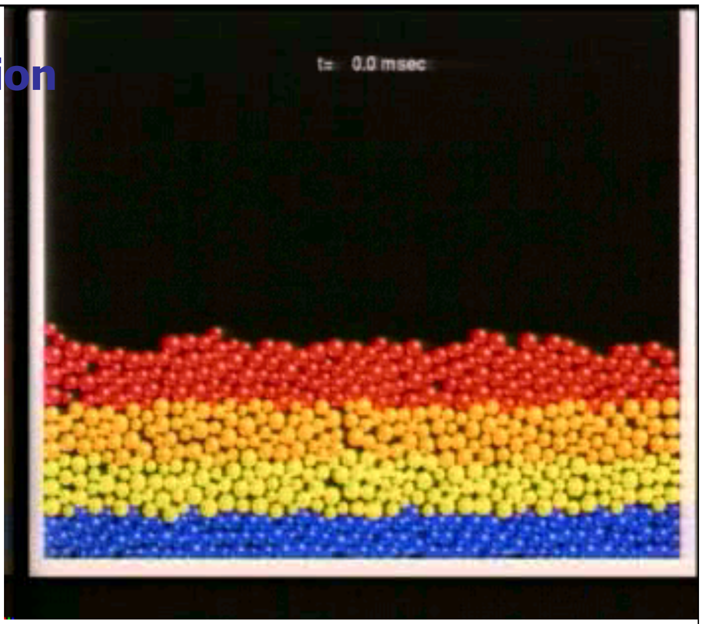


Hertz Contact model

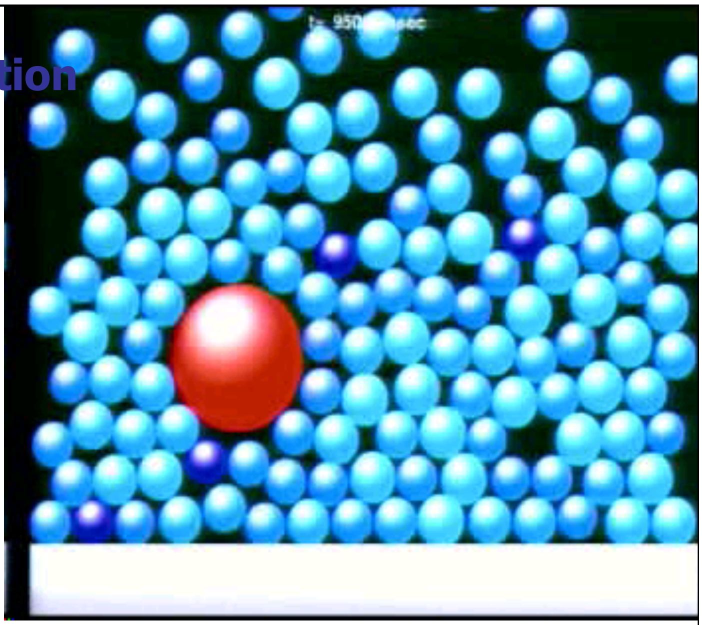
- simple ☺
- non-linear
- easy to implement

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

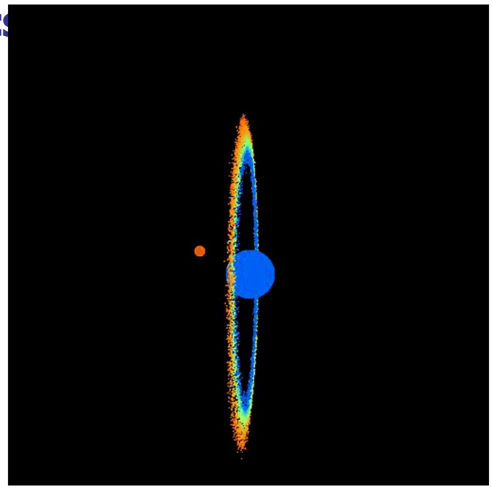
Convection



Segregation

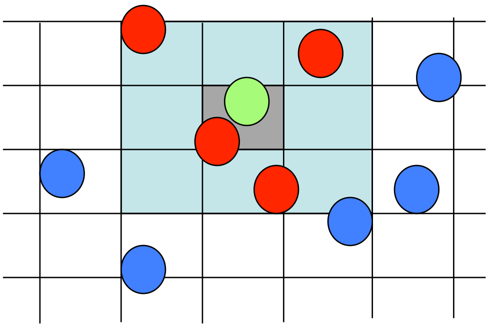


Molecular Dynamics example from astrophysics



Algorithmic trick(s) for speed-up

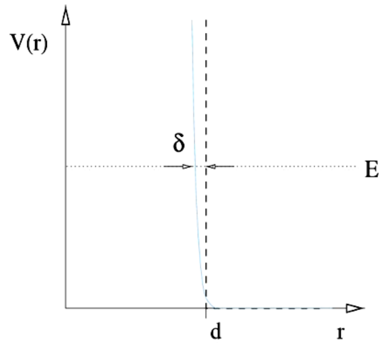
- Linked cells neighborhood search O(1) (*short range forces*)



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

What is Molecular Dynamics ?

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



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

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

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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)

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   Events (=collisions) occur in **zero-time** (instantaneously)
   Integration is *impossible* !
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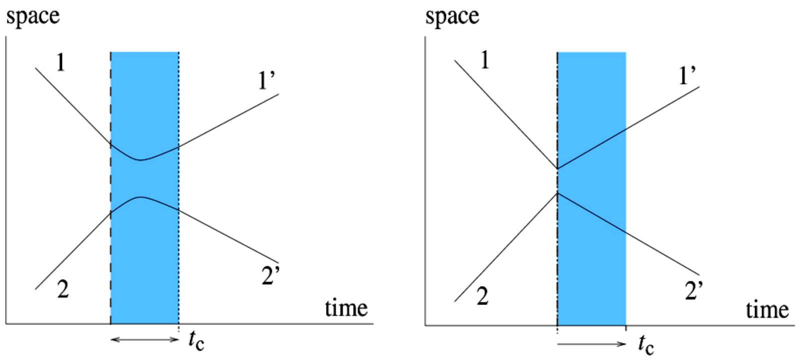

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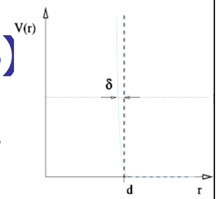


2. Solve equation of motion between collisions

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

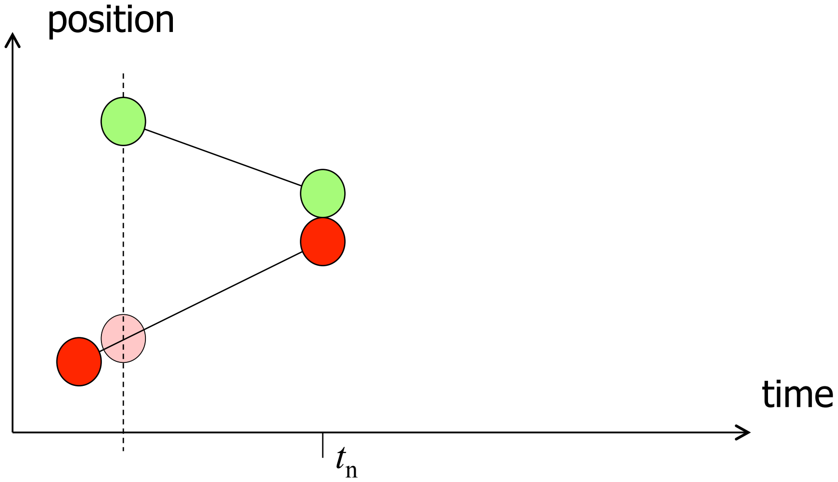
- contact $\left\|\Delta\mathbf{x}_{ij}\right\| = \left\|\mathbf{x}_i(t) - \mathbf{x}_j(t)\right\| = r_1 + r_2$

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

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

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

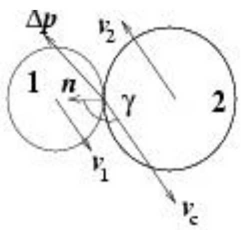
Time evolution



Rigid interaction (hard spheres)

Collision rule (translational)

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

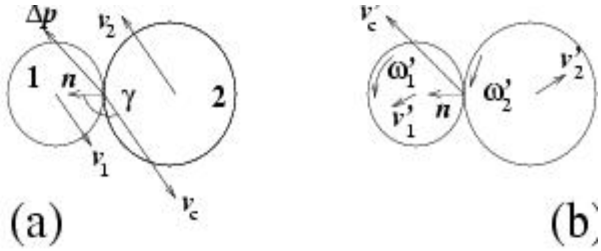


Momentum conservation + dissipation
with restitution coefficient (normal): r

Rigid interaction (hard spheres)

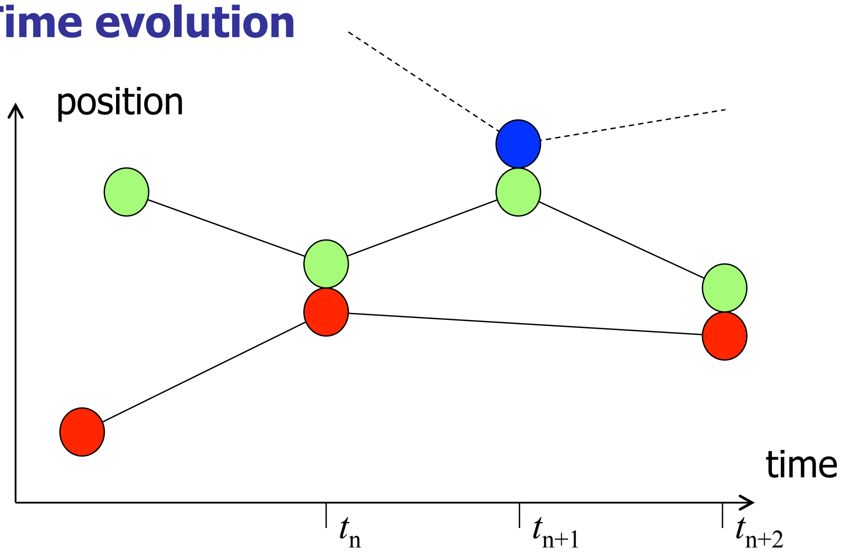
Collision rule (translational and rotational)

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



Restitution coefficient (normal): r (tangential) r_t

Time evolution



Algorithm (ED serial)

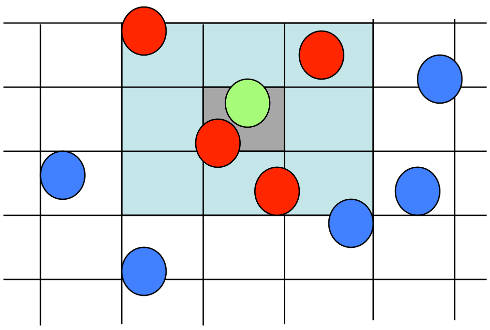
0. Initialize

- 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

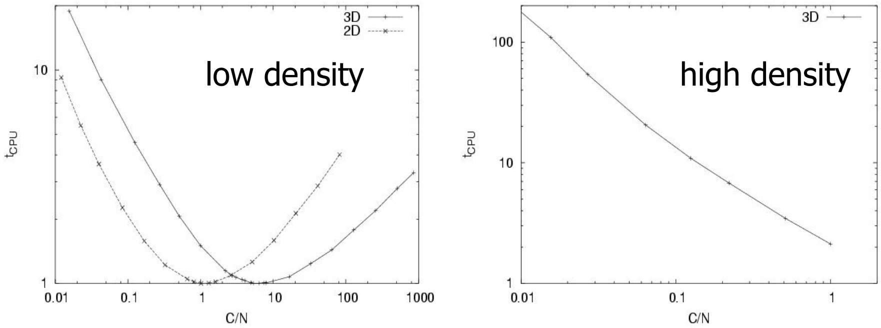
- Linked cells neighborhood search O(1) (*short range forces*)



- Linked cells update not needed !

Performance

- Short range contacts
- Linked cells neighbourhood search



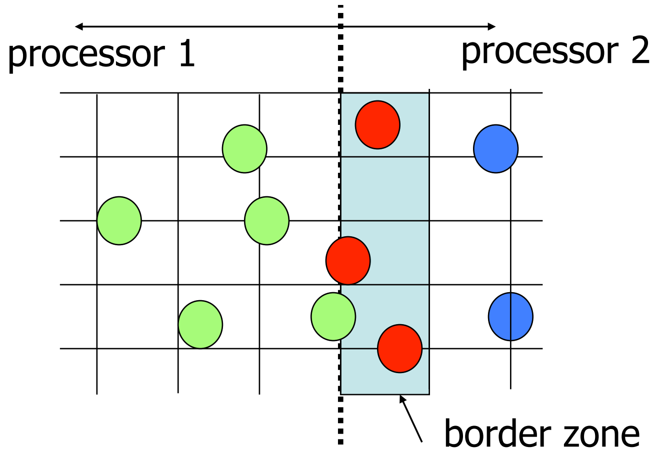
Cells per particle

Algorithm (parallel)

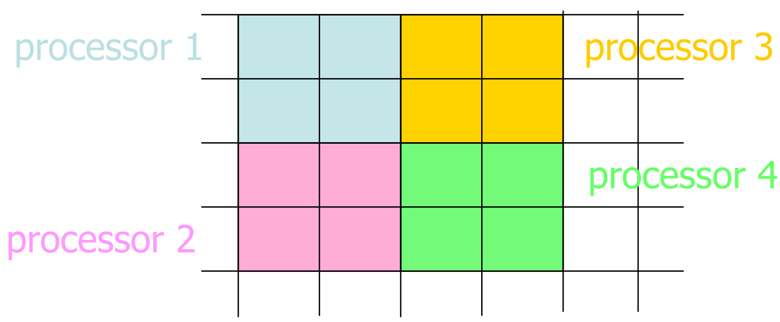
0. Initialize

- 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



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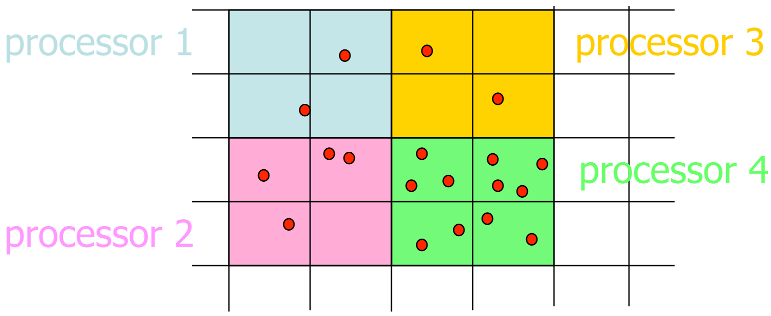
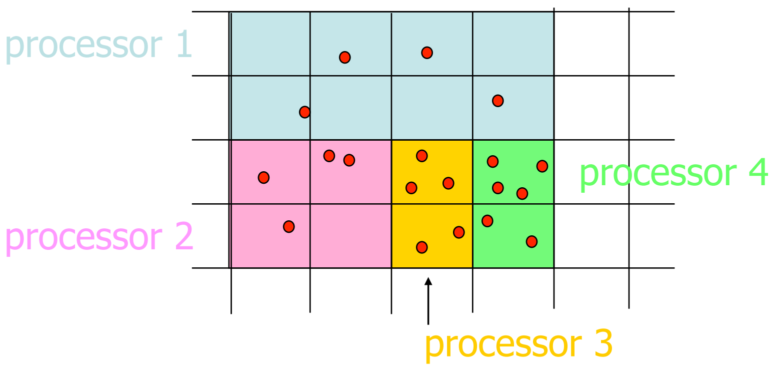


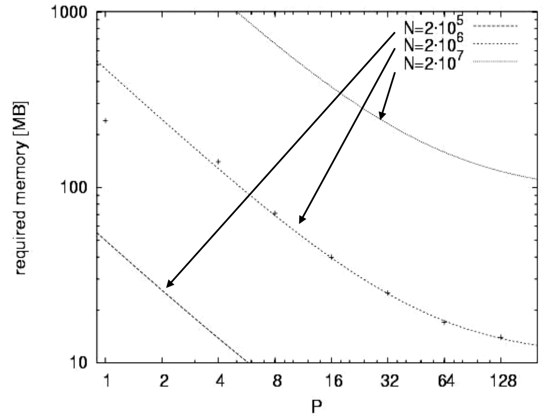
Parallelization – load balancing



Performance (fixed N)

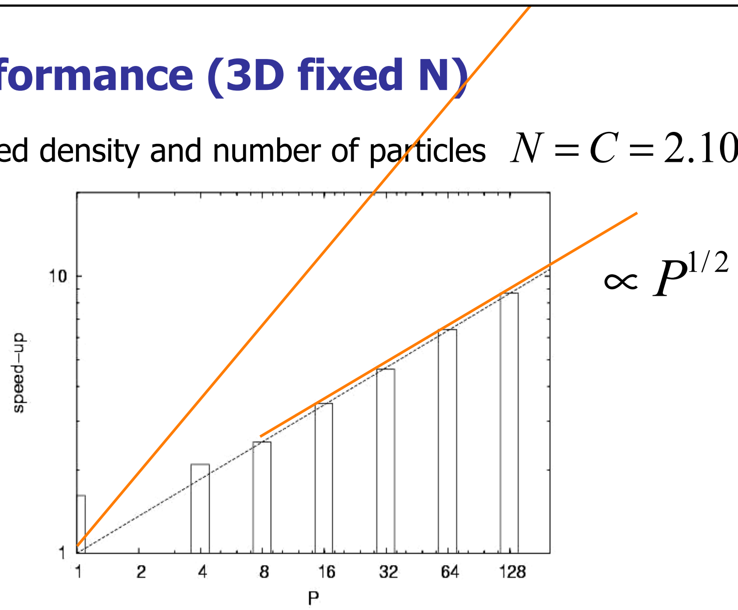
$$\propto N\left(\frac{c_1}{P}+\frac{c_2}{\sqrt[3]{P}}+c_3\right)$$

- Required memory per processor [MByte]



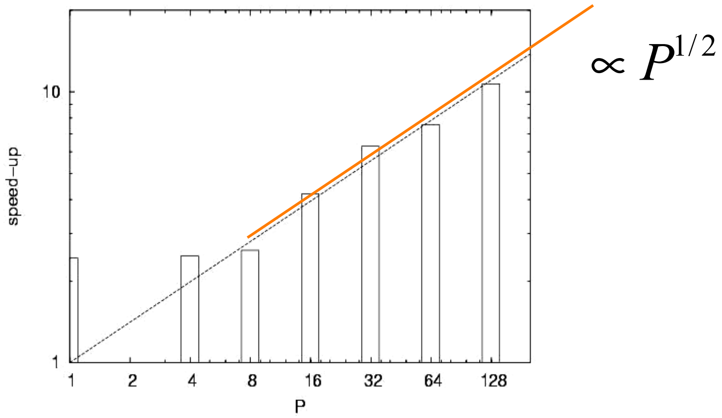
Performance (3D fixed N)

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



Performance (3D fixed N/P)

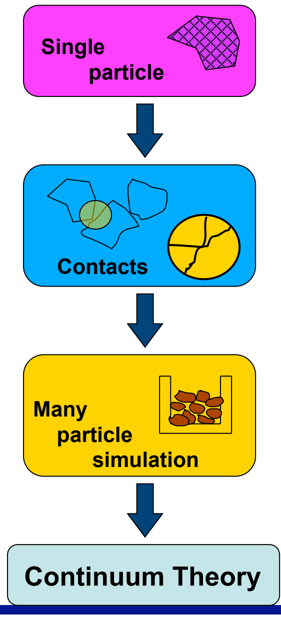
- Fixed number of particles per processor $N/P = 4.10^4$



The End (Technical)

Overview MultiScale

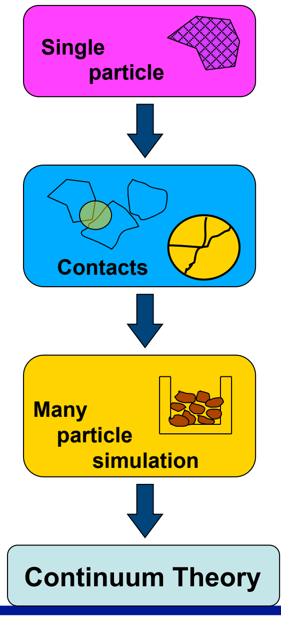
- Introduction
- Contact models
- Many particle simulation
- Local coarse graining
- Continuum Theory



Goal:

Large Scale systems
Applications

Continuum Theory



Continuum theory

mass conservation:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

momentum conservation:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k) = -\frac{\partial}{\partial x_i}P + \frac{\partial}{\partial x_j}\sigma_{ij}^{\text{dev}} + \rho g_i$$

energy balance:

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho u^2 + \tfrac{1}{2}\rho v^2\right) = -\frac{\partial}{\partial x_k}\left[\rho u_k\left(\frac{P}{\rho} + \tfrac{1}{2}u^2 + \tfrac{1}{2}v^2\right) - u_i\sigma_{ik}^{\text{dev}} - K\frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right] + \rho u_i g_i - I$$

- **Pressure *P***
- **Shear Stress** σ_{ij}^{dev}
- **Energy Dissipation Rate *I***

Continuum theory ...

Method	Abbrev.	
Finite Element Method	FEM	e.g. Structures
Finite Differences	FD	
Finite Volume	FV	
Computational Fluid Dynamics	CFD	
Smoothed Particle Hydrodynamics	SPH	e.g. astro-phys.

Particle based methods ...

Method	Abbrev.	Theory
Molecular dynamics (soft particles)	MD	...
Event Driven (hard particles)	ED	(Kinetic Theory)
Smoothed Particle Hydrodynamics	SPH	Astro-Phys.
Dissipative Particle Dynamics	DPD	Viscous+Random
Etc.		

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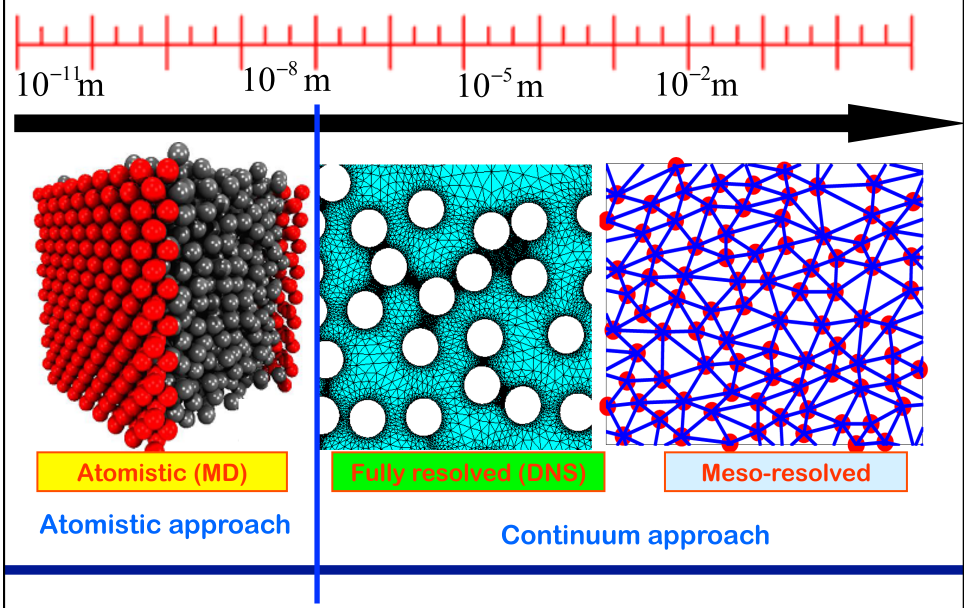
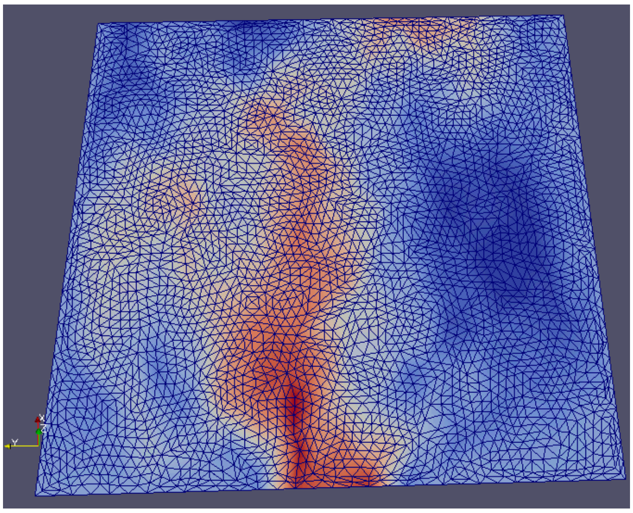
Multiscale modeling



Example 3b: Fluidization DEM-FEM



Fluidization on moving mesh with 800 particles (with gravity)

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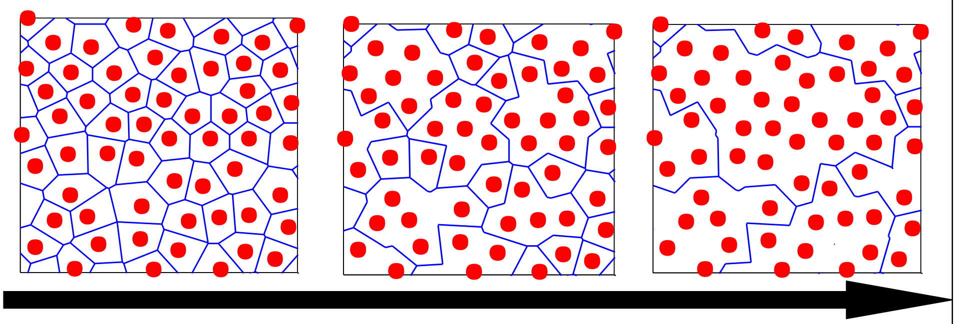
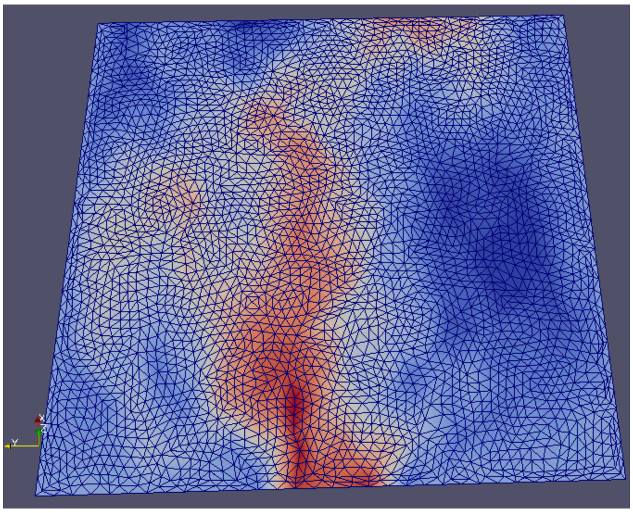
Future work



Coarse graining

- Find relations between PDF's
- Apply to the moving particles/mesh
- 3D spherical particles

Example 3b: Fluidization DEM-FEM

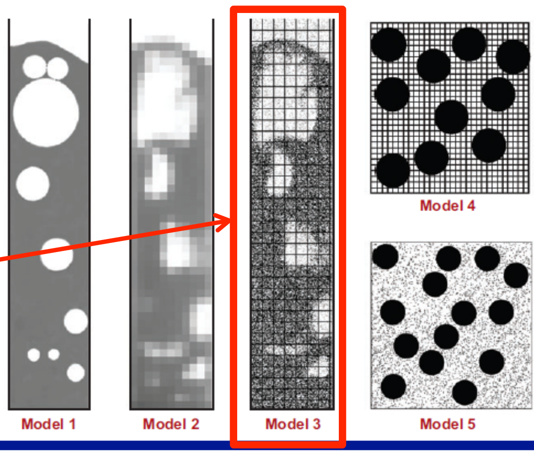


Fluidization on moving mesh with 800 particles (with gravity)

Fluid-particle simulation – which length scale?

Length scale of interest determines simulation method

Fluid resolution > particle diameter

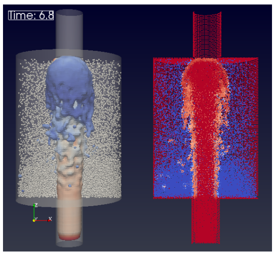


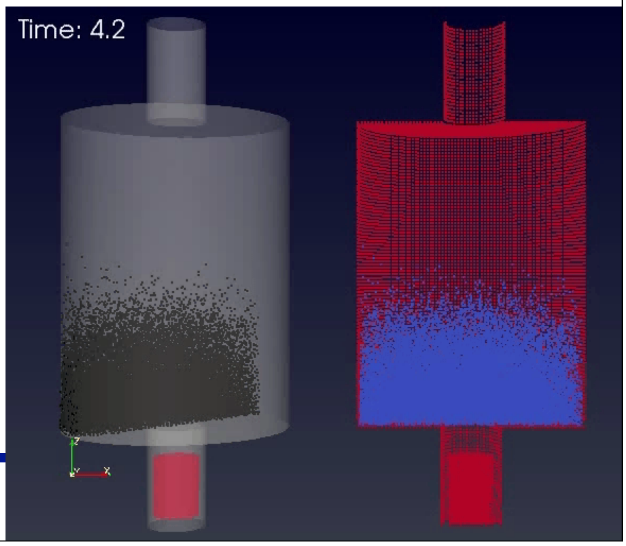
Van der Hoef, M. A., van Sint Annaland, Deen, N. G., & Kuipers, J. A. M. (2008). Numerical simulation of dense gas-solid uidized beds: A multiscale modeling strategy. Annual Review of Fluid Mechanics, 40 (1), 47{70.

Example 3a: Powder dispersion SPH-DEM

PARDEM [1&2] UNIVERSITEIT TWENTE. [1] Nestlé Research [2]

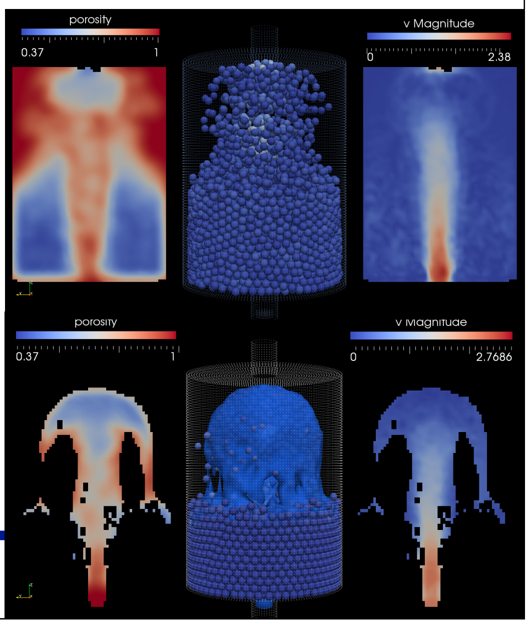
- initial results
- SPH fluid-phase
- DEM model





Simulation of powder dispersion by a liquid jet

- Application: Particle dispersion (collaboration with Nestle)
- Method: SPH-DEM
- Results:
  - **Wet** – Recovers qualitative features from experiment: Jet, dispersion …
  - **Dry** – Fails to recover some major features (e.g. bed lift regime).
  - Surface tension not modeled yet.



deterministic vs. stochastic models …

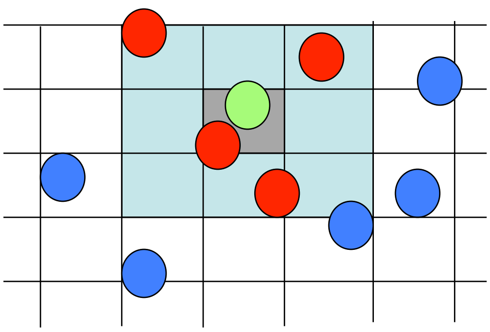
Method	Abbrev.	Theory
Molecular dynamics (soft particles)	MD	…
Event Driven (hard particles)	ED	(Kinetic Theory)

Particle method(s) first … ED …

why?

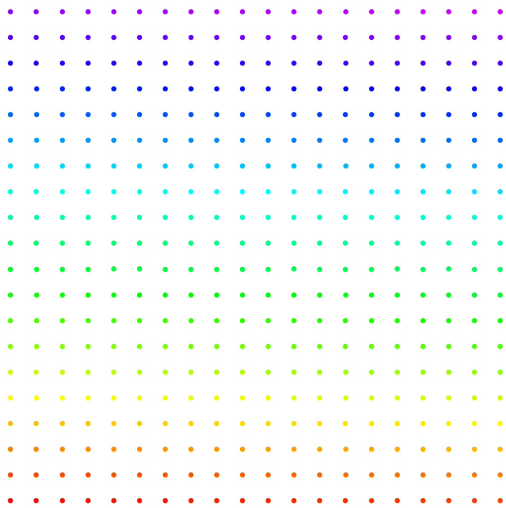
Algorithmic trick(s) for speed-up

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



- Linked cells update not needed ! <- cell-crossing events

Example 4: Agglomeration



S. Gonzalez-Briones, MSM, 2010

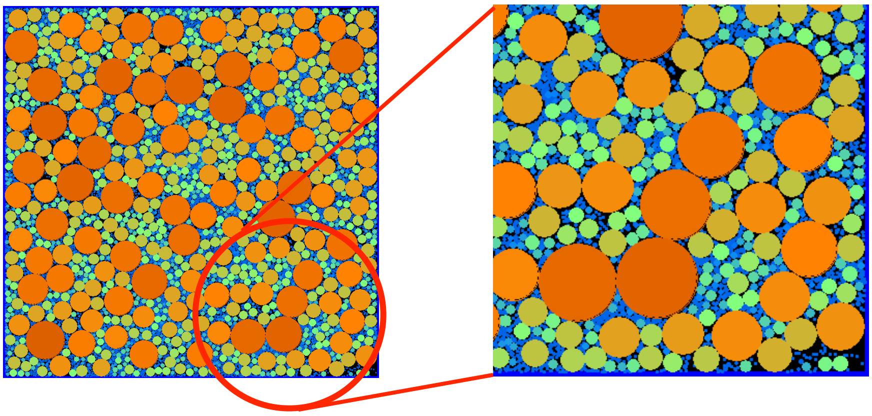
Challenge:

Fast contact detection between particles with <u>strongly different sizes</u>

Size ratio >> 10

Number of particles > 10^6

Challenge: DEM with realistic sizes



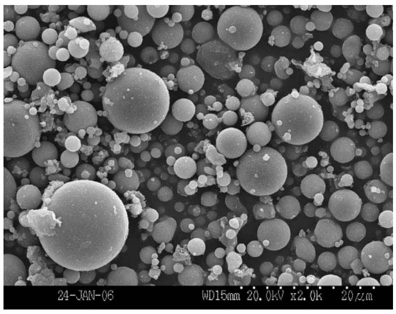
... highly polydisperse powders

Challenge:

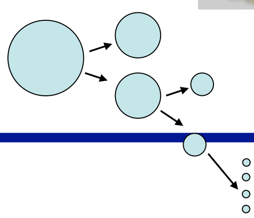
Fast contact detection between particles with strongly different sizes

Size ratio >> 10
Number of particles > 10^6

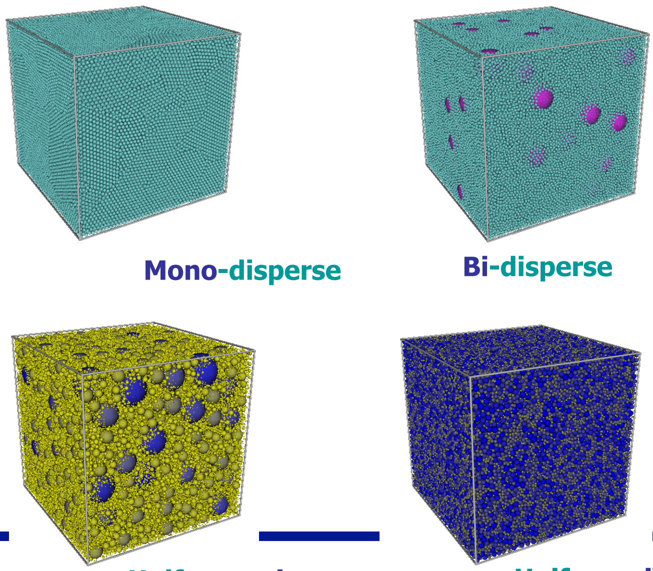
- **Breakage / Grinding**
- **Concrete**



fly ash sample at 2000x magnification, University of Kentucky, CAER



Different size distributions …



Colour by size

Mono-disperse | Bi-disperse

Uniform volume | Uniform size

Kinetic Theory – Towards Jamming

Dimensionless pressure: $Z = 1 + 4\nu g_O(\nu)$

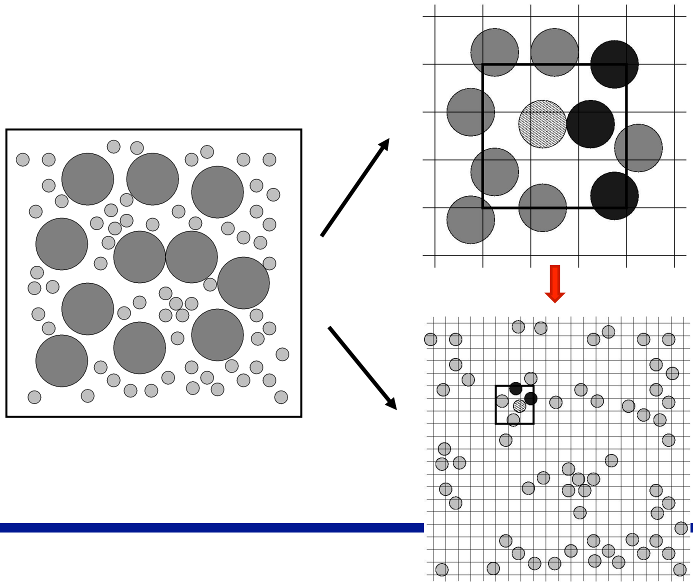
$$g_O(\nu) = \frac{(1-\nu)^2 + 3O_1(1-\nu) + O_2(3-\nu)\nu}{4(1-\nu)^3}$$

$$O_1 = \frac{\langle a \rangle \langle a^2 \rangle}{\langle a^3 \rangle} \quad \text{and} \quad O_2 = \frac{\langle a^2 \rangle^3}{\langle a^3 \rangle^2}$$

The moments are enough! 3 -> 5
… in the fluid regime and also above, towards jamming

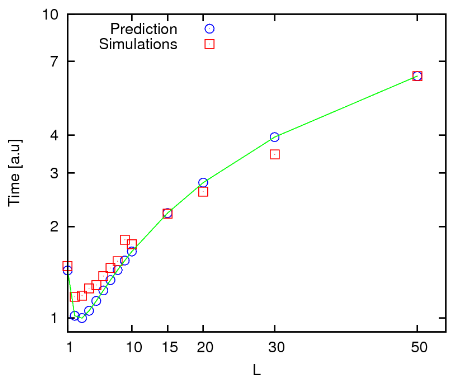
Hierarchical grid: fast, robust & flexible

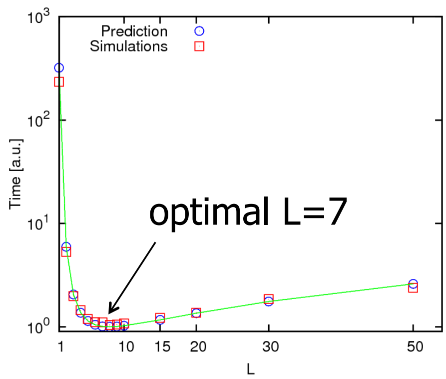
example: L=2 level grid

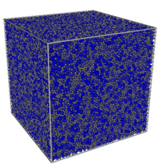


Analytical prediction vs Simulations

$$T = NL(m_L + K)$$

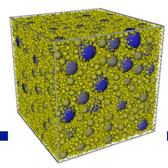






$L^* \cong 2$

uniform size



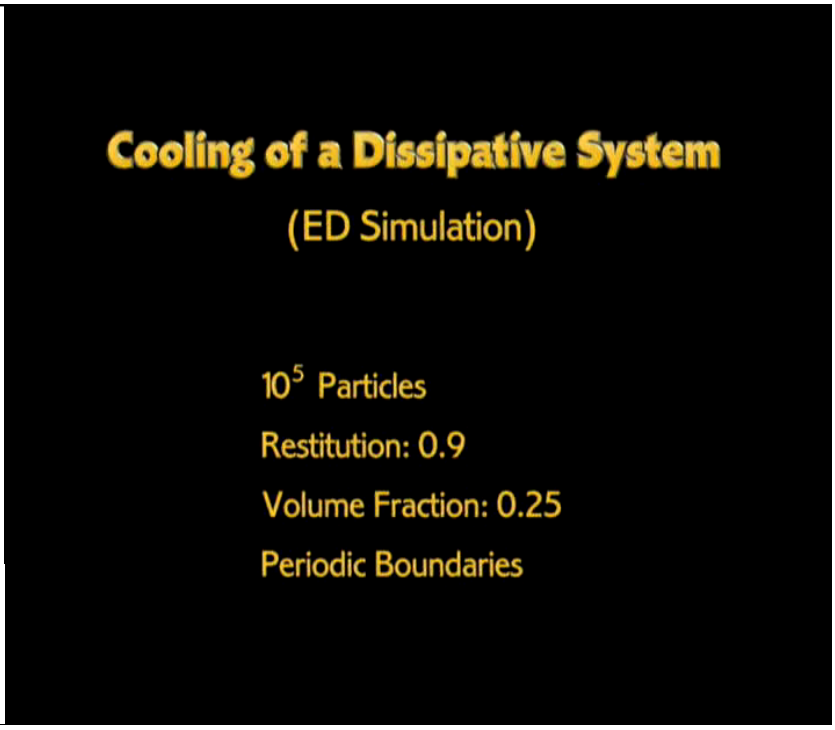
$L^* > 2$

uniform volume

Large Scales - Continuum theory

- Forget about the fluid between the particles
- Particles + dissipation/friction + collisional
  => Kinetic theory works ☺
- Challenge: Micro-Meso-Mechanics Effects
  - Structures, agglomerates, …
  - Dense & static system, …
  - Advanced contact models, …
  - Anisotropy, …

How do contacts influence the continuum behavior?



Continuum theory

mass conservation: $$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

momentum conservation: $$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k) = -\frac{\partial}{\partial x_i}P + \frac{\partial}{\partial x_j}\sigma_{ij}^{\text{dev}} + \rho g_i$$

energy balance: $$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho u^2 + \tfrac{1}{2}\rho v^2\right) = -\frac{\partial}{\partial x_k}\left[\rho u_k\left(\frac{P}{\rho} + \tfrac{1}{2}u^2 + \tfrac{1}{2}v^2\right) - u_i\sigma_{ik}^{\text{dev}} - K\frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right] + \rho u_i g_i - I$$

- **Pressure *P***
- **Shear Stress** σ_{ij}^{dev}
- **Energy Dissipation Rate *I***

Freely cooling system

homogeneous steady state: $\frac{\partial}{\partial x_i} = 0$ $\quad g_i = u_i = 0$

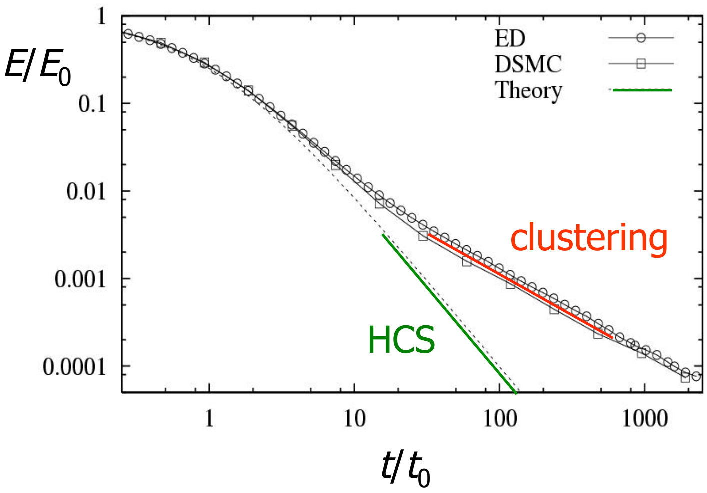
mass & momentum conservation – OK

energy balance: $\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho v^2\right) = -I$ $\quad I \propto \rho\left(1 - r^2\right)v^3$

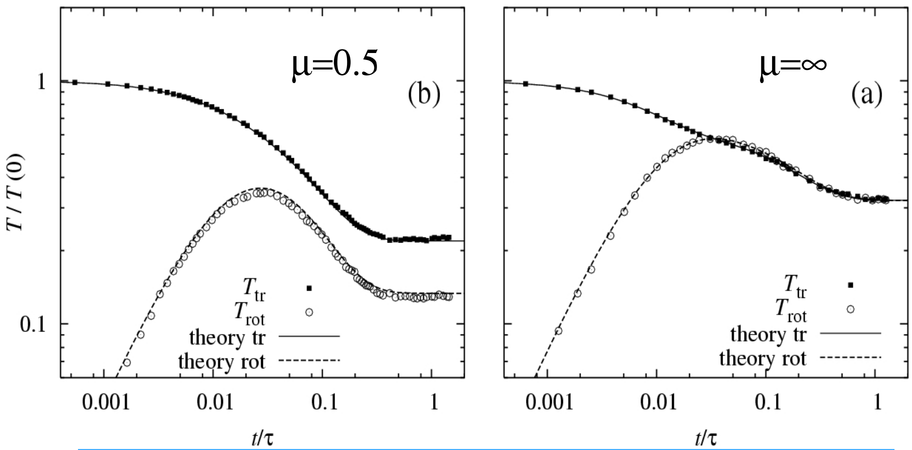
mean field (MF) solution: $$\frac{v}{v_0} = \frac{1}{1 + \alpha\left(1 - r^2\right)v_0 t}$$

$$\frac{E}{E_0} = \frac{1}{\left(1 + \alpha\left(1 - r^2\right)v_0 t\right)^2}$$

Freely cooling system (HCS)



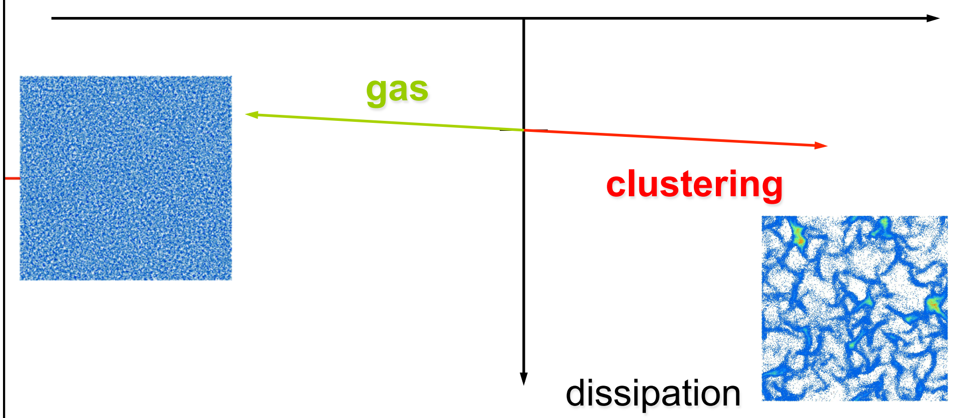
Kinetic theory with Coulomb friction



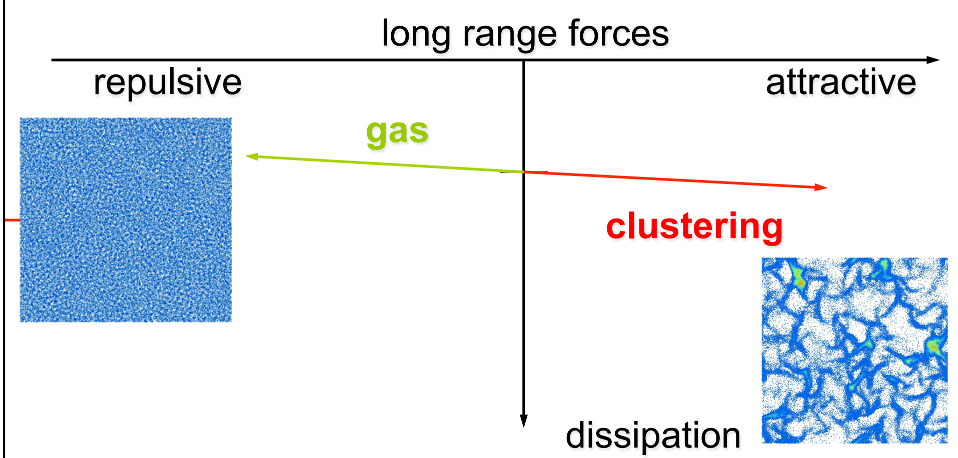
… possible, but serious hard work …

NO shortcut

Clustering/Agglomeration



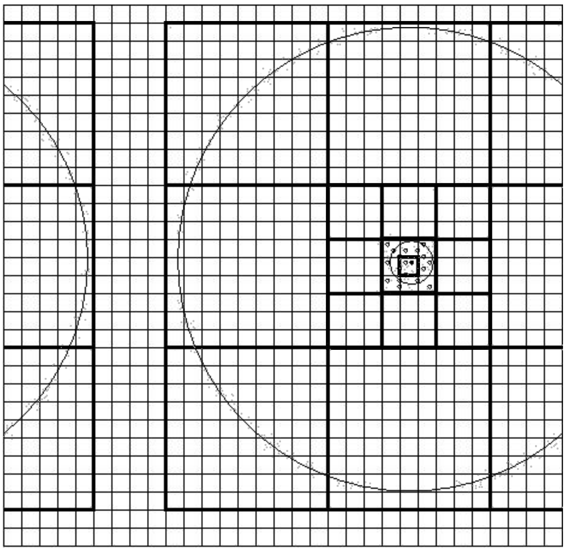
Clustering/Agglomeration



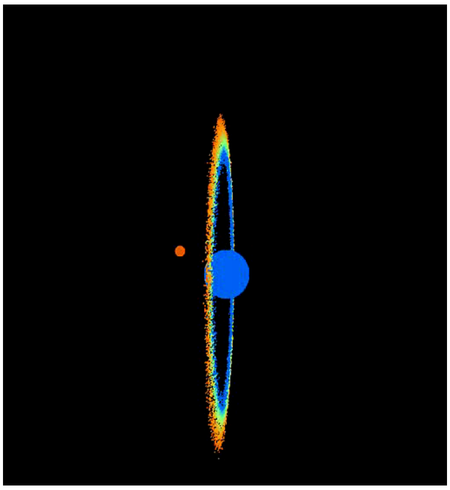
The Hierarchical Linked Cell Structure (HLC)

- particle of interest is in any H0 cell (= linked cell)
- construct H1 level (*H* =1) (= 26 H0 cells) and consider inner cut-off sphere around particle of interest
- construct H2 level (*H* =2) (= 26 H1 cells, each: 27 H0)
- construct H3 level (*H* =3) (= 26 H2 cells, each: 27 H1)
- consider outer cut-off sphere around particle of interest

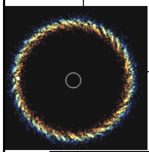
$$= N \cdot N \frac{3^D - 1}{n_{\mathrm{LC}}^D} H \propto N \log_3 N$$



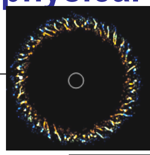
Molecular Dynamics example from astrophysics



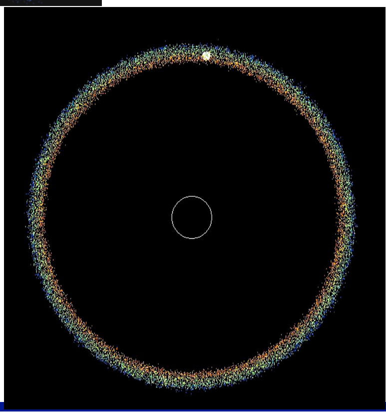
ring-shaped astrophysical systems

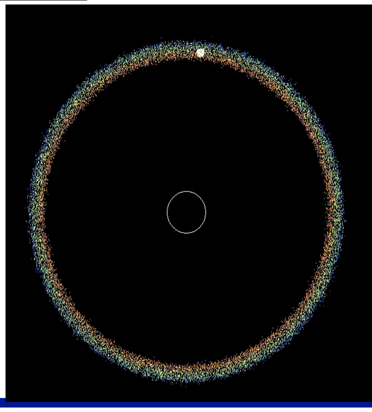


$r = 1.00 \quad c_b = -2e5$



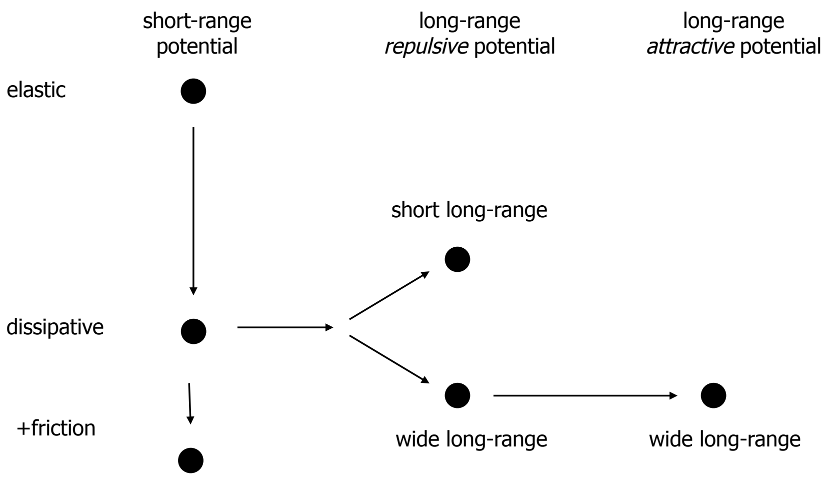
$r = 0.60 \quad c_b = -2e5$





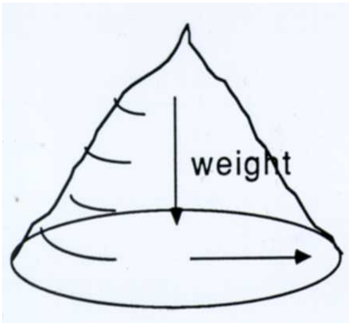
M. K. Mueller, PhD thesis, 2008

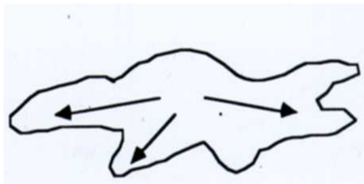
Roadmap (Homogeneous Systems) – Kinetic Theory + Extensions



Powder and Liquid Flow (differences)

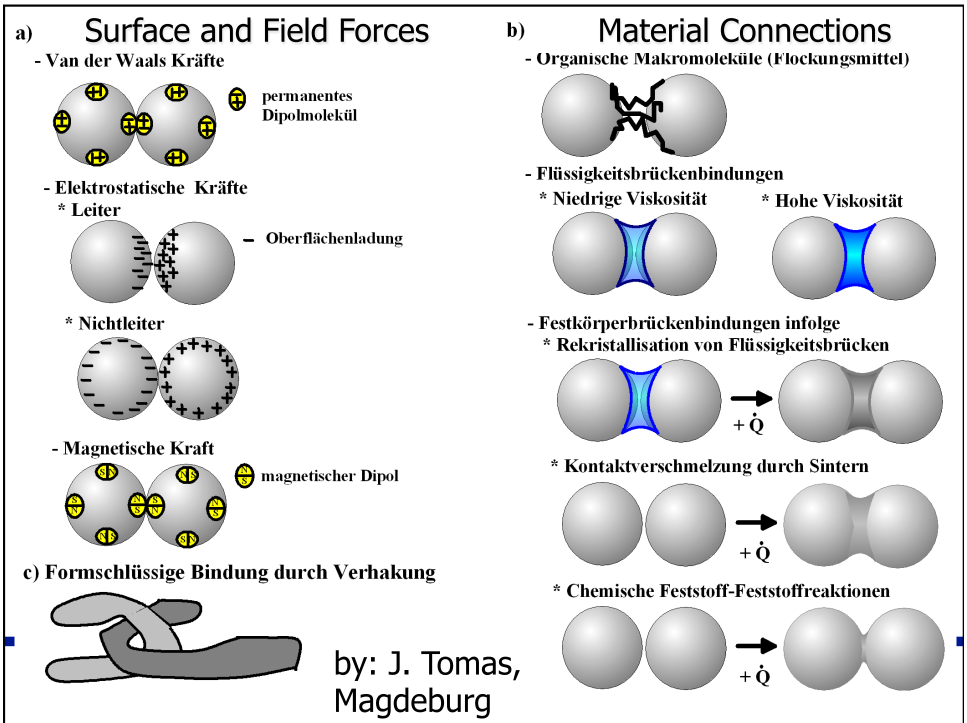
Inherent Yield Stress





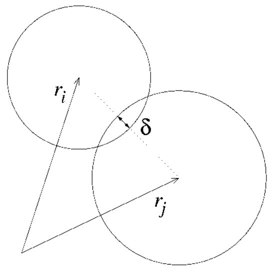
Powders heap **Liquid spreads**

Yield stress = resistance against flow



by: J. Tomas, Magdeburg

Discrete particle model



Equations of motion

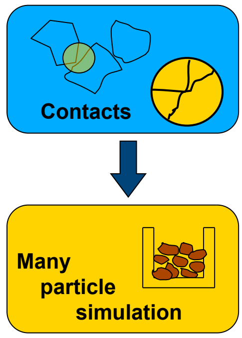
$$m_i \frac{d^2\vec{r}_i}{dt^2} = \vec{f}_i \qquad I_i \frac{d\vec{\omega}_i}{dt} = \vec{t}_i$$

Forces and torques:

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

$$\vec{t}_i = \sum_c \vec{r}_i^{\,c} \times \vec{f}_i^{\,c}$$

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



How to model Contacts?

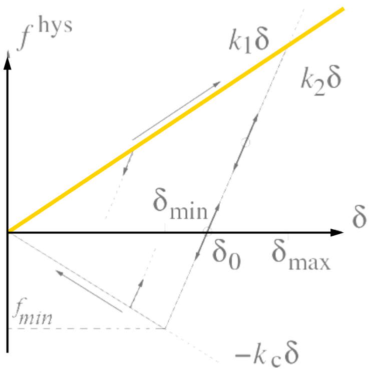
Atomistic/Molecular ...

Continuum theory + Contact Mechanics

Experiments (Nano-Ind., AFM, Mech., HSMovies)

Contact Modeling

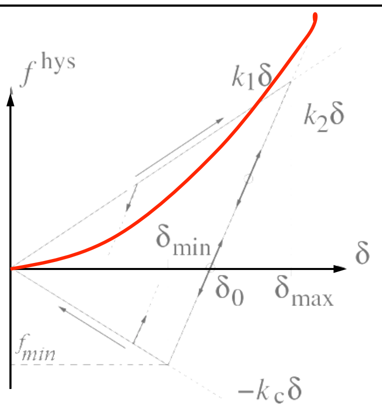
- Full/All Details ... too much!
- **Mesoscopic type Models**
- (Over-)Simplified Models



Linear Contact model

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

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

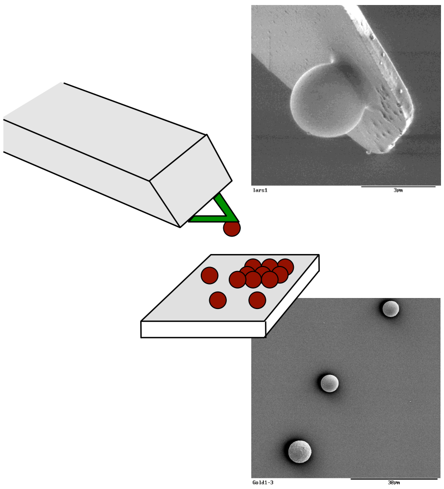


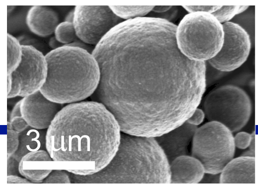
Hertz Contact model

- simple ☺
- non-linear
- easy to implement

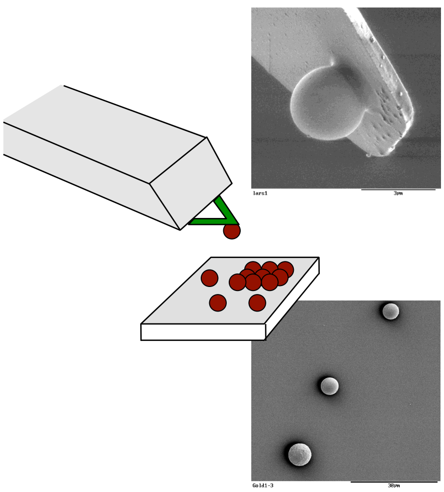
$$f_i^{hys} = \begin{cases} k_1\delta^{3/2} & \text{for un-/re-loading} \end{cases}$$

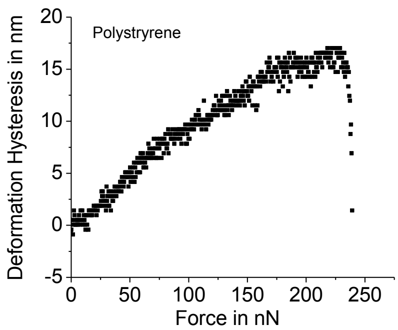
Contact force measurement (AFM)

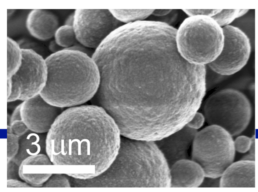




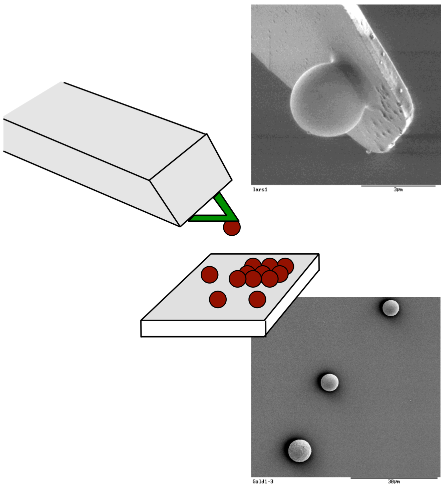
Contact force measurement (AFM)

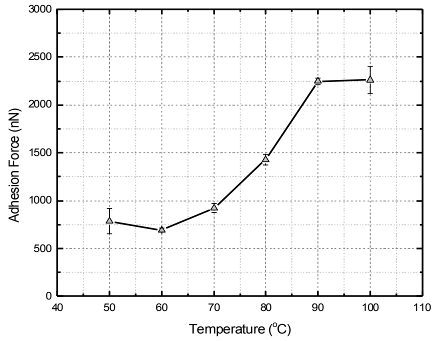


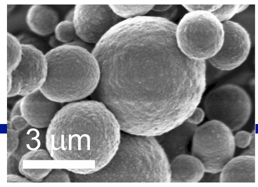




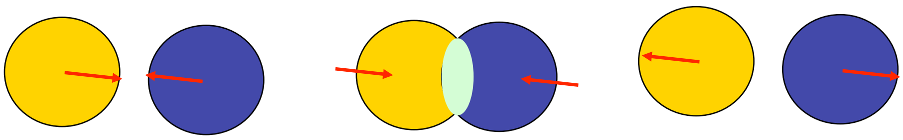
Contact force measurement (AFM)



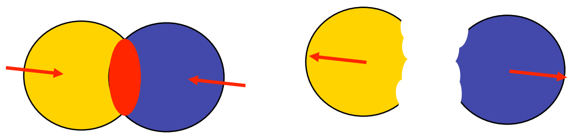




Elastic spheres

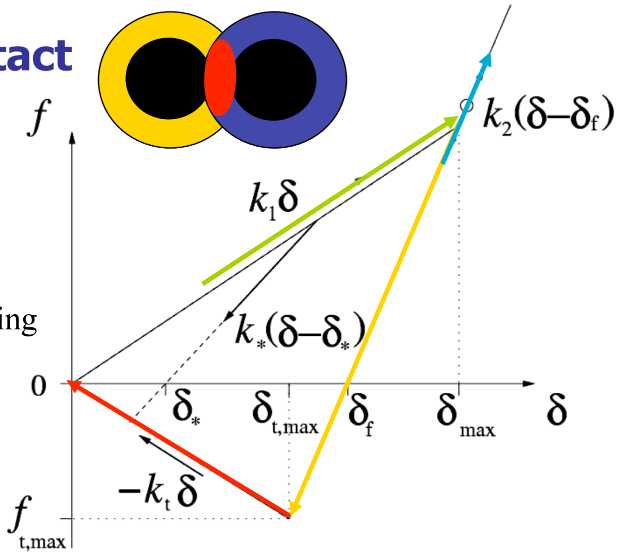


Elasto-plastic spheres



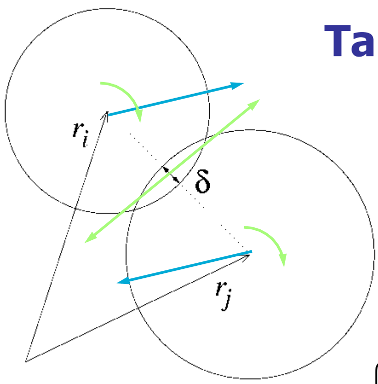
Before **During** **After**

Cohesive contact



1. **loading**
   transition to stiffness: k_2
2. **unloading**
3. **re-loading**
   elastic un/re-loading stiffness: k_2
4. **tensile failure**
   max. tensile force

Tangential contact model

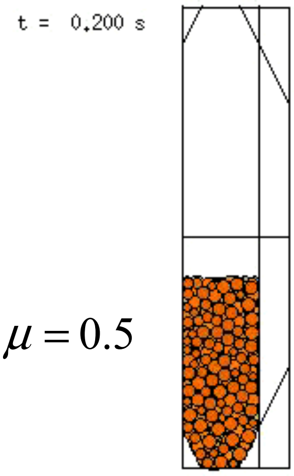


Sliding **contact points:**
- **static Coulomb friction**
- **dynamic Coulomb friction**
- **objectivity**

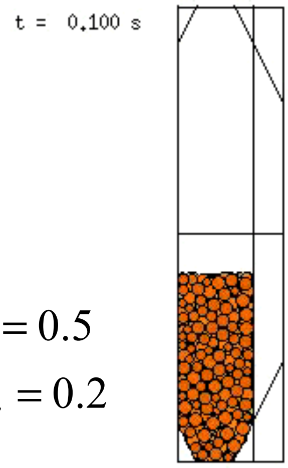
Sliding/Rolling/Torsion

$$v_t = \begin{cases} (v_i - v_j)^t + \hat{n} \times (a_i \omega_i + a_j \omega_j) & \text{sliding} \\ a_{ij} \hat{n} \times (\omega_i - \omega_j) & \text{rolling} \\ a_{ij} \hat{n}\hat{n} \cdot (\omega_i - \omega_j) & \text{torsion} \end{cases}$$

Flow with friction & rolling resistance



$\mu = 0.5$

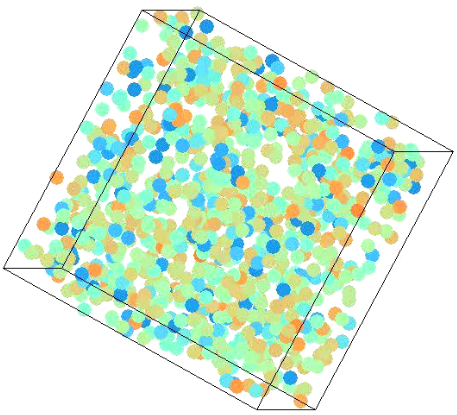


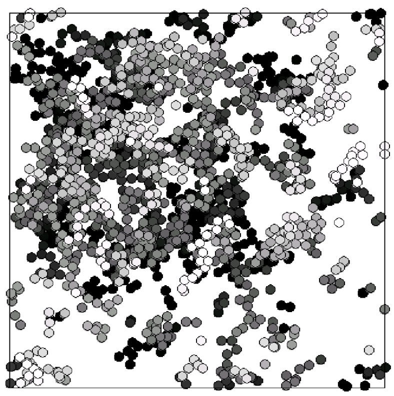
$\mu = 0.5$

$\mu_r = 0.2$

UNIVERSITY OF TWENTE.

… details of interaction

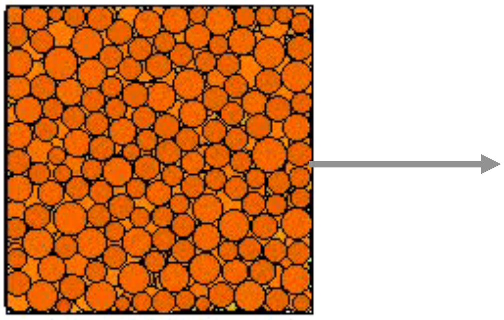




Attraction + Dissipation = Agglomeration

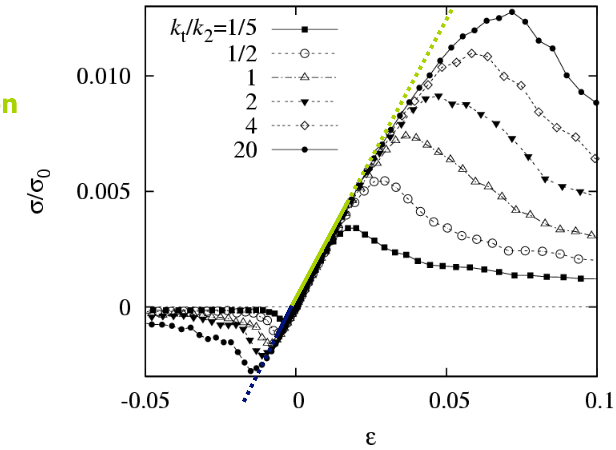
tension - uni-axial

$k_t / k_2 = 1/2$



uni-axial compression-tension

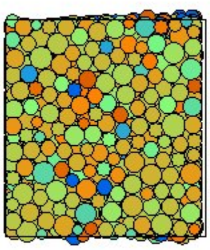
- Compression
- Tension

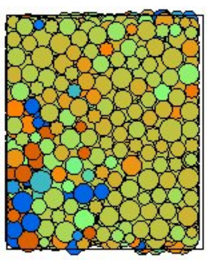


compression - uni-axial

$k_t / k_2 = 1/2$

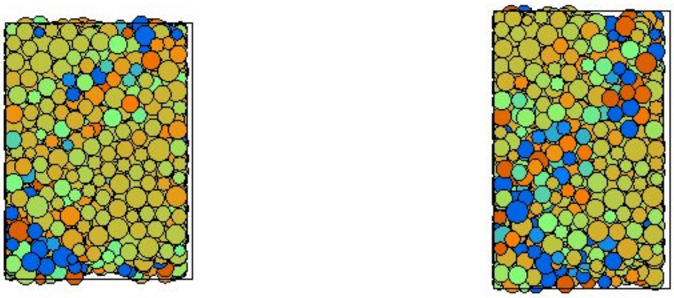
compression - uni-axial





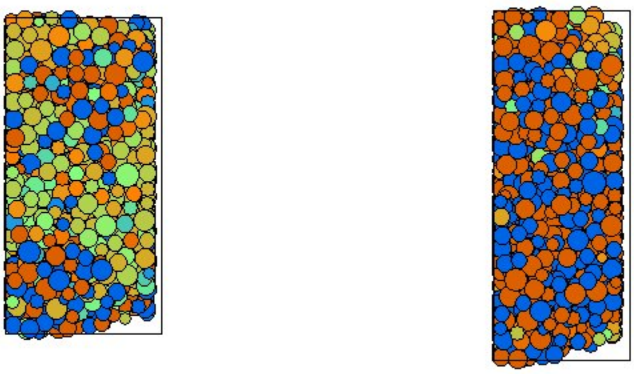
$k_t / k_2 = 1/2$

compression - uni-axial



$k_t/k_2 = 1/2$

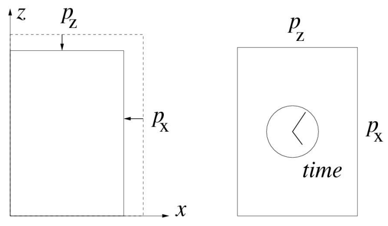
compression - uni-axial

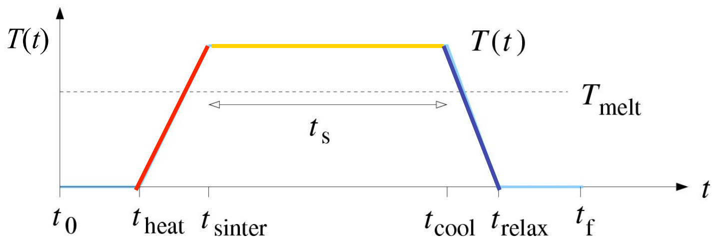


$k_t/k_2 = 1/2$

Sintering / Cementation (back to 2D)

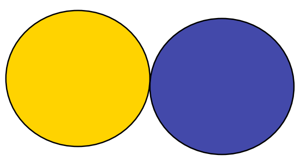
1. Preparation
2. Heating
3. Sintering / Cementation
4. Cooling
5. Relaxation
6. Testing



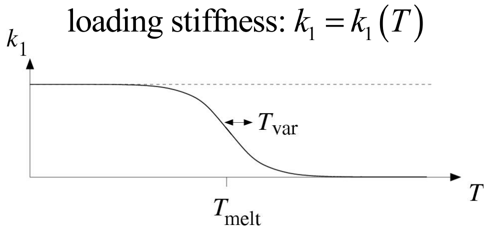


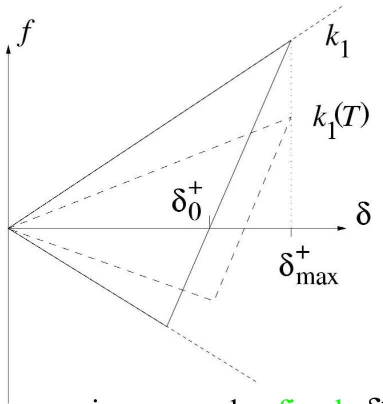
Sintering /Cementation 2

2. Heating



loading stiffness: $k_1 = k_1(T)$



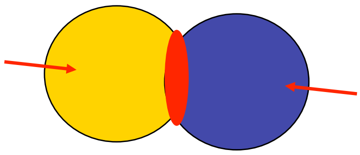


maximum overlap fixed: δ_{max}^+

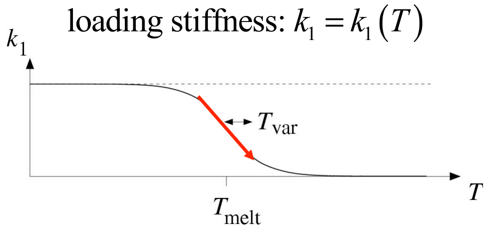
neutral overlap increasing: δ_0^+

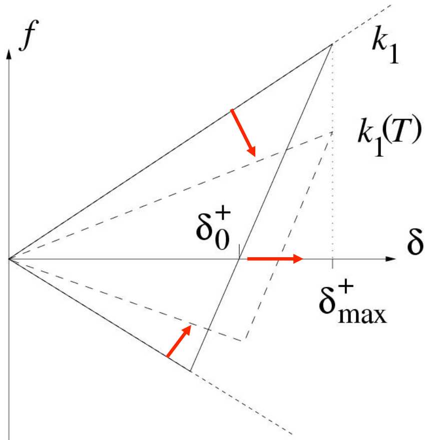
Sintering /Cem.

2. Heating



loading stiffness: $k_1 = k_1(T)$



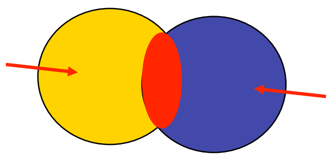


maximum overlap fixed: δ_{max}^+

neutral overlap increasing: δ_0^+

Sintering / Cem. 3

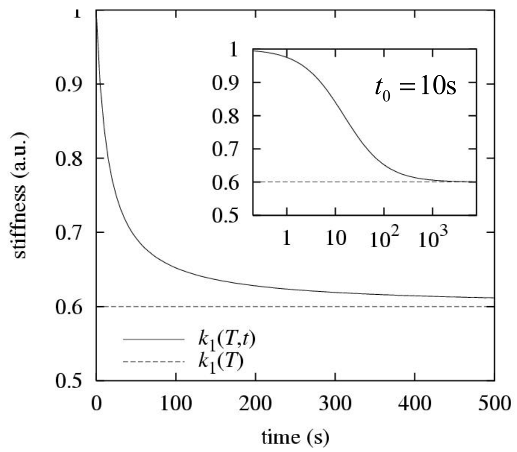
3. Sintering / Cementation - Reaction



Sintering 3

3. Sintering

- slow dynamics (t_0)
- diffusion, …
- trick: increase t_0

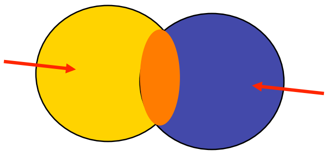


time delay:

$$\frac{\partial}{\partial t} k_1(T,t) = \pm \frac{\left[k_1(T) - k_1(T,t)\right]^2}{k_1(T)\, t_0} \qquad k_1(T,t) = k_1(T)\left\{1 - \left(\frac{1}{1 - k_1(T_0)/k_1(T)} - \frac{t}{t_0}\right)^{-1}\right\}$$

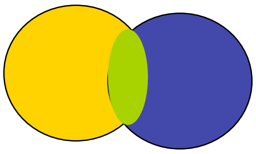
Sintering 4

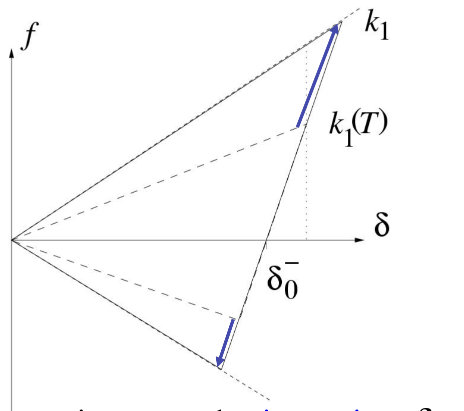
4. Cooling



Sintering 4

4. **Cooling**



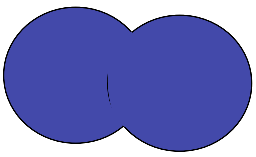


maximum overlap increasing: $\delta^{-}_{\max}$

neutral overlap fixed: δ^{-}_{0}

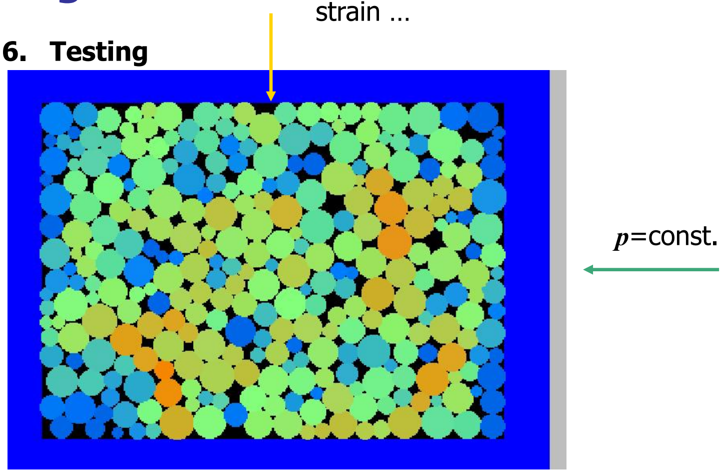
Sintering 5

5. **Relaxation**



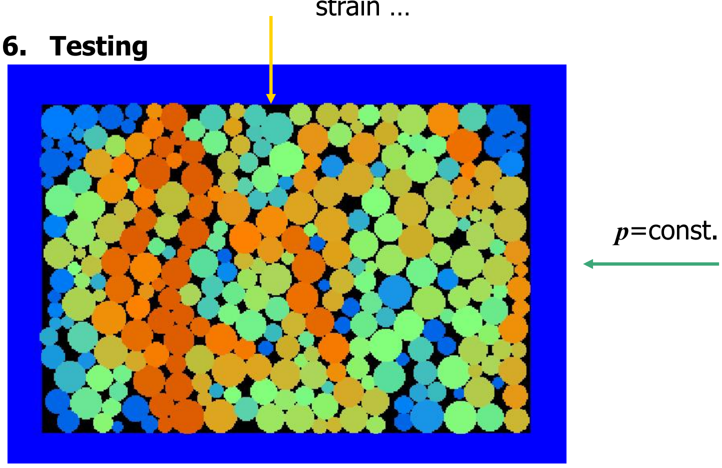
Sintering 6

6. **Testing**



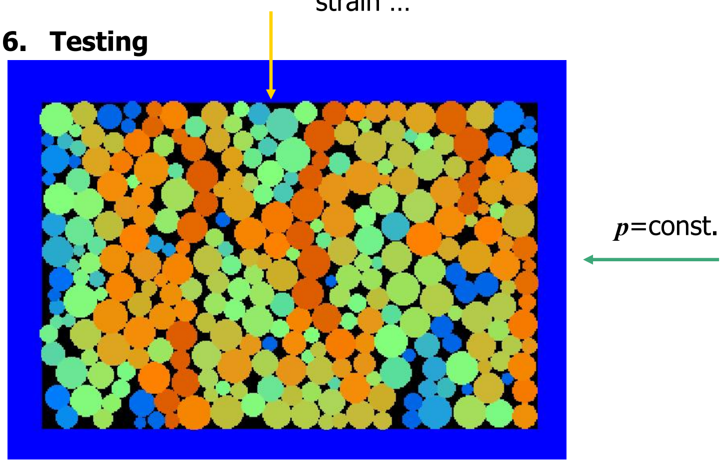
Sintering 6

6. **Testing**



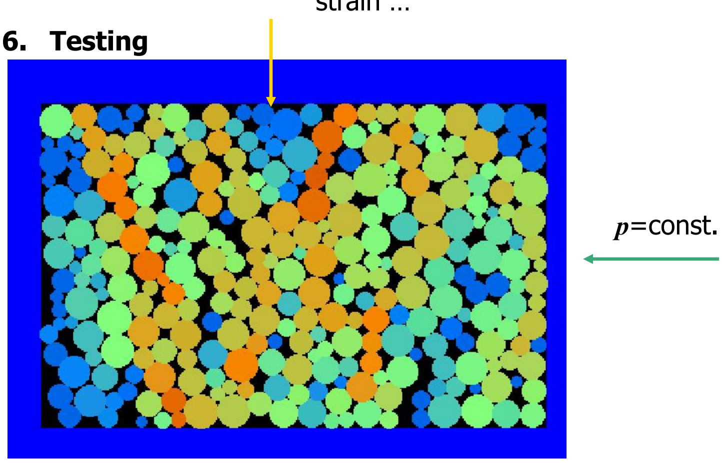
Sintering 6

6. Testing



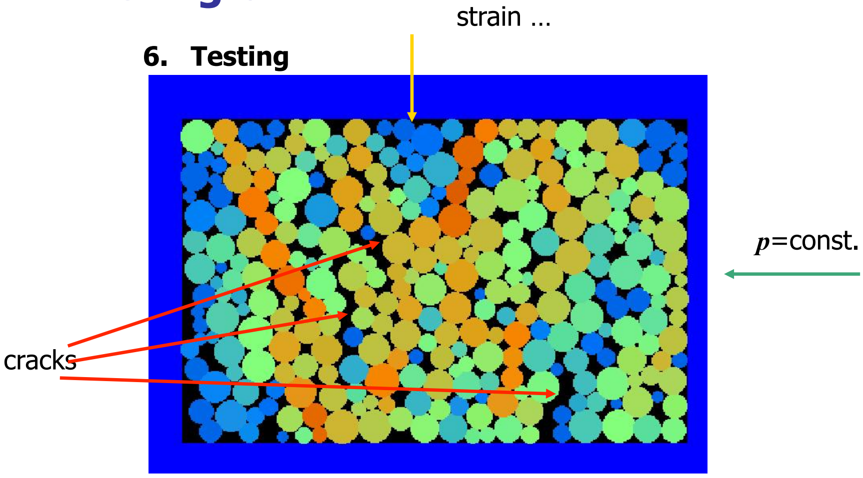
Sintering 6

6. Testing



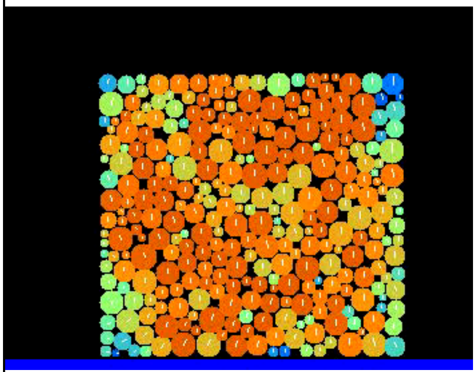
Sintering 6

6. Testing

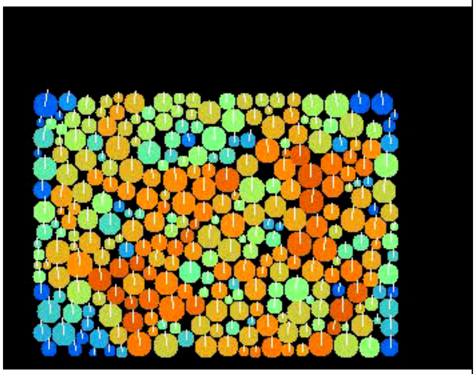


Sintering (Temperature+Pressure)

Vibration test



p=100



p=10

Micro-macro GLOBAL

- Micro-/Macro-Flow Rheology
  - micro-adhesion … macro-cohesion
  - micro-contact-friction … macro-friction-angle
- Non-Newtonian Rheology (Anisotropy?, Micro-polar?)

Biaxial box element test

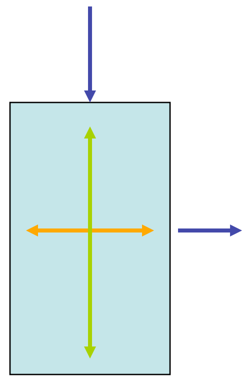
- Top wall: strain controlled

$$z(t) = z_f + \frac{z_0 - z_f}{2}(1 + \cos \omega t)$$

- Right wall: stress controlled

$$p = \text{const.}$$

- Evolution with time … ?



Constitutive model
various deformation modes

Mode 0: Isotropic $d\gamma = 0$

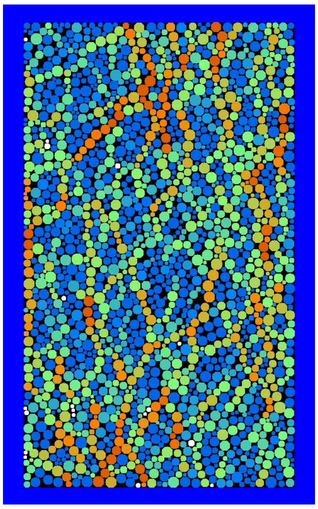
Mode 1: Uni-axial

Mode 2: Deviatoric $\varepsilon_V = 0$

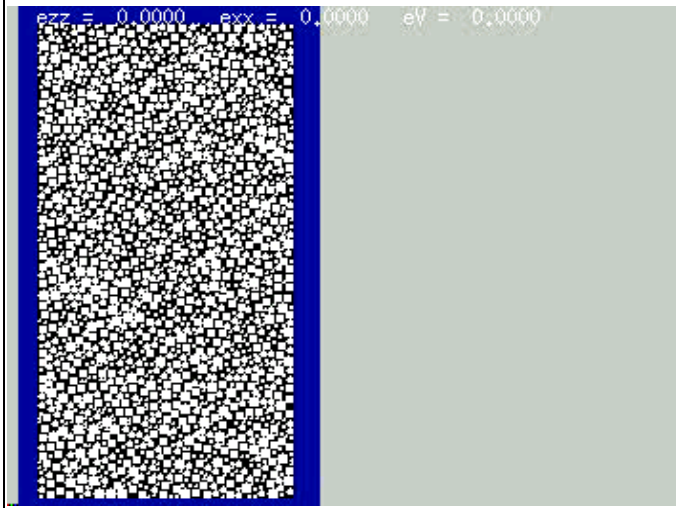
Mode 3: Bi-axial (side-stress controlled)

Mode 4: Bi-axial (isobaric, p-contolled)

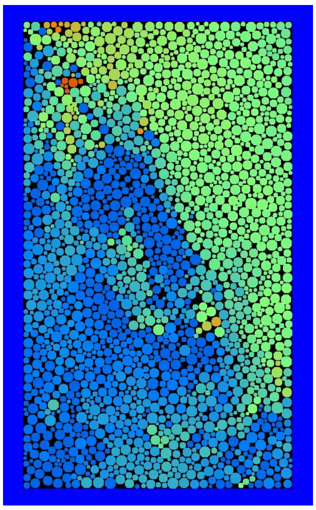
Bi-axial box (stress chains)



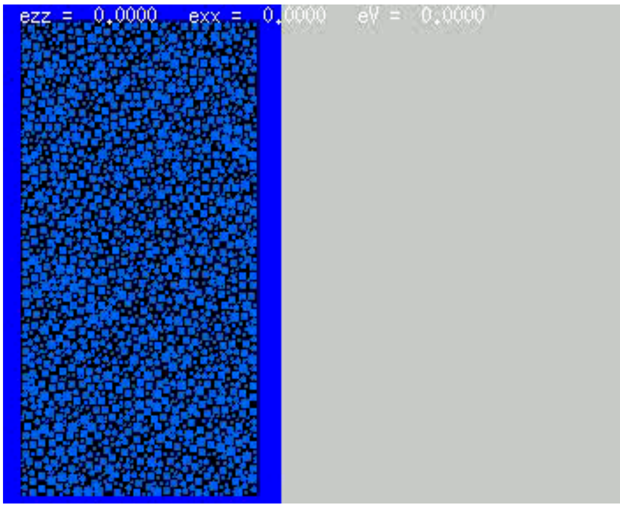
Bi-axial box (stress chains)



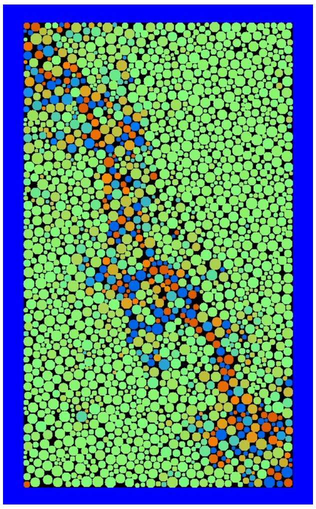
Bi-axial box (kinetic energy)



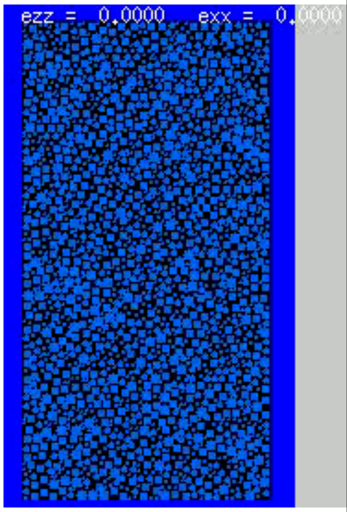
Bi-axial box (kinetic energy)



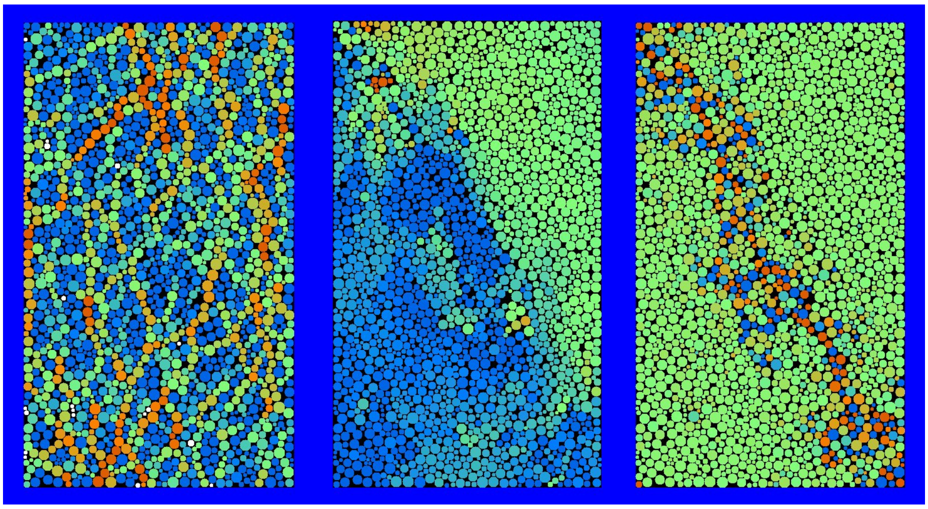
Bi-axial box (rotations)



Bi-axial box (rotations)

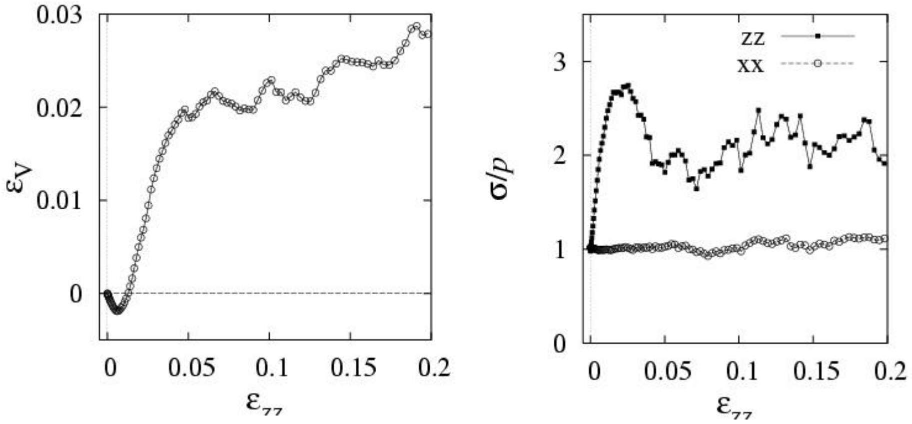


Multiple micro-mechanisms

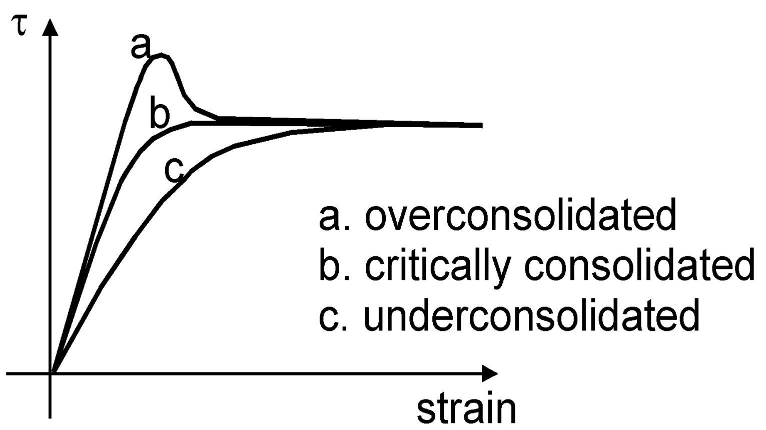


inhomogeneity & anisotropy, instabilities & structures, rotations

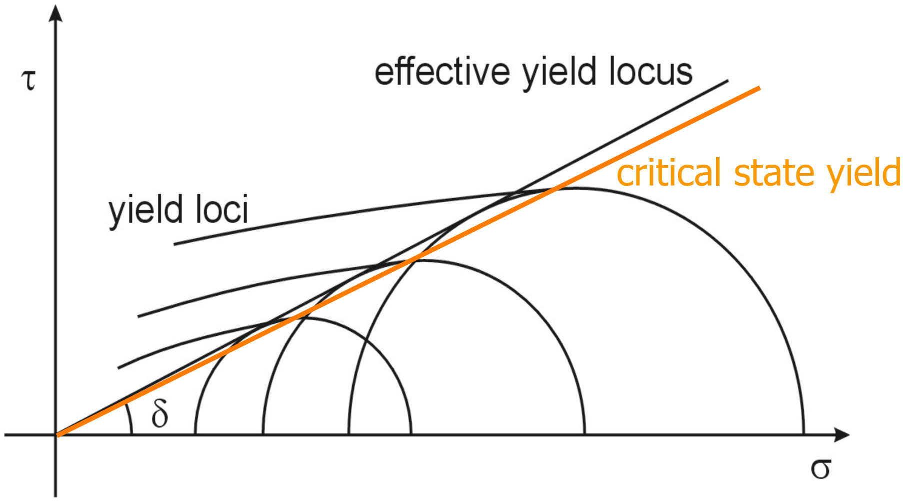
Bi-axial compression with p_x=const.



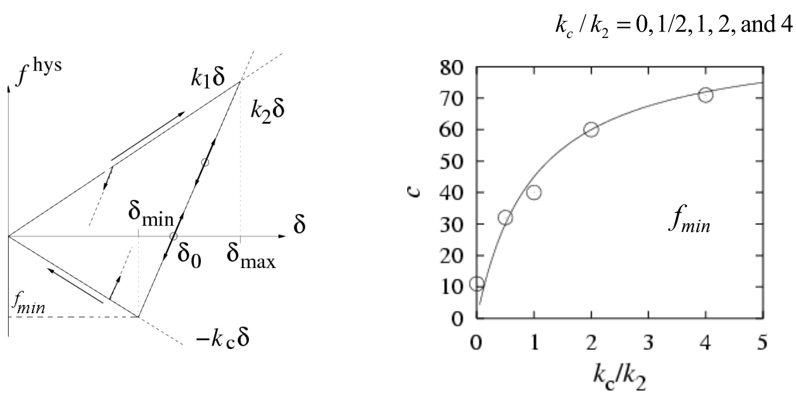
Microscopic interpretation: memory?



Yield loci

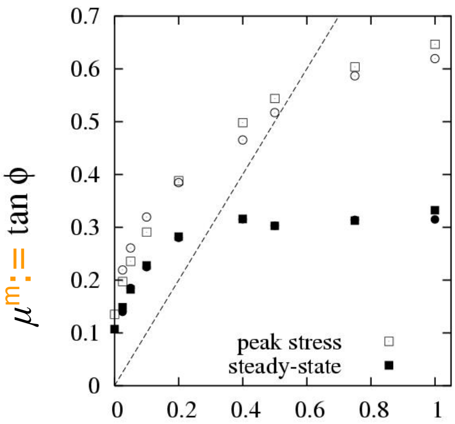


Micro-macro for cohesion



micro adhesion: f_{min} macro cohesion $c = c_0 \frac{1 - k_1/k_2}{1 + k_2/k_c}$

Micro-macro for friction



prepared μ=0

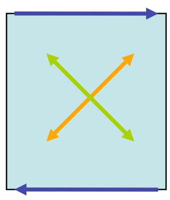
prepared μ=0.5

steady-state shear

micro contact-friction μ macro friction-angle μ^m

NOTE: each point = 5-10 simulations

Anisotropy <-> Shear ?



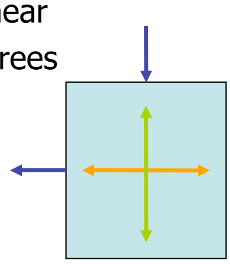
- Simple shear

$$\varepsilon = \begin{pmatrix} 0 & 2\varepsilon_s \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon_s \\ -\varepsilon_s & 0 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix}$$

Rotation + symmetric shear

- Rotate symmetric shear tensor by 45 degrees

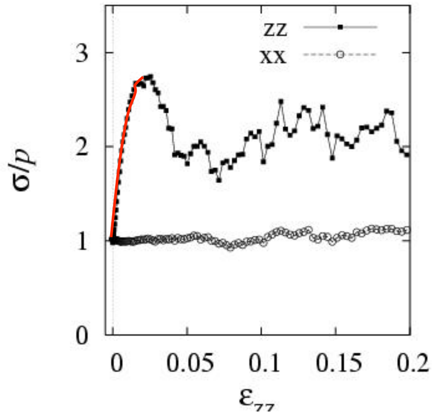
$$R_{45} \cdot \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix} \cdot R_{45}^T = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & -\varepsilon_s \end{pmatrix}$$



- Biaxial "shear": compression+extension

An-isotropy

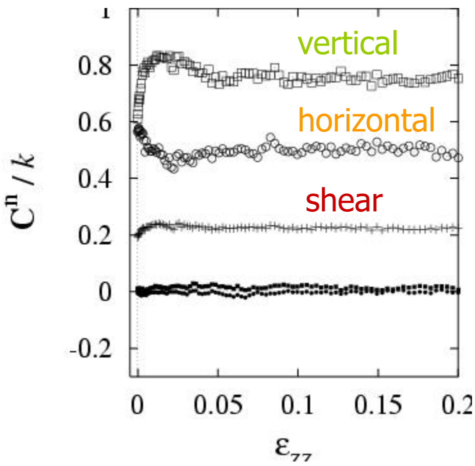
in stress

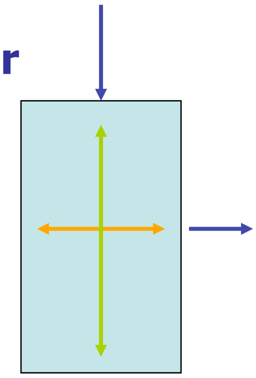


An-isotropy (Stress)

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

Stiffness/structure tensor





Different moduli:

- against shear C_2
- perpendicular C_1
- *one* shear modulus

An-isotropy (Stress & Structure)

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

An-isotropy (Stress & Structure)

Modulus

Friction

$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

$$\frac{\partial}{\partial \varepsilon_D} A = \beta_F \left(A_{\max} - A \right)$$

Constitutive model – isobaric (mode 4)
scalar! (in the biaxial box eigen-system)

Isotropic stress $0 = 2B\varepsilon_V + AS\,d\gamma$

Deviatoric stress $\delta\tau = \delta\sigma_D = A\varepsilon_V + 2GS\,d\gamma$

Anisotropy $\delta A = \beta_A \left(A^{\max} - A \right) \left| d\gamma \right|$

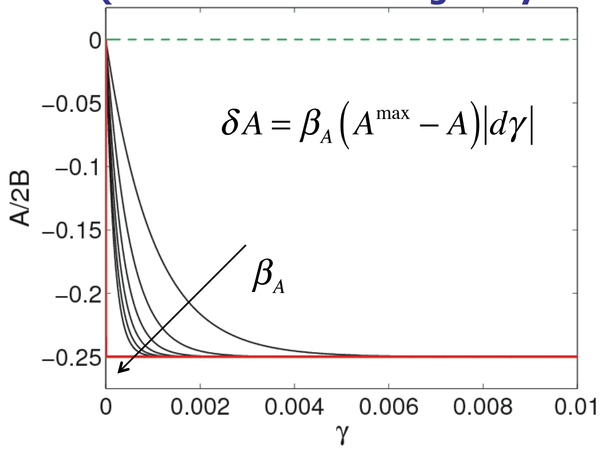
abbrev. stress-isotropy $S = 1 - \sigma_D / \sigma_D^{\max} = 1 - s_D / s_D^{\max}$

Isotropic|deviatoric strain increment $\varepsilon_V \mid d\gamma$

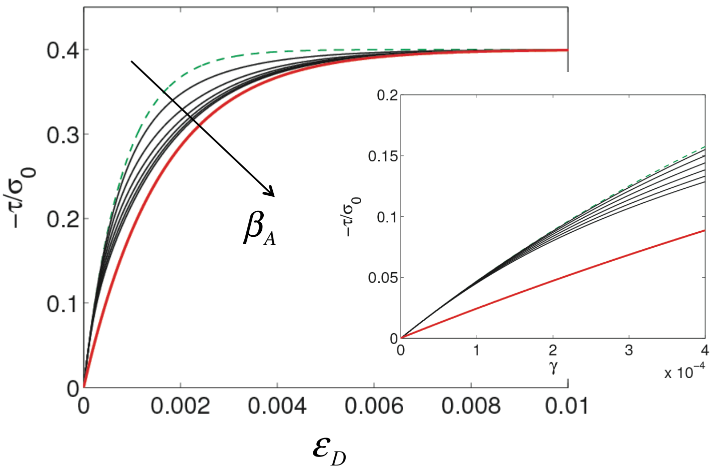
B … Bulk-, *G* … Shear-, *A* … Anisotropy-Modulus

Constitutive model – scalar

(in the biaxial box eigen-system)

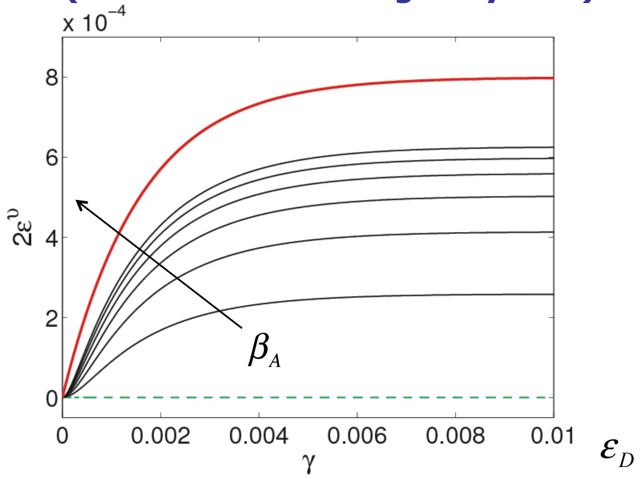


Constitutive model – scalar



Constitutive model – scalar

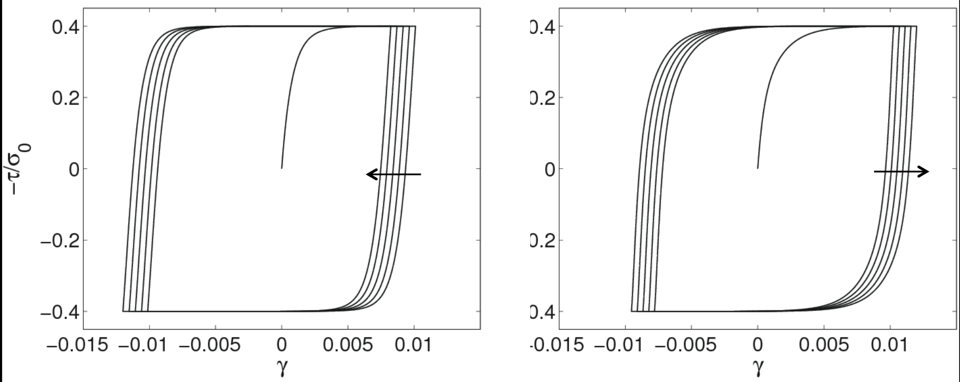
(in the biaxial box eigen-system)



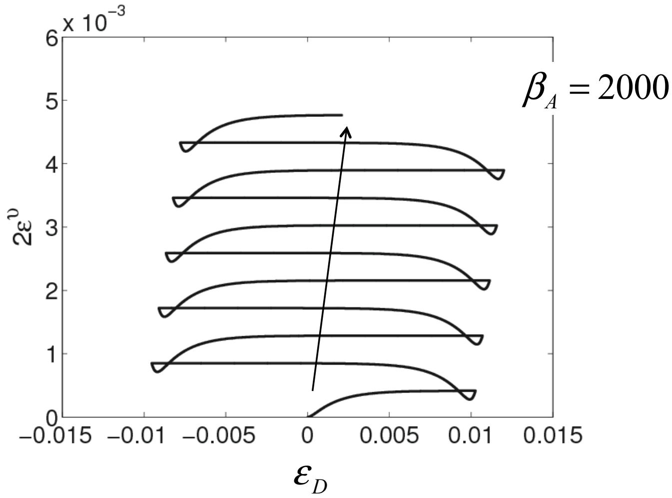
Constitutive model – cyclic loading

(in the biaxial box eigen-system)

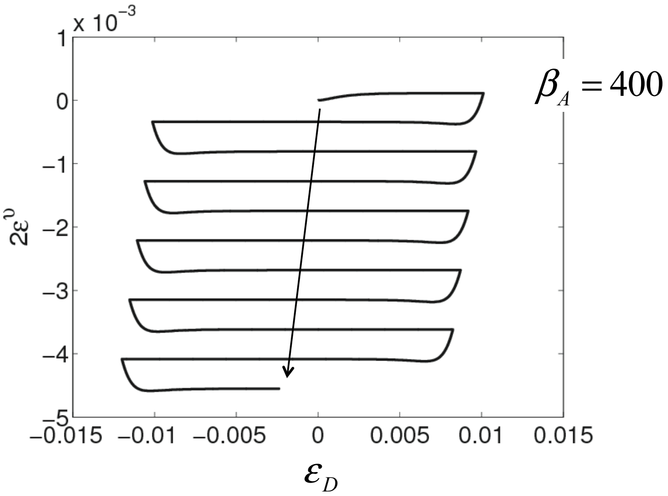
$\beta_A = 2000$ $\beta_A = 400$



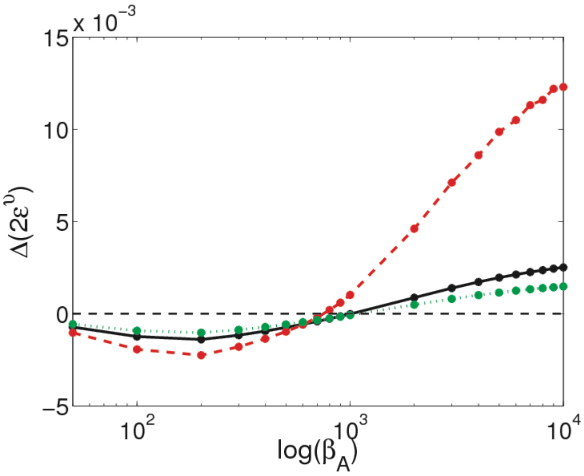
Constitutive model – scalar: dilatancy



Constitutive model – scalar: contractancy



Constitutive model – anisotropy rate



Constitutive model – scalar

(in the biaxial box eigen-system)

Bulk modulus B:
compression leads to pressure

Shear modulus G:
shear strain leads to shear stress

Anisotropy:
shear strain leads to pressure
compression leads to shear-stress

Cross-coupling of isotropic and deviatoric parts

Constitutive model – scalar

(in the biaxial box eigen-system)

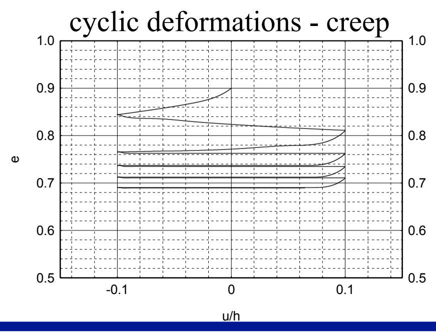
Anisotropy:

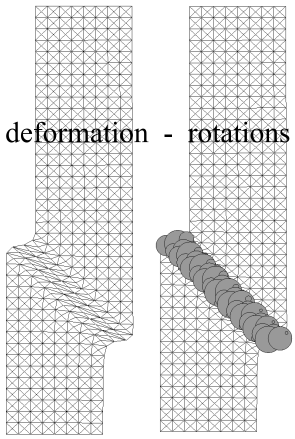
Strain-controlled:
shear strain leads to pressure
compression leads to shear-stress

Stress-controlled:
shear stress leads to dilatancy/compactancy
compression leads to shear-deformation

Hypoplastic FEM model

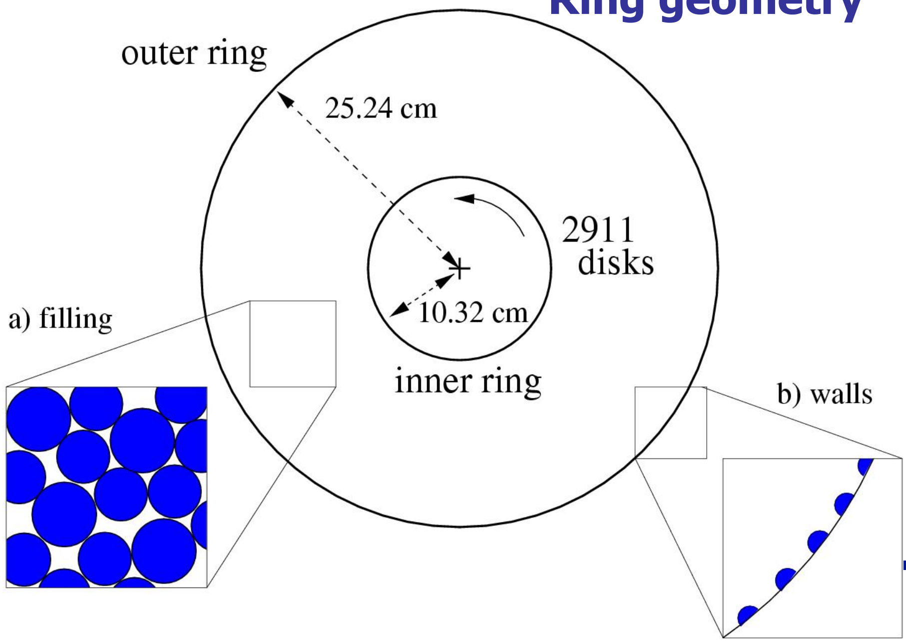
+ successful tool – few parameters
- microscopic foundations ?
- extensions & parameter identification



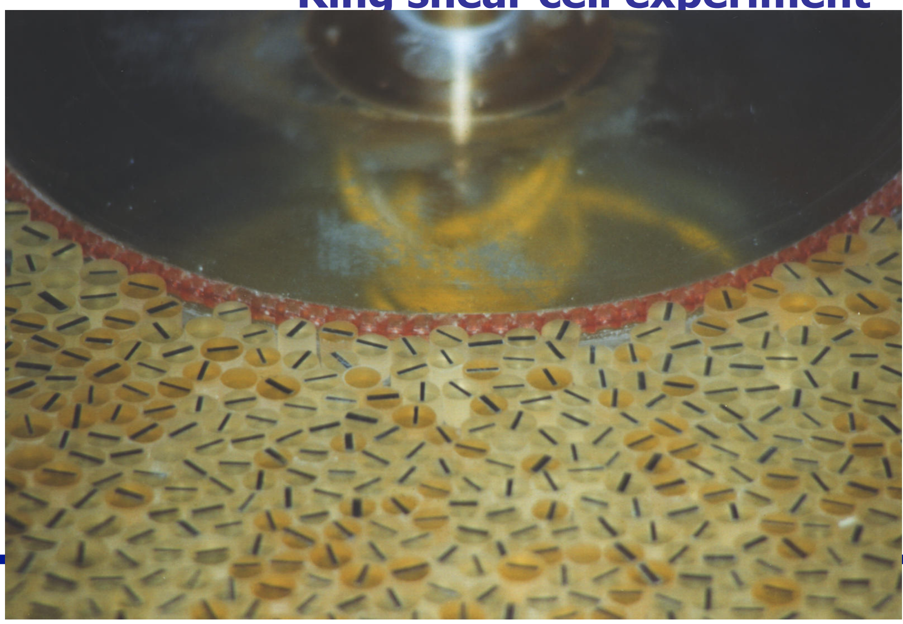


Continuum Theory

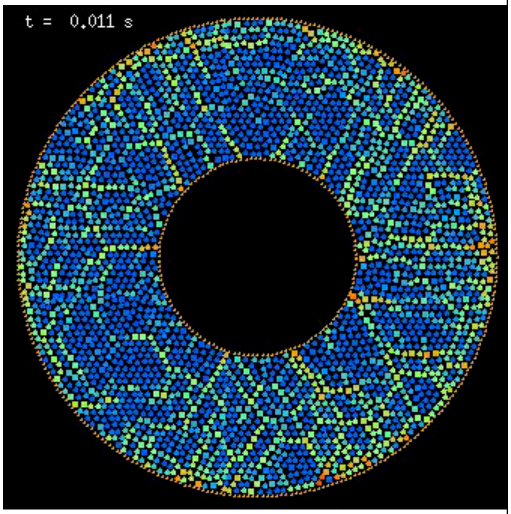
Ring geometry



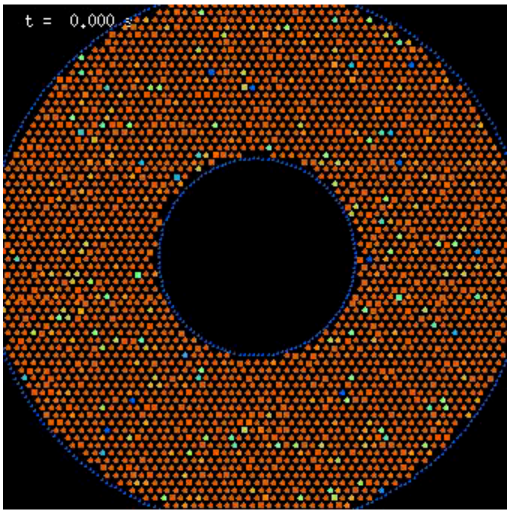
Ring shear cell experiment



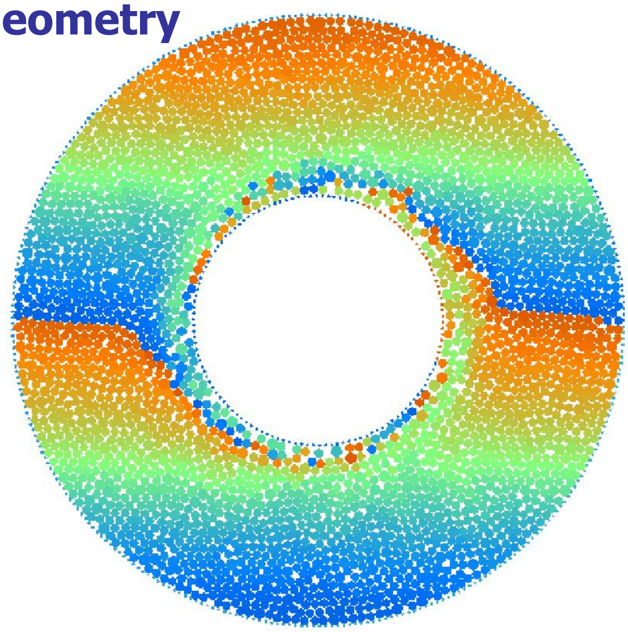
2D shear cell – force chains
= inhomogeneity
+ anisotropy



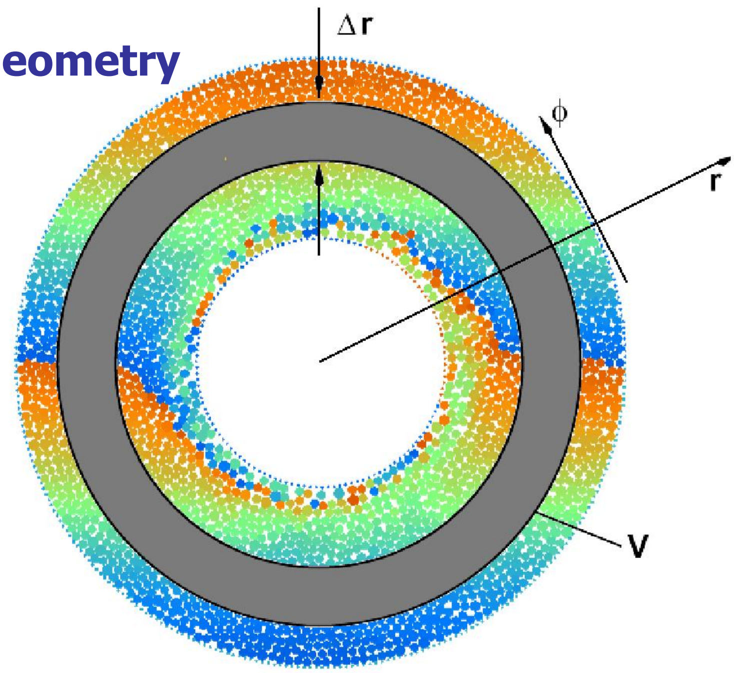
2D shear cell – energy



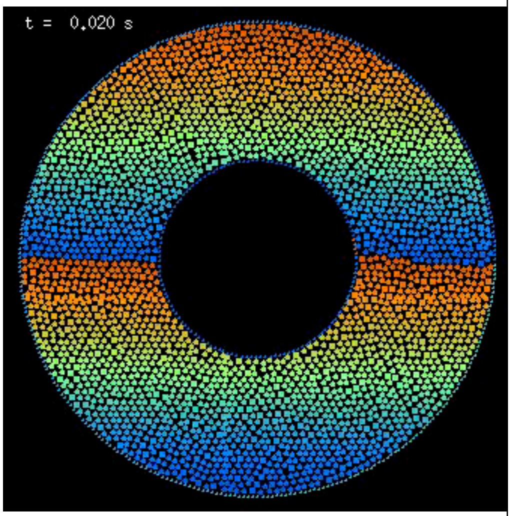
Ring geometry



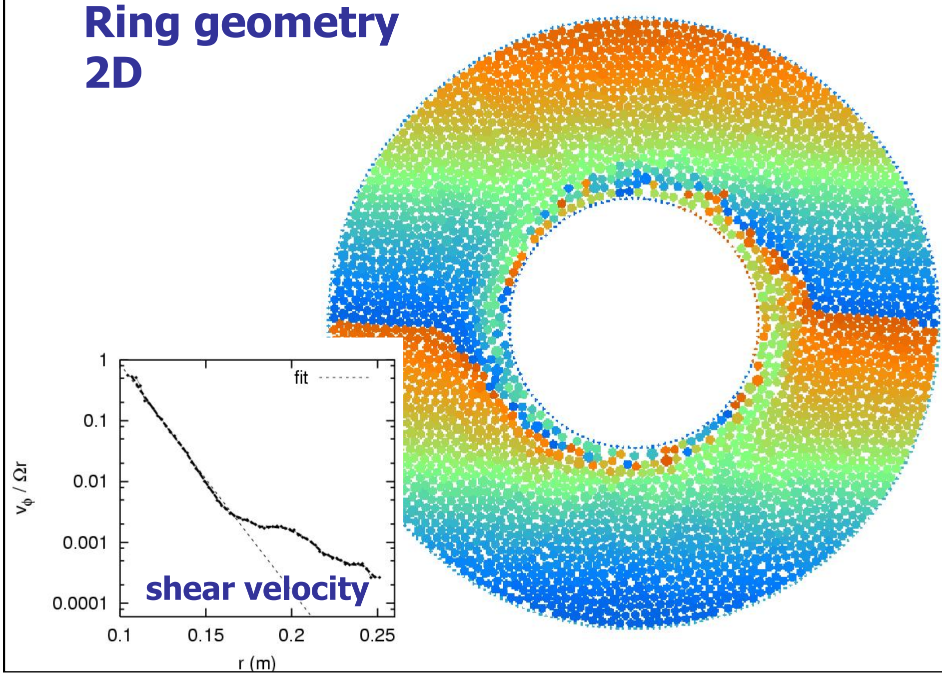
Ring geometry



2D shear cell:
- shear localization
- non-Newtonian



Ring geometry
2D



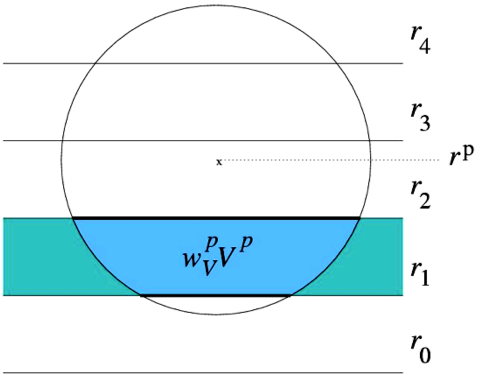
Averaging Formalism

$$Q = \langle Q^p \rangle = \frac{1}{V} \sum_{p \in V} w_V^p V^p Q^p$$

Any quantity:

$$Q^p = \sum_c Q^c$$

- Scalar
- Vector
- Tensor



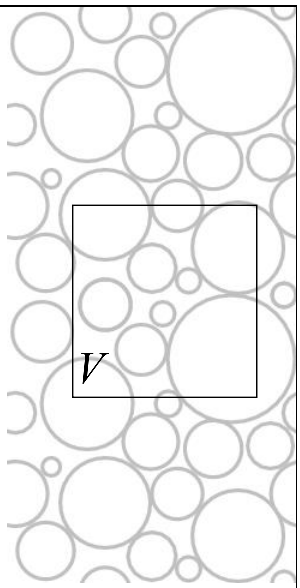
Averaging Formalism

$$Q = \langle Q^p \rangle = \frac{1}{V} \sum_{p \in V} w_V^p V^p Q^p$$

Any quantity:

$$Q^p$$

In averaging volume: V



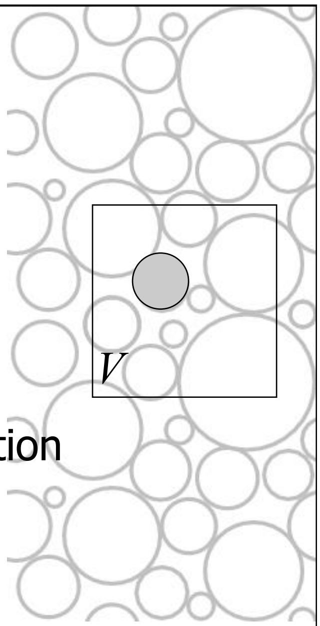
Averaging Density

$$Q = \nu = \frac{1}{V}\sum_{p\in V} w_V^p V^p$$

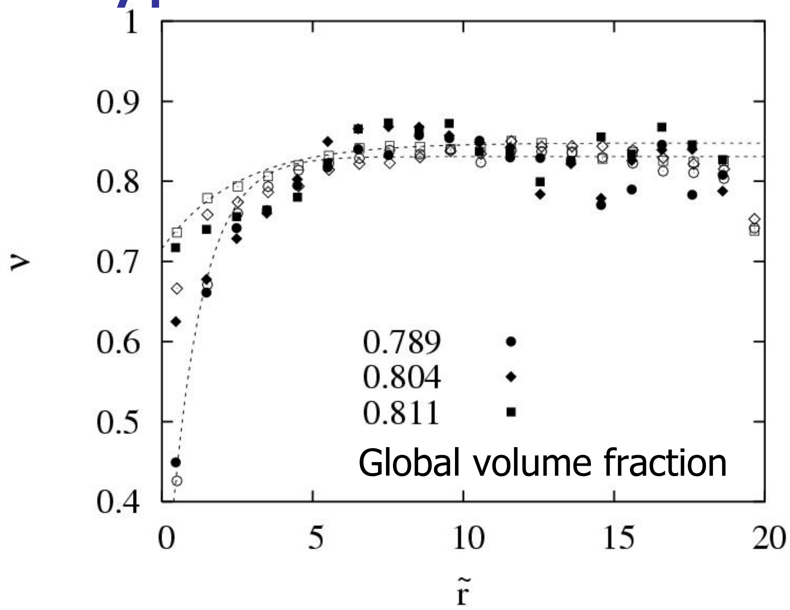
Any quantity:

$$Q^p = 1$$

- Scalar: Density/volume fraction



Density profile



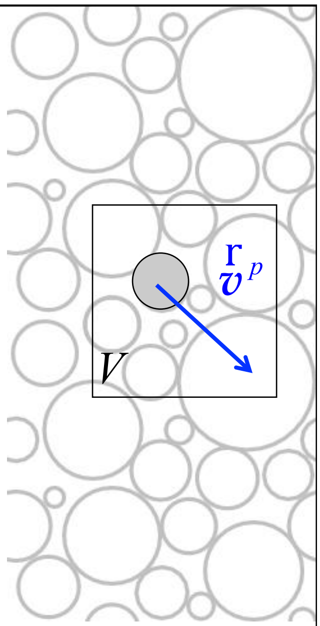
Averaging Velocity

$$Q = \nu \vec{v} = \frac{1}{V} \sum_{p \in V} w_V^p V^p \vec{v}^p$$

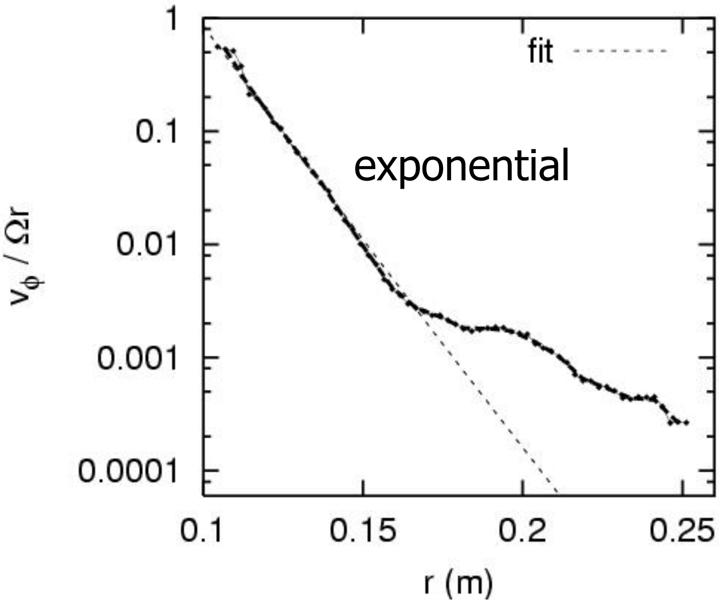
Any quantity:

$$Q^p = \vec{v}^p$$

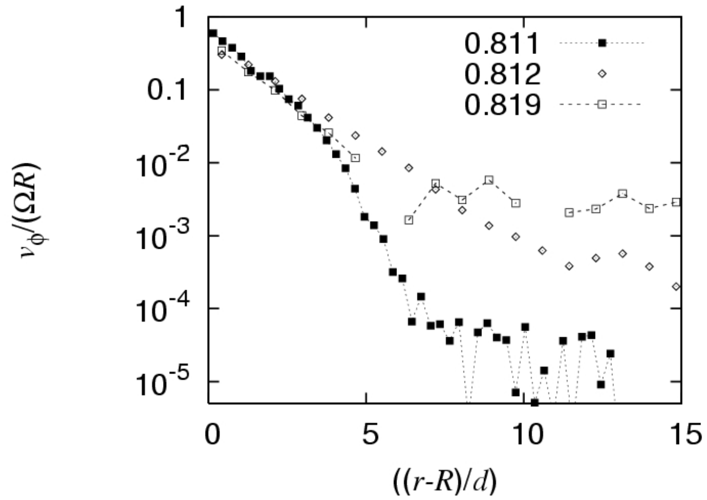
- Scalar
- Vector – velocity density



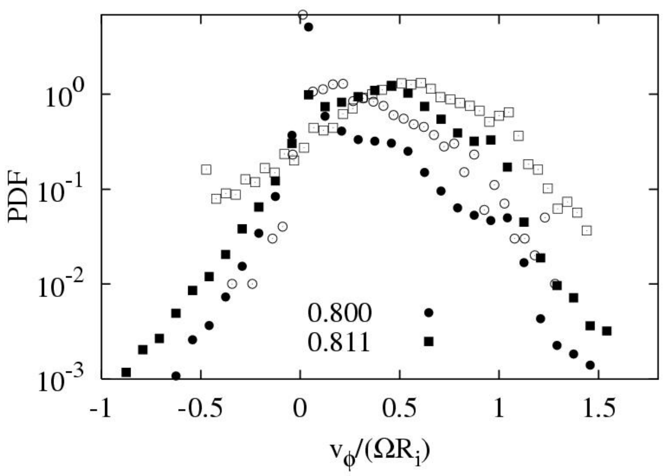
Velocity field -> velocity gradient



Velocity field -> velocity gradient



Velocity distribution



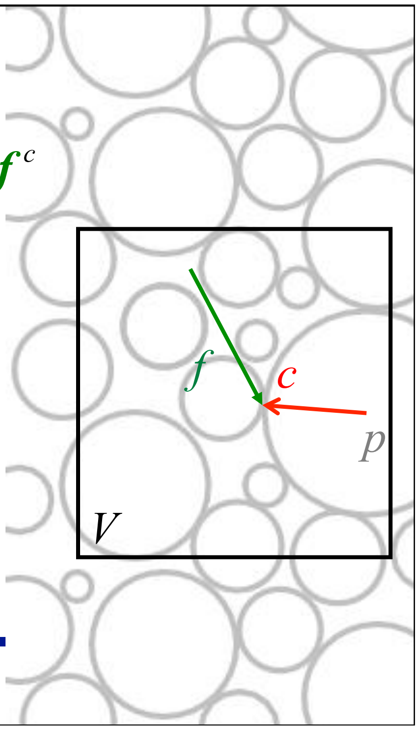
Averaging Stress

$$Q = \underline{\underline{\sigma}} = \frac{1}{V} \sum_{p \in V} \sum_{c} w_V^p \, \boldsymbol{l}^{pc} \boldsymbol{f}^{c}$$

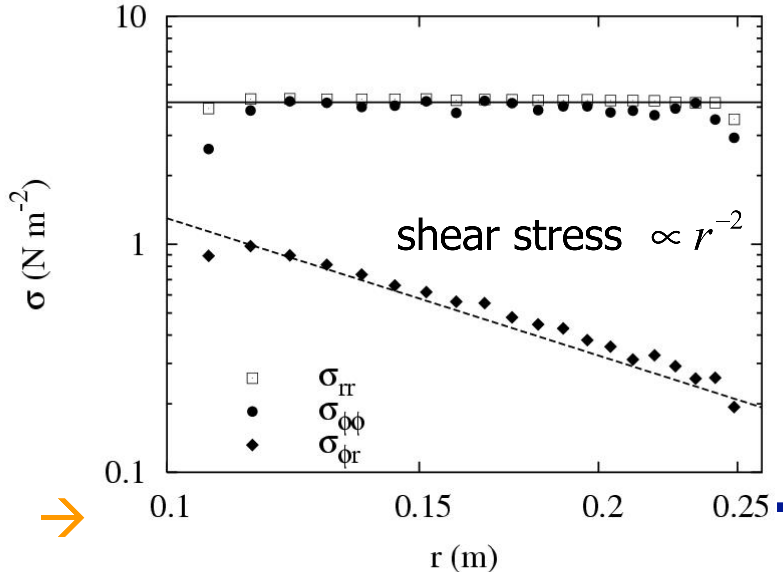
Any quantity:

$$Q^p = \underline{\underline{\sigma}}^p = \frac{1}{V^p} \sum_{c} \boldsymbol{l}^{pc} \boldsymbol{f}^{c}$$

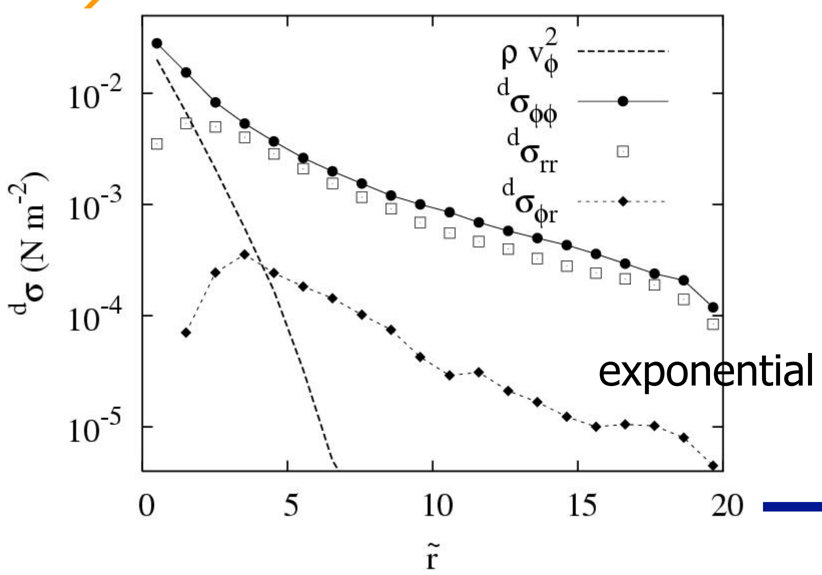
- Scalar
- Vector
- Tensor: Stress



Stress tensor (static)



Stress tensor (dynamic)



Stress equilibrium (1)

$$\Rightarrow \nabla\cdot\sigma = \frac{1}{r}\left[\frac{\partial(r\sigma_{rr})}{\partial r} - \sigma_{\phi\phi}\right]\vec{e}_r + \frac{1}{r}\left[\frac{\partial(r\sigma_{r\phi})}{\partial r} + \sigma_{\phi r}\right]\vec{e}_\phi$$

acceleration: $\vec{a} = \frac{d}{dt}\vec{v} = \frac{\partial}{\partial t}\vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v}$

$$\rho\vec{a} = \vec{\nabla}\cdot\sigma \Rightarrow \quad 0 = \rho v_\phi^2 + r\frac{\partial\sigma_{rr}}{\partial r} + (\sigma_{rr} - \sigma_{\phi\phi}),$$

$$0 = r\frac{\partial\sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r}),$$

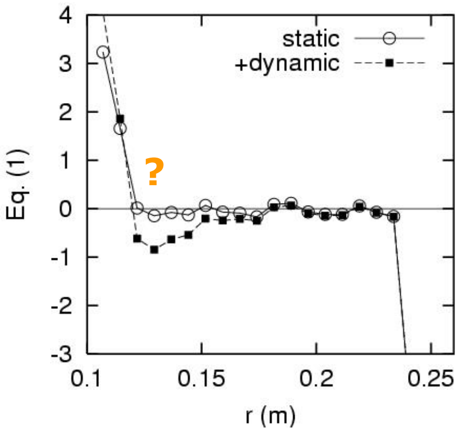
$$\Rightarrow \frac{\partial(r\sigma_{rr})}{\partial r} = \sigma_{\phi\phi} \qquad \frac{\partial(r\sigma_{r\phi})}{\partial r} = -\sigma_{\phi r}$$

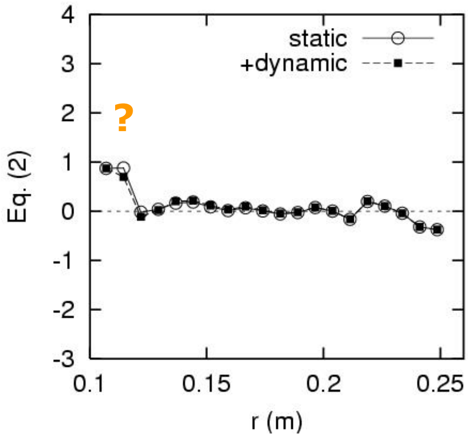
$$(\sigma_{rr} \propto \sigma_{\phi\phi} \propto r^0 \qquad \sigma_{r\phi} \propto \sigma_{\phi r} \propto r^{-2})$$

Stress equilibrium (2)

$$0 = \rho v_\phi^2 + r\frac{\partial \sigma_{rr}}{\partial r} + (\sigma_{rr} - \sigma_{\phi\phi}),$$

$$0 = r\frac{\partial \sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r}),$$





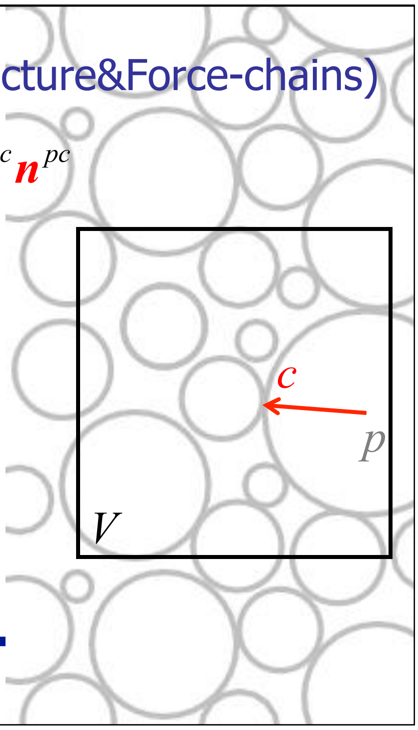
Averaging Fabric (Structure&Force-chains)

$$Q = \underline{\underline{\mathbf{F}}} = \frac{1}{V}\sum_{p\in V} w_V^p V^p \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

Any quantity:

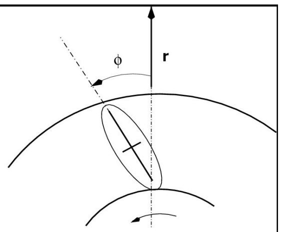
$$Q^p = \underline{\underline{\mathbf{F}}}^p = \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

- Scalar: contacts
- Vector: normal
- Contact distribution



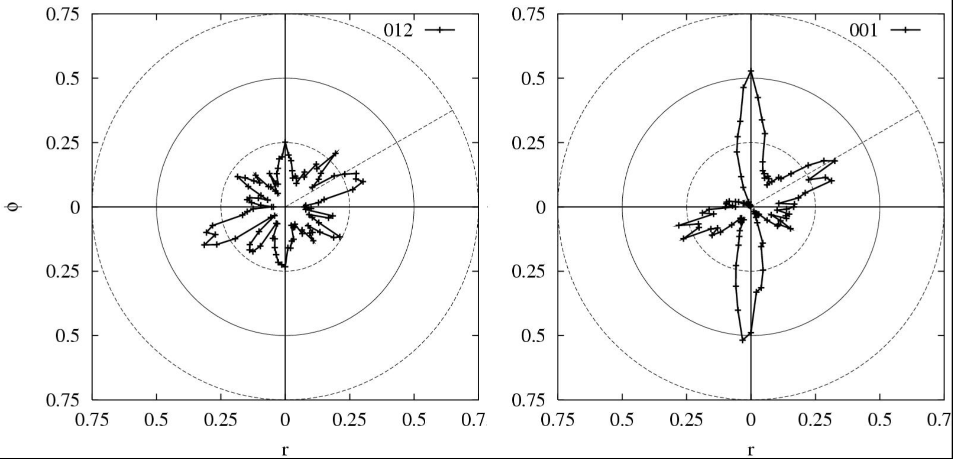
Fabric tensor

contact probability ...

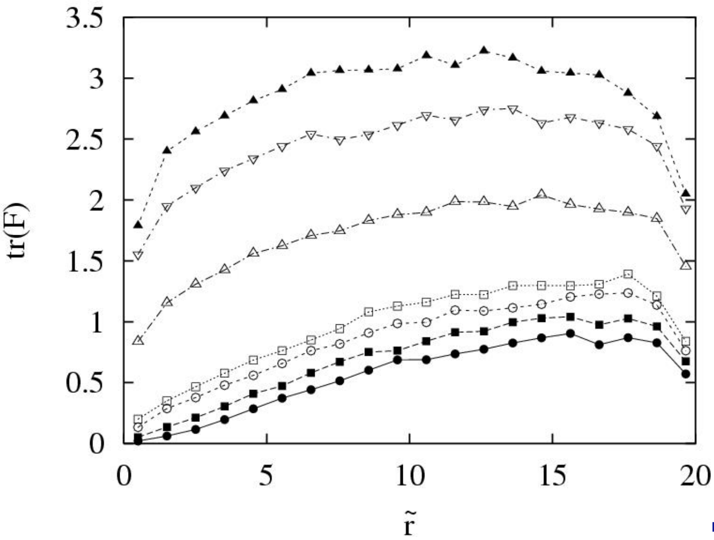


center

wall

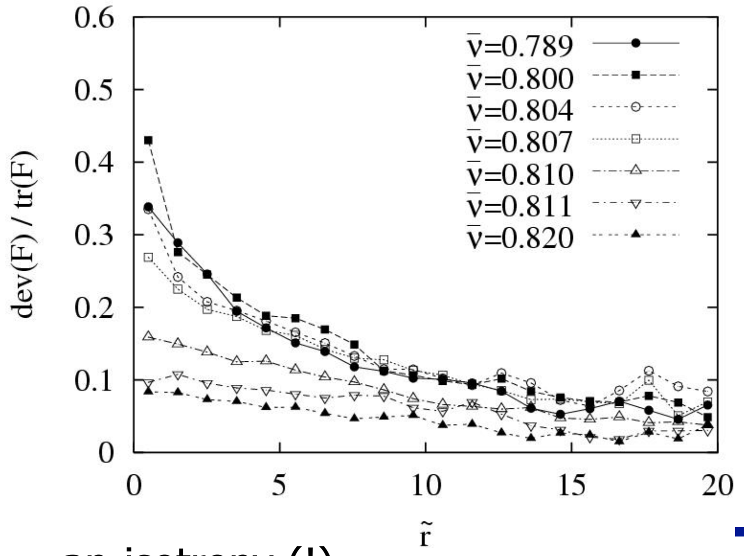


Fabric tensor (trace)



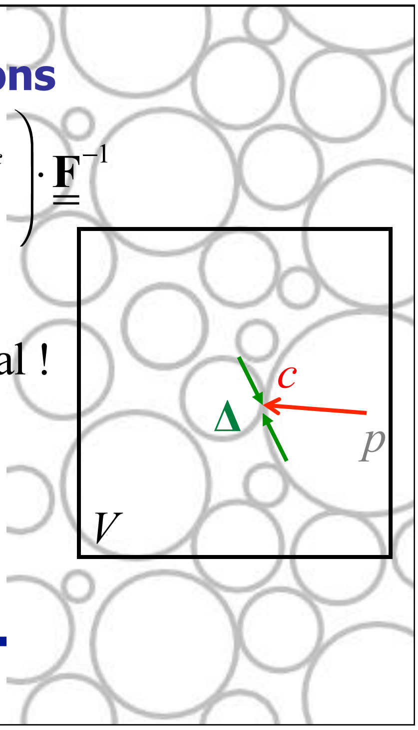
contact number density

Fabric tensor (deviator)



an-isotropy (!)

Averaging Deformations

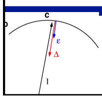


$$Q = \underline{\underline{\varepsilon}} = \frac{\pi h}{V}\left(\sum_{p\in V} w_V^p \sum_c \boldsymbol{l}^{pc} \Delta^c\right)\cdot \underline{\underline{\mathbf{F}}}^{-1}$$

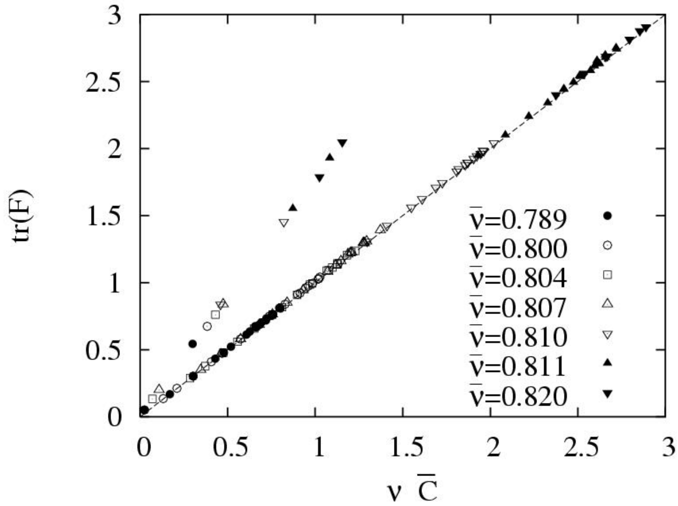
Deformation:

$$S = \left(\Delta^c - \underline{\underline{\varepsilon}} \cdot \boldsymbol{l}^{pc}\right)^2 \quad \text{minimal !}$$

- Scalar
- Vector
- Tensor: Deformation

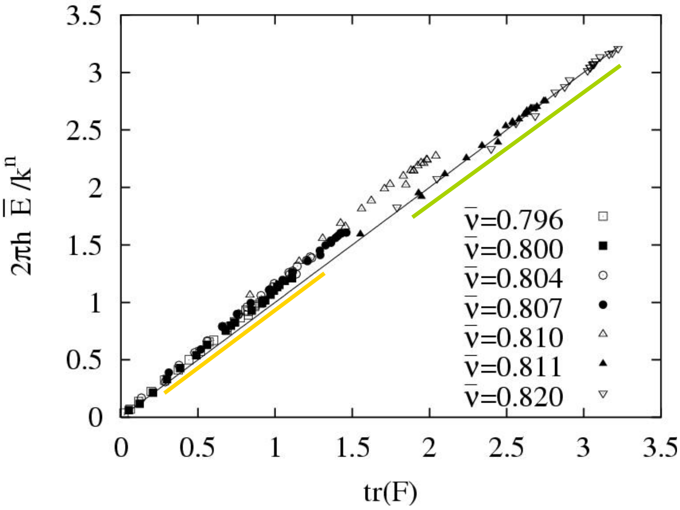


Macro (contact density)



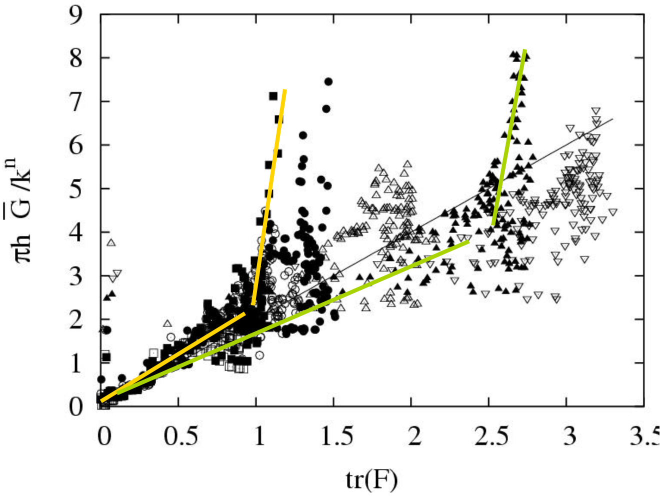
Macro (bulk modulus)

$$\overline{E} = \frac{\mathrm{tr}\,\underline{\underline{\sigma}}}{\mathrm{tr}\,\underline{\underline{\varepsilon}}}$$

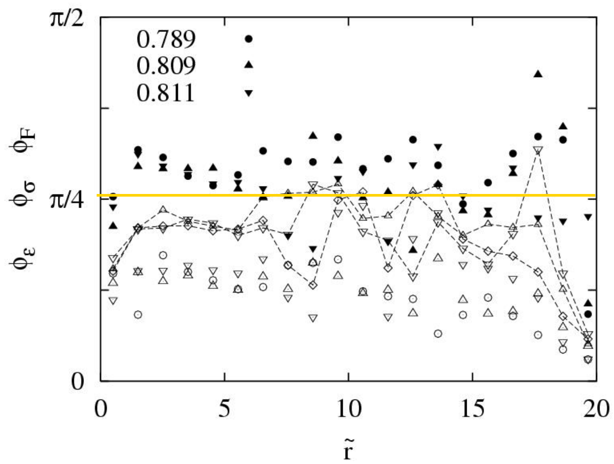


Macro (shear modulus)

$$\overline{G} = \frac{\text{dev}\underline{\underline{\sigma}}}{\text{dev}\underline{\underline{\varepsilon}}}$$



Anisotropy – not co-linear!



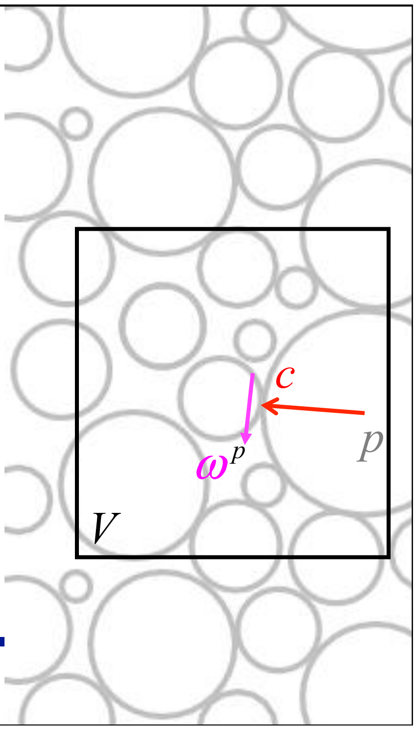
Averaging Rotations

$$Q = \nu\omega = \frac{1}{V}\sum_{p\in V}\sum_{c} w_V^p V^p \omega^p$$

Deformation:

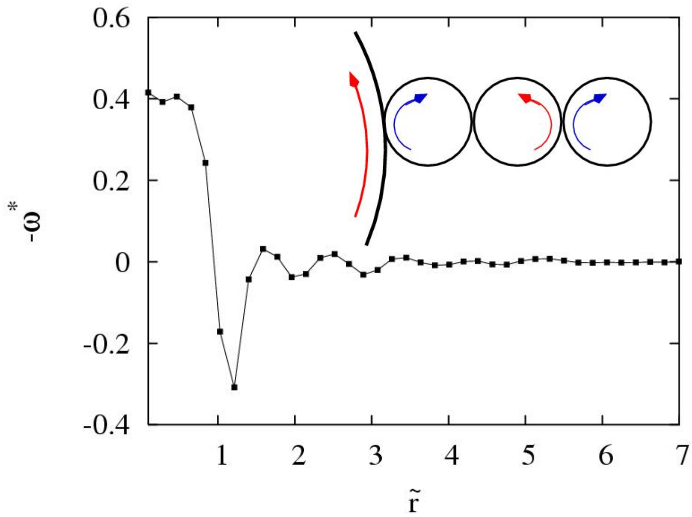
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor

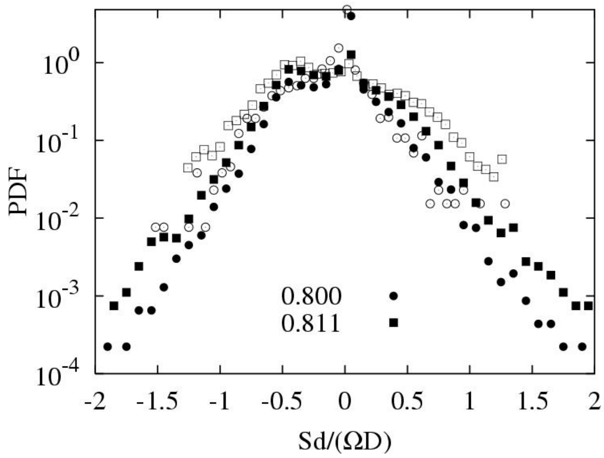


Rotations – spin density

eigen-rotation: $\omega^* = \omega - W_{r\phi}$



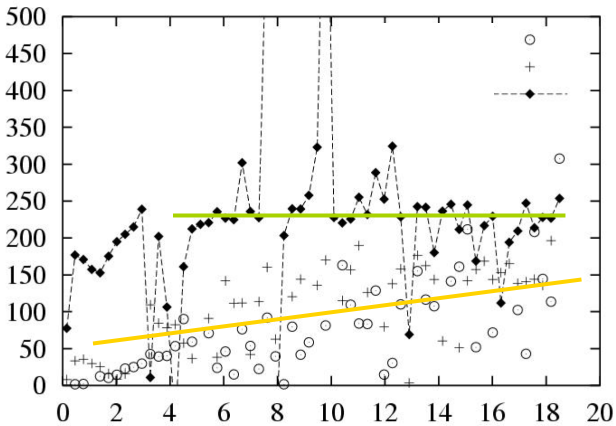
Spin distribution



Macro (torque stiffness)

$$\overline{\mu l^2} = \frac{\underline{\underline{M}}}{\underline{\underline{\kappa}}}$$

$\overline{\mu l^2}$



does global averaging make sense?

micro-macro for various deformation modes

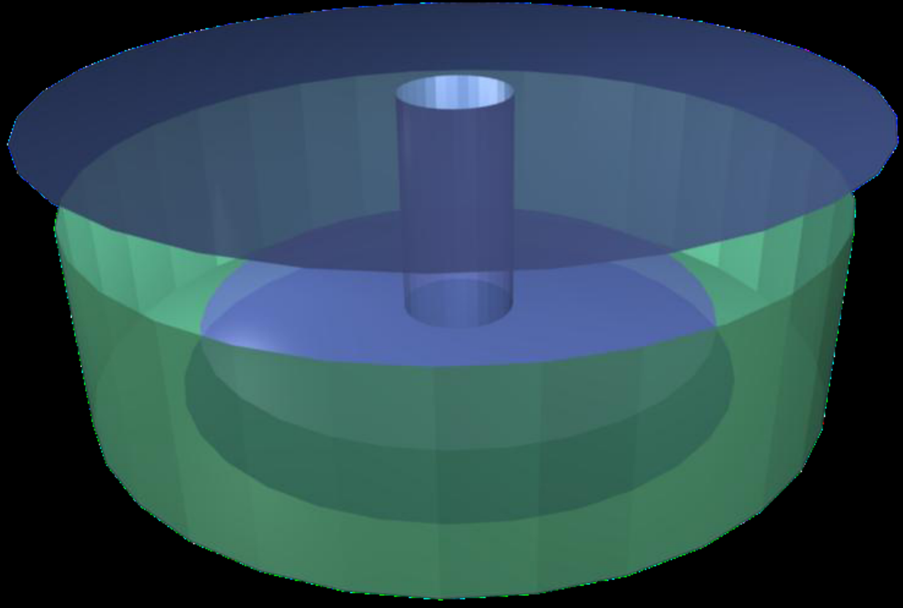
- visco-elasticity
- yield stress
- anisotropy

But: inhomogeneity is ignored

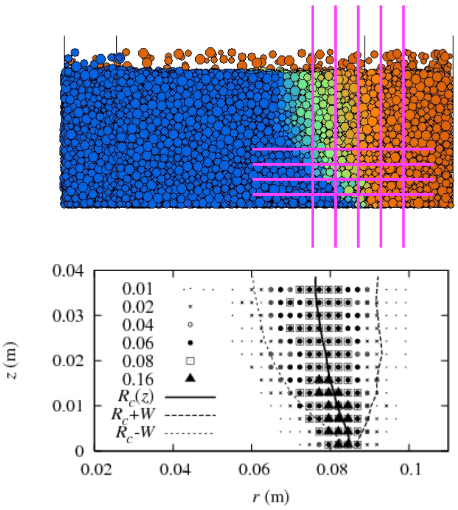
Advantages of local ring-averaging:

- shearband position known!
- long time-averaging -> slow
- space-averaging -> small

Split-bottom ring-shear cell (Leiden, 2003- ...)

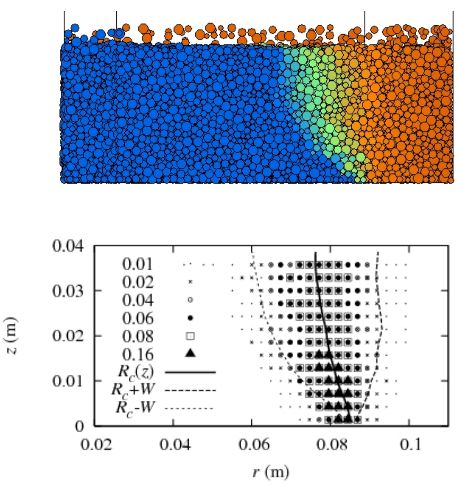


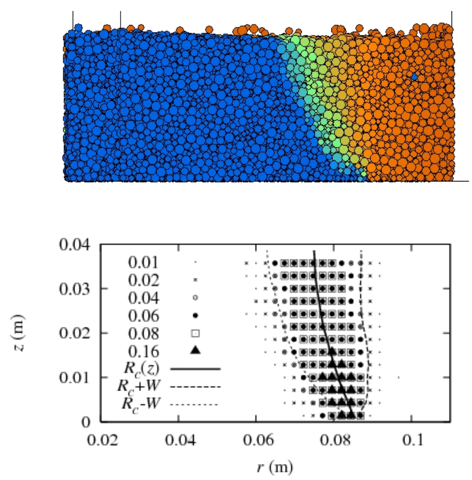
Constitutive relations – shear rate $\dot{\gamma}$



no friction

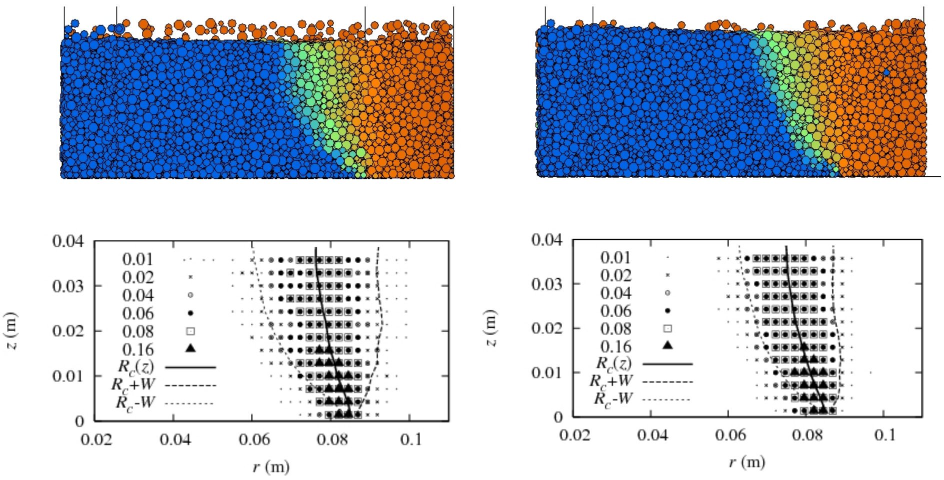
Constitutive relations – shear rate $\dot{\gamma}$





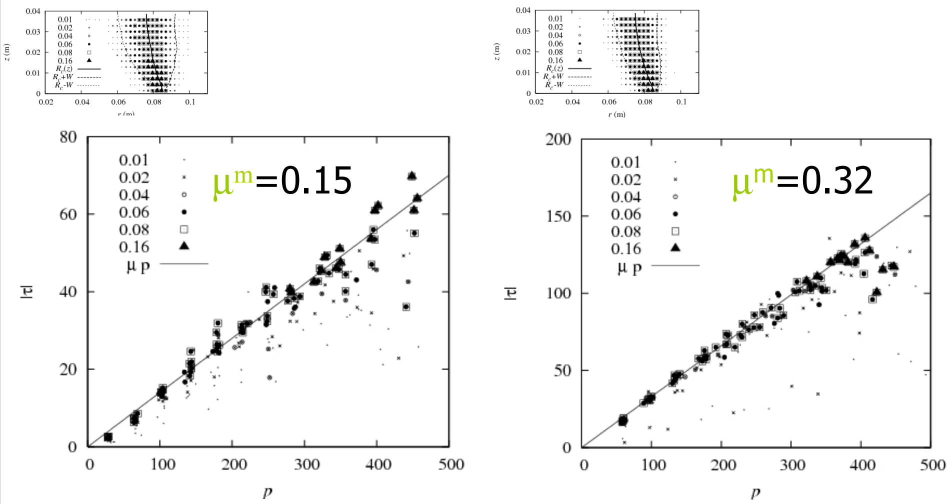
no friction friction

Constitutive relations – shear rate $\dot{\gamma}$



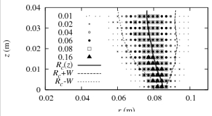
90% quantitative agreement with experiments …

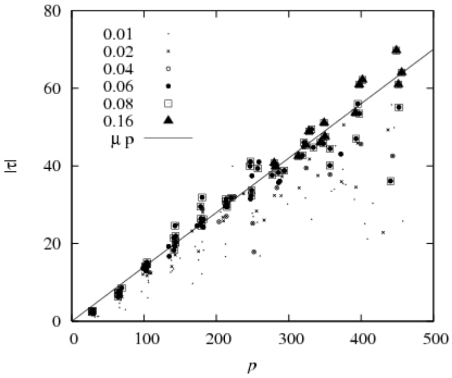
Constitutive relations: Mohr-Coulomb

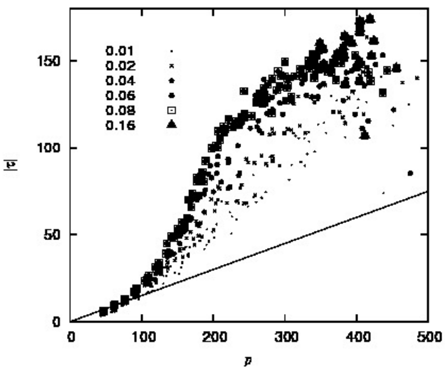


no friction μ=0 friction μ=0.4

Constitutive relations: Mohr-Coulomb







no friction/cohesion   cohesion

3D Flow behavior – steady state shear

Obtain constitutive relations from
one SINGLE simulation:

- Mohr Coulomb yield stress
- shear softening viscosity
- compression/dilatancy …
- inhomogeneity (force-chains)
- (almost always) an-isotropy
- micro-polar effects (rotations) …

Goal (see also www.pardem.eu)

DEM particle (element-test) simulations
with quantitative, predictive value

+ contact models (which? how detailed?)
+ *micro-macro transition* (LOCAL!!!)
Verification <-> Validation -> Experiments

=> Larger scale … models … continuum …

Application

From Lab- and industrial scales …

The End